

Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2022 – 06:22 pm GMT

PDB ID : 7B8W

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.26

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

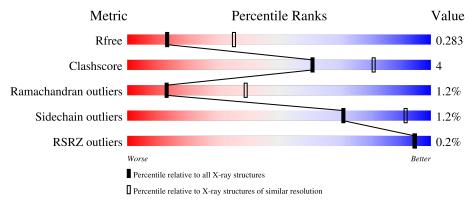
Validation Pipeline (wwPDB-VP) : 2.26

1 Overall quality at a glance (i)

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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	79%	11%	10%
1	В	310	75%	13%	11%
1	С	310	79%	10%	• 11%
1	D	310	81%	7%	12%



2 Entry composition (i)

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.

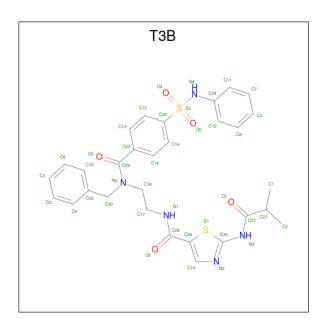
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	279	Total	С	N	О	S	0	0	0
1	A	219	2143	1378	367	379	19	0	0	U
1	В	975	Total	С	N	О	S	0	0	0
1	Ъ	275	2093	1351	356	368	18	0	0	U
1	С	276	Total	С	N	О	S	0	0	0
1		270	2116	1362	369	367	18	0	0	U
1	D	273	Total	С	N	О	S	0	0	0
1	ש	213	2112	1357	368	370	17	U	0	U

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
В	328	SER	-	expression tag	UNP P53667
В	329	MET	-	expression tag	UNP P53667
С	328	SER	-	expression tag	UNP P53667
С	329	MET	-	expression tag	UNP P53667
D	328	SER	-	expression tag	UNP P53667
D	329	MET	-	expression tag	UNP P53667

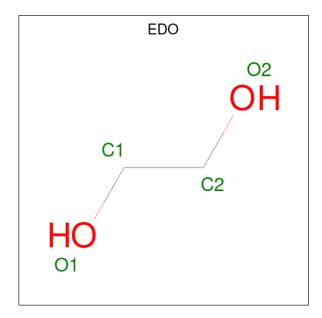
• Molecule 2 is 2-(2-methylpropanoylamino)- $\{N\}$ -[2-[(phenylmethyl)-[4-(phenylsulfamoyl)p henyl]carbonyl-amino]ethyl]-1,3-thiazole-5-carboxamide (three-letter code: T3B) (formula: $C_{30}H_{31}N_5O_5S_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	Λ	1	Total	С	N	О	S	0	0	
2	Λ	1	42	30	5	5	2	0	0	
2	B	1	Total C N O S		0	0				
2	Ъ	1	42	30	5	5	2	0	0	
2	С	1	Total	С	N	О	S	0	0	
2		1	42	30	5	5	2	0		
2	D	1	Total	С	N	О	S	0	0	
	ע	1	42	30	5	5	2			

 \bullet Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$





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.

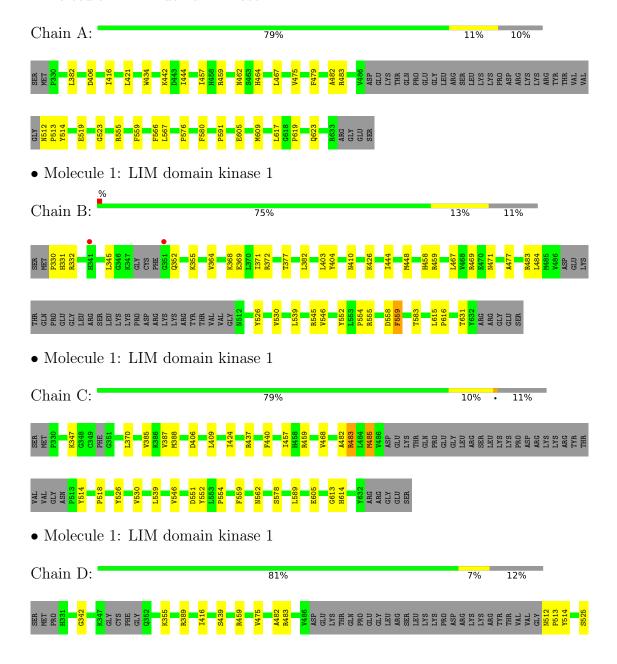
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	В	1	Total O 1 1	0	0
4	С	1	Total O 1 1	0	0
4	D	3	Total O 3 3	0	0



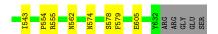
3 Residue-property plots (i)

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: LIM domain kinase 1









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	84.69Å 83.67Å 96.51Å	Donositon
a, b, c, α , β , γ	90.00° 91.97° 90.00°	Depositor
Resolution (Å)	50.15 - 2.80	Depositor
rtesolution (A)	50.10 - 2.80	EDS
% Data completeness	99.9 (50.15-2.80)	Depositor
(in resolution range)	99.9 (50.10-2.80)	EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.78 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.206 , 0.286	Depositor
it, itfree	0.210 , 0.283	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 $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.31$	Xtriage
	0.097 for k,h,-l	
Estimated twinning fraction	0.088 for -k,-h,-l	Xtriage
	0.085 for h,-k,-l	
F_o, F_c correlation	0.93	EDS
Total number of atoms	8652	wwPDB-VP
Average B, all atoms (\mathring{A}^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.

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



¹Intensities estimated from amplitudes.

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).

Mal	Mol Chain		lengths	Bond angles		
Wioi Chai	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.66	0/2200	0.80	0/2994	
1	В	0.67	0/2147	0.78	0/2923	
1	С	0.66	0/2171	0.78	0/2952	
1	D	0.65	0/2165	0.79	0/2944	
All	All	0.66	0/8683	0.79	0/11813	

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 (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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2143	0	2022	19	0
1	В	2093	0	1972	24	0
1	С	2116	0	2010	17	0
1	D	2112	0	2011	13	0
2	A	42	0	0	1	0
2	В	42	0	0	2	0
2	С	42	0	0	0	0
2	D	42	0	0	1	0
3	A	12	0	18	0	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	0	0	0
4	В	1	0	0	1	0
4	С	1	0	0	0	0
4	D	3	0	0	0	0
All	All	8652	0	8033	75	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 4.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + a 1	A4 a 2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	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: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:C:605:GLU:HA	1:C:605:GLU:OE1	2.07	0.54
1:B:558:ASP:O	1:B:559:PHE:HB2	2.09	0.54
1:C:370:LEU:HD13	1:C:409:LEU:HG	1.89	0.54
1:D:483:ARG:O	1:D:483:ARG:HD2	2.09	0.52
1:B:330:PRO:O	1:B:332:ARG:N	2.43	0.52
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:459:ARG:NH1	1:C:482:ALA:O	2.41	0.51
1:A:459:ARG:HD3	1:A:482:ALA:O	2.12	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



 $Continued\ from\ previous\ page...$

Continuea from prev		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	overlap (Å)
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: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:368:LYS:HG2	2:B:701:T3B:C5	2.46	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:387:VAL:HB	1:C:485:MET:HE1	1.99	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: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
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:C:385:VAL:HG22	1:C:388:MET:HE3	2.02	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: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: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



Continued from previous page...

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\mbox{\normalfont\AA}) \end{aligned}$
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: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
1:B:426:LYS:NZ	4:B:801:HOH:O	2.49	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	Perce	entiles
1	A	275/310 (89%)	257 (94%)	16 (6%)	2 (1%)	22	53
1	В	269/310 (87%)	244 (91%)	20 (7%)	5 (2%)	8	26
1	C	270/310 (87%)	245 (91%)	21 (8%)	4 (2%)	10	33
1	D	267/310~(86%)	242 (91%)	23 (9%)	2 (1%)	22	53
All	All	1081/1240 (87%)	988 (91%)	80 (7%)	13 (1%)	13	39

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	331	HIS
1	В	372	ARG
1	С	559	PHE
1	В	371	ILE
1	В	631	THR
1	С	578	SER
1	D	578	SER
1	A	406	ASP
1	С	347	LYS
1	С	406	ASP



Continued from previous page...

Mol	Chain	Res	Type
1	D	574	ASN
1	A	523	GLY
1	В	559	PHE

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	219/279~(78%)	218 (100%)	1 (0%)	88	96	
1	В	211/279 (76%)	208 (99%)	3 (1%)	67	90	
1	С	$214/279 \ (77\%)$	210 (98%)	4 (2%)	57	85	
1	D	216/279 (77%)	214 (99%)	2 (1%)	78	94	
All	All	860/1116 (77%)	850 (99%)	10 (1%)	71	92	

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	617	LEU
1	В	377	THR
1	В	545	ARG
1	В	555	ARG
1	С	483	ARG
1	С	485	MET
1	С	514	TYR
1	С	539	LEU
1	D	439	SER
1	D	525	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

\mathbf{Mol}	Chain	Res	Type
1	A	602	HIS
1	D	464	HIS



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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	ol Type Chain Res		Link	Bond lengths			Bond angles				
WIOI	Type	Chain	nes	res	ites Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	702	-	3,3,3	0.10	0	2,2,2	0.20	0	
2	ТЗВ	A	701	-	41,45,45	0.40	0	54,62,62	0.92	2 (3%)	
2	T3B	D	701	-	41,45,45	0.37	0	54,62,62	1.05	4 (7%)	
3	EDO	A	703	-	3,3,3	0.11	0	2,2,2	0.23	0	
2	T3B	В	701	-	41,45,45	0.41	0	54,62,62	0.90	3 (5%)	
3	EDO	A	704	-	3,3,3	0.12	0	2,2,2	0.26	0	
2	ТЗВ	С	701	-	41,45,45	0.37	0	54,62,62	0.90	4 (7%)	

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	702	-	-	1/1/1/1	-
2	ТЗВ	A	701	-	-	6/35/41/41	0/4/4/4



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ТЗВ	D	701	-	-	7/35/41/41	0/4/4/4
3	EDO	A	703	-	-	1/1/1/1	-
2	ТЗВ	В	701	-	-	6/35/41/41	0/4/4/4
3	EDO	A	704	-	-	1/1/1/1	-
2	ТЗВ	С	701	-	-	6/35/41/41	0/4/4/4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	701	ТЗВ	C26-C19-N2	3.46	116.03	109.09
2	С	701	ТЗВ	C26-C19-N2	3.42	115.96	109.09
2	D	701	ТЗВ	C26-C19-N2	3.31	115.74	109.09
2	D	701	T3B	C26-C28-N1	3.28	120.17	115.59
2	A	701	ТЗВ	C30-N3-C27	-3.25	121.79	129.02
2	В	701	ТЗВ	C26-C19-N2	3.23	115.57	109.09
2	В	701	ТЗВ	C30-N3-C27	-2.85	122.68	129.02
2	D	701	ТЗВ	C30-N3-C27	-2.77	122.86	129.02
2	С	701	ТЗВ	C30-N3-C27	-2.49	123.48	129.02
2	С	701	ТЗВ	C26-C28-N1	2.47	119.05	115.59
2	В	701	T3B	C26-C28-N1	2.28	118.78	115.59
2	D	701	ТЗВ	C22-C20-N5	2.17	116.63	113.13
2	С	701	ТЗВ	C25-S2-N4	-2.16	104.12	106.83

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	ТЗВ	C24-N4-S2-O4
2	В	701	ТЗВ	N1-C17-C18-N5
2	С	701	ТЗВ	N1-C17-C18-N5
2	D	701	ТЗВ	N1-C17-C18-N5
2	A	701	ТЗВ	C24-N4-S2-O5
2	В	701	ТЗВ	C24-N4-S2-O5
2	D	701	ТЗВ	C24-N4-S2-O5
2	A	701	ТЗВ	N1-C17-C18-N5
2	В	701	ТЗВ	C24-N4-S2-C25
2	D	701	ТЗВ	C24-N4-S2-C25
2	С	701	ТЗВ	C1-C21-C27-O1



Continued from previous page...

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

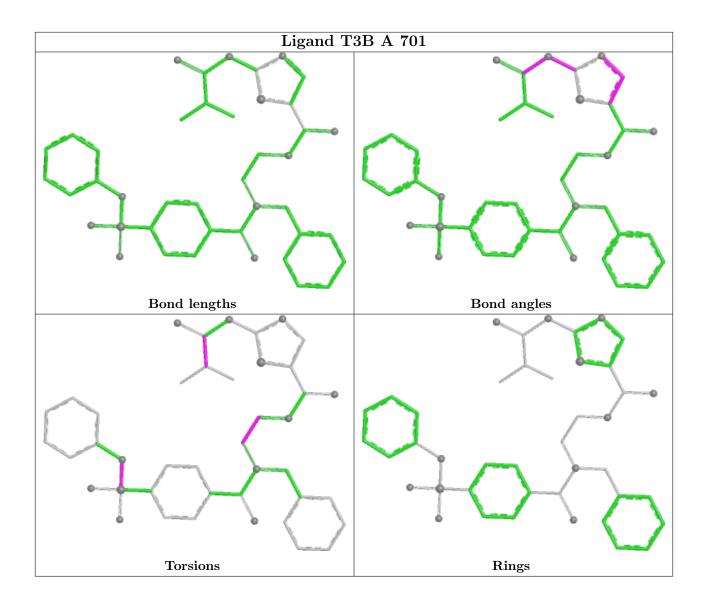
There are no ring outliers.

3 monomers are involved in 4 short contacts:

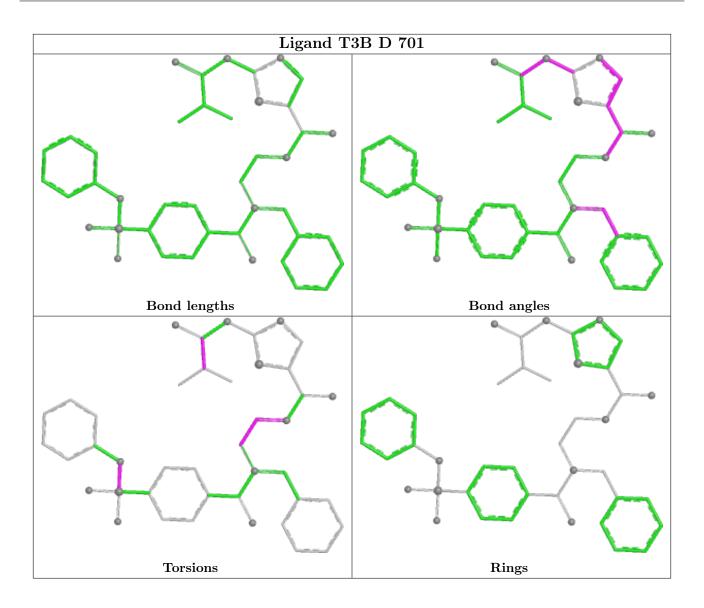
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	ТЗВ	1	0
2	D	701	ТЗВ	1	0
2	В	701	ТЗВ	2	0

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 then 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.

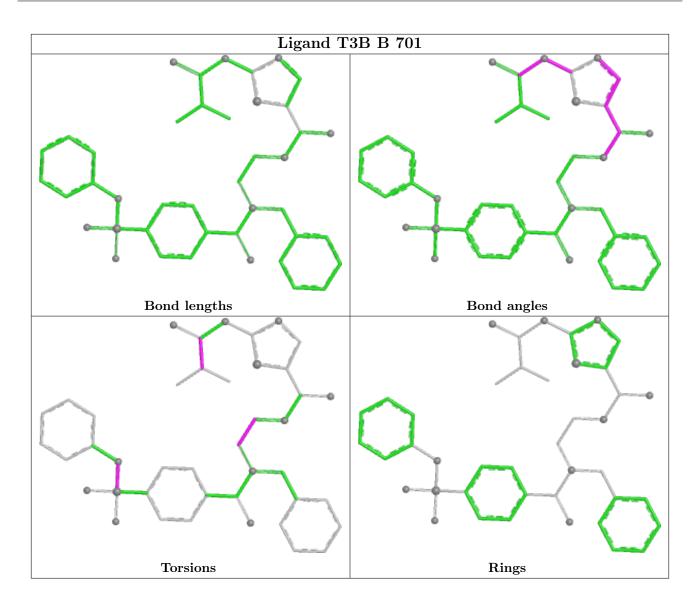




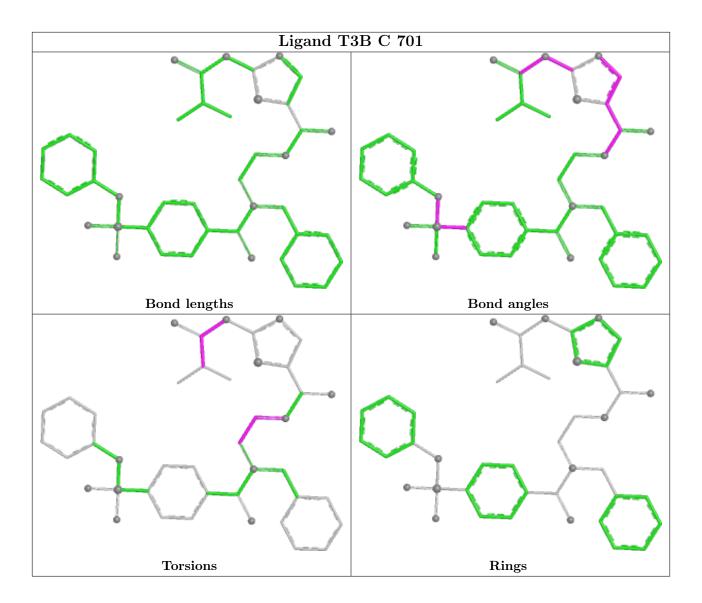












5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	279/310~(90%)	-0.48	0 100 100	28, 48, 78, 101	0
1	В	275/310 (88%)	-0.41	2 (0%) 87 84	31, 49, 77, 96	0
1	С	276/310 (89%)	-0.46	0 100 100	29, 49, 81, 117	0
1	D	273/310 (88%)	-0.46	0 100 100	29, 45, 77, 98	0
All	All	1103/1240 (88%)	-0.45	2 (0%) 95 94	28, 48, 79, 117	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	341	HIS	3.1
1	В	351	GLY	2.3

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 monosaccharides in this entry.

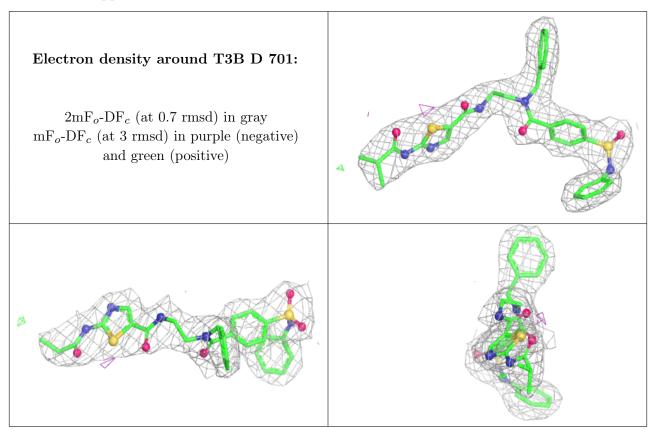
6.4 Ligands (i)

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^{th} 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.

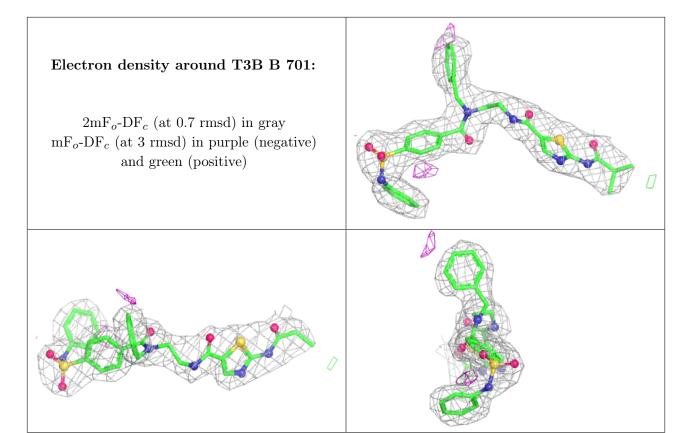


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	EDO	A	703	4/4	0.82	0.15	61,63,65,68	0
3	EDO	A	702	4/4	0.92	0.14	65,67,68,68	0
3	EDO	A	704	4/4	0.95	0.12	44,47,50,50	0
2	ТЗВ	D	701	42/42	0.97	0.15	32,41,51,54	0
2	ТЗВ	В	701	42/42	0.98	0.18	34,39,53,57	0
2	ТЗВ	С	701	42/42	0.98	0.18	31,38,49,60	0
2	ТЗВ	A	701	42/42	0.98	0.15	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.

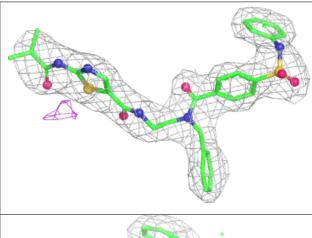


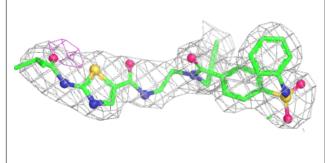


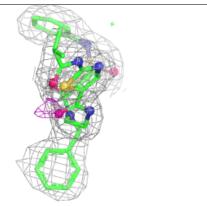


Electron density around T3B C 701:

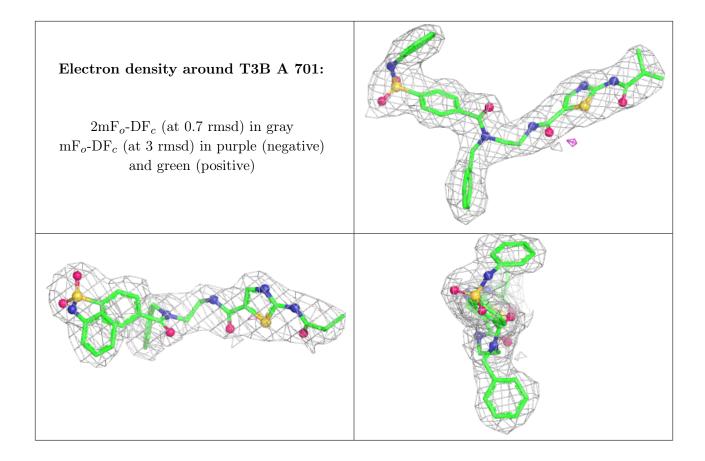
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

