



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 07:48 pm BST

PDB ID : 3TUR  
Title : Crystal Structure of M. tuberculosis LD-transpeptidase type 2 complexed with a peptidoglycan fragment  
Authors : Bianchet, M.A.; Erdemli, S.B.; Gupta, R.; Lamichhane, G.; Amzel, L.M.  
Deposited on : 2011-09-17  
Resolution : 1.72 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

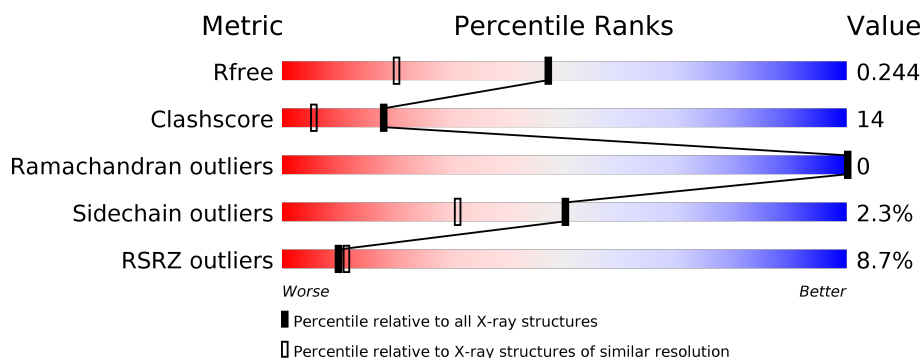
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.72 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	287	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>••</div> <div>10%</div> </div> </div>
1	B	287	<div> <div>11%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>•</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0JC	A	504[A]	-	-	-	X
2	0JC	A	504[B]	-	-	-	X
2	0JC	B	505	-	-	X	-
3	DGL	A	505[A]	-	-	-	X
3	DGL	A	505[B]	-	-	-	X
4	6CL	A	506[A]	-	-	X	X
4	6CL	A	506[B]	-	-	X	X

## 2 Entry composition [i](#)

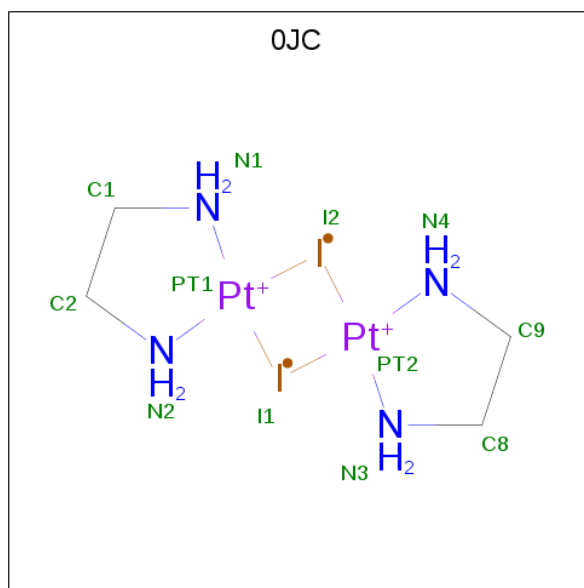
There are 6 unique types of molecules in this entry. The entry contains 4653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mycobacteria Tuberculosis LD-transpeptidase type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	3	0
			2008	1266	349	385	8			
1	B	269	Total	C	N	O	S	0	2	0
			2063	1301	357	398	7			

- Molecule 2 is Di-mu-iodobis(ethylenediamine)diplatinum(II) (three-letter code: 0JC) (formula:  $C_4H_{16}I_2N_4Pt_2$ ).



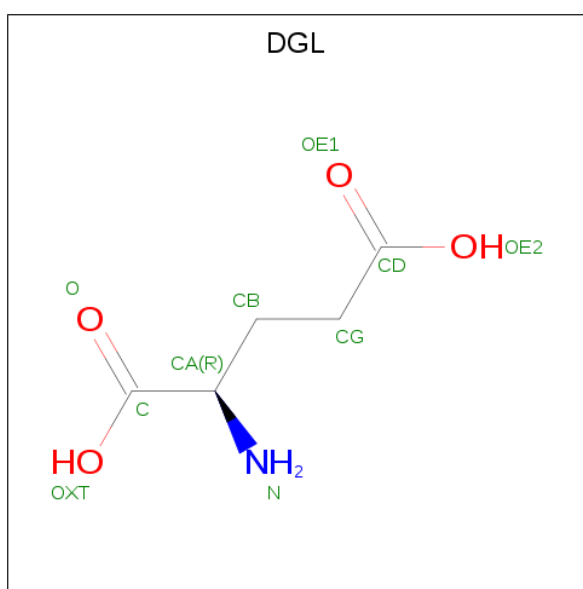
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	I	N	Pt	0	0
			6	2	1	2	1		
2	A	1	Total	C	I	N	Pt	0	1
			12	4	2	4	2		
2	A	1	Total	C	I	N	Pt	0	0
			6	2	1	2	1		
2	A	1	Total	C	I	N	Pt	0	1
			12	4	2	4	2		

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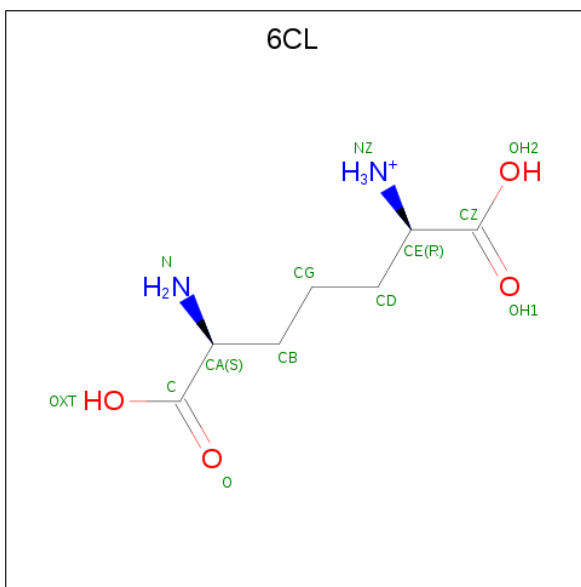
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	I	N	Pt	0	0
			6	2	1	2	1		
2	B	1	Total	C	I	N	Pt	0	0
			6	2	1	2	1		
2	B	1	Total	C	I	N	Pt	0	1
			12	4	2	4	2		
2	B	1	Total	C	I	N	Pt	0	0
			6	2	1	2	1		

- Molecule 3 is D-GLUTAMIC ACID (three-letter code: DGL) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			18	10	2	6		

- Molecule 4 is 6-CARBOXYLYSINE (three-letter code: 6CL) (formula: C<sub>7</sub>H<sub>15</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			26	14	4	8		

- Molecule 5 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Pt	0	0
			1	1		

- Molecule 6 is water.

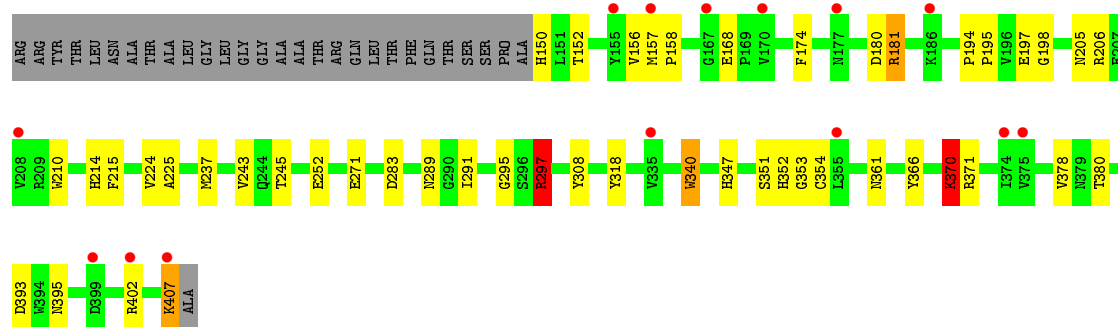
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	229	Total	O	0	1
			230	230		
6	B	241	Total	O	0	0
			241	241		

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

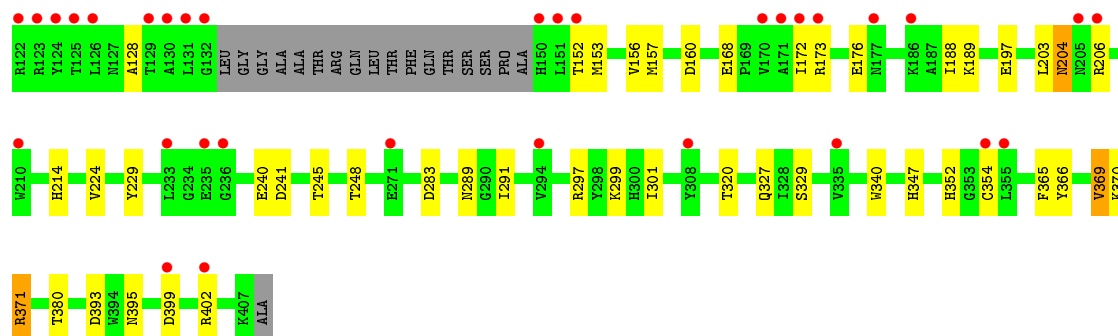
- Molecule 1: Mycobacteria Tuberculosis LD-transpeptidase type 2

Chain A: 



- Molecule 1: Mycobacteria Tuberculosis LD-transpeptidase type 2

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.13Å 120.83Å 122.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.69 – 1.72 25.87 – 1.72	Depositor EDS
% Data completeness (in resolution range)	94.3 (85.69-1.72) 94.4 (25.87-1.72)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.72Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.199 , 0.235 0.209 , 0.244	Depositor DCC
$R_{free}$ test set	4474 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.057 for -h,-l,-k 0.003 for l,-k,h 0.006 for -k,-h,-l 0.000 for k,-l,-h 0.000 for -l,h,-k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4653	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 6CL, 0JC, DGL, PT

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	1.41	10/2067 (0.5%)	1.17	7/2827 (0.2%)
1	B	1.43	7/2125 (0.3%)	1.20	10/2905 (0.3%)
All	All	1.42	17/4192 (0.4%)	1.19	17/5732 (0.3%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	LYS	CE-NZ	9.23	1.72	1.49
1	A	318	TYR	CD2-CE2	7.00	1.49	1.39
1	A	197	GLU	CG-CD	6.38	1.61	1.51
1	B	329	SER	CB-OG	6.01	1.50	1.42
1	B	370	LYS	CD-CE	5.84	1.65	1.51
1	A	252	GLU	CG-CD	5.74	1.60	1.51
1	A	308	TYR	CD2-CE2	5.65	1.47	1.39
1	B	197	GLU	CG-CD	5.63	1.60	1.51
1	B	340	TRP	CE3-CZ3	5.42	1.47	1.38
1	A	297[A]	ARG	CZ-NH1	-5.37	1.26	1.33
1	A	297[B]	ARG	CZ-NH1	-5.37	1.26	1.33
1	A	340	TRP	CE3-CZ3	5.30	1.47	1.38
1	A	225	ALA	CA-CB	5.20	1.63	1.52
1	B	365	PHE	CE2-CZ	5.16	1.47	1.37
1	A	215	PHE	CD1-CE1	5.13	1.49	1.39
1	B	370	LYS	CE-NZ	5.08	1.61	1.49
1	B	229	TYR	CD2-CE2	5.07	1.47	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	ARG	NE-CZ-NH1	-15.22	112.69	120.30
1	A	180	ASP	CB-CG-OD1	8.89	126.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	LEU	CB-CG-CD2	8.52	125.48	111.00
1	B	160	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	A	297[A]	ARG	CG-CD-NE	-7.81	95.40	111.80
1	A	297[B]	ARG	CG-CD-NE	-7.81	95.40	111.80
1	A	181	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	B	371	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	B	370	LYS	CD-CE-NZ	6.78	127.28	111.70
1	A	283	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	160	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	181	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	248	THR	CA-CB-CG2	-5.75	104.35	112.40
1	A	378	VAL	CG1-CB-CG2	-5.73	101.73	110.90
1	B	283	ASP	CB-CG-OD1	5.56	123.30	118.30
1	B	301	ILE	CG1-CB-CG2	5.07	122.55	111.40
1	B	369	VAL	CB-CA-C	5.05	120.99	111.40

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	2008	0	1910	50	0
1	B	2063	0	1951	55	0
2	A	36	0	24	10	0
2	B	30	0	20	17	0
3	A	18	0	14	3	0
4	A	26	0	24	33	0
5	B	1	0	0	0	0
6	A	230	0	0	2	1
6	B	241	0	0	11	1
All	All	4653	0	3943	110	2

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 14.

All (110) 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:370:LYS:CE	1:A:370:LYS:NZ	1.72	1.53
2:B:504[A]:0JC:I1	6:B:838:HOH:O	2.26	1.22
2:B:502:0JC:H6	6:B:718:HOH:O	1.45	1.14
4:A:506[B]:6CL:HA	1:B:352:HIS:H	1.10	1.12
1:A:157[A]:MET:HG3	1:A:158:PRO:HA	1.32	1.09
1:A:354:CYS:SG	4:A:506[A]:6CL:HG2	1.96	1.05
1:A:352:HIS:H	4:A:506[A]:6CL:HA	1.14	1.04
1:A:237:MET:HG3	2:A:503:0JC:I1	2.33	0.99
3:A:505[B]:DGL:OE2	4:A:506[B]:6CL:C	2.06	0.98
3:A:505[B]:DGL:OE2	4:A:506[B]:6CL:O	1.85	0.94
1:A:237:MET:CG	2:A:503:0JC:I1	2.85	0.93
1:B:153:MET:HG2	2:B:505:0JC:I1	2.39	0.93
1:A:289:ASN:HD21	1:A:380:THR:H	1.11	0.91
1:B:173:ARG:NH1	2:B:504[B]:0JC:I1	2.74	0.91
1:B:240:GLU:OE2	2:B:505:0JC:N2	2.06	0.90
1:B:153:MET:CE	2:B:505:0JC:I1	2.90	0.89
4:A:506[B]:6CL:HB3	1:B:354:CYS:HB2	1.52	0.89
1:B:291:ILE:H	1:B:395:ASN:HD21	1.19	0.89
1:A:291:ILE:H	1:A:395:ASN:HD21	1.13	0.88
1:A:214:HIS:CG	2:A:504[B]:0JC:N2	2.29	0.85
1:B:204:ASN:HD22	1:B:206:ARG:H	1.24	0.85
1:A:354:CYS:HB2	4:A:506[A]:6CL:HB3	1.61	0.82
1:B:289:ASN:HD21	1:B:380:THR:H	1.26	0.80
1:B:240:GLU:CD	2:B:505:0JC:N2	2.36	0.79
4:A:506[B]:6CL:HA	1:B:352:HIS:N	1.95	0.78
2:B:504[A]:0JC:I1	6:B:782:HOH:O	2.71	0.78
1:B:240:GLU:OE1	2:B:505:0JC:N2	2.18	0.77
1:A:347:HIS:ND1	2:A:501:0JC:I1	2.88	0.76
4:A:506[B]:6CL:HG2	1:B:354:CYS:SG	2.25	0.76
1:B:299[B]:LYS:HE3	6:B:810:HOH:O	1.86	0.74
1:A:157[A]:MET:CG	1:A:158:PRO:HA	2.13	0.74
4:A:506[B]:6CL:CD	1:B:352:HIS:HB2	2.19	0.73
1:B:297:ARG:HD2	6:B:839:HOH:O	1.90	0.72
1:B:153:MET:HE2	2:B:505:0JC:I1	2.57	0.72
1:A:347:HIS:HB3	2:A:501:0JC:I1	2.61	0.71
1:A:354:CYS:H	4:A:506[A]:6CL:CB	2.06	0.69
4:A:506[B]:6CL:HB3	1:B:354:CYS:CB	2.23	0.69
1:B:299[B]:LYS:NZ	6:B:816:HOH:O	2.25	0.67
2:B:504[B]:0JC:H6	6:B:623:HOH:O	1.95	0.65
1:B:128:ALA:HB2	1:B:156:VAL:HG13	1.77	0.65
4:A:506[B]:6CL:CA	1:B:352:HIS:H	2.01	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:CYS:CB	4:A:506[A]:6CL:HB3	2.28	0.65
1:A:352:HIS:HB2	4:A:506[A]:6CL:HD3	1.78	0.64
4:A:506[B]:6CL:HD3	1:B:352:HIS:C	2.18	0.64
1:B:297:ARG:CD	6:B:839:HOH:O	2.46	0.64
1:A:354:CYS:H	4:A:506[A]:6CL:HB3	1.64	0.63
1:B:152:THR:HG23	1:B:176:GLU:HB2	1.82	0.62
1:B:369:VAL:HB	6:B:620:HOH:O	1.99	0.62
1:B:297:ARG:NH1	1:B:297:ARG:HG3	2.15	0.61
1:B:214:HIS:HB3	2:B:503:OJC:I1	2.72	0.60
4:A:506[B]:6CL:HD2	1:B:352:HIS:HB2	1.84	0.60
1:B:153:MET:CG	2:B:505:OJC:I1	3.11	0.57
1:B:299[B]:LYS:HG3	1:B:366:TYR:OH	2.05	0.57
1:A:224:VAL:HB	1:A:245:THR:HG22	1.85	0.57
1:A:156:VAL:HG12	1:A:243:VAL:CG1	2.35	0.57
1:A:347:HIS:ND1	2:A:501:OJC:N1	2.52	0.56
1:B:173:ARG:CZ	2:B:504[B]:OJC:I1	3.23	0.56
1:A:352:HIS:HB2	4:A:506[A]:6CL:CD	2.34	0.56
1:B:153:MET:HE1	2:B:505:OJC:I1	2.65	0.55
1:A:352:HIS:N	4:A:506[A]:6CL:HA	2.00	0.55
1:B:128:ALA:HB2	1:B:156:VAL:CG1	2.35	0.55
1:A:157[B]:MET:CE	2:A:502[B]:OJC:I1	3.25	0.54
1:B:204:ASN:ND2	1:B:206:ARG:H	1.98	0.54
1:A:156:VAL:HG12	1:A:243:VAL:HG11	1.90	0.53
1:B:157:MET:CE	2:B:504[B]:OJC:I1	3.27	0.53
1:B:224:VAL:HB	1:B:245:THR:HG22	1.90	0.52
1:B:297:ARG:NE	6:B:839:HOH:O	2.43	0.52
1:B:168:GLU:OE2	1:B:371:ARG:HD2	2.10	0.51
4:A:506[B]:6CL:CB	1:B:354:CYS:H	2.23	0.50
1:A:352:HIS:CB	4:A:506[A]:6CL:HD3	2.42	0.50
1:A:181:ARG:HH21	1:A:205:ASN:HD22	1.61	0.49
1:A:402:ARG:HD3	6:A:791:HOH:O	2.12	0.49
1:A:353:GLY:HA3	4:A:506[A]:6CL:HZ1	1.77	0.49
1:A:354:CYS:SG	4:A:506[A]:6CL:CG	2.86	0.48
1:A:347:HIS:CG	2:A:501:OJC:I1	3.36	0.48
1:B:128:ALA:CB	1:B:156:VAL:HG13	2.42	0.48
1:B:172:ILE:HD13	1:B:188:ILE:HD13	1.95	0.48
1:B:291:ILE:N	1:B:395:ASN:HD21	2.00	0.48
1:A:158:PRO:HG3	1:A:168:GLU:HG2	1.96	0.47
1:A:289:ASN:HD21	1:A:380:THR:N	1.95	0.47
1:A:157[A]:MET:HG3	1:A:158:PRO:CA	2.24	0.47
1:A:297[A]:ARG:NH2	1:A:297[A]:ARG:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:HH11	1:B:297:ARG:HG3	1.80	0.46
1:A:158:PRO:HB3	1:A:371:ARG:NH2	2.31	0.44
1:B:297:ARG:CG	1:B:297:ARG:NH1	2.80	0.44
1:A:295:GLY:O	1:A:297[A]:ARG:NH1	2.50	0.44
1:B:399:ASP:OD1	1:B:402:ARG:NH2	2.51	0.44
1:A:237:MET:HG2	2:A:503:OJC:I1	2.75	0.44
1:A:353:GLY:N	4:A:506[A]:6CL:HB2	2.32	0.44
1:A:351:SER:HB2	4:A:506[A]:6CL:C	2.48	0.44
1:A:152:THR:HG21	1:A:174:PHE:HB3	1.98	0.44
1:A:407:LYS:HD3	1:A:407:LYS:HA	1.69	0.43
1:B:152:THR:CG2	1:B:176:GLU:HB2	2.47	0.43
1:A:340:TRP:HB2	1:B:320:THR:HG23	2.00	0.43
1:A:150:HIS:N	2:A:503:OJC:H5	2.34	0.43
1:B:347:HIS:HB3	2:B:502:OJC:I1	2.88	0.43
1:B:327:GLN:OE1	6:B:746:HOH:O	2.21	0.43
1:A:198:GLY:HA3	1:A:210:TRP:CZ2	2.54	0.43
4:A:506[B]:6CL:HB2	1:B:354:CYS:H	1.83	0.43
1:A:361:ASN:HD22	1:A:361:ASN:HA	1.67	0.42
1:A:352:HIS:N	4:A:506[A]:6CL:HB2	2.34	0.42
4:A:506[B]:6CL:HD3	1:B:352:HIS:HB2	1.98	0.42
1:A:371:ARG:HG2	6:A:617:HOH:O	2.20	0.42
1:A:297[B]:ARG:NH2	1:A:366:TYR:O	2.54	0.41
1:A:352:HIS:ND1	3:A:505[A]:DGL:CD	2.84	0.41
4:A:506[B]:6CL:CB	1:B:352:HIS:H	2.34	0.41
4:A:506[B]:6CL:N	1:B:352:HIS:ND1	2.69	0.41
4:A:506[B]:6CL:CD	1:B:352:HIS:CB	2.97	0.40
1:A:194:PRO:HA	1:A:195:PRO:HD3	1.98	0.40
4:A:506[B]:6CL:HB2	1:B:352:HIS:N	2.37	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:781:HOH:O	6:B:781:HOH:O[7_455]	2.14	0.06
6:A:677:HOH:O	6:A:677:HOH:O[8_555]	2.15	0.05

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	259/287 (90%)	255 (98%)	4 (2%)	0	100	100
1	B	267/287 (93%)	259 (97%)	8 (3%)	0	100	100
All	All	526/574 (92%)	514 (98%)	12 (2%)	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	215/232 (93%)	208 (97%)	7 (3%)	38	17
1	B	218/232 (94%)	214 (98%)	4 (2%)	59	41
All	All	433/464 (93%)	422 (98%)	11 (2%)	50	27

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ARG
1	A	271	GLU
1	A	297[A]	ARG
1	A	297[B]	ARG
1	A	370	LYS
1	A	393	ASP
1	A	407	LYS
1	B	189	LYS

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Mol	Chain	Res	Type
1	B	204	ASN
1	B	241	ASP
1	B	393	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	289	ASN
1	A	361	ASN
1	A	379	ASN
1	A	395	ASN
1	B	150	HIS
1	B	204	ASN
1	B	244	GLN
1	B	289	ASN
1	B	361	ASN
1	B	379	ASN
1	B	395	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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
4	6CL	A	506[B]	-	4,12,12	0.60	0	3,15,15	0.98	0
2	0JC	A	504[A]	1	3,6,14	0.48	0	2,7,22	0.48	0
2	0JC	A	504[B]	1	3,6,14	0.47	0	2,7,22	0.60	0
2	0JC	A	503	1	3,6,14	0.52	0	2,7,22	0.21	0
2	0JC	B	504[B]	1	3,6,14	0.43	0	2,7,22	2.57	1 (50%)
2	0JC	A	502[B]	1	3,6,14	0.26	0	2,7,22	0.41	0
2	0JC	B	502	1	3,6,14	0.42	0	2,7,22	0.58	0
2	0JC	B	504[A]	1	3,6,14	0.45	0	2,7,22	0.62	0
2	0JC	A	501	1	3,6,14	0.63	0	2,7,22	0.44	0
2	0JC	B	505	1	3,6,14	0.51	0	2,7,22	0.90	0
2	0JC	A	502[A]	1	3,6,14	0.65	0	2,7,22	0.77	0
2	0JC	B	503	-	3,6,14	0.59	0	2,7,22	0.60	0
4	6CL	A	506[A]	-	4,12,12	1.52	1 (25%)	3,15,15	0.95	0

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
4	6CL	A	506[B]	-	-	4/6/14/14	-
2	0JC	A	504[A]	1	-	-	0/1/1/3
2	0JC	A	504[B]	1	-	-	0/1/1/3
2	0JC	B	502	1	-	-	0/1/1/3
2	0JC	B	504[B]	1	-	-	0/1/1/3
2	0JC	A	502[B]	1	-	-	0/1/1/3
2	0JC	B	504[A]	1	-	-	0/1/1/3
2	0JC	A	501	1	-	-	0/1/1/3
2	0JC	B	505	1	-	-	0/1/1/3
2	0JC	A	502[A]	1	-	-	0/1/1/3
2	0JC	A	503	1	-	-	0/1/1/3
2	0JC	B	503	-	-	-	0/1/1/3
4	6CL	A	506[A]	-	-	4/6/14/14	-

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	506[A]	6CL	CE-NZ	-2.23	1.42	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504[B]	0JC	C2-C1-N1	-3.62	93.16	108.12

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506[B]	6CL	N-CA-CB-CG
4	A	506[B]	6CL	C-CA-CB-CG
4	A	506[A]	6CL	N-CA-CB-CG
4	A	506[A]	6CL	C-CA-CB-CG
4	A	506[B]	6CL	CA-CB-CG-CD
4	A	506[A]	6CL	CA-CB-CG-CD
4	A	506[A]	6CL	CE-CD-CG-CB
4	A	506[B]	6CL	CE-CD-CG-CB

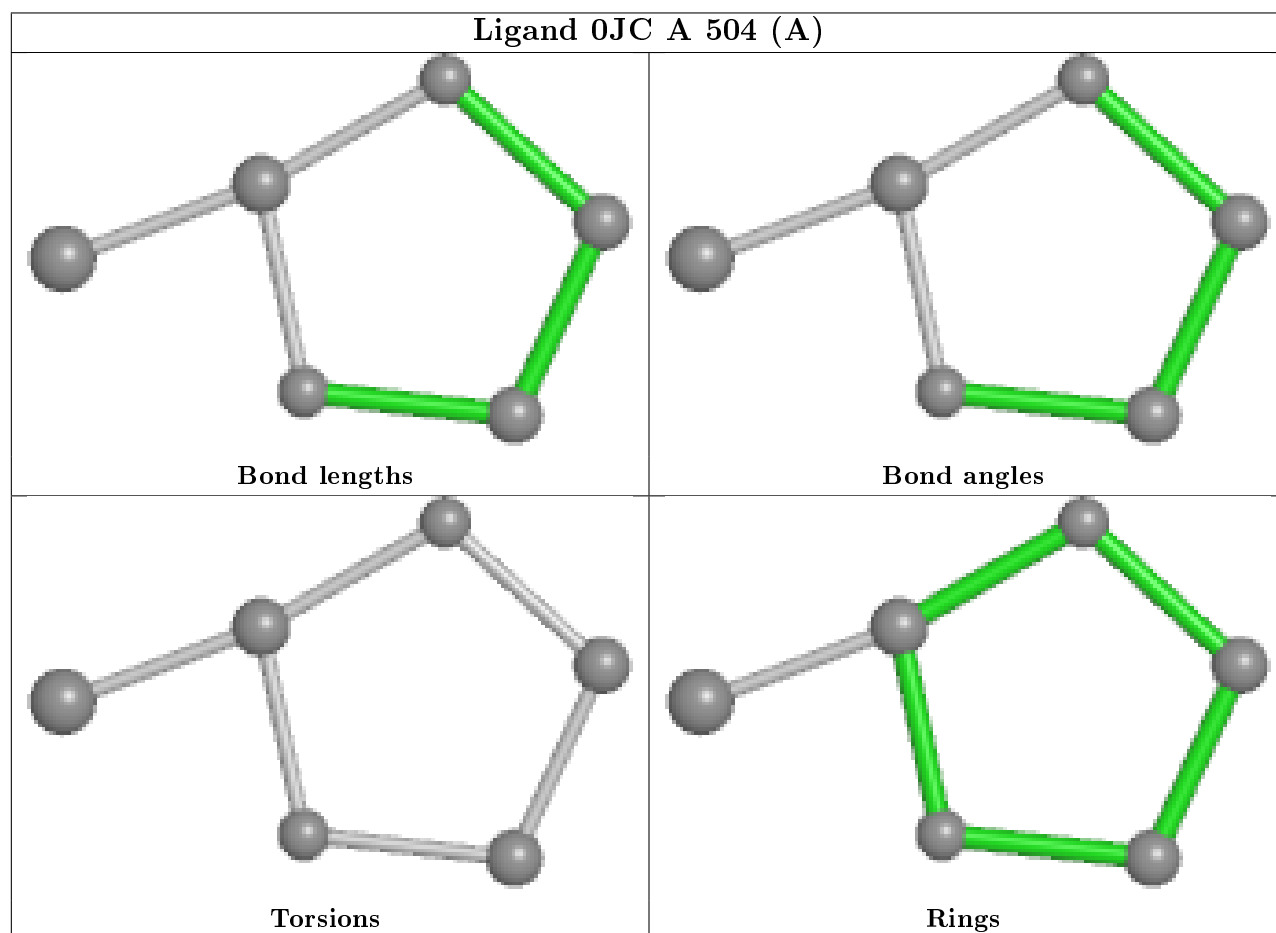
There are no ring outliers.

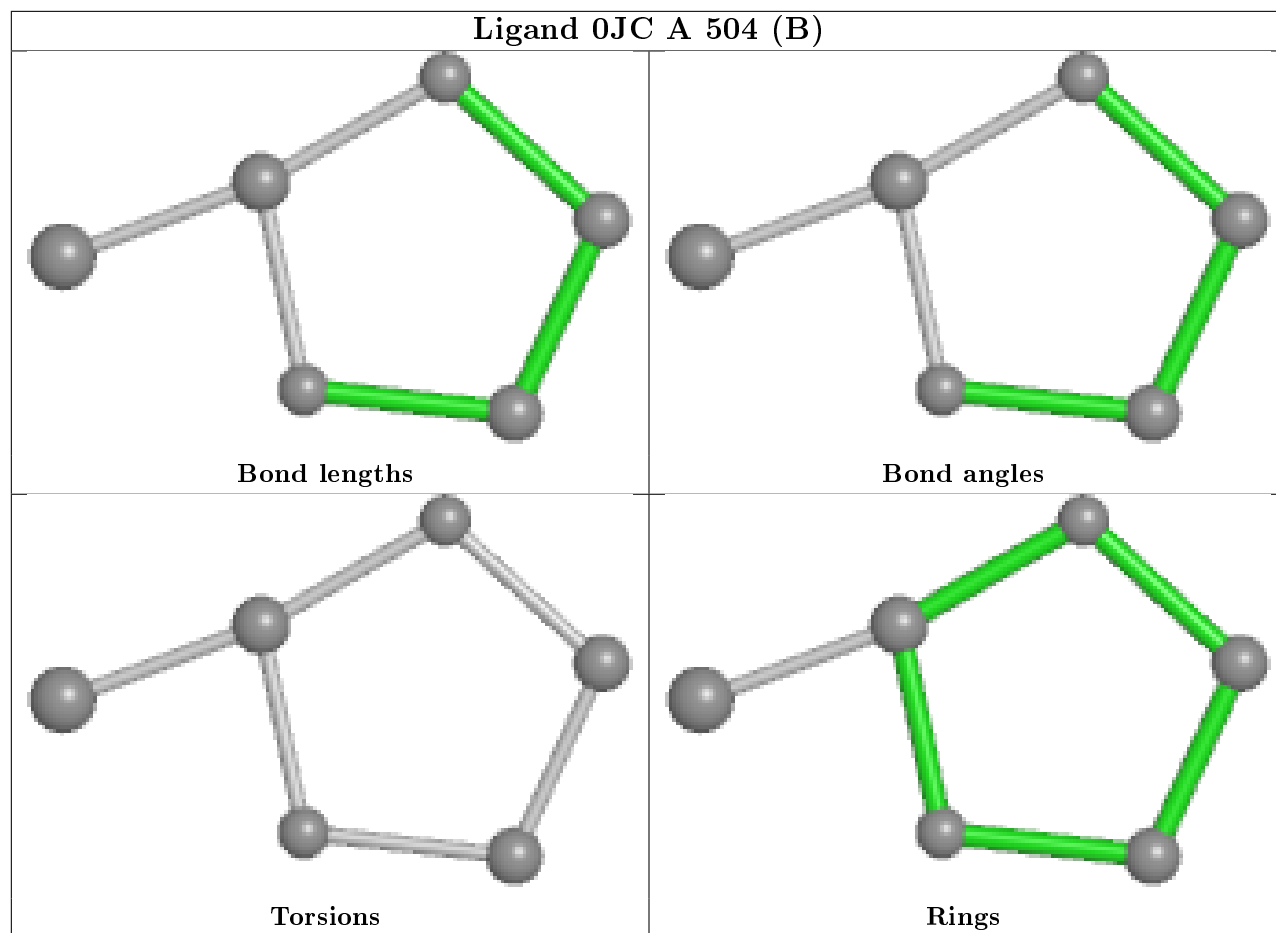
11 monomers are involved in 60 short contacts:

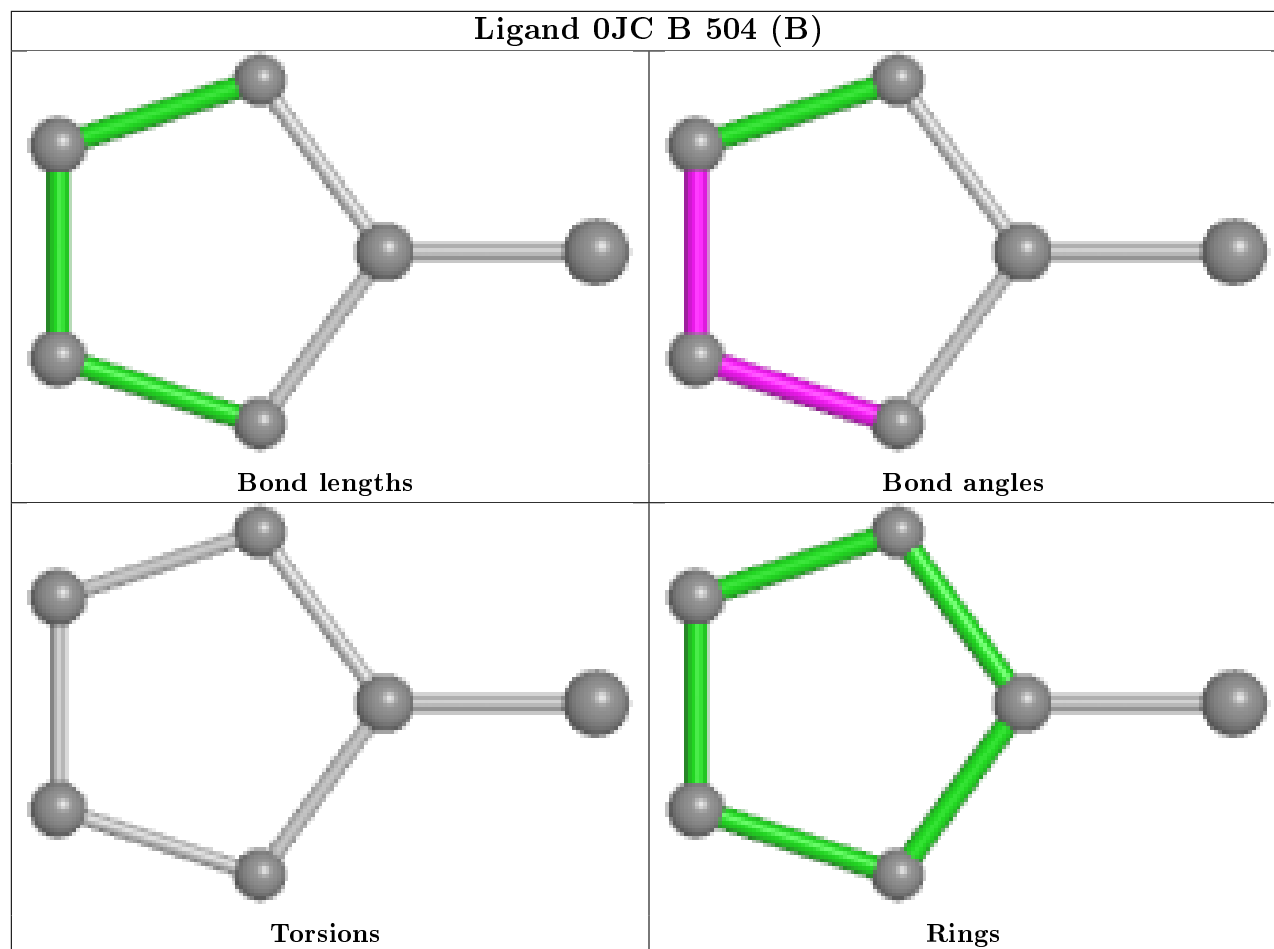
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506[B]	6CL	18	0
2	A	504[B]	0JC	1	0
2	A	503	0JC	4	0
2	B	504[B]	0JC	4	0
2	A	502[B]	0JC	1	0
2	B	502	0JC	2	0
2	B	504[A]	0JC	2	0
2	A	501	0JC	4	0
2	B	505	0JC	8	0
2	B	503	0JC	1	0
4	A	506[A]	6CL	15	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	258/287 (89%)	0.33	14 (5%) 25 28	25, 33, 53, 61	0
1	B	269/287 (93%)	0.60	32 (11%) 4 5	25, 34, 56, 76	1 (0%)
All	All	527/574 (91%)	0.47	46 (8%) 10 11	25, 33, 55, 76	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	ARG	8.3
1	B	124	TYR	8.2
1	B	131	LEU	6.8
1	B	150	HIS	6.2
1	B	123	ARG	6.2
1	B	126	LEU	6.0
1	B	129	THR	5.6
1	A	399	ASP	3.5
1	A	375	VAL	3.3
1	A	374	ILE	3.3
1	B	235	GLU	3.3
1	B	294	VAL	3.3
1	B	236	GLY	3.3
1	A	208	VAL	3.2
1	A	155	TYR	3.1
1	B	125	THR	3.1
1	B	355	LEU	3.0
1	B	233	LEU	3.0
1	B	172	ILE	2.9
1	A	407	LYS	2.8
1	B	151	LEU	2.8
1	B	177	ASN	2.7
1	B	186	LYS	2.7
1	B	335	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	186	LYS	2.6
1	B	399	ASP	2.6
1	B	402	ARG	2.6
1	A	157[A]	MET	2.5
1	B	132	GLY	2.5
1	B	205	ASN	2.5
1	B	271	GLU	2.4
1	A	167	GLY	2.4
1	B	170	VAL	2.4
1	A	355	LEU	2.3
1	B	354	CYS	2.3
1	B	210	TRP	2.2
1	A	335	VAL	2.2
1	B	308	TYR	2.2
1	B	130	ALA	2.2
1	B	171	ALA	2.2
1	B	173	ARG	2.1
1	B	152	THR	2.1
1	A	170	VAL	2.1
1	A	402	ARG	2.1
1	B	206	ARG	2.1
1	A	177	ASN	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	6CL	A	506[B]	13/13	0.65	0.66	38,43,49,50	13

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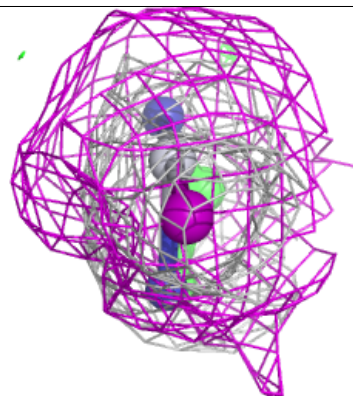
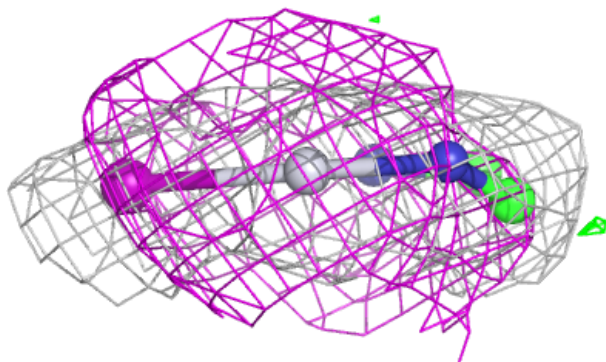
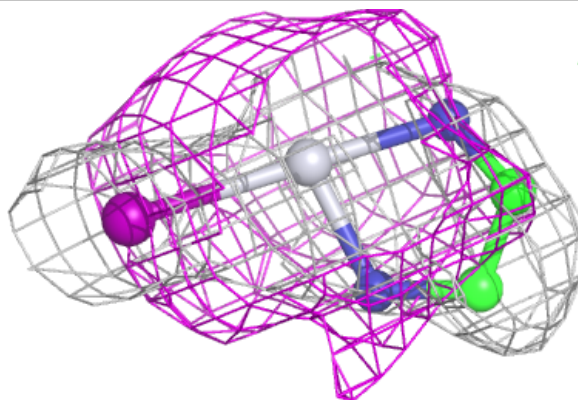
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	0JC	A	501	6/12	0.65	0.33	49,52,56,59	6
4	6CL	A	506[A]	13/13	0.65	0.66	31,40,43,45	13
3	DGL	A	505[A]	9/10	0.69	0.67	46,55,57,57	9
3	DGL	A	505[B]	9/10	0.69	0.67	48,62,64,65	9
2	0JC	A	504[A]	6/12	0.76	0.49	95,97,109,110	6
2	0JC	A	504[B]	6/12	0.76	0.49	101,103,112,114	6
2	0JC	B	503	6/12	0.81	0.31	138,138,139,146	5
2	0JC	B	505	6/12	0.89	0.27	67,75,76,84	6
2	0JC	A	502[B]	6/12	0.91	0.23	54,57,61,88	6
2	0JC	A	502[A]	6/12	0.91	0.23	101,102,109,115	6
2	0JC	B	504[A]	6/12	0.95	0.20	13,34,41,45	6
2	0JC	B	504[B]	6/12	0.95	0.20	14,45,67,83	6
2	0JC	A	503	6/12	0.96	0.12	69,70,72,78	6
5	PT	B	501	1/1	0.97	0.08	82,82,82,82	1
2	0JC	B	502	6/12	0.98	0.22	61,66,68,85	6

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.

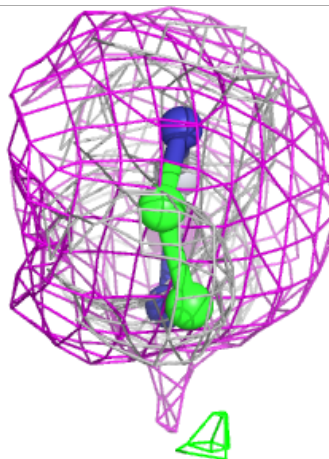
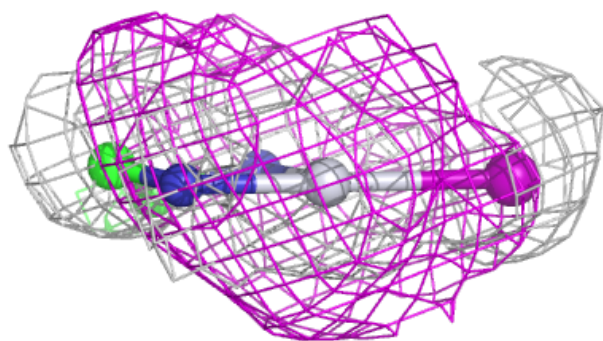
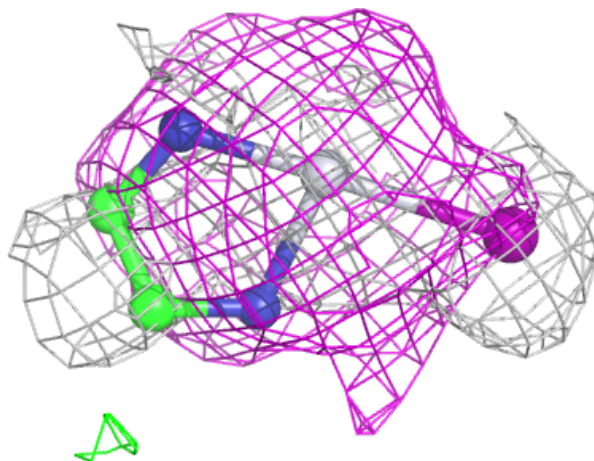
**Electron density around 0JC A 504 (A):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 0JC A 504 (B):**

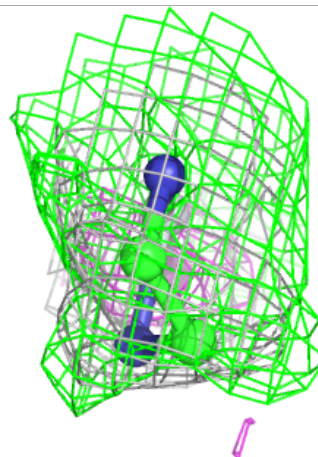
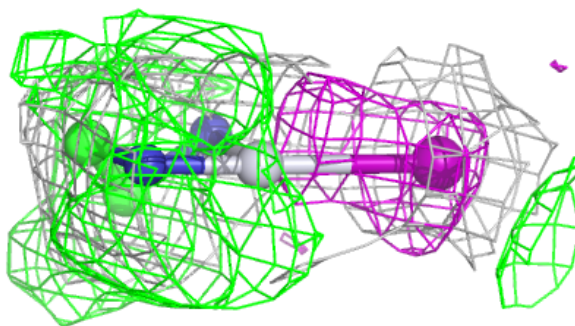
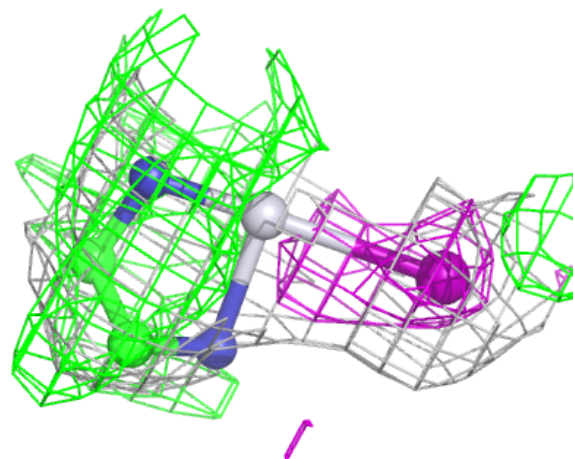
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around 0JC B 504 (B):**

$2mF_o-DF_c$  (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.