



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:49 am BST

PDB ID : 4U0N  
Title : Structure of the *Vibrio cholerae* di-nucleotide cyclase (DncV) deletion mutant D-loop  
Authors : Xiang, Y.; Zhu, D.Y.  
Deposited on : 2014-07-12  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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

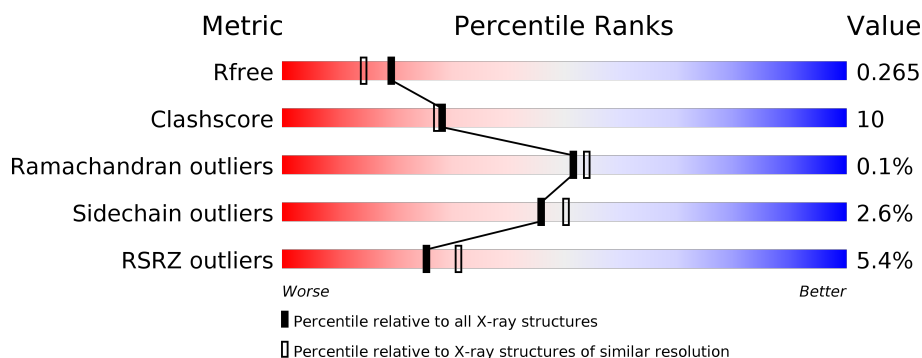
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	391	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	B	391	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6498 atoms, of which 58 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 Cyclic AMP-GMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2984	1883	515	570	16			
1	B	373	Total	C	N	O	S	0	0	0
			2984	1883	515	570	16			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP Q9KVG7
A	?	-	PHE	deletion	UNP Q9KVG7
A	?	-	GLN	deletion	UNP Q9KVG7
A	?	-	LYS	deletion	UNP Q9KVG7
A	?	-	LYS	deletion	UNP Q9KVG7
A	?	-	GLN	deletion	UNP Q9KVG7
A	?	-	ILE	deletion	UNP Q9KVG7
A	?	-	ALA	deletion	UNP Q9KVG7
A	?	-	LEU	deletion	UNP Q9KVG7
A	?	-	GLU	deletion	UNP Q9KVG7
A	?	-	ALA	deletion	UNP Q9KVG7
A	?	-	ASN	deletion	UNP Q9KVG7
A	?	-	ARG	deletion	UNP Q9KVG7
A	?	-	SER	deletion	UNP Q9KVG7
A	?	-	PHE	deletion	UNP Q9KVG7
A	?	-	VAL	deletion	UNP Q9KVG7
A	?	-	LYS	deletion	UNP Q9KVG7
A	?	-	GLY	deletion	UNP Q9KVG7
A	?	-	ALA	deletion	UNP Q9KVG7
A	?	-	ILE	deletion	UNP Q9KVG7
A	?	-	PHE	deletion	UNP Q9KVG7
A	?	-	GLU	deletion	UNP Q9KVG7
A	?	-	SER	deletion	UNP Q9KVG7
A	?	-	TYR	deletion	UNP Q9KVG7
A	?	-	VAL	deletion	UNP Q9KVG7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP Q9KVG7
A	?	-	ASP	deletion	UNP Q9KVG7
A	?	-	SER	deletion	UNP Q9KVG7
A	?	-	ILE	deletion	UNP Q9KVG7
A	?	-	THR	deletion	UNP Q9KVG7
A	?	-	ASP	deletion	UNP Q9KVG7
A	?	-	ASP	deletion	UNP Q9KVG7
A	?	-	SER	deletion	UNP Q9KVG7
A	?	-	GLU	deletion	UNP Q9KVG7
A	?	-	THR	deletion	UNP Q9KVG7
A	?	-	TYR	deletion	UNP Q9KVG7
A	384	LEU	-	expression tag	UNP Q9KVG7
A	385	GLU	-	expression tag	UNP Q9KVG7
A	386	HIS	-	expression tag	UNP Q9KVG7
A	387	HIS	-	expression tag	UNP Q9KVG7
A	388	HIS	-	expression tag	UNP Q9KVG7
A	389	HIS	-	expression tag	UNP Q9KVG7
A	390	HIS	-	expression tag	UNP Q9KVG7
A	391	HIS	-	expression tag	UNP Q9KVG7
B	?	-	GLU	deletion	UNP Q9KVG7
B	?	-	PHE	deletion	UNP Q9KVG7
B	?	-	GLN	deletion	UNP Q9KVG7
B	?	-	LYS	deletion	UNP Q9KVG7
B	?	-	LYS	deletion	UNP Q9KVG7
B	?	-	GLN	deletion	UNP Q9KVG7
B	?	-	ILE	deletion	UNP Q9KVG7
B	?	-	ALA	deletion	UNP Q9KVG7
B	?	-	LEU	deletion	UNP Q9KVG7
B	?	-	GLU	deletion	UNP Q9KVG7
B	?	-	ALA	deletion	UNP Q9KVG7
B	?	-	ASN	deletion	UNP Q9KVG7
B	?	-	ARG	deletion	UNP Q9KVG7
B	?	-	SER	deletion	UNP Q9KVG7
B	?	-	PHE	deletion	UNP Q9KVG7
B	?	-	VAL	deletion	UNP Q9KVG7
B	?	-	LYS	deletion	UNP Q9KVG7
B	?	-	GLY	deletion	UNP Q9KVG7
B	?	-	ALA	deletion	UNP Q9KVG7
B	?	-	ILE	deletion	UNP Q9KVG7
B	?	-	PHE	deletion	UNP Q9KVG7
B	?	-	GLU	deletion	UNP Q9KVG7
B	?	-	SER	deletion	UNP Q9KVG7

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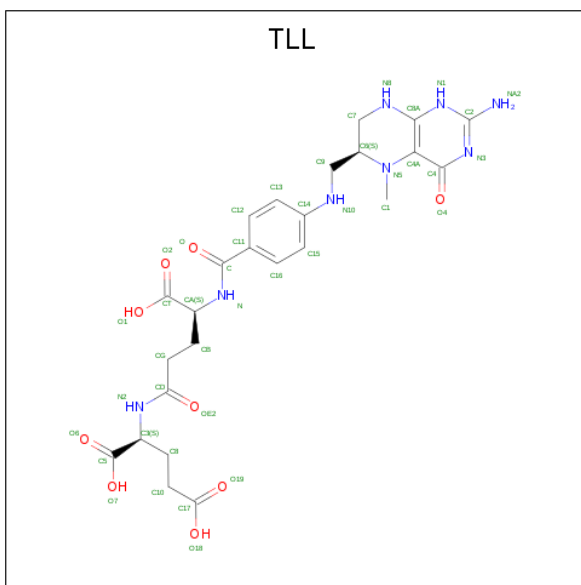
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	deletion	UNP Q9KVG7
B	?	-	VAL	deletion	UNP Q9KVG7
B	?	-	ALA	deletion	UNP Q9KVG7
B	?	-	ASP	deletion	UNP Q9KVG7
B	?	-	SER	deletion	UNP Q9KVG7
B	?	-	ILE	deletion	UNP Q9KVG7
B	?	-	THR	deletion	UNP Q9KVG7
B	?	-	ASP	deletion	UNP Q9KVG7
B	?	-	ASP	deletion	UNP Q9KVG7
B	?	-	SER	deletion	UNP Q9KVG7
B	?	-	GLU	deletion	UNP Q9KVG7
B	?	-	THR	deletion	UNP Q9KVG7
B	?	-	TYR	deletion	UNP Q9KVG7
B	384	LEU	-	expression tag	UNP Q9KVG7
B	385	GLU	-	expression tag	UNP Q9KVG7
B	386	HIS	-	expression tag	UNP Q9KVG7
B	387	HIS	-	expression tag	UNP Q9KVG7
B	388	HIS	-	expression tag	UNP Q9KVG7
B	389	HIS	-	expression tag	UNP Q9KVG7
B	390	HIS	-	expression tag	UNP Q9KVG7
B	391	HIS	-	expression tag	UNP Q9KVG7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is N-[4-({[(6S)-2-amino-5-methyl-4-oxo-1,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)benzoyl]-L-gamma-glutamyl-L-glutamic acid (three-letter code: TLL) (formula: C<sub>25</sub>H<sub>32</sub>N<sub>8</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 71	C 25	H 29	N 8	O 9	0	0
3	B	1	Total 71	C 25	H 29	N 8	O 9	0	0

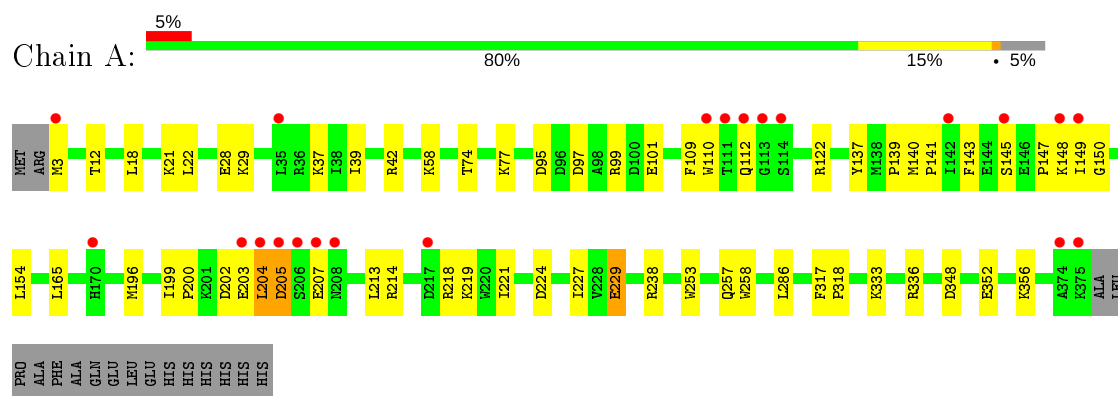
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	184	Total O 184 184	0	0
4	B	202	Total O 202 202	0	0

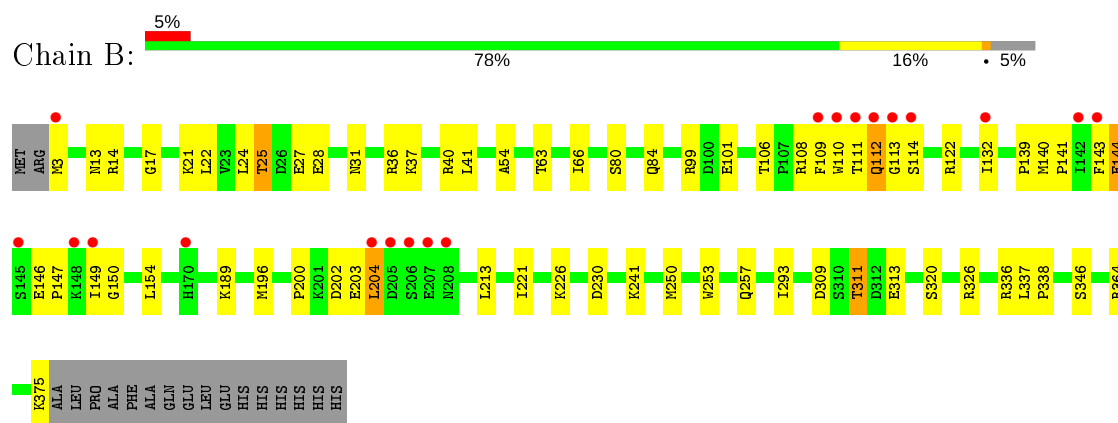
### 3 Residue-property plots [i](#)

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: Cyclic AMP-GMP synthase



#### • Molecule 1: Cyclic AMP-GMP synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.61Å 49.25Å 122.23Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	37.73 – 2.10 38.18 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.73-2.10) 99.2 (38.18-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.77 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.217 , 0.264 0.218 , 0.265	Depositor DCC
$R_{free}$ test set	2557 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6836e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TLL

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	0.25	0/3044	0.43	0/4105
1	B	0.26	0/3044	0.46	0/4105
All	All	0.26	0/6088	0.45	0/8210

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2984	0	2976	58	0
1	B	2984	0	2976	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	42	29	29	12	0
3	B	42	29	29	7	0
4	A	184	0	0	8	0
4	B	202	0	0	9	0
All	All	6440	58	6010	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 10.

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:109:PHE:O	3:A:402:TLL:H16	1.54	1.08
1:A:109:PHE:O	3:A:402:TLL:C16	2.12	0.98
1:A:101:GLU:HG3	1:A:148:LYS:HD2	1.52	0.92
1:B:250:MET:SD	4:B:566:HOH:O	2.32	0.85
1:B:109:PHE:O	3:B:402:TLL:H16	1.78	0.83
1:A:213:LEU:HD21	1:A:221:ILE:HD11	1.68	0.76
1:A:205:ASP:HB2	3:A:402:TLL:C2	2.15	0.75
1:A:109:PHE:H	3:A:402:TLL:H16	1.52	0.74
1:B:108:ARG:HE	1:B:139:PRO:HG3	1.53	0.74
1:A:12:THR:HG22	1:A:286:LEU:HD12	1.70	0.72
1:B:140:MET:HB3	1:B:141:PRO:HD2	1.71	0.71
3:A:402:TLL:O2	4:A:684:HOH:O	2.08	0.70
1:B:36:ARG:NH1	1:B:112:GLN:OE1	2.26	0.69
1:B:140:MET:HG2	1:B:149:ILE:HD12	1.76	0.68
1:A:109:PHE:O	3:A:402:TLL:C15	2.42	0.68
1:A:336:ARG:NH2	4:A:502:HOH:O	2.26	0.67
1:B:25:THR:HG22	1:B:27:GLU:H	1.60	0.67
1:B:109:PHE:H	3:B:402:TLL:H16	1.62	0.65
1:B:150:GLY:HA3	4:B:611:HOH:O	1.96	0.64
1:B:109:PHE:O	3:B:402:TLL:C16	2.46	0.64
1:A:213:LEU:HD11	1:A:221:ILE:HD13	1.79	0.64
1:B:101:GLU:HG3	1:B:149:ILE:HD11	1.79	0.63
1:A:101:GLU:CG	1:A:148:LYS:HD2	2.27	0.63
1:A:3:MET:SD	1:A:348:ASP:HA	2.39	0.63
1:B:143:PHE:CD2	1:B:147:PRO:HB3	2.33	0.62
1:A:112:GLN:NE2	1:B:375:LYS:HD3	2.15	0.62
1:A:21:LYS:NZ	4:A:610:HOH:O	2.31	0.61
1:A:140:MET:HB3	1:A:141:PRO:HD2	1.82	0.61
1:A:112:GLN:HE22	1:B:375:LYS:HD3	1.66	0.61
1:B:110:TRP:CE3	1:B:112:GLN:HA	2.36	0.61
1:A:109:PHE:N	3:A:402:TLL:H16	2.17	0.60
1:B:146:GLU:HG3	1:B:147:PRO:HD2	1.82	0.59
1:B:25:THR:HG22	1:B:27:GLU:N	2.18	0.59
1:A:149:ILE:H	1:A:149:ILE:HD12	1.68	0.59
1:B:21:LYS:O	1:B:122:ARG:HD3	2.02	0.58
1:B:146:GLU:CG	1:B:147:PRO:HD2	2.32	0.58
1:B:109:PHE:N	3:B:402:TLL:H16	2.18	0.58
1:A:213:LEU:HD21	1:A:221:ILE:CD1	2.35	0.57
1:A:143:PHE:CD1	1:A:147:PRO:HB3	2.38	0.57
1:B:37:LYS:HG3	3:B:402:TLL:O19	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ARG:NH2	4:B:661:HOH:O	2.37	0.56
1:A:352:GLU:HG3	1:A:356:LYS:HE2	1.87	0.56
1:B:309:ASP:OD1	1:B:311:THR:HB	2.05	0.56
1:A:333:LYS:HE3	4:A:683:HOH:O	2.07	0.55
1:A:205:ASP:HB2	3:A:402:TLL:NA2	2.22	0.55
1:B:250:MET:HE3	1:B:293:ILE:HG22	1.88	0.55
1:B:204:LEU:O	1:B:204:LEU:HD13	2.06	0.55
1:B:139:PRO:HG2	4:B:633:HOH:O	2.07	0.54
1:B:189:LYS:NZ	4:B:501:HOH:O	2.24	0.54
1:B:250:MET:HE3	1:B:293:ILE:CG2	2.38	0.54
1:B:40:ARG:HG2	1:B:109:PHE:CD1	2.43	0.54
1:A:140:MET:SD	1:A:149:ILE:HD13	2.47	0.54
1:A:39:ILE:HD13	1:A:165:LEU:CD1	2.37	0.54
1:A:101:GLU:HG3	1:A:148:LYS:CD	2.33	0.54
1:B:143:PHE:CB	1:B:147:PRO:HA	2.40	0.52
1:A:150:GLY:HA3	4:A:565:HOH:O	2.09	0.52
1:B:112:GLN:C	1:B:114:SER:N	2.62	0.52
1:B:22:LEU:O	1:B:122:ARG:HG3	2.10	0.52
1:A:12:THR:CG2	1:A:286:LEU:HD12	2.40	0.51
1:A:21:LYS:O	1:A:122:ARG:HD3	2.11	0.51
1:A:200:PRO:HG2	1:A:203:GLU:O	2.11	0.51
1:B:41:LEU:HD21	3:B:402:TLL:H8	1.92	0.51
1:B:25:THR:CG2	1:B:27:GLU:H	2.23	0.50
1:B:154:LEU:HB3	1:B:196:MET:SD	2.51	0.50
1:A:28:GLU:OE2	1:A:122:ARG:NH2	2.44	0.49
1:A:39:ILE:HD13	1:A:165:LEU:HD13	1.93	0.49
1:B:213:LEU:HD21	1:B:221:ILE:HD11	1.93	0.49
1:B:80:SER:O	1:B:84:GLN:HG3	2.12	0.49
1:A:154:LEU:HB3	1:A:196:MET:SD	2.52	0.49
1:A:238:ARG:NH2	4:A:614:HOH:O	2.46	0.48
1:A:147:PRO:HG2	1:A:149:ILE:O	2.13	0.48
1:A:202:ASP:OD1	1:A:202:ASP:N	2.31	0.47
1:B:336:ARG:HD2	4:B:517:HOH:O	2.12	0.47
1:A:258:TRP:CZ2	1:A:333:LYS:HG3	2.50	0.47
1:A:253:TRP:O	1:A:257:GLN:HG2	2.15	0.46
1:B:147:PRO:HG2	1:B:149:ILE:O	2.14	0.46
1:A:22:LEU:O	1:A:122:ARG:HG3	2.15	0.46
1:A:110:TRP:CH2	1:A:229:GLU:HG3	2.51	0.46
1:B:28:GLU:OE1	1:B:122:ARG:NH1	2.48	0.46
1:B:63:THR:OG1	1:B:66:ILE:HG12	2.16	0.46
1:B:364:ARG:NH2	4:B:546:HOH:O	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LYS:HB2	1:A:99:ARG:HD2	1.98	0.45
1:B:146:GLU:HG3	1:B:147:PRO:CD	2.47	0.45
1:B:140:MET:CG	1:B:149:ILE:HD12	2.47	0.45
1:B:13:ASN:HB3	1:B:17:GLY:HA3	1.99	0.44
1:A:219:LYS:NZ	4:A:507:HOH:O	2.49	0.44
1:A:58:LYS:HB2	1:A:99:ARG:CD	2.47	0.44
1:A:74:THR:O	1:A:77:LYS:HG2	2.18	0.44
1:B:253:TRP:O	1:B:257:GLN:HG2	2.18	0.44
1:B:226:LYS:HE3	1:B:230:ASP:OD2	2.18	0.44
1:A:199:ILE:HD13	3:A:402:TLL:H71	2.00	0.43
1:B:140:MET:SD	1:B:149:ILE:HB	2.58	0.43
1:A:18:LEU:O	1:A:22:LEU:HG	2.19	0.43
1:A:109:PHE:C	3:A:402:TLL:H16	2.34	0.43
1:B:200:PRO:HG2	1:B:203:GLU:O	2.19	0.43
1:B:36:ARG:HB3	4:B:631:HOH:O	2.18	0.43
1:A:109:PHE:O	3:A:402:TLL:H15	2.17	0.43
1:A:224:ASP:HB3	1:A:227:ILE:HG13	2.00	0.42
1:B:144:GLU:N	1:B:144:GLU:OE2	2.50	0.42
1:B:24:LEU:HD12	1:B:122:ARG:HG2	2.01	0.42
1:B:337:LEU:N	1:B:338:PRO:HD2	2.33	0.42
1:B:241:LYS:NZ	4:B:608:HOH:O	2.51	0.42
1:A:29:LYS:HB3	1:A:29:LYS:HE3	1.71	0.42
1:B:132:ILE:HG13	1:B:132:ILE:O	2.19	0.42
1:A:95:ASP:OD1	1:A:97:ASP:HB3	2.19	0.42
1:B:54:ALA:O	1:B:99:ARG:HD3	2.19	0.42
1:A:317:PHE:HA	1:A:318:PRO:HD3	1.92	0.41
1:B:146:GLU:CD	1:B:147:PRO:HD2	2.40	0.41
1:A:257:GLN:HB2	1:A:258:TRP:CE3	2.55	0.41
1:B:143:PHE:HB2	1:B:147:PRO:HA	2.02	0.41
1:A:137:TYR:O	1:A:139:PRO:HD3	2.20	0.41
1:A:42:ARG:HG2	1:A:165:LEU:HG	2.02	0.41
1:B:27:GLU:O	1:B:31:ASN:ND2	2.47	0.41
1:A:204:LEU:HD13	1:A:204:LEU:O	2.21	0.41
1:B:3:MET:O	1:B:346:SER:HA	2.21	0.41
1:A:214:ARG:HD3	4:A:596:HOH:O	2.21	0.40
1:A:37:LYS:HG3	3:A:402:TLL:O19	2.22	0.40
1:B:109:PHE:C	3:B:402:TLL:H16	2.39	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	371/391 (95%)	361 (97%)	10 (3%)	0	100	100
1	B	371/391 (95%)	358 (96%)	12 (3%)	1 (0%)	41	41
All	All	742/782 (95%)	719 (97%)	22 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	113	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/344 (96%)	323 (98%)	6 (2%)	59	65
1	B	329/344 (96%)	318 (97%)	11 (3%)	38	40
All	All	658/688 (96%)	641 (97%)	17 (3%)	46	50

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	SER
1	A	204	LEU
1	A	205	ASP
1	A	207	GLU
1	A	218	ARG

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Mol	Chain	Res	Type
1	A	229	GLU
1	B	25	THR
1	B	106	THR
1	B	111	THR
1	B	112	GLN
1	B	144	GLU
1	B	202	ASP
1	B	204	LEU
1	B	311	THR
1	B	313	GLU
1	B	320	SER
1	B	326	ARG

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

Mol	Chain	Res	Type
1	A	112	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
3	TLL	A	402	-	33,44,44	4.39	13 (39%)	34,61,61	2.60	15 (44%)
3	TLL	B	402	-	33,44,44	4.39	15 (45%)	34,61,61	2.54	15 (44%)

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
3	TLL	A	402	-	-	6/25/48/48	0/3/3/3
3	TLL	B	402	-	-	6/25/48/48	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	TLL	C4-C4A	12.82	1.58	1.41
3	A	402	TLL	C4-C4A	12.49	1.58	1.41
3	A	402	TLL	C4-N3	11.05	1.52	1.33
3	B	402	TLL	C4-N3	10.97	1.52	1.33
3	A	402	TLL	C12-C13	8.51	1.54	1.38
3	B	402	TLL	C12-C13	7.92	1.53	1.38
3	B	402	TLL	C15-C14	7.57	1.52	1.39
3	A	402	TLL	C15-C14	7.35	1.51	1.39
3	A	402	TLL	C16-C11	6.83	1.51	1.39
3	B	402	TLL	C16-C11	6.69	1.50	1.39
3	A	402	TLL	O4-C4	6.51	1.40	1.24
3	B	402	TLL	O4-C4	6.43	1.40	1.24
3	A	402	TLL	C-N	5.33	1.45	1.34
3	B	402	TLL	C-N	5.27	1.45	1.34
3	B	402	TLL	CD-N2	5.18	1.45	1.34
3	A	402	TLL	C2-NA2	5.11	1.44	1.33
3	A	402	TLL	CD-N2	4.95	1.44	1.34
3	B	402	TLL	C2-NA2	4.90	1.43	1.33
3	A	402	TLL	C4A-C8A	-4.55	1.32	1.41
3	B	402	TLL	C4A-C8A	-4.28	1.32	1.41
3	A	402	TLL	C3-N2	-2.77	1.43	1.46
3	B	402	TLL	C3-N2	-2.73	1.43	1.46
3	B	402	TLL	C13-C14	-2.36	1.35	1.39
3	B	402	TLL	C12-C11	-2.36	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	TLL	C15-C16	-2.34	1.34	1.38
3	A	402	TLL	C15-C16	-2.33	1.34	1.38
3	A	402	TLL	C12-C11	-2.05	1.35	1.39
3	B	402	TLL	C4A-N5	2.04	1.46	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	TLL	C2-N1-C8A	7.82	132.08	114.54
3	A	402	TLL	C2-N1-C8A	7.64	131.67	114.54
3	A	402	TLL	N3-C2-N1	-5.25	117.19	125.42
3	B	402	TLL	N3-C2-N1	-5.23	117.21	125.42
3	B	402	TLL	C1-N5-C4A	4.23	119.05	113.30
3	A	402	TLL	C1-N5-C4A	4.16	118.96	113.30
3	B	402	TLL	C9-N10-C14	-4.02	111.75	122.14
3	A	402	TLL	C9-N10-C14	-3.52	113.03	122.14
3	A	402	TLL	CB-CA-N	3.44	115.21	110.19
3	A	402	TLL	C4-C4A-C8A	3.28	117.00	114.44
3	B	402	TLL	NA2-C2-N3	3.28	122.35	117.25
3	A	402	TLL	NA2-C2-N3	3.15	122.16	117.25
3	A	402	TLL	O-C-C11	-3.13	115.35	120.94
3	B	402	TLL	CA-N-C	2.94	126.13	122.34
3	B	402	TLL	O-C-C11	-2.90	115.76	120.94
3	A	402	TLL	C15-C14-N10	-2.87	115.02	120.97
3	B	402	TLL	C8-C3-N2	-2.80	106.12	110.19
3	A	402	TLL	CA-N-C	2.75	125.88	122.34
3	B	402	TLL	CB-CA-N	2.71	114.14	110.19
3	A	402	TLL	C4A-C4-N3	-2.50	118.01	123.14
3	B	402	TLL	C6-C9-N10	2.32	118.27	112.23
3	A	402	TLL	CB-CG-CD	-2.28	107.95	113.04
3	B	402	TLL	C4-C4A-C8A	2.28	116.22	114.44
3	B	402	TLL	C4A-C4-N3	-2.20	118.62	123.14
3	A	402	TLL	NA2-C2-N1	2.19	120.65	117.25
3	B	402	TLL	C15-C14-N10	-2.13	116.56	120.97
3	A	402	TLL	C8-C3-N2	-2.13	107.09	110.19
3	B	402	TLL	CB-CG-CD	-2.09	108.36	113.04
3	A	402	TLL	C16-C11-C	-2.08	113.88	120.62
3	B	402	TLL	NA2-C2-N1	2.05	120.44	117.25

There are no chirality outliers.

All (12) torsion outliers are listed below:



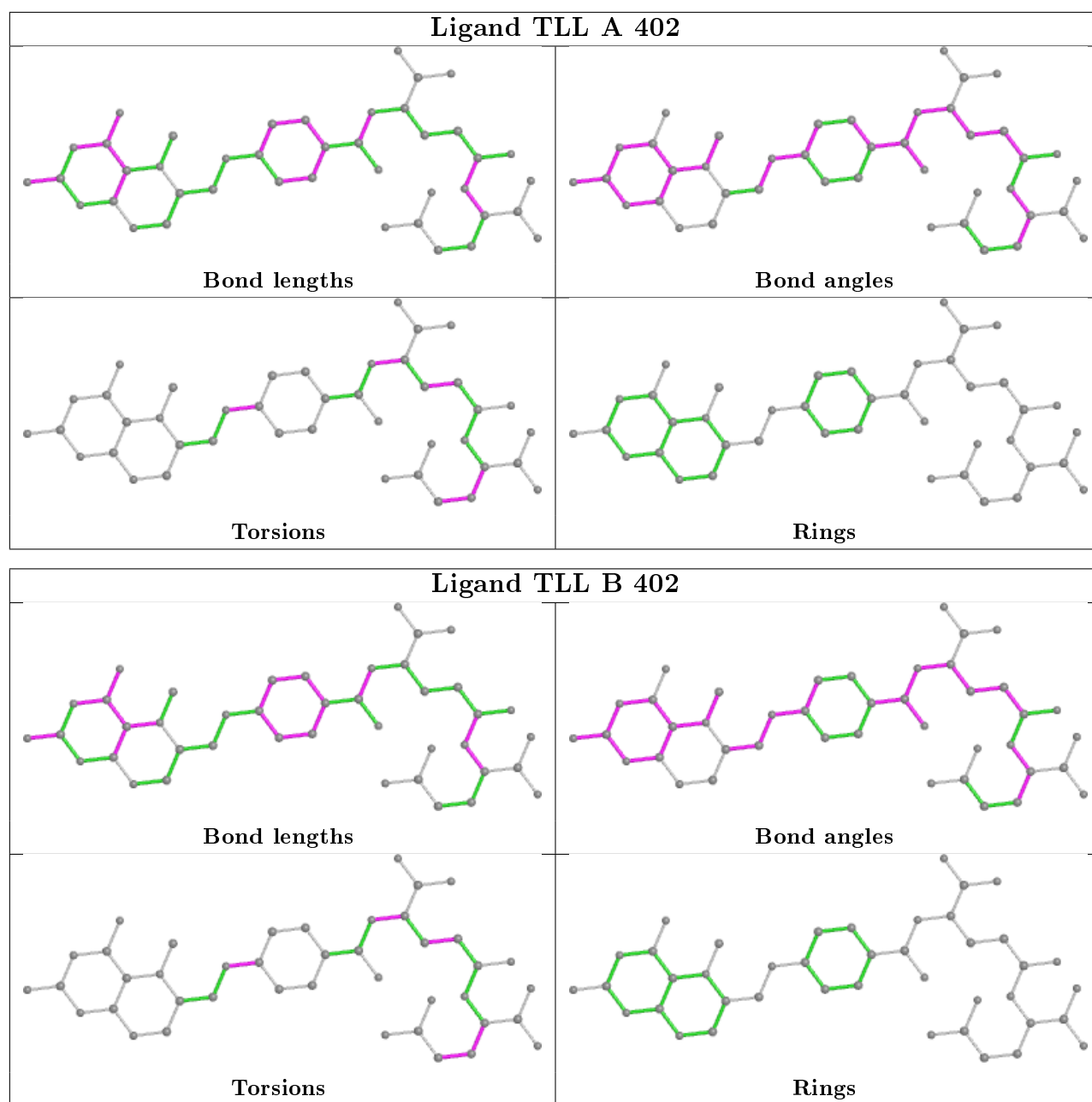
Mol	Chain	Res	Type	Atoms
3	B	402	TLL	CB-CA-N-C
3	A	402	TLL	CB-CA-N-C
3	A	402	TLL	N2-C3-C8-C10
3	A	402	TLL	CA-CB-CG-CD
3	B	402	TLL	N2-C3-C8-C10
3	B	402	TLL	CA-CB-CG-CD
3	B	402	TLL	C13-C14-N10-C9
3	B	402	TLL	C17-C10-C8-C3
3	A	402	TLL	C17-C10-C8-C3
3	A	402	TLL	C13-C14-N10-C9
3	B	402	TLL	C15-C14-N10-C9
3	A	402	TLL	C15-C14-N10-C9

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	TLL	12	0
3	B	402	TLL	7	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	373/391 (95%)	0.11	21 (5%) 24 29	17, 31, 65, 84	0
1	B	373/391 (95%)	0.09	19 (5%) 28 33	16, 30, 66, 91	0
All	All	746/782 (95%)	0.10	40 (5%) 25 31	16, 30, 66, 91	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	LEU	7.6
1	B	113	GLY	6.4
1	B	206	SER	6.0
1	B	111	THR	6.0
1	B	112	GLN	6.0
1	B	204	LEU	5.6
1	B	149	ILE	5.1
1	A	170	HIS	4.5
1	B	145	SER	4.3
1	A	149	ILE	4.3
1	B	142	ILE	4.2
1	A	148	LYS	4.2
1	A	111	THR	4.0
1	A	206	SER	3.9
1	A	208	ASN	3.7
1	A	203	GLU	3.4
1	B	205	ASP	3.3
1	A	145	SER	3.3
1	B	207	GLU	3.3
1	A	112	GLN	3.2
1	B	170	HIS	3.2
1	A	205	ASP	3.2
1	A	110	TRP	3.1
1	A	207	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	374	ALA	2.8
1	B	110	TRP	2.8
1	B	143	PHE	2.8
1	B	3	MET	2.7
1	A	113	GLY	2.7
1	A	3	MET	2.6
1	B	114	SER	2.6
1	B	132	ILE	2.5
1	B	148	LYS	2.4
1	A	114	SER	2.4
1	A	142	ILE	2.3
1	A	35	LEU	2.2
1	B	109	PHE	2.2
1	A	217	ASP	2.2
1	A	375	LYS	2.1
1	B	208	ASN	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 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.

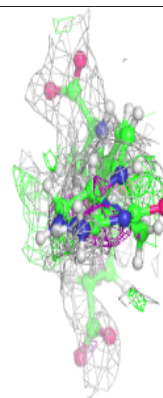
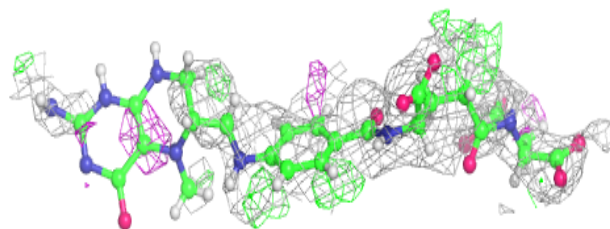
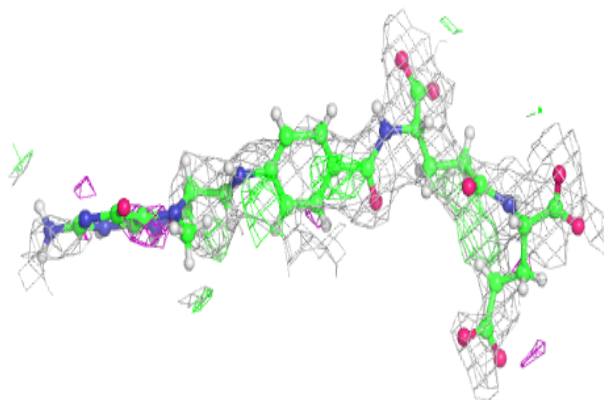
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TLL	A	402	42/42	0.67	0.36	51,93,130,133	0
3	TLL	B	402	42/42	0.72	0.36	47,81,128,131	0
2	MG	B	401	1/1	0.81	0.09	37,37,37,37	0
2	MG	A	401	1/1	0.97	0.04	39,39,39,39	0

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.

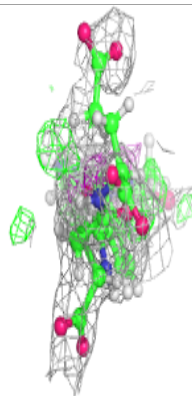
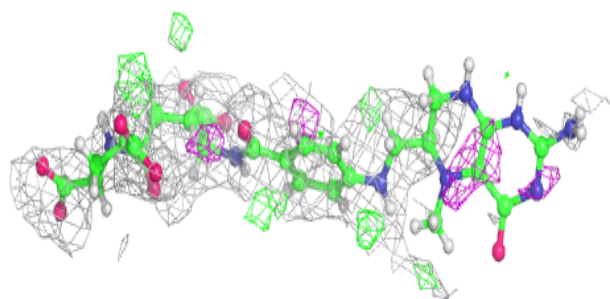
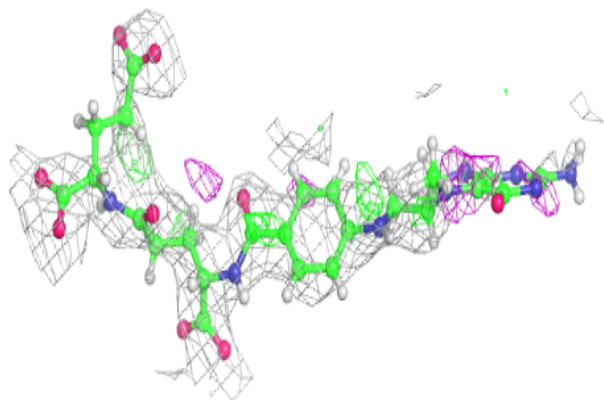
**Electron density around TLL A 402:**

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



**Electron density around TLL B 402:**

$2mF_o-DF_c$  (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.