



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:36 AM UTC

PDB ID : 3ZHS / pdb_00003zhs
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis KGD, first post-decarboxylation intermediate from alpha-ketoglutarate
Authors : Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.
Deposited on : 2012-12-24
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

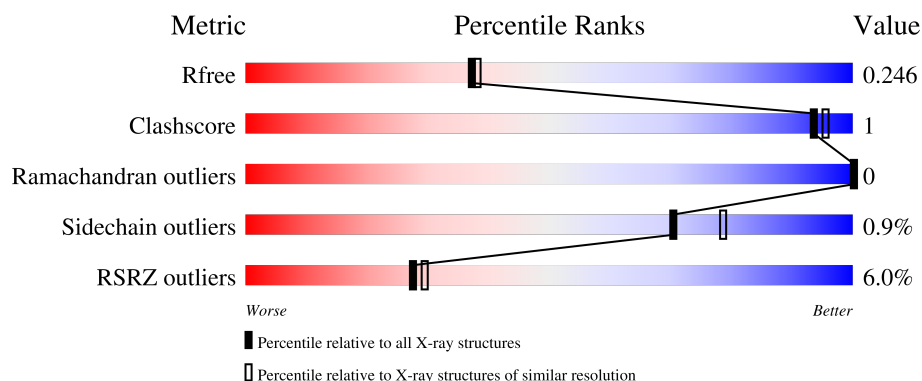
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	868	4% 88% 6% 6%
1	B	868	6% 89% 5% 6%
1	C	868	6% 88% 5% 7%
1	D	868	7% 88% 5% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26258 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	817	Total	C	N	O	S	0	0	0
			6319	3983	1114	1200	22			
1	B	813	Total	C	N	O	S	0	0	0
			6254	3946	1106	1179	23			
1	C	808	Total	C	N	O	S	0	0	0
			6280	3962	1108	1187	23			
1	D	810	Total	C	N	O	S	0	0	0
			6225	3926	1102	1173	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 (4S)-4-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-(2-{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}ethyl)-4-methyl-1,3lambda 5 -thiazol-2-yl}-4-hydroxybutanoic acid (CCD ID: TD6) (formula: C₁₆H₂₅N₄O₁₀P₂S).



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

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

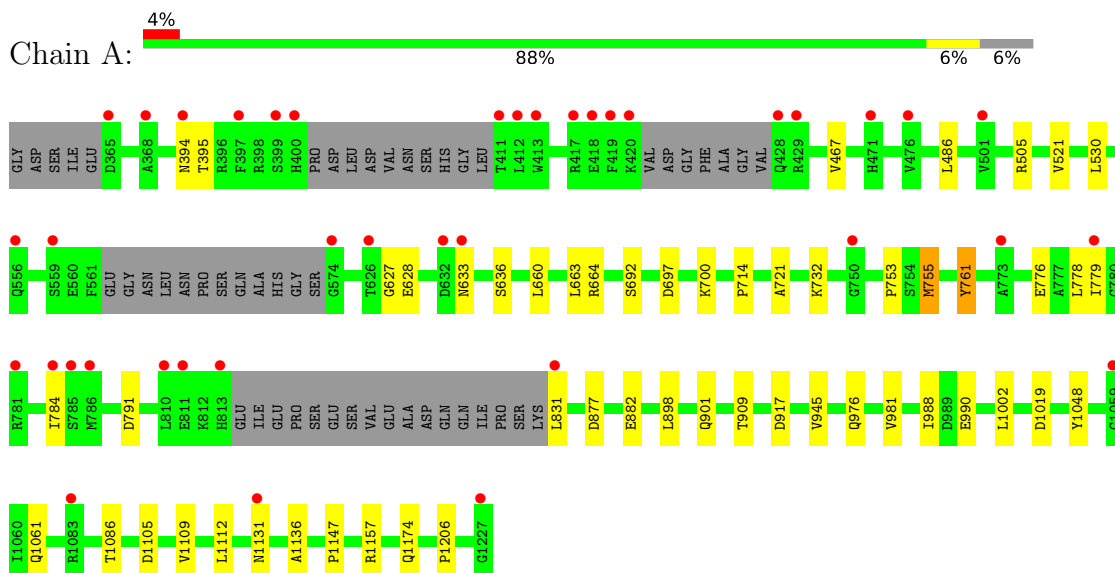
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	316	Total 316	O 316	0	0
5	B	241	Total 241	O 241	0	0
5	C	272	Total 272	O 272	0	0
5	D	211	Total 211	O 211	0	0

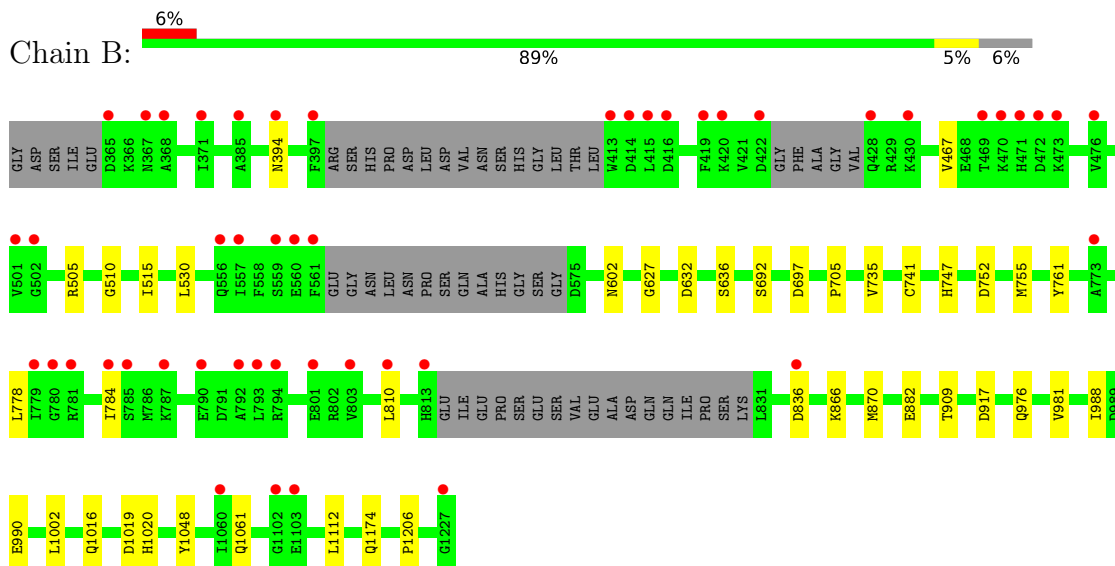
3 Residue-property plots [i](#)

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.

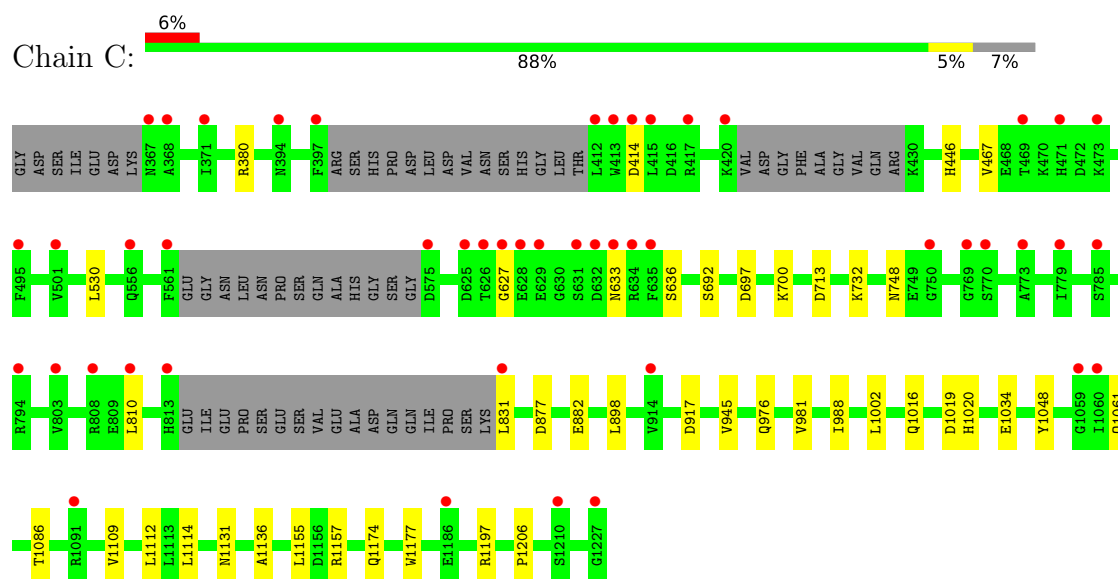
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



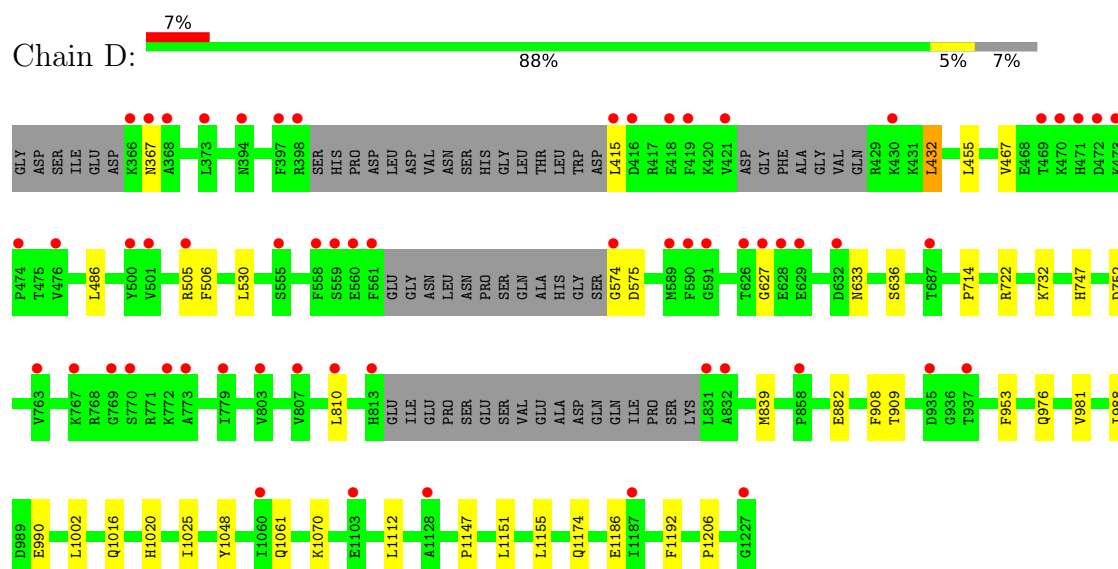
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.85Å 83.71Å 159.94Å 99.89° 99.03° 100.20°	Depositor
Resolution (Å)	30.75 – 2.10 30.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.75-2.10) 94.5 (30.75-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.200 , 0.228 0.215 , 0.246	Depositor DCC
R_{free} test set	10967 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26258	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, TD6, 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	0.86	1/6448 (0.0%)	1.21	15/8749 (0.2%)
1	B	0.85	1/6381 (0.0%)	1.22	9/8661 (0.1%)
1	C	0.85	0/6407	1.23	10/8684 (0.1%)
1	D	0.85	1/6351 (0.0%)	1.23	12/8615 (0.1%)
All	All	0.85	3/25587 (0.0%)	1.22	46/34709 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	839	MET	SD-CE	-6.72	1.62	1.79
1	B	515	ILE	CA-C	5.07	1.58	1.52
1	A	755	MET	SD-CE	5.03	1.92	1.79

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	836	ASP	CA-CB-CG	7.88	120.48	112.60
1	A	394	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	791	ASP	CA-CB-CG	5.83	118.42	112.60
1	D	575	ASP	CA-C-N	5.60	129.49	120.30
1	D	575	ASP	C-N-CA	5.60	129.49	120.30
1	D	627	GLY	CA-C-N	5.56	127.73	120.28
1	D	627	GLY	C-N-CA	5.56	127.73	120.28
1	A	1147	PRO	CA-C-N	5.55	128.03	120.54
1	A	1147	PRO	C-N-CA	5.55	128.03	120.54
1	C	627	GLY	CA-C-N	5.55	128.03	120.54
1	C	627	GLY	C-N-CA	5.55	128.03	120.54
1	B	632	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	627	GLY	CA-C-N	5.48	127.89	120.38
1	A	627	GLY	C-N-CA	5.48	127.89	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	877	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	761	TYR	CA-CB-CG	-5.40	104.19	113.90
1	B	761	TYR	CA-CB-CG	-5.38	104.22	113.90
1	C	877	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	602	ASN	N-CA-C	5.37	113.05	108.22
1	C	414	ASP	CA-C-N	5.36	129.67	120.72
1	C	414	ASP	C-N-CA	5.36	129.67	120.72
1	D	752	ASP	CB-CA-C	5.28	115.19	110.44
1	D	1186	GLU	CA-C-N	5.27	127.90	120.42
1	D	1186	GLU	C-N-CA	5.27	127.90	120.42
1	C	917	ASP	CA-C-N	5.21	127.79	120.28
1	C	917	ASP	C-N-CA	5.21	127.79	120.28
1	D	1147	PRO	CA-C-N	5.21	127.57	120.54
1	D	1147	PRO	C-N-CA	5.21	127.57	120.54
1	A	917	ASP	CA-C-N	5.15	127.70	120.28
1	A	917	ASP	C-N-CA	5.15	127.70	120.28
1	A	700	LYS	CA-C-N	5.14	127.42	120.38
1	A	700	LYS	C-N-CA	5.14	127.42	120.38
1	B	752	ASP	CB-CA-C	5.10	115.03	110.44
1	B	627	GLY	CA-C-N	5.09	127.35	120.38
1	B	627	GLY	C-N-CA	5.09	127.35	120.38
1	D	953	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	1105	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	700	LYS	CA-C-N	5.06	127.31	120.38
1	C	700	LYS	C-N-CA	5.06	127.31	120.38
1	B	917	ASP	CA-C-N	5.05	127.56	120.28
1	B	917	ASP	C-N-CA	5.05	127.56	120.28
1	D	1025	ILE	CA-C-N	5.05	127.56	120.28
1	D	1025	ILE	C-N-CA	5.05	127.56	120.28
1	C	748	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	395	THR	CA-C-N	5.03	127.27	120.38
1	A	395	THR	C-N-CA	5.03	127.27	120.38

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	6319	0	6087	24	0
1	B	6254	0	6025	16	0
1	C	6280	0	6099	19	0
1	D	6225	0	6004	17	0
2	A	33	0	21	0	0
2	B	33	0	21	1	0
2	C	33	0	21	0	0
2	D	33	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	316	0	0	1	0
5	B	241	0	0	0	0
5	C	272	0	0	0	0
5	D	211	0	0	1	0
All	All	26258	0	24299	68	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 (68) 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:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.77	0.65
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.84	0.59
1:A:1157:ARG:NH2	1:C:1086:THR:O	2.33	0.58
1:C:1109:VAL:HG21	1:C:1136:ALA:HB2	1.84	0.58
1:C:380:ARG:NH1	1:D:455:LEU:O	2.33	0.56
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.89	0.54
1:D:1151:LEU:O	1:D:1155:LEU:HG	2.08	0.52
1:B:505:ARG:HA	1:B:747:HIS:O	2.09	0.52
1:D:415:LEU:HA	1:D:432:LEU:HD12	1.91	0.52
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.91	0.52
1:B:882:GLU:HB2	1:B:1048:TYR:HE2	1.75	0.51
1:A:486:LEU:HD11	1:A:714:PRO:HG3	1.93	0.50
1:A:1086:THR:O	1:C:1157:ARG:NH2	2.40	0.50
1:A:753:PRO:HB2	1:A:761:TYR:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:LEU:HD22	1:B:636:SER:HA	1.94	0.49
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.94	0.48
1:A:778:LEU:HB3	1:A:784:ILE:HG12	1.96	0.48
1:A:909:THR:HG21	1:B:755:MET:HE1	1.96	0.47
1:C:446:HIS:ND1	1:C:713:ASP:OD2	2.47	0.47
1:D:506:PHE:CZ	1:D:574:GLY:HA2	2.50	0.46
1:A:1109:VAL:HG21	1:A:1136:ALA:HB2	1.97	0.46
1:A:755:MET:HE1	1:B:909:THR:HG21	1.97	0.46
1:A:628:GLU:HG2	1:A:664:ARG:O	2.16	0.46
1:A:1019:ASP:OD1	1:B:990:GLU:OE1	2.34	0.46
1:C:530:LEU:HD22	1:C:636:SER:HA	1.98	0.45
1:D:882:GLU:HB2	1:D:1048:TYR:HE2	1.81	0.45
1:D:722:ARG:NH1	5:D:3087:HOH:O	2.50	0.45
1:A:692:SER:HB2	1:A:697:ASP:OD2	2.17	0.45
1:D:633:ASN:O	1:D:732:LYS:HE3	2.17	0.45
1:A:776:GLU:HA	1:A:779:ILE:HD12	1.99	0.44
1:A:882:GLU:HB2	1:A:1048:TYR:HE2	1.82	0.44
1:D:486:LEU:HD11	1:D:714:PRO:HG3	1.99	0.44
1:C:1112:LEU:HD23	1:C:1114:LEU:HD11	2.00	0.44
1:D:530:LEU:HD22	1:D:636:SER:HA	2.00	0.44
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.52	0.44
1:D:1002:LEU:HB3	1:D:1061:GLN:HB2	2.00	0.43
1:A:660:LEU:HA	1:A:663:LEU:HD12	2.01	0.43
1:A:1174:GLN:OE1	1:A:1206:PRO:HA	2.18	0.43
1:D:505:ARG:HA	1:D:747:HIS:O	2.19	0.43
1:D:1155:LEU:HD11	1:D:1192:PHE:CZ	2.54	0.43
1:D:1174:GLN:OE1	1:D:1206:PRO:HA	2.19	0.43
1:B:705:PRO:HG2	1:B:735:VAL:HG13	2.01	0.42
1:C:692:SER:HB2	1:C:697:ASP:OD2	2.20	0.42
1:C:633:ASN:O	1:C:732:LYS:HE2	2.19	0.42
1:B:1016:GLN:HB3	1:B:1020:HIS:HB2	2.01	0.42
1:A:990:GLU:OE1	1:B:1019:ASP:OD1	2.38	0.42
1:C:1112:LEU:CD2	1:C:1155:LEU:HD22	2.46	0.42
1:C:1019:ASP:OD1	1:D:990:GLU:OE1	2.37	0.42
1:C:1002:LEU:HB3	1:C:1061:GLN:CB	2.50	0.42
1:C:1016:GLN:HB3	1:C:1020:HIS:HB2	2.02	0.42
1:B:866:LYS:HG3	1:B:870:MET:HE2	2.02	0.42
1:D:1016:GLN:HB3	1:D:1020:HIS:HB2	2.01	0.42
1:A:521:VAL:HG23	1:A:721:ALA:HB1	2.02	0.41
1:A:898:LEU:O	1:A:945:VAL:HA	2.20	0.41
1:B:1002:LEU:HB3	1:B:1061:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ARG:HG2	5:A:3024:HOH:O	2.21	0.41
1:B:1174:GLN:OE1	1:B:1206:PRO:HA	2.21	0.41
1:C:898:LEU:O	1:C:945:VAL:HA	2.19	0.41
1:C:1174:GLN:OE1	1:C:1206:PRO:HA	2.20	0.41
1:A:633:ASN:O	1:A:732:LYS:HE2	2.21	0.41
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.56	0.41
1:A:901:GLN:OE1	2:B:2001:TD6:H6'	2.21	0.40
1:C:882:GLU:HB2	1:C:1048:TYR:HE2	1.86	0.40
1:B:692:SER:HB2	1:B:697:ASP:OD2	2.22	0.40
1:B:778:LEU:HB3	1:B:784:ILE:HG12	2.02	0.40
1:B:510:GLY:O	1:B:741:CYS:HB2	2.22	0.40
1:A:530:LEU:HD22	1:A:636:SER:HA	2.03	0.40
1:A:1002:LEU:HB3	1:A:1061:GLN:HB2	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	807/868 (93%)	786 (97%)	21 (3%)	0	100	100
1	B	803/868 (92%)	784 (98%)	19 (2%)	0	100	100
1	C	798/868 (92%)	777 (97%)	21 (3%)	0	100	100
1	D	800/868 (92%)	779 (97%)	21 (3%)	0	100	100
All	All	3208/3472 (92%)	3126 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	649/726 (89%)	644 (99%)	5 (1%)	73	81
1	B	638/726 (88%)	633 (99%)	5 (1%)	73	81
1	C	649/726 (89%)	643 (99%)	6 (1%)	70	78
1	D	634/726 (87%)	627 (99%)	7 (1%)	65	74
All	All	2570/2904 (88%)	2547 (99%)	23 (1%)	70	78

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

Mol	Chain	Res	Type
1	A	467	VAL
1	A	831	LEU
1	A	976	GLN
1	A	1112	LEU
1	A	1131	ASN
1	B	394	ASN
1	B	467	VAL
1	B	810	LEU
1	B	976	GLN
1	B	1112	LEU
1	C	467	VAL
1	C	810	LEU
1	C	831	LEU
1	C	976	GLN
1	C	1034	GLU
1	C	1131	ASN
1	D	367	ASN
1	D	432	LEU
1	D	467	VAL
1	D	810	LEU
1	D	909	THR
1	D	976	GLN
1	D	1112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	497	GLN
1	A	503	GLN
1	A	1001	GLN
1	A	1030	GLN
1	B	497	GLN
1	B	503	GLN
1	B	524	GLN
1	B	797	GLN
1	B	1001	GLN
1	B	1061	GLN
1	B	1219	GLN
1	C	503	GLN
1	C	524	GLN
1	C	556	GLN
1	C	797	GLN
1	C	947	ASN
1	C	1001	GLN
1	C	1030	GLN
1	C	1219	GLN
1	D	503	GLN
1	D	524	GLN
1	D	556	GLN
1	D	797	GLN
1	D	933	ASN
1	D	1001	GLN
1	D	1030	GLN
1	D	1061	GLN

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 oligosaccharides 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	TD6	C	2001	3	31,34,34	1.42	6 (19%)	38,50,50	1.55	9 (23%)
2	TD6	B	2001	3	31,34,34	1.44	6 (19%)	38,50,50	1.55	8 (21%)
2	TD6	D	2001	3	31,34,34	1.64	6 (19%)	38,50,50	1.59	8 (21%)
2	TD6	A	2001	3	31,34,34	1.39	5 (16%)	38,50,50	1.56	9 (23%)

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	TD6	C	2001	3	-	7/25/26/26	0/2/2/2
2	TD6	B	2001	3	-	6/25/26/26	0/2/2/2
2	TD6	D	2001	3	-	6/25/26/26	0/2/2/2
2	TD6	A	2001	3	-	5/25/26/26	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	TD6	PA-O3A	-5.94	1.53	1.59
2	C	2001	TD6	PA-O3A	-4.35	1.54	1.59
2	B	2001	TD6	PA-O3A	-4.28	1.54	1.59
2	A	2001	TD6	C5-C4	4.04	1.43	1.35
2	A	2001	TD6	PA-O3A	-4.02	1.55	1.59
2	D	2001	TD6	C5-S1	-3.82	1.66	1.74
2	B	2001	TD6	C5-S1	-3.49	1.67	1.74
2	C	2001	TD6	C5-S1	-3.39	1.67	1.74
2	D	2001	TD6	C5-C4	3.08	1.41	1.35
2	D	2001	TD6	OL2-CLC	-2.90	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	TD6	C11-C2	2.81	1.55	1.51
2	B	2001	TD6	C11-C2	2.77	1.55	1.51
2	B	2001	TD6	C5-C4	2.75	1.41	1.35
2	D	2001	TD6	OL3-CLC	2.75	1.31	1.22
2	B	2001	TD6	OL2-CLC	-2.73	1.21	1.30
2	A	2001	TD6	OL3-CLC	2.70	1.30	1.22
2	C	2001	TD6	OL3-CLC	2.66	1.30	1.22
2	C	2001	TD6	C5-C4	2.60	1.40	1.35
2	C	2001	TD6	OL2-CLC	-2.48	1.22	1.30
2	B	2001	TD6	OL3-CLC	2.47	1.30	1.22
2	A	2001	TD6	OL2-CLC	-2.45	1.22	1.30
2	A	2001	TD6	C5-S1	-2.40	1.69	1.74
2	D	2001	TD6	C11-C2	2.13	1.54	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	TD6	O2A-PA-O3A	-3.73	97.20	107.27
2	D	2001	TD6	O2A-PA-O3A	-3.50	97.82	107.27
2	C	2001	TD6	O2A-PA-O3A	-3.47	97.89	107.27
2	A	2001	TD6	O2A-PA-O3A	-3.37	98.16	107.27
2	C	2001	TD6	OL3-CLC-C13	-3.28	112.68	123.09
2	A	2001	TD6	C7'-N3-C4	3.27	129.41	123.95
2	A	2001	TD6	OL3-CLC-C13	-3.17	113.03	123.09
2	D	2001	TD6	C7'-N3-C4	3.06	129.06	123.95
2	C	2001	TD6	OL2-CLC-C13	3.04	123.62	114.00
2	B	2001	TD6	OL3-CLC-C13	-3.04	113.47	123.09
2	D	2001	TD6	OL3-CLC-C13	-2.95	113.74	123.09
2	A	2001	TD6	OL2-CLC-C13	2.93	123.25	114.00
2	D	2001	TD6	OL2-CLC-C13	2.92	123.23	114.00
2	D	2001	TD6	O7-PA-O1A	2.89	120.40	108.94
2	B	2001	TD6	OL2-CLC-C13	2.88	123.10	114.00
2	B	2001	TD6	O7-PA-O1A	2.77	119.93	108.94
2	C	2001	TD6	O3A-PA-O1A	2.75	118.97	110.70
2	A	2001	TD6	O1B-PB-O3A	-2.73	95.46	104.64
2	C	2001	TD6	C7'-N3-C4	2.63	128.36	123.95
2	A	2001	TD6	O7-PA-O1A	2.62	119.34	108.94
2	D	2001	TD6	O3A-PA-O1A	2.60	118.53	110.70
2	B	2001	TD6	C7'-N3-C4	2.60	128.29	123.95
2	D	2001	TD6	O1B-PB-O3A	-2.47	96.35	104.64
2	B	2001	TD6	O1B-PB-O3A	-2.46	96.38	104.64
2	A	2001	TD6	O3A-PA-O1A	2.45	118.08	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	TD6	O7-PA-O1A	2.35	118.25	108.94
2	A	2001	TD6	C6-C5-S1	2.32	124.28	119.29
2	C	2001	TD6	C7'-C5'-C4'	2.29	126.54	122.36
2	C	2001	TD6	O1B-PB-O3A	-2.26	97.06	104.64
2	B	2001	TD6	O3A-PA-O1A	2.23	117.42	110.70
2	B	2001	TD6	C13-CLB-C11	2.08	117.70	114.48
2	D	2001	TD6	O3B-PB-O2B	2.06	118.85	110.83
2	A	2001	TD6	O3B-PB-O2B	2.02	118.69	110.83
2	C	2001	TD6	O3B-PB-O2B	2.00	118.65	110.83

There are no chirality outliers.

All (24) torsion outliers are listed below:

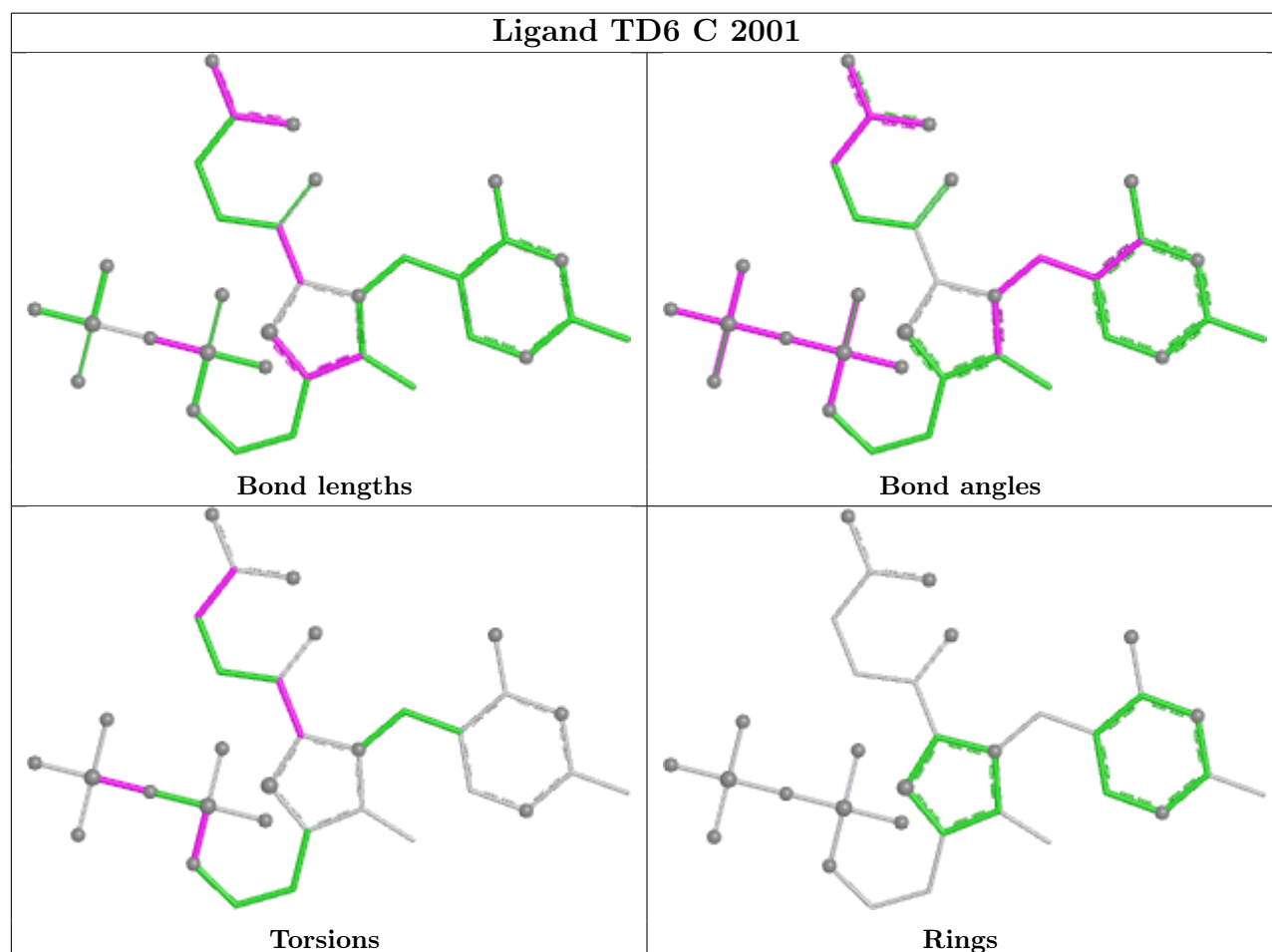
Mol	Chain	Res	Type	Atoms
2	A	2001	TD6	OL1-C11-C2-S1
2	A	2001	TD6	OL1-C11-C2-N3
2	B	2001	TD6	OL1-C11-C2-N3
2	C	2001	TD6	OL1-C11-C2-S1
2	C	2001	TD6	OL1-C11-C2-N3
2	D	2001	TD6	OL1-C11-C2-S1
2	D	2001	TD6	OL1-C11-C2-N3
2	A	2001	TD6	PA-O3A-PB-O2B
2	C	2001	TD6	PA-O3A-PB-O2B
2	D	2001	TD6	PA-O3A-PB-O2B
2	B	2001	TD6	OL1-C11-C2-S1
2	B	2001	TD6	PA-O3A-PB-O1B
2	C	2001	TD6	PA-O3A-PB-O1B
2	D	2001	TD6	PA-O3A-PB-O1B
2	C	2001	TD6	C7-O7-PA-O1A
2	B	2001	TD6	PA-O3A-PB-O2B
2	B	2001	TD6	CLB-C13-CLC-OL2
2	D	2001	TD6	CLB-C13-CLC-OL2
2	A	2001	TD6	CLB-C13-CLC-OL2
2	C	2001	TD6	CLB-C13-CLC-OL3
2	C	2001	TD6	CLB-C13-CLC-OL2
2	A	2001	TD6	CLB-C13-CLC-OL3
2	B	2001	TD6	CLB-C13-CLC-OL3
2	D	2001	TD6	CLB-C13-CLC-OL3

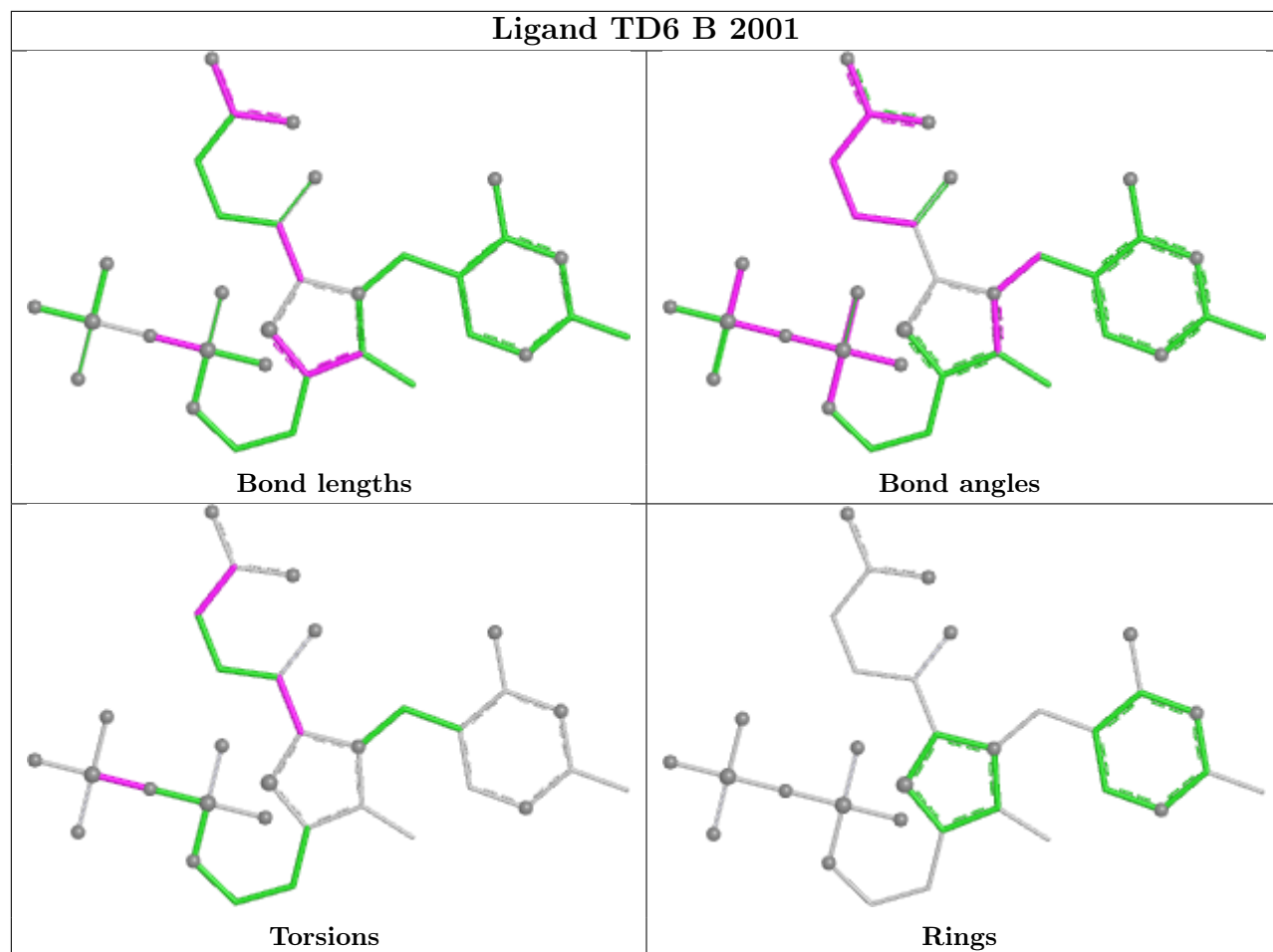
There are no ring outliers.

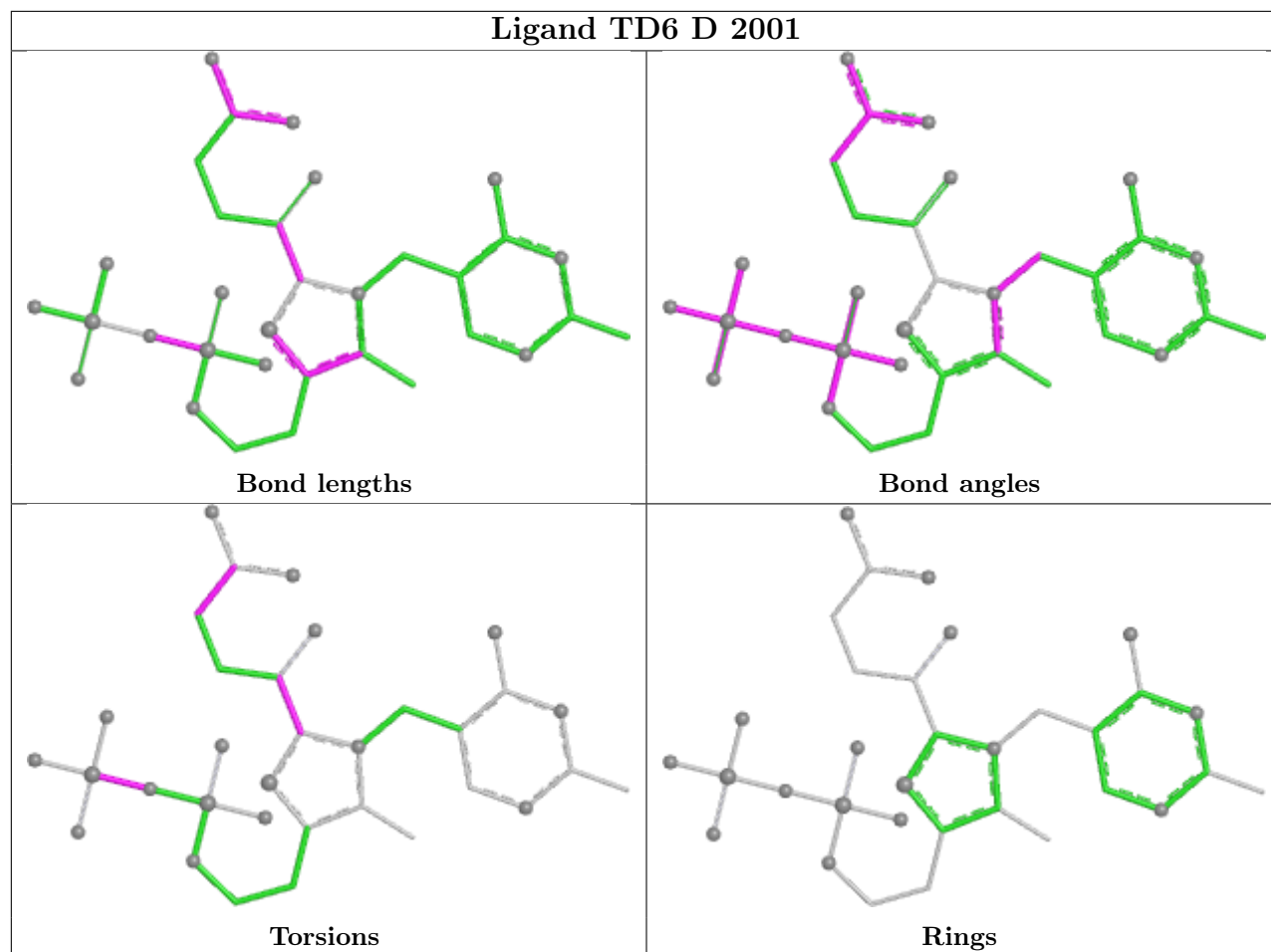
1 monomer is involved in 1 short contact:

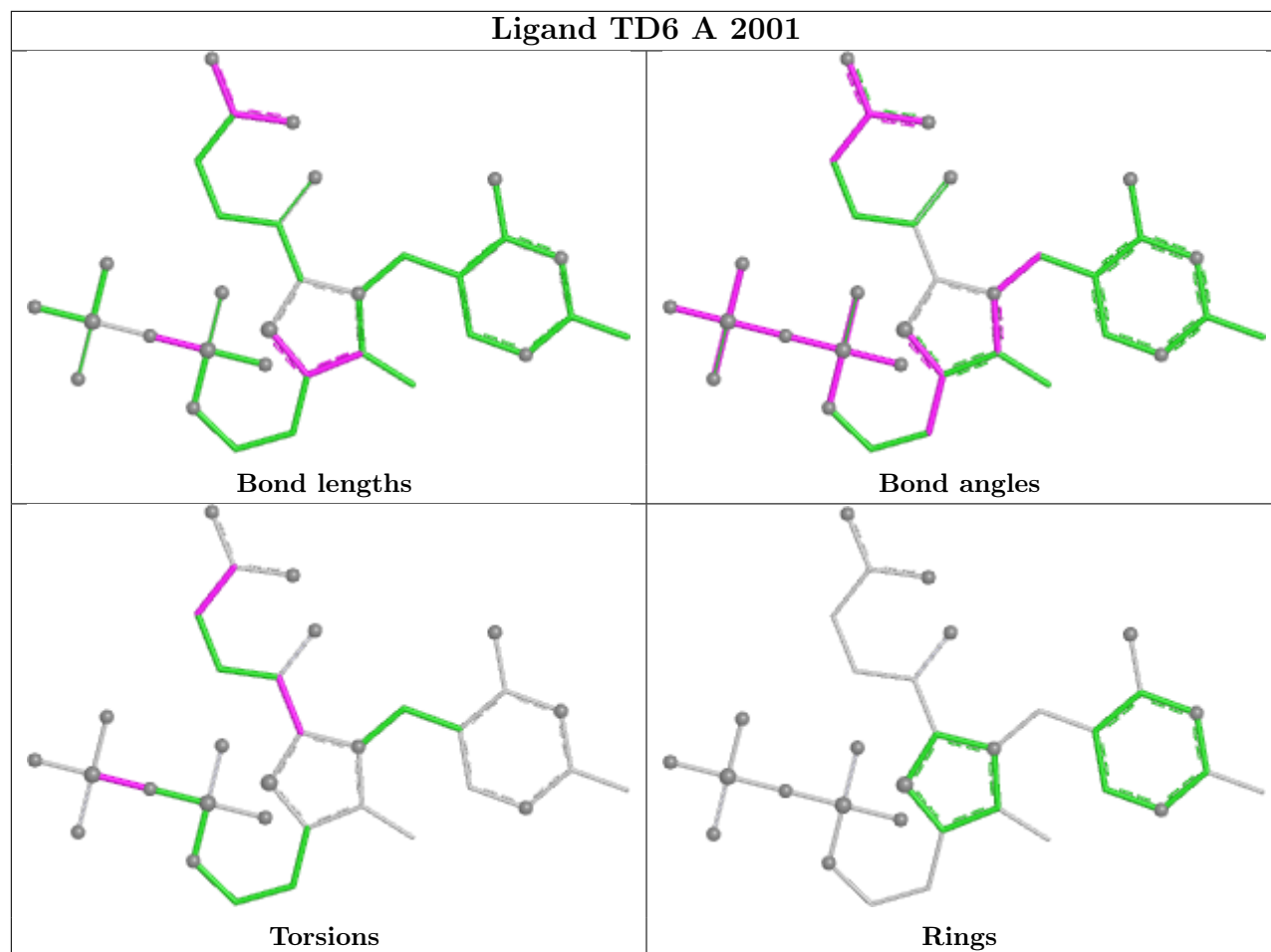
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	TD6	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	817/868 (94%)	0.31	39 (4%) 35 38	15, 32, 59, 82	0
1	B	813/868 (93%)	0.44	49 (6%) 27 29	15, 32, 66, 101	0
1	C	808/868 (93%)	0.49	48 (5%) 28 30	18, 35, 64, 92	0
1	D	810/868 (93%)	0.59	59 (7%) 21 22	17, 35, 66, 96	0
All	All	3248/3472 (93%)	0.46	195 (6%) 27 29	15, 33, 64, 101	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	561	PHE	6.3
1	A	365	ASP	6.1
1	D	574	GLY	5.9
1	B	413	TRP	5.7
1	D	421	VAL	5.3
1	A	411	THR	5.1
1	B	810	LEU	4.9
1	C	626	THR	4.9
1	D	935	ASP	4.9
1	C	813	HIS	4.8
1	A	813	HIS	4.8
1	B	422	ASP	4.8
1	C	413	TRP	4.6
1	B	1102	GLY	4.5
1	C	810	LEU	4.2
1	D	415	LEU	4.2
1	B	780	GLY	4.2
1	D	813	HIS	4.2
1	B	561	PHE	4.2
1	D	810	LEU	4.2
1	C	831	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	779	ILE	4.1
1	C	629	GLU	4.0
1	C	501	VAL	4.0
1	C	750	GLY	4.0
1	B	813	HIS	3.9
1	D	398	ARG	3.9
1	C	628	GLU	3.9
1	B	472	ASP	3.8
1	C	785	SER	3.8
1	C	412	LEU	3.8
1	B	365	ASP	3.7
1	C	367	ASN	3.7
1	B	501	VAL	3.7
1	D	471	HIS	3.7
1	D	807	VAL	3.6
1	D	831	LEU	3.6
1	C	633	ASN	3.6
1	D	476	VAL	3.5
1	D	419	PHE	3.5
1	A	400	HIS	3.5
1	D	470	LYS	3.5
1	A	501	VAL	3.5
1	C	368	ALA	3.4
1	C	575	ASP	3.4
1	D	1227	GLY	3.4
1	B	368	ALA	3.3
1	C	1227	GLY	3.2
1	B	470	LYS	3.2
1	C	632	ASP	3.2
1	B	794	ARG	3.2
1	A	420	LYS	3.2
1	D	416	ASP	3.1
1	D	368	ALA	3.1
1	D	367	ASN	3.1
1	D	770	SER	3.1
1	D	469	THR	3.1
1	D	472	ASP	3.1
1	D	632	ASP	3.1
1	B	473	LYS	3.0
1	A	574	GLY	3.0
1	B	560	GLU	3.0
1	B	414	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	781	ARG	3.0
1	A	399	SER	3.0
1	D	394	ASN	3.0
1	A	626	THR	3.0
1	B	476	VAL	2.9
1	D	628	GLU	2.9
1	A	368	ALA	2.9
1	D	366	LYS	2.9
1	C	803	VAL	2.9
1	D	501	VAL	2.9
1	A	785	SER	2.9
1	C	1210	SER	2.9
1	C	808	ARG	2.9
1	B	793	LEU	2.8
1	C	779	ILE	2.8
1	C	631	SER	2.8
1	C	469	THR	2.8
1	B	785	SER	2.8
1	C	394	ASN	2.8
1	A	1083	ARG	2.8
1	B	397	PHE	2.8
1	A	810	LEU	2.8
1	B	420	LYS	2.8
1	D	1103	GLU	2.8
1	A	750	GLY	2.8
1	B	419	PHE	2.8
1	B	792	ALA	2.8
1	D	763	VAL	2.8
1	C	770	SER	2.7
1	C	914	VAL	2.7
1	D	589	MET	2.7
1	B	790	GLU	2.7
1	A	428	GLN	2.7
1	B	428	GLN	2.7
1	A	394	ASN	2.7
1	A	633	ASN	2.7
1	B	784	ILE	2.7
1	D	773	ALA	2.7
1	C	414	ASP	2.7
1	C	397	PHE	2.6
1	A	471	HIS	2.6
1	B	394	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	471	HIS	2.6
1	C	473	LYS	2.6
1	D	626	THR	2.6
1	B	415	LEU	2.6
1	A	556	GLN	2.6
1	D	560	GLU	2.6
1	D	1128	ALA	2.6
1	D	1187	ILE	2.6
1	A	773	ALA	2.6
1	C	634	ARG	2.6
1	C	415	LEU	2.6
1	C	495	PHE	2.5
1	D	397	PHE	2.5
1	D	803	VAL	2.5
1	A	831	LEU	2.5
1	D	430	LYS	2.5
1	D	937	THR	2.5
1	B	371	ILE	2.5
1	C	371	ILE	2.5
1	D	779	ILE	2.5
1	D	832	ALA	2.5
1	A	784	ILE	2.5
1	B	556	GLN	2.4
1	C	556	GLN	2.4
1	B	773	ALA	2.4
1	C	773	ALA	2.4
1	D	772	LYS	2.4
1	A	1059	GLY	2.4
1	D	505	ARG	2.4
1	C	635	PHE	2.4
1	D	590	PHE	2.4
1	C	1060	ILE	2.4
1	B	430	LYS	2.4
1	B	1227	GLY	2.4
1	D	591	GLY	2.3
1	A	786	MET	2.3
1	D	767	LYS	2.3
1	C	769	GLY	2.3
1	A	632	ASP	2.3
1	A	429	ARG	2.3
1	A	476	VAL	2.3
1	A	413	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	625	ASP	2.3
1	D	500	TYR	2.3
1	C	420	LYS	2.3
1	D	555	SER	2.3
1	A	419	PHE	2.3
1	C	561	PHE	2.3
1	D	858	PRO	2.3
1	B	385	ALA	2.3
1	A	1227	GLY	2.3
1	A	412	LEU	2.3
1	B	1103	GLU	2.2
1	B	559	SER	2.2
1	A	779	ILE	2.2
1	B	801	GLU	2.2
1	C	1186	GLU	2.2
1	B	787	LYS	2.2
1	D	1060	ILE	2.2
1	B	416	ASP	2.2
1	D	627	GLY	2.2
1	C	794	ARG	2.2
1	D	473	LYS	2.2
1	D	687	THR	2.2
1	C	1059	GLY	2.2
1	C	1091	ARG	2.2
1	B	557	ILE	2.1
1	D	418	GLU	2.1
1	C	471	HIS	2.1
1	D	559	SER	2.1
1	B	367	ASN	2.1
1	B	469	THR	2.1
1	B	1060	ILE	2.1
1	D	769	GLY	2.1
1	A	417	ARG	2.1
1	B	502	GLY	2.1
1	C	627	GLY	2.1
1	B	803	VAL	2.1
1	A	418	GLU	2.1
1	D	629	GLU	2.1
1	A	1131	ASN	2.1
1	A	397	PHE	2.1
1	D	373	LEU	2.0
1	B	836	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	781	ARG	2.0
1	A	811	GLU	2.0
1	D	558	PHE	2.0
1	A	559	SER	2.0
1	C	417	ARG	2.0
1	D	474	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

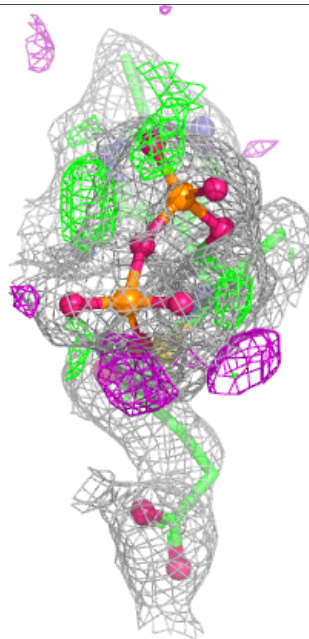
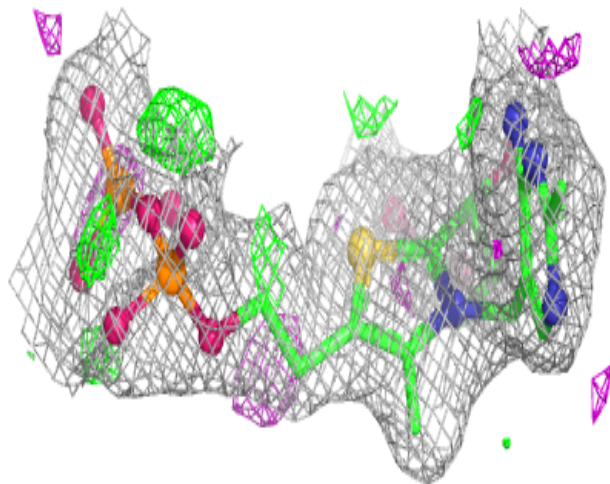
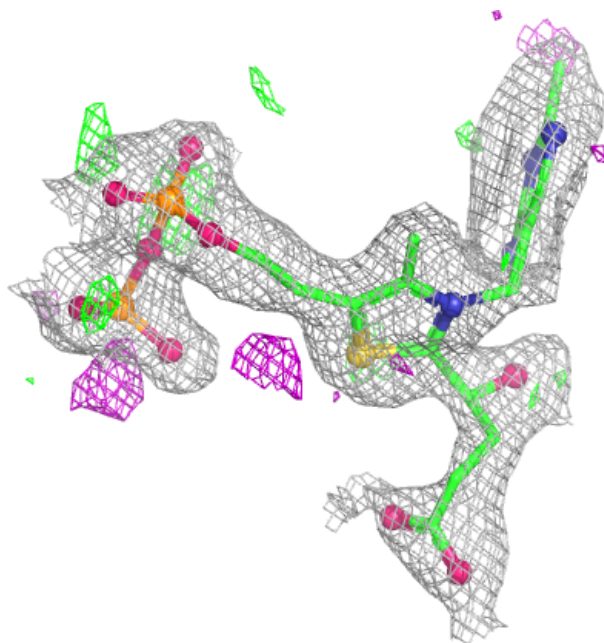
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TD6	B	2001	33/33	0.96	0.09	12,23,48,50	0
2	TD6	C	2001	33/33	0.96	0.09	19,23,46,49	0
4	CA	C	2003	1/1	0.96	0.06	33,33,33,33	0
2	TD6	D	2001	33/33	0.97	0.08	13,24,48,53	0
3	MG	B	2002	1/1	0.97	0.03	17,17,17,17	0
3	MG	D	2002	1/1	0.97	0.05	19,19,19,19	0
2	TD6	A	2001	33/33	0.97	0.07	15,21,46,48	0
3	MG	A	2002	1/1	0.99	0.05	12,12,12,12	0
4	CA	A	2003	1/1	0.99	0.04	29,29,29,29	0
4	CA	B	2003	1/1	0.99	0.04	29,29,29,29	0
3	MG	C	2002	1/1	0.99	0.06	14,14,14,14	0
4	CA	D	2003	1/1	0.99	0.04	31,31,31,31	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.

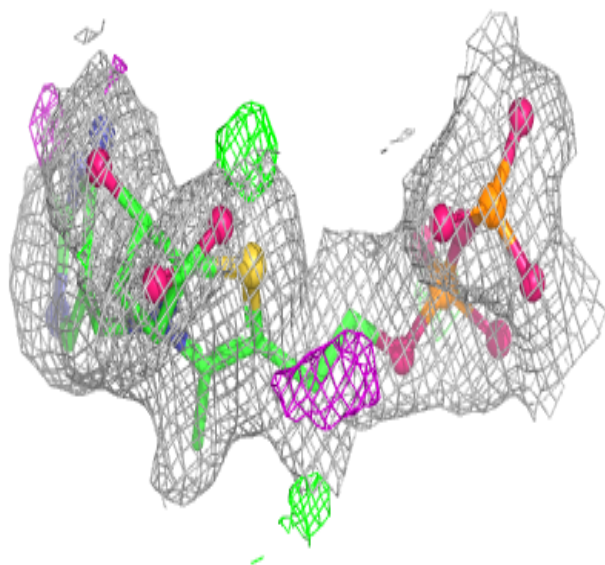
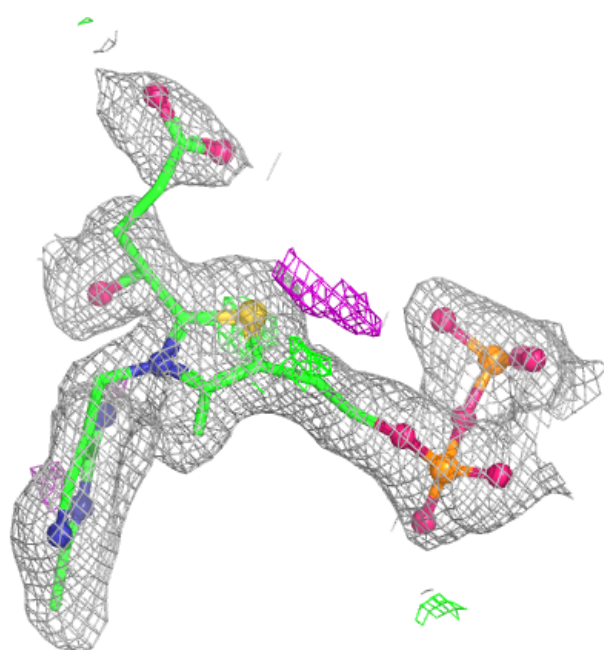
Electron density around TD6 B 2001:

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



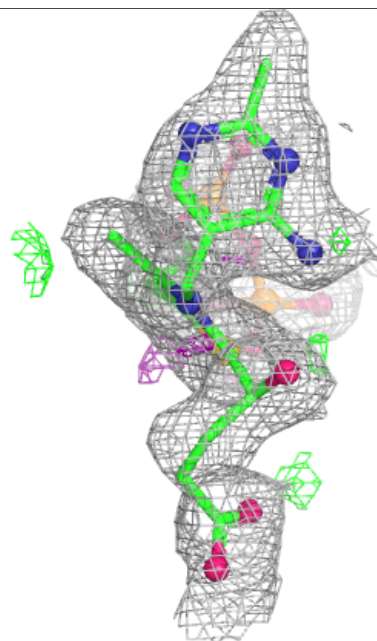
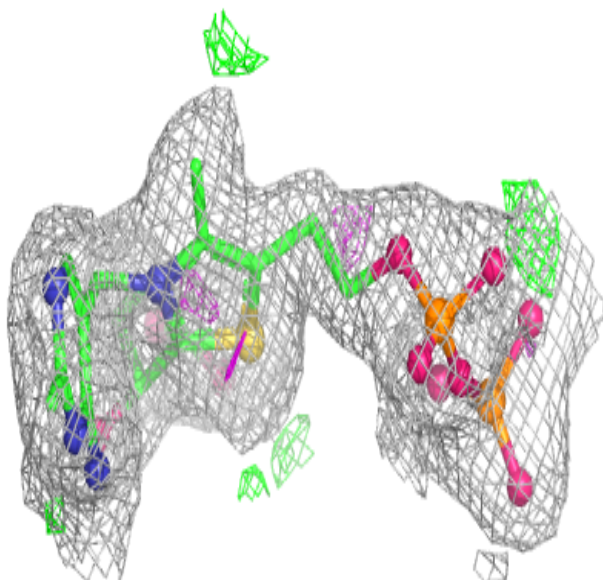
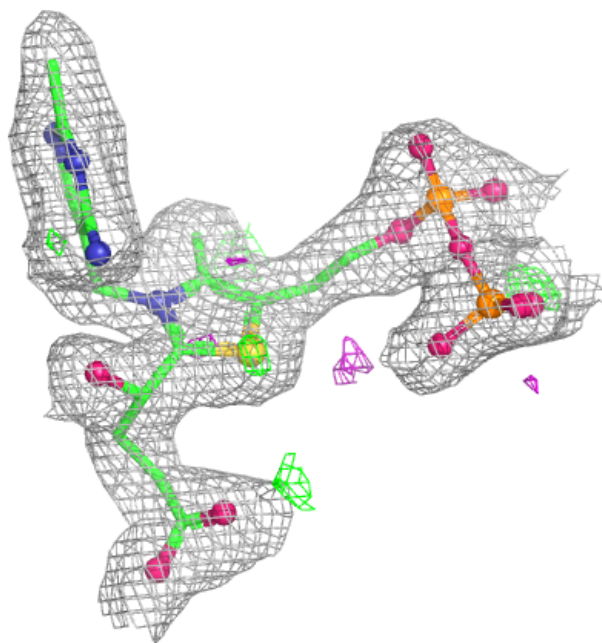
Electron density around TD6 C 2001:

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



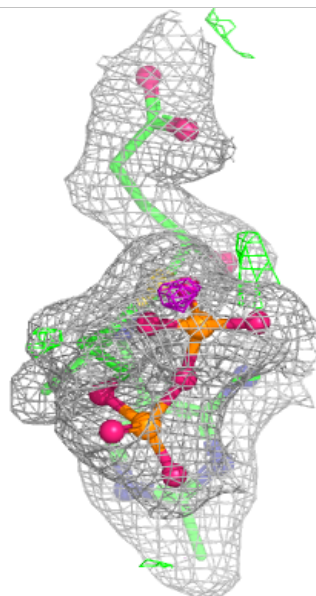
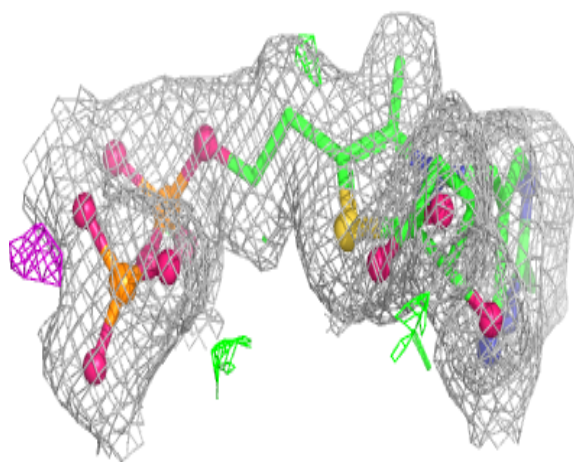
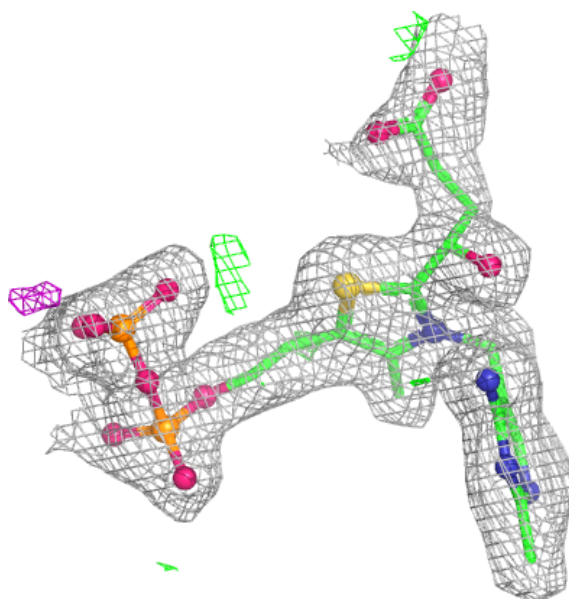
Electron density around TD6 D 2001:

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



Electron density around TD6 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.