



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:42 AM UTC

PDB ID : 4U0N / pdb_00004u0n
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

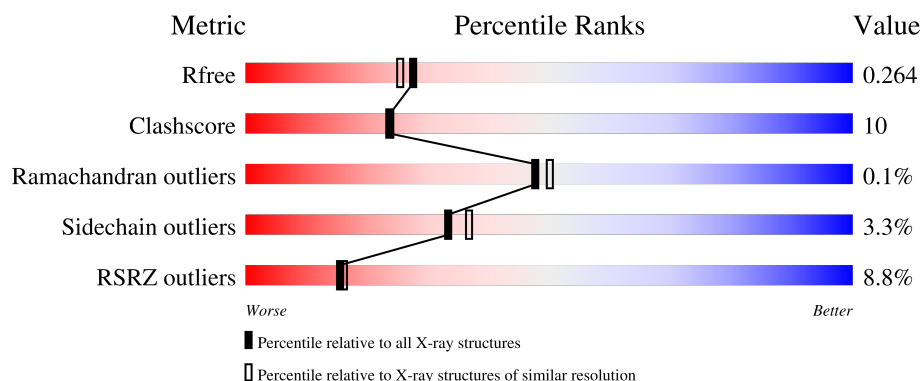
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	391	8% 79% 16% • 5%
1	B	391	9% 77% 16% • 5%

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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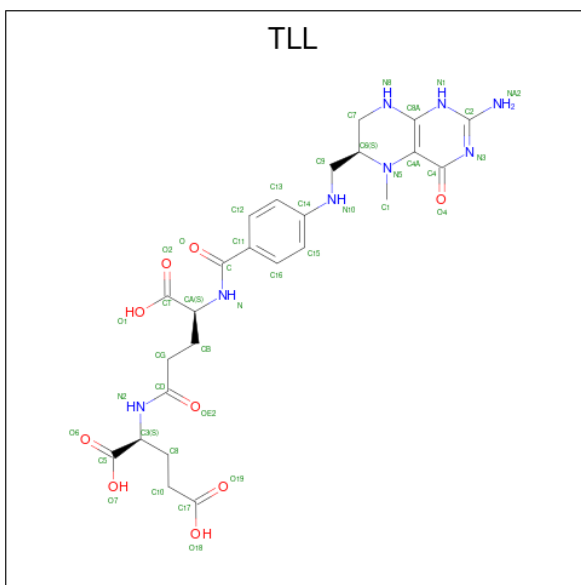
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	deletion	UNP Q9KVG7
B	?	-	VAL	deletion	UNP Q9KVG7
B	?	-	ALA	deletion	UNP Q9KVG7
B	?	-	ASP	deletion	UNP Q9KVG7
B	?	-	SER	deletion	UNP Q9KVG7
B	?	-	ILE	deletion	UNP Q9KVG7
B	?	-	THR	deletion	UNP 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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	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 (CCD ID: TLL) (formula: C₂₅H₃₂N₈O₉).



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

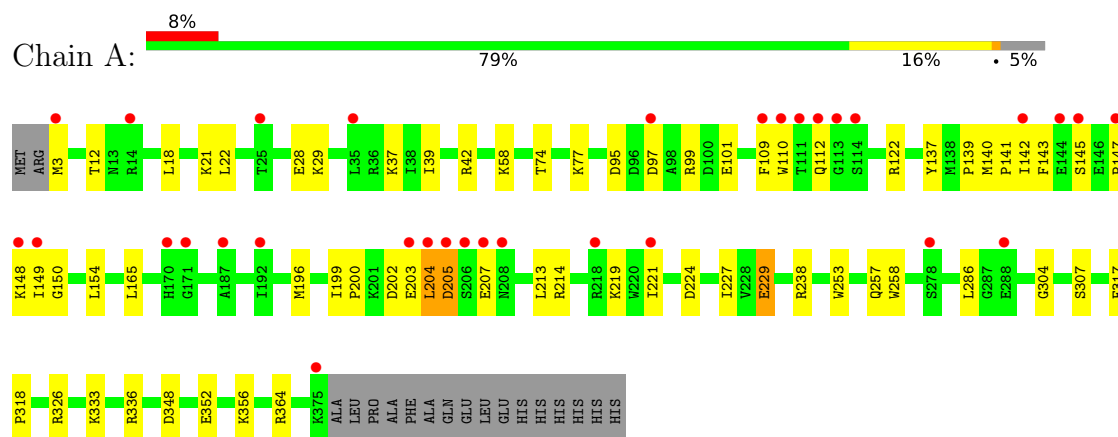
- Molecule 4 is water.

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

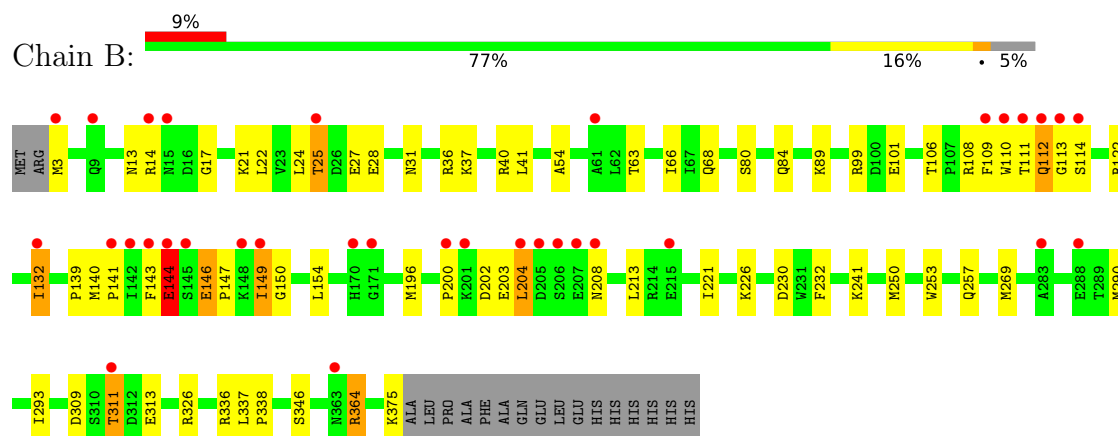
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: 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, α , β , γ	73.61Å 49.25Å 122.23Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	37.73 – 2.10 37.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.73-2.10) 99.2 (37.73-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 , 0.264	Depositor DCC
R_{free} test set	2557 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6498	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: TLL, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/3044	0.74	3/4105 (0.1%)
1	B	0.32	0/3044	0.78	4/4105 (0.1%)
All	All	0.31	0/6088	0.76	7/8210 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	GLU	CA-C-N	8.68	128.32	119.56
1	B	146	GLU	C-N-CA	8.68	128.32	119.56
1	B	208	ASN	N-CA-C	7.31	122.38	113.17
1	A	307	SER	CA-C-N	5.63	125.31	119.56
1	A	307	SER	C-N-CA	5.63	125.31	119.56
1	A	304	GLY	N-CA-C	-5.27	106.11	112.48
1	B	144	GLU	N-CA-C	-5.27	101.53	109.85

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	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	122	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 (122) 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
1:B:250:MET:HE3	1:B:293:ILE:CG2	2.21	0.70
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:250:MET:HE3	1:B:293:ILE:HG21	1.77	0.66
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:B:89:LYS:NZ	4:B:503:HOH:O	2.31	0.63
1:A:3:MET:SD	1:A:348:ASP:HA	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:250:MET:HE2	1:B:290:MET:HE1	1.84	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
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:B:112:GLN:C	1:B:114:SER:N	2.62	0.56
1:B:250:MET:HE2	1:B:290:MET:CE	2.36	0.55
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:204:LEU:HD13	1:B:204:LEU:O	2.06	0.55
1:B:139:PRO:HG2	4:B:633:HOH:O	2.07	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: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:80:SER:O	1:B:84:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LEU:HD21	1:B:221:ILE:HD11	1.93	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:B:250:MET:HE3	1:B:293:ILE:HG22	1.93	0.48
1:A:147:PRO:HG2	1:A:149:ILE:O	2.13	0.48
1:A:109:PHE:C	3:A:402:TLL:H16	2.34	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:146:GLU:CD	1:B:147:PRO:HD2	2.40	0.46
1:A:21:LYS:NZ	4:A:610:HOH:O	2.31	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
1:A:58:LYS:HB2	1:A:99:ARG:HD2	1.98	0.45
1:B:109:PHE:C	3:B:402:TLL:H16	2.39	0.45
1:B:140:MET:CG	1:B:149:ILE:HD12	2.47	0.45
1:B:146:GLU:HG3	1:B:147:PRO:CD	2.47	0.45
1:B:13:ASN:HB3	1:B:17:GLY:HA3	1.99	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: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:24:LEU:HD12	1:B:122:ARG:HG2	2.01	0.42
1:B:144:GLU:OE2	1:B:144:GLU:N	2.50	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:HE3	1:A:29:LYS:HB3	1.71	0.42
1:B:132:ILE:O	1:B:132:ILE:HG13	2.19	0.42
1:A:95:ASP:OD1	1:A:97:ASP:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:42:ARG:HG2	1:A:165:LEU:HG	2.02	0.41
1:A:137:TYR:O	1:A:139:PRO:HD3	2.20	0.41
1:A:219:LYS:NZ	4:A:507:HOH:O	2.49	0.41
1:B:27:GLU:O	1:B:31:ASN:ND2	2.47	0.41
1:A:204:LEU:O	1:A:204:LEU:HD13	2.21	0.41
1:B:3:MET:O	1:B:346:SER:HA	2.21	0.41
1:B:232:PHE:CE1	1:B:269:MET:HE3	2.56	0.40
1:A:37:LYS:HG3	3:A:402:TLL:O19	2.22	0.40
1:A:214:ARG:HD3	4:A:596:HOH:O	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	371/391 (95%)	361 (97%)	10 (3%)	0	100	100
1	B	371/391 (95%)	358 (96%)	12 (3%)	1 (0%)	36	36
All	All	742/782 (95%)	719 (97%)	22 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	113	GLY

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	329/344 (96%)	321 (98%)	8 (2%)	43	49
1	B	329/344 (96%)	315 (96%)	14 (4%)	26	27
All	All	658/688 (96%)	636 (97%)	22 (3%)	33	37

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ILE
1	A	145	SER
1	A	204	LEU
1	A	205	ASP
1	A	207	GLU
1	A	229	GLU
1	A	326	ARG
1	A	364	ARG
1	B	25	THR
1	B	68	GLN
1	B	106	THR
1	B	111	THR
1	B	112	GLN
1	B	132	ILE
1	B	144	GLU
1	B	149	ILE
1	B	202	ASP
1	B	204	LEU
1	B	311	THR
1	B	313	GLU
1	B	326	ARG
1	B	364	ARG

Sometimes 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 oligosaccharides 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	B	402	-	42,44,44	3.69	13 (30%)	47,61,61	1.84	13 (27%)
3	TLL	A	402	-	42,44,44	3.72	13 (30%)	47,61,61	1.88	15 (31%)

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	B	402	-	-	13/35/48/48	0/3/3/3
3	TLL	A	402	-	-	14/35/48/48	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	TLL	C12-C13	9.54	1.54	1.38
3	A	402	TLL	O4-C4	9.46	1.40	1.23
3	B	402	TLL	O4-C4	9.35	1.40	1.23
3	A	402	TLL	C8A-N8	9.20	1.41	1.32
3	B	402	TLL	C8A-N8	9.18	1.41	1.32
3	B	402	TLL	C12-C13	8.88	1.53	1.38
3	A	402	TLL	C4-N3	8.36	1.52	1.38
3	B	402	TLL	C4-N3	8.27	1.52	1.38
3	A	402	TLL	C16-C11	7.64	1.51	1.39
3	B	402	TLL	C15-C14	7.57	1.52	1.39
3	B	402	TLL	C16-C11	7.48	1.50	1.39
3	A	402	TLL	C15-C14	7.35	1.51	1.39
3	B	402	TLL	CD-N2	5.22	1.45	1.34
3	A	402	TLL	C-N	4.99	1.45	1.34
3	A	402	TLL	CD-N2	4.98	1.44	1.34
3	B	402	TLL	C-N	4.93	1.45	1.34
3	A	402	TLL	C2-NA2	4.25	1.44	1.34
3	B	402	TLL	C2-NA2	4.07	1.43	1.34
3	B	402	TLL	C7-N8	-3.99	1.42	1.46
3	A	402	TLL	C7-N8	-3.53	1.42	1.46
3	B	402	TLL	C12-C11	-2.74	1.35	1.39
3	B	402	TLL	C15-C16	-2.66	1.34	1.38
3	A	402	TLL	C15-C16	-2.66	1.34	1.38
3	A	402	TLL	C12-C11	-2.40	1.35	1.39
3	B	402	TLL	C13-C14	-2.38	1.35	1.39
3	A	402	TLL	C6-N5	-2.24	1.45	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	TLL	C2-N1-C8A	4.32	132.08	119.75
3	A	402	TLL	C2-N1-C8A	4.18	131.67	119.75
3	B	402	TLL	C9-N10-C14	-4.03	111.75	122.00
3	A	402	TLL	CT-CA-N	-3.57	102.28	110.57
3	A	402	TLL	C9-N10-C14	-3.52	113.03	122.00
3	B	402	TLL	CT-CA-N	-3.38	102.74	110.57
3	A	402	TLL	N1-C2-N3	-3.35	117.19	123.32
3	B	402	TLL	N1-C2-N3	-3.34	117.21	123.32
3	A	402	TLL	O-C-C11	-2.80	115.35	120.90
3	A	402	TLL	N1-C8A-N8	2.77	122.49	117.28
3	A	402	TLL	C15-C14-N10	-2.63	115.02	120.96
3	B	402	TLL	O1-CT-O2	-2.60	118.19	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	TLL	O-C-C11	-2.60	115.76	120.90
3	B	402	TLL	C1-N5-C6	2.59	125.69	117.97
3	B	402	TLL	O1-CT-CA	2.52	122.04	113.51
3	A	402	TLL	O1-CT-CA	2.51	122.02	113.51
3	A	402	TLL	O7-C5-C3	2.45	121.81	113.51
3	B	402	TLL	C8-C3-N2	-2.42	106.12	110.91
3	A	402	TLL	C1-N5-C6	2.38	125.06	117.97
3	B	402	TLL	O7-C5-C3	2.37	121.52	113.51
3	B	402	TLL	O7-C5-O6	-2.34	118.78	124.08
3	A	402	TLL	CB-CG-CD	-2.29	107.95	113.06
3	A	402	TLL	O7-C5-O6	-2.27	118.92	124.08
3	A	402	TLL	O1-CT-O2	-2.26	118.94	124.08
3	A	402	TLL	CB-CA-N	2.17	115.21	110.91
3	B	402	TLL	CB-CG-CD	-2.11	108.36	113.06
3	A	402	TLL	C16-C11-C	-2.07	113.88	120.60
3	B	402	TLL	N1-C8A-N8	2.07	121.17	117.28

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	TLL	CB-CA-N-C
3	B	402	TLL	CB-CA-N-C
3	A	402	TLL	N2-C3-C8-C10
3	A	402	TLL	C5-C3-C8-C10
3	A	402	TLL	CA-CB-CG-CD
3	B	402	TLL	N2-C3-C8-C10
3	B	402	TLL	N2-C3-C5-O6
3	A	402	TLL	N2-C3-C5-O6
3	A	402	TLL	N2-C3-C5-O7
3	B	402	TLL	N2-C3-C5-O7
3	B	402	TLL	C13-C14-N10-C9
3	A	402	TLL	CB-CA-CT-O1
3	B	402	TLL	CA-CB-CG-CD
3	A	402	TLL	C8-C3-C5-O7
3	A	402	TLL	C13-C14-N10-C9
3	A	402	TLL	CB-CA-CT-O2
3	A	402	TLL	C8-C3-C5-O6
3	B	402	TLL	C8-C3-C5-O7
3	B	402	TLL	C8-C3-C5-O6
3	B	402	TLL	C15-C14-N10-C9
3	B	402	TLL	CB-CA-CT-O1

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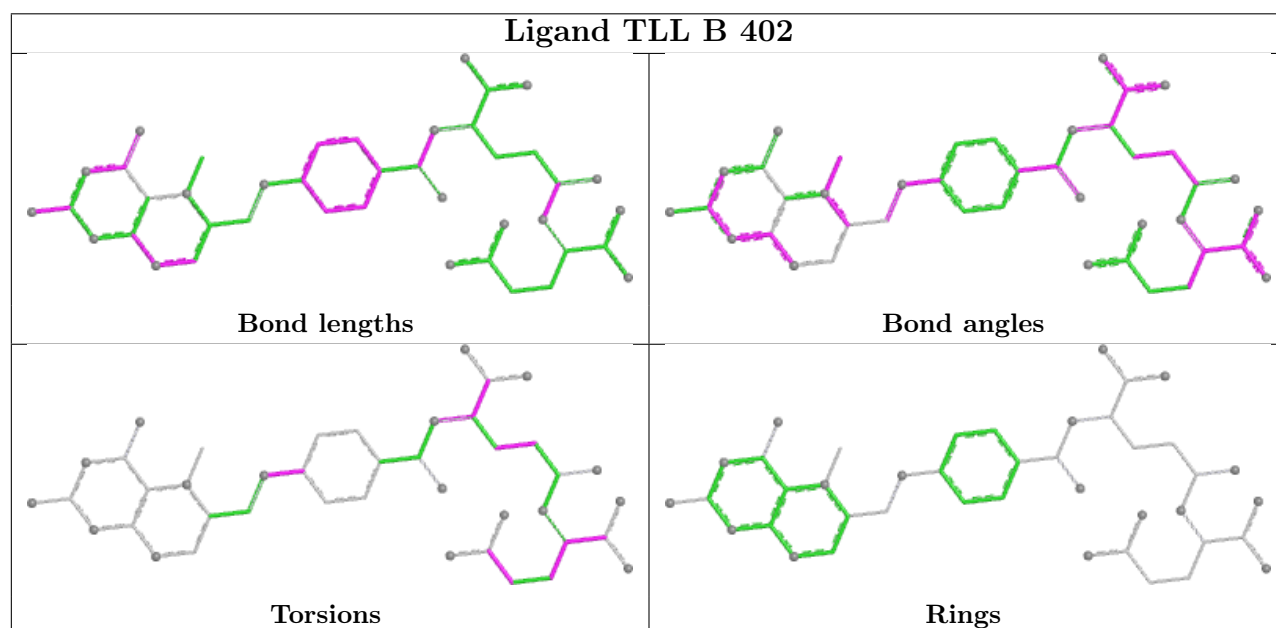
Mol	Chain	Res	Type	Atoms
3	B	402	TLL	C8-C10-C17-O18
3	A	402	TLL	C15-C14-N10-C9
3	B	402	TLL	C8-C10-C17-O19
3	A	402	TLL	C8-C10-C17-O19
3	A	402	TLL	C8-C10-C17-O18
3	B	402	TLL	CB-CA-CT-O2

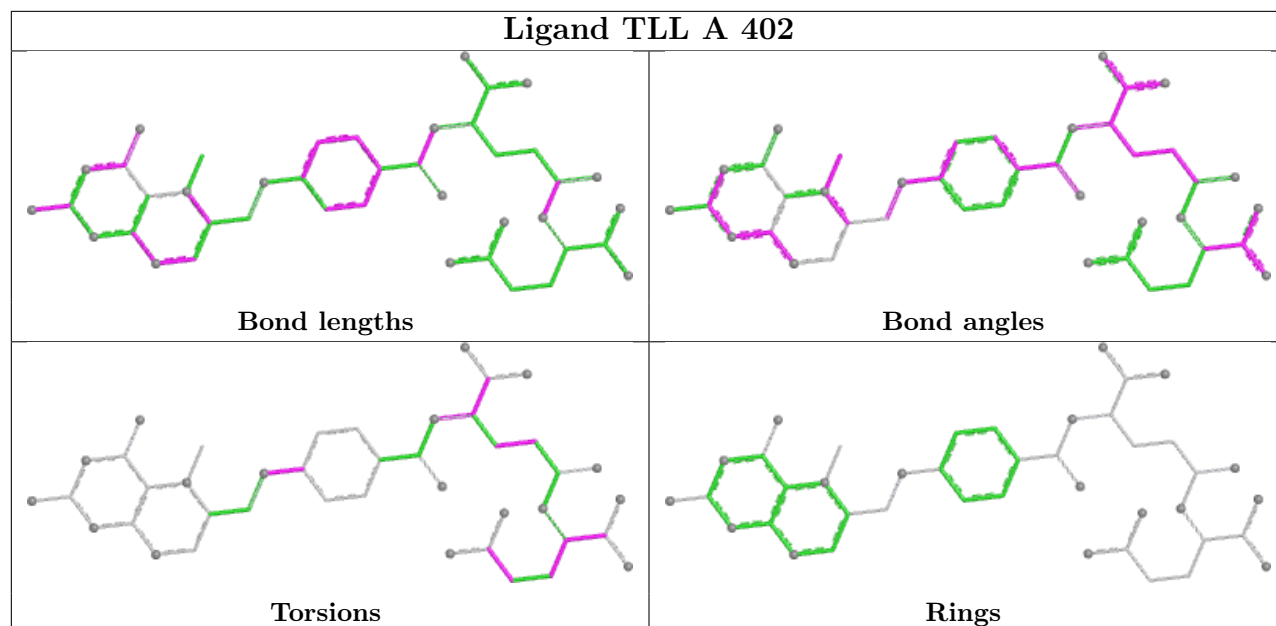
There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	TLL	7	0
3	A	402	TLL	12	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	373/391 (95%)	0.56	32 (8%) 16 17	17, 31, 65, 84	0
1	B	373/391 (95%)	0.54	34 (9%) 15 15	16, 30, 66, 91	0
All	All	746/782 (95%)	0.55	66 (8%) 15 16	16, 30, 66, 91	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	GLN	8.6
1	B	113	GLY	7.6
1	B	111	THR	6.9
1	A	170	HIS	6.1
1	A	204	LEU	5.9
1	B	142	ILE	5.7
1	B	204	LEU	5.6
1	B	149	ILE	5.2
1	B	206	SER	5.0
1	A	149	ILE	4.8
1	A	110	TRP	4.7
1	B	148	LYS	4.3
1	A	114	SER	4.3
1	B	114	SER	4.3
1	A	113	GLY	4.1
1	B	205	ASP	4.1
1	B	110	TRP	4.0
1	A	148	LYS	4.0
1	B	132	ILE	3.9
1	B	145	SER	3.8
1	B	143	PHE	3.8
1	B	208	ASN	3.8
1	A	142	ILE	3.7
1	A	208	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	109	PHE	3.5
1	B	109	PHE	3.5
1	A	206	SER	3.5
1	B	170	HIS	3.4
1	A	203	GLU	3.3
1	A	3	MET	3.3
1	B	288	GLU	3.2
1	A	278	SER	3.0
1	B	283	ALA	3.0
1	B	311	THR	3.0
1	A	207	GLU	2.8
1	A	145	SER	2.8
1	B	201	LYS	2.7
1	B	171	GLY	2.6
1	B	25	THR	2.6
1	A	35	LEU	2.6
1	A	288	GLU	2.5
1	A	187	ALA	2.5
1	A	205	ASP	2.4
1	A	218	ARG	2.4
1	B	3	MET	2.4
1	A	147	PRO	2.4
1	B	15	ASN	2.3
1	B	215	GLU	2.3
1	A	111	THR	2.3
1	A	112	GLN	2.3
1	A	221	ILE	2.3
1	A	375	LYS	2.3
1	B	61	ALA	2.2
1	B	207	GLU	2.1
1	A	144	GLU	2.1
1	A	192	ILE	2.1
1	A	25	THR	2.1
1	B	14	ARG	2.1
1	B	144	GLU	2.1
1	B	9	GLN	2.1
1	A	14	ARG	2.1
1	B	141	PRO	2.1
1	B	200	PRO	2.1
1	B	363	ASN	2.0
1	A	171	GLY	2.0
1	A	97	ASP	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 [i](#)

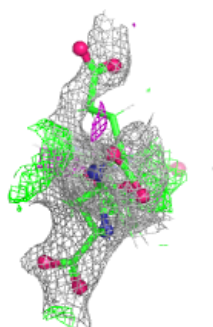
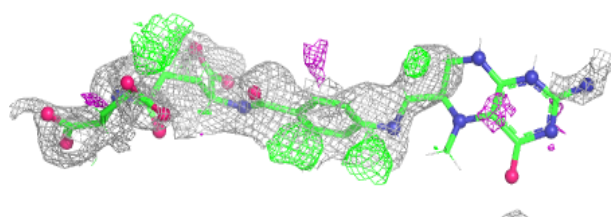
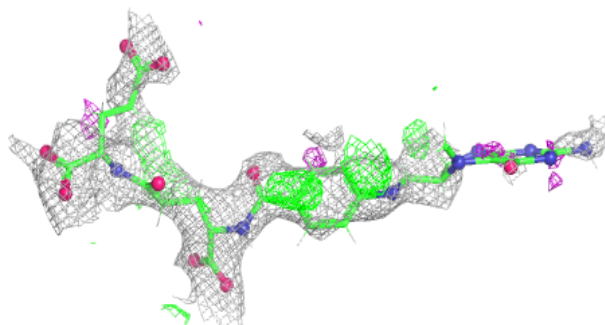
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TLL	A	402	42/42	0.64	0.22	51,93,130,133	0
3	TLL	B	402	42/42	0.65	0.20	47,81,128,131	0
2	MG	B	401	1/1	0.88	0.08	37,37,37,37	0
2	MG	A	401	1/1	0.96	0.06	39,39,39,39	0

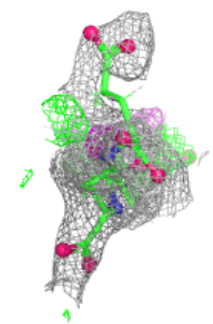
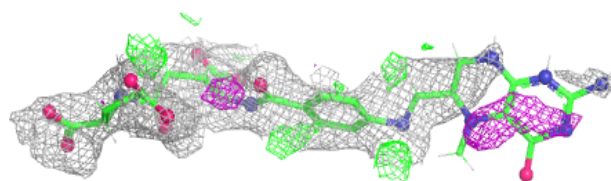
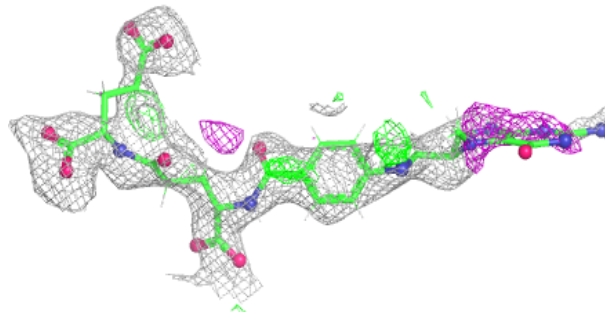
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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.