Full wwPDB X-ray Structure Validation Report (i)

Oct 29, 2024 – 02:06 pm GMT

PDB ID	:	9FIQ
Title	:	Structure-guided discovery of selective USP7 inhibitors with in vivo activity
Authors	:	Baker, L.M.; Murray, J.; Hubbard, R.E.; Whitehead, N.
Deposited on	:	2024-05-29
Resolution	:	2.86 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

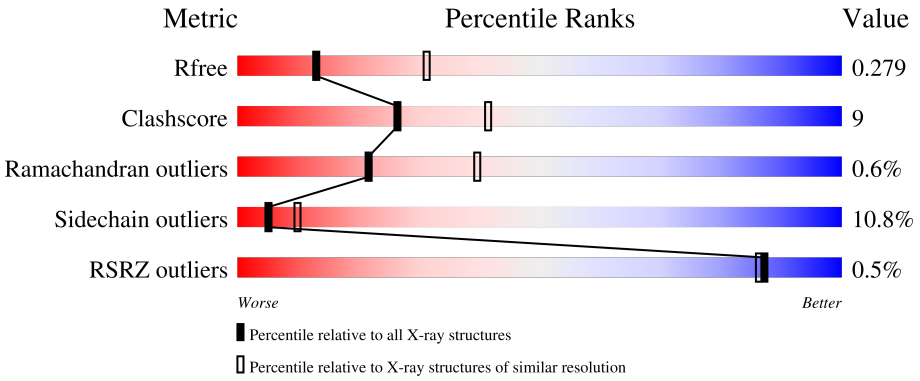
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

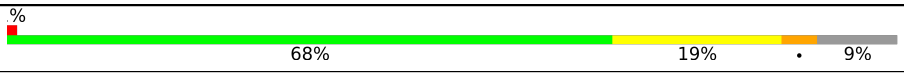
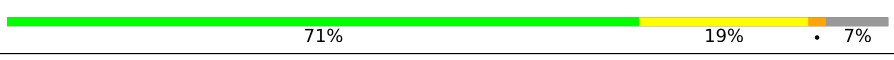
The reported resolution of this entry is 2.86 Å.

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}	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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	355	
1	B	355	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10715 atoms, of which 5307 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.

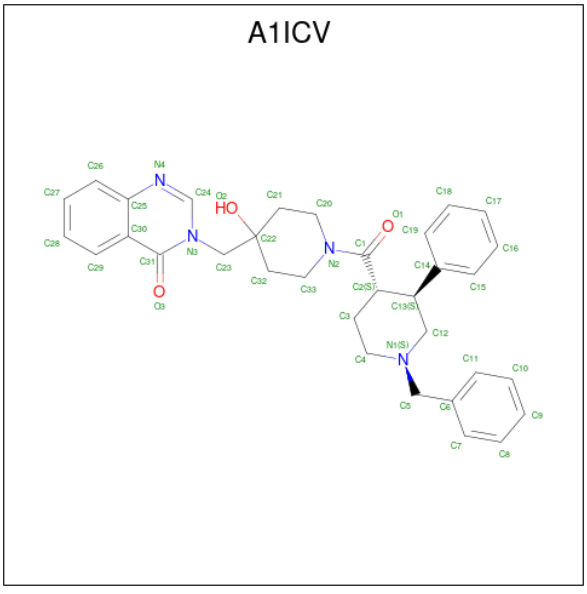
- Molecule 1 is a protein called Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	324	Total	C	H	N	O	S	71	0	0
			5234	1674	2598	443	504	15			
1	B	329	Total	C	H	N	O	S	76	0	0
			5311	1698	2637	452	508	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	GLY	-	expression tag	UNP Q93009
B	206	GLY	-	expression tag	UNP Q93009

- Molecule 2 is 3-[[4-oxidanyl-1-[(3 {S},4 {S})-3-phenyl-1-(phenylmethyl)piperidin-4-yl]carbonyl-piperidin-4-yl]methyl]quinazolin-4-one (three-letter code: A1ICV) (formula: $C_{33}H_{36}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	1	0
			76	33	36	4	3		
2	B	1	Total	C	H	N	O	1	0
			76	33	36	4	3		

- Molecule 3 is water.

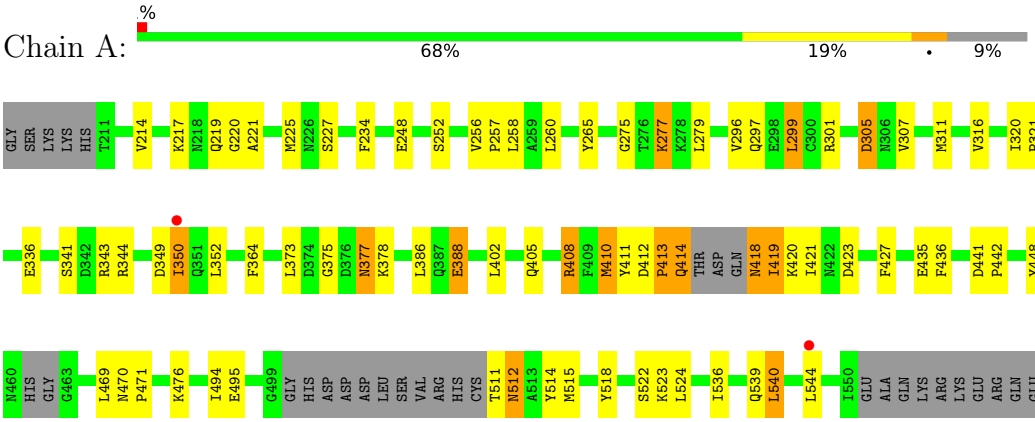
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	10	Total	O	0	0
			10	10		

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.

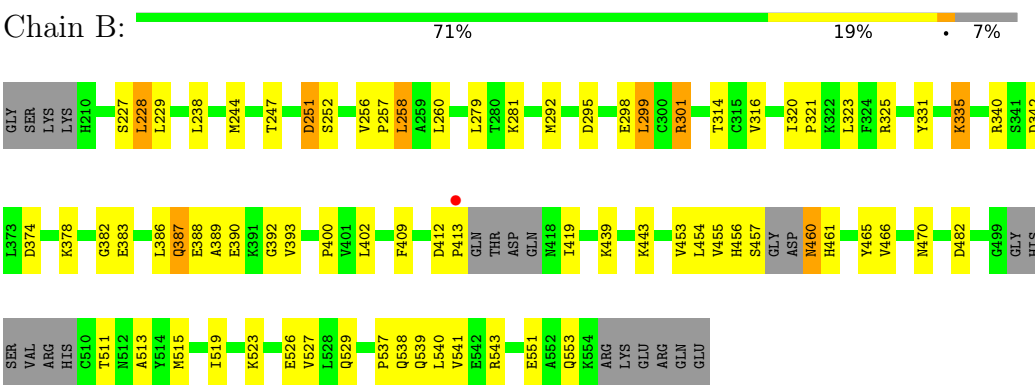
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

Chain A:



• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.75Å 70.46Å 77.95Å 90.00° 92.91° 90.00°	Depositor
Resolution (Å)	43.73 – 2.86 43.73 – 2.86	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.73-2.86) 96.5 (43.73-2.86)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.197 , 0.278 0.198 , 0.279	Depositor DCC
R_{free} test set	986 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	90.8	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.033 for h,-k,-l 0.014 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10715	wwPDB-VP
Average B, all atoms (Å^2)	92.0	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 35.21 % 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 6.0427e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: A1ICV

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	0.37	0/2689	0.77	0/3625
1	B	0.38	0/2729	0.84	0/3678
All	All	0.37	0/5418	0.81	0/7303

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	460	ASN	Peptide

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	2636	2598	2585	41	0
1	B	2674	2637	2620	56	0
2	A	40	36	0	1	0
2	B	40	36	0	0	0
3	A	8	0	0	0	0
3	B	10	0	0	1	0
All	All	5408	5307	5205	97	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 9.

All (97) 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:B:335:LYS:NZ	1:B:388:GLU:HB3	1.50	1.26
1:B:335:LYS:HD2	1:B:388:GLU:CB	1.68	1.24
1:B:335:LYS:HD2	1:B:388:GLU:HB2	1.04	1.01
1:B:335:LYS:CD	1:B:388:GLU:HB2	1.91	0.99
1:B:335:LYS:CE	1:B:388:GLU:HB3	1.93	0.98
1:B:335:LYS:CD	1:B:388:GLU:CB	2.43	0.95
1:B:335:LYS:HZ2	1:B:388:GLU:HB3	1.05	0.92
1:B:301:ARG:NH1	3:B:701:HOH:O	1.97	0.90
1:B:335:LYS:HG3	1:B:389:ALA:HA	1.65	0.79
1:B:526:GLU:O	1:B:529:GLN:NE2	2.17	0.78
1:A:375:GLY:HA2	1:A:378:LYS:HG3	1.67	0.75
1:A:227:SER:HB3	1:A:454:LEU:CD1	2.18	0.74
1:B:335:LYS:CE	1:B:388:GLU:CB	2.66	0.73
1:B:455:VAL:HG13	1:B:511:THR:HB	1.72	0.71
1:B:335:LYS:HE3	1:B:389:ALA:N	2.05	0.70
1:B:537:PRO:O	1:B:541:VAL:HG23	1.92	0.69
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.75	0.68
1:B:335:LYS:HZ2	1:B:388:GLU:CB	1.96	0.68
1:B:335:LYS:HG3	1:B:389:ALA:CA	2.26	0.66
1:B:251:ASP:OD1	1:B:251:ASP:C	2.33	0.66
1:A:234:PHE:CD1	1:A:471:PRO:HB3	2.34	0.63
1:A:227:SER:HB3	1:A:454:LEU:HD12	1.81	0.61
1:B:252:SER:HA	1:B:258:LEU:HD12	1.83	0.59
1:B:335:LYS:HD2	1:B:388:GLU:CA	2.32	0.57
1:B:378:LYS:HD2	1:B:386:LEU:HB3	1.87	0.57
1:B:335:LYS:HE3	1:B:389:ALA:H	1.70	0.56
1:B:252:SER:HA	1:B:258:LEU:CD1	2.34	0.56
1:A:225:MET:HG3	1:A:299:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:NE	1:B:342:ASP:OD1	2.40	0.55
1:B:335:LYS:HD2	1:B:388:GLU:C	2.27	0.55
1:B:386:LEU:O	1:B:387:GLN:NE2	2.41	0.54
1:B:331:TYR:CZ	1:B:392:GLY:HA3	2.42	0.54
1:A:410:MET:O	1:A:419:ILE:N	2.39	0.54
1:B:455:VAL:CG1	1:B:511:THR:HB	2.35	0.54
1:A:411:TYR:HA	1:A:418:ASN:HA	1.90	0.53
1:B:227:SER:HB3	1:B:454:LEU:CD1	2.39	0.52
1:A:375:GLY:HA2	1:A:378:LYS:HE3	1.90	0.52
1:B:295:ASP:O	1:B:298:GLU:HB2	2.10	0.52
1:A:297:GLN:OE1	1:A:405:GLN:HG2	2.11	0.51
1:A:220:GLY:O	1:A:221:ALA:HB3	2.11	0.51
1:A:414:GLN:OE1	1:A:418:ASN:N	2.44	0.51
1:A:408:ARG:NH1	1:A:423:ASP:O	2.44	0.50
1:A:320:ILE:HB	1:A:321:PRO:CD	2.42	0.50
1:B:454:LEU:HB2	1:B:515:MET:HB3	1.93	0.49
1:B:335:LYS:CD	1:B:388:GLU:C	2.80	0.49
1:B:323:LEU:HA	1:B:400:PRO:HG2	1.95	0.49
1:B:335:LYS:HG3	1:B:389:ALA:N	2.28	0.49
1:A:375:GLY:HA2	1:A:378:LYS:CG	2.40	0.49
1:A:350:ILE:HD11	1:A:352:LEU:HD21	1.94	0.48
1:A:301:ARG:CZ	1:A:301:ARG:HA	2.44	0.48
1:B:335:LYS:NZ	1:B:388:GLU:CB	2.46	0.48
1:B:453:VAL:HG12	1:B:455:VAL:HG23	1.94	0.48
1:B:382:GLY:O	1:B:383:GLU:HB3	2.14	0.48
1:A:256:VAL:HB	1:A:257:PRO:HD3	1.95	0.47
1:A:512:ASN:C	1:A:512:ASN:HD22	2.18	0.47
2:A:601:A1ICV:C9	1:B:460:ASN:HA	2.44	0.47
1:B:331:TYR:CE1	1:B:392:GLY:HA3	2.50	0.47
1:B:400:PRO:HB3	1:B:523:LYS:HG3	1.96	0.47
1:B:456:HIS:HD2	1:B:465:TYR:CZ	2.33	0.46
1:B:301:ARG:N	1:B:301:ARG:HD2	2.30	0.46
1:B:256:VAL:HB	1:B:257:PRO:HD3	1.98	0.46
1:B:455:VAL:HB	1:B:466:VAL:O	2.16	0.46
1:A:421:ILE:N	1:A:421:ILE:HD12	2.31	0.45
1:A:301:ARG:O	1:A:305:ASP:HB2	2.17	0.45
1:B:538:GLN:O	1:B:539:GLN:C	2.54	0.45
1:A:375:GLY:HA2	1:A:378:LYS:CE	2.47	0.44
1:B:247:THR:O	1:B:543:ARG:NH1	2.50	0.44
1:B:256:VAL:N	1:B:257:PRO:CD	2.81	0.44
1:A:373:LEU:O	1:A:388:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:GLY:C	1:A:377:ASN:H	2.21	0.44
1:A:217:LYS:HB2	1:A:275:GLY:HA2	2.00	0.43
1:B:251:ASP:OD1	1:B:252:SER:N	2.52	0.43
1:A:307:VAL:HG13	1:A:311:MET:HE3	2.00	0.43
1:A:248:GLU:HG2	1:A:539:GLN:CD	2.39	0.43
1:A:364:PHE:HB3	1:A:436:PHE:CE1	2.54	0.43
1:A:427:PHE:CE1	1:A:494:ILE:HG23	2.54	0.43
1:A:454:LEU:HB3	1:A:514:TYR:CZ	2.53	0.43
1:A:265:TYR:CD2	1:A:544:LEU:HD13	2.53	0.43
1:B:519:ILE:HD13	1:B:527:VAL:HG11	2.00	0.43
1:A:325:ARG:HG2	1:A:326:GLY:N	2.34	0.42
1:A:412:ASP:O	1:A:413:PRO:C	2.57	0.42
1:B:372:GLN:NE2	1:B:390:GLU:OE1	2.51	0.42
1:A:405:GLN:NE2	1:A:515:MET:SD	2.90	0.42
1:B:325:ARG:HD3	1:B:346:ASP:OD2	2.20	0.42
1:A:252:SER:HA	1:A:258:LEU:HD12	2.02	0.42
1:A:256:VAL:N	1:A:257:PRO:CD	2.83	0.42
1:B:540:LEU:O	1:B:541:VAL:C	2.57	0.42
1:B:228:LEU:HD12	1:B:299:LEU:HD13	2.02	0.42
1:A:219:GLN:HE21	1:A:277:LYS:HD2	1.86	0.41
1:B:374:ASP:HB2	1:B:388:GLU:OE1	2.20	0.41
1:B:454:LEU:O	1:B:513:ALA:HA	2.20	0.41
1:A:441:ASP:OD1	1:A:442:PRO:HD2	2.20	0.41
1:A:448:TYR:HB3	1:A:518:TYR:HB3	2.03	0.41
1:A:375:GLY:CA	1:A:378:LYS:HE3	2.51	0.41
1:A:408:ARG:O	1:A:420:LYS:HA	2.21	0.41
1:A:536:ILE:HG23	1:A:540:LEU:HD13	2.03	0.41
1:B:335:LYS:HZ2	1:B:374:ASP:HB3	1.86	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	316/355 (89%)	284 (90%)	30 (10%)	2 (1%)	22 40
1	B	321/355 (90%)	302 (94%)	17 (5%)	2 (1%)	22 40
All	All	637/710 (90%)	586 (92%)	47 (7%)	4 (1%)	22 40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	ASP
1	A	413	PRO
1	B	335	LYS
1	B	482	ASP

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	294/321 (92%)	258 (88%)	36 (12%)	4 7
1	B	297/321 (92%)	269 (91%)	28 (9%)	7 14
All	All	591/642 (92%)	527 (89%)	64 (11%)	5 10

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	VAL
1	A	260	LEU
1	A	277	LYS
1	A	279	LEU
1	A	296	VAL
1	A	299	LEU
1	A	305	ASP
1	A	316	VAL
1	A	325	ARG
1	A	327	LYS
1	A	336	GLU
1	A	341	SER

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Mol	Chain	Res	Type
1	A	343	ARG
1	A	344	ARG
1	A	349	ASP
1	A	350	ILE
1	A	377	ASN
1	A	386	LEU
1	A	388	GLU
1	A	402	LEU
1	A	408	ARG
1	A	410	MET
1	A	414	GLN
1	A	418	ASN
1	A	419	ILE
1	A	435	GLU
1	A	469	LEU
1	A	470	ASN
1	A	476	LYS
1	A	495	GLU
1	A	511	THR
1	A	512	ASN
1	A	522	SER
1	A	523	LYS
1	A	524	LEU
1	A	540	LEU
1	B	228	LEU
1	B	229	LEU
1	B	238	LEU
1	B	244	MET
1	B	251	ASP
1	B	258	LEU
1	B	260	LEU
1	B	279	LEU
1	B	281	LYS
1	B	292	MET
1	B	299	LEU
1	B	301	ARG
1	B	314	THR
1	B	316	VAL
1	B	387	GLN
1	B	393	VAL
1	B	402	LEU
1	B	409	PHE

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Mol	Chain	Res	Type
1	B	412	ASP
1	B	413	PRO
1	B	419	ILE
1	B	439	LYS
1	B	443	LYS
1	B	457	SER
1	B	461	HIS
1	B	470	ASN
1	B	551	GLU
1	B	553	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	309	ASN
1	A	377	ASN
1	A	438	GLN
1	A	447	ASN
1	A	496	HIS
1	A	512	ASN
1	B	237	GLN
1	B	384	HIS
1	B	387	GLN
1	B	418	ASN
1	B	456	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	A1ICV	B	601	-	45,45,45	0.43	0	57,64,64	2.16	10 (17%)
2	A1ICV	A	601	-	45,45,45	0.46	0	57,64,64	1.87	10 (17%)

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	A1ICV	B	601	-	-	6/21/46/46	0/6/6/6
2	A1ICV	A	601	-	-	5/21/46/46	0/6/6/6

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	A1ICV	C2-C1-N2	7.53	133.30	118.99
2	A	601	A1ICV	C13-C2-C1	7.14	121.82	111.19
2	B	601	A1ICV	O1-C1-N2	-6.75	113.77	121.67
2	B	601	A1ICV	C13-C2-C1	5.59	119.52	111.19
2	B	601	A1ICV	O1-C1-C2	-5.13	112.84	121.88
2	A	601	A1ICV	C4-C3-C2	-5.08	103.05	111.59
2	B	601	A1ICV	C4-C3-C2	-5.00	103.19	111.59
2	A	601	A1ICV	C3-C2-C13	-4.24	104.85	109.58
2	B	601	A1ICV	C3-C2-C1	4.14	115.69	109.50
2	A	601	A1ICV	C2-C1-N2	4.03	126.64	118.99
2	A	601	A1ICV	C4-N1-C12	3.68	115.15	109.52
2	A	601	A1ICV	O1-C1-C2	-3.67	115.42	121.88
2	A	601	A1ICV	O1-C1-N2	-3.19	117.94	121.67
2	B	601	A1ICV	C30-C31-N3	3.05	115.58	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	A1ICV	C32-C22-C21	-2.82	106.56	109.85
2	A	601	A1ICV	C30-C31-N3	2.81	115.44	113.80
2	B	601	A1ICV	C14-C13-C2	2.80	118.12	112.84
2	B	601	A1ICV	C3-C2-C13	-2.63	106.65	109.58
2	A	601	A1ICV	C14-C13-C2	2.52	117.59	112.84
2	A	601	A1ICV	C3-C4-N1	2.37	114.79	111.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

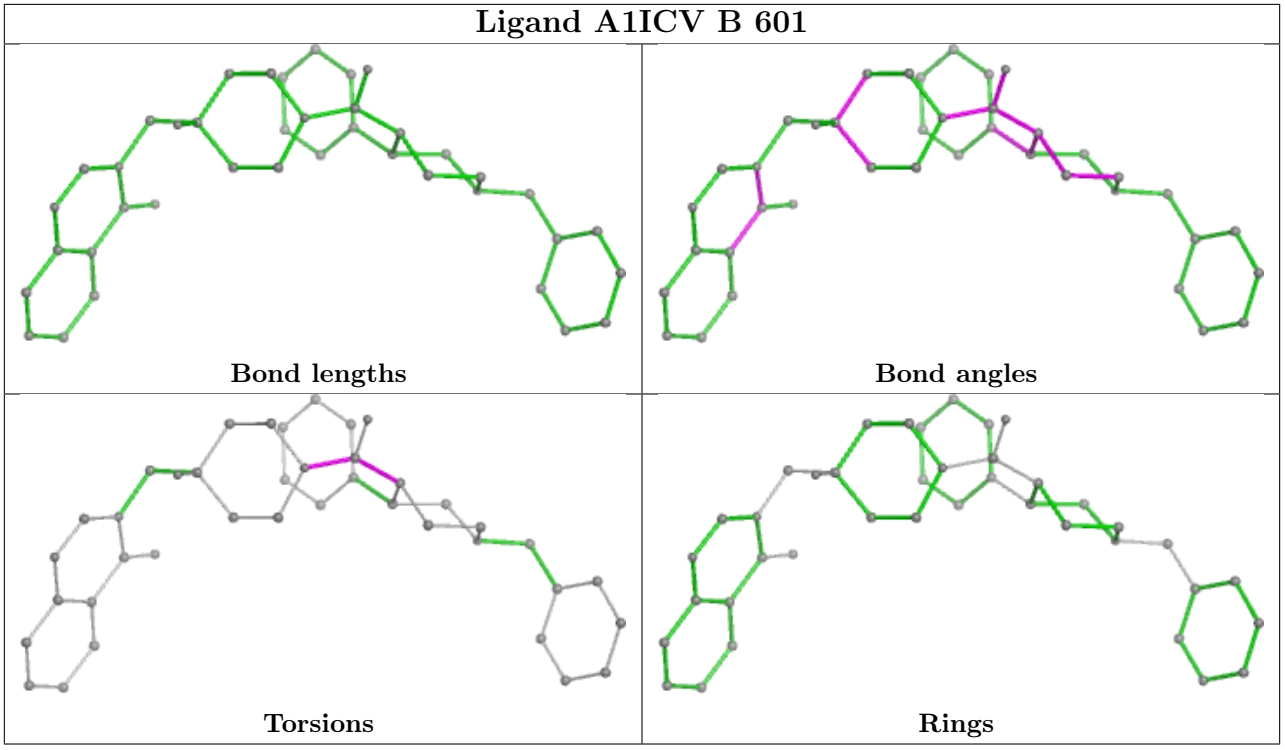
Mol	Chain	Res	Type	Atoms
2	A	601	A1ICV	O1-C1-C2-C13
2	A	601	A1ICV	N2-C1-C2-C13
2	B	601	A1ICV	O1-C1-C2-C13
2	B	601	A1ICV	N2-C1-C2-C13
2	B	601	A1ICV	O1-C1-N2-C20
2	B	601	A1ICV	C2-C1-N2-C20
2	A	601	A1ICV	C6-C5-N1-C4
2	A	601	A1ICV	C6-C5-N1-C12
2	B	601	A1ICV	C2-C1-N2-C33
2	B	601	A1ICV	O1-C1-N2-C33
2	A	601	A1ICV	C32-C22-C23-N3

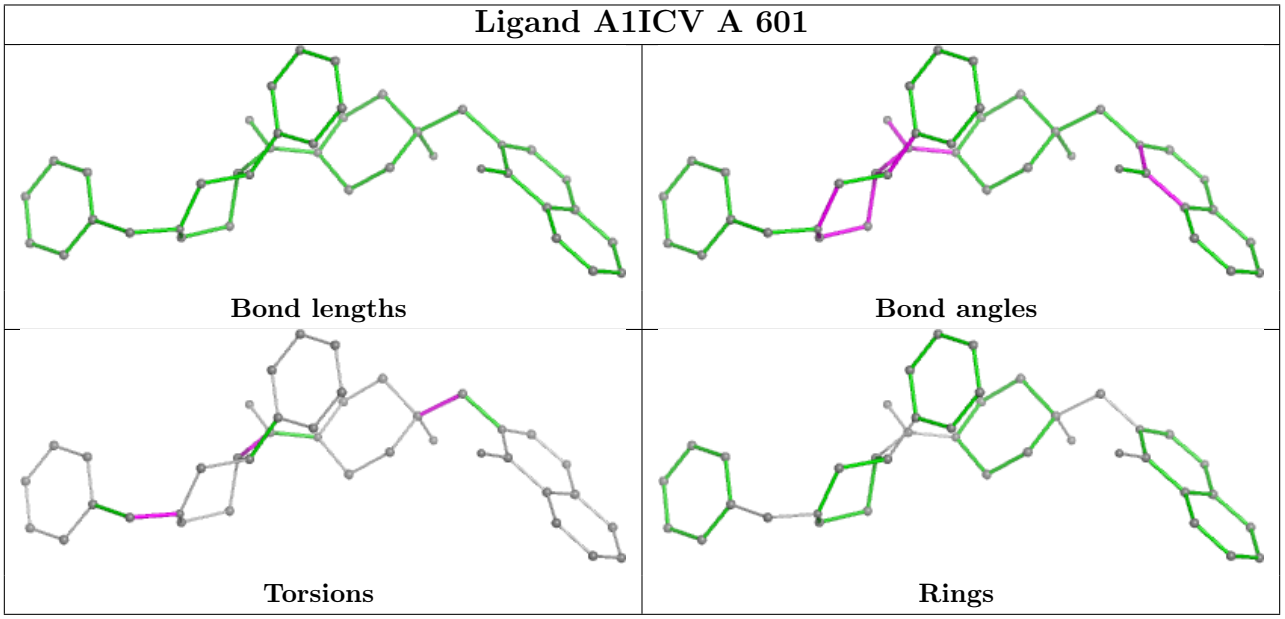
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	A1ICV	1	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

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	324/355 (91%)	-0.58	2 (0%)	85	84	57, 90, 138, 173	0
1	B	329/355 (92%)	-0.61	1 (0%)	90	90	49, 85, 128, 180	0
All	All	653/710 (91%)	-0.59	3 (0%)	87	86	49, 88, 137, 180	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	ILE	2.7
1	B	413	PRO	2.3
1	A	544	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

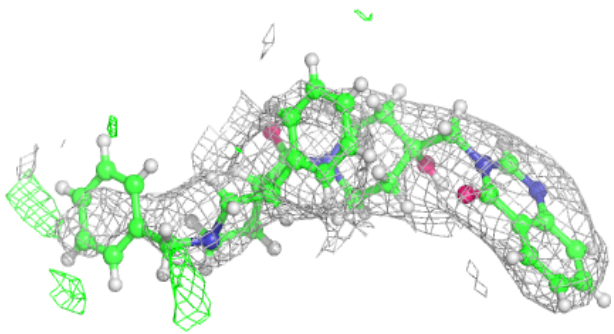
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

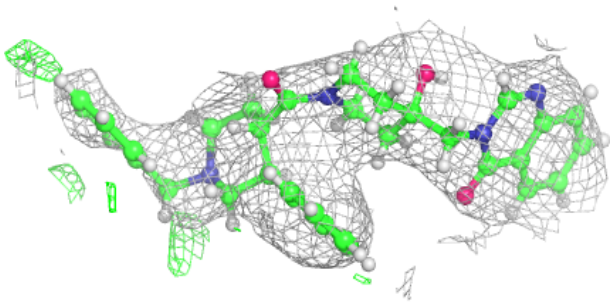
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1ICV	A	601	40/40	0.92	0.12	43,92,130,133	1
2	A1ICV	B	601	40/40	0.94	0.10	47,85,142,161	1

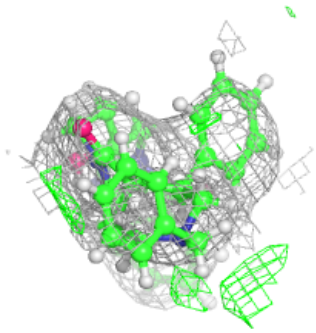
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1ICV A 601:

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

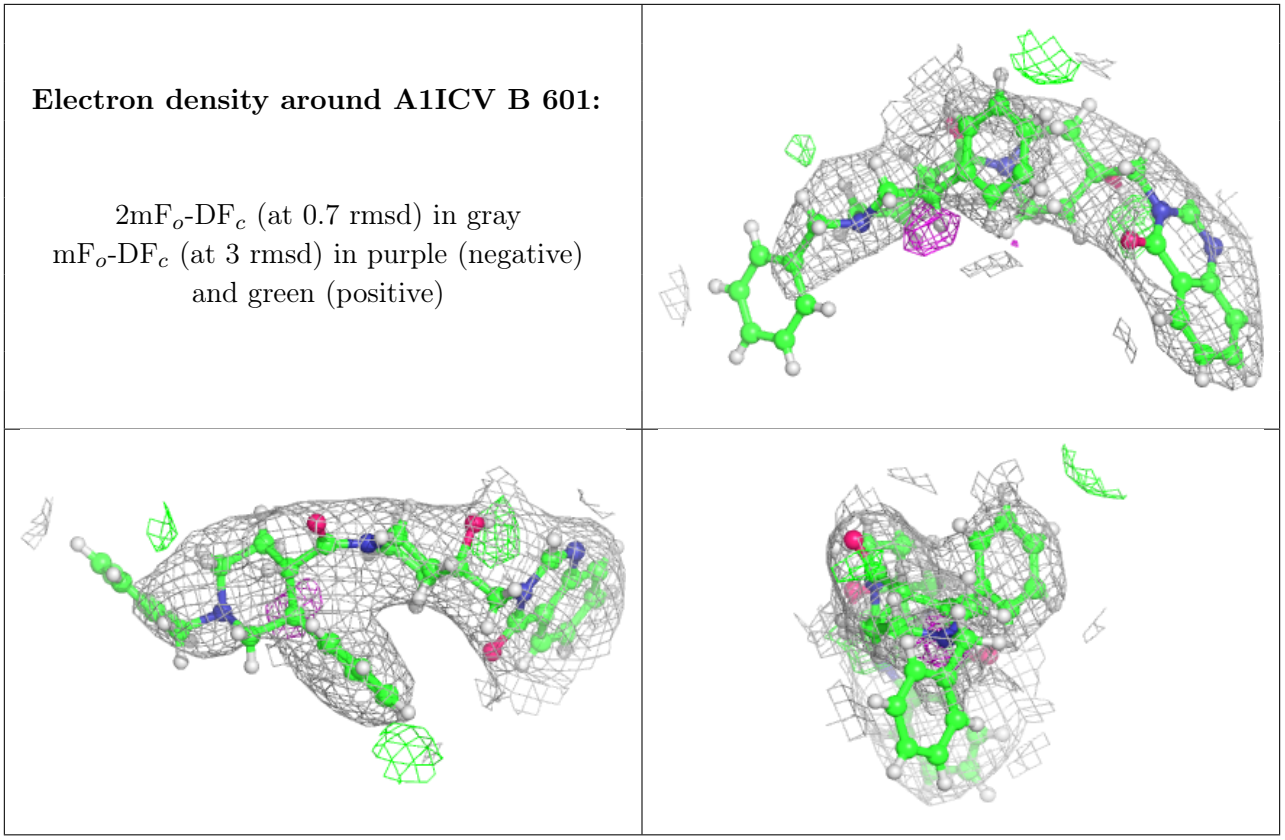






Electron density around A1ICV B 601:

$2mF_o$-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.