Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 09:29 am GMT

PDB ID	:	3ZHU
Title	:	Crystal structure of the SucA domain of Mycobacterium smegmatis KGD, second post-decarboxylation intermediate from 2-oxoadipate
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:

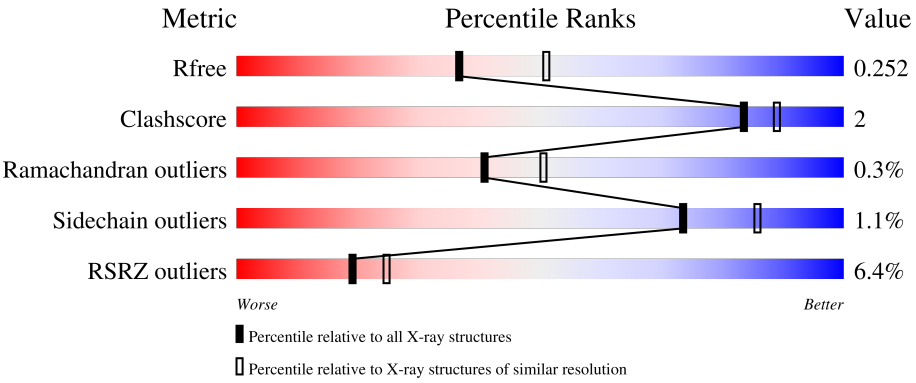
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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	8% 92% 6%
1	B	868	5% 90% 6%
1	C	868	4% 91% 6%
1	D	868	7% 92% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27180 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.

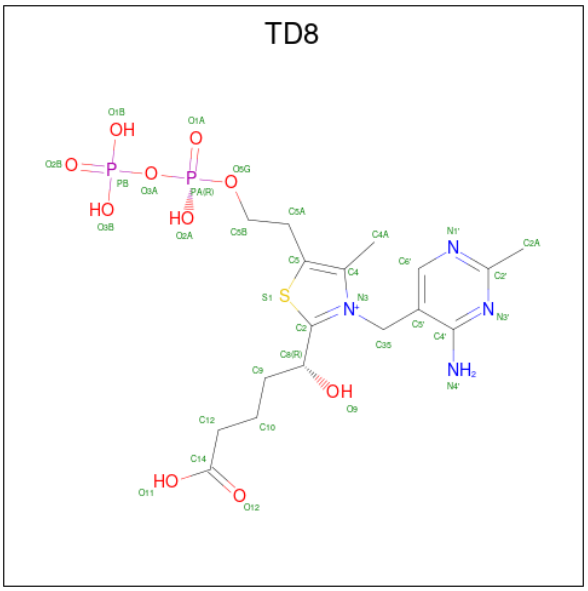
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	847	Total	C	N	O	S	0	1	0
			6531	4106	1156	1245	24			
1	B	836	Total	C	N	O	S	0	0	0
			6463	4067	1142	1230	24			
1	C	845	Total	C	N	O	S	0	1	0
			6530	4108	1157	1241	24			
1	D	852	Total	C	N	O	S	0	0	0
			6578	4138	1163	1253	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 (5R)-5-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-4-methyl-5-(2-{[(phosphonatooxy)phosphinato]oxy}ethyl)-1,3-thiazol-3-ium-2-yl}-5-hydroxypentanoate (three-letter code: TD8) (formula: $C_{17}H_{27}N_4O_{10}P_2S$).



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

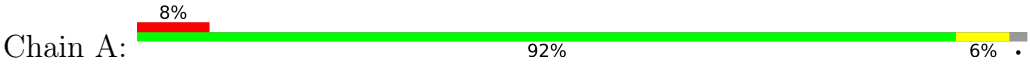
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	239	Total O 239 239	0	0
5	B	204	Total O 204 204	0	0
5	C	298	Total O 298 298	0	0
5	D	193	Total O 193 193	0	0

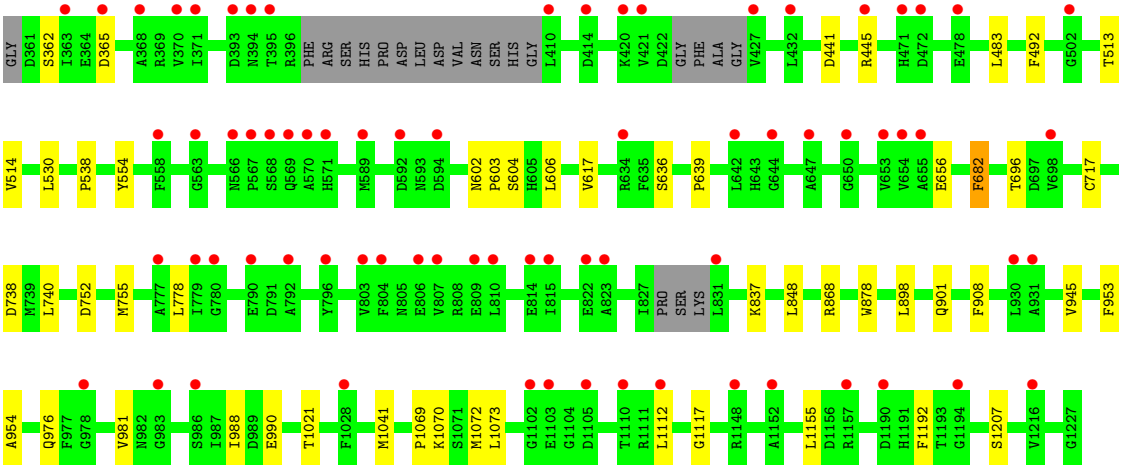
3 Residue-property plots (i)

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

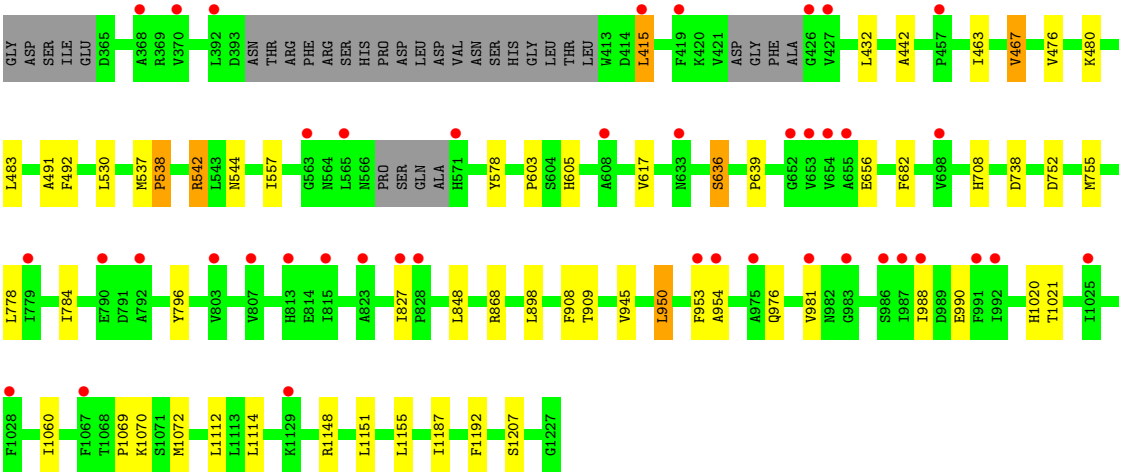
Chain A:





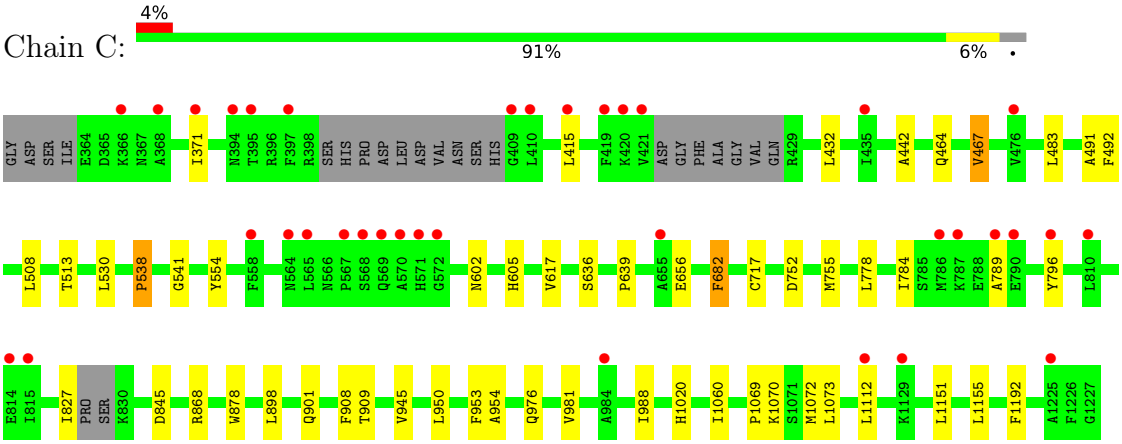
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

Chain B:



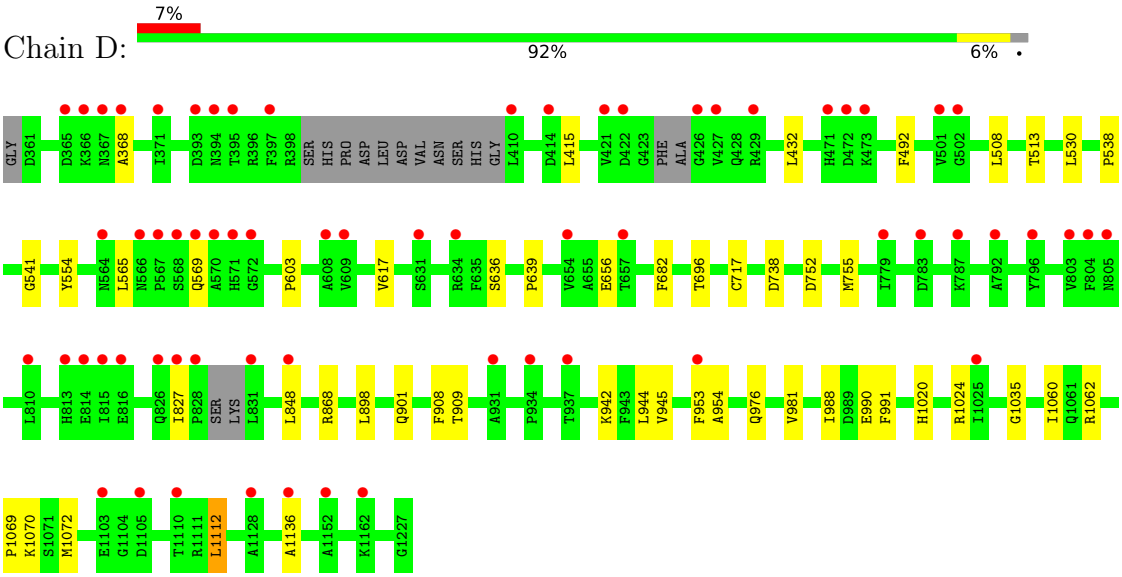
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

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	79.78Å 82.29Å 163.04Å 99.19° 99.10° 100.71°	Depositor
Resolution (Å)	40.36 – 2.30 40.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (40.36-2.30) 96.7 (40.36-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.200 , 0.235 0.214 , 0.252	Depositor DCC
R_{free} test set	8505 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	27180	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.56% 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: CA, TD8, 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	0.49	0/6663	0.63	0/9034
1	B	0.50	0/6594	0.63	0/8940
1	C	0.51	0/6661	0.63	0/9032
1	D	0.49	0/6710	0.62	0/9097
All	All	0.50	0/26628	0.63	0/36103

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	6531	0	6302	25	0
1	B	6463	0	6253	34	0
1	C	6530	0	6308	32	0
1	D	6578	0	6362	27	0
2	A	34	0	22	6	0
2	B	34	0	22	2	0
2	C	34	0	22	1	0
2	D	34	0	22	4	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	239	0	0	0	0
5	B	204	0	0	2	0
5	C	298	0	0	2	0
5	D	193	0	0	2	0
All	All	27180	0	25313	121	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 (121) 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	1.66	0.78
1:C:827:ILE:HA	1:C:1060:ILE:HD11	1.69	0.71
1:C:492:PHE:HD1	1:C:554:TYR:HE1	1.38	0.71
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.73	0.70
1:D:827:ILE:HA	1:D:1060:ILE:HD11	1.74	0.70
1:C:371:ILE:HD12	1:D:368:ALA:HB1	1.78	0.66
1:A:1112:LEU:HD21	1:A:1155:LEU:HD22	1.78	0.64
1:C:508:LEU:HD13	1:C:541:GLY:HA3	1.82	0.61
1:D:848:LEU:HD12	1:D:868:ARG:HD3	1.82	0.60
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.84	0.59
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.83	0.59
1:B:537:MET:O	1:B:542:ARG:NH2	2.35	0.58
1:A:848:LEU:HD12	1:A:868:ARG:HD3	1.85	0.58
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.85	0.58
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.85	0.58
1:C:492:PHE:CD1	1:C:554:TYR:HE1	2.21	0.57
2:A:2001:TD8:H5BA	1:B:950:LEU:HD11	1.86	0.57
1:A:901:GLN:OE1	2:B:2001:TD8:H6'	2.06	0.56
1:B:476:VAL:HG12	1:B:480:LYS:HE3	1.88	0.56
1:C:1020:HIS:HD2	5:C:3230:HOH:O	1.89	0.55
1:B:442:ALA:HB1	1:B:467:VAL:HG13	1.88	0.55
1:C:950:LEU:CD1	2:D:2001:TD8:H5BA	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:901[A]:GLN:OE1	2:D:2001:TD8:H6'	2.07	0.55
1:C:950:LEU:HD11	2:D:2001:TD8:H5BA	1.89	0.55
1:C:442:ALA:HB1	1:C:467:VAL:HG13	1.89	0.54
1:D:1069:PRO:CB	1:D:1072:MET:HB3	2.37	0.54
2:A:2001:TD8:C2	2:A:2001:TD8:HN4A	2.20	0.54
1:D:1069:PRO:HB2	1:D:1072:MET:HB3	1.89	0.54
1:A:606:LEU:HG	2:A:2001:TD8:N4'	2.23	0.54
1:B:1069:PRO:HB2	1:B:1072:MET:HB3	1.90	0.54
1:A:1069:PRO:CB	1:A:1072:MET:HB3	2.39	0.53
1:B:1069:PRO:CB	1:B:1072:MET:HB3	2.39	0.53
1:C:492:PHE:HD1	1:C:554:TYR:CE1	2.22	0.53
1:A:492:PHE:HD1	1:A:554:TYR:HE1	1.56	0.53
1:D:492:PHE:HD1	1:D:554:TYR:HE1	1.55	0.53
1:C:1069:PRO:HB2	1:C:1072:MET:HB3	1.90	0.52
1:A:1069:PRO:HB2	1:A:1072:MET:HB3	1.91	0.52
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	1.91	0.52
1:B:1151:LEU:O	1:B:1155:LEU:HG	2.10	0.52
2:C:2001:TD8:H6'	1:D:901:GLN:OE1	2.10	0.51
1:A:441:ASP:HA	1:A:445:ARG:HG3	1.93	0.51
1:C:1069:PRO:CB	1:C:1072:MET:HB3	2.40	0.51
1:C:492:PHE:CD1	1:C:554:TYR:CE1	2.98	0.51
1:B:483:LEU:HD22	1:B:778:LEU:HD12	1.93	0.51
1:C:415:LEU:HA	1:C:432:LEU:HB3	1.93	0.51
1:C:483:LEU:HD22	1:C:778:LEU:HD12	1.93	0.51
1:D:603:PRO:HG3	1:D:990:GLU:HB3	1.93	0.51
1:D:1020:HIS:HD2	5:D:3165:HOH:O	1.93	0.50
1:A:908:PHE:CZ	1:A:1070:LYS:HG2	2.45	0.50
1:B:491:ALA:HB3	1:B:796:TYR:CD2	2.46	0.50
1:A:362:SER:H	1:A:365:ASP:HB3	1.76	0.50
2:A:2001:TD8:H5BA	1:B:950:LEU:CD1	2.42	0.50
2:D:2001:TD8:C2	2:D:2001:TD8:HN4A	2.25	0.50
1:B:415:LEU:HA	1:B:432:LEU:HB3	1.94	0.50
1:B:538:PRO:HD2	5:B:3032:HOH:O	2.12	0.50
1:D:513:THR:HG21	1:D:717:CYS:SG	2.52	0.49
1:B:1155:LEU:HD11	1:B:1192:PHE:CZ	2.47	0.49
1:C:784:ILE:HD12	1:C:789:ALA:HB2	1.94	0.49
1:A:483:LEU:HD22	1:A:778:LEU:HD12	1.95	0.49
1:A:603:PRO:HG3	1:A:990:GLU:HB3	1.94	0.49
1:A:1155:LEU:HD11	1:A:1192:PHE:CZ	2.47	0.48
1:B:1021:THR:HG21	1:B:1207:SER:HB3	1.94	0.48
1:B:530:LEU:HD22	1:B:636:SER:HA	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:PRO:HD2	5:C:3037:HOH:O	2.13	0.48
1:D:656:GLU:HB3	1:D:954:ALA:HB2	1.96	0.48
2:A:2001:TD8:HN4A	2:A:2001:TD8:C8	2.27	0.47
1:B:656:GLU:HB3	1:B:954:ALA:HB2	1.95	0.47
1:B:1148:ARG:HG3	1:B:1187:ILE:HD12	1.95	0.47
1:C:513:THR:HG21	1:C:717:CYS:SG	2.55	0.47
1:C:530:LEU:HD22	1:C:636:SER:HA	1.96	0.47
1:D:1112:LEU:HD12	1:D:1136:ALA:HB3	1.96	0.47
1:C:656:GLU:HB3	1:C:954:ALA:HB2	1.97	0.47
1:A:513:THR:HG21	1:A:717:CYS:SG	2.55	0.47
1:A:752:ASP:O	1:A:755:MET:HE2	2.15	0.46
1:D:752:ASP:O	1:D:755:MET:HE2	2.15	0.46
1:D:508:LEU:HD13	1:D:541:GLY:HA3	1.98	0.46
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.51	0.46
1:D:565:LEU:HB3	1:D:569:GLN:HB3	1.98	0.46
1:D:1024:ARG:HB2	5:D:3168:HOH:O	2.16	0.46
1:C:1155:LEU:HD11	1:C:1192:PHE:CZ	2.51	0.46
1:A:898:LEU:O	1:A:945:VAL:HA	2.16	0.45
1:A:530:LEU:HD22	1:A:636:SER:HA	1.98	0.45
1:B:898:LEU:O	1:B:945:VAL:HA	2.16	0.45
1:B:1020:HIS:HD2	5:B:3160:HOH:O	1.99	0.45
1:B:480:LYS:HE2	1:B:784:ILE:HG23	1.99	0.45
1:C:908:PHE:CZ	1:C:1070:LYS:HG2	2.52	0.45
1:D:898:LEU:O	1:D:945:VAL:HA	2.17	0.45
1:B:491:ALA:HB3	1:B:796:TYR:CE2	2.52	0.44
1:A:656:GLU:HB3	1:A:954:ALA:HB2	1.99	0.44
1:C:752:ASP:O	1:C:755:MET:HE2	2.16	0.44
1:B:463:ILE:O	1:B:467:VAL:HB	2.18	0.44
1:A:696:THR:HG21	1:A:738:ASP:HB2	2.01	0.43
1:B:492:PHE:HZ	1:B:557:ILE:HG21	1.84	0.42
1:A:1021:THR:HG21	1:A:1207:SER:HB3	2.01	0.42
1:C:845:ASP:OD1	1:C:868:ARG:NE	2.46	0.42
1:C:898:LEU:O	1:C:945:VAL:HA	2.18	0.42
2:B:2001:TD8:C8	2:B:2001:TD8:HN4A	2.31	0.42
1:C:491:ALA:HB3	1:C:796:TYR:CD2	2.55	0.42
1:D:1035:GLY:O	1:D:1062:ARG:HD3	2.20	0.42
1:B:542:ARG:HE	1:B:542:ARG:HB2	1.70	0.42
1:B:603:PRO:HG3	1:B:990:GLU:HB3	2.01	0.42
1:A:604:SER:O	2:A:2001:TD8:N4'	2.43	0.42
1:B:617:VAL:HG11	1:B:639:PRO:HG3	2.02	0.41
1:D:492:PHE:CD1	1:D:554:TYR:HE1	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:MET:HE2	1:A:1117:GLY:HA3	2.03	0.41
1:B:848:LEU:HD12	1:B:868:ARG:HD3	2.01	0.41
1:C:617:VAL:HG11	1:C:639:PRO:HG3	2.03	0.41
1:B:752:ASP:O	1:B:755:MET:HE2	2.21	0.41
1:D:942:LYS:HE3	1:D:944:LEU:HD21	2.02	0.41
1:A:878:TRP:HB3	1:A:1073:LEU:HD23	2.02	0.41
1:D:617:VAL:HG11	1:D:639:PRO:HG3	2.03	0.41
1:D:696:THR:HG21	1:D:738:ASP:HB2	2.02	0.41
1:C:878:TRP:HB3	1:C:1073:LEU:HD23	2.03	0.41
1:B:542:ARG:HG2	1:B:578:TYR:HA	2.03	0.40
1:D:415:LEU:HA	1:D:432:LEU:HB3	2.03	0.40
1:B:708:HIS:HA	1:B:738:ASP:HB3	2.02	0.40
1:D:530:LEU:HD22	1:D:636:SER:HA	2.02	0.40
1:D:603:PRO:HD3	1:D:991:PHE:CZ	2.57	0.40
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.56	0.40
1:A:617:VAL:HG11	1:A:639:PRO:HG3	2.03	0.40
1:C:1151:LEU:O	1:C:1155:LEU:HG	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	840/868 (97%)	821 (98%)	17 (2%)	2 (0%)	47	58
1	B	828/868 (95%)	806 (97%)	19 (2%)	3 (0%)	34	42
1	C	838/868 (96%)	818 (98%)	17 (2%)	3 (0%)	34	42
1	D	844/868 (97%)	821 (97%)	22 (3%)	1 (0%)	51	64
All	All	3350/3472 (96%)	3266 (98%)	75 (2%)	9 (0%)	41	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	636	SER
1	C	605	HIS
1	B	605	HIS
1	A	682	PHE
1	C	682	PHE
1	B	538	PRO
1	C	538	PRO
1	D	538	PRO
1	A	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	671/726 (92%)	664 (99%)	7 (1%)	76	87
1	B	668/726 (92%)	658 (98%)	10 (2%)	65	79
1	C	672/726 (93%)	665 (99%)	7 (1%)	76	87
1	D	679/726 (94%)	674 (99%)	5 (1%)	84	92
All	All	2690/2904 (93%)	2661 (99%)	29 (1%)	73	86

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	514	VAL
1	A	602	ASN
1	A	682	PHE
1	A	740	LEU
1	A	837	LYS
1	A	953	PHE
1	A	976	GLN
1	B	415	LEU
1	B	467	VAL
1	B	542	ARG
1	B	544	ASN
1	B	682	PHE
1	B	909	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	950	LEU
1	B	953	PHE
1	B	976	GLN
1	B	1114	LEU
1	C	464	GLN
1	C	467	VAL
1	C	602	ASN
1	C	682	PHE
1	C	909	THR
1	C	953	PHE
1	C	976	GLN
1	D	682	PHE
1	D	909	THR
1	D	953	PHE
1	D	976	GLN
1	D	1112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	TD8	A	2001	3	30,35,35	1.09	1 (3%)	36,51,51	2.15	12 (33%)
2	TD8	C	2001	3	30,35,35	1.11	2 (6%)	36,51,51	2.32	8 (22%)
2	TD8	B	2001	3	30,35,35	1.37	2 (6%)	36,51,51	2.16	10 (27%)
2	TD8	D	2001	3	30,35,35	1.08	1 (3%)	36,51,51	2.03	8 (22%)

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	TD8	A	2001	3	-	3/22/27/27	0/2/2/2
2	TD8	C	2001	3	-	12/22/27/27	0/2/2/2
2	TD8	B	2001	3	-	7/22/27/27	0/2/2/2
2	TD8	D	2001	3	-	7/22/27/27	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	TD8	C5A-C5	5.53	1.53	1.50
2	D	2001	TD8	O9-C8	-3.94	1.33	1.42
2	A	2001	TD8	O9-C8	-3.86	1.34	1.42
2	C	2001	TD8	O9-C8	-3.75	1.34	1.42
2	B	2001	TD8	O9-C8	-3.56	1.34	1.42
2	C	2001	TD8	C5A-C5	2.59	1.52	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2001	TD8	C5A-C5-C4	9.87	135.35	127.43
2	B	2001	TD8	C5A-C5-C4	8.43	134.20	127.43
2	A	2001	TD8	C5A-C5-C4	8.34	134.13	127.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2001	TD8	C5A-C5-C4	7.09	133.12	127.43
2	D	2001	TD8	C2A-C2'-N1'	4.00	121.54	117.14
2	C	2001	TD8	C2A-C2'-N1'	3.66	121.16	117.14
2	C	2001	TD8	N1'-C2'-N3'	-3.52	119.49	125.54
2	B	2001	TD8	C2A-C2'-N1'	3.46	120.94	117.14
2	D	2001	TD8	N1'-C2'-N3'	-3.33	119.81	125.54
2	B	2001	TD8	C6'-N1'-C2'	3.22	121.44	115.96
2	B	2001	TD8	N1'-C2'-N3'	-3.16	120.10	125.54
2	C	2001	TD8	C6'-N1'-C2'	3.13	121.28	115.96
2	D	2001	TD8	C6'-N1'-C2'	3.09	121.22	115.96
2	C	2001	TD8	C4A-C4-C5	-3.04	120.96	127.60
2	A	2001	TD8	C2A-C2'-N1'	3.01	120.45	117.14
2	A	2001	TD8	N1'-C2'-N3'	-2.84	120.65	125.54
2	B	2001	TD8	C5-C4-N3	2.76	113.42	107.66
2	D	2001	TD8	C4A-C4-C5	-2.73	121.64	127.60
2	B	2001	TD8	C4A-C4-C5	-2.71	121.68	127.60
2	C	2001	TD8	C5-C4-N3	2.66	113.21	107.66
2	A	2001	TD8	C4A-C4-C5	-2.64	121.82	127.60
2	A	2001	TD8	C6'-N1'-C2'	2.59	120.38	115.96
2	A	2001	TD8	C4A-C4-N3	2.47	125.80	122.69
2	C	2001	TD8	C4A-C4-N3	2.43	125.75	122.69
2	D	2001	TD8	C5-C4-N3	2.37	112.62	107.66
2	A	2001	TD8	O3B-PB-O1B	2.35	116.61	107.64
2	D	2001	TD8	C4A-C4-N3	2.35	125.64	122.69
2	B	2001	TD8	C10-C9-C8	-2.33	106.75	113.82
2	A	2001	TD8	O9-C8-C9	2.29	118.40	109.55
2	B	2001	TD8	O1B-PB-O3A	2.23	112.11	104.64
2	A	2001	TD8	C5'-C6'-N1'	-2.18	120.18	123.82
2	A	2001	TD8	C6'-C5'-C4'	2.18	118.68	115.72
2	C	2001	TD8	O12-C14-C12	-2.17	116.12	123.08
2	B	2001	TD8	C5'-C6'-N1'	-2.08	120.35	123.82
2	D	2001	TD8	O5G-PA-O1A	-2.08	100.94	109.07
2	A	2001	TD8	C10-C9-C8	-2.05	107.59	113.82
2	A	2001	TD8	C5-C4-N3	2.05	111.95	107.66
2	B	2001	TD8	O9-C8-C9	2.01	117.32	109.55

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	TD8	C2-C8-C9-C10
2	B	2001	TD8	C2-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2001	TD8	PA-O3A-PB-O1B
2	B	2001	TD8	PA-O3A-PB-O3B
2	B	2001	TD8	C5-C5A-C5B-O5G
2	C	2001	TD8	C2-C8-C9-C10
2	C	2001	TD8	O9-C8-C9-C10
2	C	2001	TD8	C5B-O5G-PA-O3A
2	C	2001	TD8	PA-O3A-PB-O1B
2	C	2001	TD8	C5-C5A-C5B-O5G
2	D	2001	TD8	C2-C8-C9-C10
2	D	2001	TD8	O9-C8-C9-C10
2	D	2001	TD8	C9-C10-C12-C14
2	C	2001	TD8	PA-O3A-PB-O3B
2	B	2001	TD8	C5B-O5G-PA-O3A
2	C	2001	TD8	C5B-O5G-PA-O1A
2	C	2001	TD8	C5B-O5G-PA-O2A
2	D	2001	TD8	C10-C12-C14-O11
2	D	2001	TD8	C12-C10-C9-C8
2	D	2001	TD8	C10-C12-C14-O12
2	C	2001	TD8	C10-C12-C14-O12
2	A	2001	TD8	C10-C12-C14-O11
2	A	2001	TD8	C10-C12-C14-O12
2	B	2001	TD8	C10-C12-C14-O11
2	D	2001	TD8	N3-C35-C5'-C4'
2	C	2001	TD8	PA-O3A-PB-O2B
2	C	2001	TD8	C10-C12-C14-O11
2	B	2001	TD8	C10-C12-C14-O12
2	C	2001	TD8	C12-C10-C9-C8

There are no ring outliers.

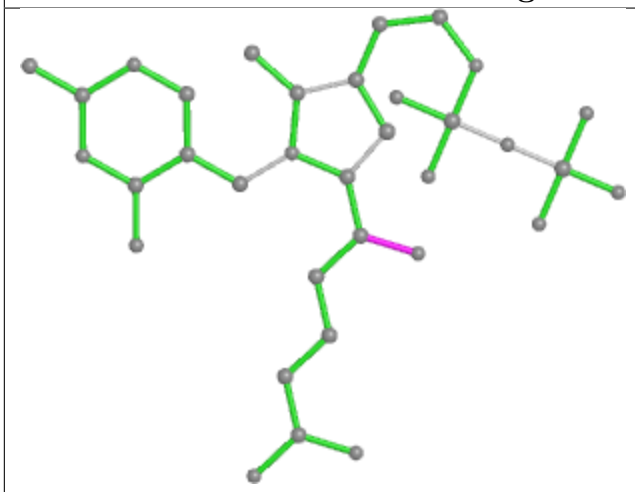
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	TD8	6	0
2	C	2001	TD8	1	0
2	B	2001	TD8	2	0
2	D	2001	TD8	4	0

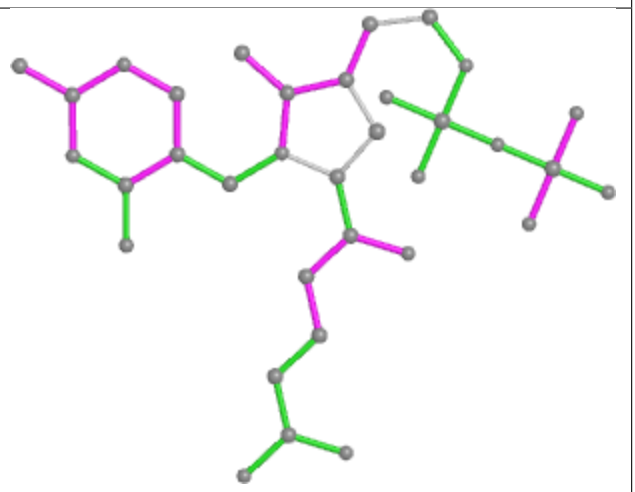
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

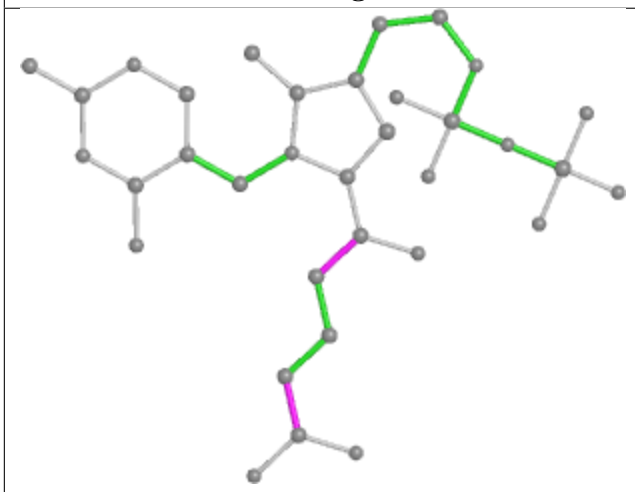
Ligand TD8 A 2001



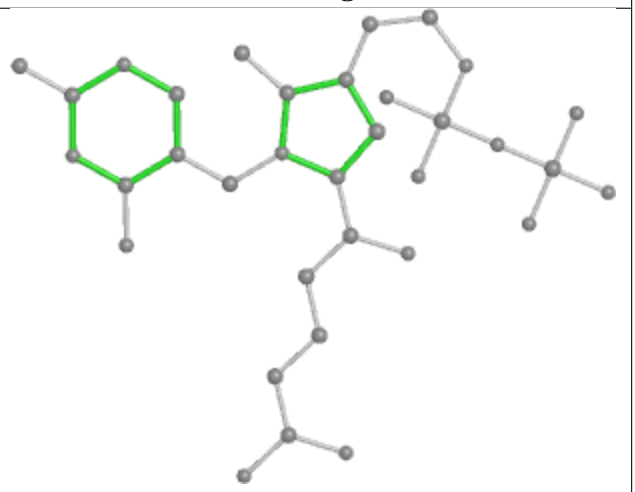
Bond lengths



Bond angles

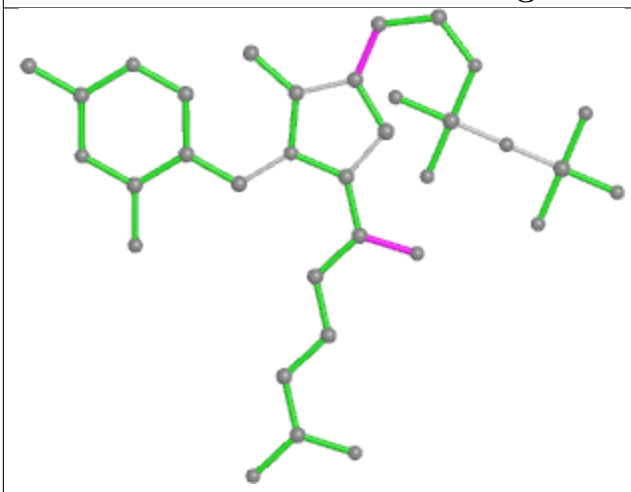


Torsions

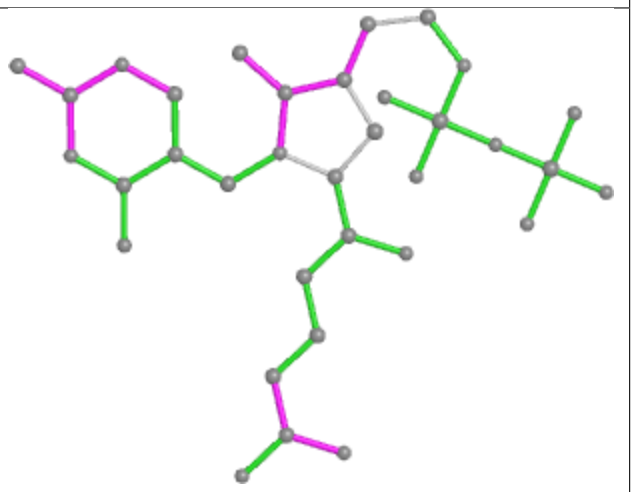


Rings

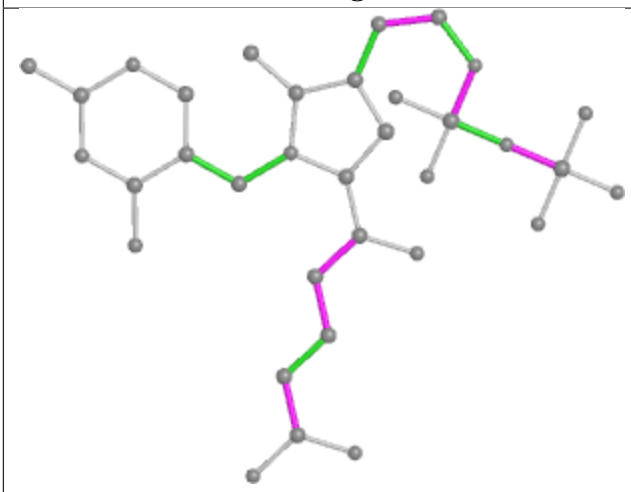
Ligand TD8 C 2001



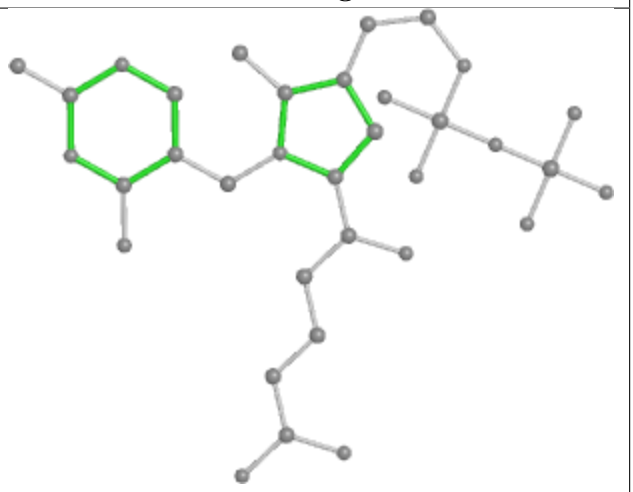
Bond lengths



Bond angles

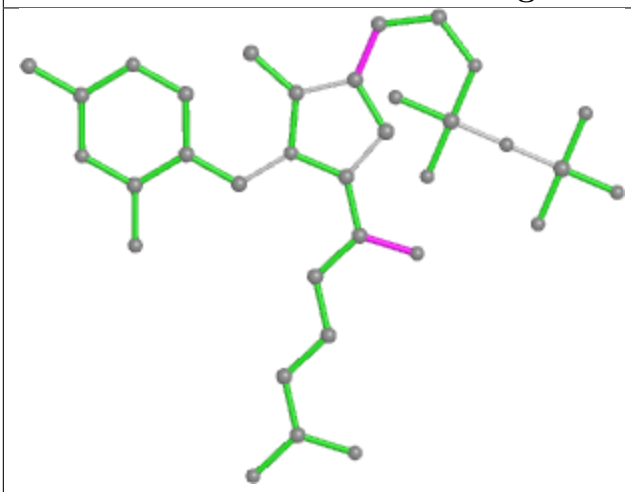


Torsions

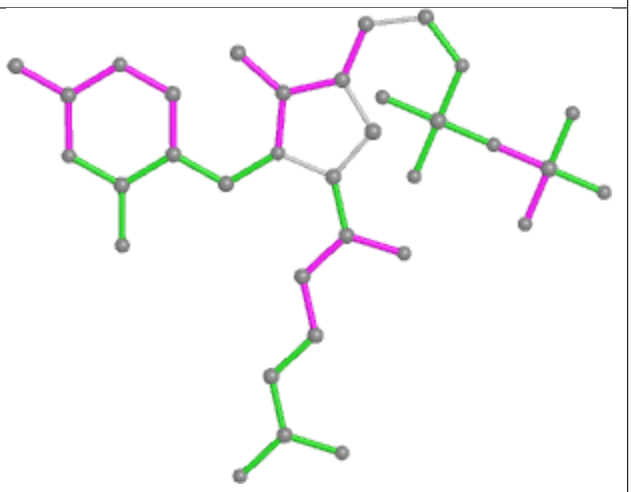


Rings

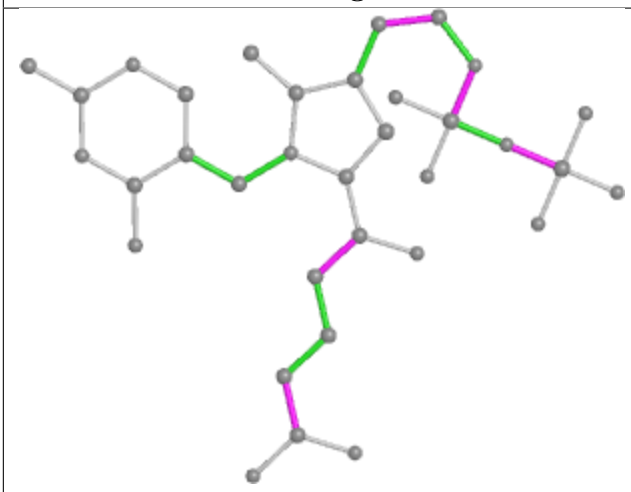
Ligand TD8 B 2001



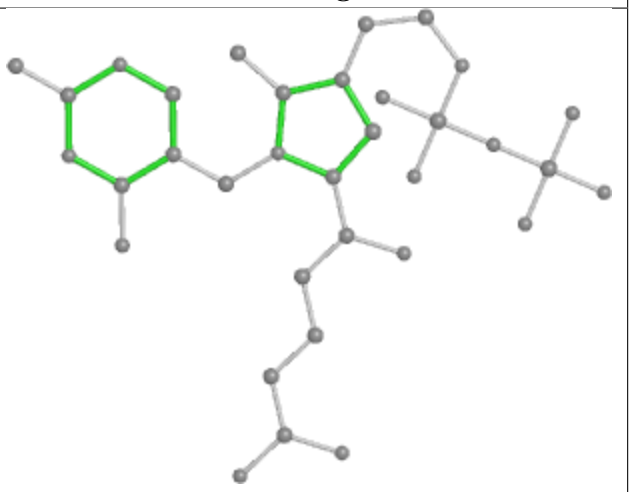
Bond lengths



Bond angles

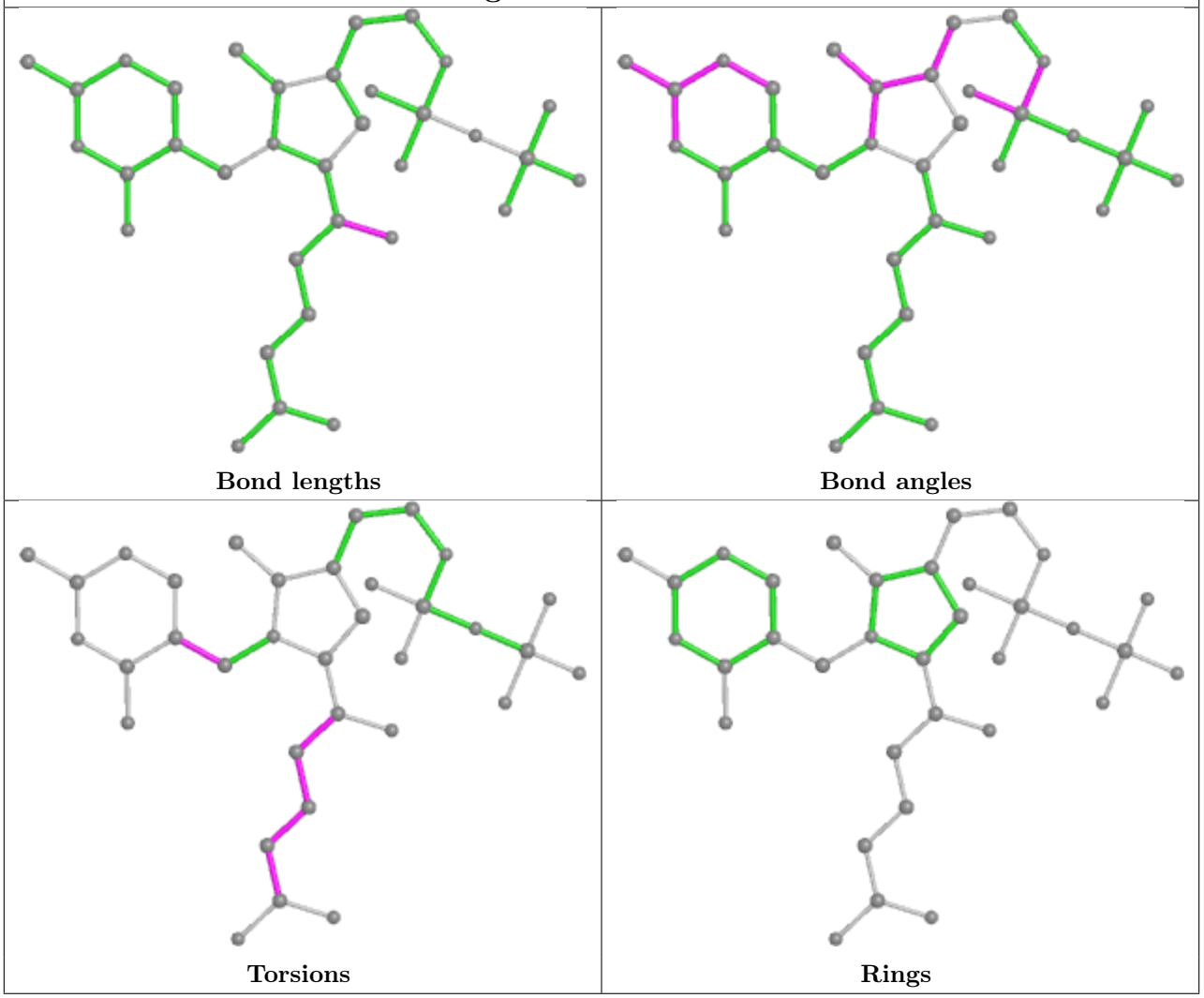


Torsions



Rings

Ligand TD8 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	847/868 (97%)	0.47	73 (8%)	10	14	23, 41, 74, 103	0
1	B	836/868 (96%)	0.26	42 (5%)	28	35	22, 36, 65, 94	0
1	C	845/868 (97%)	0.28	36 (4%)	35	42	22, 36, 65, 114	0
1	D	852/868 (98%)	0.46	65 (7%)	13	18	22, 40, 73, 109	0
All	All	3380/3472 (97%)	0.37	216 (6%)	19	25	22, 38, 70, 114	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	421	VAL	10.6
1	A	570	ALA	7.6
1	A	569	GLN	7.3
1	C	570	ALA	7.2
1	C	420	LYS	6.4
1	A	571	HIS	6.0
1	A	568	SER	5.9
1	A	502	GLY	5.8
1	B	368	ALA	5.8
1	D	368	ALA	5.7
1	A	410	LEU	5.5
1	C	569	GLN	5.5
1	A	779	ILE	5.3
1	D	427	VAL	5.0
1	B	571	HIS	4.9
1	C	397	PHE	4.8
1	C	419	PHE	4.8
1	C	571	HIS	4.8
1	D	803	VAL	4.8
1	A	368	ALA	4.7
1	A	807	VAL	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	371	ILE	4.6
1	D	426	GLY	4.6
1	A	394	ASN	4.4
1	A	567	PRO	4.4
1	A	370	VAL	4.4
1	D	568	SER	4.3
1	A	566	ASN	4.2
1	C	790	GLU	4.2
1	D	410	LEU	4.2
1	D	571	HIS	4.1
1	A	790	GLU	4.1
1	C	394	ASN	4.1
1	A	427	VAL	4.0
1	B	426	GLY	4.0
1	B	815	ILE	4.0
1	D	567	PRO	4.0
1	D	365	ASP	3.8
1	D	796	TYR	3.8
1	D	816	GLU	3.7
1	D	569	GLN	3.7
1	D	1152	ALA	3.7
1	C	568	SER	3.6
1	D	570	ALA	3.6
1	D	471	HIS	3.6
1	B	953	PHE	3.6
1	C	565	LEU	3.6
1	B	807	VAL	3.5
1	D	831	LEU	3.5
1	A	810	LEU	3.5
1	A	815	ILE	3.4
1	D	395	THR	3.4
1	A	698	VAL	3.4
1	A	1152	ALA	3.4
1	C	395	THR	3.3
1	C	415	LEU	3.3
1	C	368	ALA	3.2
1	D	394	ASN	3.2
1	A	1148	ARG	3.2
1	D	564	ASN	3.2
1	D	827	ILE	3.2
1	A	803	VAL	3.2
1	C	366	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	653	VAL	3.1
1	B	792	ALA	3.1
1	B	655	ALA	3.0
1	D	473	LYS	3.0
1	A	809	GLU	3.0
1	A	831	LEU	3.0
1	B	633	ASN	3.0
1	B	827	ILE	2.9
1	A	558	PHE	2.9
1	A	421	VAL	2.9
1	A	395	THR	2.9
1	A	589	MET	2.9
1	C	815	ILE	2.8
1	D	366	LYS	2.8
1	A	780	GLY	2.8
1	B	823	ALA	2.8
1	B	563	GLY	2.8
1	A	592	ASP	2.8
1	B	986	SER	2.8
1	B	790	GLU	2.8
1	D	804	PHE	2.8
1	D	828	PRO	2.8
1	D	631	SER	2.7
1	B	392	LEU	2.7
1	B	983	GLY	2.7
1	B	652	GLY	2.7
1	A	1190	ASP	2.7
1	D	779	ILE	2.7
1	D	414	ASP	2.7
1	D	848	LEU	2.7
1	C	409	GLY	2.7
1	D	393	ASP	2.7
1	D	783	ASP	2.7
1	A	823	ALA	2.6
1	D	813	HIS	2.6
1	B	698	VAL	2.6
1	B	803	VAL	2.6
1	D	934	PRO	2.6
1	C	435	ILE	2.6
1	A	414	ASP	2.6
1	A	472	ASP	2.6
1	C	655	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	983	GLY	2.6
1	D	654	VAL	2.6
1	B	565	LEU	2.6
1	C	558	PHE	2.6
1	C	984	ALA	2.6
1	D	502	GLY	2.6
1	D	421	VAL	2.5
1	D	810	LEU	2.5
1	A	420	LYS	2.5
1	A	1110	THR	2.5
1	D	805	ASN	2.5
1	A	1157	ARG	2.5
1	D	367	ASN	2.5
1	A	796	TYR	2.5
1	B	457	PRO	2.5
1	B	427	VAL	2.5
1	B	987	ILE	2.5
1	A	654	VAL	2.4
1	A	655	ALA	2.4
1	B	1028	PHE	2.4
1	C	814	GLU	2.4
1	C	810	LEU	2.4
1	B	608	ALA	2.4
1	D	1103	GLU	2.4
1	C	410	LEU	2.4
1	A	478	GLU	2.4
1	C	1225	ALA	2.4
1	B	779	ILE	2.4
1	D	1110	THR	2.4
1	A	432	LEU	2.4
1	D	397	PHE	2.4
1	D	815	ILE	2.3
1	D	931	ALA	2.3
1	D	937	THR	2.3
1	D	953	PHE	2.3
1	A	471	HIS	2.3
1	D	422	ASP	2.3
1	D	792	ALA	2.3
1	A	986	SER	2.3
1	B	1129	LYS	2.3
1	A	634	ARG	2.3
1	A	822	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	501	VAL	2.3
1	C	564	ASN	2.3
1	B	954	ALA	2.3
1	A	814	GLU	2.2
1	B	981	VAL	2.2
1	D	826	GLN	2.2
1	A	445	ARG	2.2
1	B	988	ILE	2.2
1	C	796	TYR	2.2
1	B	1067	PHE	2.2
1	D	1105	ASP	2.2
1	A	806	GLU	2.2
1	B	370	VAL	2.2
1	A	931	ALA	2.2
1	B	1025	ILE	2.2
1	C	786	MET	2.2
1	D	787	LYS	2.2
1	A	653	VAL	2.2
1	A	1105	ASP	2.2
1	D	472	ASP	2.2
1	B	813	HIS	2.2
1	A	371	ILE	2.2
1	B	828	PRO	2.2
1	A	1194	GLY	2.2
1	A	363	ILE	2.2
1	B	992	ILE	2.2
1	A	1112	LEU	2.2
1	A	563	GLY	2.2
1	C	787	LYS	2.1
1	D	572	GLY	2.2
1	C	476	VAL	2.1
1	D	429	ARG	2.1
1	A	792	ALA	2.1
1	C	789	ALA	2.1
1	D	814	GLU	2.1
1	A	365	ASP	2.1
1	C	1129	LYS	2.1
1	D	1128	ALA	2.1
1	D	1136	ALA	2.1
1	A	594	ASP	2.1
1	A	930	LEU	2.1
1	A	393	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	654	VAL	2.1
1	C	572	GLY	2.1
1	A	642	LEU	2.1
1	A	647	ALA	2.1
1	A	777	ALA	2.1
1	A	650	GLY	2.1
1	A	978	GLY	2.1
1	B	419	PHE	2.1
1	C	1112	LEU	2.1
1	D	657	THR	2.1
1	D	1162	LYS	2.1
1	D	609	VAL	2.1
1	C	567	PRO	2.1
1	C	371	ILE	2.0
1	D	566	ASN	2.0
1	A	1102	GLY	2.0
1	D	608	ALA	2.0
1	A	804	PHE	2.0
1	A	1028	PHE	2.0
1	B	991	PHE	2.0
1	D	1025	ILE	2.0
1	A	644	GLY	2.0
1	A	1216	VAL	2.0
1	A	1103	GLU	2.0
1	B	415	LEU	2.0
1	D	634	ARG	2.0
1	B	975	ALA	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,

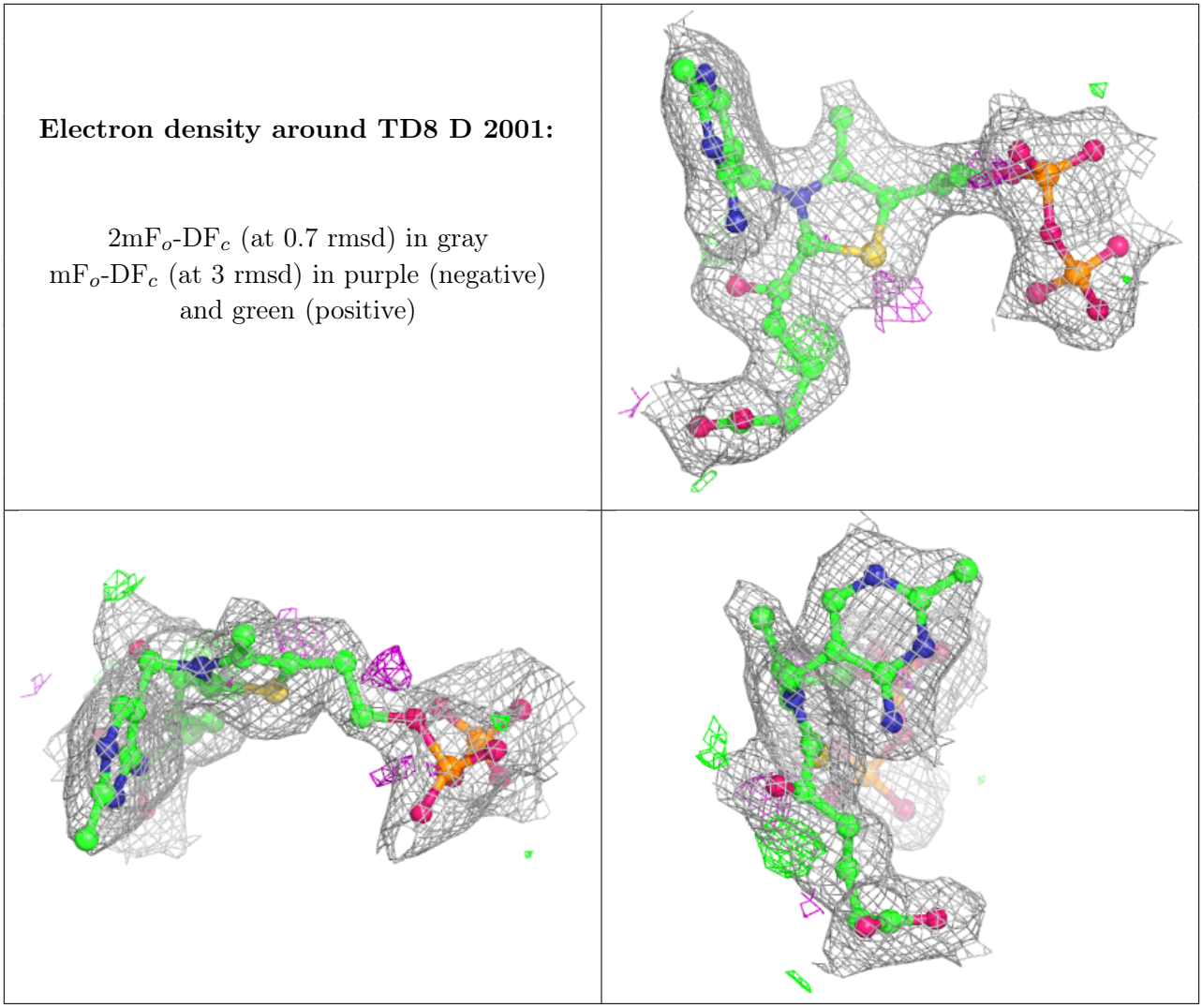
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	2002	1/1	0.95	0.12	26,26,26,26	0
2	TD8	D	2001	34/34	0.96	0.14	19,26,41,43	0
2	TD8	C	2001	34/34	0.96	0.14	16,28,44,48	0
4	CA	A	2003	1/1	0.96	0.07	41,41,41,41	0
2	TD8	A	2001	34/34	0.97	0.14	16,30,40,41	0
3	MG	D	2002	1/1	0.97	0.09	25,25,25,25	0
2	TD8	B	2001	34/34	0.97	0.13	17,28,34,37	0
4	CA	D	2003	1/1	0.97	0.08	41,41,41,41	0
3	MG	C	2002	1/1	0.98	0.10	12,12,12,12	0
4	CA	B	2003	1/1	0.99	0.04	29,29,29,29	0
4	CA	C	2003	1/1	0.99	0.10	28,28,28,28	0
3	MG	B	2002	1/1	0.99	0.05	17,17,17,17	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.

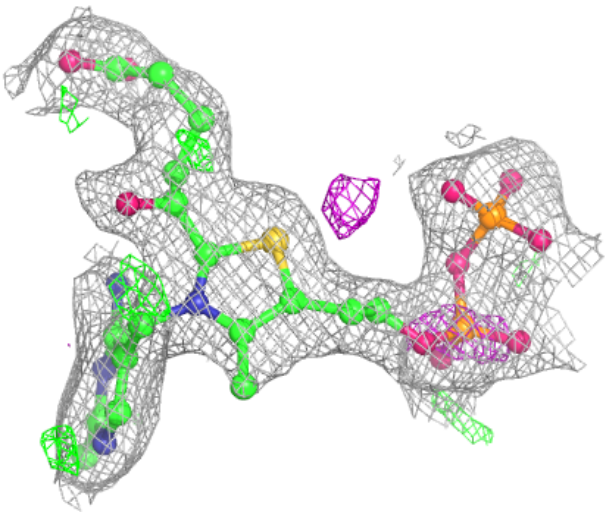
Electron density around TD8 D 2001:

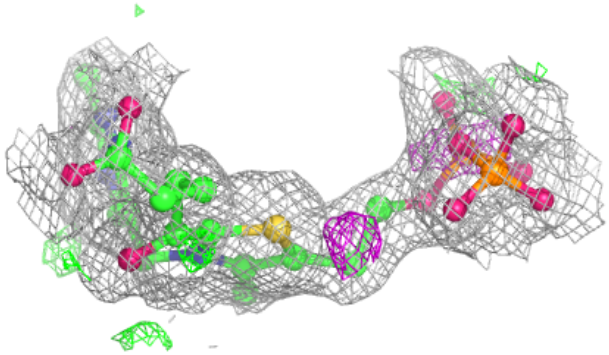
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

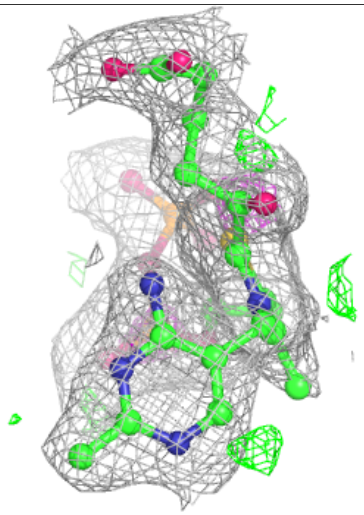


Electron density around TD8 C 2001:

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

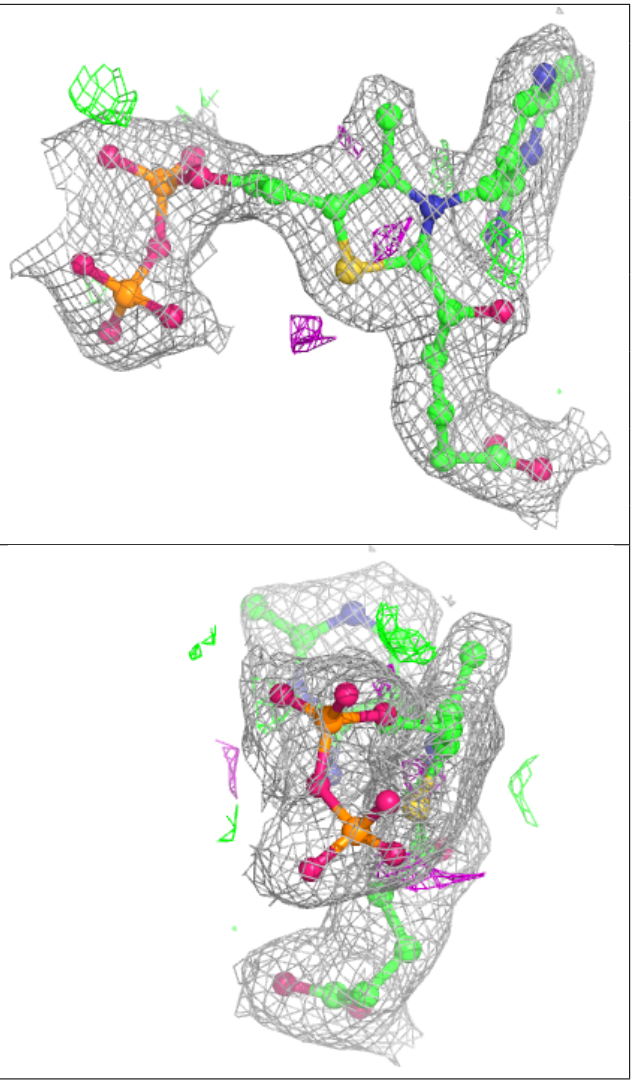






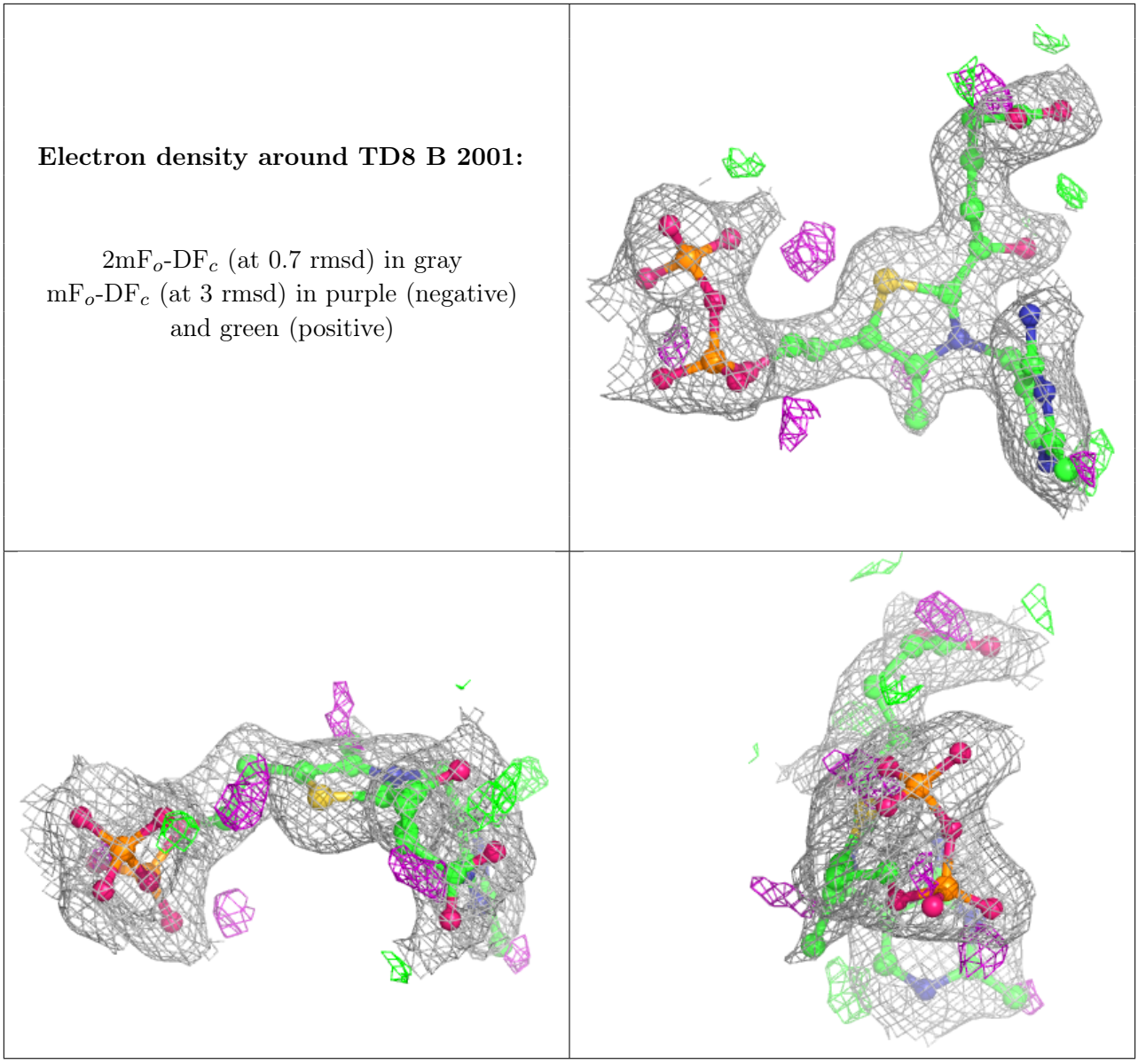
Electron density around TD8 A 2001:

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



Electron density around TD8 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

There are no such residues in this entry.