



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:45 PM UTC

PDB ID : 2YID / pdb_00002yid
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 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

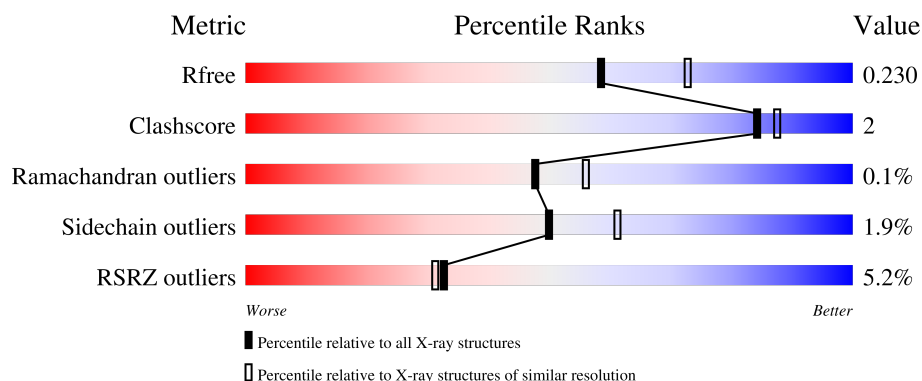
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	868	6% 90% 6% ••
1	B	868	4% 88% 7% •
1	C	868	4% 89% 7% •
1	D	868	6% 90% 8% •

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
1	A	844	Total	C	N	O	S	0	0	0
			6519	4099	1154	1242	24			
1	B	837	Total	C	N	O	S	0	1	0
			6475	4074	1141	1236	24			
1	C	843	Total	C	N	O	S	0	1	0
			6537	4112	1162	1239	24			
1	D	852	Total	C	N	O	S	0	0	0
			6586	4143	1164	1255	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 (4E)-4-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-(2-{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}ethyl)-4-methyl-1,3-thiazol-2(3H)-ylidene}-4-hydroxybutanoic acid (CCD ID: TD7) (formula: C₁₆H₂₄N₄O₁₀P₂S).

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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

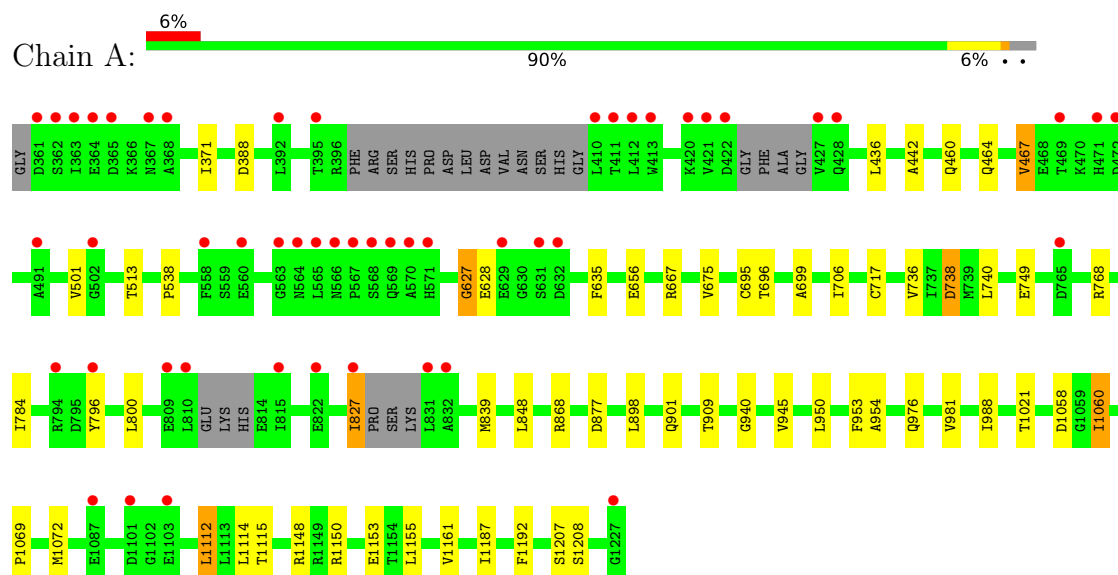
- Molecule 5 is water.

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

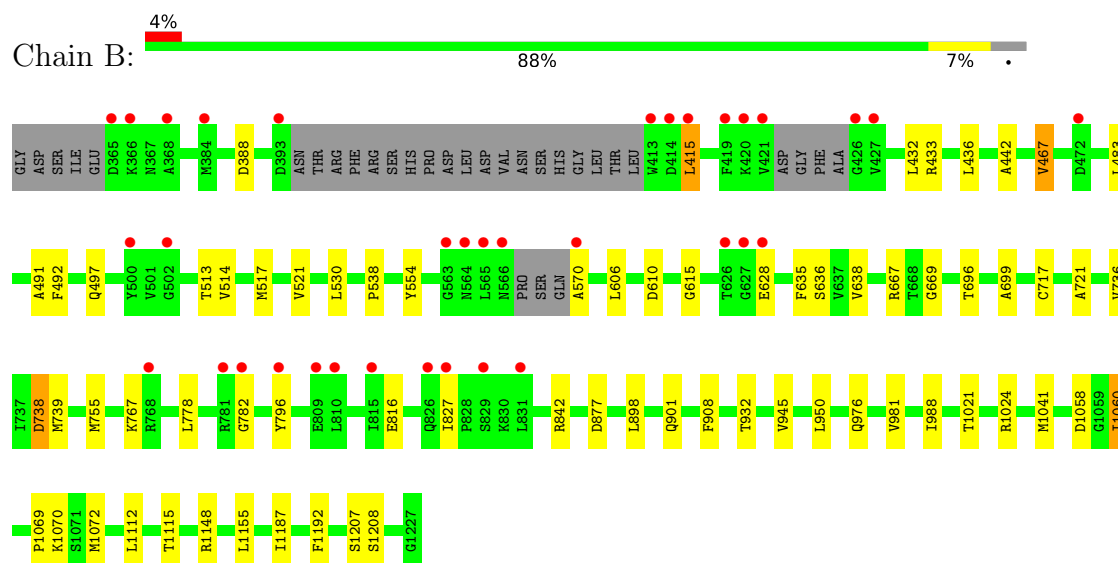
3 Residue-property plots [i](#)

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.

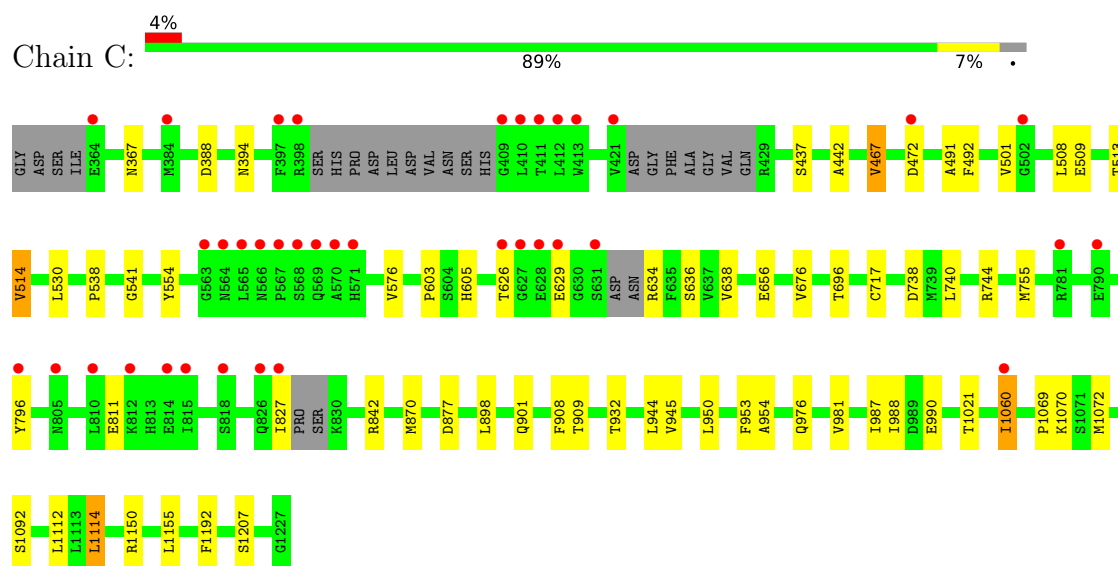
• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



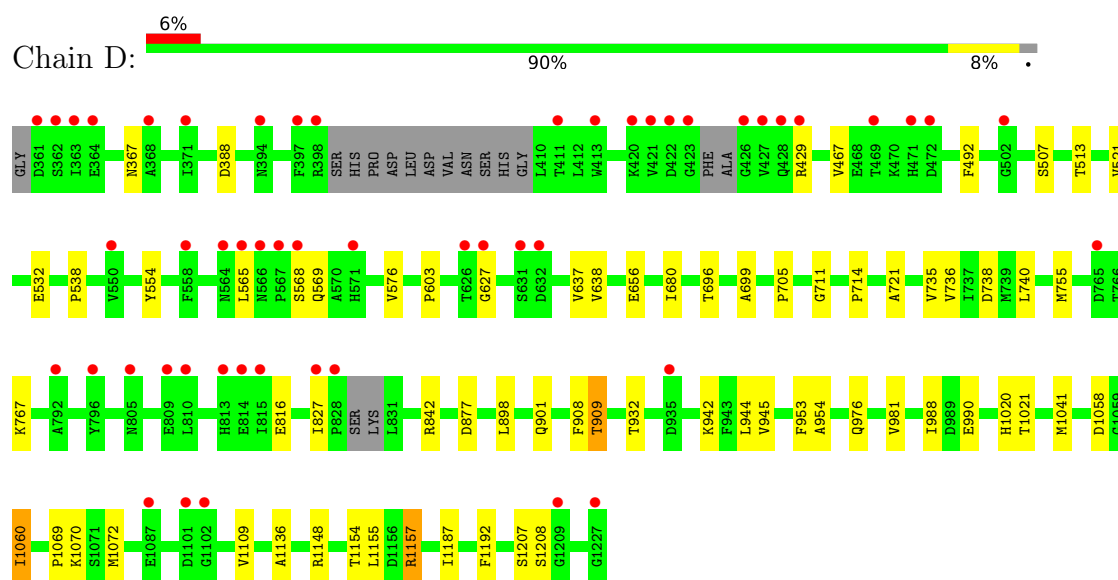
• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



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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 32.94 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.7 (32.94-2.25) 95.7 (32.94-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.192 , 0.223 (Not available) , 0.230	Depositor DCC
R_{free} test set	9064 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
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

Xtriage'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	0.85	0/6647	1.22	8/9010 (0.1%)
1	B	0.85	3/6609 (0.0%)	1.23	13/8961 (0.1%)
1	C	0.88	2/6668 (0.0%)	1.21	9/9037 (0.1%)
1	D	0.87	1/6718 (0.0%)	1.21	9/9106 (0.1%)
All	All	0.86	6/26642 (0.0%)	1.22	39/36114 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	870	MET	SD-CE	-6.20	1.64	1.79
1	B	610	ASP	CA-C	5.88	1.59	1.52
1	D	680	ILE	CA-CB	5.48	1.61	1.55
1	C	987	ILE	CG1-CD1	5.29	1.72	1.51
1	B	517	MET	SD-CE	-5.23	1.66	1.79
1	B	1041	MET	SD-CE	-5.09	1.66	1.79

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	953	PHE	CA-CB-CG	6.54	120.34	113.80
1	B	638	VAL	N-CA-C	6.46	115.01	107.77
1	B	738	ASP	CA-CB-CG	6.24	118.84	112.60
1	C	388	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	877	ASP	CA-CB-CG	5.93	118.53	112.60
1	C	472	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	388	ASP	CA-CB-CG	5.83	118.43	112.60
1	D	388	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	638	VAL	N-CA-C	5.78	114.24	107.77
1	D	627	GLY	CA-C-N	5.70	128.23	120.54
1	D	627	GLY	C-N-CA	5.70	128.23	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	877	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	388	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	638	VAL	N-CA-C	5.63	114.08	107.77
1	A	627	GLY	CA-C-N	5.53	128.00	120.54
1	A	627	GLY	C-N-CA	5.53	128.00	120.54
1	A	940	GLY	N-CA-C	-5.50	108.14	114.69
1	A	738	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	570	ALA	CA-C-N	5.45	128.58	120.90
1	B	570	ALA	C-N-CA	5.45	128.58	120.90
1	B	615	GLY	CA-C-N	5.41	127.47	120.44
1	B	615	GLY	C-N-CA	5.41	127.47	120.44
1	B	877	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	953	PHE	CA-CB-CG	5.37	119.17	113.80
1	B	1024	ARG	CA-C-N	5.30	127.43	120.60
1	B	1024	ARG	C-N-CA	5.30	127.43	120.60
1	C	877	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	1058	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	782	GLY	CA-C-N	5.19	127.55	120.54
1	B	782	GLY	C-N-CA	5.19	127.55	120.54
1	C	576	VAL	CA-C-N	5.14	127.68	120.28
1	C	576	VAL	C-N-CA	5.14	127.68	120.28
1	D	953	PHE	CA-CB-CG	5.13	118.93	113.80
1	C	437	SER	CA-C-N	5.11	126.99	120.56
1	C	437	SER	C-N-CA	5.11	126.99	120.56
1	D	576	VAL	CA-C-N	5.06	127.56	120.28
1	D	576	VAL	C-N-CA	5.06	127.56	120.28
1	D	1058	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	1058	ASP	CA-CB-CG	5.03	117.63	112.60

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	6519	0	6303	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6475	0	6261	30	0
1	C	6537	0	6327	31	0
1	D	6586	0	6377	30	0
2	A	33	0	20	2	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
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	1	0
5	C	228	0	0	1	0
5	D	131	0	0	3	0
All	All	26987	0	25348	118	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 (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:MET:HE3	1:A:839:MET:HA	1.68	0.74
1:B:827:ILE:HA	1:B:1060:ILE:HD11	1.78	0.65
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:D:1041:MET:HE2	5:D:3123:HOH:O	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.88	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
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
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:B:514:VAL:HG23	1:B:739:MET:HE1	1.92	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:898:LEU:O	1:D:945:VAL:HA	2.13	0.48
1:D:1020:HIS:HD2	5:D:3110:HOH:O	1.96	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:C11	2:A:2001:TD7:H4'1	2.27	0.47
1:A:898:LEU:O	1:A:945:VAL:HA	2.13	0.47
1:A:1148:ARG:HG3	1:A:1187:ILE:HD12	1.97	0.47
1:C:898:LEU:O	1:C:945:VAL:HA	2.14	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
2:D:2001:TD7:C11	2:D:2001:TD7:H4'1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1041:MET:CE	5:D:3123:HOH:O	2.62	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
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:909:THR:CG2	1:B:755:MET:HE1	2.48	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:842:ARG:NH2	1:D:932:THR:O	2.51	0.42
1:D:565:LEU:HB3	1:D:569:GLN:HB2	2.01	0.42
1:D:1155:LEU:HD11	1:D:1192:PHE:CZ	2.54	0.42
1:A:749:GLU:N	1:A:749:GLU:CD	2.77	0.42
1:A:1069:PRO:HB2	1:A:1072:MET:HB3	2.01	0.42
1:B:635:PHE:CG	1:B:669:GLY:HA3	2.54	0.42
1:C:629:GLU:HG3	1:C:944:LEU:HD22	2.00	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: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:492:PHE:CD1	1:C:554:TYR:CE1	3.03	0.42
1:C:1069:PRO:HB2	1:C:1072:MET:HB3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:491:ALA:HB3	1:C:796:TYR:CE2	2.55	0.42
1:A:627:GLY:HA2	1:A:635:PHE:CD1	2.55	0.41
1:A:1150:ARG:NH1	1:A:1153:GLU:OE1	2.53	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: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:C:755:MET:HE1	1:D:909:THR:CG2	2.50	0.41
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.55	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:C:909:THR:CG2	1:D:755:MET:HE1	2.50	0.41
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.56	0.41
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%)	48	56
1	B	830/868 (96%)	807 (97%)	22 (3%)	1 (0%)	48	56
1	C	834/868 (96%)	811 (97%)	21 (2%)	2 (0%)	43	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	844/868 (97%)	820 (97%)	23 (3%)	1 (0%)	48 56
All	All	3342/3472 (96%)	3249 (97%)	88 (3%)	5 (0%)	48 56

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 ⓘ

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%)	657 (98%)	15 (2%)	45 56
1	B	670/726 (92%)	659 (98%)	11 (2%)	55 66
1	C	674/726 (93%)	662 (98%)	12 (2%)	51 63
1	D	681/726 (94%)	668 (98%)	13 (2%)	50 61
All	All	2697/2904 (93%)	2646 (98%)	51 (2%)	50 61

All (51) 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	501	VAL
1	A	740	LEU
1	A	768	ARG
1	A	784	ILE
1	A	827	ILE
1	A	950	LEU

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Mol	Chain	Res	Type
1	A	976	GLN
1	A	1060	ILE
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	767	LYS
1	B	816	GLU
1	B	950	LEU
1	B	976	GLN
1	B	1060	ILE
1	B	1112	LEU
1	B	1115	THR
1	B	1208	SER
1	C	367	ASN
1	C	394	ASN
1	C	467	VAL
1	C	501	VAL
1	C	514	VAL
1	C	740	LEU
1	C	811	GLU
1	C	950	LEU
1	C	976	GLN
1	C	1060	ILE
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	740	LEU
1	D	767	LYS
1	D	816	GLU
1	D	909	THR
1	D	976	GLN
1	D	1060	ILE
1	D	1157	ARG
1	D	1208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	479	GLN
1	A	556	GLN
1	A	1001	GLN
1	A	1061	GLN
1	A	1107	ASN
1	B	566	ASN
1	B	985	GLN
1	B	1107	ASN
1	C	556	GLN
1	C	966	ASN
1	C	1001	GLN
1	C	1061	GLN
1	C	1107	ASN
1	D	556	GLN
1	D	813	HIS
1	D	985	GLN
1	D	1001	GLN
1	D	1061	GLN
1	D	1107	ASN

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	TD7	B	2001	3	32,34,34	1.57	4 (12%)	40,50,50	1.67	9 (22%)
2	TD7	A	2001	3	32,34,34	1.64	6 (18%)	40,50,50	1.67	10 (25%)
2	TD7	C	2001	3	32,34,34	1.58	5 (15%)	40,50,50	1.77	10 (25%)
2	TD7	D	2001	3	32,34,34	1.60	5 (15%)	40,50,50	1.68	10 (25%)

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	-	4/22/26/26	0/2/2/2
2	TD7	A	2001	3	-	7/22/26/26	0/2/2/2
2	TD7	C	2001	3	-	7/22/26/26	0/2/2/2
2	TD7	D	2001	3	-	8/22/26/26	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	TD7	OL1-C11	4.26	1.44	1.32
2	C	2001	TD7	OL1-C11	4.24	1.44	1.32
2	A	2001	TD7	OL1-C11	4.23	1.44	1.32
2	D	2001	TD7	OL1-C11	4.10	1.43	1.32
2	A	2001	TD7	C2-N3	-3.90	1.31	1.39
2	C	2001	TD7	C2-N3	-3.57	1.32	1.39
2	D	2001	TD7	C2-N3	-3.57	1.32	1.39
2	B	2001	TD7	C2-N3	-3.52	1.32	1.39
2	D	2001	TD7	PB-O2B	3.51	1.61	1.50
2	A	2001	TD7	PB-O2B	3.46	1.61	1.50
2	B	2001	TD7	PB-O2B	3.45	1.61	1.50
2	C	2001	TD7	PB-O2B	3.26	1.60	1.50
2	D	2001	TD7	C4-N3	-3.11	1.34	1.39
2	B	2001	TD7	C4-N3	-2.66	1.34	1.39
2	C	2001	TD7	PB-O3B	-2.43	1.45	1.54
2	A	2001	TD7	C4-N3	-2.41	1.35	1.39
2	C	2001	TD7	C4-N3	-2.37	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	TD7	PB-O3B	-2.20	1.46	1.54
2	D	2001	TD7	PB-O3B	-2.17	1.46	1.54
2	A	2001	TD7	C2-S1	-2.09	1.69	1.74

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	TD7	CM2-C2'-N1'	4.90	122.42	117.20
2	A	2001	TD7	C4-C5-S1	-3.94	107.05	110.63
2	D	2001	TD7	CM2-C2'-N1'	3.92	121.37	117.20
2	B	2001	TD7	C6'-N1'-C2'	3.75	122.24	116.07
2	B	2001	TD7	C4-C5-S1	-3.67	107.29	110.63
2	B	2001	TD7	CM2-C2'-N1'	3.55	120.98	117.20
2	A	2001	TD7	C6'-N1'-C2'	3.46	121.76	116.07
2	D	2001	TD7	OL1-C11-CLB	3.41	123.22	114.08
2	C	2001	TD7	C4-C5-S1	-3.40	107.53	110.63
2	A	2001	TD7	OL1-C11-CLB	3.40	123.17	114.08
2	C	2001	TD7	OL1-C11-CLB	3.22	122.69	114.08
2	D	2001	TD7	C4-C5-S1	-3.06	107.84	110.63
2	C	2001	TD7	C6'-N1'-C2'	3.02	121.03	116.07
2	B	2001	TD7	OL1-C11-CLB	3.01	122.15	114.08
2	D	2001	TD7	C6'-N1'-C2'	2.96	120.94	116.07
2	B	2001	TD7	C5'-C6'-N1'	-2.86	119.17	123.83
2	B	2001	TD7	N1'-C2'-N3'	-2.86	120.78	125.53
2	C	2001	TD7	CM4-C4-N3	2.78	126.35	122.27
2	C	2001	TD7	C5'-C6'-N1'	-2.71	119.42	123.83
2	A	2001	TD7	C5'-C6'-N1'	-2.71	119.42	123.83
2	B	2001	TD7	C7'-N3-C4	-2.69	121.57	124.98
2	A	2001	TD7	N1'-C2'-N3'	-2.66	121.11	125.53
2	C	2001	TD7	N1'-C2'-N3'	-2.63	121.16	125.53
2	D	2001	TD7	CLB-C13-CLC	-2.61	106.73	113.67
2	C	2001	TD7	C2'-N3'-C4'	2.56	122.03	118.10
2	D	2001	TD7	C5'-C6'-N1'	-2.54	119.70	123.83
2	A	2001	TD7	CLB-C13-CLC	-2.52	106.98	113.67
2	D	2001	TD7	N1'-C2'-N3'	-2.51	121.36	125.53
2	A	2001	TD7	CM4-C4-N3	2.42	125.81	122.27
2	C	2001	TD7	CLB-C13-CLC	-2.41	107.28	113.67
2	D	2001	TD7	CM4-C4-N3	2.40	125.78	122.27
2	A	2001	TD7	CM2-C2'-N1'	2.34	119.69	117.20
2	D	2001	TD7	C7-C6-C5	-2.33	105.42	112.73
2	A	2001	TD7	C7'-N3-C2	-2.31	123.28	126.13
2	B	2001	TD7	O3B-PB-O3A	2.14	111.82	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	TD7	C2'-N3'-C4'	2.13	121.38	118.10
2	C	2001	TD7	C7-C6-C5	-2.03	106.37	112.73
2	A	2001	TD7	C7-C6-C5	-2.02	106.40	112.73
2	B	2001	TD7	O3A-PB-O2B	-2.01	100.45	111.04

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	TD7	CLC-C13-CLB-C11
2	C	2001	TD7	CLC-C13-CLB-C11
2	D	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	B	2001	TD7	PA-O3A-PB-O3B
2	D	2001	TD7	PA-O3A-PB-O3B
2	A	2001	TD7	C7-O7-PA-O1A
2	C	2001	TD7	C7-O7-PA-O1A
2	D	2001	TD7	C7-O7-PA-O1A
2	B	2001	TD7	PA-O3A-PB-O2B
2	D	2001	TD7	PA-O3A-PB-O2B
2	D	2001	TD7	CLB-C13-CLC-OL2
2	C	2001	TD7	CLB-C13-CLC-OL2
2	A	2001	TD7	CLB-C13-CLC-OL2
2	A	2001	TD7	CLB-C13-CLC-OL3
2	C	2001	TD7	CLB-C13-CLC-OL3
2	D	2001	TD7	CLB-C13-CLC-OL3
2	B	2001	TD7	CLB-C13-CLC-OL2
2	A	2001	TD7	OL1-C11-CLB-C13
2	C	2001	TD7	C2-C11-CLB-C13
2	D	2001	TD7	C2-C11-CLB-C13
2	B	2001	TD7	CLB-C13-CLC-OL3
2	D	2001	TD7	OL1-C11-CLB-C13
2	C	2001	TD7	OL1-C11-CLB-C13

There are no ring outliers.

4 monomers are involved in 8 short contacts:

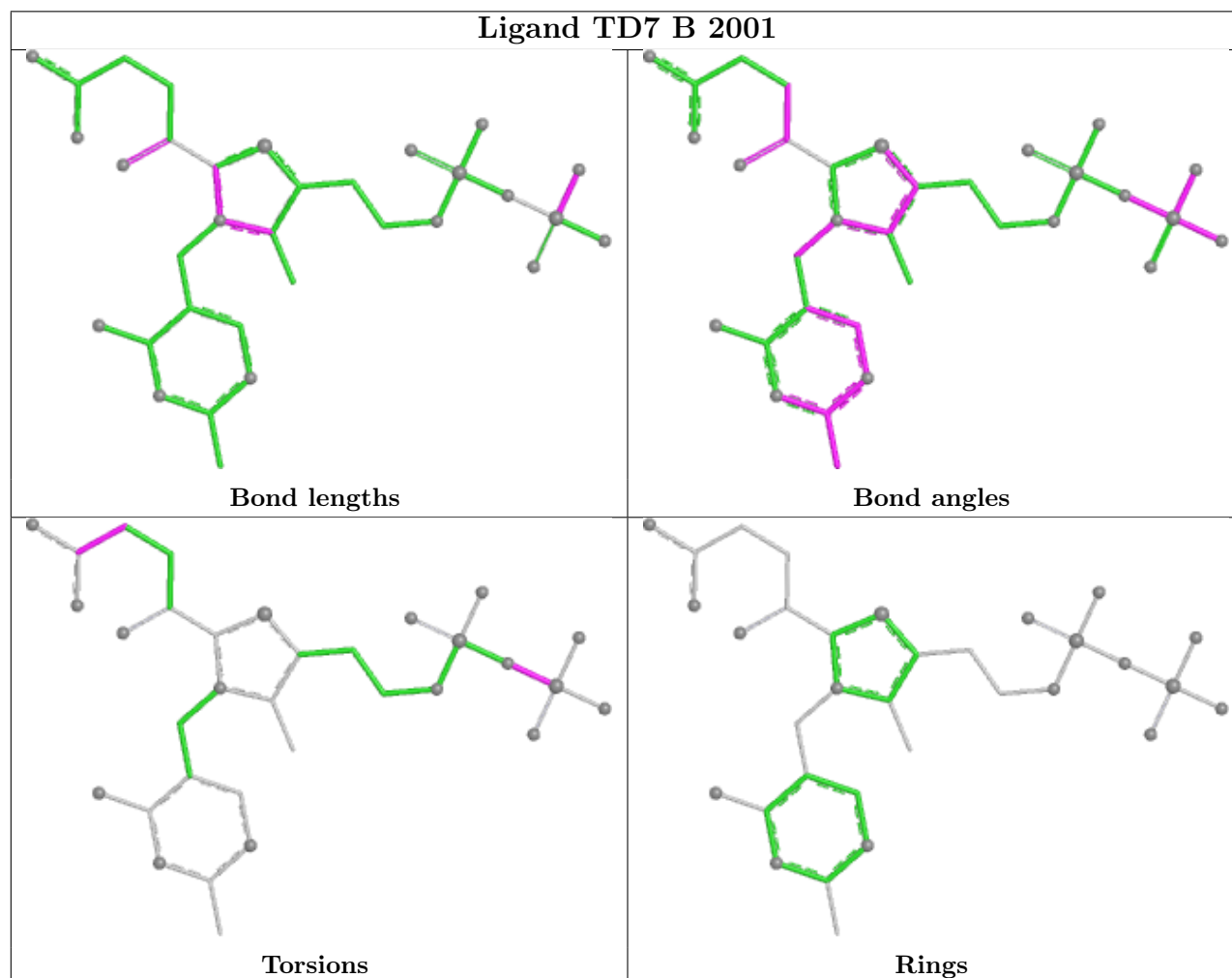
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	TD7	2	0

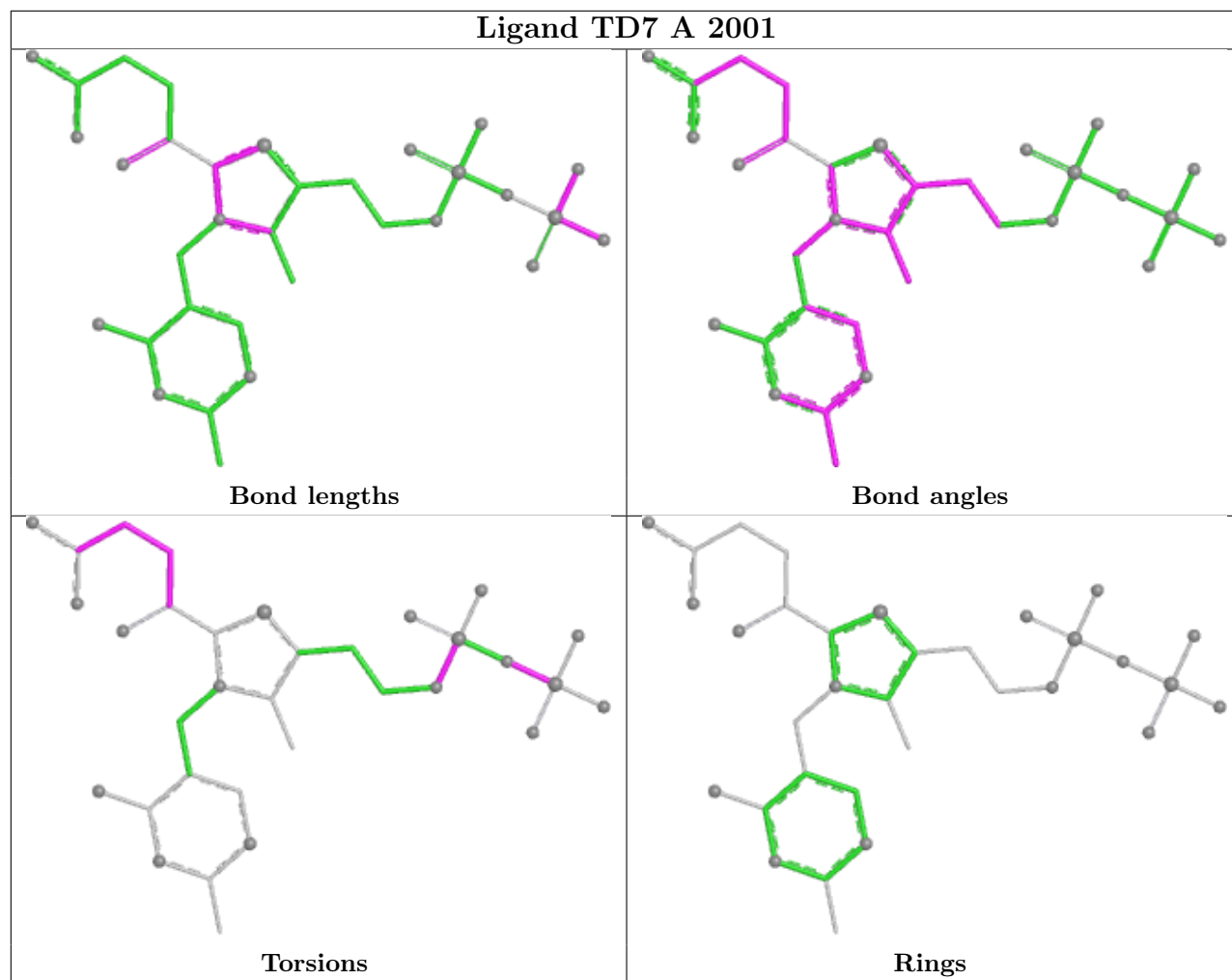
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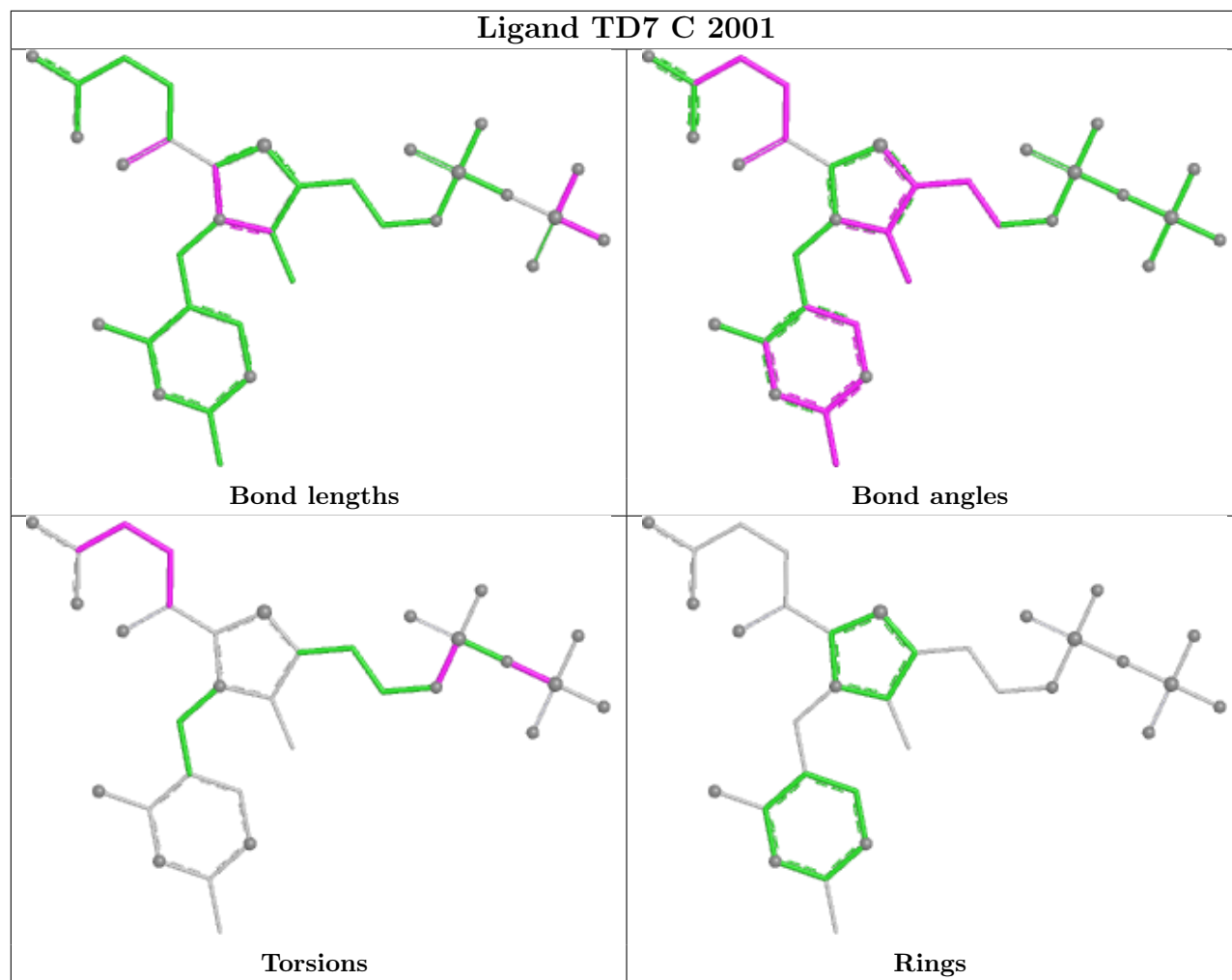
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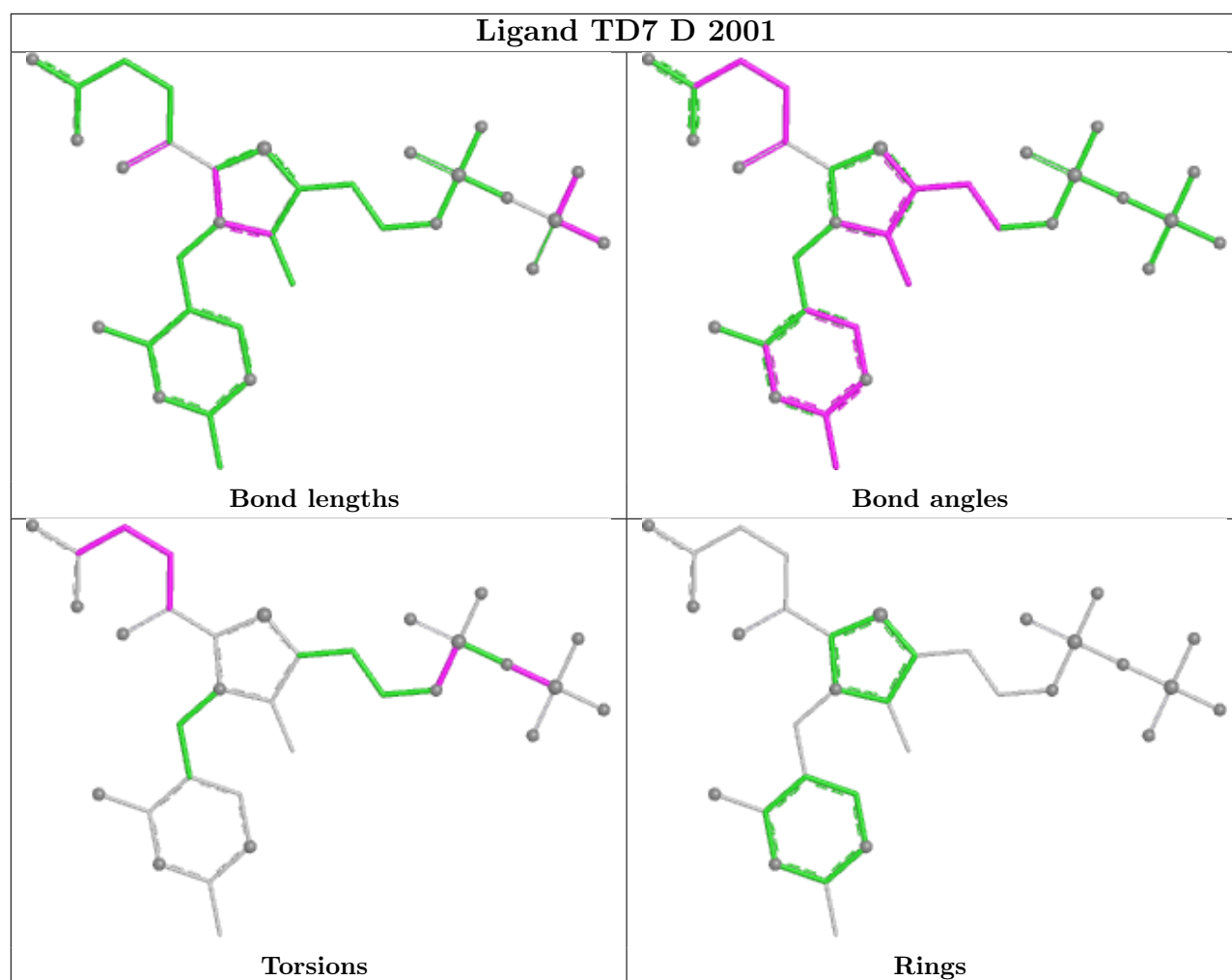
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	TD7	2	0
2	C	2001	TD7	2	0
2	D	2001	TD7	2	0

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%)	0.36	51 (6%) 27 25	14, 31, 65, 94	0
1	B	837/868 (96%)	0.21	35 (4%) 40 40	11, 30, 61, 89	1 (0%)
1	C	843/868 (97%)	0.16	38 (4%) 38 37	7, 28, 63, 93	1 (0%)
1	D	852/868 (98%)	0.32	52 (6%) 27 25	14, 31, 67, 91	0
All	All	3376/3472 (97%)	0.26	176 (5%) 33 31	7, 30, 64, 94	2 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	568	SER	8.0
1	A	827	ILE	7.2
1	C	631	SER	6.1
1	A	831	LEU	5.6
1	A	502	GLY	5.4
1	A	796	TYR	5.4
1	B	570	ALA	5.2
1	C	568	SER	5.1
1	D	422	ASP	4.9
1	A	571	HIS	4.9
1	B	564	ASN	4.9
1	D	398	ARG	4.9
1	A	565	LEU	4.6
1	A	566	ASN	4.6
1	D	427	VAL	4.6
1	C	398	ARG	4.5
1	D	568	SER	4.4
1	C	827	ILE	4.4
1	A	364	GLU	4.3
1	A	363	ILE	4.3
1	D	364	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	472	ASP	4.2
1	D	361	ASP	4.2
1	A	810	LEU	4.1
1	A	815	ILE	4.1
1	A	569	GLN	4.1
1	D	565	LEU	4.1
1	C	815	ILE	4.0
1	C	565	LEU	4.0
1	D	502	GLY	4.0
1	C	564	ASN	4.0
1	D	426	GLY	4.0
1	B	627	GLY	3.9
1	D	814	GLU	3.9
1	B	427	VAL	3.9
1	B	827	ILE	3.8
1	D	363	ILE	3.8
1	D	796	TYR	3.8
1	B	413	TRP	3.7
1	B	502	GLY	3.7
1	D	815	ILE	3.6
1	D	423	GLY	3.6
1	B	626	THR	3.6
1	A	567	PRO	3.6
1	C	626	THR	3.6
1	A	832	ALA	3.6
1	D	827	ILE	3.6
1	C	502	GLY	3.5
1	C	570	ALA	3.5
1	D	472	ASP	3.5
1	A	570	ALA	3.5
1	A	395	THR	3.4
1	D	828	PRO	3.4
1	C	796	TYR	3.3
1	D	411	THR	3.3
1	B	781	ARG	3.3
1	A	361	ASP	3.2
1	B	565	LEU	3.2
1	C	421	VAL	3.2
1	A	413	TRP	3.2
1	C	411	THR	3.2
1	A	564	ASN	3.2
1	A	411	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	629	GLU	3.1
1	A	427	VAL	3.1
1	A	365	ASP	3.1
1	A	632	ASP	3.1
1	C	409	GLY	3.1
1	B	421	VAL	3.1
1	C	814	GLU	3.1
1	B	566	ASN	3.1
1	D	564	ASN	3.0
1	C	364	GLU	3.0
1	A	1227	GLY	3.0
1	A	362	SER	3.0
1	B	426	GLY	2.9
1	C	627	GLY	2.9
1	C	569	GLN	2.9
1	A	765	ASP	2.9
1	C	397	PHE	2.9
1	C	566	ASN	2.9
1	D	632	ASP	2.9
1	C	810	LEU	2.8
1	C	629	GLU	2.8
1	D	428	GLN	2.8
1	B	796	TYR	2.8
1	A	410	LEU	2.8
1	D	813	HIS	2.8
1	A	472	ASP	2.8
1	B	810	LEU	2.8
1	C	413	TRP	2.7
1	D	362	SER	2.7
1	A	809	GLU	2.7
1	D	420	LYS	2.7
1	D	631	SER	2.7
1	C	790	GLU	2.7
1	C	781	ARG	2.7
1	C	571	HIS	2.6
1	A	428	GLN	2.6
1	A	822	GLU	2.6
1	D	1227	GLY	2.6
1	C	567	PRO	2.6
1	A	367	ASN	2.6
1	A	412	LEU	2.6
1	A	1087	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	794	ARG	2.6
1	D	429	ARG	2.6
1	B	815	ILE	2.6
1	C	628	GLU	2.6
1	B	365	ASP	2.6
1	B	829	SER	2.6
1	D	792	ALA	2.5
1	D	394	ASN	2.5
1	D	413	TRP	2.5
1	A	368	ALA	2.5
1	D	368	ALA	2.5
1	A	471	HIS	2.5
1	D	471	HIS	2.5
1	D	627	GLY	2.5
1	B	368	ALA	2.4
1	A	421	VAL	2.4
1	B	420	LYS	2.4
1	D	571	HIS	2.4
1	A	560	GLU	2.4
1	B	414	ASP	2.3
1	D	566	ASN	2.3
1	D	1101	ASP	2.3
1	D	421	VAL	2.3
1	C	412	LEU	2.3
1	B	366	LYS	2.3
1	B	563	GLY	2.3
1	B	419	PHE	2.3
1	D	397	PHE	2.3
1	A	1101	ASP	2.3
1	C	818	SER	2.3
1	C	410	LEU	2.3
1	D	567	PRO	2.3
1	A	558	PHE	2.2
1	D	558	PHE	2.2
1	A	469	THR	2.2
1	C	563	GLY	2.2
1	D	1102	GLY	2.2
1	B	809	GLU	2.2
1	C	1060	ILE	2.2
1	B	415	LEU	2.2
1	D	1209	GLY	2.2
1	C	812	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	826	GLN	2.2
1	A	631	SER	2.2
1	D	469	THR	2.2
1	B	500	TYR	2.2
1	A	392	LEU	2.2
1	D	371	ILE	2.1
1	D	550	VAL	2.1
1	D	809	GLU	2.1
1	B	826	GLN	2.1
1	B	393	ASP	2.1
1	C	472	ASP	2.1
1	C	805	ASN	2.1
1	A	563	GLY	2.1
1	A	491	ALA	2.1
1	A	420	LYS	2.1
1	D	805	ASN	2.1
1	B	782	GLY	2.1
1	B	384	MET	2.1
1	B	831	LEU	2.1
1	D	810	LEU	2.1
1	D	765	ASP	2.1
1	C	384	MET	2.0
1	A	422	ASP	2.0
1	D	935	ASP	2.0
1	B	768	ARG	2.0
1	A	1103	GLU	2.0
1	B	628	GLU	2.0
1	D	626	THR	2.0
1	D	1087	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 oligosaccharides in this entry.

6.4 Ligands

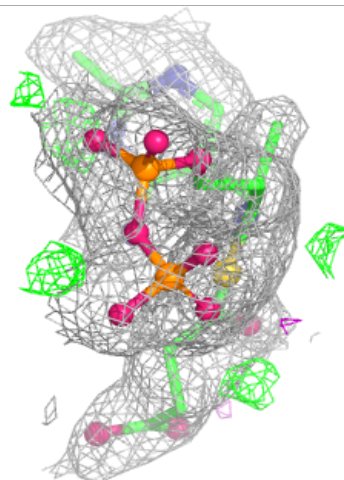
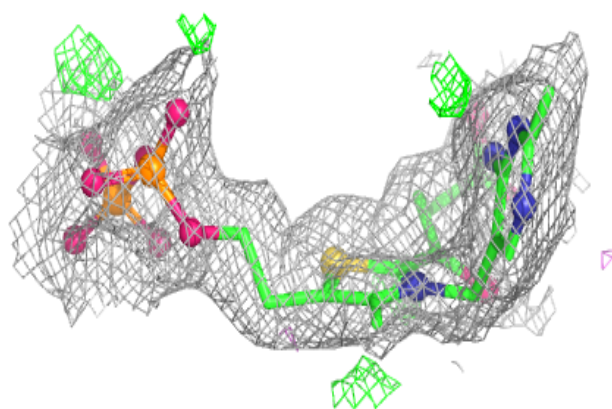
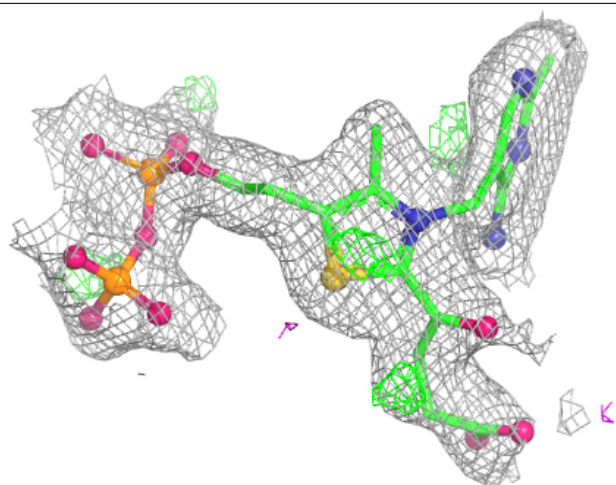
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TD7	A	2001	33/33	0.98	0.07	11,20,45,48	0
2	TD7	B	2001	33/33	0.98	0.06	9,19,42,44	0
2	TD7	C	2001	33/33	0.98	0.06	12,19,41,42	0
2	TD7	D	2001	33/33	0.98	0.06	9,18,37,44	0
4	CA	A	2003	1/1	0.98	0.05	33,33,33,33	0
4	CA	C	2003	1/1	0.98	0.06	27,27,27,27	0
3	MG	D	2002	1/1	0.99	0.02	8,8,8,8	0
3	MG	B	2002	1/1	0.99	0.02	12,12,12,12	0
4	CA	B	2003	1/1	0.99	0.04	30,30,30,30	0
3	MG	C	2002	1/1	0.99	0.02	8,8,8,8	0
4	CA	D	2003	1/1	0.99	0.10	29,29,29,29	0
3	MG	A	2002	1/1	1.00	0.03	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.

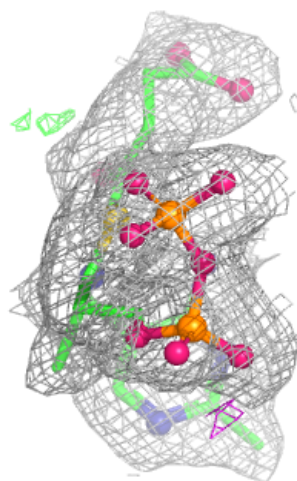
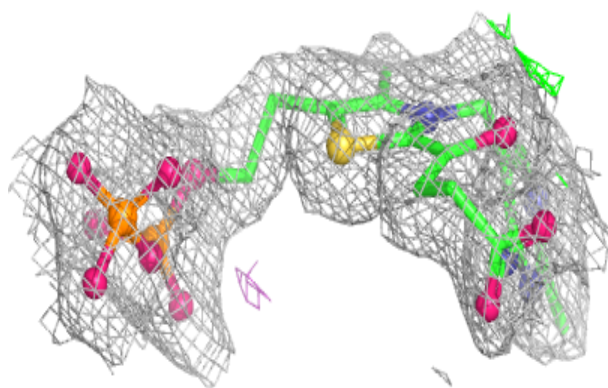
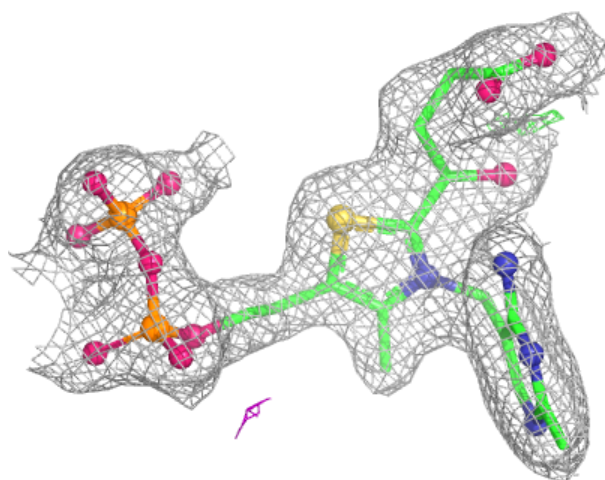
Electron density around TD7 A 2001:

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



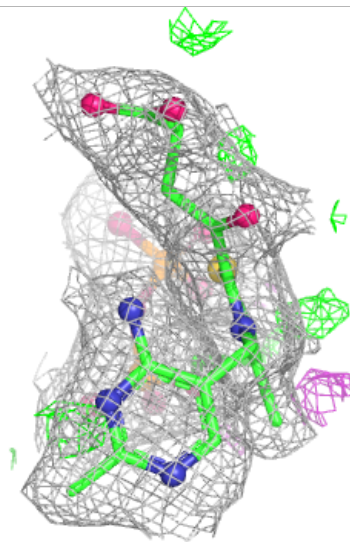
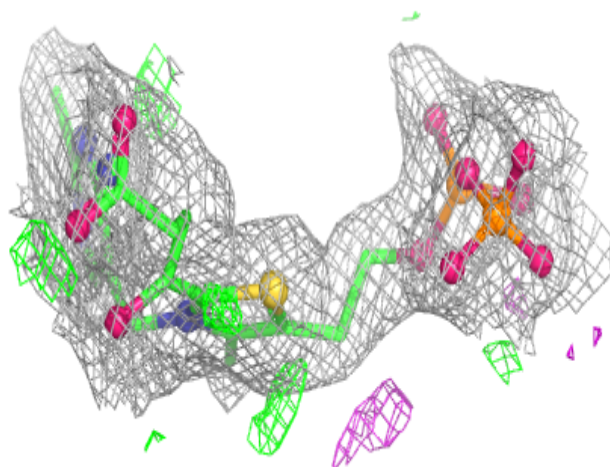
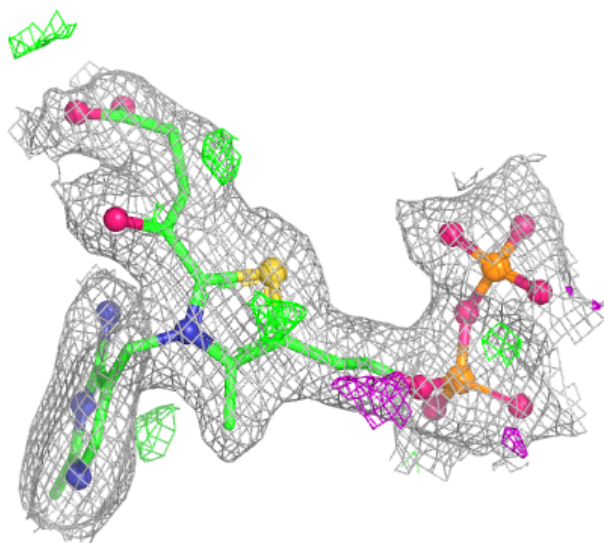
Electron density around TD7 B 2001:

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



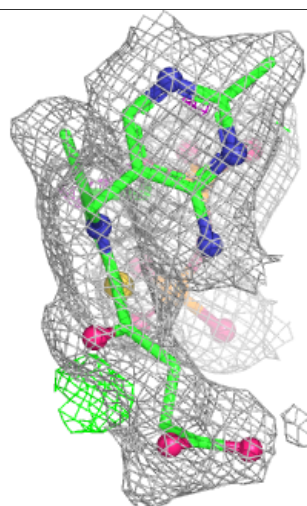
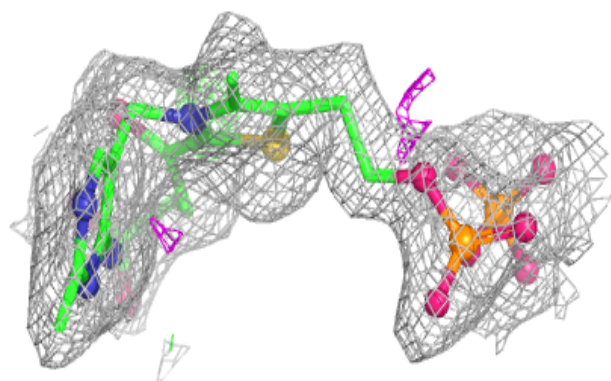
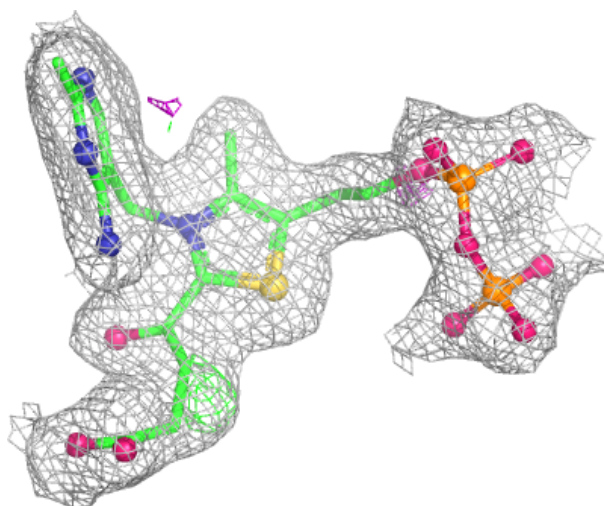
Electron density around TD7 C 2001:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.