



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 07:28 AM EDT

PDB ID : 9FIR / pdb_00009fir
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 : 2.76 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

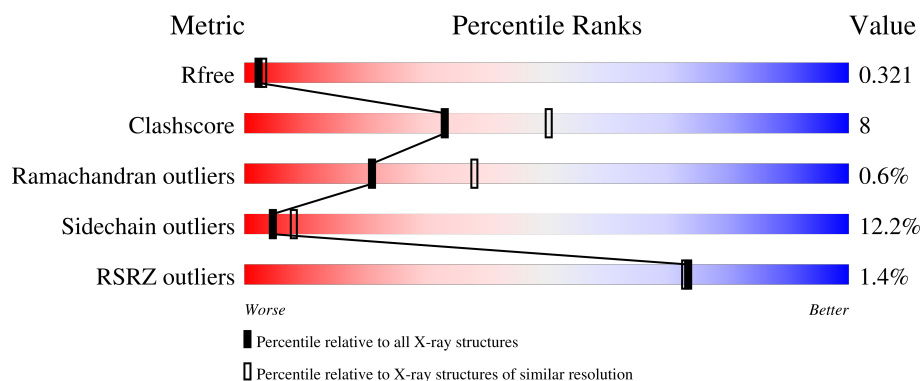
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	355	
1	B	355	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10628 atoms, of which 5250 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.

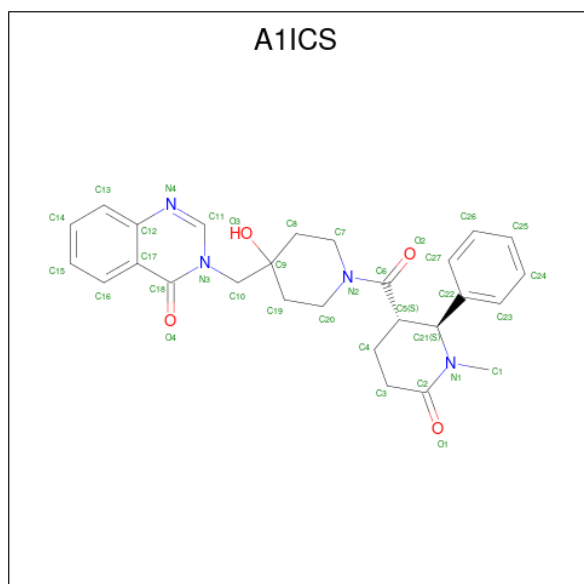
- Molecule 1 is a protein called Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	326	Total	C	H	N	O	S	71	0	0
			5252	1675	2610	446	505	16			
1	B	322	Total	C	H	N	O	S	73	0	0
			5191	1655	2580	445	496	15			

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-[[1-[(2 {S},3 {S})-1-methyl-6-oxidanylidene-2-phenyl-piperidin-3-yl]carbonyl-4-oxidanyl-piperidin-4-yl]methyl]quinazolin-4-one (CCD ID: A1ICS) (formula: C₂₇H₃₀N₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	4	0
			65	27	30	4	4		
2	B	1	Total	C	H	N	O	4	0
			65	27	30	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	32	Total	O	0	0
			32	32		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.94Å 66.78Å 76.31Å 90.00° 94.60° 90.00°	Depositor
Resolution (Å)	54.40 – 2.76 54.40 – 2.76	Depositor EDS
% Data completeness (in resolution range)	96.7 (54.40-2.76) 96.7 (54.40-2.76)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.214 , 0.322 0.214 , 0.321	Depositor DCC
R_{free} test set	926 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10628	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1ICS

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	0.91	1/2693 (0.0%)	1.44	19/3627 (0.5%)
1	B	0.87	0/2663	1.42	17/3587 (0.5%)
All	All	0.89	1/5356 (0.0%)	1.43	36/7214 (0.5%)

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	A	0	3
1	B	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	VAL	C-O	-5.06	1.18	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	VAL	N-CA-CB	9.15	120.23	110.62
1	B	453	VAL	N-CA-CB	-8.62	101.72	112.15
1	A	423	ASP	CA-CB-CG	8.57	121.17	112.60
1	A	244	MET	CG-SD-CE	8.27	119.10	100.90
1	A	474	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	268	GLN	CG-CD-NE2	-7.13	105.70	116.40
1	A	268	GLN	OE1-CD-NE2	7.00	129.60	122.60
1	B	542	GLU	CB-CA-C	-6.56	100.31	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ASN	CB-CA-C	6.21	121.14	111.13
1	A	483	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	460	ASN	CB-CA-C	-5.83	99.50	109.65
1	A	432	PRO	N-CA-CB	-5.82	97.14	103.25
1	A	271	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	246	PRO	N-CA-CB	-5.67	98.59	102.73
1	A	489	THR	CA-CB-OG1	-5.59	101.21	109.60
1	B	448	TYR	N-CA-CB	-5.50	101.26	110.83
1	B	410	MET	CG-SD-CE	5.49	112.97	100.90
1	B	474	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	400	PRO	N-CA-C	-5.35	106.10	113.53
1	B	283	PHE	CA-CB-CG	5.30	119.10	113.80
1	B	464	HIS	CA-CB-CG	-5.28	108.52	113.80
1	A	380	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	483	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	489	THR	OG1-CB-CG2	5.17	119.64	109.30
1	B	423	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	236	ASN	CB-CA-C	-5.14	102.26	110.79
1	A	473	GLY	N-CA-C	-5.13	108.17	115.30
1	B	231	THR	OG1-CB-CG2	-5.10	99.10	109.30
1	B	225	MET	CA-C-N	-5.07	113.85	120.44
1	B	225	MET	C-N-CA	-5.07	113.85	120.44
1	A	296	VAL	CA-C-O	-5.05	116.16	121.41
1	A	316	VAL	CB-CA-C	5.05	119.57	111.29
1	B	361	PHE	CB-CA-C	5.04	118.79	110.88
1	A	297	GLN	N-CA-CB	5.03	117.60	110.06
1	A	354	ILE	N-CA-CB	-5.01	107.53	111.64
1	B	448	TYR	CB-CA-C	5.00	118.93	109.37

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	ARG	Sidechain
1	A	344	ARG	Sidechain
1	A	549	ARG	Sidechain
1	B	325	ARG	Sidechain
1	B	424	ARG	Sidechain

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	2642	2610	2597	39	0
1	B	2611	2580	2565	46	0
2	A	35	30	0	4	0
2	B	35	30	0	0	0
3	A	23	0	0	2	0
3	B	32	0	0	8	0
All	All	5378	5250	5162	82	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 8.

All (82) 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:548:LYS:NZ	3:B:702:HOH:O	1.99	0.94
1:B:462:GLY:O	3:B:701:HOH:O	1.87	0.93
1:B:532:THR:HG21	3:B:715:HOH:O	1.70	0.89
1:A:295:ASP:HB2	2:A:601:A1ICS:O3	1.73	0.88
1:B:378:LYS:HB2	1:B:387:GLN:O	1.86	0.76
1:A:329:VAL:HG23	1:A:396:LEU:HD11	1.69	0.74
1:A:482:ASP:OD2	1:B:460:ASN:ND2	2.24	0.70
1:B:374:ASP:HB3	1:B:388:GLU:HB3	1.75	0.68
1:B:220:GLY:O	3:B:703:HOH:O	2.13	0.66
1:A:329:VAL:CG2	1:A:396:LEU:HD11	2.26	0.65
1:A:464:HIS:CE1	1:B:460:ASN:OD1	2.51	0.63
1:B:375:GLY:O	1:B:376:ASP:C	2.40	0.63
1:A:329:VAL:HG23	1:A:396:LEU:CD1	2.32	0.60
1:B:351:GLN:HB3	1:B:407:MET:HE3	1.82	0.60
1:A:407:MET:HG2	2:A:601:A1ICS:C15	2.32	0.58
1:B:362:GLU:HA	1:B:365:VAL:HG12	1.85	0.58
1:B:379:TYR:N	1:B:387:GLN:O	2.28	0.58
1:B:540:LEU:O	1:B:541:VAL:C	2.48	0.57
1:B:333:GLN:O	1:B:389:ALA:HB1	2.05	0.57
1:B:343:ARG:NH2	3:B:707:HOH:O	2.39	0.56
1:A:350:ILE:HD11	1:A:352:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LYS:HG2	1:B:273:PRO:HB2	1.88	0.54
1:B:410:MET:O	1:B:418:ASN:HA	2.09	0.53
1:B:464:HIS:CE1	3:B:723:HOH:O	2.61	0.53
1:B:464:HIS:HE1	3:B:723:HOH:O	1.91	0.53
1:A:490:LYS:HG3	1:A:494:ILE:HD12	1.91	0.53
1:A:304:LEU:HD22	1:A:320:ILE:CD1	2.39	0.52
1:A:469:LEU:HD12	1:A:480:PHE:CD1	2.45	0.52
1:A:407:MET:HG2	2:A:601:A1ICS:C14	2.40	0.52
1:B:463:GLY:HA3	1:B:465:TYR:CE1	2.45	0.51
1:A:431:LEU:HD22	1:A:518:TYR:CZ	2.46	0.51
1:A:408:ARG:NH1	1:A:423:ASP:O	2.44	0.49
1:B:227:SER:HB3	1:B:467:VAL:HB	1.94	0.49
1:B:370:VAL:CG1	1:B:390:GLU:HB2	2.42	0.49
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.94	0.49
1:B:354:ILE:HG21	1:B:406:LEU:HB3	1.94	0.49
1:B:256:VAL:HB	1:B:257:PRO:HD3	1.96	0.48
1:A:227:SER:HB3	1:A:454:LEU:CD1	2.43	0.48
1:B:492:GLU:HA	1:B:496:HIS:ND1	2.28	0.48
1:A:235:THR:O	1:A:238:LEU:HB3	2.14	0.48
1:B:377:ASN:OD1	1:B:377:ASN:N	2.47	0.48
1:B:374:ASP:CB	1:B:388:GLU:HB3	2.43	0.47
1:A:470:ASN:O	1:A:470:ASN:CG	2.58	0.47
1:B:328:MET:HE3	1:B:347:TYR:CD2	2.50	0.47
1:B:459:ASP:OD1	1:B:463:GLY:O	2.33	0.46
1:A:307:VAL:HG13	1:A:311:MET:HE3	1.97	0.46
2:A:601:A1ICS:O3	2:A:601:A1ICS:C11	2.64	0.45
1:B:351:GLN:HB3	1:B:407:MET:CE	2.46	0.45
1:A:225:MET:HG3	1:A:299:LEU:HD11	1.99	0.45
1:A:460:ASN:HD22	1:A:460:ASN:HA	1.61	0.45
1:B:514:TYR:OH	3:B:704:HOH:O	2.20	0.45
1:A:550:ILE:O	1:A:553:GLN:HG2	2.17	0.44
1:B:225:MET:O	1:B:226:ASN:C	2.57	0.44
1:B:228:LEU:HD12	1:B:299:LEU:HD13	1.99	0.44
1:B:374:ASP:HA	1:B:388:GLU:HB3	1.99	0.44
1:B:553:GLN:O	1:B:553:GLN:HG3	2.18	0.44
1:A:340:ARG:HB3	3:A:716:HOH:O	2.17	0.44
1:B:373:LEU:HD22	1:B:389:ALA:O	2.18	0.43
1:A:464:HIS:ND1	1:B:460:ASN:OD1	2.51	0.43
1:A:546:GLU:O	1:A:549:ARG:HB2	2.19	0.43
1:A:248:GLU:H	1:A:248:GLU:HG2	1.50	0.43
1:A:304:LEU:HD22	1:A:320:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LYS:NZ	1:A:495:GLU:OE1	2.45	0.43
1:A:256:VAL:O	1:A:257:PRO:C	2.61	0.43
1:B:225:MET:HE3	1:B:283:PHE:HZ	1.82	0.43
1:A:352:LEU:HD22	1:A:363:SER:HB3	2.01	0.42
1:B:399:PRO:O	1:B:448:TYR:OH	2.34	0.42
1:A:260:LEU:HD13	1:A:307:VAL:CG2	2.50	0.42
1:A:297:GLN:HE21	1:A:351:GLN:NE2	2.18	0.42
1:A:452:ALA:HA	1:A:468:TYR:O	2.20	0.41
1:B:375:GLY:O	1:B:377:ASN:N	2.53	0.41
1:A:296:VAL:O	1:A:297:GLN:C	2.62	0.41
1:A:396:LEU:C	1:A:397:THR:HG23	2.45	0.41
1:A:231:THR:HG21	1:A:517:VAL:HG21	2.03	0.41
1:A:231:THR:CG2	3:A:708:HOH:O	2.69	0.41
1:A:258:LEU:HD22	1:A:258:LEU:O	2.21	0.41
1:B:352:LEU:HD23	1:B:352:LEU:HA	1.95	0.41
1:B:537:PRO:O	1:B:541:VAL:HG23	2.21	0.40
1:B:381:ALA:O	1:B:383:GLU:N	2.54	0.40
1:A:325:ARG:C	1:A:325:ARG:HD2	2.47	0.40
1:B:455:VAL:HG13	1:B:511:THR:HB	2.04	0.40
1:A:221:ALA:HB2	1:B:221:ALA:HB2	2.03	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	318/355 (90%)	301 (95%)	16 (5%)	1 (0%)	36	56
1	B	314/355 (88%)	292 (93%)	19 (6%)	3 (1%)	12	24
All	All	632/710 (89%)	593 (94%)	35 (6%)	4 (1%)	21	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	382	GLY
1	B	376	ASP
1	B	381	ALA
1	A	552	ALA

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	294/321 (92%)	257 (87%)	37 (13%)	4	8
1	B	290/321 (90%)	256 (88%)	34 (12%)	5	9
All	All	584/642 (91%)	513 (88%)	71 (12%)	5	8

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	LEU
1	A	248	GLU
1	A	258	LEU
1	A	260	LEU
1	A	279	LEU
1	A	296	VAL
1	A	299	LEU
1	A	301	ARG
1	A	316	VAL
1	A	327	LYS
1	A	336	GLU
1	A	343	ARG
1	A	350	ILE
1	A	354	ILE
1	A	360	ILE
1	A	365	VAL
1	A	374	ASP
1	A	378	LYS
1	A	388	GLU
1	A	393	VAL

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Mol	Chain	Res	Type
1	A	402	LEU
1	A	420	LYS
1	A	421	ILE
1	A	432	PRO
1	A	435	GLU
1	A	438	GLN
1	A	459	ASP
1	A	476	LYS
1	A	483	ASP
1	A	487	ARG
1	A	490	LYS
1	A	495	GLU
1	A	511	THR
1	A	523	LYS
1	A	540	LEU
1	A	549	ARG
1	A	554	LYS
1	B	222	THR
1	B	228	LEU
1	B	238	LEU
1	B	240	LYS
1	B	244	MET
1	B	251	ASP
1	B	257	PRO
1	B	271	ASP
1	B	272	LYS
1	B	277	LYS
1	B	279	LEU
1	B	280	THR
1	B	287	THR
1	B	299	LEU
1	B	308	GLU
1	B	316	VAL
1	B	332	ILE
1	B	373	LEU
1	B	374	ASP
1	B	376	ASP
1	B	377	ASN
1	B	387	GLN
1	B	388	GLU
1	B	393	VAL
1	B	402	LEU

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Mol	Chain	Res	Type
1	B	410	MET
1	B	419	ILE
1	B	440	THR
1	B	443	LYS
1	B	454	LEU
1	B	455	VAL
1	B	457	SER
1	B	469	LEU
1	B	472	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	306	ASN
1	A	351	GLN
1	A	438	GLN
1	A	460	ASN
1	A	529	GLN
1	A	545	GLN
1	B	237	GLN
1	B	293	GLN
1	B	403	HIS
1	B	422	ASN
1	B	447	ASN
1	B	464	HIS
1	B	497	ASN
1	B	512	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	A1ICS	A	601	-	39,39,39	0.68	0	48,57,57	1.66	7 (14%)
2	A1ICS	B	601	-	39,39,39	0.84	1 (2%)	48,57,57	1.92	9 (18%)

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	A1ICS	A	601	-	-	7/17/46/46	0/5/5/5
2	A1ICS	B	601	-	-	5/17/46/46	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	A1ICS	C8-C9	-2.57	1.50	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	A1ICS	O2-C6-N2	-5.78	114.71	121.61
2	B	601	A1ICS	C4-C5-C6	5.48	117.62	109.64
2	B	601	A1ICS	O3-C9-C8	-4.93	96.44	108.25
2	B	601	A1ICS	O2-C6-C5	-4.81	113.35	121.85
2	A	601	A1ICS	C4-C5-C6	4.55	116.27	109.64
2	A	601	A1ICS	C9-C10-N3	-4.43	105.44	113.99
2	B	601	A1ICS	C22-C21-N1	4.24	116.80	112.23
2	B	601	A1ICS	C9-C10-N3	-3.57	107.10	113.99
2	B	601	A1ICS	C17-C18-N3	3.23	115.68	113.76
2	A	601	A1ICS	O2-C6-C5	-3.08	116.41	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	A1ICS	C22-C21-N1	2.83	115.29	112.23
2	B	601	A1ICS	O2-C6-N2	-2.70	118.39	121.61
2	B	601	A1ICS	C1-N1-C21	2.38	121.69	117.19
2	B	601	A1ICS	C11-N3-C18	-2.37	120.12	121.89
2	A	601	A1ICS	C3-C4-C5	-2.21	107.03	111.45
2	A	601	A1ICS	O3-C9-C8	-2.14	103.11	108.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

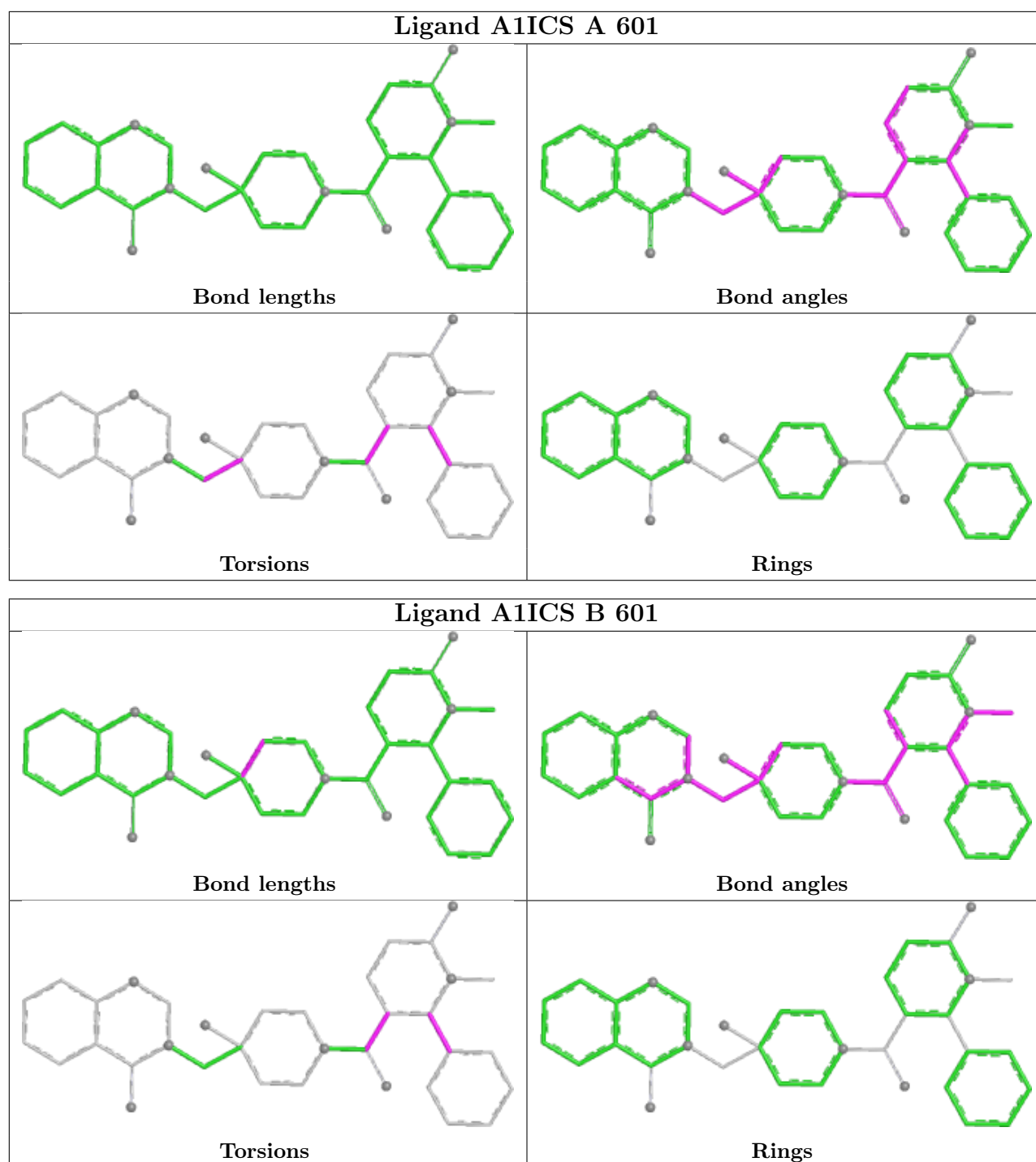
Mol	Chain	Res	Type	Atoms
2	A	601	A1ICS	N1-C21-C22-C27
2	B	601	A1ICS	N1-C21-C22-C27
2	B	601	A1ICS	N1-C21-C22-C23
2	A	601	A1ICS	N1-C21-C22-C23
2	A	601	A1ICS	C5-C21-C22-C27
2	B	601	A1ICS	C5-C21-C22-C27
2	A	601	A1ICS	C4-C5-C6-O2
2	B	601	A1ICS	C4-C5-C6-O2
2	B	601	A1ICS	C5-C21-C22-C23
2	A	601	A1ICS	C5-C21-C22-C23
2	A	601	A1ICS	C4-C5-C6-N2
2	A	601	A1ICS	N3-C10-C9-C8

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	A1ICS	4	0

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



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, 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	326/355 (91%)	-0.05	5 (1%) 72 71	28, 55, 92, 129	0
1	B	322/355 (90%)	0.14	4 (1%) 76 76	29, 58, 116, 161	0
All	All	648/710 (91%)	0.04	9 (1%) 73 73	28, 56, 106, 161	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	LEU	3.6
1	A	511	THR	2.8
1	B	260	LEU	2.6
1	A	460	ASN	2.3
1	B	379	TYR	2.1
1	B	410	MET	2.1
1	A	510	CYS	2.1
1	A	459	ASP	2.0
1	A	481	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,

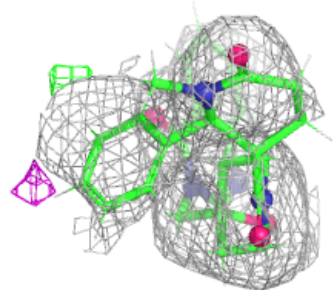
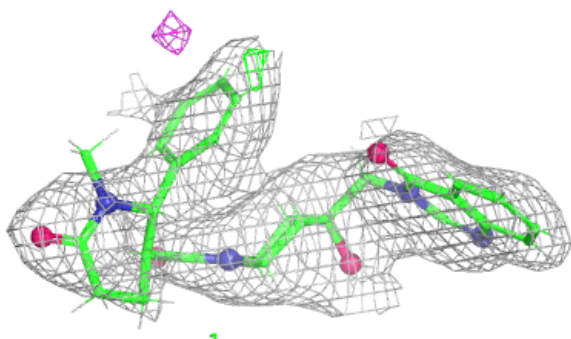
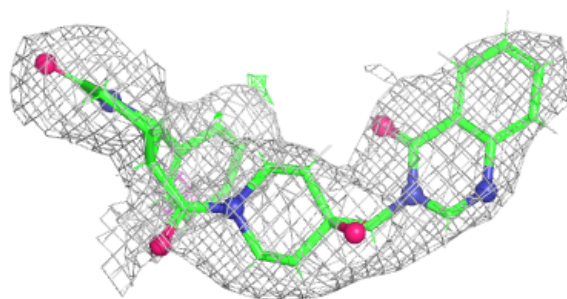
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1ICS	B	601	35/35	0.90	0.12	40,57,72,84	4
2	A1ICS	A	601	35/35	0.91	0.12	44,66,85,90	4

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.

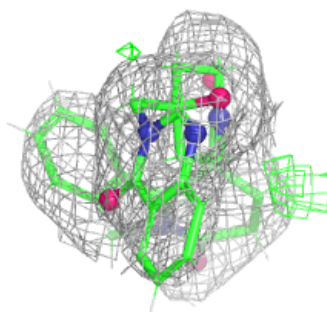
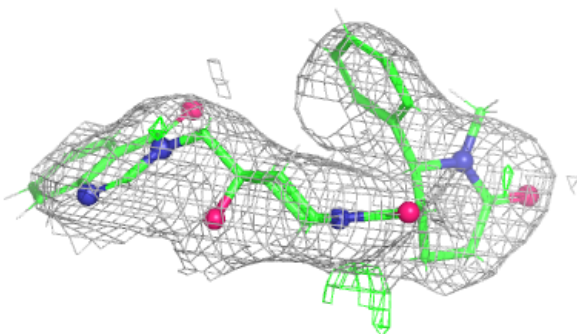
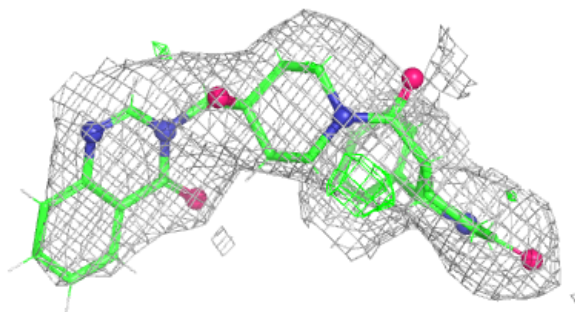
Electron density around A1ICS B 601:

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



Electron density around A1ICS 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.