



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:46 PM UTC

PDB ID : 3ZHU / pdb_00003zhu
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	:	4-5-2 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

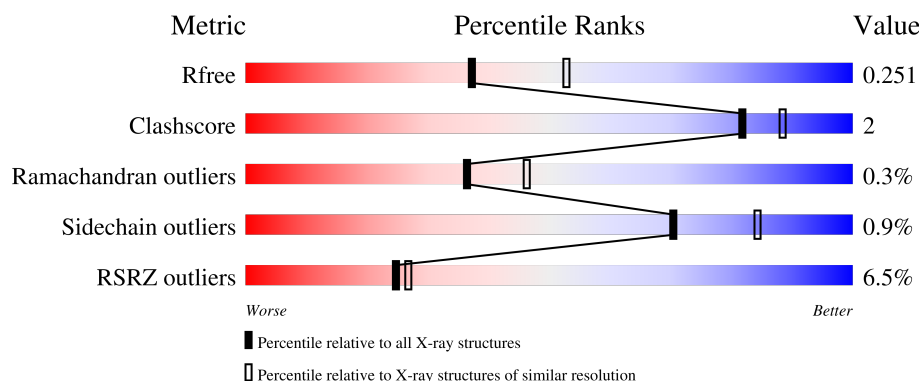
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	8% 91% 7%
1	B	868	4% 89% 6%
1	C	868	6% 90% 7%
1	D	868	8% 92% 6%

2 Entry composition

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.

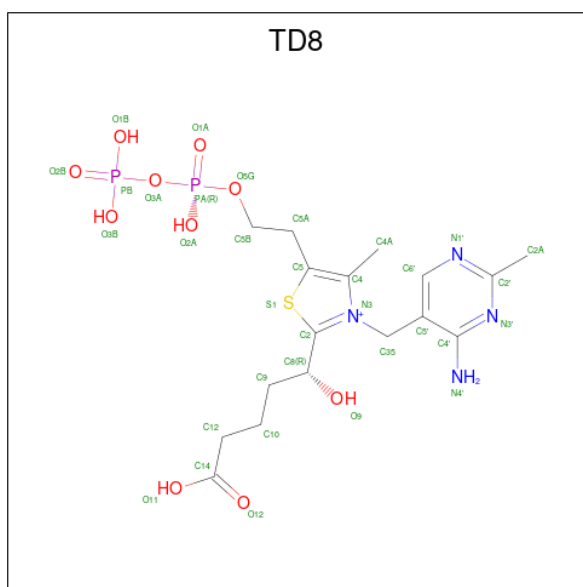
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

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-[(phosphonatoxy)phosphinato]oxy)ethyl)-1,3-thiazol-3-ium-2-yl}-5-hydroxypentanoate (CCD ID: TD8) (formula: C₁₇H₂₇N₄O₁₀P₂S).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

Continued on next page...

Continued from previous page...

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

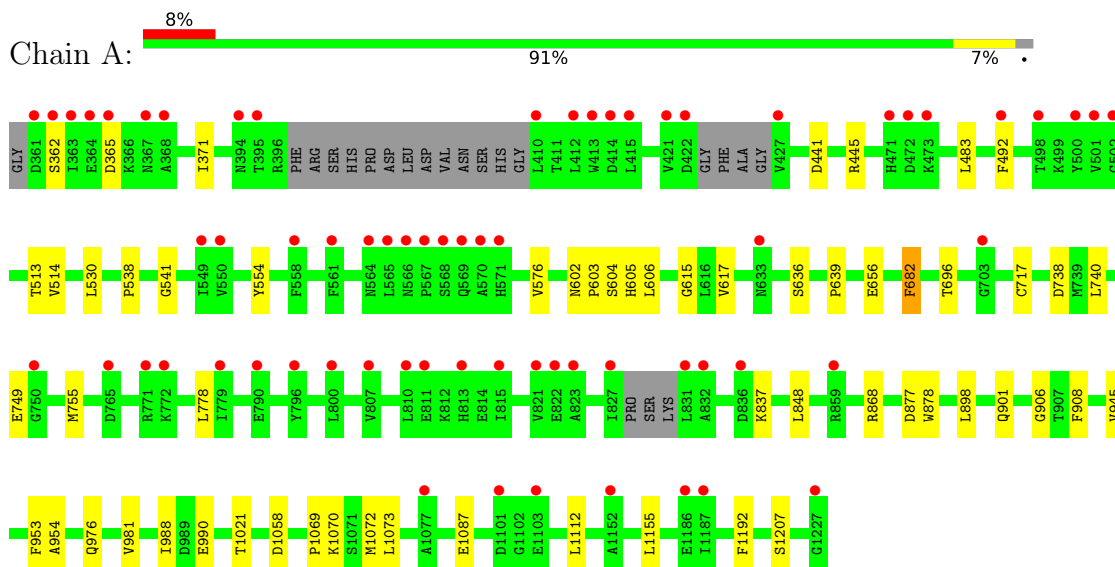
- Molecule 5 is water.

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

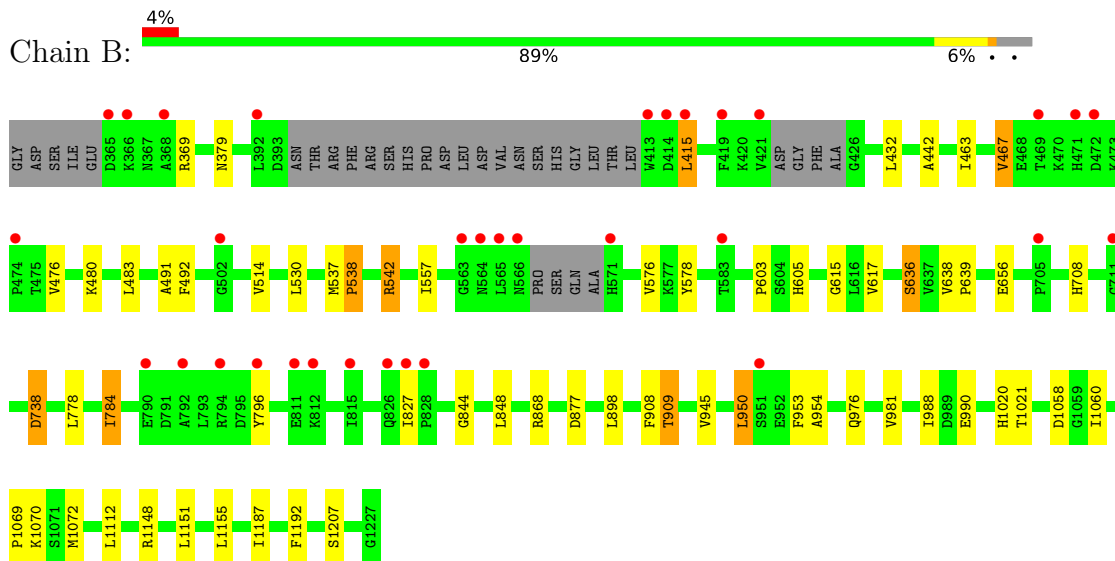
3 Residue-property plots [i](#)

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.

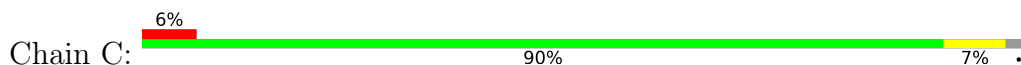
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

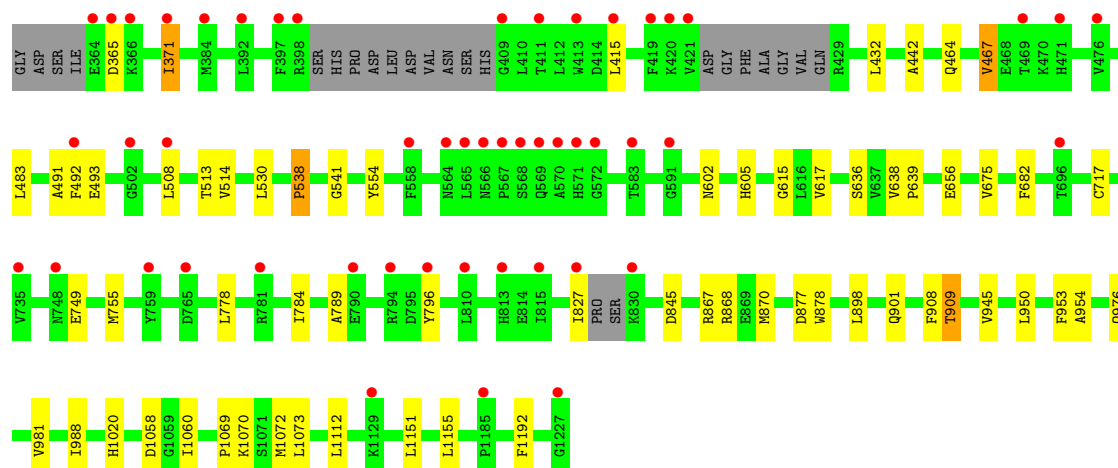


• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

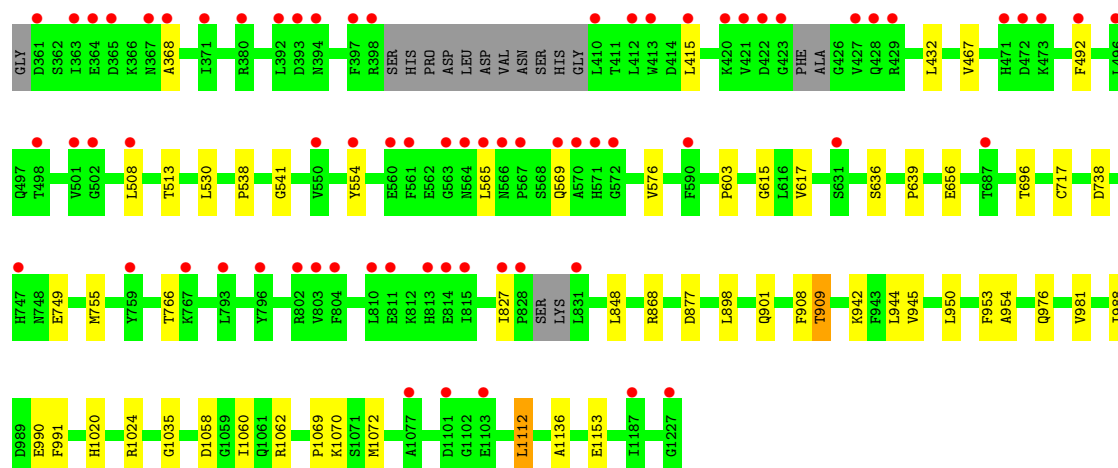


• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME





• 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	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
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.200 , 0.235 0.214 , 0.251	Depositor DCC
R_{free} test set	8506 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 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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.*

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: MG, TD8, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.84	0/6663	1.27	15/9034 (0.2%)
1	B	0.87	0/6594	1.26	14/8940 (0.2%)
1	C	0.87	0/6661	1.27	11/9032 (0.1%)
1	D	0.85	0/6710	1.27	11/9097 (0.1%)
All	All	0.86	0/26628	1.27	51/36103 (0.1%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	682	PHE	CA-CB-CG	6.69	120.49	113.80
1	A	877	ASP	CA-CB-CG	6.41	119.01	112.60
1	D	877	ASP	CA-CB-CG	6.37	118.97	112.60
1	B	877	ASP	CA-CB-CG	6.14	118.75	112.60
1	D	766	THR	CA-C-N	5.98	129.32	120.95
1	D	766	THR	C-N-CA	5.98	129.32	120.95
1	C	365	ASP	CA-C-N	5.84	128.42	120.54
1	C	365	ASP	C-N-CA	5.84	128.42	120.54
1	C	675	VAL	N-CA-CB	5.79	117.60	111.00
1	D	1153	GLU	CA-C-N	5.76	127.93	120.44
1	D	1153	GLU	C-N-CA	5.76	127.93	120.44
1	C	877	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	602	ASN	N-CA-C	5.72	113.28	108.13
1	A	541	GLY	CA-C-N	5.46	127.55	120.44
1	A	541	GLY	C-N-CA	5.46	127.55	120.44
1	A	615	GLY	CA-C-N	5.44	127.51	120.44
1	A	615	GLY	C-N-CA	5.44	127.51	120.44
1	C	953	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	953	PHE	CA-CB-CG	5.43	119.23	113.80
1	B	638	VAL	N-CA-C	5.39	113.80	107.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	906	GLY	CA-C-N	5.36	127.47	120.28
1	A	906	GLY	C-N-CA	5.36	127.47	120.28
1	B	576	VAL	CA-C-N	5.34	127.97	120.28
1	B	576	VAL	C-N-CA	5.34	127.97	120.28
1	D	953	PHE	CA-CB-CG	5.34	119.14	113.80
1	C	615	GLY	CA-C-N	5.33	127.37	120.44
1	C	615	GLY	C-N-CA	5.33	127.37	120.44
1	B	738	ASP	CA-CB-CG	5.33	117.92	112.60
1	B	615	GLY	CA-C-N	5.26	127.28	120.44
1	B	615	GLY	C-N-CA	5.26	127.28	120.44
1	D	1058	ASP	CA-CB-CG	5.26	117.86	112.60
1	D	615	GLY	CA-C-N	5.24	127.25	120.44
1	D	615	GLY	C-N-CA	5.24	127.25	120.44
1	B	379	ASN	CA-CB-CG	5.24	117.84	112.60
1	B	1058	ASP	CA-CB-CG	5.23	117.83	112.60
1	C	1058	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	1058	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	576	VAL	CA-C-N	5.19	127.76	120.28
1	A	576	VAL	C-N-CA	5.19	127.76	120.28
1	C	493	GLU	CB-CG-CD	5.17	121.39	112.60
1	C	638	VAL	N-CA-C	5.17	113.56	107.77
1	A	605	HIS	CA-C-N	5.15	128.08	120.82
1	A	605	HIS	C-N-CA	5.15	128.08	120.82
1	B	953	PHE	CA-CB-CG	5.14	118.94	113.80
1	D	576	VAL	CA-C-N	5.12	127.65	120.28
1	D	576	VAL	C-N-CA	5.12	127.65	120.28
1	C	602	ASN	N-CA-C	5.07	112.69	108.13
1	B	369	ARG	CA-C-N	5.03	127.00	120.56
1	B	369	ARG	C-N-CA	5.03	127.00	120.56
1	B	844	GLY	CA-C-N	5.03	127.02	120.28
1	B	844	GLY	C-N-CA	5.03	127.02	120.28

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	26	0
1	B	6463	0	6253	35	0
1	C	6530	0	6308	38	0
1	D	6578	0	6362	31	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
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	127	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 (127) 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:A:755:MET:HE1	1:B:909:THR:HG21	1.83	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⁷	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
1:C:901[A]:GLN:OE1	2:D:2001:TD8:H6 ⁷	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 ⁷	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 ⁷	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:PRO:HD2	5:B:3032:HOH:O	2.12	0.50
1:A:755:MET:HE1	1:B:909:THR:CG2	2.41	0.49
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
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:C:909:THR:CG2	1:D:755:MET:HE1	2.45	0.47
1:C:554:TYR:OH	1:C:796:TYR:OH	2.23	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:C:755:MET:HE1	1:D:909:THR:HG21	1.98	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:C:909:THR:HG21	1:D:755:MET:HE1	1.98	0.44
1:A:656:GLU:HB3	1:A:954:ALA:HB2	1.99	0.44
1:C:755:MET:HE1	1:D:909:THR:CG2	2.47	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:867:ARG:HA	1:C:870:MET:HE3	2.01	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
1:C:749:GLU:CD	1:C:749:GLU:N	2.79	0.41
1:A:749:GLU:N	1:A:749:GLU:CD	2.79	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: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:D:749:GLU:CD	1:D:749:GLU:N	2.79	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%)	43	55
1	B	828/868 (95%)	806 (97%)	19 (2%)	3 (0%)	30	38
1	C	838/868 (96%)	818 (98%)	17 (2%)	3 (0%)	30	38
1	D	844/868 (97%)	821 (97%)	22 (3%)	1 (0%)	48	60
All	All	3350/3472 (96%)	3266 (98%)	75 (2%)	9 (0%)	36	46

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 ⓘ

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%)	665 (99%)	6 (1%)	70	84
1	B	668/726 (92%)	660 (99%)	8 (1%)	63	79
1	C	672/726 (93%)	666 (99%)	6 (1%)	70	84
1	D	679/726 (94%)	674 (99%)	5 (1%)	76	87
All	All	2690/2904 (93%)	2665 (99%)	25 (1%)	70	84

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	ILE
1	A	514	VAL
1	A	740	LEU
1	A	837	LYS
1	A	976	GLN
1	A	1087	GLU
1	B	415	LEU
1	B	467	VAL
1	B	514	VAL
1	B	542	ARG
1	B	784	ILE
1	B	909	THR
1	B	950	LEU
1	B	976	GLN
1	C	371	ILE
1	C	464	GLN
1	C	467	VAL
1	C	514	VAL
1	C	909	THR
1	C	976	GLN
1	D	467	VAL
1	D	909	THR
1	D	950	LEU
1	D	976	GLN
1	D	1112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	679	GLN
1	A	947	ASN
1	A	1001	GLN
1	A	1061	GLN
1	A	1107	ASN
1	B	556	GLN
1	B	679	GLN
1	B	912	HIS
1	B	1061	GLN
1	B	1107	ASN
1	C	367	ASN
1	C	1061	GLN
1	C	1107	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	679	GLN
1	D	966	ASN
1	D	1107	ASN

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 oligosaccharides 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	C	2001	3	32,35,35	1.79	3 (9%)	39,51,51	1.76	10 (25%)
2	TD8	A	2001	3	32,35,35	1.70	3 (9%)	39,51,51	1.76	12 (30%)
2	TD8	B	2001	3	32,35,35	1.73	4 (12%)	39,51,51	1.77	12 (30%)
2	TD8	D	2001	3	32,35,35	1.61	2 (6%)	39,51,51	1.67	7 (17%)

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	C	2001	3	-	14/26/27/27	0/2/2/2
2	TD8	A	2001	3	-	5/26/27/27	0/2/2/2
2	TD8	B	2001	3	-	8/26/27/27	0/2/2/2
2	TD8	D	2001	3	-	9/26/27/27	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	TD8	C5-C4	7.22	1.50	1.35
2	A	2001	TD8	C5-C4	6.99	1.49	1.35
2	C	2001	TD8	C5-C4	6.96	1.49	1.35
2	D	2001	TD8	C5-C4	6.71	1.49	1.35
2	D	2001	TD8	O9-C8	-4.16	1.33	1.42
2	A	2001	TD8	O9-C8	-4.08	1.34	1.42
2	C	2001	TD8	PA-O3A	3.98	1.63	1.59
2	C	2001	TD8	O9-C8	-3.97	1.34	1.42
2	B	2001	TD8	O9-C8	-3.76	1.34	1.42
2	B	2001	TD8	PA-O3A	2.76	1.62	1.59
2	A	2001	TD8	PA-O3A	2.24	1.61	1.59
2	B	2001	TD8	C35-N3	2.04	1.49	1.47

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	TD8	C2A-C2'-N1'	4.07	121.54	117.20
2	B	2001	TD8	C4-C5-S1	-3.87	106.56	110.56
2	C	2001	TD8	C2A-C2'-N1'	3.72	121.16	117.20
2	C	2001	TD8	N1'-C2'-N3'	-3.63	119.49	125.53
2	B	2001	TD8	C2A-C2'-N1'	3.52	120.94	117.20
2	A	2001	TD8	O9-C8-C9	3.49	118.40	109.14
2	D	2001	TD8	N1'-C2'-N3'	-3.44	119.81	125.53
2	B	2001	TD8	N1'-C2'-N3'	-3.27	120.10	125.53
2	B	2001	TD8	C6'-N1'-C2'	3.27	121.44	116.07
2	C	2001	TD8	C6'-N1'-C2'	3.17	121.28	116.07
2	D	2001	TD8	C6'-N1'-C2'	3.13	121.22	116.07
2	C	2001	TD8	C4-C5-S1	-3.09	107.36	110.56
2	B	2001	TD8	O9-C8-C9	3.09	117.32	109.14
2	A	2001	TD8	C2A-C2'-N1'	3.05	120.45	117.20
2	A	2001	TD8	C4A-C4-N3	2.95	125.80	121.95
2	A	2001	TD8	N1'-C2'-N3'	-2.94	120.65	125.53
2	C	2001	TD8	C4A-C4-N3	2.91	125.75	121.95
2	C	2001	TD8	C5A-C5-C4	2.86	135.35	128.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	TD8	C4-C5-S1	-2.85	107.61	110.56
2	D	2001	TD8	C4A-C4-N3	2.83	125.64	121.95
2	C	2001	TD8	C4A-C4-C5	-2.65	120.96	127.75
2	A	2001	TD8	C6'-N1'-C2'	2.62	120.38	116.07
2	A	2001	TD8	C6'-C5'-C4'	2.55	118.68	115.55
2	C	2001	TD8	O9-C8-C9	2.50	115.76	109.14
2	B	2001	TD8	C5A-C5-C4	2.40	134.20	128.17
2	D	2001	TD8	C4A-C4-C5	-2.38	121.64	127.75
2	A	2001	TD8	C5A-C5-C4	2.37	134.13	128.17
2	B	2001	TD8	C4A-C4-C5	-2.37	121.68	127.75
2	A	2001	TD8	O3B-PB-O1B	2.35	116.61	107.80
2	A	2001	TD8	C4A-C4-C5	-2.31	121.82	127.75
2	A	2001	TD8	C5B-C5A-C5	-2.28	105.59	112.73
2	A	2001	TD8	C5'-C6'-N1'	-2.24	120.18	123.83
2	B	2001	TD8	O1B-PB-O3A	2.23	112.11	104.64
2	C	2001	TD8	O12-C14-C12	-2.20	116.12	123.09
2	B	2001	TD8	C4A-C4-N3	2.19	124.81	121.95
2	D	2001	TD8	C4-C5-S1	-2.15	108.34	110.56
2	B	2001	TD8	C5'-C6'-N1'	-2.14	120.35	123.83
2	B	2001	TD8	O5G-C5B-C5A	2.11	117.09	108.63
2	C	2001	TD8	O11-C14-C12	2.04	120.44	114.00
2	B	2001	TD8	C5B-C5A-C5	-2.03	106.35	112.73
2	D	2001	TD8	O5G-PA-O1A	-2.02	100.94	108.94

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	TD8	S1-C2-C8-O9
2	B	2001	TD8	C2-C8-C9-C10
2	B	2001	TD8	PA-O3A-PB-O1B
2	B	2001	TD8	PA-O3A-PB-O3B
2	C	2001	TD8	C2-C8-C9-C10
2	C	2001	TD8	C5B-O5G-PA-O2A
2	C	2001	TD8	C5B-O5G-PA-O3A
2	C	2001	TD8	PA-O3A-PB-O1B
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	O9-C8-C9-C10
2	A	2001	TD8	C2-C8-C9-C10
2	B	2001	TD8	S1-C2-C8-O9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	2001	TD8	S1-C2-C8-O9
2	C	2001	TD8	PA-O3A-PB-O3B
2	D	2001	TD8	S1-C2-C8-O9
2	B	2001	TD8	C5-C5A-C5B-O5G
2	C	2001	TD8	C5-C5A-C5B-O5G
2	C	2001	TD8	C5B-O5G-PA-O1A
2	D	2001	TD8	C12-C10-C9-C8
2	D	2001	TD8	C10-C12-C14-O11
2	A	2001	TD8	C10-C12-C14-O11
2	A	2001	TD8	C10-C12-C14-O12
2	D	2001	TD8	C10-C12-C14-O12
2	B	2001	TD8	C10-C12-C14-O11
2	C	2001	TD8	PA-O3A-PB-O2B
2	B	2001	TD8	C10-C12-C14-O12
2	C	2001	TD8	C10-C12-C14-O12
2	C	2001	TD8	C10-C12-C14-O11
2	D	2001	TD8	N3-C35-C5'-C4'
2	C	2001	TD8	C12-C10-C9-C8
2	A	2001	TD8	N3-C2-C8-O9
2	B	2001	TD8	N3-C2-C8-O9
2	C	2001	TD8	N3-C2-C8-O9
2	D	2001	TD8	N3-C2-C8-O9

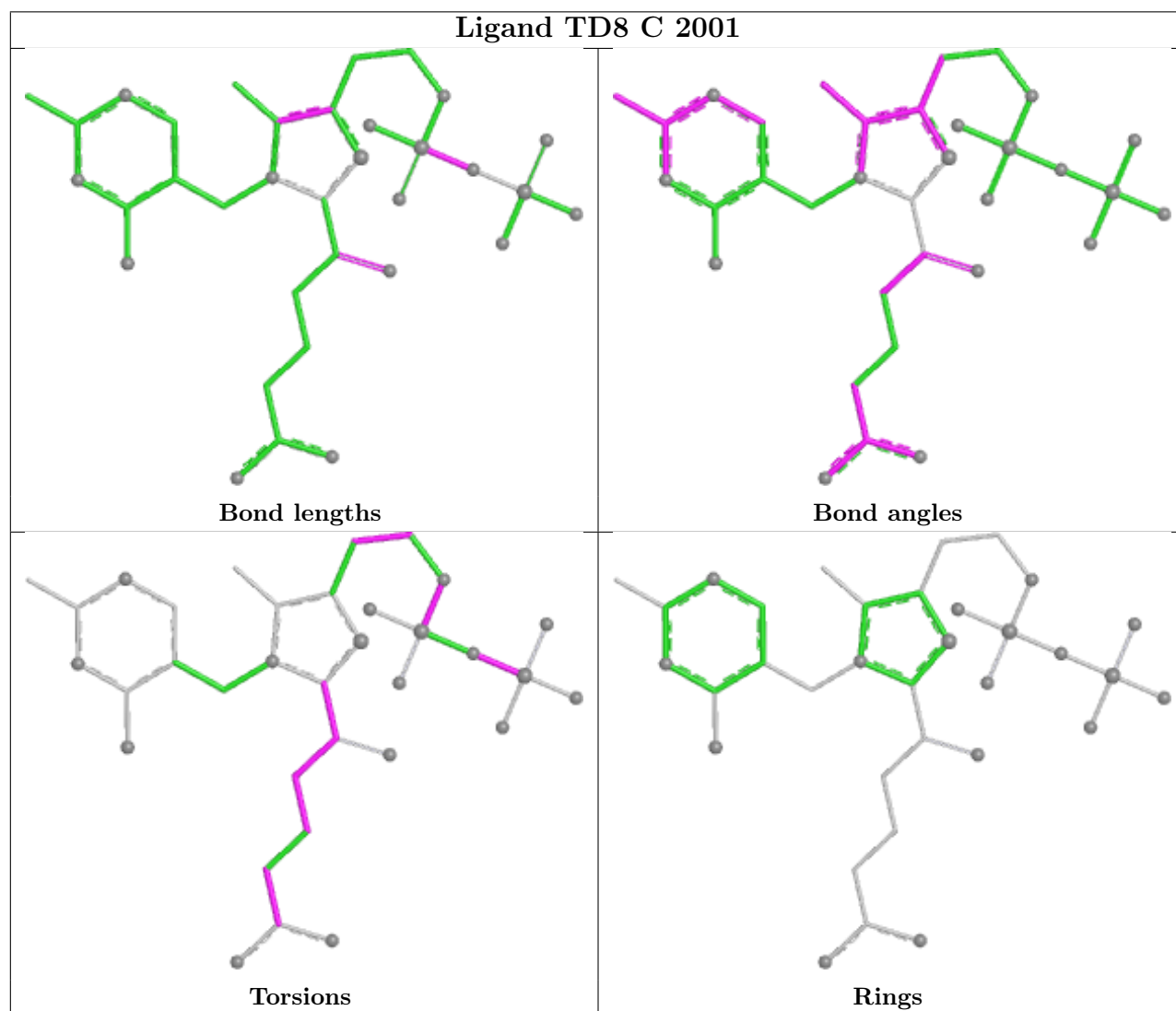
There are no ring outliers.

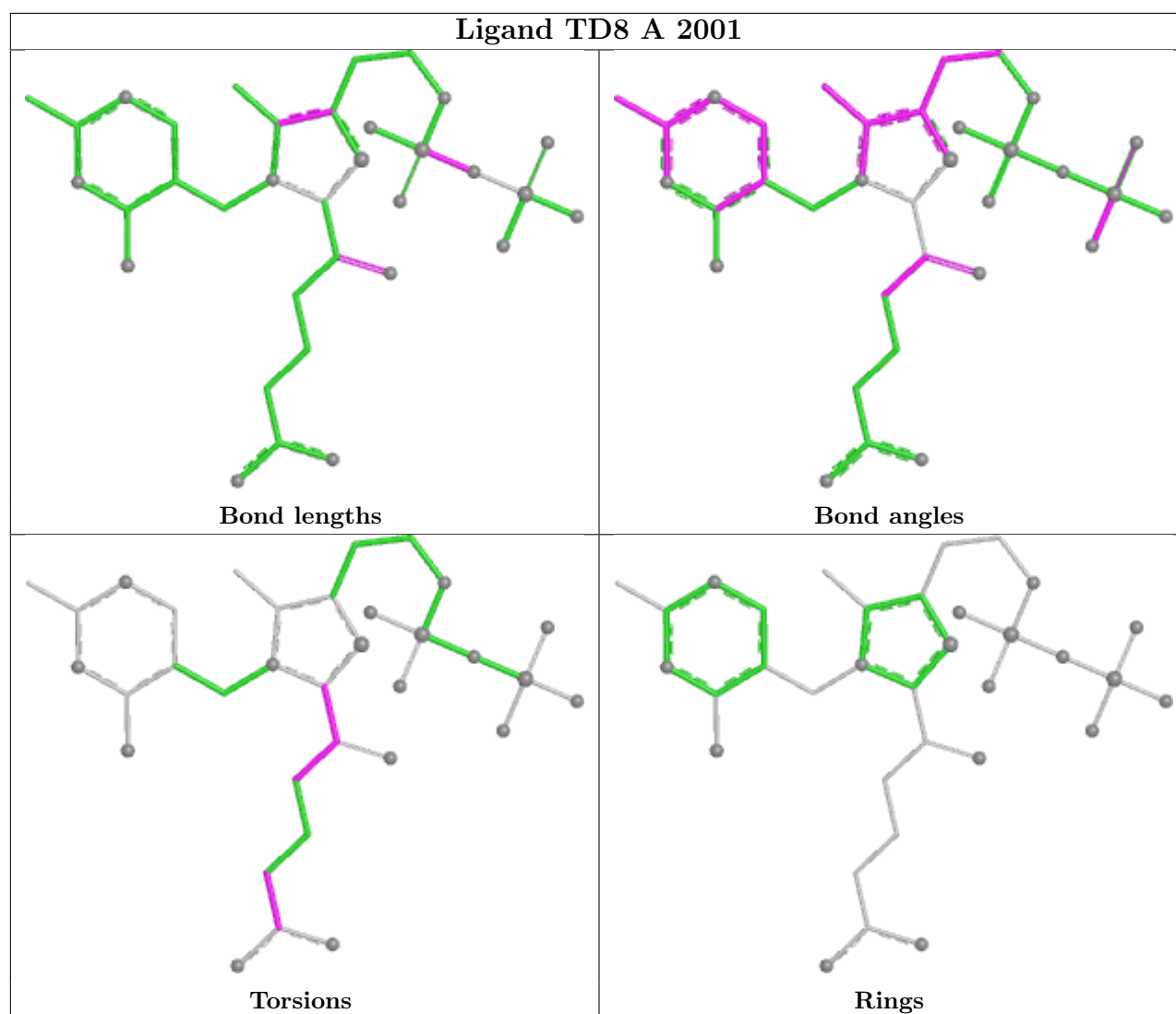
4 monomers are involved in 13 short contacts:

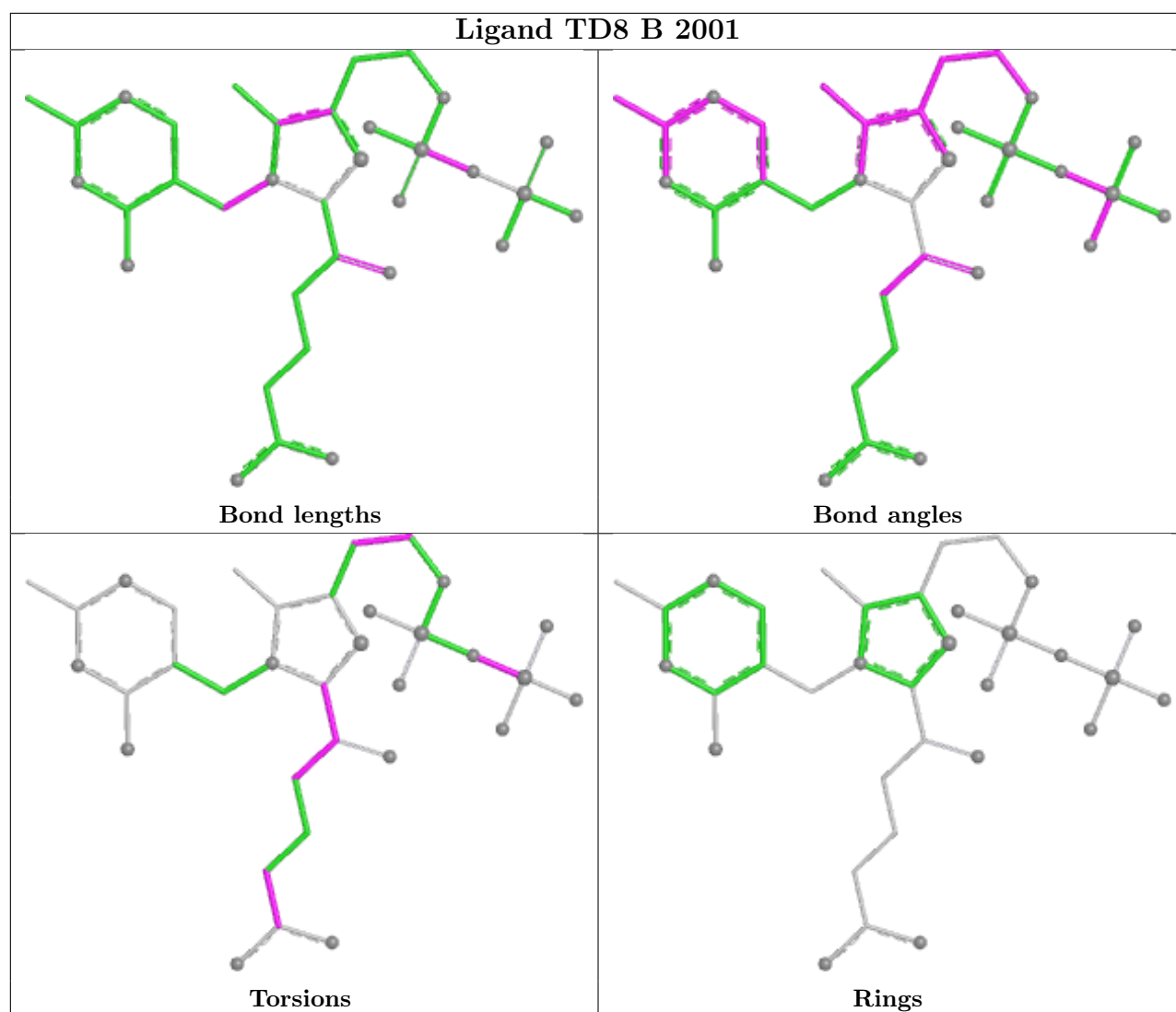
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	TD8	1	0
2	A	2001	TD8	6	0
2	B	2001	TD8	2	0
2	D	2001	TD8	4	0

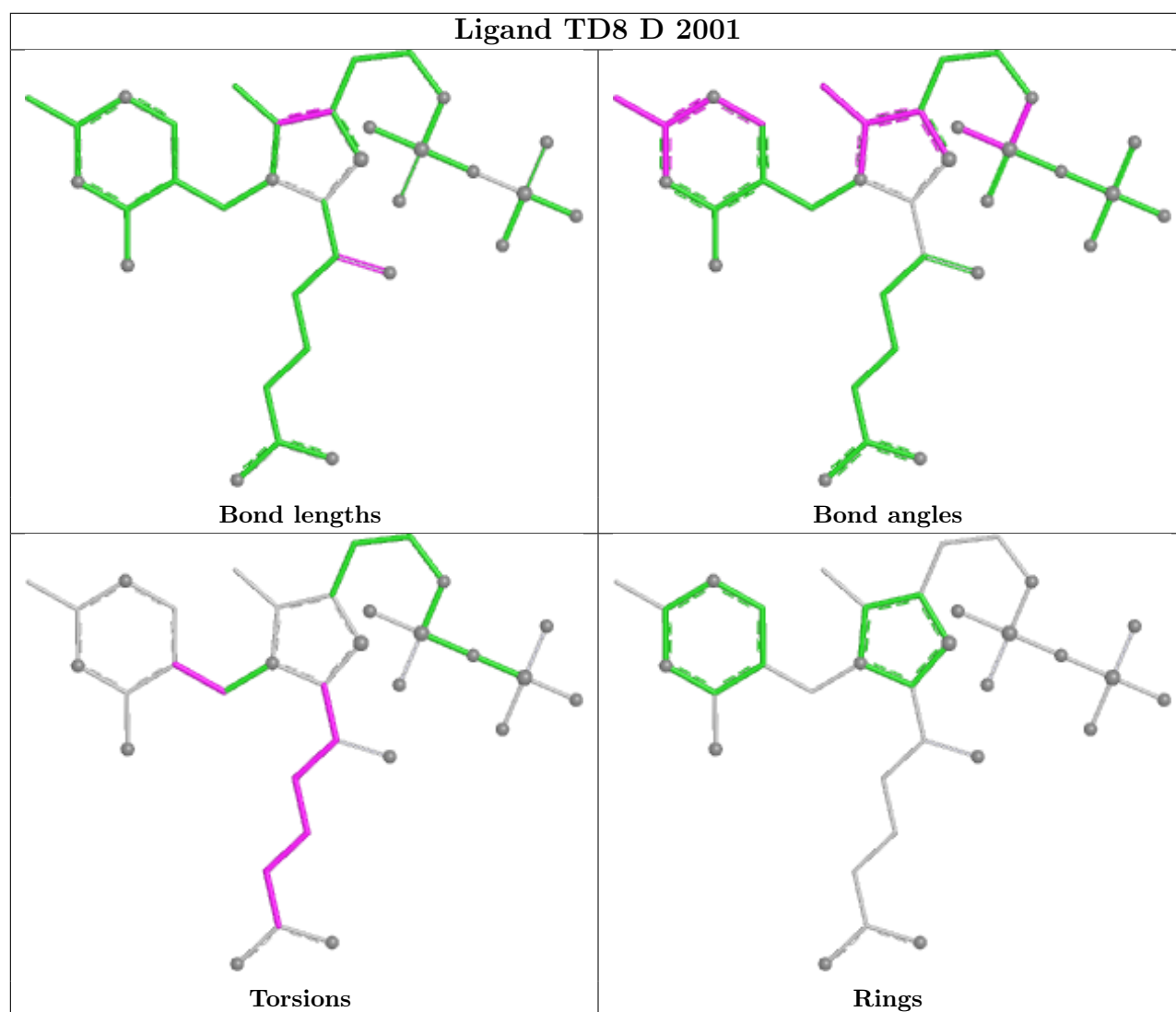
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	847/868 (97%)	0.70	67 (7%) 18 20	20, 41, 74, 103	1 (0%)
1	B	836/868 (96%)	0.46	33 (3%) 43 45	22, 36, 65, 94	0
1	C	845/868 (97%)	0.47	50 (5%) 28 30	13, 36, 65, 114	1 (0%)
1	D	852/868 (98%)	0.67	70 (8%) 17 19	22, 40, 73, 109	0
All	All	3380/3472 (97%)	0.58	220 (6%) 25 27	13, 38, 70, 114	2 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	568	SER	6.6
1	B	413	TRP	6.0
1	A	827	ILE	5.8
1	C	421	VAL	5.7
1	C	827	ILE	5.2
1	D	398	ARG	5.2
1	A	502	GLY	5.0
1	C	790	GLU	5.0
1	A	363	ILE	4.7
1	C	413	TRP	4.6
1	B	368	ALA	4.5
1	D	422	ASP	4.5
1	A	571	HIS	4.4
1	C	420	LYS	4.4
1	D	828	PRO	4.4
1	A	1227	GLY	4.3
1	A	831	LEU	4.3
1	A	566	ASN	4.3
1	B	827	ILE	4.3
1	D	803	VAL	4.2
1	C	565	LEU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	364	GLU	4.2
1	A	564	ASN	4.2
1	D	565	LEU	4.1
1	C	564	ASN	4.1
1	D	363	ILE	4.0
1	A	394	ASN	4.0
1	B	472	ASP	4.0
1	D	423	GLY	3.9
1	A	395	THR	3.9
1	D	827	ILE	3.9
1	C	569	GLN	3.9
1	C	568	SER	3.9
1	A	807	VAL	3.8
1	D	564	ASN	3.8
1	D	1227	GLY	3.8
1	A	569	GLN	3.7
1	B	365	ASP	3.7
1	D	796	TYR	3.7
1	D	413	TRP	3.6
1	D	364	GLU	3.6
1	B	421	VAL	3.6
1	A	567	PRO	3.6
1	A	570	ALA	3.6
1	A	810	LEU	3.5
1	A	472	ASP	3.5
1	D	361	ASP	3.5
1	C	419	PHE	3.5
1	B	563	GLY	3.5
1	A	796	TYR	3.5
1	A	565	LEU	3.4
1	A	558	PHE	3.4
1	D	502	GLY	3.4
1	D	427	VAL	3.4
1	A	427	VAL	3.4
1	A	368	ALA	3.4
1	D	572	GLY	3.4
1	D	392	LEU	3.3
1	B	415	LEU	3.3
1	A	832	ALA	3.3
1	D	410	LEU	3.3
1	C	796	TYR	3.3
1	C	570	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	471	HIS	3.2
1	C	571	HIS	3.2
1	D	815	ILE	3.2
1	D	811	GLU	3.1
1	A	1101	ASP	3.1
1	B	564	ASN	3.1
1	D	368	ALA	3.1
1	C	567	PRO	3.1
1	A	815	ILE	3.1
1	C	409	GLY	3.1
1	D	472	ASP	3.0
1	C	398	ARG	3.0
1	B	414	ASP	3.0
1	D	367	ASN	3.0
1	A	500	TYR	3.0
1	A	361	ASP	3.0
1	B	566	ASN	3.0
1	A	790	GLU	3.0
1	D	1077	ALA	2.9
1	D	831	LEU	2.9
1	A	413	TRP	2.9
1	A	362	SER	2.9
1	D	567	PRO	2.9
1	C	558	PHE	2.9
1	A	364	GLU	2.9
1	D	429	ARG	2.8
1	B	565	LEU	2.8
1	D	561	PHE	2.8
1	B	711	GLY	2.8
1	C	566	ASN	2.8
1	D	394	ASN	2.8
1	A	779	ILE	2.8
1	D	371	ILE	2.8
1	B	469	THR	2.7
1	C	415	LEU	2.7
1	C	502	GLY	2.7
1	A	412	LEU	2.7
1	D	393	ASP	2.7
1	A	1187	ILE	2.7
1	C	830	LYS	2.7
1	D	631	SER	2.7
1	D	415	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	571	HIS	2.7
1	C	397	PHE	2.7
1	A	498	THR	2.7
1	C	371	ILE	2.7
1	B	815	ILE	2.6
1	D	569	GLN	2.6
1	A	1077	ALA	2.6
1	D	471	HIS	2.6
1	A	410	LEU	2.6
1	D	428	GLN	2.6
1	A	772	LYS	2.6
1	D	498	THR	2.6
1	B	828	PRO	2.6
1	B	366	LYS	2.6
1	C	759	TYR	2.6
1	B	811	GLU	2.5
1	C	392	LEU	2.5
1	D	1103	GLU	2.5
1	D	687	THR	2.5
1	C	815	ILE	2.5
1	D	810	LEU	2.5
1	A	367	ASN	2.5
1	A	765	ASP	2.5
1	B	790	GLU	2.5
1	C	810	LEU	2.5
1	A	822	GLU	2.5
1	D	759	TYR	2.5
1	A	415	LEU	2.5
1	B	571	HIS	2.5
1	C	1185	PRO	2.5
1	D	563	GLY	2.5
1	C	492	PHE	2.4
1	A	823	ALA	2.4
1	D	397	PHE	2.4
1	C	1129	LYS	2.4
1	C	411	THR	2.4
1	C	735	VAL	2.4
1	A	836	ASP	2.4
1	D	1101	ASP	2.4
1	A	561	PHE	2.4
1	C	384	MET	2.4
1	C	476	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	471	HIS	2.4
1	B	826	GLN	2.4
1	A	422	ASP	2.3
1	C	591	GLY	2.3
1	A	501	VAL	2.3
1	D	804	PHE	2.3
1	C	813	HIS	2.3
1	B	792	ALA	2.3
1	D	1187	ILE	2.3
1	D	501	VAL	2.3
1	C	366	LYS	2.3
1	D	566	ASN	2.3
1	B	474	PRO	2.3
1	A	703	GLY	2.3
1	C	572	GLY	2.3
1	D	554	TYR	2.3
1	D	814	GLU	2.3
1	C	765	ASP	2.2
1	B	502	GLY	2.2
1	D	802	ARG	2.2
1	A	813	HIS	2.2
1	A	549	ILE	2.2
1	D	590	PHE	2.2
1	B	794	ARG	2.2
1	C	1227	GLY	2.2
1	A	811	GLU	2.2
1	C	583	THR	2.2
1	A	550	VAL	2.2
1	D	421	VAL	2.2
1	D	550	VAL	2.2
1	C	365	ASP	2.2
1	C	748	ASN	2.2
1	A	750	GLY	2.2
1	A	1103	GLU	2.2
1	A	1186	GLU	2.2
1	A	1152	ALA	2.2
1	B	796	TYR	2.2
1	A	859	ARG	2.2
1	B	392	LEU	2.2
1	A	492	PHE	2.2
1	B	419	PHE	2.2
1	D	365	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	747	HIS	2.1
1	B	951	SER	2.1
1	C	781	ARG	2.1
1	D	380	ARG	2.1
1	B	812	LYS	2.1
1	C	469	THR	2.1
1	D	767	LYS	2.1
1	D	412	LEU	2.1
1	B	471	HIS	2.1
1	A	821	VAL	2.1
1	C	794	ARG	2.1
1	C	696	THR	2.1
1	D	420	LYS	2.1
1	D	473	LYS	2.1
1	A	800	LEU	2.1
1	D	508	LEU	2.1
1	A	421	VAL	2.1
1	A	771	ARG	2.1
1	A	633	ASN	2.0
1	D	496	LEU	2.0
1	D	793	LEU	2.0
1	D	492	PHE	2.0
1	B	583	THR	2.0
1	D	560	GLU	2.0
1	D	570	ALA	2.0
1	D	813	HIS	2.0
1	A	365	ASP	2.0
1	A	414	ASP	2.0
1	C	508	LEU	2.0
1	B	705	PRO	2.0
1	A	473	LYS	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

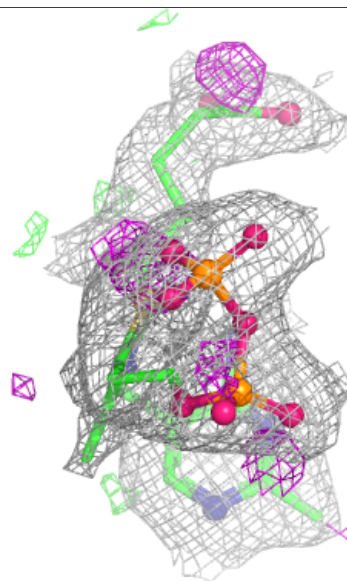
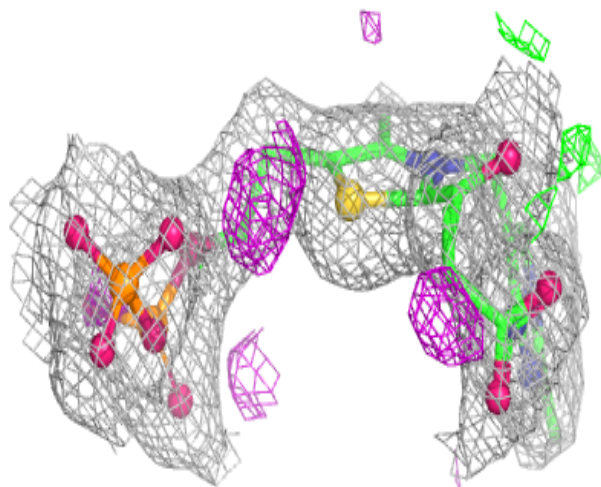
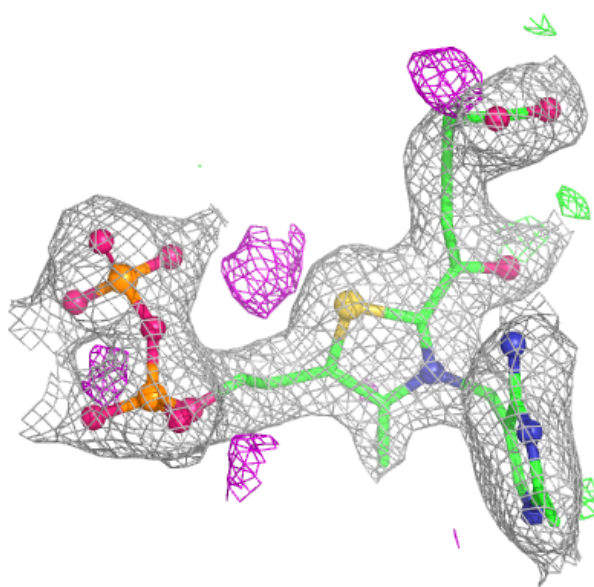
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TD8	B	2001	34/34	0.96	0.08	17,28,34,37	0
2	TD8	C	2001	34/34	0.96	0.09	16,28,44,48	0
2	TD8	D	2001	34/34	0.96	0.08	19,26,41,43	0
4	CA	A	2003	1/1	0.96	0.09	41,41,41,41	0
3	MG	A	2002	1/1	0.97	0.03	26,26,26,26	0
2	TD8	A	2001	34/34	0.97	0.08	16,30,40,41	0
4	CA	D	2003	1/1	0.97	0.11	41,41,41,41	0
4	CA	C	2003	1/1	0.98	0.09	28,28,28,28	0
3	MG	D	2002	1/1	0.98	0.03	25,25,25,25	0
4	CA	B	2003	1/1	0.99	0.05	29,29,29,29	0
3	MG	B	2002	1/1	0.99	0.04	17,17,17,17	0
3	MG	C	2002	1/1	0.99	0.02	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.

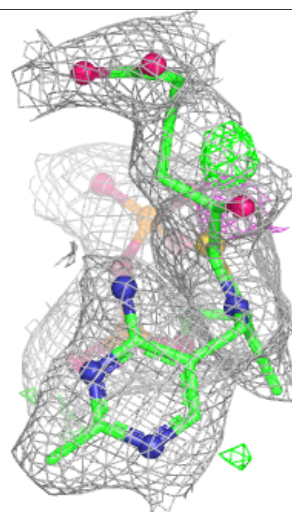
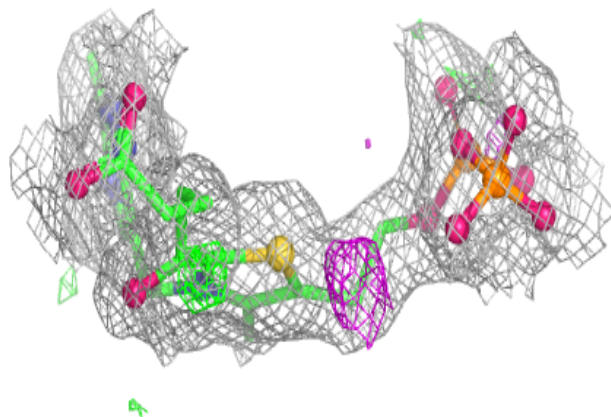
Electron density around TD8 B 2001:

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



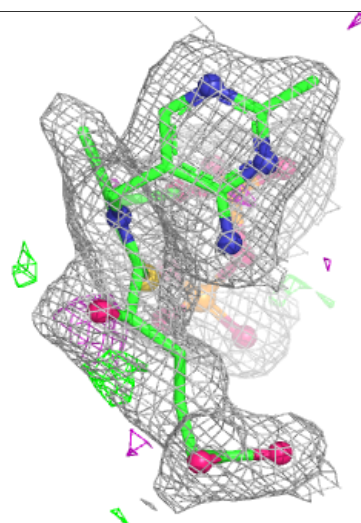
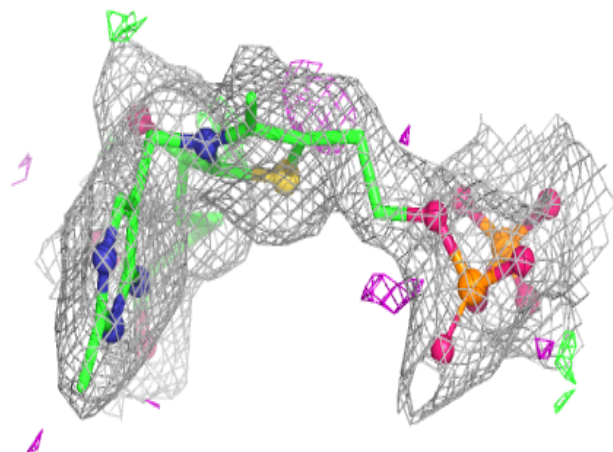
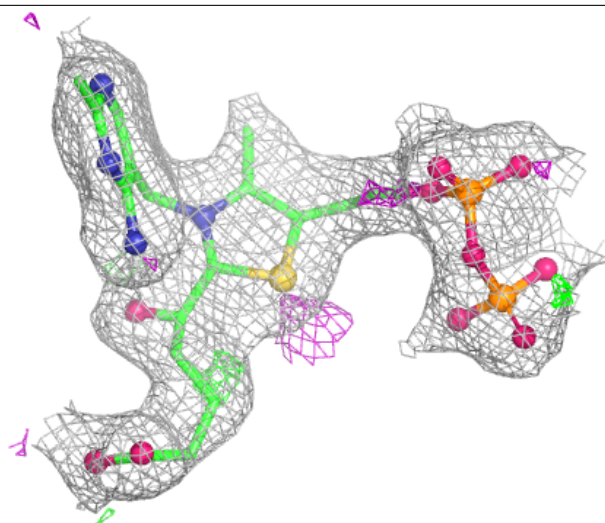
Electron density around TD8 C 2001:

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



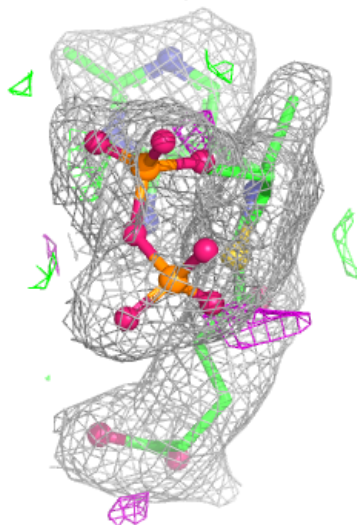
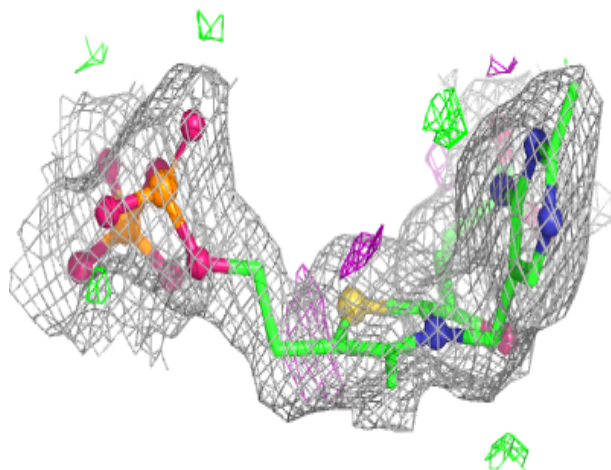
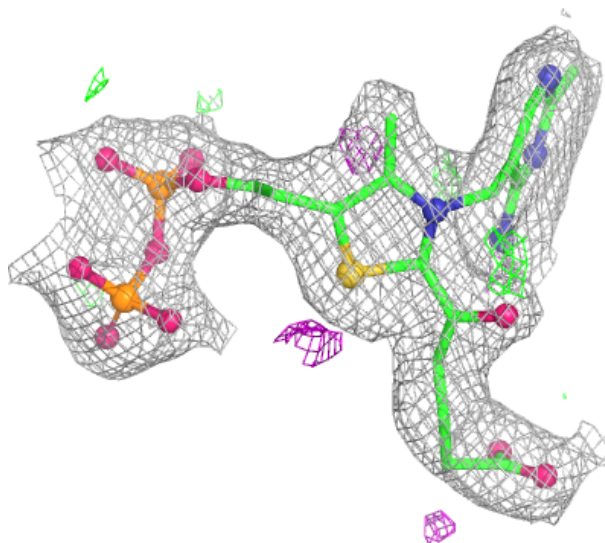
Electron density around TD8 D 2001:

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



Electron density around TD8 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 [i](#)

There are no such residues in this entry.