



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:39 PM UTC

PDB ID : 7B8W / pdb_00007b8w
Title : Structure of LIMK1 Kinase domain with allosteric inhibitor TH-470
Authors : Lee, H.; Yosaatmadja, Y.; Burgess-Brown, N.A.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Elkins, J.M.
Deposited on : 2020-12-13
Resolution : 2.80 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

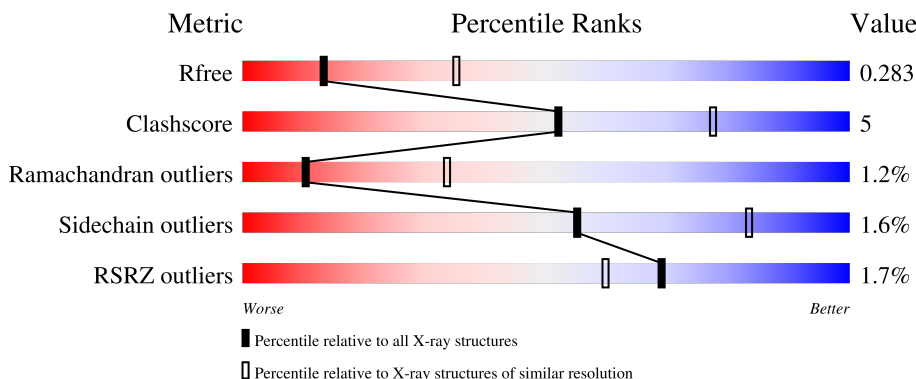
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	310	2% 78%12%10%
1	B	310	2% 73%15%11%
1	C	310	2% 78%11%11%
1	D	310	% 79%8%12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8652 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.

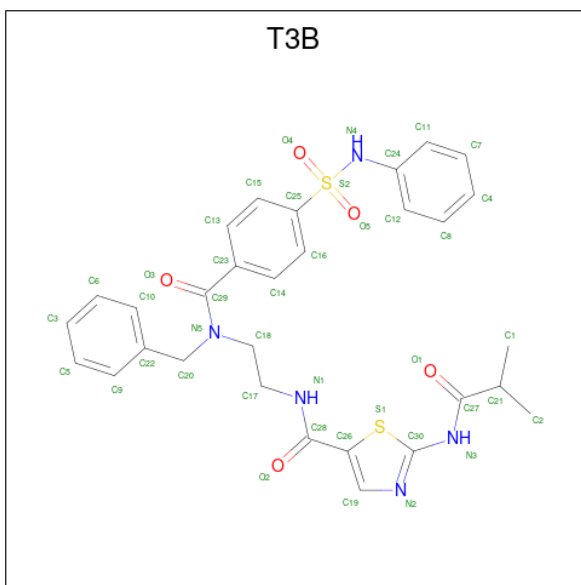
- Molecule 1 is a protein called LIM domain kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2143	1378	367	379	19			
1	B	275	Total	C	N	O	S	0	0	0
			2093	1351	356	368	18			
1	C	276	Total	C	N	O	S	0	0	0
			2116	1362	369	367	18			
1	D	273	Total	C	N	O	S	0	0	0
			2112	1357	368	370	17			

There are 8 discrepancies between the modelled and reference sequences:

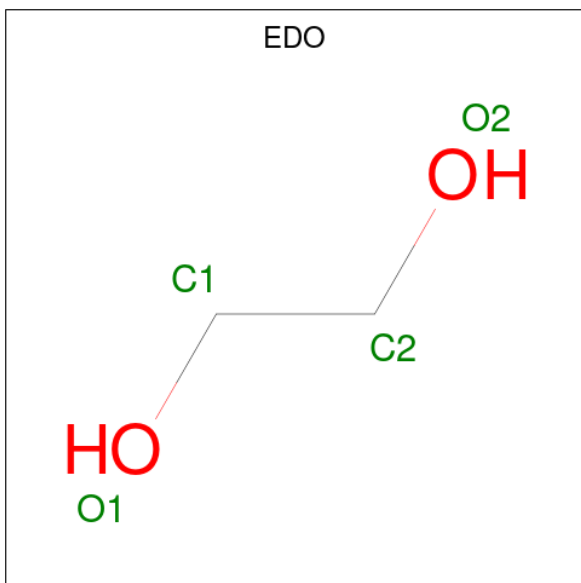
Chain	Residue	Modelled	Actual	Comment	Reference
A	328	SER	-	expression tag	UNP P53667
A	329	MET	-	expression tag	UNP P53667
B	328	SER	-	expression tag	UNP P53667
B	329	MET	-	expression tag	UNP P53667
C	328	SER	-	expression tag	UNP P53667
C	329	MET	-	expression tag	UNP P53667
D	328	SER	-	expression tag	UNP P53667
D	329	MET	-	expression tag	UNP P53667

- Molecule 2 is 2-(2-methylpropanoylamino)- {N}-[2-[(phenylmethyl)-[4-(phenylsulfamoyl)phenyl]carbonyl-amino]ethyl]-1,3-thiazole-5-carboxamide (CCD ID: T3B) (formula: C₃₀H₃₁N₅O₅S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			42	30	5	5	2		
2	B	1	Total	C	N	O	S	0	0
			42	30	5	5	2		
2	C	1	Total	C	N	O	S	0	0
			42	30	5	5	2		
2	D	1	Total	C	N	O	S	0	0
			42	30	5	5	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

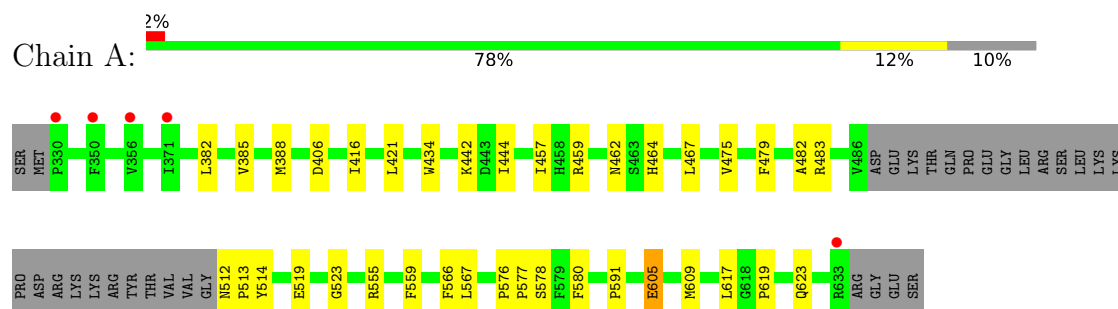
- Molecule 4 is water.

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

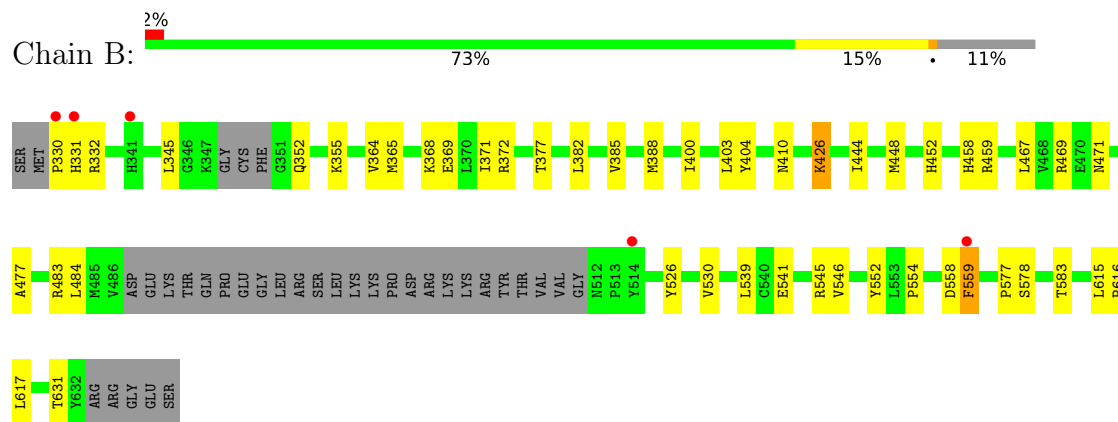
3 Residue-property plots

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: LIM domain kinase 1



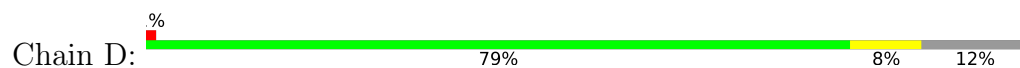
• Molecule 1: LIM domain kinase 1

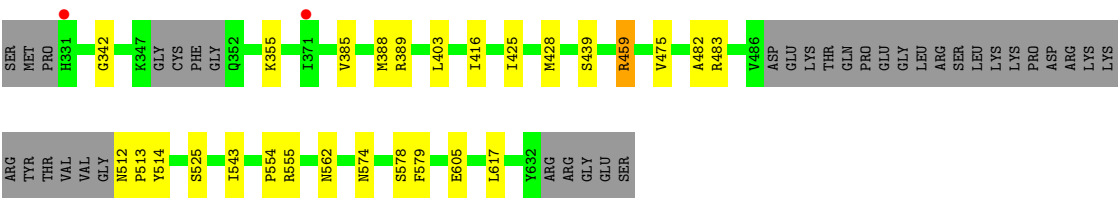


• Molecule 1: LIM domain kinase 1



• Molecule 1: LIM domain kinase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.69Å 83.67Å 96.51Å 90.00° 91.97° 90.00°	Depositor
Resolution (Å)	50.15 – 2.80 50.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.15-2.80) 99.9 (50.15-2.80)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.206 , 0.286 0.210 , 0.283	Depositor DCC
R_{free} test set	1574 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.097 for k,h,-l 0.088 for -k,-h,-l 0.085 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8652	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: T3B, EDO

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	1.02	0/2200	1.46	0/2994
1	B	1.03	0/2147	1.46	4/2923 (0.1%)
1	C	1.02	0/2171	1.45	0/2952
1	D	1.01	0/2165	1.44	0/2944
All	All	1.02	0/8683	1.45	4/11813 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	541	GLU	CA-C-N	5.62	127.58	120.72
1	B	541	GLU	C-N-CA	5.62	127.58	120.72
1	B	452	HIS	CA-C-N	5.10	127.36	120.38
1	B	452	HIS	C-N-CA	5.10	127.36	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2143	0	2022	21	0
1	B	2093	0	1972	27	0
1	C	2116	0	2010	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2112	0	2011	16	0
2	A	42	0	0	1	0
2	B	42	0	0	2	0
2	C	42	0	0	0	0
2	D	42	0	0	1	0
3	A	12	0	18	0	0
4	A	3	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
All	All	8652	0	8033	85	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 5.

All (85) 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:416:ILE:HG13	1:A:475:VAL:HG21	1.63	0.81
1:A:555:ARG:NH1	1:A:559:PHE:O	2.23	0.72
1:C:551:ASP:OD2	1:D:389:ARG:NH2	2.23	0.70
1:D:512:ASN:HB3	1:D:513:PRO:HD2	1.72	0.69
1:D:512:ASN:HB3	1:D:513:PRO:CD	2.23	0.68
1:A:605:GLU:HA	1:A:605:GLU:OE1	1.94	0.66
1:C:387:VAL:HB	1:C:485:MET:HE1	1.79	0.64
1:C:457:ILE:HG22	1:C:459:ARG:HG3	1.84	0.60
1:A:605:GLU:O	1:A:609:MET:HG2	2.02	0.59
2:A:701:T3B:S1	2:A:701:T3B:O1	2.61	0.57
1:D:514:TYR:O	1:D:555:ARG:NH2	2.37	0.57
2:B:701:T3B:S1	2:B:701:T3B:O1	2.63	0.56
1:C:554:PRO:HB2	1:C:562:ASN:HB3	1.88	0.55
1:D:342:GLY:HA2	1:D:355:LYS:O	2.07	0.55
1:B:459:ARG:NH1	1:B:484:LEU:HB2	2.22	0.55
1:B:615:LEU:HB3	1:B:616:PRO:HD2	1.88	0.54
1:B:385:VAL:HA	1:B:388:MET:HE3	1.90	0.54
1:C:605:GLU:HA	1:C:605:GLU:OE1	2.07	0.54
1:C:370:LEU:HD13	1:C:409:LEU:HG	1.89	0.54
1:B:558:ASP:O	1:B:559:PHE:HB2	2.09	0.53
1:D:483:ARG:O	1:D:483:ARG:HD2	2.09	0.52
1:B:365:MET:HE2	1:B:400:ILE:HD13	1.92	0.52
1:B:330:PRO:O	1:B:332:ARG:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ILE:HG22	1:A:459:ARG:HG3	1.91	0.52
1:C:437:ARG:O	1:C:440:PHE:HB2	2.11	0.51
1:C:384:GLU:HB3	1:C:485:MET:HE2	1.93	0.51
1:C:459:ARG:NH1	1:C:482:ALA:O	2.41	0.51
1:C:385:VAL:HA	1:C:388:MET:HE3	1.93	0.50
1:A:459:ARG:HD3	1:A:482:ALA:O	2.12	0.49
1:C:387:VAL:CB	1:C:485:MET:HE1	2.41	0.49
1:B:483:ARG:HD2	1:B:483:ARG:O	2.13	0.49
1:D:543:ILE:HG12	1:D:579:PHE:CE2	2.48	0.48
1:B:369:GLU:HB3	1:B:410:ASN:OD1	2.13	0.48
1:A:483:ARG:O	1:A:483:ARG:HG3	2.14	0.48
1:A:519:GLU:OE1	1:A:591:PRO:HG3	2.14	0.48
1:A:512:ASN:CB	1:A:513:PRO:HD2	2.44	0.47
1:D:459:ARG:HD3	1:D:482:ALA:O	2.14	0.47
1:A:514:TYR:O	1:A:555:ARG:NH2	2.47	0.47
1:B:546:VAL:CG2	1:B:552:TYR:HB3	2.45	0.47
2:D:701:T3B:S1	2:D:701:T3B:O1	2.71	0.47
1:D:385:VAL:HA	1:D:388:MET:HE3	1.97	0.47
1:B:552:TYR:O	1:B:554:PRO:HD3	2.15	0.46
1:D:512:ASN:CB	1:D:513:PRO:CD	2.90	0.46
1:B:577:PRO:O	1:B:578:SER:OG	2.33	0.46
1:B:368:LYS:HG2	2:B:701:T3B:C5	2.46	0.46
1:B:426:LYS:NZ	4:B:801:HOH:O	2.49	0.46
1:A:467:LEU:HD21	1:A:479:PHE:HZ	1.81	0.45
1:D:416:ILE:HG13	1:D:475:VAL:HG21	1.98	0.45
1:C:459:ARG:HD3	1:C:482:ALA:O	2.17	0.45
1:C:526:TYR:HB2	1:C:530:VAL:HG11	1.99	0.45
1:B:615:LEU:HB3	1:B:616:PRO:CD	2.47	0.45
1:B:459:ARG:HH11	1:B:484:LEU:HB2	1.80	0.45
1:C:483:ARG:NH1	1:C:485:MET:SD	2.90	0.45
1:C:546:VAL:CG2	1:C:552:TYR:HB3	2.47	0.45
1:D:554:PRO:HB2	1:D:562:ASN:HB3	1.97	0.44
1:D:403:LEU:C	1:D:403:LEU:HD23	2.43	0.44
1:A:421:LEU:HD22	1:A:444:ILE:HD11	1.99	0.43
1:D:605:GLU:HA	1:D:605:GLU:OE1	2.19	0.43
1:A:619:PRO:O	1:A:623:GLN:N	2.50	0.43
1:D:554:PRO:CB	1:D:562:ASN:HB3	2.49	0.43
1:A:566:PHE:CD2	1:A:580:PHE:CE1	3.07	0.43
1:B:355:LYS:HE2	1:B:364:VAL:HG11	2.01	0.43
1:B:345:LEU:O	1:B:352:GLN:NE2	2.50	0.43
1:B:403:LEU:HD23	1:B:404:TYR:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LYS:HD2	1:A:605:GLU:HB2	2.00	0.43
1:A:567:LEU:HD23	1:A:567:LEU:HA	1.92	0.43
1:B:546:VAL:HG22	1:B:552:TYR:HB3	2.00	0.42
1:B:467:LEU:HD12	1:B:477:ALA:HB2	2.01	0.42
1:C:613:GLY:O	1:C:614:HIS:HB2	2.20	0.42
1:B:469:ARG:HD2	1:B:471:ASN:HD21	1.85	0.41
1:C:424:ILE:HD12	1:C:468:VAL:HG21	2.01	0.41
1:A:577:PRO:O	1:A:578:SER:OG	2.36	0.41
1:B:458:HIS:O	1:B:459:ARG:HB2	2.20	0.41
1:A:434:TRP:CD2	1:A:576:PRO:HD3	2.55	0.41
1:B:526:TYR:HB2	1:B:530:VAL:HG11	2.02	0.41
1:C:518:PRO:HG2	1:C:589:LEU:CD2	2.51	0.41
1:A:385:VAL:HA	1:A:388:MET:HE3	2.03	0.41
1:A:462:ASN:OD1	1:A:464:HIS:HB2	2.21	0.41
1:B:382:LEU:HD12	1:B:382:LEU:HA	1.95	0.41
1:B:539:LEU:HB2	1:B:583:THR:HG23	2.02	0.41
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.95	0.40
1:B:526:TYR:HB2	1:B:530:VAL:CG1	2.51	0.40
1:D:425:ILE:HA	1:D:428:MET:HE3	2.03	0.40
1:B:444:ILE:O	1:B:448:MET:HG2	2.20	0.40
1:C:518:PRO:HG2	1:C:589:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

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	275/310 (89%)	257 (94%)	16 (6%)	2 (1%)	18	47
1	B	269/310 (87%)	244 (91%)	20 (7%)	5 (2%)	6	22
1	C	270/310 (87%)	245 (91%)	21 (8%)	4 (2%)	8	28
1	D	267/310 (86%)	242 (91%)	23 (9%)	2 (1%)	18	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1081/1240 (87%)	988 (91%)	80 (7%)	13 (1%)	10	34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	331	HIS
1	B	372	ARG
1	C	559	PHE
1	B	371	ILE
1	B	631	THR
1	C	578	SER
1	D	578	SER
1	A	406	ASP
1	C	347	LYS
1	C	406	ASP
1	D	574	ASN
1	A	523	GLY
1	B	559	PHE

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	219/279 (78%)	217 (99%)	2 (1%)	70	89
1	B	211/279 (76%)	207 (98%)	4 (2%)	50	81
1	C	214/279 (77%)	210 (98%)	4 (2%)	50	81
1	D	216/279 (77%)	212 (98%)	4 (2%)	50	81
All	All	860/1116 (77%)	846 (98%)	14 (2%)	55	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	605	GLU
1	A	617	LEU

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Mol	Chain	Res	Type
1	B	377	THR
1	B	426	LYS
1	B	545	ARG
1	B	617	LEU
1	C	514	TYR
1	C	519	GLU
1	C	539	LEU
1	C	609	MET
1	D	439	SER
1	D	459	ARG
1	D	525	SER
1	D	617	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	ASN
1	A	602	HIS
1	B	464	HIS
1	B	471	ASN
1	B	473	ASN
1	B	620	GLN
1	C	436	GLN
1	C	464	HIS
1	C	473	ASN
1	D	464	HIS
1	D	610	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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	EDO	A	704	-	3,3,3	0.12	0	2,2,2	0.19	0
2	T3B	A	701	-	45,45,45	0.35	0	62,62,62	0.77	3 (4%)
3	EDO	A	703	-	3,3,3	0.10	0	2,2,2	0.16	0
2	T3B	C	701	-	45,45,45	0.31	0	62,62,62	0.79	3 (4%)
2	T3B	D	701	-	45,45,45	0.27	0	62,62,62	0.99	4 (6%)
3	EDO	A	702	-	3,3,3	0.10	0	2,2,2	0.13	0
2	T3B	B	701	-	45,45,45	0.31	0	62,62,62	0.85	3 (4%)

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	EDO	A	704	-	-	1/1/1/1	-
2	T3B	A	701	-	-	6/41/41/41	0/4/4/4
3	EDO	A	703	-	-	1/1/1/1	-
2	T3B	C	701	-	-	6/41/41/41	0/4/4/4
2	T3B	D	701	-	-	7/41/41/41	0/4/4/4
3	EDO	A	702	-	-	1/1/1/1	-
2	T3B	B	701	-	-	6/41/41/41	0/4/4/4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	T3B	C19-C26-C28	3.41	135.96	130.64
2	D	701	T3B	C19-C26-C28	3.41	135.95	130.64
2	D	701	T3B	C21-C27-N3	3.05	119.00	115.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	T3B	C19-C26-C28	2.99	135.30	130.64
2	D	701	T3B	C26-C28-N1	2.58	120.17	117.09
2	A	701	T3B	C21-C27-N3	2.27	117.99	115.03
2	A	701	T3B	C27-N3-C30	-2.26	121.79	124.54
2	C	701	T3B	C25-S2-N4	-2.22	104.12	106.88
2	D	701	T3B	C22-C20-N5	2.21	116.63	113.15
2	C	701	T3B	C21-C27-N3	2.12	117.80	115.03
2	A	701	T3B	S1-C30-N3	-2.04	120.99	123.72
2	B	701	T3B	C23-C29-N5	2.02	121.18	118.66
2	B	701	T3B	C21-C27-N3	2.01	117.65	115.03

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	T3B	C24-N4-S2-C25
2	A	701	T3B	C24-N4-S2-O4
2	B	701	T3B	N1-C17-C18-N5
2	C	701	T3B	C21-C27-N3-C30
2	C	701	T3B	N1-C17-C18-N5
2	D	701	T3B	N1-C17-C18-N5
2	B	701	T3B	C24-N4-S2-O5
2	A	701	T3B	C24-N4-S2-O5
2	D	701	T3B	C24-N4-S2-O5
2	A	701	T3B	N1-C17-C18-N5
2	B	701	T3B	C24-N4-S2-C25
2	D	701	T3B	C24-N4-S2-C25
2	C	701	T3B	C1-C21-C27-O1
2	D	701	T3B	C1-C21-C27-N3
2	D	701	T3B	C1-C21-C27-O1
2	C	701	T3B	C1-C21-C27-N3
2	B	701	T3B	C24-N4-S2-O4
2	D	701	T3B	C24-N4-S2-O4
2	A	701	T3B	C1-C21-C27-O1
2	A	701	T3B	C1-C21-C27-N3
2	B	701	T3B	C1-C21-C27-O1
2	C	701	T3B	O1-C27-N3-C30
3	A	702	EDO	O1-C1-C2-O2
2	B	701	T3B	C1-C21-C27-N3
2	C	701	T3B	C18-C17-N1-C28
3	A	704	EDO	O1-C1-C2-O2
3	A	703	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	D	701	T3B	C18-C17-N1-C28

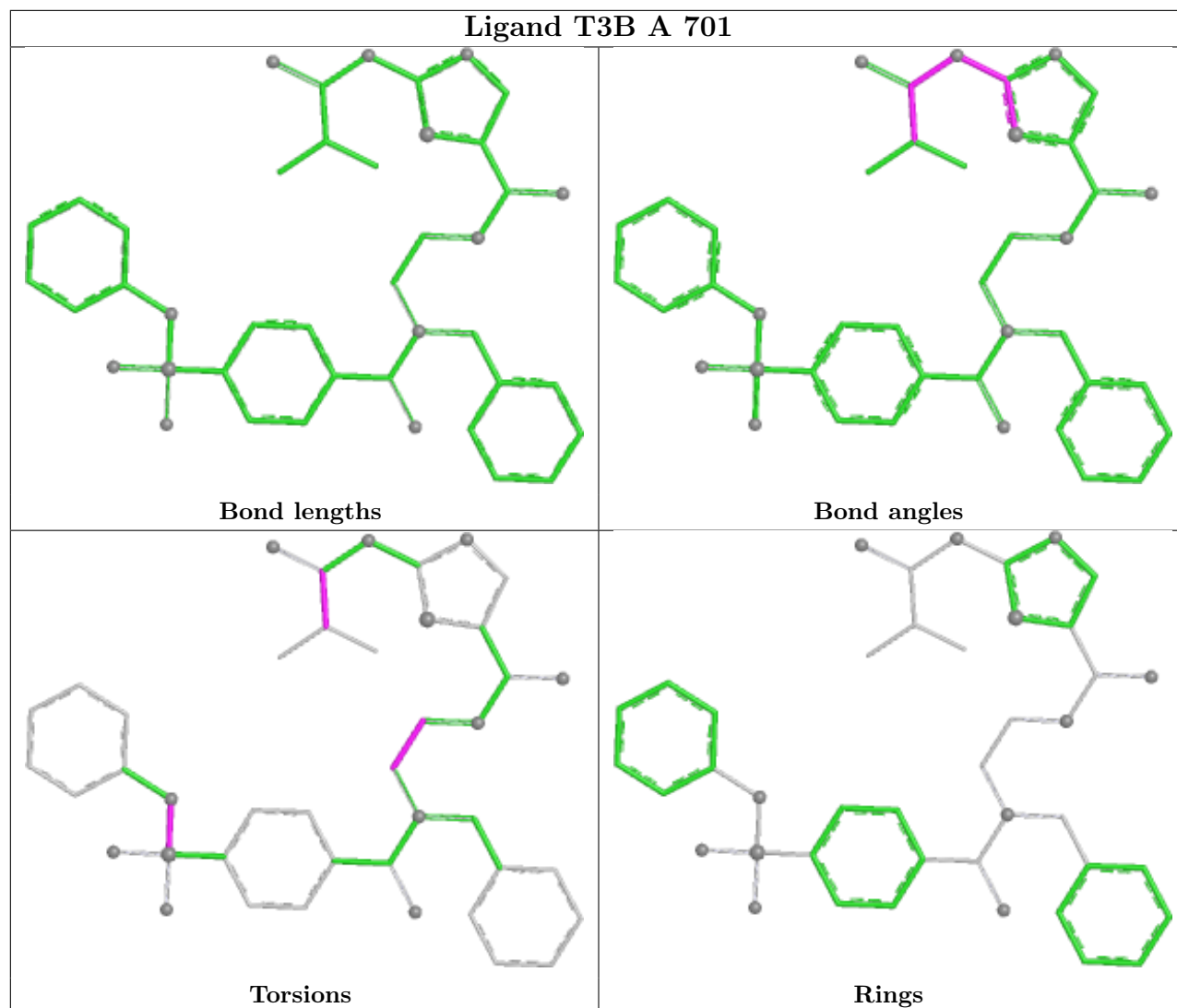
There are no ring outliers.

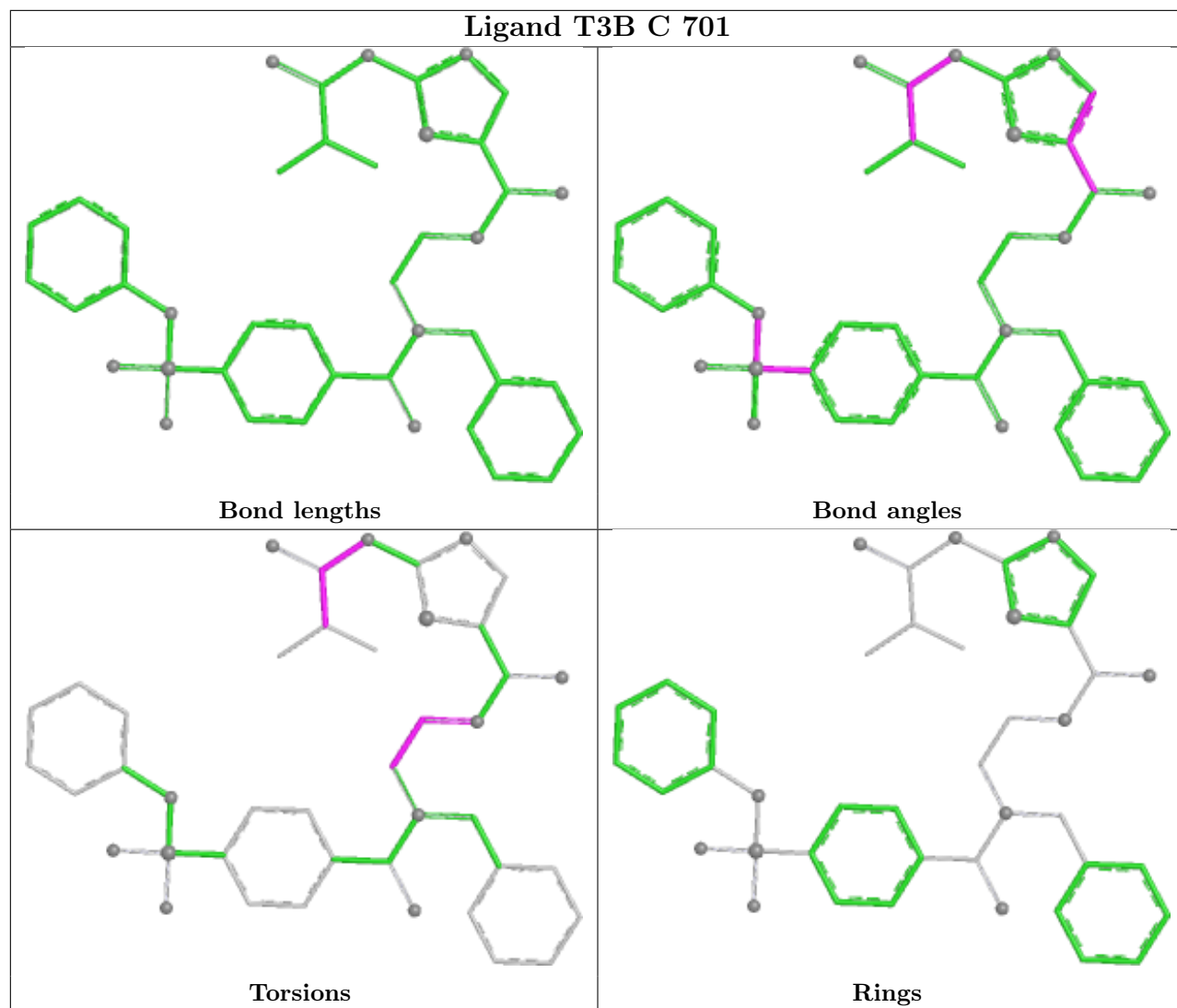
3 monomers are involved in 4 short contacts:

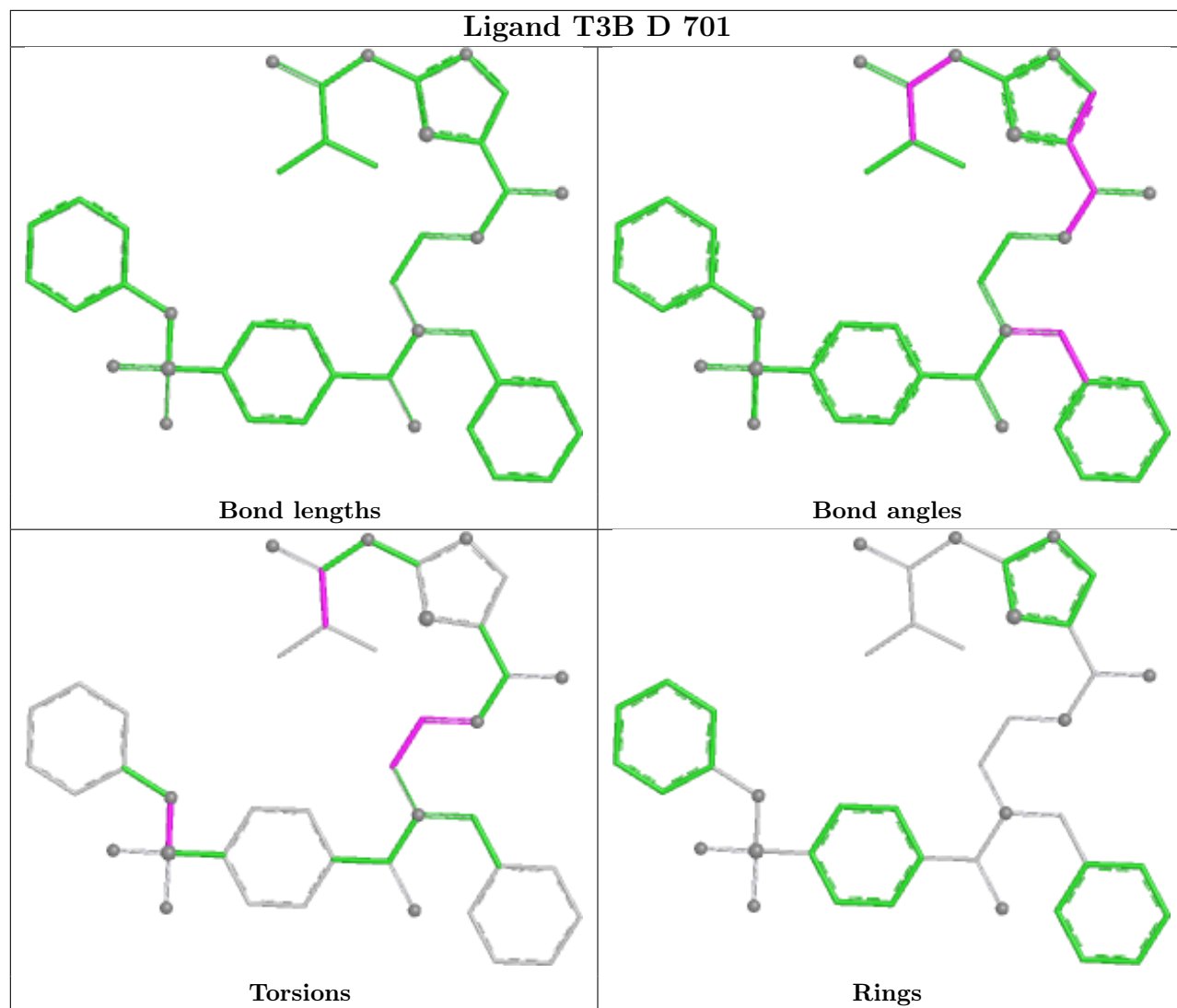
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	T3B	1	0
2	D	701	T3B	1	0
2	B	701	T3B	2	0

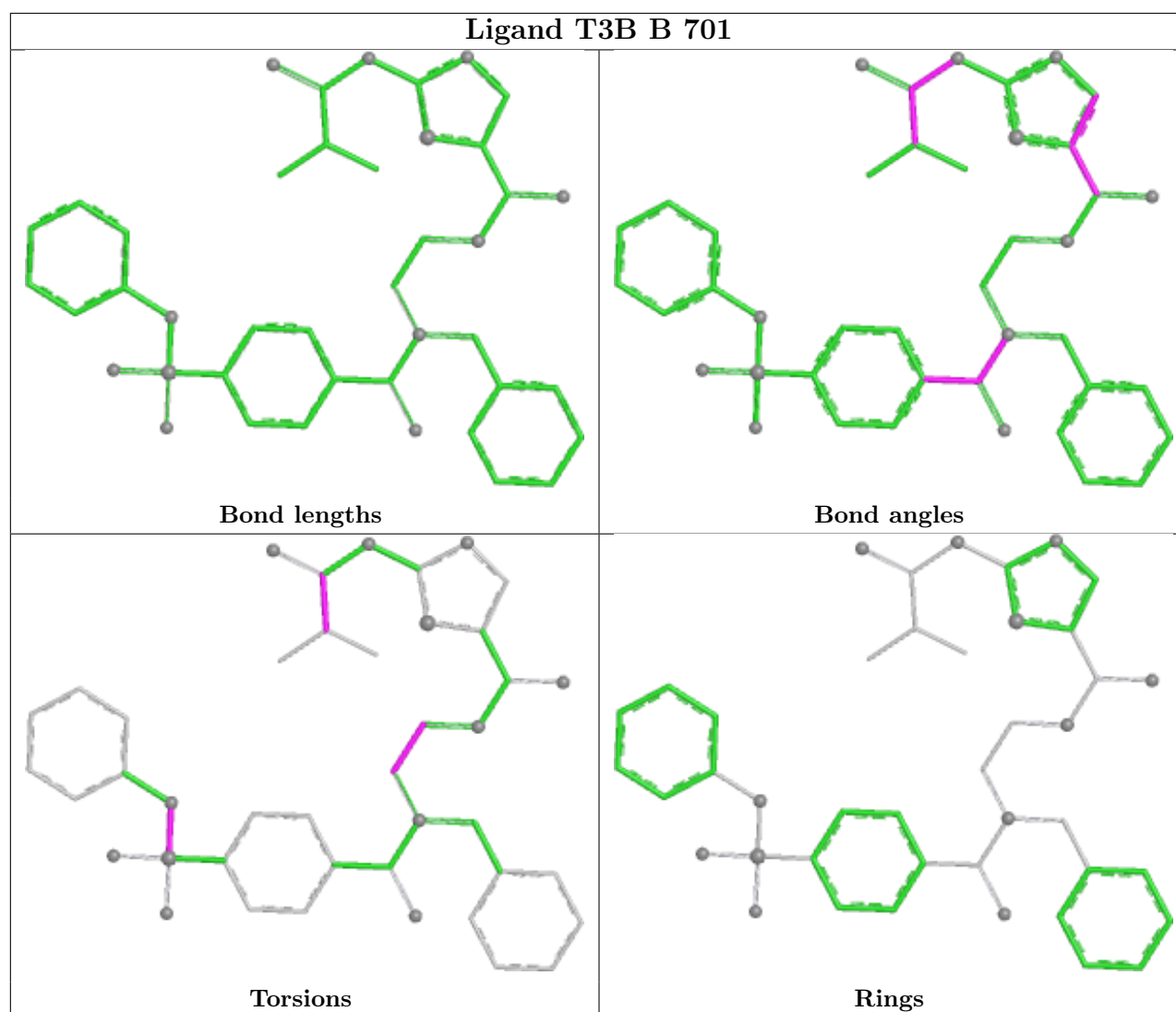
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand T3B A 701









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	279/310 (90%)	-0.04	5 (1%) 67 58	28, 48, 78, 101	0
1	B	275/310 (88%)	-0.01	5 (1%) 67 58	31, 49, 77, 96	0
1	C	276/310 (89%)	-0.04	7 (2%) 58 48	29, 49, 81, 117	0
1	D	273/310 (88%)	-0.14	2 (0%) 84 77	29, 45, 77, 98	0
All	All	1103/1240 (88%)	-0.06	19 (1%) 69 60	28, 48, 79, 117	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	PRO	4.7
1	D	371	ILE	3.7
1	B	341	HIS	3.7
1	C	330	PRO	3.2
1	B	330	PRO	3.1
1	A	356	VAL	2.8
1	B	331	HIS	2.8
1	D	331	HIS	2.7
1	A	350	PHE	2.7
1	C	513	PRO	2.5
1	C	349	CYS	2.5
1	A	371	ILE	2.4
1	B	559	PHE	2.4
1	B	514	TYR	2.4
1	C	351	GLY	2.3
1	C	341	HIS	2.3
1	A	633	ARG	2.2
1	C	514	TYR	2.1
1	C	347	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 [i](#)

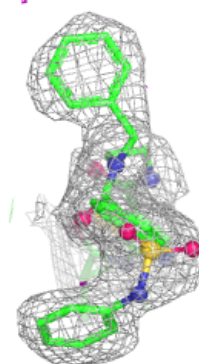
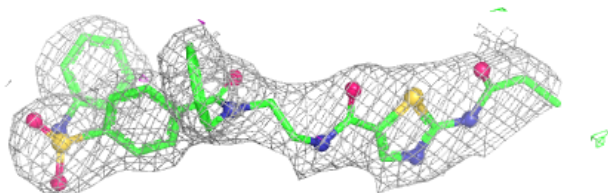
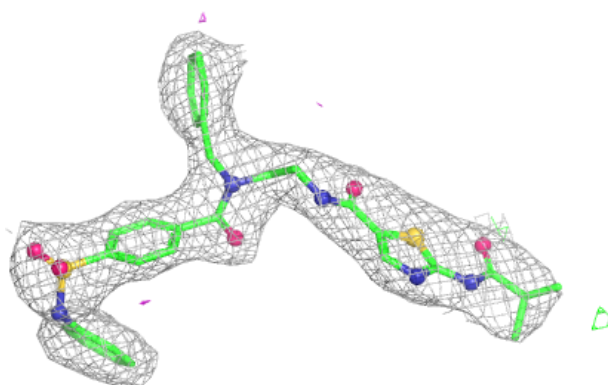
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	A	702	4/4	0.76	0.25	65,67,68,68	0
3	EDO	A	703	4/4	0.86	0.15	61,63,65,68	0
3	EDO	A	704	4/4	0.93	0.11	44,47,50,50	0
2	T3B	B	701	42/42	0.96	0.07	34,39,53,57	0
2	T3B	C	701	42/42	0.96	0.08	31,38,49,60	0
2	T3B	D	701	42/42	0.96	0.08	32,41,51,54	0
2	T3B	A	701	42/42	0.97	0.07	30,38,49,52	0

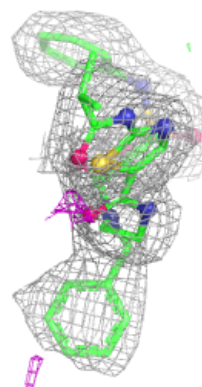
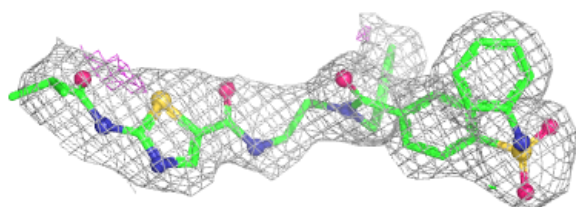
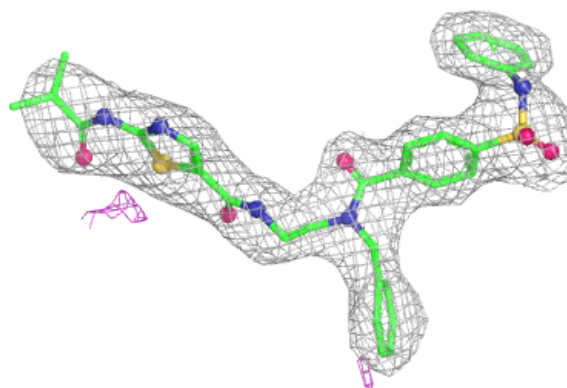
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around T3B B 701:

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

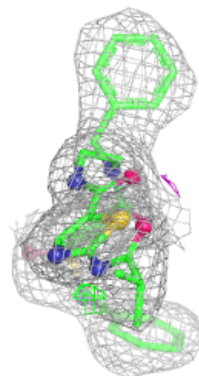
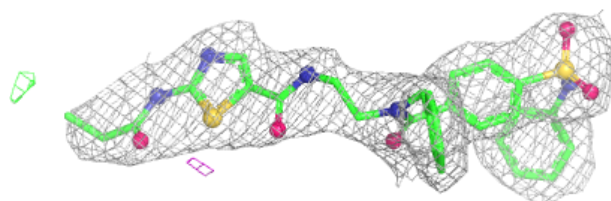
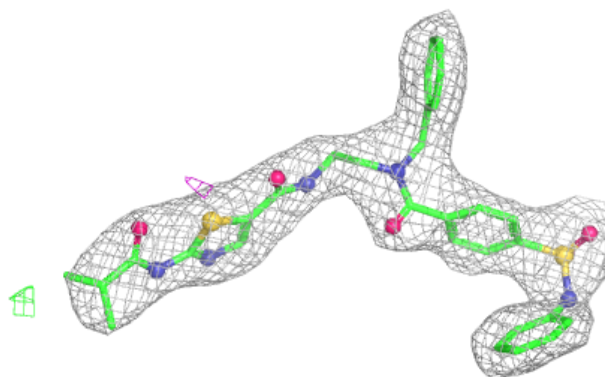
**Electron density around T3B C 701:**

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

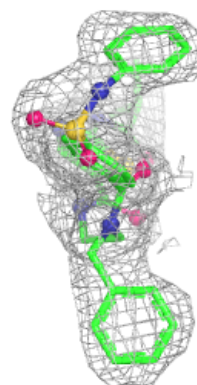
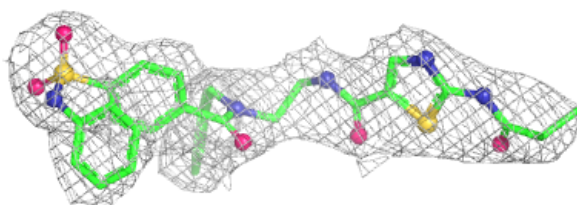
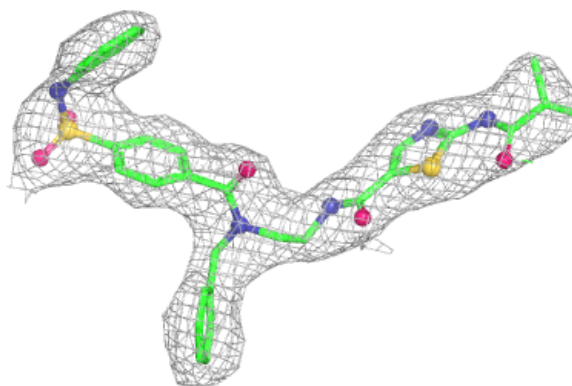


Electron density around T3B D 701:

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

**Electron density around T3B A 701:**

$2mF_o-DF_c$ (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.