Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 12:58 AM EDT

PDB ID	:	7U36
Title	:	Crystal structure of human GSK3B in complex with ARN1484
Authors	:	Tripathi, S.K.; Balboni, B.; Giabbai, B.; Storici, P.; Girotto, S.; Cavalli, A.
Deposited on	:	2022-02-25
Resolution	:	2.75 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:

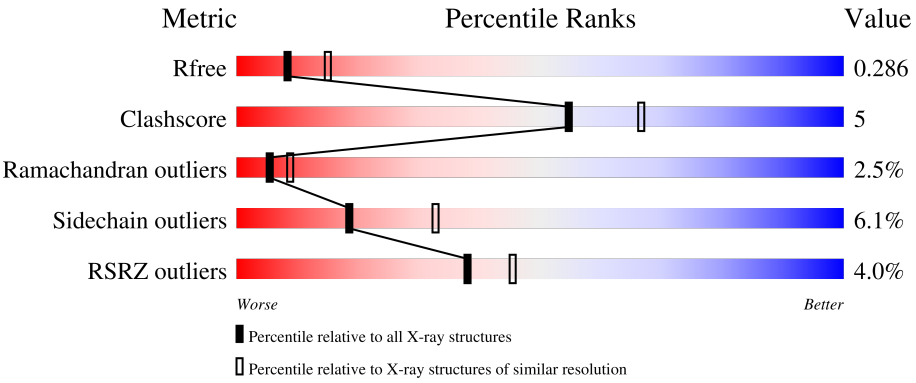
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	351	6% 86% 11%
1	B	351	2% 80% 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5654 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.

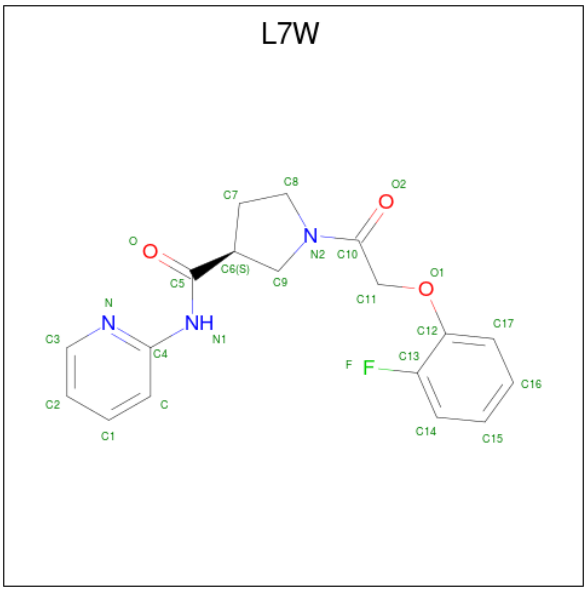
- Molecule 1 is a protein called Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2807	1806	482	508	11			
1	B	346	Total	C	N	O	S	0	0	0
			2770	1783	473	503	11			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is (3S)-1-[(2-fluorophenoxy)acetyl]-N-(pyridin-2-yl)pyrrolidine-3-carboxamide (three-letter code: L7W) (formula: $C_{18}H_{18}FN_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			25	18	1	3	3		
3	B	1	Total	C	F	N	O	0	0
			25	18	1	3	3		

- Molecule 4 is water.

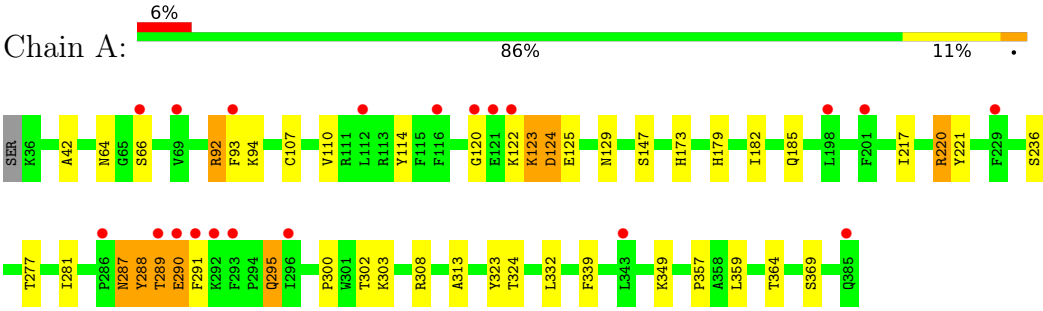
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	9	Total	O	0	0
			9	9		

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.

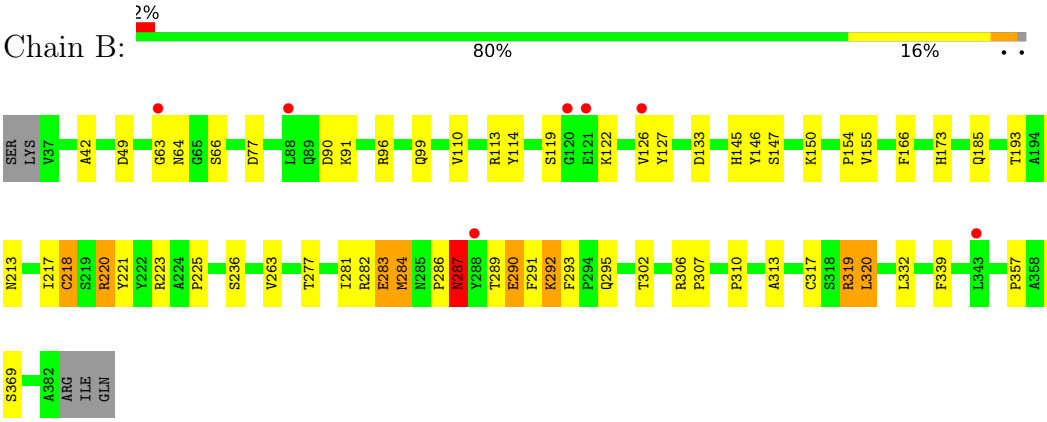
• Molecule 1: Glycogen synthase kinase-3 beta

Chain A:



• Molecule 1: Glycogen synthase kinase-3 beta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.20Å 85.31Å 178.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.08 – 2.75 76.96 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (77.08-2.75) 99.9 (76.96-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.238 , 0.275 0.251 , 0.286	Depositor DCC
R_{free} test set	1550 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å^2)	59.1	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5654	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L7W, CL

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	0.44	0/2878	0.69	0/3915
1	B	0.44	0/2841	0.69	0/3867
All	All	0.44	0/5719	0.69	0/7782

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2807	0	2836	23	0
1	B	2770	0	2791	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
4	A	16	0	0	0	0
4	B	9	0	0	0	0
All	All	5654	0	5627	59	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 (59) 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:266:LEU:O	1:A:270:ILE:HG12	1.81	0.80
1:B:306:ARG:HG3	1:B:307:PRO:HD2	1.72	0.71
1:A:120:GLY:O	1:A:123:LYS:CG	2.40	0.69
1:A:120:GLY:O	1:A:123:LYS:HG3	1.92	0.69
1:A:295:GLN:HE21	1:A:295:GLN:N	1.92	0.68
1:B:319:ARG:HG2	1:B:319:ARG:NH1	2.15	0.61
1:B:306:ARG:HG3	1:B:307:PRO:CD	2.34	0.58
1:B:90:ASP:O	1:B:91:LYS:HB2	2.05	0.57
1:B:289:THR:O	1:B:290:GLU:HG3	2.05	0.57
1:B:286:PRO:O	1:B:287:ASN:HB2	2.06	0.56
1:A:123:LYS:HB3	1:A:125:GLU:HG2	1.88	0.56
1:A:277:THR:O	1:A:281:ILE:HD12	2.06	0.56
1:A:120:GLY:O	1:A:123:LYS:HG2	2.06	0.55
1:B:113:ARG:HD2	1:B:133:ASP:OD1	2.06	0.55
1:B:166:PHE:HZ	1:B:320:LEU:HD21	1.71	0.55
1:A:270:ILE:HD13	1:A:323:TYR:OH	2.07	0.54
1:B:277:THR:O	1:B:281:ILE:HD12	2.08	0.54
1:B:319:ARG:HH11	1:B:319:ARG:CG	2.20	0.54
1:B:205:LYS:NZ	1:B:213:ASN:OD1	2.25	0.53
1:A:123:LYS:HD2	1:A:125:GLU:CD	2.30	0.52
1:B:319:ARG:NH1	1:B:319:ARG:CG	2.73	0.52
1:A:289:THR:O	1:A:290:GLU:HG2	2.11	0.50
1:B:289:THR:O	1:B:290:GLU:CG	2.59	0.50
1:A:220:ARG:HG2	1:A:221:TYR:CD1	2.47	0.49
1:B:126:VAL:HG13	1:B:127:TYR:N	2.27	0.49
1:A:42:ALA:HB1	1:A:114:TYR:HB3	1.95	0.49
1:B:220:ARG:HG2	1:B:221:TYR:CD1	2.48	0.49
1:A:92:ARG:NH2	1:B:295:GLN:HB2	2.28	0.48
1:B:126:VAL:CG1	1:B:127:TYR:N	2.75	0.48
1:B:42:ALA:HB1	1:B:114:TYR:HB3	1.96	0.47
1:B:96:ARG:NH1	1:B:205:LYS:HD3	2.29	0.47
1:A:332:LEU:HD22	1:A:369:SER:HB3	1.96	0.47
1:B:283:GLU:O	1:B:284:MET:C	2.54	0.46
1:B:146:TYR:CE2	1:B:154:PRO:HD3	2.51	0.46
1:B:286:PRO:O	1:B:287:ASN:CB	2.63	0.45
1:A:179:HIS:HB3	1:A:182:ILE:CD1	2.46	0.45
1:A:123:LYS:HD2	1:A:125:GLU:OE2	2.16	0.44
1:B:290:GLU:O	1:B:292:LYS:N	2.49	0.44
1:A:300:PRO:HG2	1:A:303:LYS:HE3	1.99	0.44
1:B:313:ALA:HB2	1:B:339:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:HIS:ND1	1:B:145:HIS:C	2.71	0.44
1:B:225:PRO:CB	1:B:284:MET:HE3	2.47	0.44
1:A:122:LYS:O	1:A:124:ASP:N	2.46	0.44
1:B:289:THR:O	1:B:290:GLU:CB	2.66	0.43
1:A:313:ALA:HB2	1:A:339:PHE:CE1	2.53	0.43
1:B:286:PRO:C	1:B:287:ASN:HD22	2.21	0.43
1:A:173:HIS:CE1	1:A:236:SER:HB3	2.55	0.42
1:B:173:HIS:CE1	1:B:236:SER:HB3	2.55	0.41
1:B:217:ILE:O	1:B:218:CYS:CB	2.68	0.41
1:A:287:ASN:O	1:A:288:TYR:C	2.58	0.41
1:B:155:VAL:HG11	1:B:310:PRO:HG2	2.01	0.41
1:B:320:LEU:HD12	1:B:320:LEU:HA	1.76	0.41
1:B:217:ILE:O	1:B:223:ARG:NH1	2.53	0.41
1:B:225:PRO:CB	1:B:284:MET:CE	2.98	0.41
1:B:332:LEU:HD22	1:B:369:SER:HB3	2.02	0.41
1:A:357:PRO:O	1:A:359:LEU:HG	2.21	0.41
1:B:357:PRO:O	1:B:359:LEU:HG	2.20	0.40
1:A:289:THR:O	1:A:290:GLU:CB	2.69	0.40
1:B:193:THR:HB	1:B:195:VAL:HG23	2.03	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	348/351 (99%)	317 (91%)	26 (8%)	5 (1%)	11 19
1	B	344/351 (98%)	309 (90%)	23 (7%)	12 (4%)	3 5
All	All	692/702 (99%)	626 (90%)	49 (7%)	17 (2%)	5 9

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	A	123	LYS
1	A	290	GLU
1	B	64	ASN
1	B	66	SER
1	B	283	GLU
1	B	284	MET
1	B	291	PHE
1	A	288	TYR
1	B	122	LYS
1	B	287	ASN
1	B	290	GLU
1	B	292	LYS
1	A	287	ASN
1	B	218	CYS
1	B	293	PHE
1	B	63	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	312/313 (100%)	292 (94%)	20 (6%)	17 31
1	B	308/313 (98%)	290 (94%)	18 (6%)	20 35
All	All	620/626 (99%)	582 (94%)	38 (6%)	18 33

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	92	ARG
1	A	93	PHE
1	A	94	LYS
1	A	107	CYS
1	A	110	VAL
1	A	124	ASP

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Mol	Chain	Res	Type
1	A	129	ASN
1	A	147	SER
1	A	185	GLN
1	A	217	ILE
1	A	220	ARG
1	A	289	THR
1	A	291	PHE
1	A	295	GLN
1	A	302	THR
1	A	308	ARG
1	A	324	THR
1	A	349	LYS
1	A	364	THR
1	B	49	ASP
1	B	77	ASP
1	B	99	GLN
1	B	110	VAL
1	B	119	SER
1	B	147	SER
1	B	150	LYS
1	B	185	GLN
1	B	205	LYS
1	B	220	ARG
1	B	263	VAL
1	B	282	ARG
1	B	287	ASN
1	B	302	THR
1	B	317	CYS
1	B	319	ARG
1	B	320	LEU
1	B	364	THR

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	64	ASN
1	A	129	ASN
1	A	151	GLN
1	A	295	GLN
1	B	64	ASN
1	B	129	ASN
1	B	285	ASN

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Mol	Chain	Res	Type
1	B	287	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

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	L7W	A	402	-	27,27,27	1.38	1 (3%)	35,36,36	1.81	9 (25%)
3	L7W	B	402	-	27,27,27	1.32	1 (3%)	35,36,36	1.78	8 (22%)

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	L7W	A	402	-	-	11/17/26/26	0/3/3/3
3	L7W	B	402	-	-	5/17/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	L7W	C12-C13	6.22	1.51	1.38
3	B	402	L7W	C12-C13	5.72	1.50	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	L7W	C11-O1-C12	4.34	126.56	117.60
3	A	402	L7W	C14-C13-C12	-4.22	117.45	122.12
3	A	402	L7W	C11-O1-C12	3.87	125.61	117.60
3	A	402	L7W	F-C13-C12	3.57	123.44	118.05
3	B	402	L7W	O-C5-C6	-3.52	117.54	122.12
3	B	402	L7W	C7-C6-C5	-3.48	106.02	112.66
3	A	402	L7W	C3-N-C4	3.41	122.05	117.22
3	B	402	L7W	C3-N-C4	3.36	121.98	117.22
3	B	402	L7W	C-C4-N	-3.08	117.76	122.57
3	A	402	L7W	C-C4-N	-3.05	117.81	122.57
3	A	402	L7W	C7-C6-C9	2.67	105.97	102.45
3	B	402	L7W	C14-C13-C12	-2.56	119.29	122.12
3	B	402	L7W	C11-C10-N2	2.37	122.42	116.93
3	A	402	L7W	O1-C12-C17	-2.16	119.30	123.97
3	A	402	L7W	O2-C10-C11	-2.13	115.51	120.66
3	A	402	L7W	C7-C6-C5	-2.10	108.66	112.66
3	B	402	L7W	C6-C5-N1	2.09	118.09	115.02

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	L7W	O2-C10-N2-C8
3	A	402	L7W	O2-C10-N2-C9
3	A	402	L7W	C11-C10-N2-C8
3	A	402	L7W	C11-C10-N2-C9
3	A	402	L7W	C13-C12-O1-C11
3	B	402	L7W	C13-C12-O1-C11
3	A	402	L7W	N2-C10-C11-O1
3	A	402	L7W	O2-C10-C11-O1
3	B	402	L7W	N2-C10-C11-O1
3	A	402	L7W	O-C5-C6-C7
3	A	402	L7W	N1-C5-C6-C7
3	A	402	L7W	C17-C12-O1-C11
3	B	402	L7W	C17-C12-O1-C11

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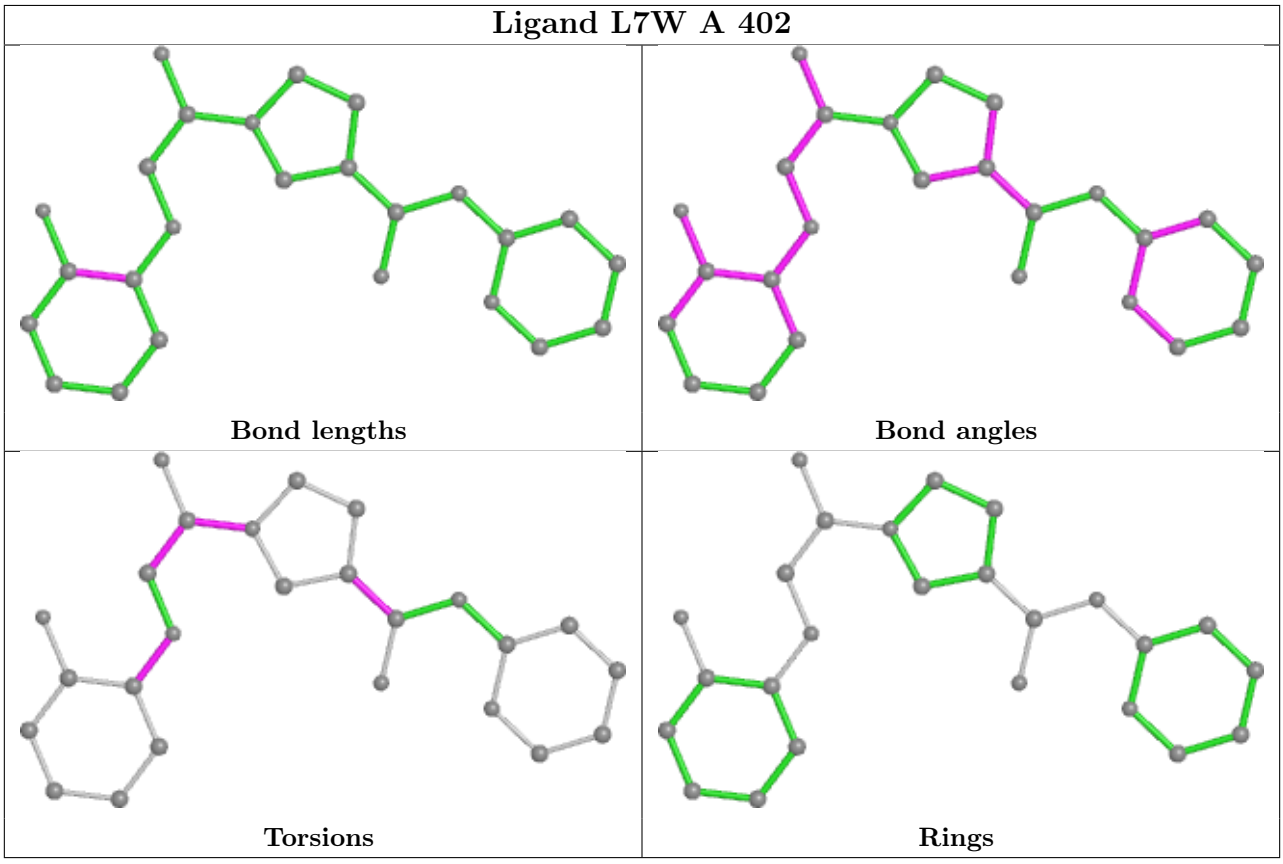
Mol	Chain	Res	Type	Atoms
3	B	402	L7W	O2-C10-C11-O1
3	A	402	L7W	N1-C5-C6-C9
3	B	402	L7W	C10-C11-O1-C12

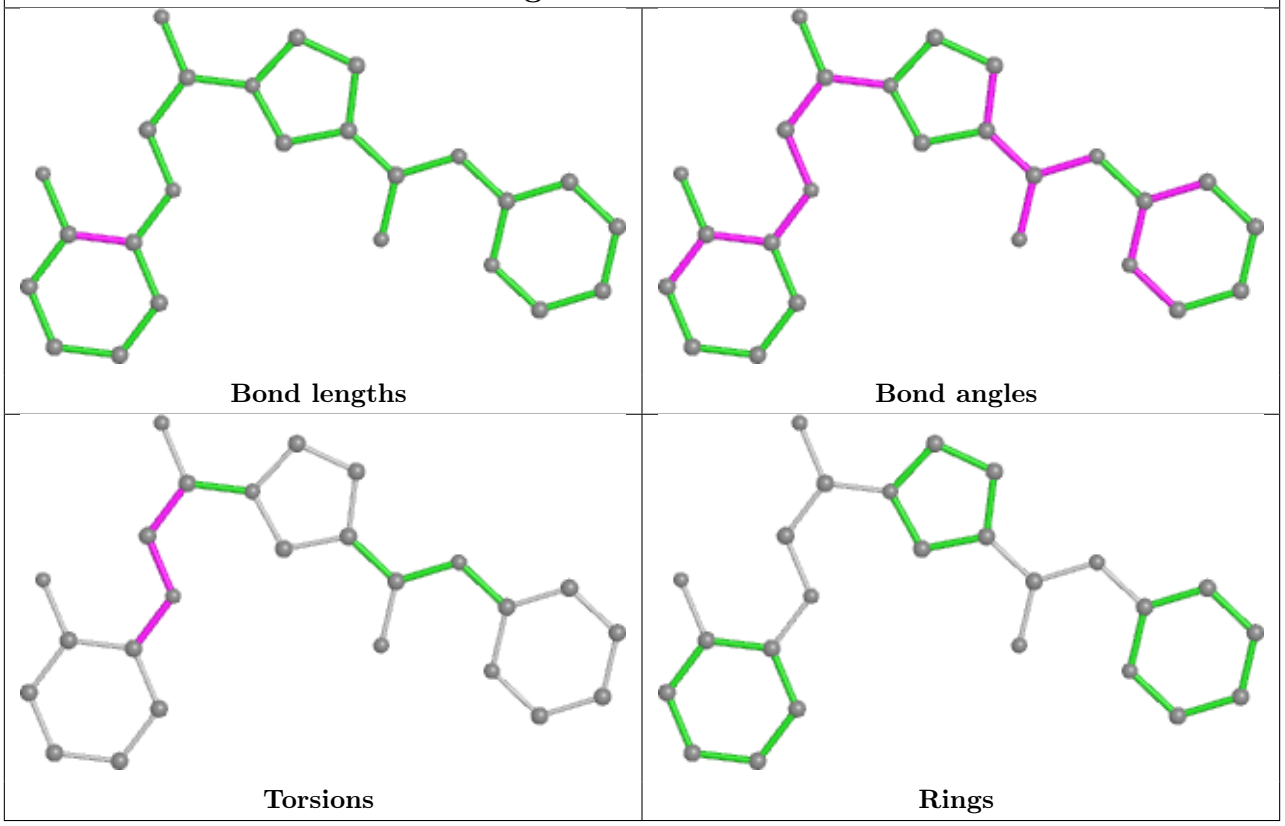
There are no ring outliers.

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 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.



Ligand L7W B 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	OWAB(Å^2)	Q<0.9
1	A	350/351 (99%)	0.70	21 (6%) 21 26	51, 69, 116, 149	0
1	B	346/351 (98%)	0.55	7 (2%) 65 73	50, 67, 117, 146	0
All	All	696/702 (99%)	0.63	28 (4%) 38 45	50, 68, 118, 149	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	GLY	6.5
1	A	291	PHE	6.5
1	A	121	GLU	5.4
1	B	288	TYR	5.1
1	B	120	GLY	4.4
1	A	122	LYS	4.2
1	A	93	PHE	3.3
1	A	289	THR	3.2
1	A	290	GLU	3.1
1	A	229	PHE	3.0
1	B	63	GLY	3.0
1	A	198	LEU	2.8
1	B	121	GLU	2.6
1	A	112	LEU	2.5
1	A	385	GLN	2.5
1	A	286	PRO	2.5
1	A	66	SER	2.5
1	A	69	VAL	2.4
1	A	201	PHE	2.4
1	B	126	VAL	2.4
1	A	293	PHE	2.3
1	A	292	LYS	2.3
1	A	296	ILE	2.2
1	B	343	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	88	LEU	2.1
1	A	266	LEU	2.1
1	A	116	PHE	2.1
1	A	343	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

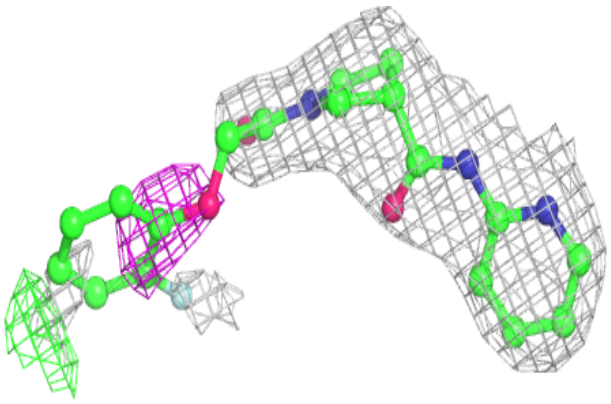
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

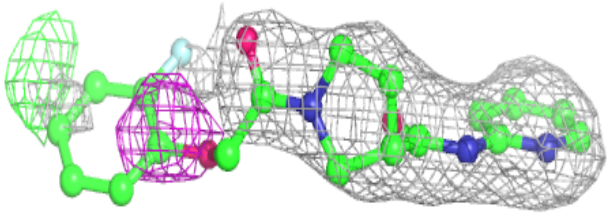
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	A	401	1/1	0.47	0.32	85,85,85,85	0
3	L7W	B	402	25/25	0.86	0.42	67,95,133,136	0
3	L7W	A	402	25/25	0.90	0.34	57,75,112,114	0
2	CL	B	401	1/1	0.96	0.14	60,60,60,60	0

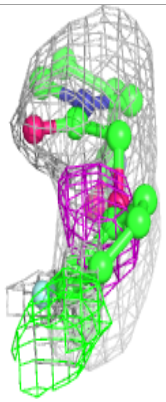
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around L7W 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)

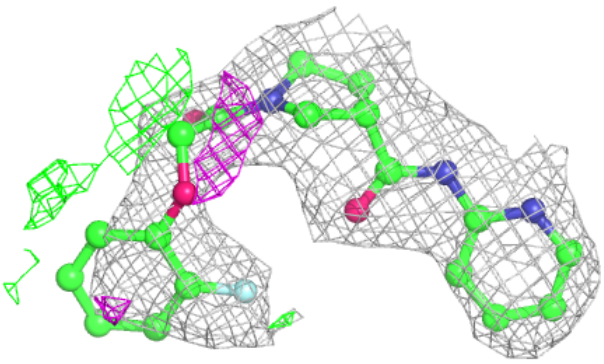


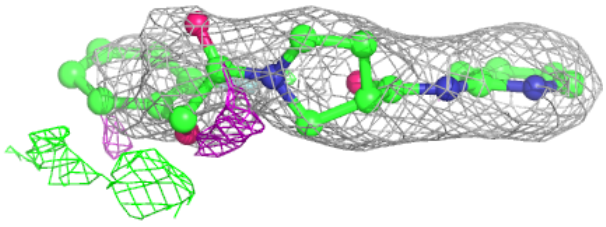


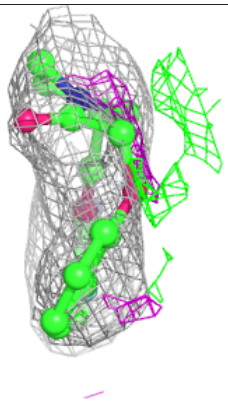


Electron density around L7W A 402:

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







6.5 Other polymers (i)

There are no such residues in this entry.