



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:50 AM UTC

PDB ID : 8S3X / pdb_00008s3x
Title : LIM Domain Kinase 2 (LIMK2) bound to compound 52
Authors : Mathea, S.; Chatterjee, D.; Preuss, F.; Ple, K.; Knapp, S.
Deposited on : 2024-02-20
Resolution : 2.59 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

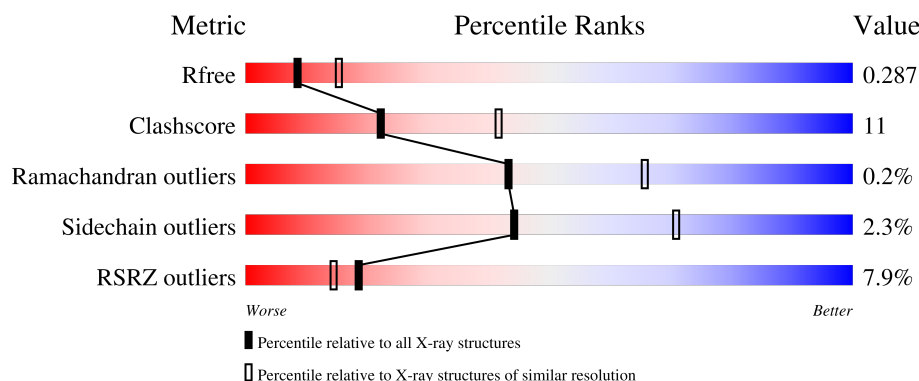
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	305	5% 69% 19% 12%
1	B	305	9% 72% 18% 10%
1	C	305	6% 66% 23% 10%
1	D	305	9% 65% 21% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8159 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.

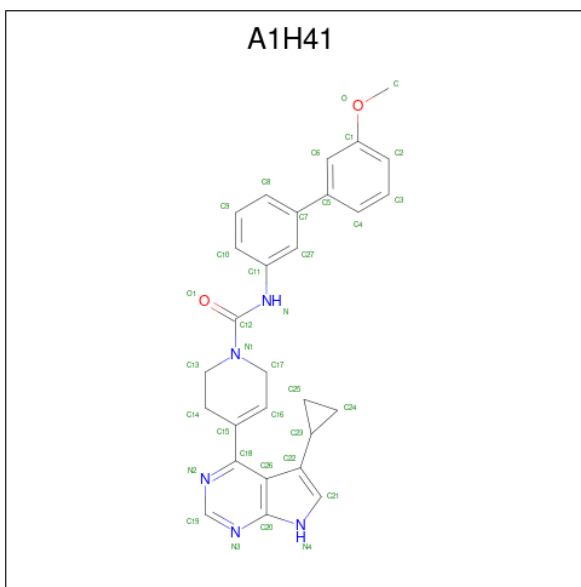
- Molecule 1 is a protein called LIM domain kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2007	1313	319	361	14			
1	B	275	Total	C	N	O	S	0	0	0
			2061	1346	331	369	15			
1	C	273	Total	C	N	O	S	0	0	0
			2054	1345	327	368	14			
1	D	263	Total	C	N	O	S	0	0	0
			1884	1227	308	336	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	SER	-	expression tag	UNP P53671
A	329	MET	-	expression tag	UNP P53671
B	328	SER	-	expression tag	UNP P53671
B	329	MET	-	expression tag	UNP P53671
C	328	SER	-	expression tag	UNP P53671
C	329	MET	-	expression tag	UNP P53671
D	328	SER	-	expression tag	UNP P53671
D	329	MET	-	expression tag	UNP P53671

- Molecule 2 is 4-(5-cyclopropyl-7 {H}-pyrrolo[2,3-d]pyrimidin-4-yl)- {N}-[3-(3-methoxy phenyl)phenyl]-3,6-dihydro-2 {H}-pyridine-1-carboxamide (CCD ID: A1H41) (formula: C₂₈H₂₇N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	28	5	2		
2	B	1	Total	C	N	O	0	0
			35	28	5	2		
2	C	1	Total	C	N	O	0	0
			35	28	5	2		
2	D	1	Total	C	N	O	0	0
			35	28	5	2		

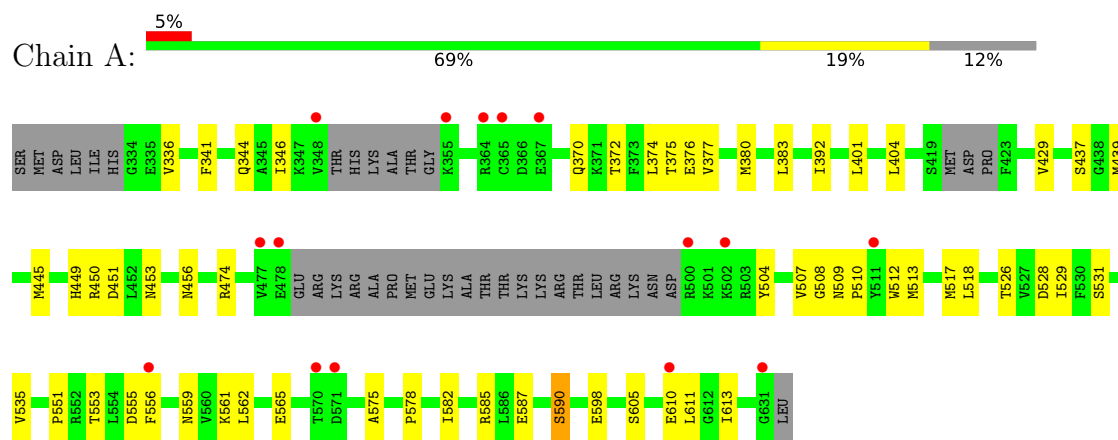
- Molecule 3 is water.

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

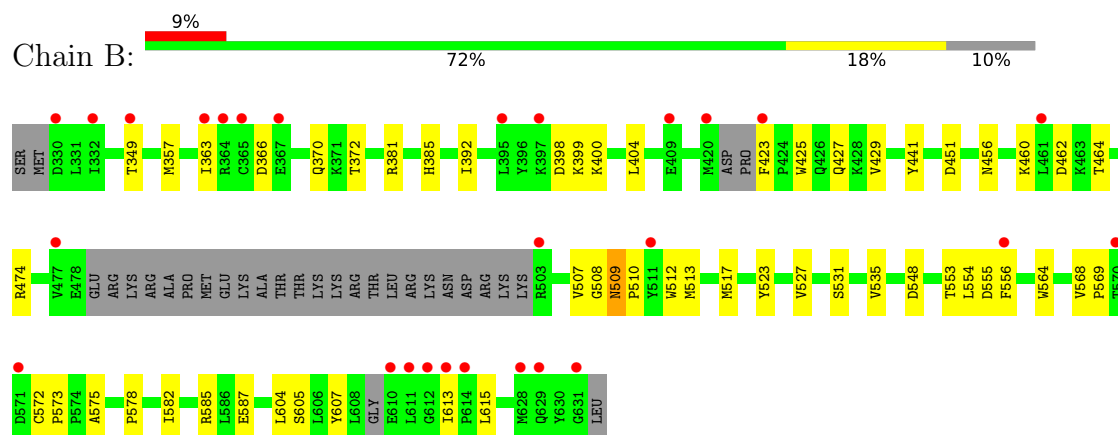
3 Residue-property plots [i](#)

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.

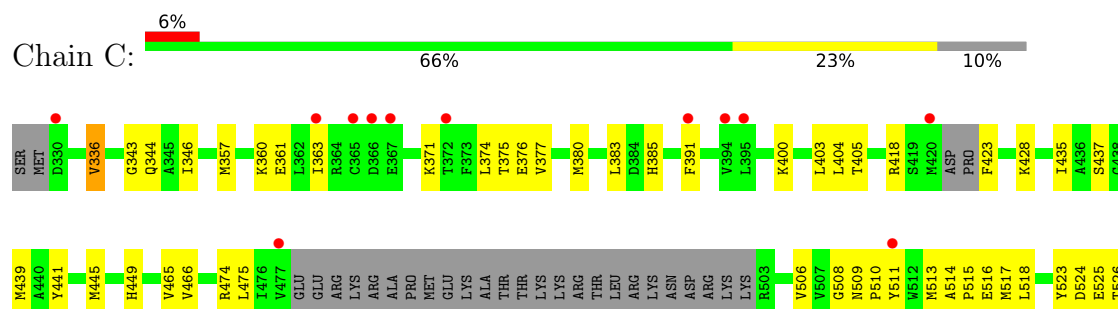
• Molecule 1: LIM domain kinase 2

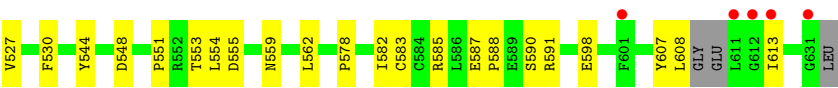


• Molecule 1: LIM domain kinase 2

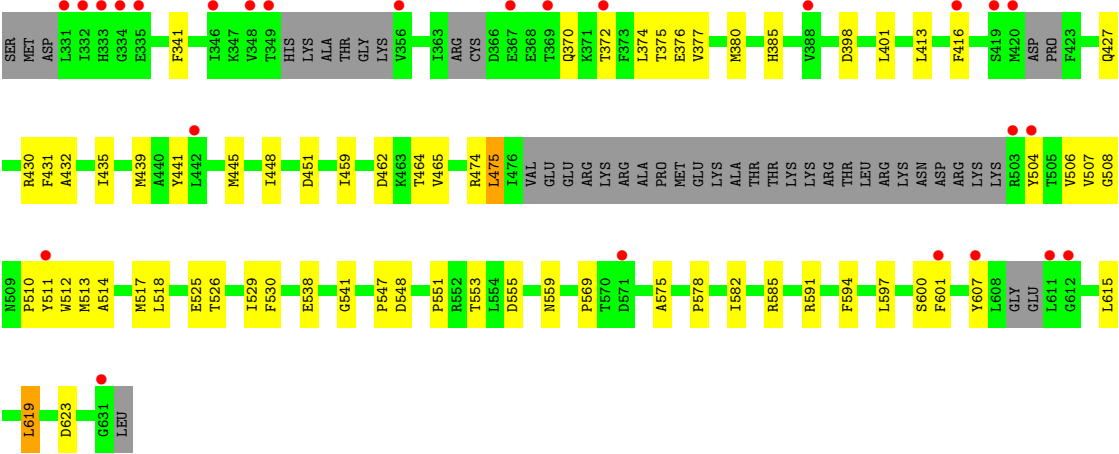


• Molecule 1: LIM domain kinase 2





● Molecule 1: LIM domain kinase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.91Å 86.92Å 103.30Å 90.00° 94.38° 90.00°	Depositor
Resolution (Å)	45.83 – 2.59 45.83 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.83-2.59) 99.5 (45.83-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.239 , 0.287 0.238 , 0.287	Depositor DCC
R_{free} test set	2381 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8159	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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 41.57 % 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 2.3141e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1H41

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	0.26	0/2054	0.46	0/2800
1	B	0.26	0/2110	0.45	0/2874
1	C	0.28	0/2103	0.46	0/2866
1	D	0.24	0/1930	0.43	0/2638
All	All	0.26	0/8197	0.45	0/11178

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)	H(added)	Clashes	Symm-Clashes
1	A	2007	0	1890	37	0
1	B	2061	0	1938	33	0
1	C	2054	0	1943	51	0
1	D	1884	0	1640	49	0
2	A	35	0	0	0	0
2	B	35	0	0	0	0
2	C	35	0	0	0	0
2	D	35	0	0	0	0
3	A	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	3	0	0	1	0
3	D	3	0	0	1	0
All	All	8159	0	7411	165	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 11.

All (165) 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:D:435:ILE:HG13	1:D:465:VAL:HG11	1.54	0.88
1:D:370:GLN:HG2	1:D:401:LEU:HD12	1.56	0.87
1:B:553:THR:OG1	1:B:555:ASP:OD1	2.02	0.77
1:B:363:ILE:HG22	1:B:400:LYS:HD2	1.67	0.75
1:D:441:TYR:HE1	1:D:445:MET:HE2	1.52	0.72
1:B:357:MET:HE2	1:B:404:LEU:HD12	1.71	0.71
1:A:553:THR:OG1	1:A:555:ASP:OD1	2.08	0.71
1:D:607:TYR:HD1	1:D:615:LEU:HD11	1.56	0.71
1:D:385:HIS:HB2	1:D:441:TYR:CE2	2.24	0.71
1:D:607:TYR:HD1	1:D:615:LEU:CD1	2.06	0.69
1:C:511:TYR:CZ	1:C:548:ASP:HB3	2.28	0.68
1:D:513:MET:HE2	1:D:518:LEU:HD21	1.76	0.68
1:C:508:GLY:O	1:C:510:PRO:HD3	1.95	0.67
1:D:582:ILE:O	1:D:585:ARG:HG3	1.95	0.67
1:C:361:GLU:OE2	1:C:400:LYS:NZ	2.25	0.67
1:D:432:ALA:HB1	1:D:601:PHE:CE2	2.30	0.66
1:D:513:MET:HB3	1:D:517:MET:HE3	1.75	0.66
1:D:508:GLY:O	1:D:510:PRO:HD3	1.96	0.65
1:D:432:ALA:HB1	1:D:601:PHE:HE2	1.59	0.65
1:C:513:MET:HB3	1:C:517:MET:HE3	1.78	0.64
1:D:441:TYR:CE1	1:D:445:MET:HE2	2.33	0.64
1:B:509:ASN:HB3	1:B:512:TRP:HZ3	1.64	0.63
1:C:376:GLU:O	1:C:380:MET:HG3	1.99	0.62
1:D:615:LEU:HD23	1:D:619:LEU:HB3	1.82	0.61
1:B:587:GLU:H	1:B:587:GLU:CD	2.08	0.61
1:B:509:ASN:HB3	1:B:512:TRP:CZ3	2.35	0.61
1:C:511:TYR:CE1	1:C:548:ASP:HB3	2.36	0.60
1:D:385:HIS:HB2	1:D:441:TYR:CD2	2.36	0.59
1:D:511:TYR:CE2	1:D:548:ASP:HB3	2.38	0.59
1:A:504:TYR:HB2	1:C:554:LEU:HG	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:HIS:HB2	1:D:441:TYR:HE2	1.68	0.58
1:A:449:HIS:O	1:A:450:ARG:HB2	2.01	0.58
1:C:374:LEU:O	1:C:377:VAL:HG12	2.03	0.58
1:D:475:LEU:HD12	1:D:506:VAL:HG22	1.85	0.58
1:B:474:ARG:HB2	1:B:513:MET:HE1	1.85	0.58
1:C:336:VAL:HA	1:C:346:ILE:HD13	1.85	0.58
1:C:391:PHE:HD2	1:C:405:THR:HG22	1.68	0.57
1:C:475:LEU:HD12	1:C:506:VAL:HG22	1.86	0.57
1:C:385:HIS:HB2	1:C:441:TYR:CD2	2.39	0.57
1:D:374:LEU:HA	1:D:377:VAL:HG23	1.85	0.57
1:C:357:MET:HE2	1:C:404:LEU:HG	1.86	0.56
1:C:582:ILE:O	1:C:585:ARG:HG3	2.06	0.56
1:C:551:PRO:HB3	1:C:562:LEU:HD13	1.87	0.56
1:B:607:TYR:CD2	1:B:615:LEU:HD13	2.41	0.56
1:C:435:ILE:HG13	1:C:465:VAL:HG11	1.89	0.55
1:A:392:ILE:HB	1:A:404:LEU:HB3	1.89	0.55
1:D:526:THR:HA	1:D:529:ILE:HD12	1.88	0.55
1:C:553:THR:OG1	1:C:555:ASP:OD1	2.16	0.54
1:D:511:TYR:CZ	1:D:548:ASP:HB3	2.43	0.54
1:B:423:PHE:CE1	1:B:427:GLN:HB3	2.43	0.53
1:C:587:GLU:HB2	1:C:590:SER:OG	2.08	0.53
1:B:508:GLY:O	1:B:510:PRO:HD3	2.09	0.53
1:C:377:VAL:HG23	1:C:391:PHE:HE1	1.74	0.53
1:B:582:ILE:HB	1:B:585:ARG:HE	1.74	0.53
1:C:524:ASP:OD1	1:C:526:THR:OG1	2.22	0.53
1:D:439:MET:HG2	1:D:594:PHE:CZ	2.42	0.53
1:D:451:ASP:OD1	1:D:474:ARG:HG3	2.10	0.52
1:B:460:LYS:HD3	1:B:464:THR:HB	1.92	0.52
1:D:600:SER:HB3	1:D:619:LEU:HD11	1.92	0.51
1:A:374:LEU:HA	1:A:377:VAL:HG23	1.92	0.51
1:A:383:LEU:HD23	1:A:445:MET:HG3	1.92	0.51
1:B:513:MET:HB3	1:B:517:MET:HE3	1.93	0.50
1:D:427:GLN:HA	1:D:430:ARG:HB2	1.92	0.50
1:B:381:ARG:HD2	1:B:392:ILE:O	2.11	0.50
1:C:588:PRO:O	1:C:591:ARG:HG3	2.11	0.50
1:A:611:LEU:HB2	1:A:613:ILE:HD12	1.93	0.50
1:C:514:ALA:HA	1:C:530:PHE:CD2	2.46	0.50
1:A:474:ARG:HB2	1:A:513:MET:HE1	1.94	0.49
1:A:474:ARG:NH1	1:A:508:GLY:HA3	2.28	0.49
1:D:607:TYR:CD1	1:D:615:LEU:HD11	2.42	0.49
1:D:553:THR:OG1	1:D:555:ASP:OD1	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:SER:O	1:B:535:VAL:HG23	2.13	0.48
1:C:513:MET:HE2	1:C:518:LEU:HD21	1.95	0.48
1:C:380:MET:HE2	1:C:391:PHE:CE1	2.49	0.48
1:C:582:ILE:HB	1:C:585:ARG:HE	1.78	0.48
1:A:582:ILE:O	1:A:585:ARG:HG3	2.13	0.48
1:D:511:TYR:HB2	1:D:547:PRO:HG2	1.95	0.48
1:D:551:PRO:HB2	1:D:559:ASN:HB3	1.96	0.48
1:A:341:PHE:CG	1:A:507:VAL:HG11	2.49	0.47
1:B:510:PRO:HD2	3:D:803:HOH:O	2.14	0.47
1:D:529:ILE:HG21	1:D:591:ARG:HB3	1.97	0.47
1:A:508:GLY:O	1:A:510:PRO:HD3	2.15	0.47
1:C:510:PRO:HA	1:C:513:MET:HG3	1.96	0.46
1:C:445:MET:HA	1:C:445:MET:HE2	1.96	0.46
1:C:474:ARG:HD3	1:C:509:ASN:H	1.80	0.46
1:A:513:MET:HB3	1:A:517:MET:HE2	1.97	0.46
1:A:561:LYS:O	1:A:565:GLU:HG3	2.16	0.46
1:D:372:THR:O	1:D:375:THR:OG1	2.29	0.46
1:A:518:LEU:O	1:C:554:LEU:HD13	2.16	0.46
1:C:515:PRO:HD3	1:C:530:PHE:CE2	2.51	0.46
1:B:554:LEU:HD22	1:D:504:TYR:HB2	1.98	0.45
1:D:575:ALA:C	1:D:578:PRO:HD2	2.40	0.45
1:B:564:TRP:HA	1:B:568:VAL:HG23	1.98	0.45
1:B:555:ASP:O	1:B:556:PHE:HB2	2.17	0.45
1:A:439:MET:HE2	1:A:528:ASP:HB3	1.98	0.45
1:B:451:ASP:OD1	1:B:474:ARG:HG3	2.16	0.45
1:A:526:THR:HA	1:A:529:ILE:HD12	1.97	0.44
1:B:474:ARG:NH1	1:B:508:GLY:HA3	2.32	0.44
1:A:344:GLN:HG3	1:A:346:ILE:HD11	2.00	0.44
1:C:517:MET:HE2	3:C:802:HOH:O	2.16	0.44
1:B:398:ASP:C	1:B:399:LYS:HG3	2.42	0.44
1:B:575:ALA:C	1:B:578:PRO:HD2	2.42	0.44
1:D:341:PHE:CG	1:D:507:VAL:HG11	2.53	0.44
1:D:462:ASP:CG	1:D:464:THR:HG1	2.25	0.44
1:A:437:SER:HB3	1:A:598:GLU:OE2	2.18	0.44
1:C:516:GLU:OE2	1:C:527:VAL:HG12	2.18	0.44
1:C:344:GLN:NE2	1:C:361:GLU:OE1	2.51	0.44
1:B:451:ASP:O	1:B:456:ASN:ND2	2.40	0.44
1:C:607:TYR:HA	1:C:613:ILE:O	2.18	0.44
1:D:601:PHE:CD1	1:D:601:PHE:N	2.86	0.44
1:B:507:VAL:HG22	1:D:551:PRO:HA	2.00	0.43
1:A:453:ASN:HB2	1:A:512:TRP:CE2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:TYR:HB2	1:B:527:VAL:CG1	2.48	0.43
1:A:562:LEU:HD12	1:A:562:LEU:HA	1.78	0.43
1:C:513:MET:HE2	1:C:518:LEU:CD2	2.49	0.43
1:D:575:ALA:N	1:D:623:ASP:OD2	2.48	0.42
1:A:376:GLU:CB	1:A:380:MET:HE3	2.49	0.42
1:C:360:LYS:HB2	1:C:403:LEU:HB2	2.00	0.42
1:C:423:PHE:CE2	1:C:428:LYS:HG2	2.54	0.42
1:A:518:LEU:C	1:C:554:LEU:HD13	2.45	0.42
1:D:448:ILE:HG23	1:D:525:GLU:HA	2.00	0.42
1:D:512:TRP:NE1	1:D:538:GLU:OE2	2.46	0.42
1:A:370:GLN:NE2	1:A:401:LEU:HB2	2.34	0.42
1:A:451:ASP:O	1:A:456:ASN:ND2	2.40	0.42
1:B:385:HIS:HB2	1:B:441:TYR:CD2	2.54	0.42
1:A:474:ARG:HB2	1:A:513:MET:CE	2.49	0.42
1:A:575:ALA:C	1:A:578:PRO:HD2	2.44	0.42
1:D:385:HIS:CG	1:D:441:TYR:HD2	2.38	0.42
1:A:531:SER:O	1:A:535:VAL:HG23	2.19	0.42
1:A:587:GLU:HB2	1:A:590:SER:OG	2.20	0.42
1:C:343:GLY:HA2	1:C:363:ILE:HG23	2.01	0.42
1:D:374:LEU:HA	1:D:377:VAL:CG2	2.49	0.42
1:D:376:GLU:O	1:D:380:MET:HG3	2.20	0.42
1:B:564:TRP:HA	1:B:568:VAL:CG2	2.50	0.42
1:B:425:TRP:CD2	1:B:573:PRO:HD3	2.55	0.42
1:A:559:ASN:OD1	1:A:562:LEU:HB2	2.19	0.41
1:C:523:TYR:HB2	1:C:527:VAL:CG1	2.50	0.41
1:D:514:ALA:HA	1:D:530:PHE:CD1	2.55	0.41
1:A:341:PHE:CD1	1:A:507:VAL:HG11	2.55	0.41
1:B:425:TRP:CZ2	1:B:572:CYS:HA	2.54	0.41
1:C:583:CYS:O	1:C:591:ARG:HD3	2.20	0.41
1:D:541:GLY:HA2	1:D:569:PRO:HD3	2.03	0.41
1:D:601:PHE:N	1:D:601:PHE:HD1	2.17	0.41
1:C:371:LYS:O	1:C:375:THR:HG23	2.20	0.41
1:A:437:SER:HB3	1:A:598:GLU:HG3	2.01	0.41
1:A:551:PRO:HB2	1:A:559:ASN:HB3	2.02	0.41
1:C:380:MET:HE2	1:C:391:PHE:CD1	2.55	0.41
1:C:418:ARG:HD3	1:C:544:TYR:CZ	2.55	0.41
1:D:597:LEU:O	1:D:601:PHE:CD1	2.74	0.41
1:B:366:ASP:O	1:B:370:GLN:HG3	2.20	0.41
1:C:439:MET:HE1	1:C:449:HIS:HB2	2.03	0.41
1:A:372:THR:O	1:A:375:THR:OG1	2.31	0.40
1:A:610:GLU:O	1:A:611:LEU:HD23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:SER:HB3	1:C:598:GLU:HG3	2.03	0.40
1:A:555:ASP:O	1:A:556:PHE:HB2	2.20	0.40
1:B:460:LYS:HB2	1:B:462:ASP:OD1	2.21	0.40
1:C:346:ILE:HD13	1:C:346:ILE:HA	1.94	0.40
1:C:380:MET:HA	1:C:383:LEU:HG	2.03	0.40
1:C:404:LEU:HD12	1:C:404:LEU:HA	1.79	0.40
1:C:559:ASN:CG	1:C:562:LEU:HB2	2.47	0.40
1:C:578:PRO:O	1:C:582:ILE:HG23	2.21	0.40
1:D:416:PHE:CD2	1:D:431:PHE:HE2	2.39	0.40
1:A:439:MET:HE1	1:A:449:HIS:HB2	2.04	0.40
1:B:568:VAL:HA	1:B:569:PRO:HD3	1.95	0.40
1:D:413:LEU:HD12	1:D:459:ILE:HD11	2.04	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	260/305 (85%)	241 (93%)	18 (7%)	1 (0%)	30	51
1	B	267/305 (88%)	254 (95%)	12 (4%)	1 (0%)	30	51
1	C	265/305 (87%)	250 (94%)	15 (6%)	0	100	100
1	D	251/305 (82%)	236 (94%)	15 (6%)	0	100	100
All	All	1043/1220 (86%)	981 (94%)	60 (6%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	ASN
1	B	509	ASN

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	200/270 (74%)	196 (98%)	4 (2%)	48	74
1	B	204/270 (76%)	197 (97%)	7 (3%)	32	60
1	C	205/270 (76%)	201 (98%)	4 (2%)	48	74
1	D	166/270 (62%)	163 (98%)	3 (2%)	51	76
All	All	775/1080 (72%)	757 (98%)	18 (2%)	44	71

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	VAL
1	A	429	VAL
1	A	590	SER
1	A	605	SER
1	B	349	THR
1	B	372	THR
1	B	429	VAL
1	B	548	ASP
1	B	604	LEU
1	B	605	SER
1	B	613	ILE
1	C	336	VAL
1	C	466	VAL
1	C	525	GLU
1	C	608	LEU
1	D	398	ASP
1	D	475	LEU
1	D	619	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	519	ASN
1	B	344	GLN
1	B	542	GLN
1	C	344	GLN
1	C	519	ASN
1	D	427	GLN
1	D	624	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 ⓘ

4 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	$\# Z > 2$
2	A1H41	B	701	-	39,40,40	0.18	0	48,57,57	0.52	1 (2%)
2	A1H41	C	701	-	39,40,40	0.19	0	48,57,57	0.54	1 (2%)
2	A1H41	D	701	-	39,40,40	0.20	0	48,57,57	0.54	1 (2%)
2	A1H41	A	701	-	39,40,40	0.22	0	48,57,57	0.67	2 (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
2	A1H41	B	701	-	-	0/20/34/34	0/6/6/6
2	A1H41	C	701	-	-	0/20/34/34	0/6/6/6
2	A1H41	D	701	-	-	1/20/34/34	0/6/6/6
2	A1H41	A	701	-	-	1/20/34/34	0/6/6/6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	A1H41	C15-C18-N2	-2.92	111.00	115.78
2	A	701	A1H41	C15-C18-N2	-2.87	111.09	115.78
2	C	701	A1H41	C15-C18-N2	-2.38	111.89	115.78
2	B	701	A1H41	C15-C18-N2	-2.38	111.89	115.78
2	A	701	A1H41	C14-C15-C18	2.37	121.94	118.51

There are no chirality outliers.

All (2) torsion outliers are listed below:

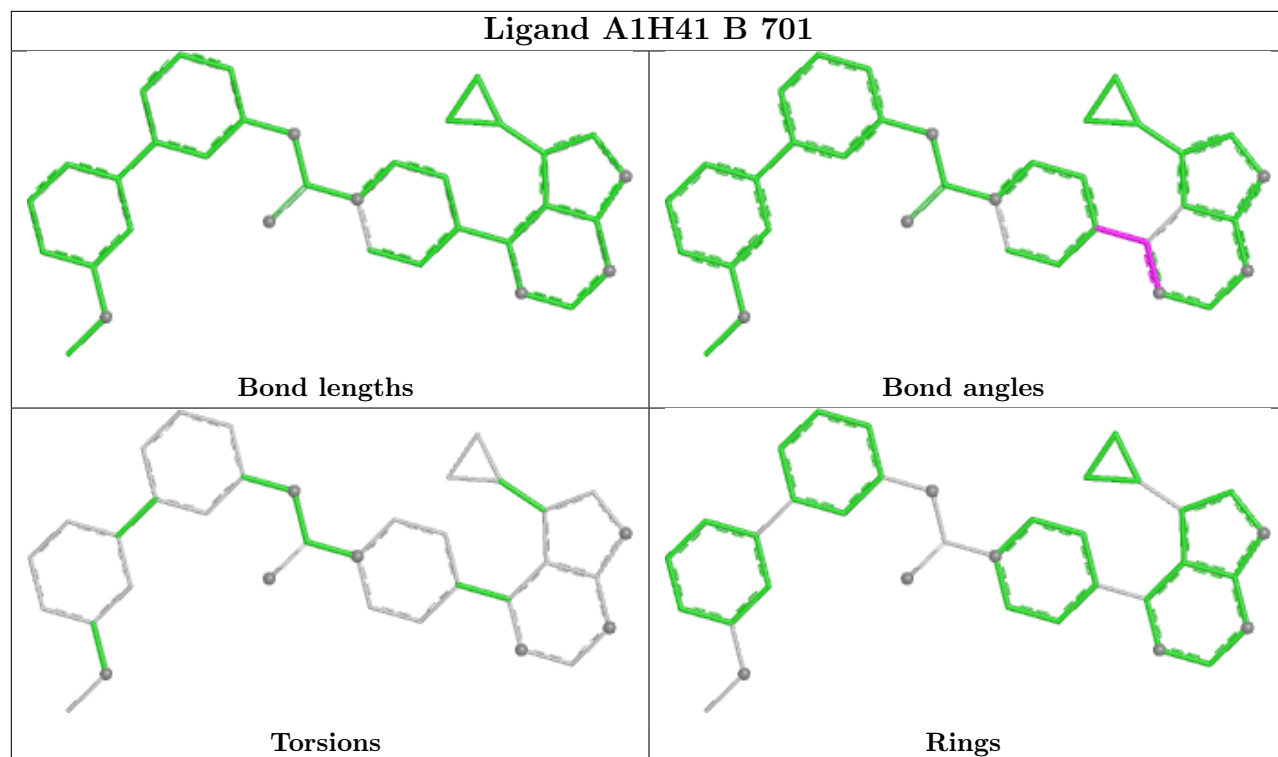
Mol	Chain	Res	Type	Atoms
2	A	701	A1H41	C21-C22-C23-C24
2	D	701	A1H41	C21-C22-C23-C25

There are no ring outliers.

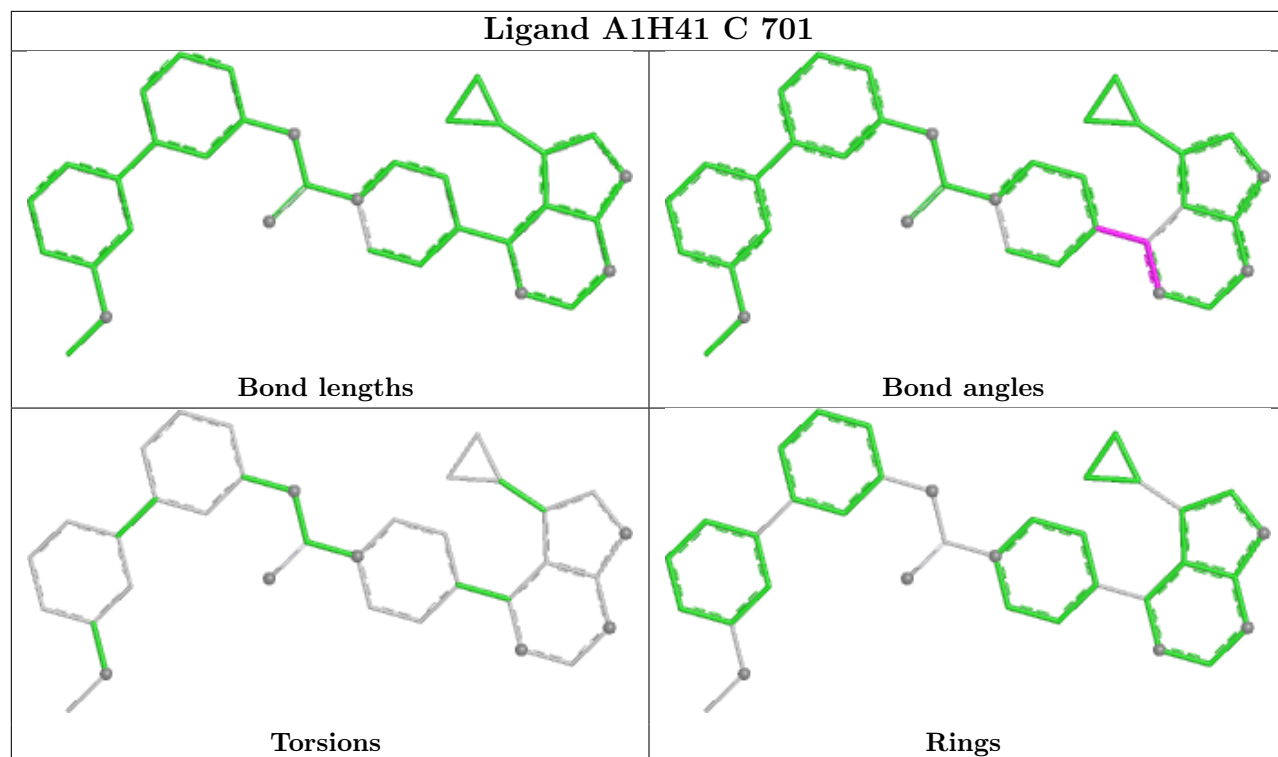
No monomer is involved in short contacts.

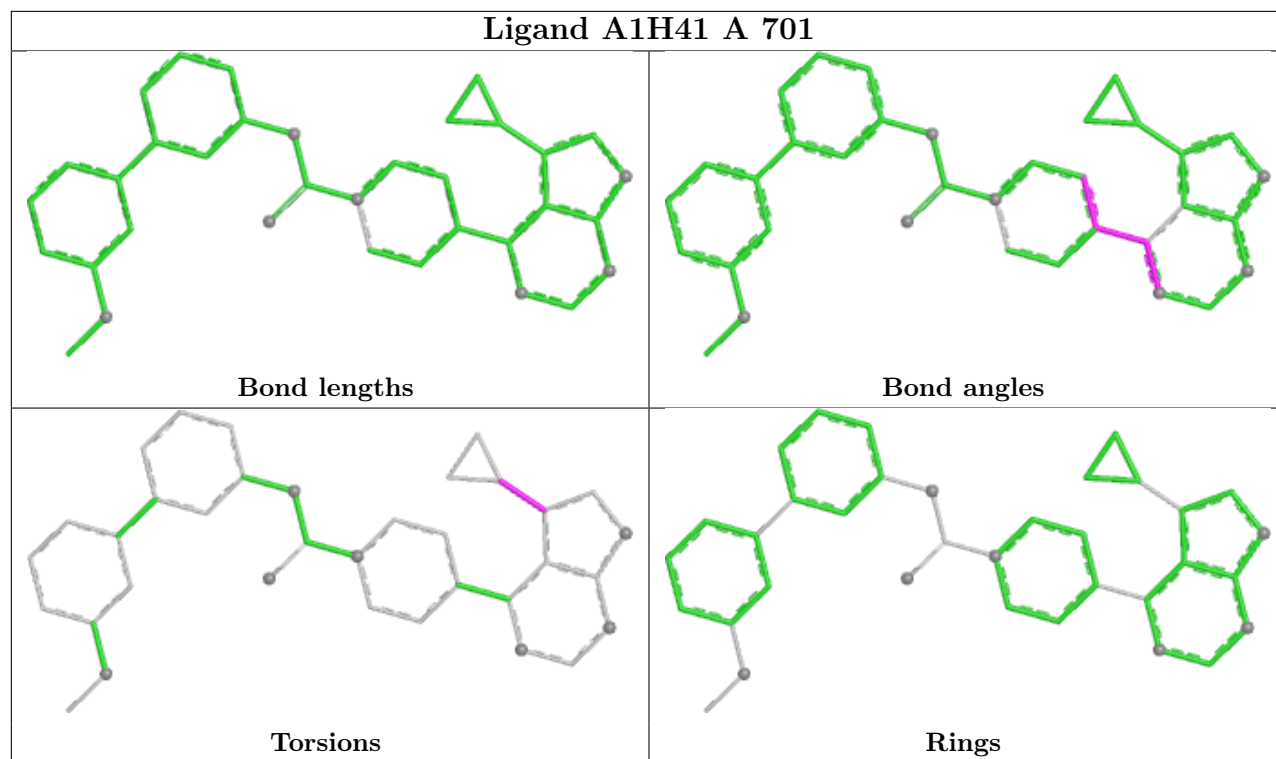
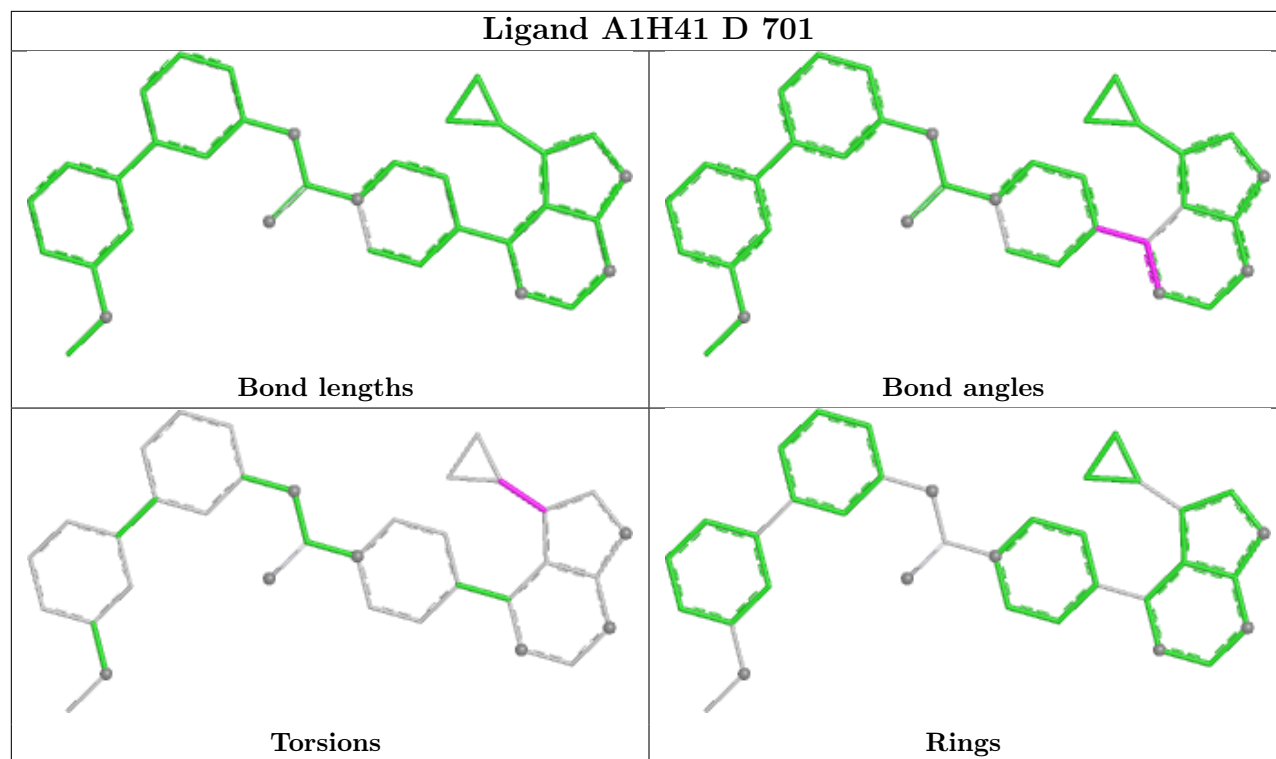
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A1H41 B 701



Ligand A1H41 C 701





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	268/305 (87%)	0.47	15 (5%)	30 24	34, 49, 71, 102	0
1	B	275/305 (90%)	0.69	27 (9%)	13 10	31, 49, 76, 93	0
1	C	273/305 (89%)	0.55	17 (6%)	26 21	39, 52, 74, 100	0
1	D	263/305 (86%)	0.84	26 (9%)	13 10	46, 64, 85, 100	0
All	All	1079/1220 (88%)	0.64	85 (7%)	18 14	31, 53, 79, 102	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	611	LEU	5.2
1	C	420	MET	4.5
1	B	363	ILE	4.0
1	D	511	TYR	4.0
1	B	330	ASP	3.9
1	C	363	ILE	3.8
1	B	365	CYS	3.8
1	A	631	GLY	3.5
1	A	610	GLU	3.5
1	C	365	CYS	3.4
1	D	332	ILE	3.4
1	D	611	LEU	3.4
1	C	612	GLY	3.4
1	B	571	ASP	3.4
1	B	631	GLY	3.3
1	D	356	VAL	3.3
1	D	420	MET	3.3
1	B	364	ARG	3.2
1	B	409	GLU	3.0
1	D	419	SER	3.0
1	B	570	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	631	GLY	2.9
1	A	355	LYS	2.9
1	B	610	GLU	2.9
1	B	477	VAL	2.9
1	B	332	ILE	2.8
1	D	331	LEU	2.8
1	B	420	MET	2.8
1	A	478	GLU	2.8
1	D	504	TYR	2.7
1	D	372	THR	2.7
1	B	367	GLU	2.7
1	D	333	HIS	2.7
1	C	391	PHE	2.7
1	D	631	GLY	2.7
1	B	611	LEU	2.7
1	A	556	PHE	2.6
1	B	461	LEU	2.6
1	D	346	ILE	2.6
1	C	511	TYR	2.6
1	B	503	ARG	2.6
1	D	335	GLU	2.6
1	D	348	VAL	2.5
1	A	500	ARG	2.5
1	A	348	VAL	2.5
1	A	477	VAL	2.5
1	A	570	THR	2.5
1	B	511	TYR	2.4
1	D	607	TYR	2.4
1	D	416	PHE	2.4
1	C	477	VAL	2.4
1	B	397	LYS	2.4
1	C	367	GLU	2.4
1	D	369	THR	2.4
1	D	612	GLY	2.4
1	B	423	PHE	2.4
1	A	511	TYR	2.3
1	C	601	PHE	2.3
1	B	612	GLY	2.3
1	C	613	ILE	2.3
1	A	367	GLU	2.3
1	C	330	ASP	2.3
1	B	349	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	364	ARG	2.2
1	B	614	PRO	2.2
1	B	629	GLN	2.2
1	D	334	GLY	2.2
1	C	395	LEU	2.2
1	D	349	THR	2.2
1	D	503	ARG	2.2
1	B	395	LEU	2.2
1	C	394	VAL	2.1
1	C	372	THR	2.1
1	A	571	ASP	2.1
1	D	571	ASP	2.1
1	D	601	PHE	2.1
1	D	388	VAL	2.1
1	A	502	LYS	2.1
1	A	365	CYS	2.1
1	D	442	LEU	2.0
1	D	367	GLU	2.0
1	B	628	MET	2.0
1	B	556	PHE	2.0
1	B	613	ILE	2.0
1	C	366	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
2	A1H41	D	701	35/35	0.90	0.14	42,50,66,66	0

Continued on next page...

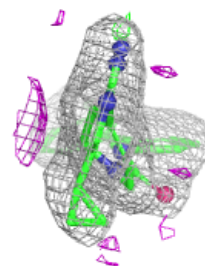
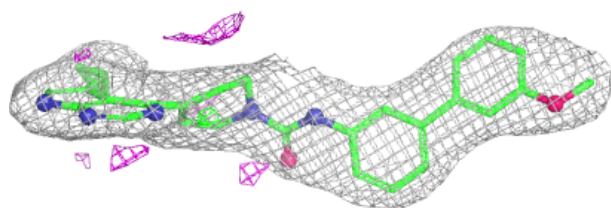
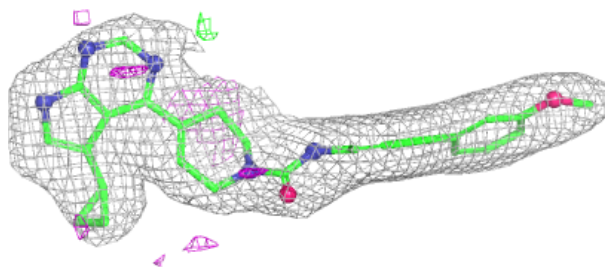
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1H41	C	701	35/35	0.91	0.12	39,43,49,50	0
2	A1H41	A	701	35/35	0.94	0.10	30,38,52,56	0
2	A1H41	B	701	35/35	0.95	0.09	31,36,47,50	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.

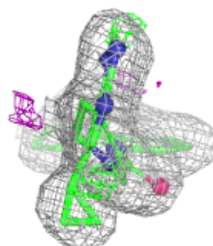
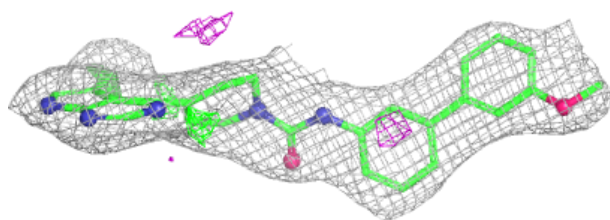
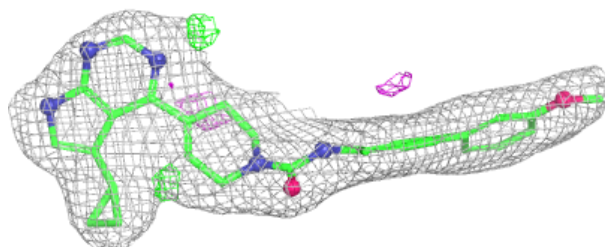
Electron density around A1H41 D 701:

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

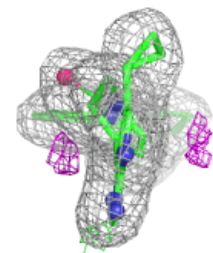
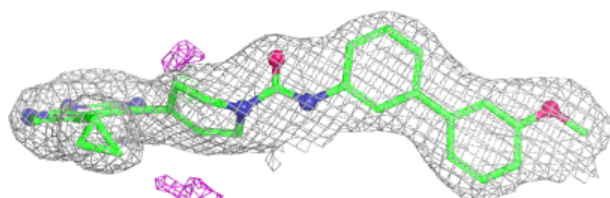
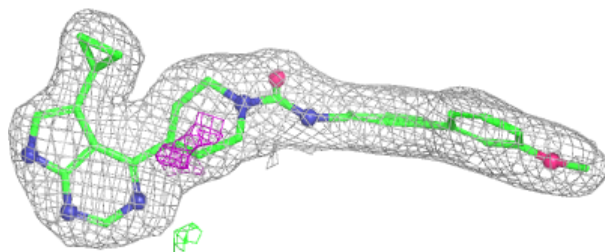


Electron density around A1H41 C 701:

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

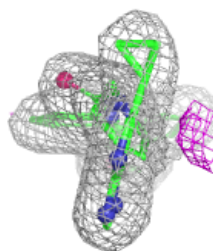
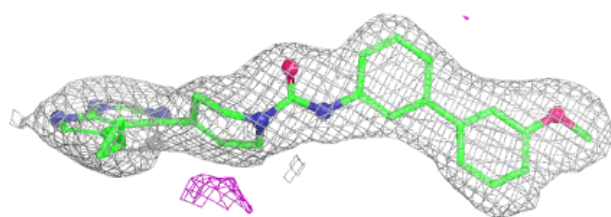
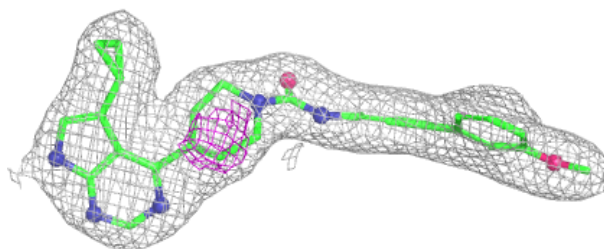
**Electron density around A1H41 A 701:**

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



Electron density around A1H41 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.