



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:52 pm BST

PDB ID : 2YID
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis alpha-ketoglutarate decarboxylase in complex with the enamine-ThDP intermediate
Authors : Wagner, T.; Bellinzoni, M.; Wehenkel, A.M.; O'Hare, H.M.; Alzari, P.M.
Deposited on : 2011-05-11
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

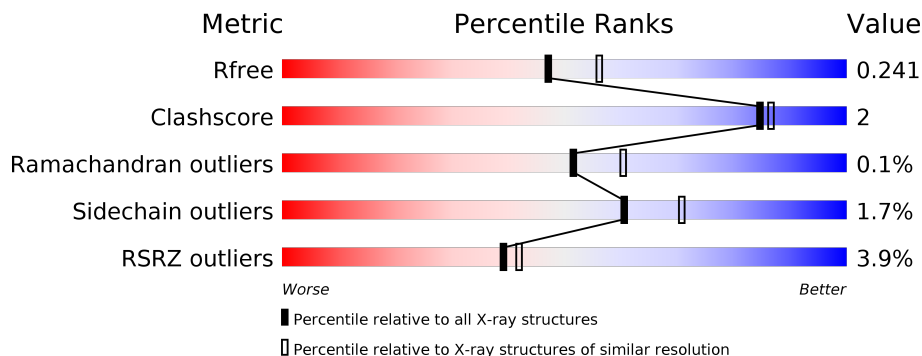
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on 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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">91% 6% •</p>
1	B	868	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 90%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">90% 6% •</p>
1	C	868	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">91% 6% •</p>
1	D	868	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">91% 7% •</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26987 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.

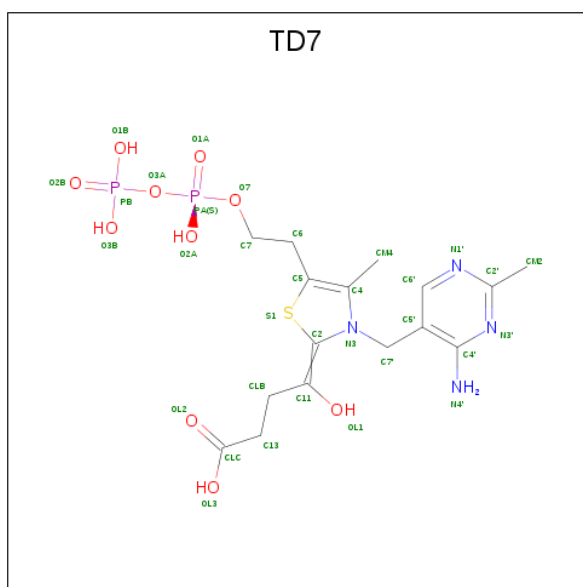
- Molecule 1 is a protein called 2-OXOGLUTARATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	844	6519	4099	1154	1242	24	0	0	0
1	B	837	6475	4074	1141	1236	24	0	1	0
1	C	843	6537	4112	1162	1239	24	0	1	0
1	D	852	6586	4143	1164	1255	24	0	0	0

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 (4E)-4-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-(2-[[S]-hydroxy(phosphonoxy)phosphoryl]oxy)ethyl)-4-methyl-1,3-thiazol-2(3H)-ylidene}-4-hydroxybutanoic acid (three-letter code: TD7) (formula: C₁₆H₂₄N₄O₁₀P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	33	16	4	10	2	1	0	0
2	B	1	33	16	4	10	2	1	0	0
2	C	1	33	16	4	10	2	1	0	0
2	D	1	33	16	4	10	2	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

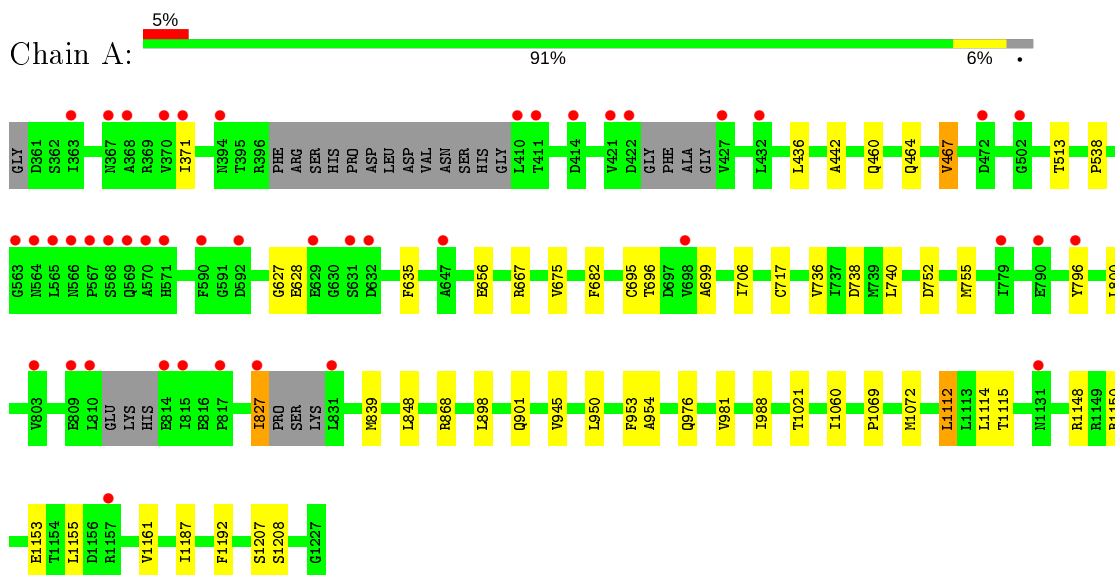
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	203	Total O 203 203	0	0
5	B	168	Total O 168 168	0	0
5	C	228	Total O 228 228	0	0
5	D	131	Total O 131 131	0	0

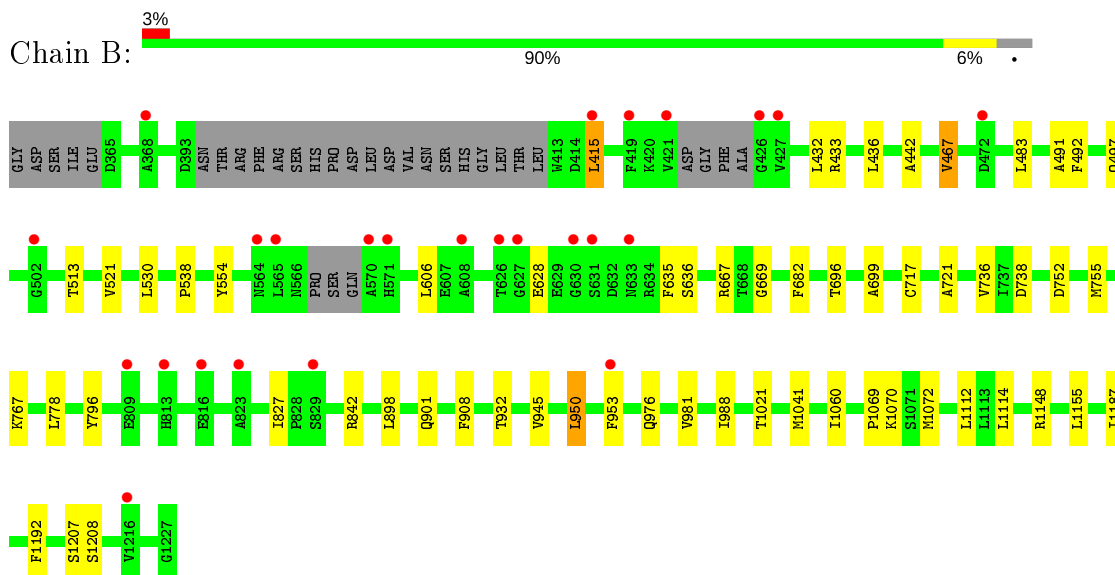
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

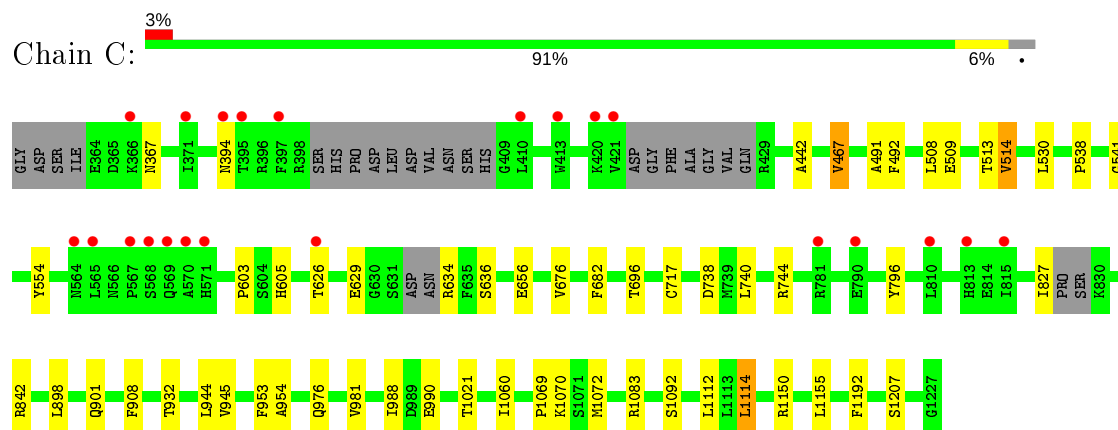
- Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



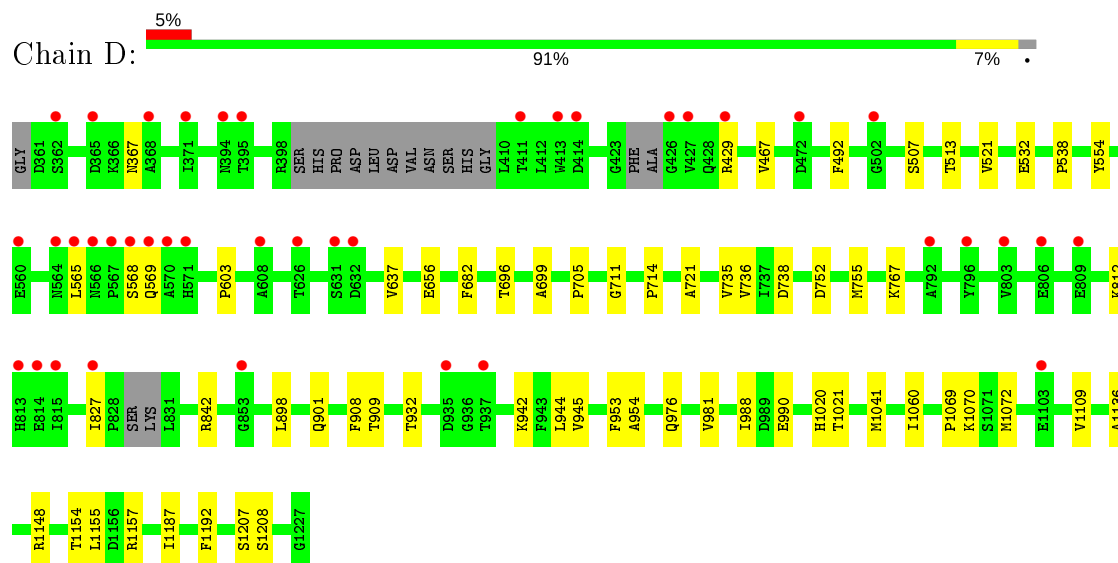
- Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



- Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.84Å 82.29Å 163.48Å 99.23° 99.03° 100.63°	Depositor
Resolution (Å)	32.94 – 2.25 40.37 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.7 (32.94-2.25) 95.7 (40.37-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.24Å)	Xtrriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.192 , 0.223 0.208 , 0.241	Depositor DCC
R_{free} test set	9064 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtrriage
Anisotropy	0.381	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26987	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.66% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, TD7, 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	0.50	0/6647	0.62	0/9010
1	B	0.50	0/6609	0.62	0/8961
1	C	0.52	0/6668	0.61	0/9037
1	D	0.51	0/6718	0.62	0/9106
All	All	0.50	0/26642	0.62	0/36114

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 [i](#)

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	6519	0	6303	27	0
1	B	6475	0	6261	31	0
1	C	6537	0	6327	29	0
1	D	6586	0	6377	29	0
2	A	33	0	20	3	0
2	B	33	0	20	2	0
2	C	33	0	20	2	0
2	D	33	0	20	2	0
3	A	1	0	0	0	0

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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	203	0	0	1	0
5	B	168	0	0	2	0
5	C	228	0	0	1	0
5	D	131	0	0	3	0
All	All	26987	0	25348	119	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 (119) 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:827:ILE:HA	1:B:1060:ILE:HD11	1.78	0.65
1:D:1041:MET:HE2	5:D:3123:HOH:O	1.96	0.64
1:C:827:ILE:HA	1:C:1060:ILE:HD11	1.78	0.63
1:A:1112:LEU:HD12	1:A:1161:VAL:HG21	1.79	0.63
1:C:492:PHE:CD1	1:C:554:TYR:HE1	2.18	0.62
1:C:513:THR:HG21	1:C:717:CYS:SG	2.40	0.61
1:C:901[A]:GLN:OE1	2:D:2001:TD7:H6'	2.01	0.60
1:B:415:LEU:HA	1:B:432:LEU:HB3	1.86	0.58
1:C:442:ALA:HB1	1:C:467:VAL:HG13	1.86	0.58
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.85	0.57
1:A:827:ILE:HA	1:A:1060:ILE:HD11	1.86	0.57
1:D:827:ILE:HA	1:D:1060:ILE:HD11	1.86	0.57
1:B:696:THR:HG21	1:B:738:ASP:HB2	1.87	0.55
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.88	0.54
1:D:603:PRO:HG3	1:D:990:GLU:HB3	1.88	0.54
1:C:492:PHE:HD1	1:C:554:TYR:HE1	1.55	0.54
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.89	0.53
1:B:415:LEU:HD23	1:B:433:ARG:HA	1.90	0.53
1:B:491:ALA:HB3	1:B:796:TYR:CE2	2.44	0.53
1:A:839:MET:HE3	1:A:839:MET:HA	1.91	0.53
2:C:2001:TD7:H6'	1:D:901:GLN:OE1	2.09	0.53
1:D:1021:THR:HG21	1:D:1207:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:705:PRO:HG2	1:D:735:VAL:HG13	1.92	0.52
1:B:442:ALA:HB1	1:B:467:VAL:HG13	1.90	0.51
1:C:603:PRO:HG3	1:C:990:GLU:HB3	1.91	0.51
1:D:492:PHE:HD1	1:D:554:TYR:HE2	1.59	0.51
1:C:696:THR:HG21	1:C:738:ASP:HB2	1.93	0.50
1:B:898:LEU:O	1:B:945:VAL:HA	2.12	0.50
1:D:696:THR:HG21	1:D:738:ASP:HB2	1.93	0.50
2:A:2001:TD7:H6'	1:B:901[A]:GLN:OE1	2.12	0.49
1:A:696:THR:HG21	1:A:738:ASP:HB2	1.95	0.48
1:D:942:LYS:HE3	1:D:944:LEU:HD21	1.95	0.48
1:D:1020:HIS:HD2	5:D:3110:HOH:O	1.96	0.48
1:D:898:LEU:O	1:D:945:VAL:HA	2.13	0.48
1:B:497:GLN:HG3	5:B:3016:HOH:O	2.13	0.48
1:D:656:GLU:HB3	1:D:954:ALA:HB2	1.96	0.48
1:A:901:GLN:OE1	2:B:2001:TD7:H6'	2.14	0.48
2:A:2001:TD7:H4'1	2:A:2001:TD7:C11	2.27	0.47
1:A:1148:ARG:HG3	1:A:1187:ILE:HD12	1.97	0.47
1:A:898:LEU:O	1:A:945:VAL:HA	2.13	0.47
1:C:898:LEU:O	1:C:945:VAL:HA	2.14	0.47
2:D:2001:TD7:C11	2:D:2001:TD7:H4'1	2.27	0.47
1:A:442:ALA:HB1	1:A:467:VAL:HG13	1.95	0.47
1:A:848:LEU:HD12	1:A:868:ARG:HD2	1.97	0.47
1:C:1092:SER:H	1:C:1150:ARG:HH11	1.61	0.47
2:C:2001:TD7:C11	2:C:2001:TD7:H4'1	2.28	0.47
1:D:513:THR:HG22	1:D:714:PRO:HB3	1.97	0.47
1:B:530:LEU:HD22	1:B:636:SER:HA	1.96	0.46
1:C:491:ALA:HB3	1:C:796:TYR:CD2	2.51	0.46
1:C:508:LEU:HD13	1:C:541:GLY:HA3	1.97	0.46
1:C:842:ARG:NH2	1:C:932:THR:O	2.49	0.46
1:C:541:GLY:HA2	5:C:3017:HOH:O	2.16	0.46
1:C:514:VAL:HG21	1:C:676:VAL:HG22	1.97	0.46
1:D:513:THR:HG21	1:D:711:GLY:O	2.16	0.46
2:A:2001:TD7:HM43	1:B:950:LEU:HD11	1.97	0.46
1:B:521:VAL:HG23	1:B:721:ALA:HB1	1.98	0.46
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.97	0.46
1:B:1021:THR:HG21	1:B:1207:SER:HB3	1.98	0.46
1:D:699:ALA:CB	1:D:736:VAL:HG21	2.46	0.45
1:A:675:VAL:HG11	1:A:695:CYS:SG	2.57	0.45
1:B:492:PHE:HD1	1:B:554:TYR:HE1	1.64	0.45
1:D:1069:PRO:CB	1:D:1072:MET:HB3	2.47	0.45
1:A:1069:PRO:CB	1:A:1072:MET:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:842:ARG:NH2	1:B:932:THR:O	2.50	0.45
1:B:492:PHE:CD1	1:B:554:TYR:HE1	2.34	0.45
1:C:1021:THR:HG21	1:C:1207:SER:HB3	1.99	0.45
1:C:1114:LEU:HD13	1:C:1192:PHE:HE1	1.82	0.45
1:A:656:GLU:HB3	1:A:954:ALA:HB2	1.99	0.44
1:A:513:THR:HG21	1:A:717:CYS:SG	2.58	0.44
1:C:656:GLU:HB3	1:C:954:ALA:HB2	2.00	0.44
1:A:699:ALA:CB	1:A:736:VAL:HG21	2.48	0.44
1:B:1148:ARG:HG3	1:B:1187:ILE:HD12	1.99	0.44
1:B:1069:PRO:CB	1:B:1072:MET:HB3	2.48	0.43
1:A:796:TYR:CE2	1:A:800:LEU:HD11	2.54	0.43
1:A:1155:LEU:HD11	1:A:1192:PHE:CZ	2.54	0.43
1:B:491:ALA:HB3	1:B:796:TYR:CD2	2.53	0.43
1:D:1069:PRO:HB2	1:D:1072:MET:HB3	2.00	0.43
1:C:1069:PRO:CB	1:C:1072:MET:HB3	2.49	0.43
1:D:1041:MET:CE	5:D:3123:HOH:O	2.62	0.42
1:D:842:ARG:NH2	1:D:932:THR:O	2.51	0.42
1:D:1155:LEU:HD11	1:D:1192:PHE:CZ	2.54	0.42
1:D:565:LEU:HB3	1:D:569:GLN:HB2	2.01	0.42
1:A:1069:PRO:HB2	1:A:1072:MET:HB3	2.01	0.42
1:A:839:MET:CE	1:A:839:MET:HA	2.49	0.42
1:B:635:PHE:CG	1:B:669:GLY:HA3	2.54	0.42
1:C:908:PHE:CZ	1:C:1070:LYS:HG2	2.55	0.42
1:C:1155:LEU:HD11	1:C:1192:PHE:CZ	2.54	0.42
1:C:629:GLU:HG3	1:C:944:LEU:HD22	2.00	0.42
1:B:1069:PRO:HB2	1:B:1072:MET:HB3	2.01	0.42
1:D:521:VAL:HG23	1:D:721:ALA:HB1	2.00	0.42
1:A:1021:THR:HG21	1:A:1207:SER:HB3	2.02	0.42
1:C:1069:PRO:HB2	1:C:1072:MET:HB3	2.01	0.42
1:C:492:PHE:CD1	1:C:554:TYR:CE1	3.03	0.42
1:D:532:GLU:HB3	1:D:637:VAL:HG13	2.02	0.42
1:A:628:GLU:OE1	1:A:667:ARG:HD3	2.19	0.42
1:C:626:THR:O	1:C:634:ARG:N	2.52	0.42
1:B:606:LEU:HG	2:B:2001:TD7:N4'	2.35	0.42
1:D:1154:THR:O	1:D:1157:ARG:HB2	2.19	0.42
1:B:513:THR:HG21	1:B:717:CYS:SG	2.59	0.42
1:B:699:ALA:CB	1:B:736:VAL:HG21	2.50	0.42
1:C:530:LEU:HD22	1:C:636:SER:HA	2.02	0.42
1:D:1109:VAL:HG21	1:D:1136:ALA:HB2	2.02	0.42
1:A:752:ASP:O	1:A:755:MET:HE2	2.19	0.42
1:C:491:ALA:HB3	1:C:796:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:ARG:NH1	1:A:1153:GLU:OE1	2.53	0.41
1:A:627:GLY:HA2	1:A:635:PHE:CD1	2.55	0.41
1:C:509:GLU:HB3	1:C:744:ARG:HB3	2.01	0.41
1:A:706:ILE:HD13	5:A:3008:HOH:O	2.20	0.41
1:B:1041:MET:HE2	5:B:3157:HOH:O	2.21	0.41
1:A:460:GLN:O	1:A:464:GLN:HB2	2.21	0.41
1:B:483:LEU:HD22	1:B:778:LEU:HD22	2.03	0.41
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.55	0.41
1:D:752:ASP:O	1:D:755:MET:HE2	2.21	0.41
1:A:827:ILE:HG13	1:A:1060:ILE:HD11	2.03	0.41
1:B:1155:LEU:HD11	1:B:1192:PHE:CZ	2.55	0.41
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.56	0.41
1:B:752:ASP:O	1:B:755:MET:HE2	2.20	0.40
1:D:1148:ARG:HG3	1:D:1187:ILE:HD12	2.03	0.40
1:B:628:GLU:OE1	1:B:667:ARG:HD3	2.21	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	834/868 (96%)	811 (97%)	22 (3%)	1 (0%)	51 60
1	B	830/868 (96%)	807 (97%)	22 (3%)	1 (0%)	51 60
1	C	834/868 (96%)	811 (97%)	21 (2%)	2 (0%)	47 55
1	D	844/868 (97%)	820 (97%)	23 (3%)	1 (0%)	51 60
All	All	3342/3472 (96%)	3249 (97%)	88 (3%)	5 (0%)	51 60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	605	HIS
1	A	538	PRO
1	B	538	PRO
1	C	538	PRO
1	D	538	PRO

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	672/726 (93%)	659 (98%)	13 (2%)	57	66
1	B	670/726 (92%)	659 (98%)	11 (2%)	62	73
1	C	674/726 (93%)	663 (98%)	11 (2%)	62	73
1	D	681/726 (94%)	669 (98%)	12 (2%)	59	68
All	All	2697/2904 (93%)	2650 (98%)	47 (2%)	60	71

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	ILE
1	A	436	LEU
1	A	467	VAL
1	A	682	PHE
1	A	740	LEU
1	A	827	ILE
1	A	950	LEU
1	A	953	PHE
1	A	976	GLN
1	A	1112	LEU
1	A	1114	LEU
1	A	1115	THR
1	A	1208	SER
1	B	415	LEU
1	B	436	LEU
1	B	467	VAL
1	B	682	PHE

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Mol	Chain	Res	Type
1	B	767	LYS
1	B	950	LEU
1	B	953	PHE
1	B	976	GLN
1	B	1112	LEU
1	B	1114	LEU
1	B	1208	SER
1	C	367	ASN
1	C	394	ASN
1	C	467	VAL
1	C	514	VAL
1	C	682	PHE
1	C	740	LEU
1	C	953	PHE
1	C	976	GLN
1	C	1083	ARG
1	C	1112	LEU
1	C	1114	LEU
1	D	367	ASN
1	D	429	ARG
1	D	467	VAL
1	D	507	SER
1	D	568	SER
1	D	682	PHE
1	D	767	LYS
1	D	812	LYS
1	D	909	THR
1	D	953	PHE
1	D	976	GLN
1	D	1208	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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	TD7	B	2001	3	26,34,34	1.69	5 (19%)	32,50,50	2.42	11 (34%)
2	TD7	A	2001	3	26,34,34	1.69	6 (23%)	32,50,50	2.45	12 (37%)
2	TD7	D	2001	3	26,34,34	1.75	6 (23%)	32,50,50	2.45	13 (40%)
2	TD7	C	2001	3	26,34,34	1.62	5 (19%)	32,50,50	2.51	13 (40%)

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	TD7	B	2001	3	-	2/19/26/26	0/2/2/2
2	TD7	A	2001	3	-	5/19/26/26	0/2/2/2
2	TD7	D	2001	3	-	5/19/26/26	0/2/2/2
2	TD7	C	2001	3	-	4/19/26/26	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	TD7	OL1-C11	4.51	1.44	1.32
2	C	2001	TD7	OL1-C11	4.50	1.44	1.32
2	A	2001	TD7	OL1-C11	4.49	1.44	1.32
2	D	2001	TD7	OL1-C11	4.35	1.43	1.32
2	A	2001	TD7	C2-N3	-3.76	1.31	1.38
2	C	2001	TD7	C2-N3	-3.39	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	TD7	C2-N3	-3.39	1.32	1.38
2	D	2001	TD7	PB-O2B	3.36	1.61	1.50
2	B	2001	TD7	C2-N3	-3.34	1.32	1.38
2	A	2001	TD7	PB-O2B	3.32	1.61	1.50
2	B	2001	TD7	PB-O2B	3.31	1.61	1.50
2	D	2001	TD7	C6-C5	3.29	1.52	1.50
2	C	2001	TD7	PB-O2B	3.12	1.60	1.50
2	B	2001	TD7	C6-C5	2.79	1.52	1.50
2	D	2001	TD7	C4-N3	-2.61	1.34	1.39
2	A	2001	TD7	C6-C5	2.47	1.52	1.50
2	C	2001	TD7	PB-O3B	-2.36	1.45	1.54
2	B	2001	TD7	C4-N3	-2.28	1.34	1.39
2	A	2001	TD7	PB-O3B	-2.13	1.46	1.54
2	D	2001	TD7	PB-O3B	-2.10	1.46	1.54
2	A	2001	TD7	C4-N3	-2.10	1.35	1.39
2	C	2001	TD7	C4-N3	-2.06	1.35	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	TD7	C2-N3-C4	6.75	112.39	108.64
2	B	2001	TD7	C2-N3-C4	6.60	112.31	108.64
2	C	2001	TD7	C2-N3-C4	6.49	112.25	108.64
2	A	2001	TD7	C2-N3-C4	6.31	112.15	108.64
2	A	2001	TD7	C6-C5-C4	5.06	131.49	127.43
2	B	2001	TD7	C6-C5-C4	4.82	131.30	127.43
2	C	2001	TD7	CM2-C2'-N1'	4.80	122.42	117.14
2	C	2001	TD7	CM4-C4-C5	-4.66	117.41	127.60
2	A	2001	TD7	CM4-C4-C5	-4.52	117.72	127.60
2	D	2001	TD7	CM4-C4-C5	-4.48	117.79	127.60
2	B	2001	TD7	CM4-C4-C5	-4.38	118.02	127.60
2	B	2001	TD7	C5-C4-N3	4.34	116.72	107.66
2	A	2001	TD7	C5-C4-N3	4.17	116.38	107.66
2	D	2001	TD7	C5-C4-N3	4.16	116.36	107.66
2	C	2001	TD7	C5-C4-N3	4.09	116.22	107.66
2	D	2001	TD7	CM2-C2'-N1'	3.85	121.37	117.14
2	D	2001	TD7	C6-C5-C4	3.77	130.46	127.43
2	C	2001	TD7	C6-C5-C4	3.74	130.43	127.43
2	B	2001	TD7	C6'-N1'-C2'	3.69	122.24	115.96
2	D	2001	TD7	CLB-C11-C2	-3.61	116.27	124.34
2	C	2001	TD7	CLB-C11-C2	-3.59	116.32	124.34
2	D	2001	TD7	CLB-C13-CLC	-3.54	106.73	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	TD7	CM2-C2'-N1'	3.50	120.98	117.14
2	A	2001	TD7	CLB-C11-C2	-3.47	116.58	124.34
2	D	2001	TD7	OL1-C11-CLB	3.41	123.22	114.08
2	A	2001	TD7	C6'-N1'-C2'	3.41	121.76	115.96
2	A	2001	TD7	OL1-C11-CLB	3.40	123.17	114.08
2	A	2001	TD7	CLB-C13-CLC	-3.39	106.98	112.67
2	B	2001	TD7	CLB-C11-C2	-3.33	116.89	124.34
2	C	2001	TD7	OL1-C11-CLB	3.22	122.69	114.08
2	C	2001	TD7	CLB-C13-CLC	-3.22	107.28	112.67
2	B	2001	TD7	OL1-C11-CLB	3.01	122.15	114.08
2	C	2001	TD7	C6'-N1'-C2'	2.98	121.03	115.96
2	D	2001	TD7	C6'-N1'-C2'	2.93	120.94	115.96
2	C	2001	TD7	CM4-C4-N3	2.91	126.35	122.69
2	B	2001	TD7	C5'-C6'-N1'	-2.79	119.17	123.82
2	B	2001	TD7	N1'-C2'-N3'	-2.77	120.78	125.54
2	C	2001	TD7	C5'-C6'-N1'	-2.64	119.42	123.82
2	A	2001	TD7	C5'-C6'-N1'	-2.64	119.42	123.82
2	A	2001	TD7	N1'-C2'-N3'	-2.57	121.11	125.54
2	C	2001	TD7	N1'-C2'-N3'	-2.55	121.16	125.54
2	C	2001	TD7	C2'-N3'-C4'	2.54	122.03	118.08
2	A	2001	TD7	CM4-C4-N3	2.48	125.81	122.69
2	D	2001	TD7	C5'-C6'-N1'	-2.47	119.70	123.82
2	D	2001	TD7	CM4-C4-N3	2.46	125.78	122.69
2	D	2001	TD7	N1'-C2'-N3'	-2.43	121.36	125.54
2	A	2001	TD7	CM2-C2'-N1'	2.32	119.69	117.14
2	B	2001	TD7	O3B-PB-O3A	2.14	111.82	104.64
2	D	2001	TD7	C2'-N3'-C4'	2.12	121.38	118.08

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2001	TD7	CLC-C13-CLB-C11
2	C	2001	TD7	CLC-C13-CLB-C11
2	A	2001	TD7	CLC-C13-CLB-C11
2	A	2001	TD7	PA-O3A-PB-O2B
2	C	2001	TD7	PA-O3A-PB-O2B
2	A	2001	TD7	PA-O3A-PB-O3B
2	D	2001	TD7	PA-O3A-PB-O3B
2	B	2001	TD7	PA-O3A-PB-O3B
2	D	2001	TD7	PA-O3A-PB-O2B
2	B	2001	TD7	PA-O3A-PB-O2B

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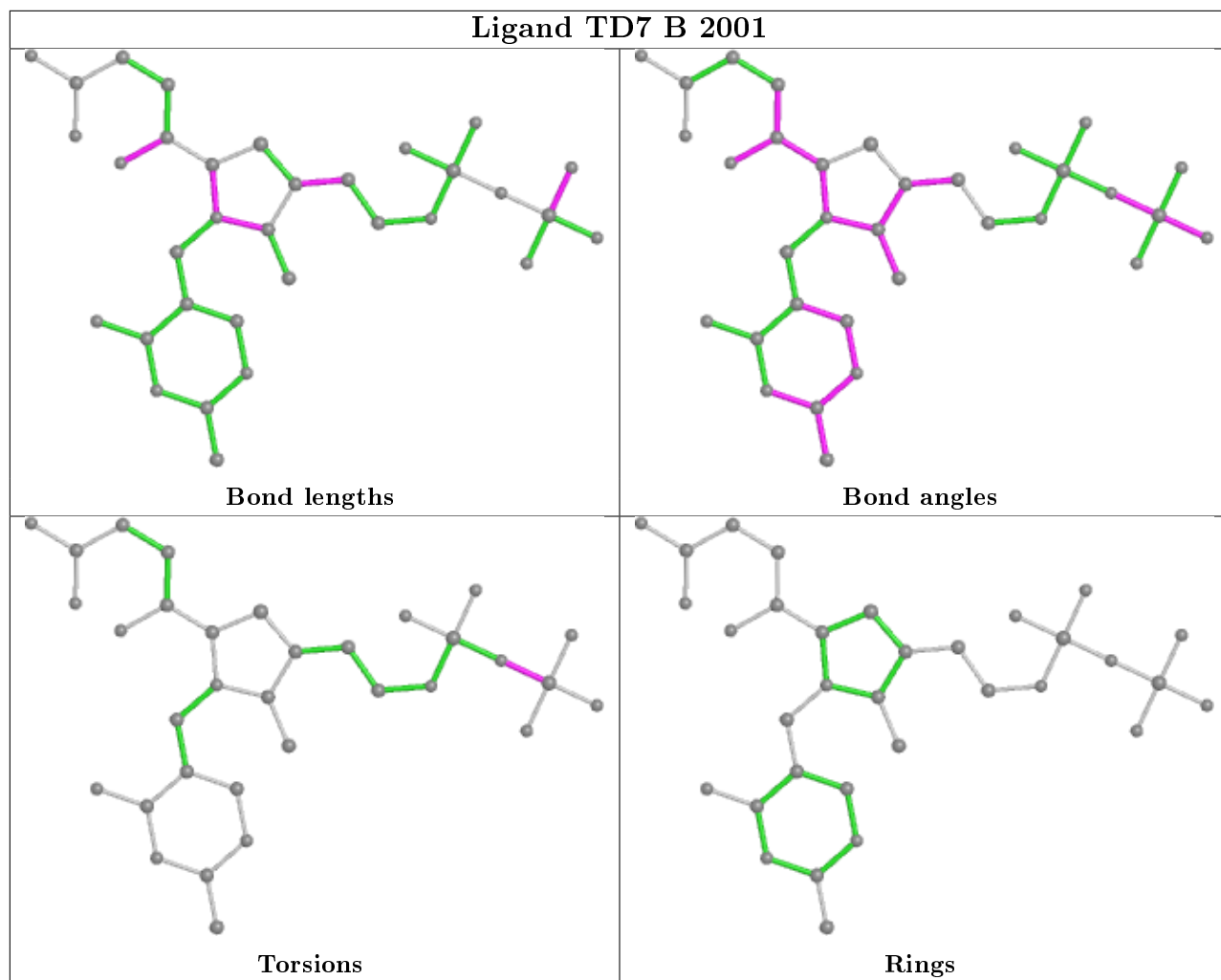
Mol	Chain	Res	Type	Atoms
2	A	2001	TD7	OL1-C11-CLB-C13
2	D	2001	TD7	OL1-C11-CLB-C13
2	A	2001	TD7	C7-O7-PA-O1A
2	C	2001	TD7	OL1-C11-CLB-C13
2	D	2001	TD7	C2-C11-CLB-C13
2	C	2001	TD7	C2-C11-CLB-C13

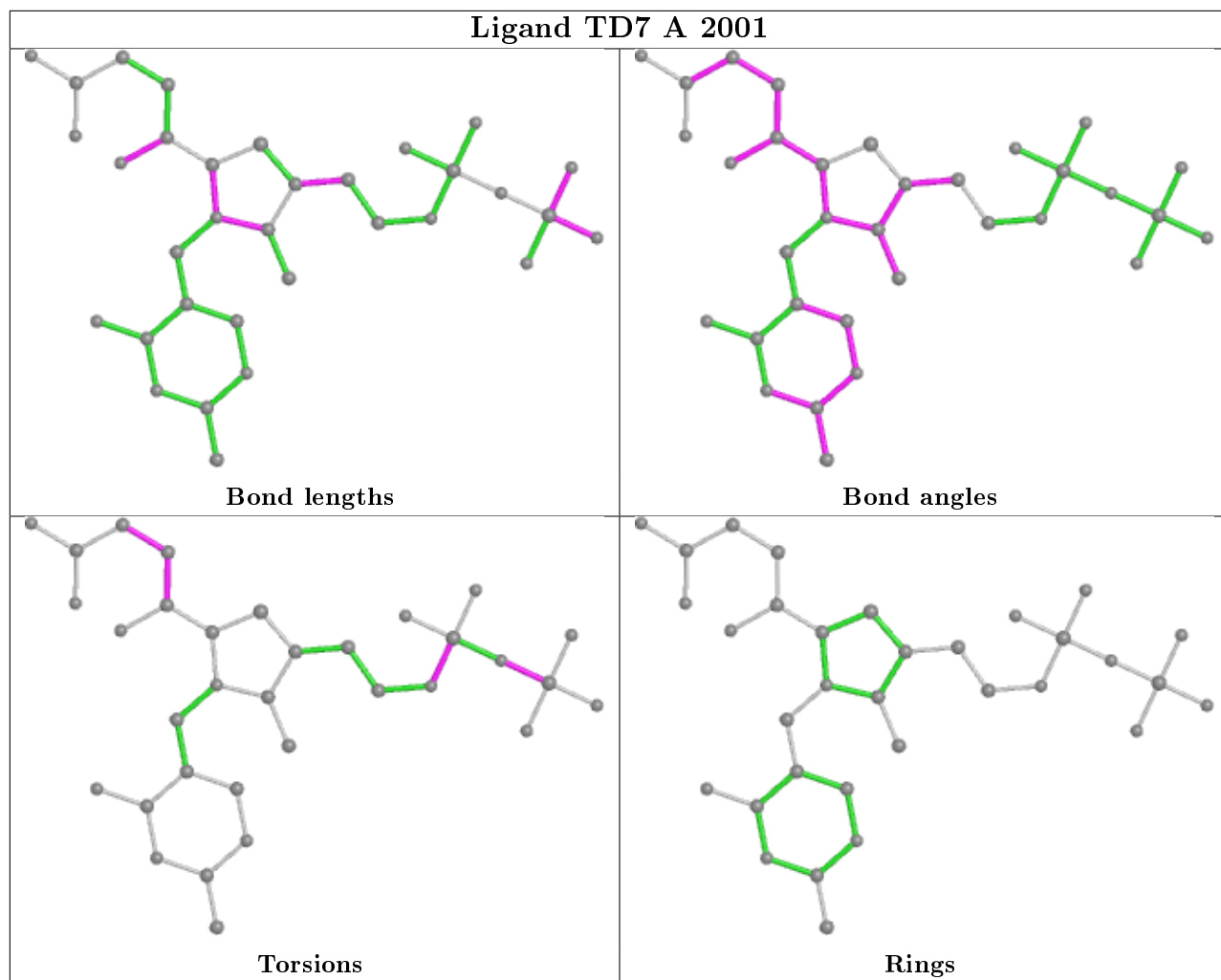
There are no ring outliers.

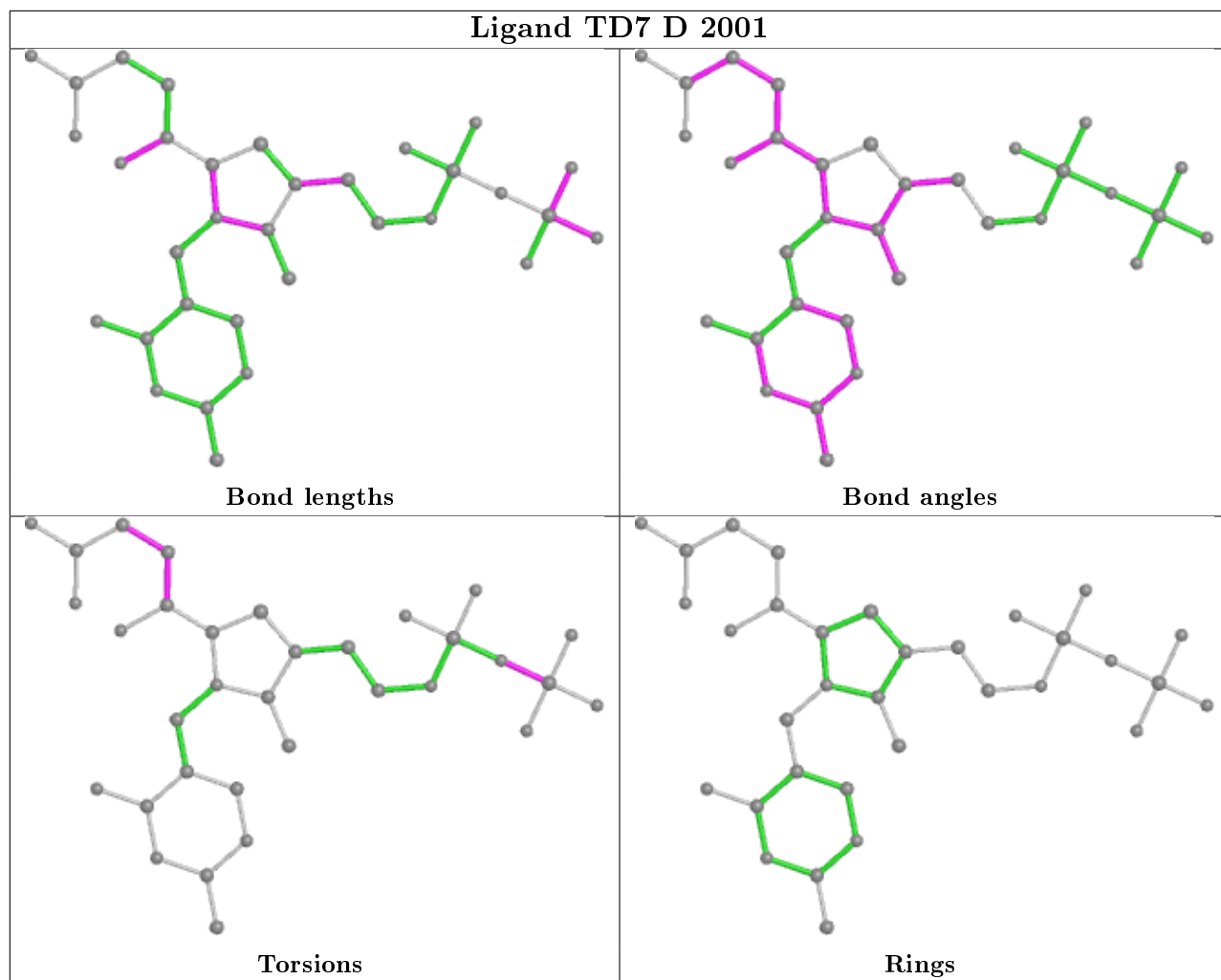
4 monomers are involved in 9 short contacts:

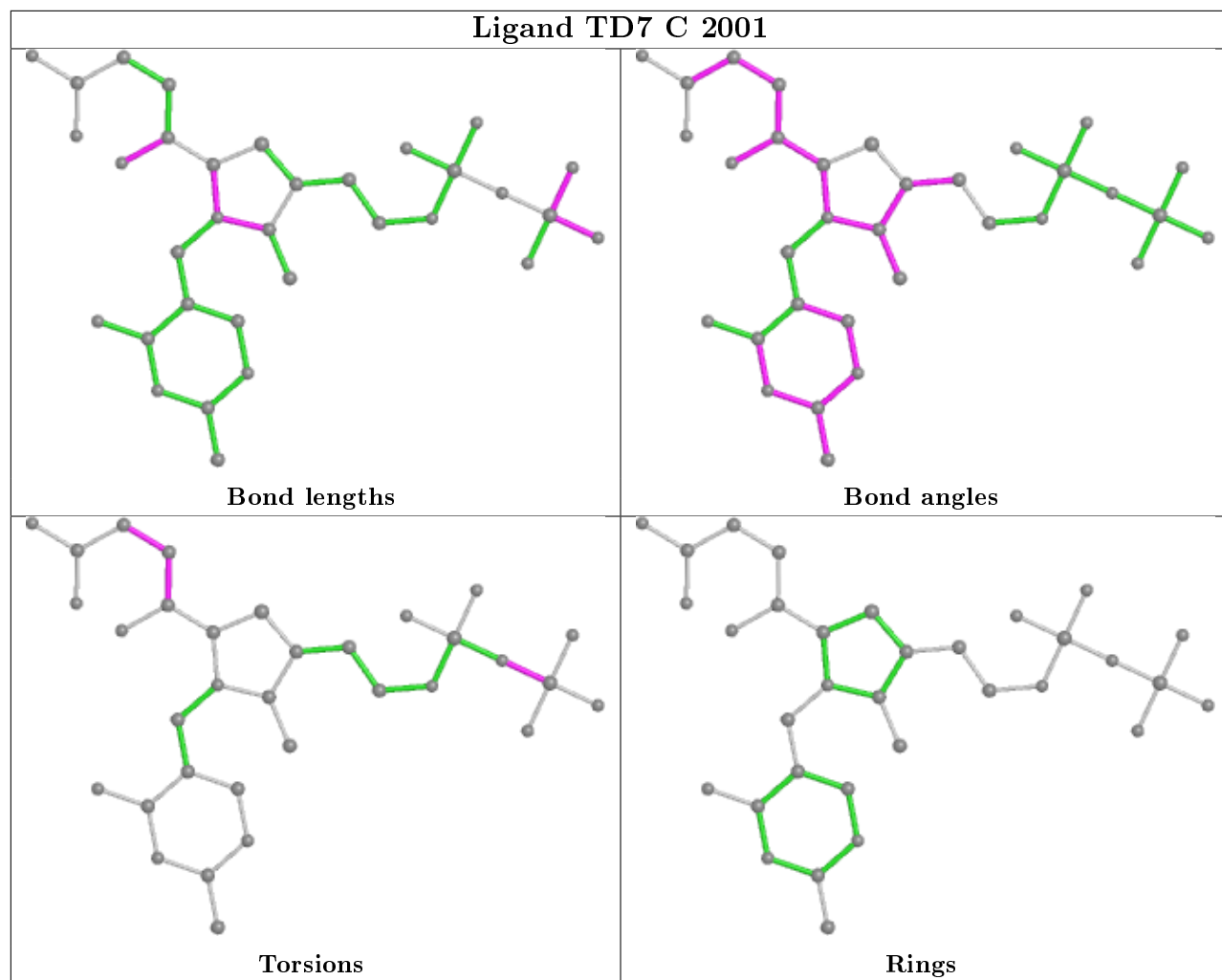
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	TD7	2	0
2	A	2001	TD7	3	0
2	D	2001	TD7	2	0
2	C	2001	TD7	2	0

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	844/868 (97%)	0.12	44 (5%) 27 30	14, 31, 65, 94	0
1	B	837/868 (96%)	-0.01	25 (2%) 50 53	14, 30, 61, 89	0
1	C	843/868 (97%)	-0.07	22 (2%) 56 59	12, 28, 63, 93	0
1	D	852/868 (98%)	0.09	40 (4%) 31 34	14, 31, 67, 91	0
All	All	3376/3472 (97%)	0.03	131 (3%) 39 42	12, 30, 64, 94	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	568	SER	7.7
1	B	570	ALA	6.6
1	C	570	ALA	6.6
1	C	421	VAL	6.5
1	D	568	SER	6.0
1	A	571	HIS	5.9
1	A	569	GLN	5.9
1	A	570	ALA	5.8
1	A	410	LEU	5.8
1	C	568	SER	5.7
1	C	569	GLN	5.7
1	C	565	LEU	5.6
1	A	567	PRO	5.6
1	D	427	VAL	5.2
1	C	567	PRO	4.8
1	D	394	ASN	4.6
1	A	502	GLY	4.5
1	B	427	VAL	4.4
1	B	426	GLY	4.3
1	D	502	GLY	4.3
1	D	631	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	813	HIS	4.2
1	D	368	ALA	4.2
1	C	397	PHE	4.1
1	D	570	ALA	4.1
1	D	569	GLN	4.1
1	B	564	ASN	4.0
1	D	796	TYR	3.8
1	C	564	ASN	3.8
1	B	626	THR	3.8
1	A	411	THR	3.7
1	A	421	VAL	3.7
1	B	472	ASP	3.7
1	B	631	SER	3.7
1	D	429	ARG	3.6
1	A	566	ASN	3.5
1	B	421	VAL	3.5
1	B	368	ALA	3.5
1	A	831	LEU	3.5
1	A	368	ALA	3.5
1	B	502	GLY	3.4
1	A	565	LEU	3.4
1	A	367	ASN	3.4
1	A	815	ILE	3.4
1	B	565	LEU	3.4
1	D	815	ILE	3.4
1	C	571	HIS	3.3
1	C	420	LYS	3.2
1	B	627	GLY	3.2
1	C	815	ILE	3.2
1	C	413	TRP	3.2
1	B	829	SER	3.2
1	C	395	THR	3.1
1	C	813	HIS	3.1
1	B	419	PHE	3.1
1	D	564	ASN	3.1
1	C	790	GLU	3.1
1	D	626	THR	3.0
1	D	632	ASP	3.0
1	D	803	VAL	3.0
1	A	394	ASN	3.0
1	A	796	TYR	3.0
1	A	814	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	565	LEU	2.9
1	D	792	ALA	2.9
1	C	626	THR	2.9
1	C	810	LEU	2.9
1	D	395	THR	2.9
1	B	571	HIS	2.9
1	A	810	LEU	2.9
1	A	472	ASP	2.9
1	A	427	VAL	2.8
1	D	813	HIS	2.8
1	D	827	ILE	2.8
1	D	571	HIS	2.7
1	B	809	GLU	2.7
1	A	817	PRO	2.7
1	A	698	VAL	2.7
1	D	371	ILE	2.6
1	B	953	PHE	2.6
1	D	411	THR	2.6
1	D	809	GLU	2.6
1	B	1216	VAL	2.6
1	D	426	GLY	2.5
1	B	633	ASN	2.5
1	D	566	ASN	2.5
1	C	366	LYS	2.5
1	C	394	ASN	2.5
1	D	414	ASP	2.5
1	A	779	ILE	2.5
1	B	816	GLU	2.4
1	A	827	ILE	2.4
1	C	781	ARG	2.4
1	B	608	ALA	2.4
1	B	630	GLY	2.4
1	D	814	GLU	2.4
1	B	415	LEU	2.4
1	A	370	VAL	2.4
1	A	631	SER	2.4
1	D	1103	GLU	2.3
1	A	590	PHE	2.3
1	D	472	ASP	2.3
1	A	432	LEU	2.3
1	A	629	GLU	2.3
1	D	853	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	560	GLU	2.3
1	A	803	VAL	2.2
1	A	564	ASN	2.2
1	B	823	ALA	2.2
1	C	410	LEU	2.2
1	A	632	ASP	2.2
1	A	647	ALA	2.2
1	D	608	ALA	2.2
1	D	362	SER	2.2
1	A	1157	ARG	2.2
1	A	414	ASP	2.2
1	A	592	ASP	2.2
1	D	567	PRO	2.1
1	A	563	GLY	2.1
1	D	806	GLU	2.1
1	D	935	ASP	2.1
1	A	363	ILE	2.1
1	A	371	ILE	2.1
1	D	413	TRP	2.1
1	A	422	ASP	2.0
1	C	371	ILE	2.0
1	A	1131	ASN	2.0
1	A	809	GLU	2.0
1	D	937	THR	2.0
1	D	365	ASP	2.0
1	A	790	GLU	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 [\(i\)](#)

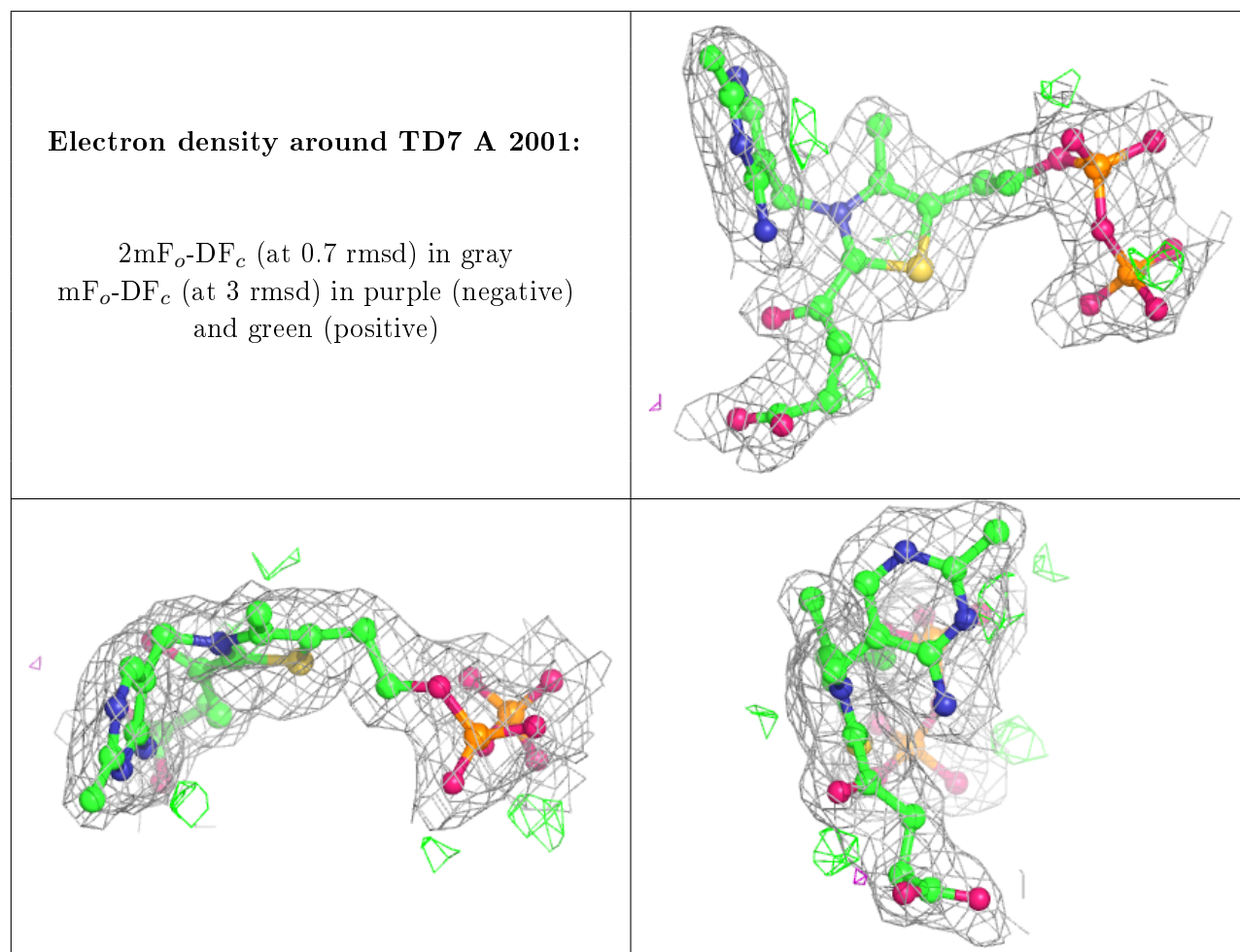
There are no carbohydrates in this entry.

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.

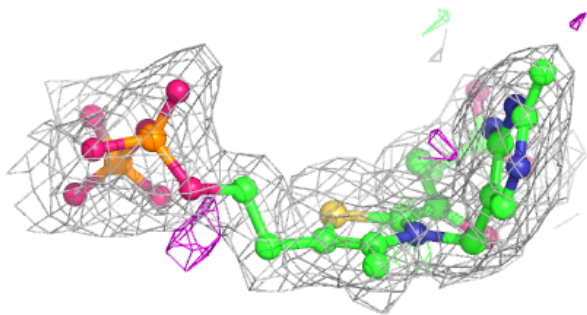
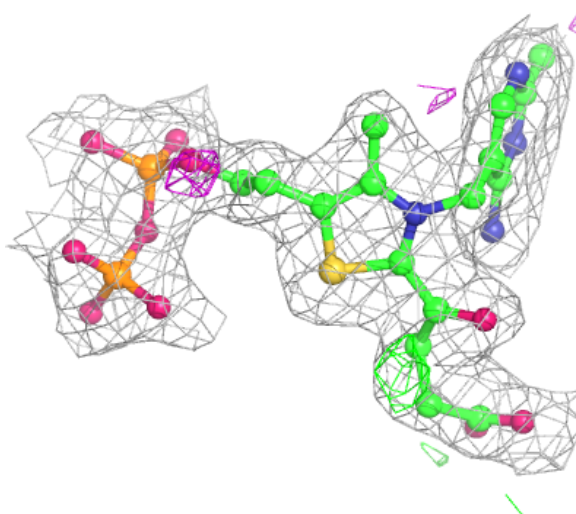
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	$Q < 0.9$
2	TD7	A	2001	33/33	0.98	0.13	11,20,45,48	0
3	MG	C	2002	1/1	0.98	0.07	8,8,8,8	0
2	TD7	D	2001	33/33	0.98	0.12	9,18,37,44	0
2	TD7	B	2001	33/33	0.98	0.12	9,19,42,44	0
3	MG	B	2002	1/1	0.98	0.06	12,12,12,12	0
4	CA	A	2003	1/1	0.98	0.04	33,33,33,33	0
2	TD7	C	2001	33/33	0.98	0.13	12,19,41,42	0
3	MG	D	2002	1/1	0.99	0.06	8,8,8,8	0
4	CA	B	2003	1/1	0.99	0.05	30,30,30,30	0
4	CA	C	2003	1/1	0.99	0.04	27,27,27,27	0
4	CA	D	2003	1/1	0.99	0.10	29,29,29,29	0
3	MG	A	2002	1/1	0.99	0.11	12,12,12,12	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.



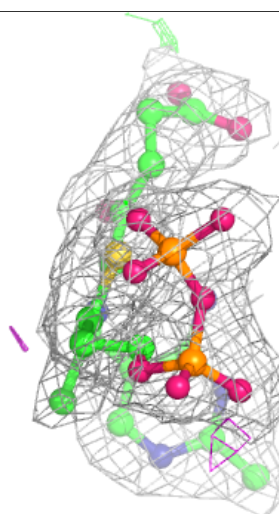
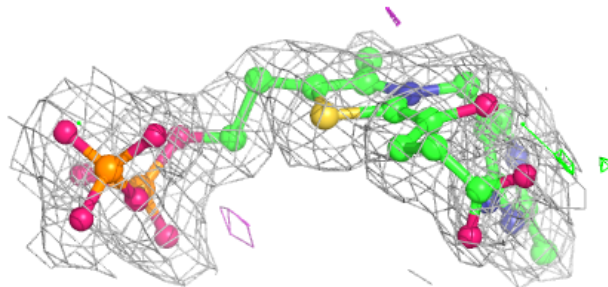
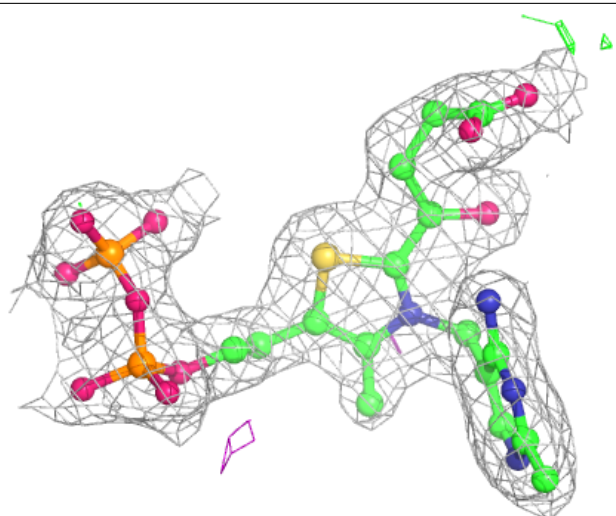
Electron density around TD7 D 2001:

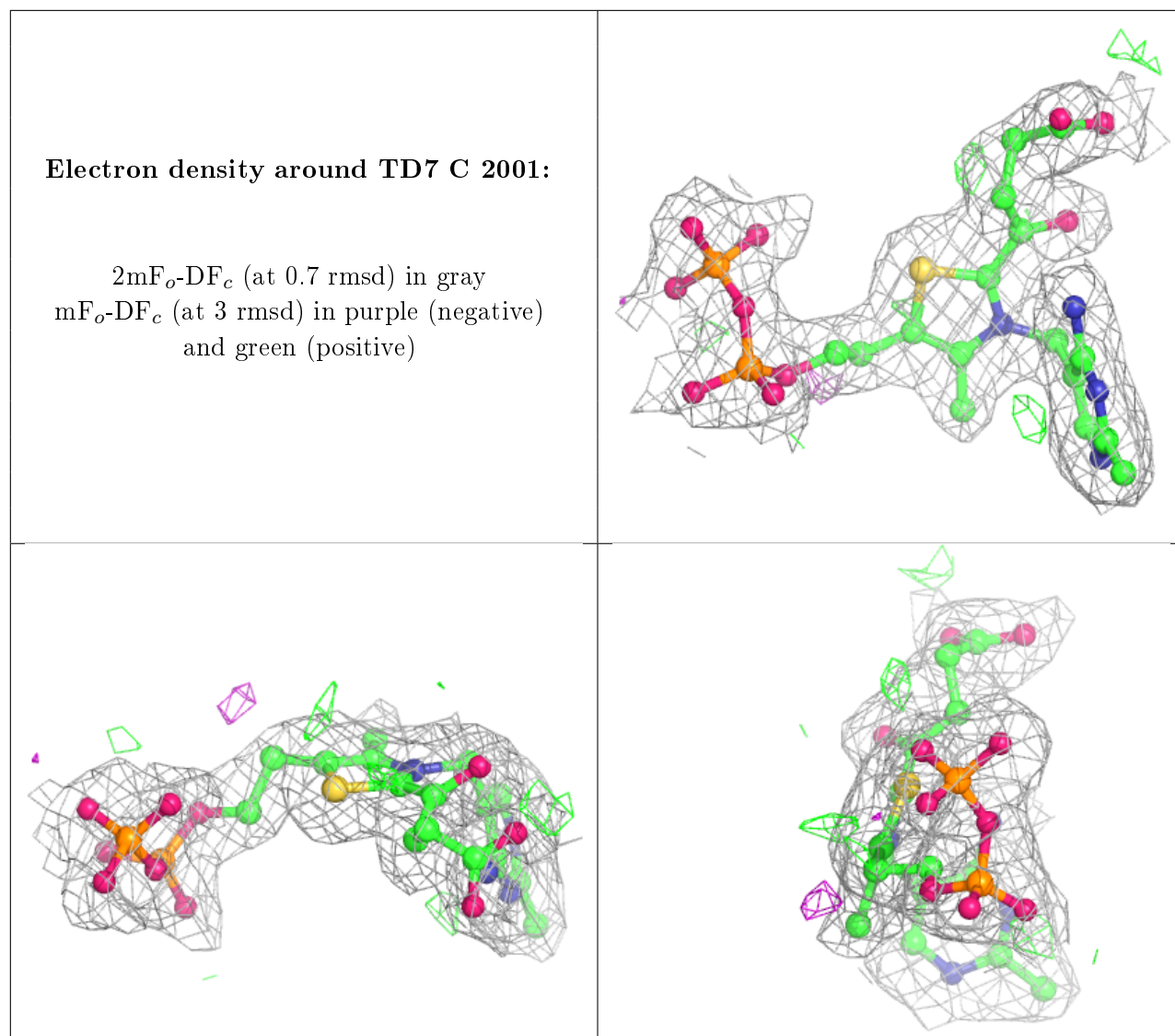
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TD7 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.