



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:48 AM UTC

PDB ID : 9R8B / pdb_00009r8b
Title : CRYSTAL STRUCTURE OF WILD-TYPE PLK1 KINASE DOMAIN IN
COMPLEX WITH THIAZOLIDINONE INHIBITOR COMPOUND 1 AND
A SELECTIVE DARPIN
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Deposited on : 2025-05-16
Resolution : 2.20 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](#) ①) 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

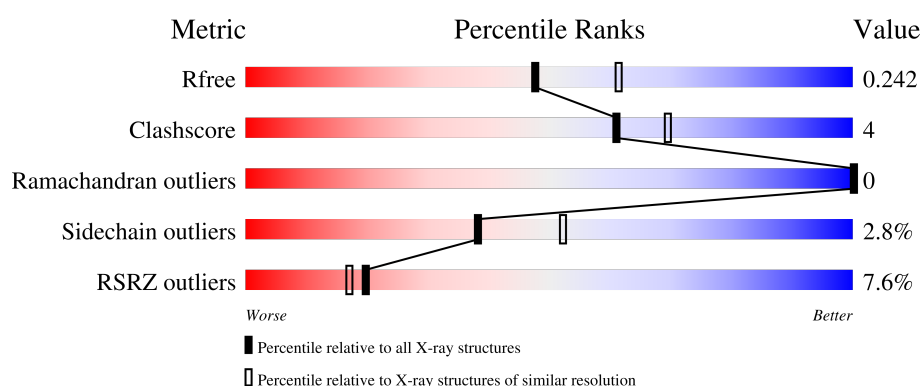
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	315	2% 85% 6% 8%
1	B	315	18% 78% 12% 9%
2	C	167	2% 71% 9% 20%
2	D	167	72% 7% 21%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Serine/threonine-protein kinase PLK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	10	0
			2402	1546	422	420	14			
1	B	287	Total	C	N	O	S	0	4	0
			2339	1505	412	410	12			

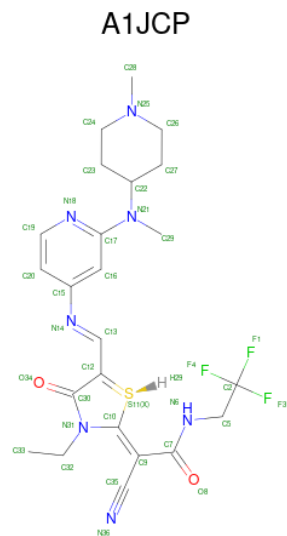
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	-	expression tag	UNP P53350
A	32	SER	-	expression tag	UNP P53350
B	31	GLY	-	expression tag	UNP P53350
B	32	SER	-	expression tag	UNP P53350

- Molecule 2 is a protein called DESIGNED ANKYRIN REPEAT PROTEIN (DARPIN), variant 3H10.

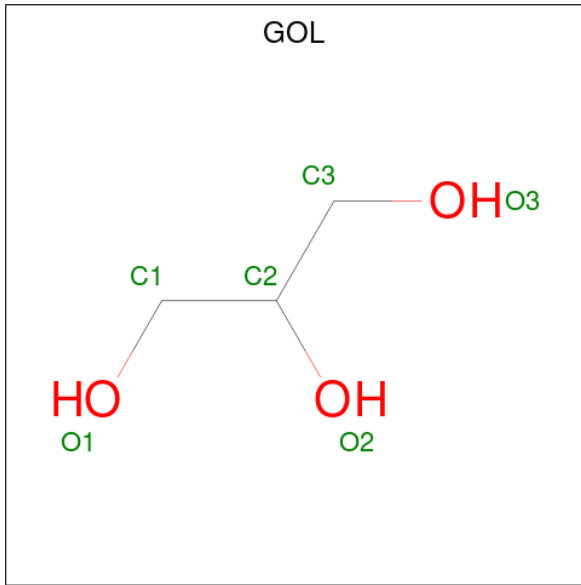
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	134	Total	C	N	O	S	0	0	0
			996	630	167	197	2			
2	D	132	Total	C	N	O	S	0	2	0
			986	622	164	197	3			

- Molecule 3 is (2 {Z})-2-cyano-2-[3-ethyl-5-[({E})-[2-[methyl-(1-methylpiperidin-4-yl)amino]pyridin-4-yl]iminomethyl]-4-oxidanylidene-1,3-thiazol-2-ylidene]- {N}-[2,2,2-tris(fluoranyl)ethyl]ethanamide (CCD ID: A1JCP) (formula: C₂₃H₂₈F₃N₇O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 36	C 23	F 3	N 7	O 2	S 1	0	0
3	B	1	Total 36	C 23	F 3	N 7	O 2	S 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Cl 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	202	Total 202	O 202	0	0
6	B	97	Total 97	O 97	0	0
6	C	44	Total 44	O 44	0	0
6	D	45	Total 45	O 45	0	0

MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	GLY	S12	D13	D27	R31	H69	G91	H92	L93	I128	V131	L132	L133	D143	LYS	PHE	GLY	LYS	THR	ALA	PHE	ASP	ILE	SER	ILE	ASP	ASN	GLY	ASN	GLU	ASP	LEU	ALA	LYS	SER	CYS	ARG	ASN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.07Å 136.90Å 140.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.54 – 2.20 68.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.4 (68.54-2.20) 92.7 (68.54-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.238 0.196 , 0.242	Depositor DCC
R_{free} test set	2826 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7196	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, A1JCP

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	1.13	1/2483 (0.0%)	1.34	4/3348 (0.1%)
1	B	1.19	4/2401 (0.2%)	1.39	3/3239 (0.1%)
2	C	1.23	4/1011 (0.4%)	1.37	1/1376 (0.1%)
2	D	1.19	1/1006 (0.1%)	1.41	0/1370
All	All	1.18	10/6901 (0.1%)	1.37	8/9333 (0.1%)

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
2	D	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	69	HIS	C-O	6.50	1.33	1.24
1	B	302	ASP	C-O	5.56	1.30	1.23
1	B	144	ARG	CD-NE	-5.55	1.38	1.46
2	C	36	ASN	C-O	5.36	1.31	1.24
1	A	112	HIS	CE1-NE2	5.33	1.37	1.32
2	C	92	HIS	CE1-NE2	5.29	1.37	1.32
1	B	175	ARG	C-O	5.27	1.30	1.24
2	D	133	LEU	C-O	5.16	1.30	1.24
2	C	69	HIS	C-N	5.15	1.40	1.33
1	B	164	CYS	C-O	5.09	1.30	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ARG	CB-CA-C	7.07	121.25	109.38
1	B	144	ARG	NE-CZ-NH2	-6.73	113.15	119.20
1	B	144	ARG	CG-CD-NE	-5.88	99.06	112.00
2	C	69	HIS	O-C-N	5.77	129.80	122.06
1	A	195	PHE	CA-C-N	5.55	127.08	120.14
1	A	195	PHE	C-N-CA	5.55	127.08	120.14
1	A	269	SER	CA-C-N	5.33	126.42	122.59
1	A	269	SER	C-N-CA	5.33	126.42	122.59

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	69	HIS	Mainchain

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	2402	0	2483	10	0
1	B	2339	0	2408	32	0
2	C	996	0	986	7	0
2	D	986	0	977	5	0
3	A	36	0	0	2	0
3	B	36	0	0	2	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	B	1	0	0	1	0
6	A	202	0	0	2	0
6	B	97	0	0	10	0
6	C	44	0	0	1	0
6	D	45	0	0	1	0
All	All	7196	0	6870	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 4.

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)
3:B:402:A1JCP:F3	3:B:402:A1JCP:C2	1.57	1.41
1:B:174:HIS:O	1:B:233:ASP:OD1	1.71	1.06
1:B:165:GLN:HB2	1:B:296[B]:ILE:HD12	1.54	0.88
1:B:168:HIS:ND1	5:B:401:CL:CL	2.49	0.81
1:A:69:GLU:OE2	6:A:1101:HOH:O	2.00	0.80
1:B:161:VAL:O	1:B:296[B]:ILE:HD11	1.88	0.72
1:B:165:GLN:CB	1:B:296[B]:ILE:HD12	2.20	0.72
1:B:201:VAL:HG23	6:B:530:HOH:O	1.92	0.69
1:B:230:PHE:CD2	6:B:505:HOH:O	2.47	0.68
1:B:98:MET:HE2	1:B:126:VAL:HG11	1.77	0.67
1:B:230:PHE:HD2	6:B:505:HOH:O	1.77	0.66
1:B:98:MET:HE2	1:B:126:VAL:CG1	2.26	0.65
2:C:93:LEU:HD11	2:C:131:VAL:HG21	1.76	0.65
1:B:165:GLN:HB2	1:B:296[B]:ILE:CD1	2.27	0.64
1:B:96:GLU:OE2	6:B:501:HOH:O	2.15	0.64
2:D:93:LEU:HD11	2:D:131:VAL:HG21	1.81	0.63
1:A:100:MET:CE	6:A:1141:HOH:O	2.47	0.62
1:B:284:LYS:NZ	1:B:302:ASP:OD1	2.33	0.60
2:D:91:GLY:HA2	2:D:128:ILE:HD12	1.86	0.58
2:C:61:GLU:OE2	2:C:61:GLU:N	2.29	0.58
1:B:174:HIS:HA	6:B:510:HOH:O	2.05	0.56
2:C:89:MET:HE2	2:C:119:LEU:HD13	1.88	0.55
1:B:173:ILE:HG13	6:B:530:HOH:O	2.06	0.55
1:B:281:LEU:HG	1:B:285:MET:HE2	1.90	0.54
1:A:98:MET:HA	1:A:98:MET:HE3	1.90	0.54
3:A:1001:A1JCP:O8	3:A:1001:A1JCP:S11	2.66	0.53
3:B:402:A1JCP:S11	3:B:402:A1JCP:O8	2.67	0.52
1:B:211:LEU:HD13	1:B:211:LEU:O	2.10	0.51
2:C:43:VAL:HG22	2:C:47:GLY:HA2	1.93	0.50
1:A:218:ILE:HG21	1:A:223:LEU:HD21	1.92	0.50
1:B:165:GLN:CA	1:B:296[B]:ILE:HD12	2.42	0.49
1:A:218:ILE:HG22	1:A:218:ILE:O	2.13	0.49
1:B:44:LEU:HD22	1:B:127:PHE:CE1	2.48	0.48
1:A:136:ARG:NH2	2:C:78:VAL:HB	2.28	0.48
1:B:157:LEU:O	1:B:161:VAL:HG23	2.13	0.48
3:A:1001:A1JCP:C35	3:A:1001:A1JCP:C32	2.92	0.47
1:B:175:ARG:C	6:B:524:HOH:O	2.58	0.46
1:A:281:LEU:HG	1:A:285:MET:HE2	1.97	0.46
2:C:117:LEU:HD11	2:C:129:VAL:HG13	1.97	0.46
1:A:93:HIS:O	1:A:97:LYS:HG3	2.16	0.46
1:B:298:GLU:O	6:B:502:HOH:O	2.21	0.46
1:B:294:PRO:HD3	6:B:506:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:HIS:O	1:B:233:ASP:CG	2.56	0.45
2:C:35:ALA:HB2	6:C:225:HOH:O	2.17	0.45
1:A:255[A]:CYS:HG	1:A:257:LYS:HB3	1.82	0.44
1:A:325:PHE:O	1:A:326:SER:OG	2.32	0.44
2:D:91:GLY:HA2	2:D:128:ILE:CD1	2.48	0.43
1:B:173:ILE:HG22	1:B:174:HIS:O	2.18	0.43
1:B:150:GLU:N	1:B:151:PRO:CD	2.82	0.43
2:D:27:ASP:O	2:D:31:ARG:HG3	2.19	0.43
1:B:175:ARG:N	6:B:510:HOH:O	2.45	0.42
1:B:132:LEU:HD23	1:B:134:ARG:NH1	2.35	0.41
1:B:211:LEU:O	1:B:212:CYS:HB2	2.22	0.40
1:B:77[B]:GLU:HG2	1:B:79:PHE:CZ	2.57	0.40
2:D:92:HIS:HB3	6:D:234:HOH:O	2.21	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	298/315 (95%)	287 (96%)	11 (4%)	0	100	100
1	B	288/315 (91%)	278 (96%)	10 (4%)	0	100	100
2	C	132/167 (79%)	132 (100%)	0	0	100	100
2	D	132/167 (79%)	132 (100%)	0	0	100	100
All	All	850/964 (88%)	829 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	270/281 (96%)	264 (98%)	6 (2%)	45	61
1	B	260/281 (92%)	250 (96%)	10 (4%)	29	40
2	C	103/130 (79%)	100 (97%)	3 (3%)	37	51
2	D	103/130 (79%)	101 (98%)	2 (2%)	50	66
All	All	736/822 (90%)	715 (97%)	21 (3%)	38	51

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	64	PHE
1	A	197[A]	LEU
1	A	197[B]	LEU
1	A	218	ILE
1	A	225	LYS
1	B	64	PHE
1	B	71	SER
1	B	173	ILE
1	B	197	LEU
1	B	200	LYS
1	B	225	LYS
1	B	248	LYS
1	B	272	LYS
1	B	286	LEU
1	B	303	GLU
2	C	98	VAL
2	C	131	VAL
2	C	145	PHE
2	D	12	SER
2	D	13	ASP

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	94	GLN
1	A	216	ASN
1	B	93	HIS
1	B	94	GLN
1	B	216	ASN
2	D	140	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 ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	A1JCP	B	402	-	35,38,38	2.46	9 (25%)	38,54,54	3.01	13 (34%)
4	GOL	B	403	-	5,5,5	0.13	0	5,5,5	0.33	0
3	A1JCP	A	1001	-	35,38,38	2.59	11 (31%)	38,54,54	2.67	15 (39%)
4	GOL	A	1002	-	5,5,5	0.16	0	5,5,5	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1JCP	B	402	-	-	0/28/57/57	0/3/3/3
4	GOL	B	403	-	-	0/4/4/4	-
3	A1JCP	A	1001	-	-	0/28/57/57	0/3/3/3
4	GOL	A	1002	-	-	2/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	A1JCP	C13-C12	-6.65	1.28	1.47
3	A	1001	A1JCP	C9-C7	6.53	1.58	1.46
3	B	402	A1JCP	C12-S11	6.48	1.85	1.74
3	B	402	A1JCP	F3-C2	6.36	1.57	1.33
3	B	402	A1JCP	C9-C7	5.89	1.57	1.46
3	A	1001	A1JCP	F1-C2	5.14	1.52	1.33
3	A	1001	A1JCP	C35-C9	4.76	1.53	1.43
3	B	402	A1JCP	C13-N14	4.43	1.36	1.28
3	B	402	A1JCP	C19-N18	4.25	1.43	1.34
3	A	1001	A1JCP	C27-C22	-4.15	1.42	1.52
3	A	1001	A1JCP	F4-C2	-3.84	1.19	1.33
3	B	402	A1JCP	C13-C12	-3.69	1.37	1.47
3	A	1001	A1JCP	C27-C26	-3.52	1.42	1.52
3	A	1001	A1JCP	C15-N14	-2.99	1.36	1.42
3	A	1001	A1JCP	C16-C17	2.91	1.43	1.39
3	A	1001	A1JCP	C13-N14	2.78	1.33	1.28
3	A	1001	A1JCP	C19-N18	2.55	1.40	1.34
3	B	402	A1JCP	F1-C2	-2.45	1.24	1.33
3	B	402	A1JCP	C27-C22	-2.32	1.46	1.52
3	B	402	A1JCP	C20-C15	2.27	1.43	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	A1JCP	C27-C22-N21	-14.70	103.25	111.91
3	A	1001	A1JCP	C27-C22-N21	-10.12	105.95	111.91
3	A	1001	A1JCP	F4-C2-C5	-6.02	95.91	111.87
3	B	402	A1JCP	C23-C22-N21	5.68	115.26	111.91
3	A	1001	A1JCP	C30-N31-C10	-4.27	112.56	116.52
3	A	1001	A1JCP	C28-N25-C26	-4.13	102.77	110.63
3	B	402	A1JCP	C32-N31-C30	-3.37	114.92	122.55
3	A	1001	A1JCP	C20-C19-N18	-3.21	120.04	123.97
3	A	1001	A1JCP	C28-N25-C24	3.20	116.72	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	A1JCP	C23-C22-N21	3.17	113.78	111.91
3	A	1001	A1JCP	C23-C24-N25	-2.96	107.38	111.20
3	B	402	A1JCP	C28-N25-C24	2.91	116.18	110.63
3	A	1001	A1JCP	C19-N18-C17	2.70	120.73	116.81
3	B	402	A1JCP	C20-C19-N18	-2.59	120.79	123.97
3	B	402	A1JCP	C16-C17-N21	2.55	124.91	121.83
3	B	402	A1JCP	C19-N18-C17	2.54	120.50	116.81
3	B	402	A1JCP	O8-C7-C9	2.53	123.86	120.93
3	A	1001	A1JCP	F4-C2-F3	2.48	115.17	106.44
3	B	402	A1JCP	C16-C17-N18	-2.39	118.84	122.82
3	B	402	A1JCP	F4-C2-C5	-2.39	105.54	111.87
3	B	402	A1JCP	C20-C15-C16	-2.28	116.74	119.44
3	A	1001	A1JCP	C16-C17-N18	-2.25	119.07	122.82
3	A	1001	A1JCP	C19-C20-C15	2.19	121.13	118.23
3	B	402	A1JCP	C32-N31-C10	2.18	129.09	124.48
3	B	402	A1JCP	C28-N25-C26	-2.13	106.58	110.63
3	A	1001	A1JCP	F1-C2-C5	2.13	117.51	111.87
3	A	1001	A1JCP	C32-N31-C10	2.07	128.87	124.48
3	A	1001	A1JCP	C16-C17-N21	2.07	124.33	121.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	GOL	C1-C2-C3-O3
4	A	1002	GOL	O2-C2-C3-O3

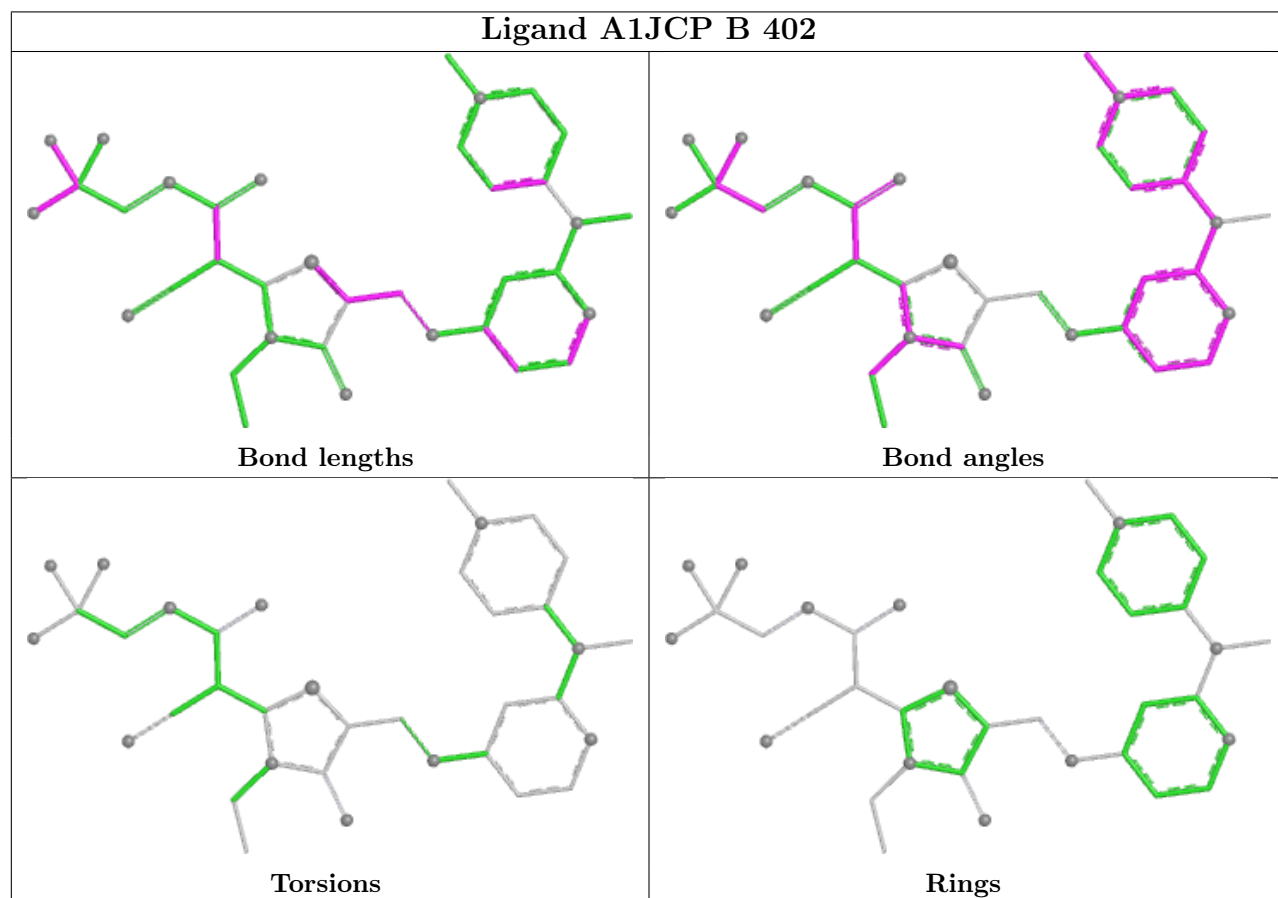
There are no ring outliers.

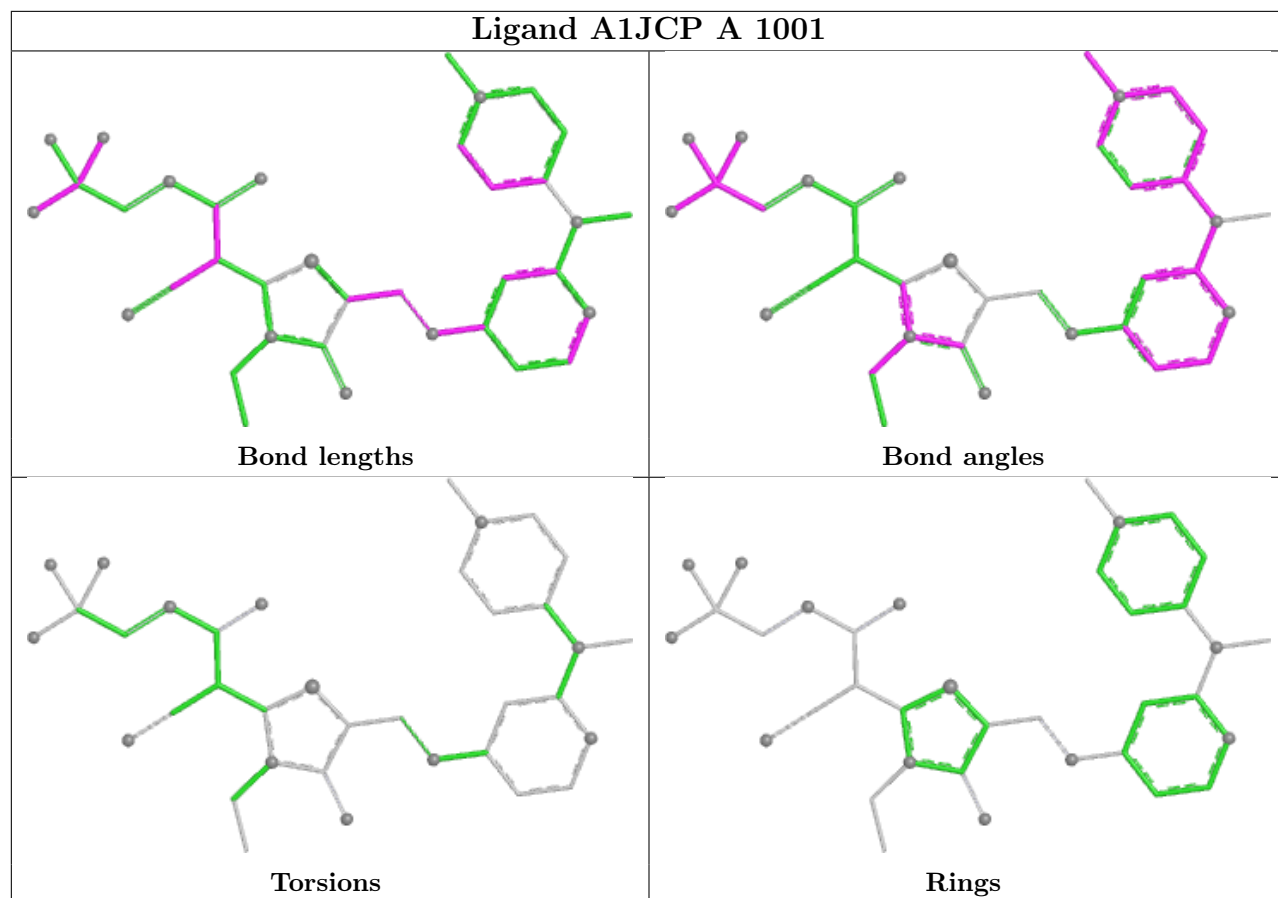
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	A1JCP	2	0
3	A	1001	A1JCP	2	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

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	290/315 (92%)	-0.16	5 (1%) 69 66	23, 46, 79, 137	10 (3%)
1	B	287/315 (91%)	1.15	56 (19%) 3 2	41, 80, 131, 180	3 (1%)
2	C	134/167 (80%)	0.03	3 (2%) 62 59	36, 53, 100, 123	0
2	D	132/167 (79%)	0.03	0 100 100	27, 53, 107, 120	2 (1%)
All	All	843/964 (87%)	0.34	64 (7%) 20 17	23, 58, 114, 180	15 (1%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	GLY	5.5
1	B	172	VAL	4.6
1	B	37	ALA	4.5
1	B	211	LEU	4.3
1	B	173	ILE	4.0
1	B	128	VAL	4.0
1	A	325	PHE	3.6
1	B	88	LEU	3.6
2	C	145	PHE	3.5
1	B	126	VAL	3.5
1	B	300	LEU	3.5
1	A	326	SER	3.4
1	B	127	PHE	3.2
1	B	118	GLY	3.1
1	B	198	ALA	3.0
1	B	160	ILE	3.0
1	B	296[A]	ILE	3.0
1	B	45	VAL	2.9
1	B	100	MET	2.9
1	B	47	PRO	2.9
1	B	38	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	227	GLY	2.9
1	B	170	ASN	2.9
1	B	167	LEU	2.8
1	B	98	MET	2.8
1	B	92	PRO	2.8
1	B	291	THR	2.7
1	B	226	LYS	2.6
1	B	232	VAL	2.6
1	B	70	ILE	2.6
1	B	90	LEU	2.6
1	B	89	LEU	2.6
1	B	196	GLY	2.5
1	B	201	VAL	2.5
1	B	294	PRO	2.5
1	B	41	PRO	2.5
1	B	87	SER	2.4
1	B	129	VAL	2.4
1	B	108	LEU	2.4
1	B	213	GLY	2.4
1	B	48	ARG	2.4
1	B	166	TYR	2.4
1	B	93	HIS	2.4
1	B	174	HIS	2.4
1	B	290	PRO	2.3
1	B	288	THR	2.3
1	B	209	LYS	2.3
1	B	105	HIS	2.3
1	B	164	CYS	2.3
1	A	37	ALA	2.3
1	B	223	LEU	2.2
1	B	81	GLY	2.2
1	B	200	LYS	2.2
1	B	102	ILE	2.2
2	C	143	ASP	2.2
1	B	323	PRO	2.2
1	A	96	GLU	2.2
1	A	90	LEU	2.1
1	B	161	VAL	2.1
1	B	130	LEU	2.1
1	B	212	CYS	2.1
1	B	208	LYS	2.1
1	B	293	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	36	ASN	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](#)

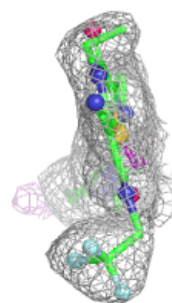
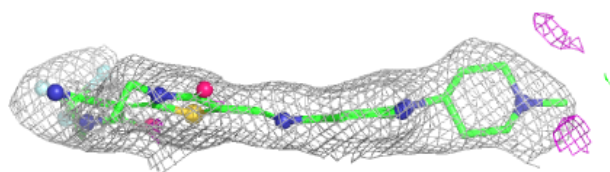
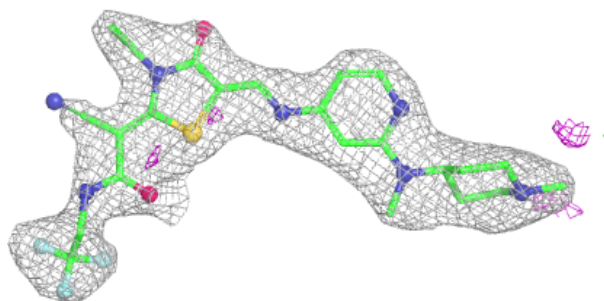
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	403	6/6	0.87	0.13	72,94,109,111	0
5	CL	B	401	1/1	0.90	0.12	82,82,82,82	0
4	GOL	A	1002	6/6	0.92	0.10	46,66,71,75	0
3	A1JCP	B	402	36/36	0.93	0.11	56,66,74,75	0
3	A1JCP	A	1001	36/36	0.95	0.10	46,52,61,61	0

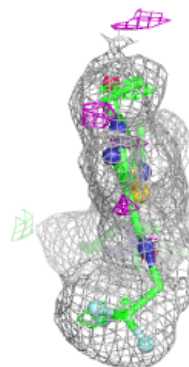
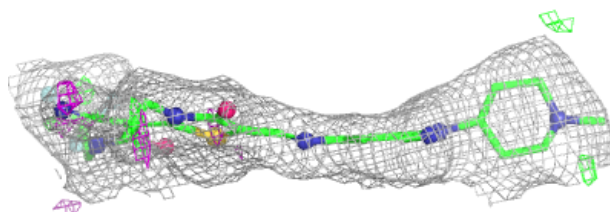
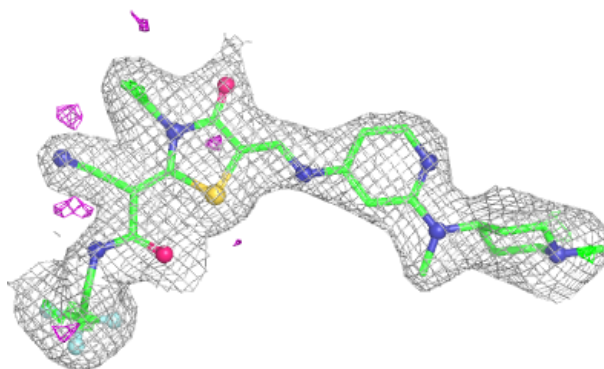
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1JCP B 402:

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

**Electron density around A1JCP A 1001:**

$2mF_o-DF_c$ (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.