



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:47 AM UTC

PDB ID : 5KKS / pdb_00005kks
Title : ROCK 1 bound to azaindole thiazole inhibitor
Authors : Jacobs, M.D.
Deposited on : 2016-06-22
Resolution : 3.30 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

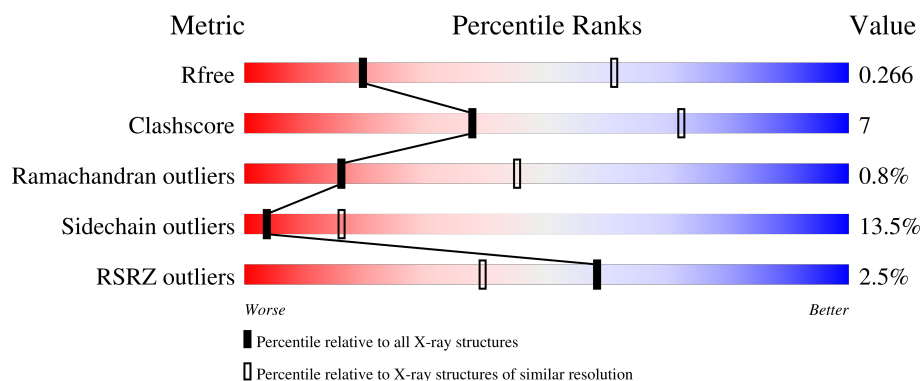
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	2% 67% 25% • 5%
1	B	415	2% 64% 27% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6570 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.

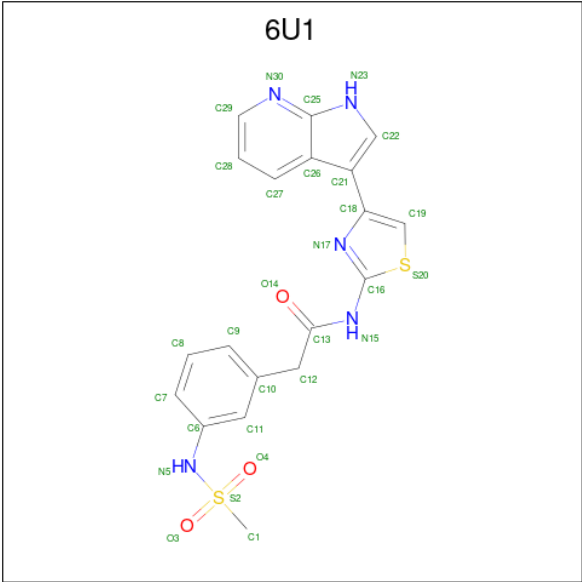
- Molecule 1 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3211	2052	535	603	21			
1	B	395	Total	C	N	O	S	0	0	0
			3200	2047	530	602	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-(methylsulfonylamino)phenyl]- {N}-[4-(1 {H}-pyrrolo[2,3-b]pyridin-3-yl)-1,3-thiazol-2-yl]ethanamide (CCD ID: 6U1) (formula: C₁₉H₁₇N₅O₃S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 30	C 19	H 1	N 5	O 3	S 2	0	0
2	B	1	Total 30	C 19	H 1	N 5	O 3	S 2	0	0

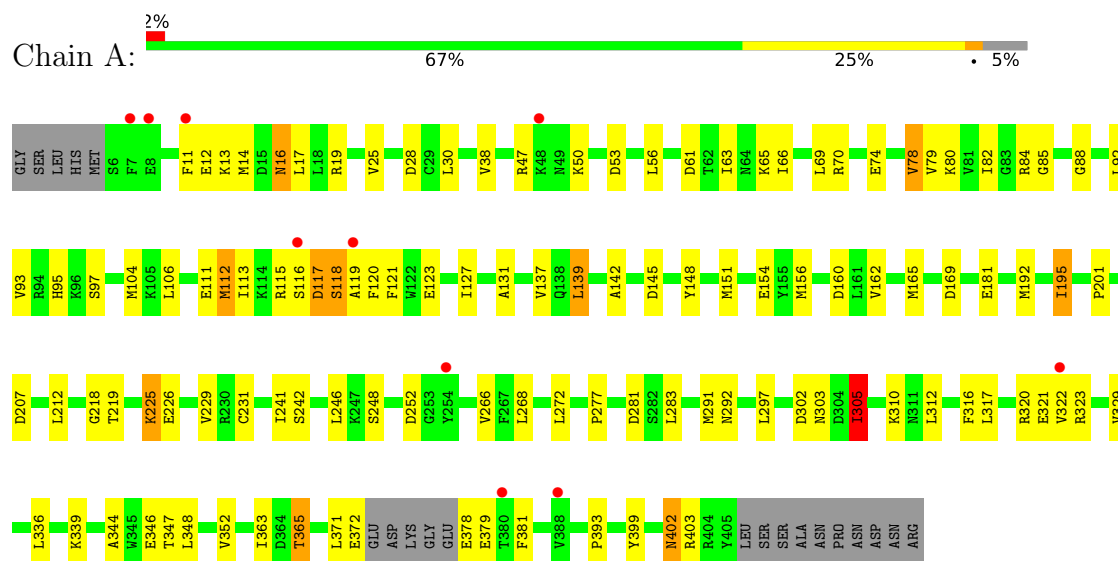
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	43	Total	O	0	0
			43	43		

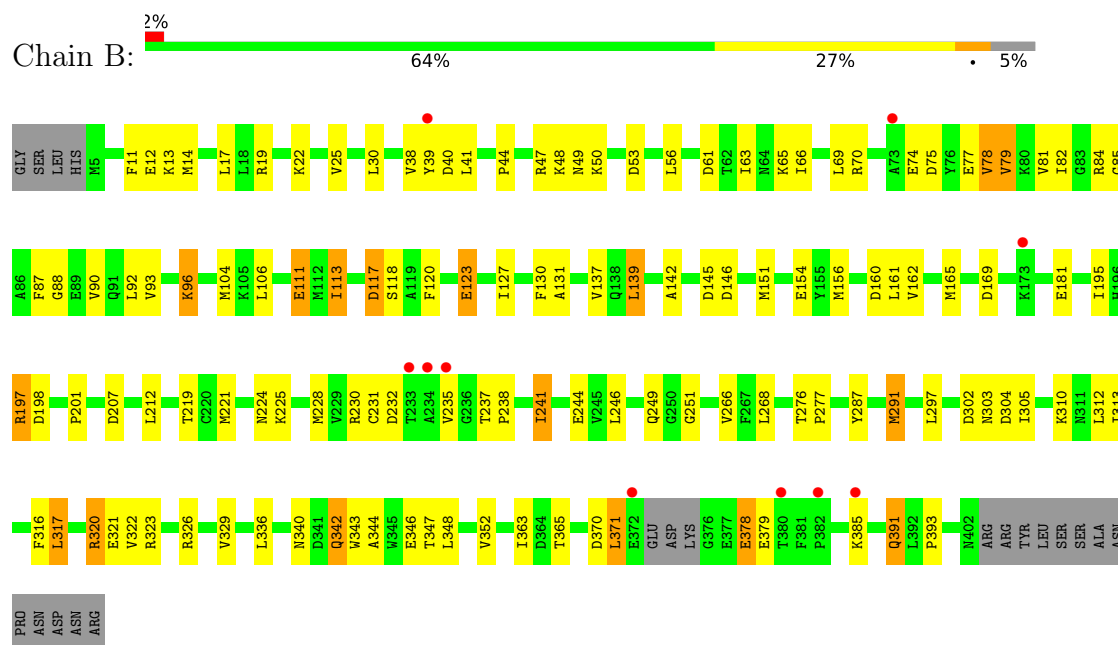
3 Residue-property plots

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	182.34Å 182.34Å 90.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.67 – 3.30 29.67 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.67-3.30) 96.9 (29.67-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.31Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.213 , 0.254 0.221 , 0.266	Depositor DCC
R_{free} test set	1230 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	89.5	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6570	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: 6U1

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	1/3287 (0.0%)	1.37	21/4441 (0.5%)
1	B	0.87	0/3276	1.36	25/4426 (0.6%)
All	All	0.88	1/6563 (0.0%)	1.37	46/8867 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	MET	SD-CE	5.20	1.92	1.79

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	ASN	CA-CB-CG	7.64	120.24	112.60
1	B	241	ILE	CA-C-N	7.58	132.19	120.68
1	B	241	ILE	C-N-CA	7.58	132.19	120.68
1	B	117	ASP	CA-CB-CG	7.50	120.10	112.60
1	A	119	ALA	CA-C-N	7.12	129.82	120.28
1	A	119	ALA	C-N-CA	7.12	129.82	120.28
1	B	145	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	160	ASP	CA-CB-CG	6.55	119.16	112.60
1	A	145	ASP	CA-CB-CG	6.53	119.13	112.60
1	B	160	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	305	ILE	N-CA-CB	5.98	117.65	110.95
1	A	117	ASP	CA-CB-CG	5.86	118.45	112.60
1	A	16	ASN	CA-CB-CG	5.83	118.43	112.60
1	B	40	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	207	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	381	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	292	ASN	CA-CB-CG	5.36	117.96	112.60
1	B	304	ASP	N-CA-C	-5.34	106.80	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	TYR	N-CA-C	5.34	117.52	109.41
1	B	320	ARG	CA-C-N	5.31	128.13	120.38
1	B	320	ARG	C-N-CA	5.31	128.13	120.38
1	B	11	PHE	CA-C-N	5.30	127.33	120.44
1	B	11	PHE	C-N-CA	5.30	127.33	120.44
1	A	320	ARG	CA-C-N	5.29	128.10	120.38
1	A	320	ARG	C-N-CA	5.29	128.10	120.38
1	A	169	ASP	N-CA-C	-5.26	98.73	107.99
1	B	378	GLU	CB-CG-CD	5.21	121.46	112.60
1	B	61	ASP	CA-C-N	5.20	127.51	120.65
1	B	61	ASP	C-N-CA	5.20	127.51	120.65
1	A	11	PHE	CA-C-N	5.19	127.19	120.44
1	A	11	PHE	C-N-CA	5.19	127.19	120.44
1	B	49	ASN	CA-CB-CG	5.19	117.79	112.60
1	B	65	LYS	CA-C-N	5.17	127.28	120.60
1	B	65	LYS	C-N-CA	5.17	127.28	120.60
1	A	207	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	232	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	44	PRO	CA-C-N	5.14	127.12	120.44
1	B	44	PRO	C-N-CA	5.14	127.12	120.44
1	A	61	ASP	CA-C-N	5.11	127.40	120.65
1	A	61	ASP	C-N-CA	5.11	127.40	120.65
1	A	195	ILE	N-CA-CB	5.08	117.86	111.46
1	A	65	LYS	CA-C-N	5.06	127.13	120.60
1	A	65	LYS	C-N-CA	5.06	127.13	120.60
1	B	169	ASP	N-CA-C	-5.05	99.09	107.99
1	B	232	ASP	CA-C-N	5.03	128.84	120.94
1	B	232	ASP	C-N-CA	5.03	128.84	120.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3211	0	3106	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3200	0	3097	58	0
2	A	29	1	0	0	0
2	B	29	1	0	1	0
3	A	56	0	0	0	0
3	B	43	0	0	0	0
All	All	6568	2	6203	89	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 7.

All (89) 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:70:ARG:HG3	1:B:14:MET:HE3	1.46	0.96
1:A:66:ILE:HD11	1:B:25:VAL:HG21	1.48	0.94
1:B:195:ILE:HG22	1:B:197:ARG:HG2	1.70	0.73
1:B:316:PHE:O	1:B:323:ARG:HD2	1.92	0.69
1:B:340:ASN:HD22	1:B:342:GLN:HG2	1.60	0.67
1:A:316:PHE:O	1:A:323:ARG:HD2	1.94	0.67
1:A:14:MET:HE3	1:B:70:ARG:HG3	1.76	0.66
1:A:95:HIS:CE1	1:A:97:SER:HB3	2.31	0.66
1:B:340:ASN:HD21	1:B:343:TRP:H	1.42	0.65
1:A:25:VAL:HG21	1:B:66:ILE:HD11	1.80	0.64
1:A:113:ILE:HD11	1:A:393:PRO:HG3	1.79	0.63
1:A:127:ILE:O	1:A:131:ALA:HB2	1.98	0.63
1:A:95:HIS:HE1	1:A:97:SER:HB3	1.65	0.61
1:A:47:ARG:HD3	1:A:53:ASP:HA	1.82	0.61
1:B:113:ILE:HD11	1:B:393:PRO:HG3	1.83	0.60
1:B:47:ARG:HD3	1:B:53:ASP:HA	1.83	0.60
1:A:69:LEU:HB2	1:B:14:MET:HE2	1.84	0.59
1:B:127:ILE:O	1:B:131:ALA:HB2	2.02	0.58
1:B:197:ARG:HE	1:B:221:MET:HG3	1.67	0.58
1:B:117:ASP:O	1:B:120:PHE:HD1	1.87	0.58
1:B:244:GLU:CD	1:B:323:ARG:HH22	2.12	0.58
1:A:120:PHE:HB2	1:A:218:GLY:O	2.04	0.57
1:A:14:MET:HE1	1:B:66:ILE:HA	1.86	0.57
1:A:19:ARG:HH12	1:B:19:ARG:HH12	1.51	0.57
1:B:344:ALA:HB3	1:B:347:THR:HG22	1.87	0.56
1:A:344:ALA:HB3	1:A:347:THR:HG22	1.87	0.56
1:A:302:ASP:HB3	1:A:305:ILE:HG12	1.88	0.56
1:A:78:VAL:HA	1:A:93:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLU:HG2	1:B:320:ARG:HD2	1.88	0.55
1:A:92:LEU:HD22	1:A:365:THR:HG23	1.88	0.55
1:A:272:LEU:HB3	1:A:305:ILE:HD12	1.89	0.54
1:B:246:LEU:O	1:B:249:GLN:HG2	2.07	0.54
1:A:241:ILE:HG21	1:A:246:LEU:HD13	1.89	0.53
1:A:112:MET:HE1	1:A:121:PHE:CD1	2.43	0.53
1:B:78:VAL:HA	1:B:93:VAL:HG12	1.89	0.53
1:B:79:VAL:HB	1:B:92:LEU:HD23	1.91	0.53
1:B:323:ARG:O	1:B:326:ARG:HD2	2.09	0.52
1:B:162:VAL:HG23	1:B:201:PRO:HB2	1.91	0.52
1:B:41:LEU:HB2	1:B:56:LEU:HD21	1.92	0.52
1:A:66:ILE:CD1	1:B:25:VAL:HG21	2.32	0.52
1:A:162:VAL:HG23	1:A:201:PRO:HB2	1.93	0.51
1:A:28:ASP:H	1:A:402:ASN:ND2	2.09	0.51
1:A:47:ARG:O	1:A:53:ASP:HB2	2.11	0.51
1:B:146:ASP:HA	1:B:391:GLN:NE2	2.26	0.50
1:A:225:LYS:HD3	1:A:226:GLU:HG3	1.94	0.50
1:B:197:ARG:HE	1:B:221:MET:CG	2.24	0.50
1:A:14:MET:HE2	1:B:69:LEU:HB2	1.92	0.50
1:B:47:ARG:O	1:B:53:ASP:HB2	2.11	0.50
1:B:266:VAL:HG13	1:B:277:PRO:HD2	1.94	0.49
1:B:340:ASN:ND2	1:B:343:TRP:H	2.09	0.49
1:A:82:ILE:HD13	1:A:92:LEU:HB2	1.94	0.49
1:A:266:VAL:HG13	1:A:277:PRO:HD2	1.95	0.48
1:A:38:VAL:HG11	1:A:63:ILE:HG21	1.94	0.48
1:B:87:PHE:HD1	1:B:111:GLU:HB3	1.79	0.48
1:B:287:TYR:CE1	1:B:291:MET:HE2	2.49	0.48
1:B:22:LYS:HG2	1:B:130:PHE:CE1	2.50	0.47
1:B:88:GLY:HA3	1:B:106:LEU:O	2.15	0.47
1:B:38:VAL:HG11	1:B:63:ILE:HG21	1.97	0.47
1:A:112:MET:O	1:A:116:SER:HB2	2.15	0.47
1:B:139:LEU:HD11	1:B:142:ALA:HB2	1.97	0.46
1:A:88:GLY:HA3	1:A:106:LEU:O	2.16	0.46
1:B:238:PRO:HA	1:B:241:ILE:HD12	1.98	0.45
1:B:81:VAL:O	1:B:371:LEU:HB2	2.17	0.45
1:B:165:MET:HE1	1:B:201:PRO:HB3	1.99	0.45
1:B:244:GLU:CG	1:B:320:ARG:HD2	2.47	0.45
1:A:181:GLU:HG2	1:A:348:LEU:HD21	1.99	0.45
1:B:342:GLN:H	1:B:342:GLN:CD	2.25	0.45
1:A:118:SER:HB3	1:A:120:PHE:HD1	1.83	0.44
1:A:30:LEU:HB3	1:B:30:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:TYR:CE2	1:A:403:ARG:HG2	2.53	0.44
1:B:39:TYR:CE1	1:B:146:ASP:HB3	2.54	0.43
1:B:84:ARG:HG3	1:B:85:GLY:H	1.82	0.43
1:B:230:ARG:HH22	1:B:251:GLY:HA3	1.83	0.43
1:B:90:VAL:HG21	2:B:501:6U1:N15	2.33	0.43
1:A:154:GLU:HG3	1:A:156:MET:HE3	2.00	0.43
1:B:82:ILE:HD13	1:B:92:LEU:HB2	2.01	0.42
1:B:181:GLU:HG2	1:B:348:LEU:HD21	2.01	0.42
1:A:104:MET:HA	1:A:151:MET:O	2.19	0.42
1:B:340:ASN:HD21	1:B:343:TRP:N	2.14	0.42
1:A:84:ARG:HG3	1:A:85:GLY:H	1.83	0.42
1:B:104:MET:HA	1:B:151:MET:O	2.20	0.41
1:B:75:ASP:O	1:B:96:LYS:HG3	2.20	0.41
1:B:123:GLU:O	1:B:127:ILE:HD12	2.20	0.41
1:B:146:ASP:HA	1:B:391:GLN:HE22	1.86	0.41
1:A:165:MET:HE1	1:A:201:PRO:HB3	2.03	0.41
1:B:154:GLU:HG3	1:B:156:MET:HE3	2.03	0.41
1:B:303:ASN:C	1:B:305:ILE:H	2.29	0.41
1:B:313:ILE:HG23	1:B:317:LEU:HD22	2.03	0.41
1:A:139:LEU:HD11	1:A:142:ALA:HB2	2.04	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	391/415 (94%)	364 (93%)	24 (6%)	3 (1%)	16	45
1	B	391/415 (94%)	368 (94%)	20 (5%)	3 (1%)	16	45
All	All	782/830 (94%)	732 (94%)	44 (6%)	6 (1%)	16	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	SER
1	B	302	ASP
1	A	115	ARG
1	A	252	ASP
1	B	118	SER
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	349/369 (95%)	301 (86%)	48 (14%)	3	15
1	B	348/369 (94%)	302 (87%)	46 (13%)	4	17
All	All	697/738 (94%)	603 (86%)	94 (14%)	4	16

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	13	LYS
1	A	16	ASN
1	A	17	LEU
1	A	50	LYS
1	A	56	LEU
1	A	74	GLU
1	A	78	VAL
1	A	79	VAL
1	A	80	LYS
1	A	111	GLU
1	A	112	MET
1	A	117	ASP
1	A	118	SER
1	A	123	GLU
1	A	137	VAL
1	A	139	LEU
1	A	195	ILE

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Mol	Chain	Res	Type
1	A	212	LEU
1	A	219	THR
1	A	225	LYS
1	A	229	VAL
1	A	231	CYS
1	A	242	SER
1	A	268	LEU
1	A	281	ASP
1	A	283	LEU
1	A	291	MET
1	A	297	LEU
1	A	303	ASN
1	A	305	ILE
1	A	310	LYS
1	A	312	LEU
1	A	317	LEU
1	A	321	GLU
1	A	322	VAL
1	A	329	VAL
1	A	336	LEU
1	A	339	LYS
1	A	346	GLU
1	A	352	VAL
1	A	363	ILE
1	A	365	THR
1	A	371	LEU
1	A	372	GLU
1	A	378	GLU
1	A	379	GLU
1	A	402	ASN
1	B	12	GLU
1	B	13	LYS
1	B	17	LEU
1	B	48	LYS
1	B	50	LYS
1	B	74	GLU
1	B	77	GLU
1	B	78	VAL
1	B	79	VAL
1	B	96	LYS
1	B	111	GLU
1	B	113	ILE

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Mol	Chain	Res	Type
1	B	123	GLU
1	B	137	VAL
1	B	139	LEU
1	B	161	LEU
1	B	197	ARG
1	B	198	ASP
1	B	212	LEU
1	B	219	THR
1	B	225	LYS
1	B	228	MET
1	B	231	CYS
1	B	235	VAL
1	B	268	LEU
1	B	276	THR
1	B	291	MET
1	B	297	LEU
1	B	310	LYS
1	B	312	LEU
1	B	317	LEU
1	B	321	GLU
1	B	322	VAL
1	B	329	VAL
1	B	336	LEU
1	B	342	GLN
1	B	346	GLU
1	B	352	VAL
1	B	363	ILE
1	B	365	THR
1	B	370	ASP
1	B	371	LEU
1	B	378	GLU
1	B	379	GLU
1	B	385	LYS
1	B	391	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	203	ASN
1	A	295	ASN
1	A	402	ASN

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Mol	Chain	Res	Type
1	B	54	ASN
1	B	64	ASN
1	B	167	ASN
1	B	203	ASN
1	B	295	ASN
1	B	340	ASN
1	B	391	GLN

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	6U1	A	501	-	31,32,32	1.32	4 (12%)	45,46,46	2.40	13 (28%)
2	6U1	B	501	-	31,32,32	1.13	3 (9%)	45,46,46	2.49	14 (31%)

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	6U1	A	501	-	-	3/17/17/17	0/4/4/4
2	6U1	B	501	-	-	4/17/17/17	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6U1	C18-N17	-3.26	1.31	1.38
2	A	501	6U1	C1-S2	3.05	1.82	1.75
2	B	501	6U1	C1-S2	2.93	1.82	1.75
2	B	501	6U1	C18-N17	-2.73	1.32	1.38
2	A	501	6U1	S2-N5	2.63	1.66	1.63
2	B	501	6U1	C6-N5	-2.45	1.39	1.43
2	A	501	6U1	C16-S20	-2.25	1.70	1.74

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	6U1	C21-C18-N17	9.50	124.04	117.20
2	A	501	6U1	C21-C18-N17	7.39	122.51	117.20
2	B	501	6U1	C26-C25-N30	-5.77	119.32	126.31
2	A	501	6U1	C16-N17-C18	5.57	117.24	109.45
2	B	501	6U1	C16-N17-C18	5.20	116.73	109.45
2	A	501	6U1	C26-C25-N30	-5.17	120.05	126.31
2	A	501	6U1	S20-C16-N17	-4.99	110.45	115.69
2	A	501	6U1	C19-C18-C21	-4.84	123.12	127.62
2	B	501	6U1	C19-C18-C21	-4.59	123.35	127.62
2	B	501	6U1	N23-C25-N30	3.91	133.03	126.69
2	B	501	6U1	O4-S2-O3	3.55	123.63	118.87
2	A	501	6U1	N23-C25-N30	3.52	132.40	126.69
2	B	501	6U1	S20-C16-N17	-3.51	112.00	115.69
2	A	501	6U1	C25-N23-C22	3.50	110.13	108.48
2	B	501	6U1	O3-S2-C1	3.30	113.48	108.26
2	A	501	6U1	C27-C26-C25	2.62	119.77	117.16
2	A	501	6U1	C12-C13-N15	2.61	117.58	114.40
2	B	501	6U1	C29-N30-C25	2.56	121.73	116.74
2	B	501	6U1	C27-C26-C25	2.56	119.71	117.16
2	A	501	6U1	O4-S2-O3	2.42	122.11	118.87
2	A	501	6U1	C26-C25-N23	-2.37	107.56	108.42
2	B	501	6U1	C12-C13-N15	2.32	117.23	114.40
2	B	501	6U1	O3-S2-N5	-2.20	102.70	107.10
2	A	501	6U1	S20-C16-N15	2.15	127.13	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	6U1	C19-C18-N17	-2.15	112.48	115.43
2	A	501	6U1	C29-N30-C25	2.14	120.91	116.74
2	B	501	6U1	C26-C25-N23	-2.12	107.65	108.42

There are no chirality outliers.

All (7) torsion outliers are listed below:

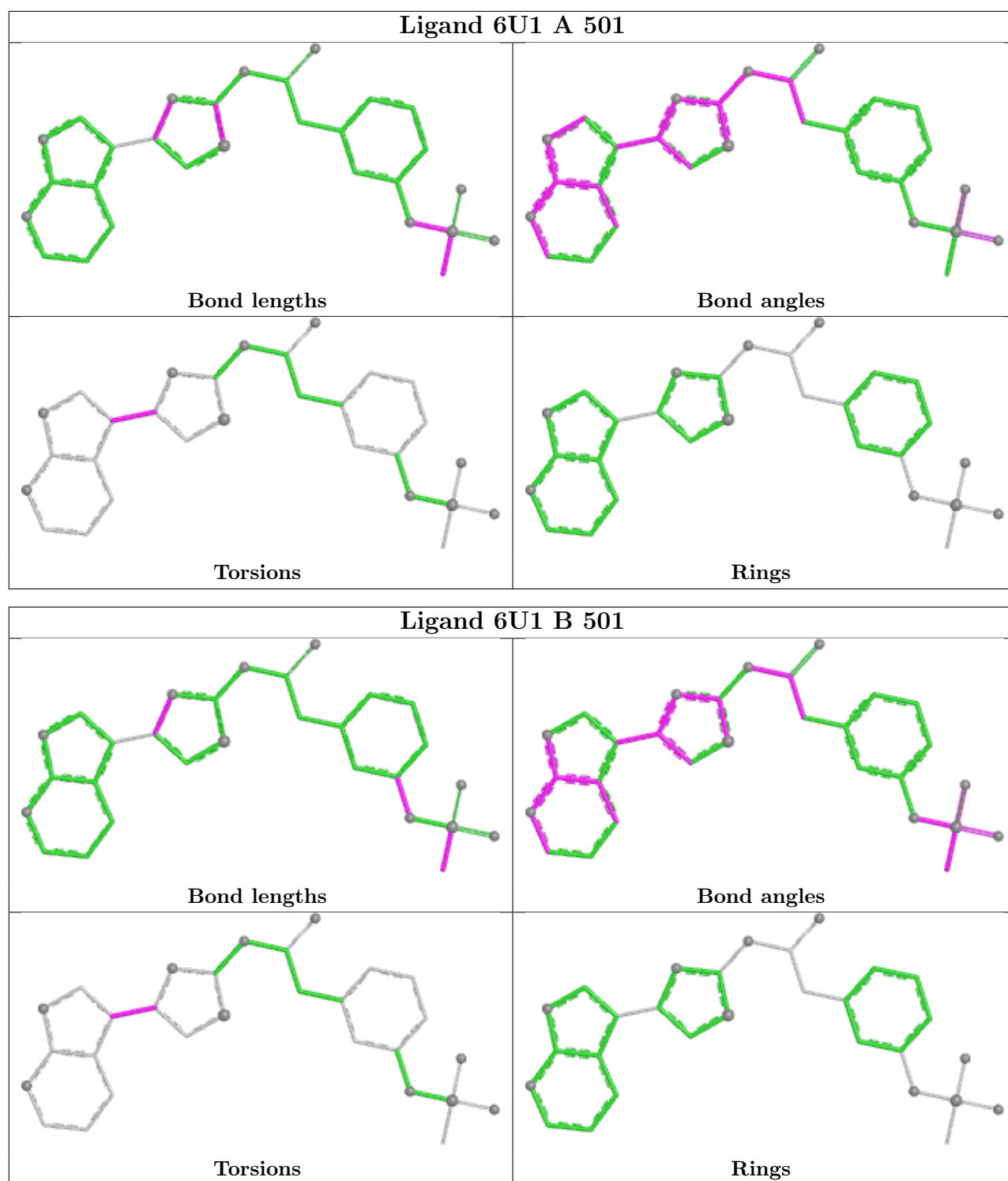
Mol	Chain	Res	Type	Atoms
2	A	501	6U1	C19-C18-C21-C26
2	B	501	6U1	C19-C18-C21-C26
2	B	501	6U1	C19-C18-C21-C22
2	B	501	6U1	N17-C18-C21-C22
2	A	501	6U1	C19-C18-C21-C22
2	B	501	6U1	N17-C18-C21-C26
2	A	501	6U1	N17-C18-C21-C22

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	6U1	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 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

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	395/415 (95%)	0.05	10 (2%) 58 39	55, 85, 137, 160	0
1	B	395/415 (95%)	0.23	10 (2%) 58 39	59, 94, 135, 159	0
All	All	790/830 (95%)	0.14	20 (2%) 58 39	55, 90, 137, 160	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	VAL	4.2
1	B	233	THR	3.4
1	B	372	GLU	3.1
1	B	380	THR	2.9
1	B	39	TYR	2.8
1	B	385	LYS	2.7
1	B	73	ALA	2.7
1	A	322	VAL	2.6
1	A	388	VAL	2.6
1	B	382	PRO	2.6
1	B	173	LYS	2.6
1	A	7	PHE	2.4
1	A	254	TYR	2.4
1	A	48	LYS	2.2
1	A	8	GLU	2.2
1	A	116	SER	2.2
1	B	234	ALA	2.2
1	A	11	PHE	2.0
1	A	119	ALA	2.0
1	A	380	THR	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](#)

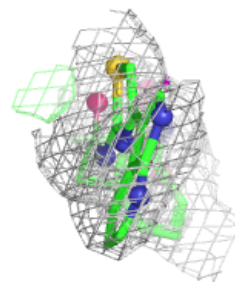
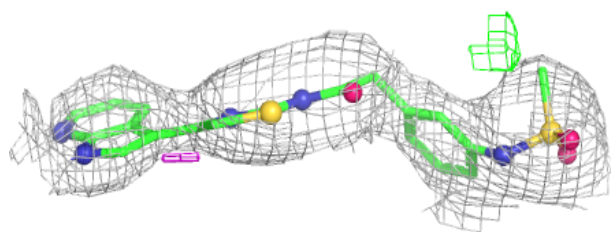
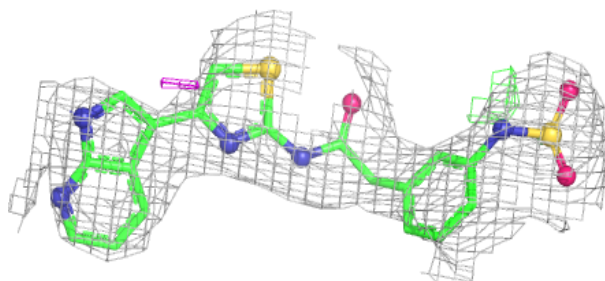
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	6U1	B	501	29/29	0.94	0.11	86,93,99,100	0
2	6U1	A	501	29/29	0.96	0.09	68,77,103,105	0

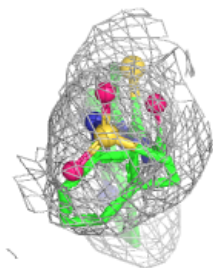
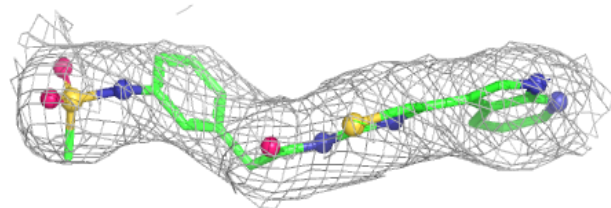
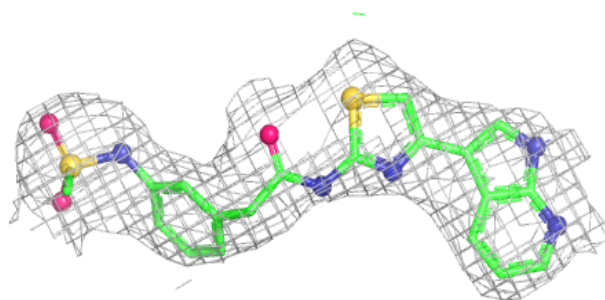
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6U1 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)

**Electron density around 6U1 A 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.