



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:14 PM UTC

PDB ID : 5KKT / pdb_00005kkt
Title : ROCK 1 bound to azaindole thiazole piperazine inhibitor
Authors : Jacobs, M.D.
Deposited on : 2016-06-22
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

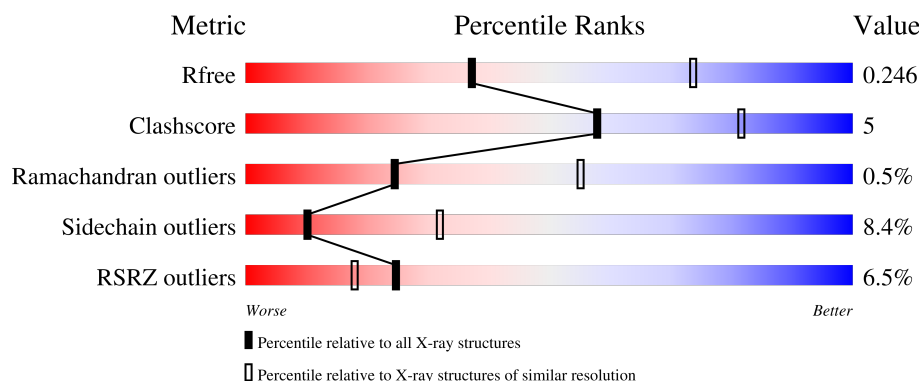
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	415	6% 76% 15% • 6%
1	B	415	7% 76% 17% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6621 atoms, of which 2 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.

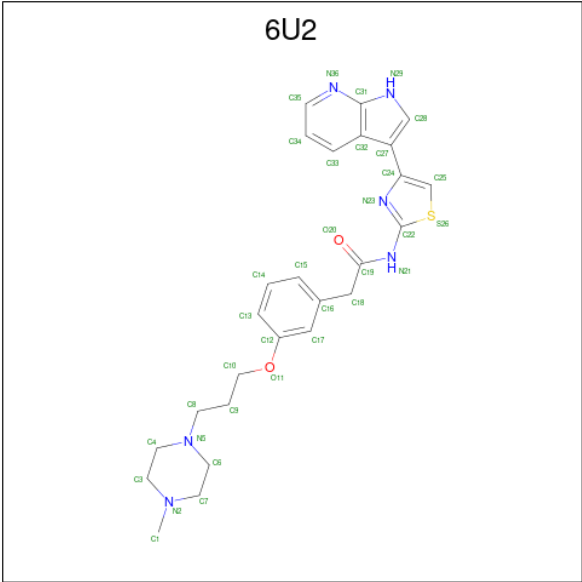
- Molecule 1 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3162	2026	526	589	21			
1	B	394	Total	C	N	O	S	0	0	0
			3195	2044	529	601	21			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q13464
A	2	SER	-	cloning artifact	UNP Q13464
A	3	LEU	-	cloning artifact	UNP Q13464
A	4	HIS	-	cloning artifact	UNP Q13464
A	5	MET	-	cloning artifact	UNP Q13464
B	1	GLY	-	cloning artifact	UNP Q13464
B	2	SER	-	cloning artifact	UNP Q13464
B	3	LEU	-	cloning artifact	UNP Q13464
B	4	HIS	-	cloning artifact	UNP Q13464
B	5	MET	-	cloning artifact	UNP Q13464

- Molecule 2 is 2-[3-[3-(4-methylpiperazin-1-yl)propoxy]phenyl]- {N}-[4-(1 {H}-pyrrolo[2,3-b]pyridin-3-yl)-1,3-thiazol-2-yl]ethanamide (CCD ID: 6U2) (formula: C₂₆H₃₀N₆O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			36	26	1	6	2	1		
2	B	1	Total	C	H	N	O	S	0	0
			36	26	1	6	2	1		

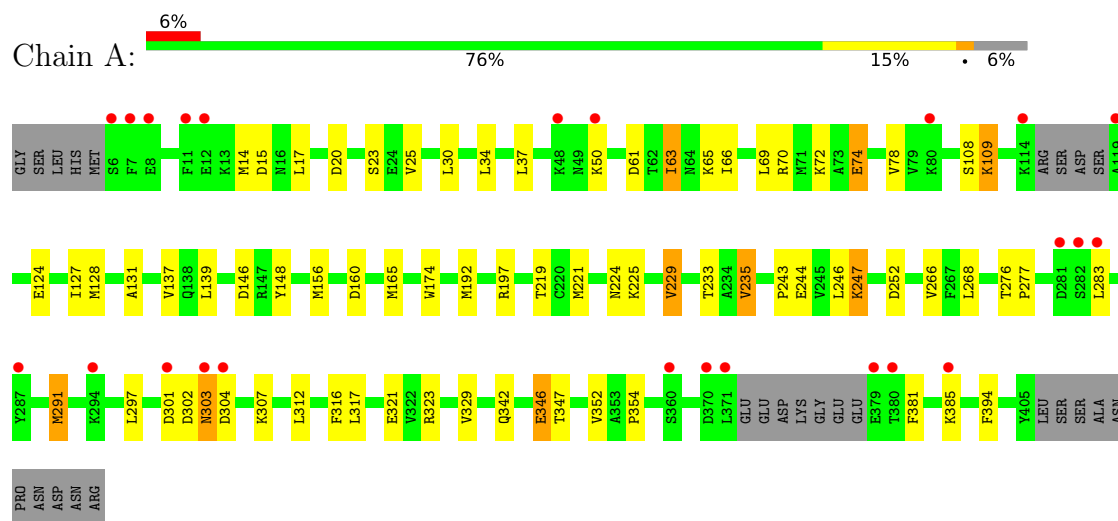
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total	O	0	0
			104	104		
3	B	88	Total	O	0	0
			88	88		

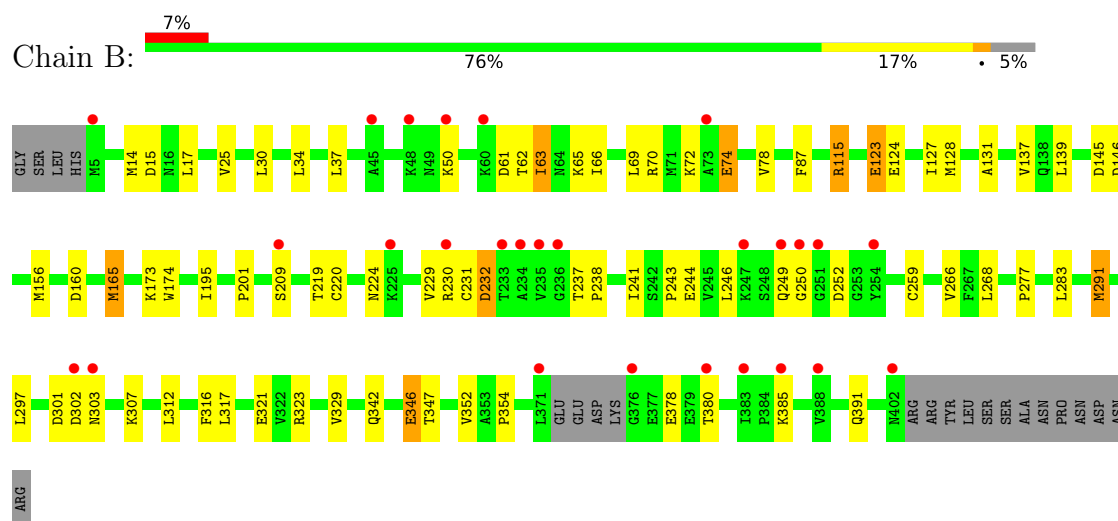
3 Residue-property plots [i](#)

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: Rho-associated protein kinase 1



- Molecule 1: Rho-associated protein kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.91Å 182.91Å 90.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.81 – 2.80 29.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.81-2.80) 98.5 (29.81-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 2.80Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.222 , 0.237 0.222 , 0.246	Depositor DCC
R_{free} test set	2076 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6621	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 3.18% 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: 6U2

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	0.88	4/3237 (0.1%)	1.33	20/4373 (0.5%)
1	B	0.85	3/3271 (0.1%)	1.33	12/4419 (0.3%)
All	All	0.87	7/6508 (0.1%)	1.33	32/8792 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	MET	SD-CE	-7.66	1.60	1.79
1	A	165	MET	SD-CE	-7.20	1.61	1.79
1	B	291	MET	SD-CE	-5.98	1.64	1.79
1	A	291	MET	SD-CE	-5.75	1.65	1.79
1	A	192	MET	SD-CE	5.47	1.93	1.79
1	A	156	MET	SD-CE	-5.10	1.66	1.79
1	B	156	MET	SD-CE	-5.08	1.66	1.79

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ASP	CA-C-N	6.52	133.99	121.54
1	A	302	ASP	C-N-CA	6.52	133.99	121.54
1	A	303	ASN	CA-CB-CG	6.04	118.64	112.60
1	A	65	LYS	CA-C-N	6.02	128.14	120.56
1	A	65	LYS	C-N-CA	6.02	128.14	120.56
1	B	65	LYS	CA-C-N	5.78	128.06	120.60
1	B	65	LYS	C-N-CA	5.78	128.06	120.60
1	A	146	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	232	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	307	LYS	CA-C-N	5.61	127.80	120.28
1	A	307	LYS	C-N-CA	5.61	127.80	120.28
1	A	381	PHE	CA-CB-CG	5.53	119.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	307	LYS	CA-C-N	5.45	127.58	120.28
1	B	307	LYS	C-N-CA	5.45	127.58	120.28
1	B	146	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	108	SER	CA-C-N	5.38	127.49	120.28
1	A	108	SER	C-N-CA	5.38	127.49	120.28
1	B	160	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	224	ASN	CA-CB-CG	5.32	117.92	112.60
1	B	302	ASP	CA-C-N	5.26	131.59	121.54
1	B	302	ASP	C-N-CA	5.26	131.59	121.54
1	A	148	TYR	CA-C-N	5.25	130.55	122.93
1	A	148	TYR	C-N-CA	5.25	130.55	122.93
1	B	224	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	301	ASP	CA-C-N	5.14	130.16	122.86
1	A	301	ASP	C-N-CA	5.14	130.16	122.86
1	A	61	ASP	CA-C-N	5.13	127.11	120.44
1	A	61	ASP	C-N-CA	5.13	127.11	120.44
1	B	61	ASP	CA-C-N	5.09	127.06	120.44
1	B	61	ASP	C-N-CA	5.09	127.06	120.44
1	A	304	ASP	CA-CB-CG	5.07	117.67	112.60

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	3162	0	3066	36	0
1	B	3195	0	3095	37	0
2	A	35	1	0	0	0
2	B	35	1	0	0	0
3	A	104	0	0	1	0
3	B	88	0	0	1	0
All	All	6619	2	6161	57	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 (57) 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:66:ILE:HD11	1:B:25:VAL:HG21	1.51	0.93
1:A:246:LEU:HD23	1:A:291:MET:HE3	1.50	0.92
1:A:316:PHE:O	1:A:323:ARG:HD2	1.85	0.77
1:B:316:PHE:O	1:B:323:ARG:HD2	1.86	0.75
1:B:243:PRO:HA	1:B:291:MET:HE1	1.73	0.71
1:A:70:ARG:HG3	1:B:14:MET:HE3	1.74	0.69
1:A:243:PRO:HA	1:A:291:MET:HE1	1.74	0.69
1:A:30:LEU:HB3	1:B:30:LEU:HB3	1.75	0.68
1:B:72:LYS:HG3	1:B:74:GLU:HG2	1.76	0.67
1:A:72:LYS:HG3	1:A:74:GLU:HG2	1.77	0.65
1:A:25:VAL:HG21	1:B:66:ILE:HD11	1.78	0.65
1:B:266:VAL:HG13	1:B:277:PRO:HD2	1.81	0.62
1:A:266:VAL:HG13	1:A:277:PRO:HD2	1.81	0.62
1:A:14:MET:HE3	1:B:70:ARG:HG3	1.83	0.60
1:A:221:MET:HG2	1:A:229:VAL:HG22	1.83	0.59
1:A:221:MET:HG2	1:A:229:VAL:CG2	2.36	0.56
1:A:124:GLU:HG2	1:A:128:MET:HE2	1.87	0.56
1:B:128:MET:HB3	1:B:139:LEU:HB2	1.88	0.55
1:B:173:LYS:HG2	3:B:641:HOH:O	2.07	0.54
1:B:124:GLU:HG2	1:B:128:MET:HE2	1.89	0.54
1:A:66:ILE:HG13	1:B:25:VAL:HG11	1.91	0.53
1:B:232:ASP:HB2	1:B:250:GLY:HA2	1.91	0.53
1:B:238:PRO:HA	1:B:241:ILE:HD12	1.90	0.53
1:A:14:MET:HE1	1:B:66:ILE:HA	1.90	0.52
1:A:128:MET:HB3	1:A:139:LEU:HB2	1.91	0.51
1:B:244:GLU:CD	1:B:323:ARG:HH22	2.18	0.51
1:A:37:LEU:HD13	1:B:37:LEU:HD13	1.92	0.51
1:A:66:ILE:HA	1:B:14:MET:HE1	1.93	0.51
1:A:109:LYS:HD2	1:A:394:PHE:CE2	2.47	0.50
1:B:246:LEU:O	1:B:249:GLN:HG2	2.10	0.50
1:A:316:PHE:O	1:A:323:ARG:CD	2.59	0.50
1:A:346:GLU:H	1:A:346:GLU:CD	2.21	0.49
1:B:243:PRO:HA	1:B:291:MET:CE	2.44	0.48
1:B:316:PHE:O	1:B:323:ARG:CD	2.60	0.47
1:B:87:PHE:HE1	1:B:115:ARG:HE	1.63	0.46
1:B:346:GLU:H	1:B:346:GLU:CD	2.22	0.46
1:A:174:TRP:CD1	1:A:354:PRO:HB3	2.51	0.45
1:A:20:ASP:HB3	1:A:23:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HG	1:B:63:ILE:HD11	1.99	0.45
1:B:123:GLU:HG3	1:B:220:CYS:O	2.16	0.45
1:A:34:LEU:HG	1:A:63:ILE:HD11	1.98	0.45
1:A:14:MET:CE	1:B:69:LEU:HB2	2.47	0.44
1:B:174:TRP:CD1	1:B:354:PRO:HB3	2.53	0.43
1:A:244:GLU:HA	1:A:247:LYS:HD3	1.99	0.43
1:A:276:THR:HB	3:A:608:HOH:O	2.19	0.43
1:A:69:LEU:CB	1:B:14:MET:HE2	2.49	0.42
1:A:197:ARG:CZ	1:A:235:VAL:HG11	2.49	0.42
1:A:14:MET:HE2	1:B:69:LEU:HB2	2.00	0.42
1:A:14:MET:HE2	1:B:69:LEU:CB	2.50	0.42
1:B:127:ILE:O	1:B:131:ALA:HB2	2.19	0.42
1:A:243:PRO:HA	1:A:291:MET:CE	2.45	0.42
1:A:69:LEU:HB2	1:B:14:MET:CE	2.50	0.41
1:B:165:MET:HE1	1:B:201:PRO:HG3	2.01	0.41
1:A:25:VAL:HG13	1:B:62:THR:CG2	2.50	0.41
1:A:127:ILE:O	1:A:131:ALA:HB2	2.21	0.41
1:A:69:LEU:HB2	1:B:14:MET:HE2	2.02	0.41
1:B:195:ILE:HG21	1:B:259:CYS:SG	2.62	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	383/415 (92%)	373 (97%)	8 (2%)	2 (0%)	24	55
1	B	390/415 (94%)	379 (97%)	9 (2%)	2 (0%)	24	55
All	All	773/830 (93%)	752 (97%)	17 (2%)	4 (0%)	24	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	B	303	ASN
1	A	252	ASP
1	B	237	THR

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	343/369 (93%)	317 (92%)	26 (8%)	12	36
1	B	348/369 (94%)	316 (91%)	32 (9%)	8	27
All	All	691/738 (94%)	633 (92%)	58 (8%)	10	32

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	17	LEU
1	A	50	LYS
1	A	63	ILE
1	A	74	GLU
1	A	78	VAL
1	A	109	LYS
1	A	137	VAL
1	A	219	THR
1	A	225	LYS
1	A	229	VAL
1	A	233	THR
1	A	235	VAL
1	A	247	LYS
1	A	268	LEU
1	A	283	LEU
1	A	297	LEU
1	A	312	LEU
1	A	317	LEU
1	A	321	GLU

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Mol	Chain	Res	Type
1	A	329	VAL
1	A	342	GLN
1	A	346	GLU
1	A	347	THR
1	A	352	VAL
1	A	385	LYS
1	B	15	ASP
1	B	17	LEU
1	B	50	LYS
1	B	63	ILE
1	B	74	GLU
1	B	78	VAL
1	B	115	ARG
1	B	123	GLU
1	B	137	VAL
1	B	145	ASP
1	B	209	SER
1	B	219	THR
1	B	229	VAL
1	B	230	ARG
1	B	231	CYS
1	B	252	ASP
1	B	268	LEU
1	B	283	LEU
1	B	297	LEU
1	B	301	ASP
1	B	312	LEU
1	B	317	LEU
1	B	321	GLU
1	B	329	VAL
1	B	342	GLN
1	B	346	GLU
1	B	347	THR
1	B	352	VAL
1	B	378	GLU
1	B	380	THR
1	B	385	LYS
1	B	391	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	91	GLN
1	A	167	ASN
1	B	16	ASN
1	B	91	GLN
1	B	167	ASN

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	6U2	B	501	-	38,39,39	0.86	1 (2%)	52,53,53	2.38	12 (23%)
2	6U2	A	501	-	38,39,39	0.94	2 (5%)	52,53,53	2.38	14 (26%)

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	6U2	B	501	-	-	9/19/29/29	0/5/5/5
2	6U2	A	501	-	-	11/19/29/29	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6U2	C22-S26	-3.02	1.69	1.74
2	A	501	6U2	C24-N23	-2.71	1.32	1.38
2	B	501	6U2	C24-N23	-2.62	1.33	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	6U2	C27-C24-N23	9.30	123.89	117.20
2	A	501	6U2	C27-C24-N23	7.87	122.86	117.20
2	B	501	6U2	C22-N23-C24	5.73	117.47	109.45
2	B	501	6U2	C32-C31-N36	-5.56	119.58	126.31
2	A	501	6U2	C22-N23-C24	5.35	116.94	109.45
2	A	501	6U2	S26-C22-N23	-5.12	110.31	115.69
2	A	501	6U2	C31-N29-C28	5.10	110.89	108.48
2	B	501	6U2	S26-C22-N23	-5.07	110.36	115.69
2	A	501	6U2	C25-C24-C27	-5.06	122.92	127.62
2	A	501	6U2	C32-C31-N36	-4.78	120.52	126.31
2	B	501	6U2	C25-C24-C27	-4.57	123.37	127.62
2	B	501	6U2	N29-C31-N36	3.91	133.02	126.69
2	A	501	6U2	N29-C31-N36	3.43	132.25	126.69
2	B	501	6U2	C18-C19-N21	3.42	118.57	114.40
2	A	501	6U2	C10-O11-C12	3.34	126.61	117.93
2	A	501	6U2	C25-S26-C22	3.32	90.98	88.40
2	A	501	6U2	C32-C31-N29	-3.27	107.23	108.42
2	B	501	6U2	C31-N29-C28	3.02	109.90	108.48
2	B	501	6U2	C35-N36-C31	2.83	122.26	116.74
2	B	501	6U2	C32-C31-N29	-2.80	107.40	108.42
2	B	501	6U2	C7-N2-C3	2.51	113.54	109.54
2	A	501	6U2	C24-C25-S26	-2.34	107.53	110.24
2	A	501	6U2	C33-C32-C31	2.33	119.48	117.16
2	A	501	6U2	C7-N2-C3	2.31	113.22	109.54
2	B	501	6U2	C6-N5-C4	2.31	113.83	108.84
2	A	501	6U2	C35-N36-C31	2.28	121.19	116.74

There are no chirality outliers.

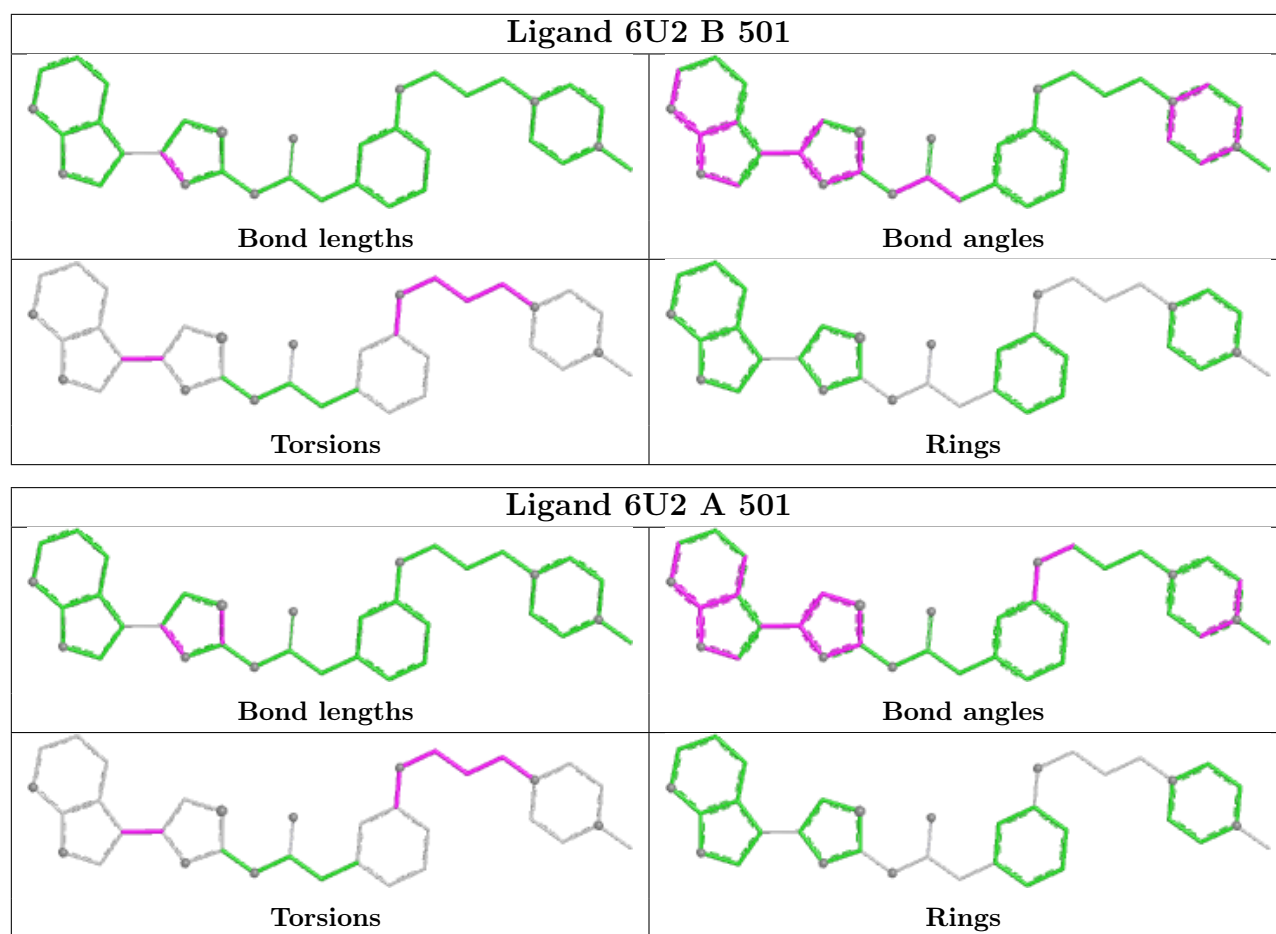
All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	6U2	C25-C24-C27-C28
2	A	501	6U2	C25-C24-C27-C32
2	A	501	6U2	O11-C10-C9-C8
2	B	501	6U2	O11-C10-C9-C8
2	A	501	6U2	C9-C8-N5-C4
2	A	501	6U2	C9-C8-N5-C6
2	B	501	6U2	C9-C8-N5-C4
2	B	501	6U2	N5-C8-C9-C10
2	A	501	6U2	N5-C8-C9-C10
2	B	501	6U2	C9-C10-O11-C12
2	A	501	6U2	C9-C10-O11-C12
2	B	501	6U2	C9-C8-N5-C6
2	A	501	6U2	C17-C12-O11-C10
2	B	501	6U2	C25-C24-C27-C32
2	B	501	6U2	C25-C24-C27-C28
2	A	501	6U2	N23-C24-C27-C32
2	A	501	6U2	N23-C24-C27-C28
2	B	501	6U2	N23-C24-C27-C28
2	B	501	6U2	C13-C12-O11-C10
2	A	501	6U2	C13-C12-O11-C10

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.



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, 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	389/415 (93%)	0.27	24 (6%) 26 20	48, 67, 108, 131	0
1	B	394/415 (94%)	0.42	27 (6%) 23 16	48, 76, 115, 138	0
All	All	783/830 (94%)	0.35	51 (6%) 25 18	48, 72, 112, 138	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	ASN	5.0
1	B	385	LYS	4.9
1	A	48	LYS	4.8
1	A	281	ASP	4.5
1	B	233	THR	4.5
1	B	225	LYS	3.8
1	A	304	ASP	3.2
1	A	11	PHE	3.2
1	B	235	VAL	3.2
1	B	302	ASP	3.1
1	A	114	LYS	3.0
1	A	7	PHE	3.0
1	B	371	LEU	3.0
1	B	376	GLY	2.9
1	A	6	SER	2.8
1	A	119	ALA	2.7
1	A	50	LYS	2.7
1	B	250	GLY	2.7
1	A	287	TYR	2.7
1	B	48	LYS	2.7
1	A	385	LYS	2.6
1	B	249	GLN	2.5
1	A	301	ASP	2.5
1	A	282	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	247	LYS	2.3
1	A	12	GLU	2.3
1	A	370	ASP	2.3
1	B	383	ILE	2.3
1	A	294	LYS	2.3
1	B	303	ASN	2.3
1	B	234	ALA	2.3
1	A	371	LEU	2.3
1	A	380	THR	2.3
1	B	73	ALA	2.3
1	B	209	SER	2.2
1	A	379	GLU	2.2
1	B	402	ASN	2.2
1	A	360	SER	2.2
1	B	236	GLY	2.2
1	A	80	LYS	2.2
1	B	45	ALA	2.2
1	B	60	LYS	2.1
1	B	380	THR	2.1
1	B	254	TYR	2.1
1	B	230	ARG	2.1
1	B	50	LYS	2.0
1	B	388	VAL	2.0
1	B	5	MET	2.0
1	A	283	LEU	2.0
1	B	251	GLY	2.0
1	A	8	GLU	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.

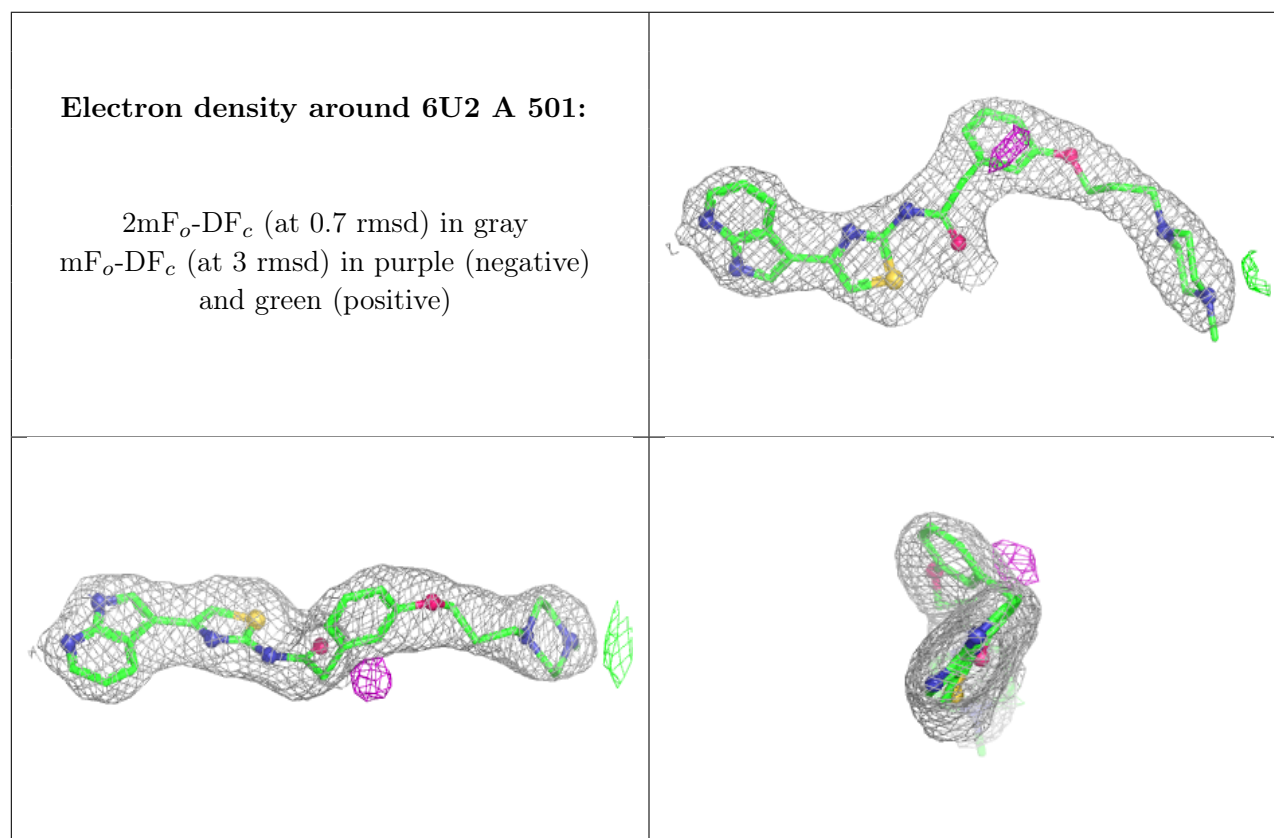
6.4 Ligands [i](#)

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.

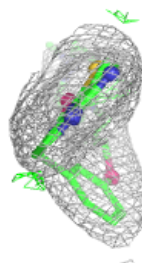
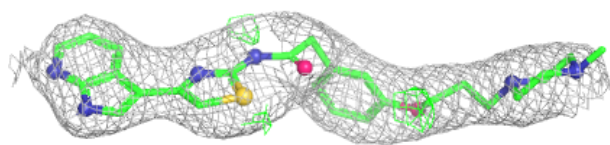
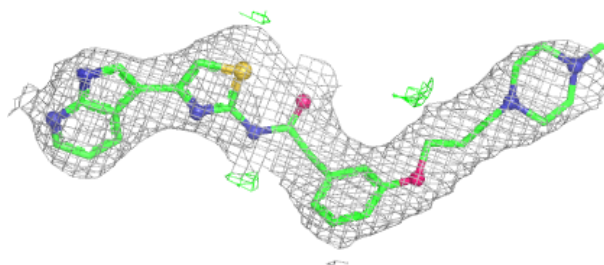
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	6U2	A	501	35/35	0.96	0.09	51,57,79,82	0
2	6U2	B	501	35/35	0.97	0.09	58,68,80,82	0

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 6U2 B 501:

$2mF_o-DF_c$ (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.