



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:38 PM UTC

PDB ID : 6CKI / pdb_00006cki
Title : Co-crystal structure of MNK2 in Complex With Inhibitor
Authors : Han, Q.
Deposited on : 2018-02-28
Resolution : 2.95 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

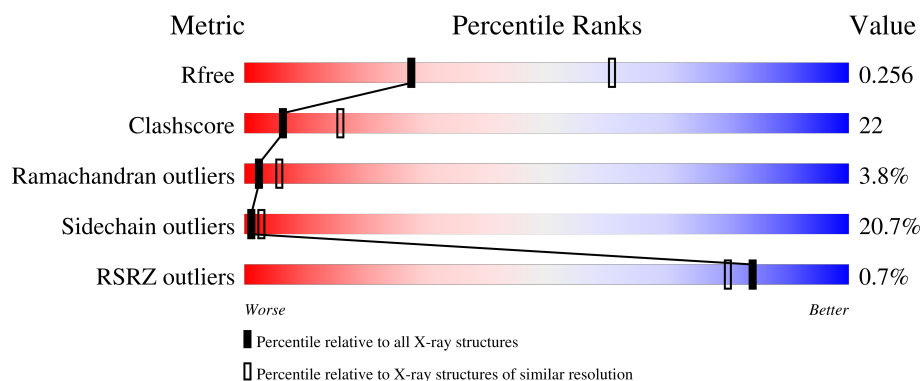
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	316	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2182 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 MAP kinase-interacting serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2154	1366	374	399	15			

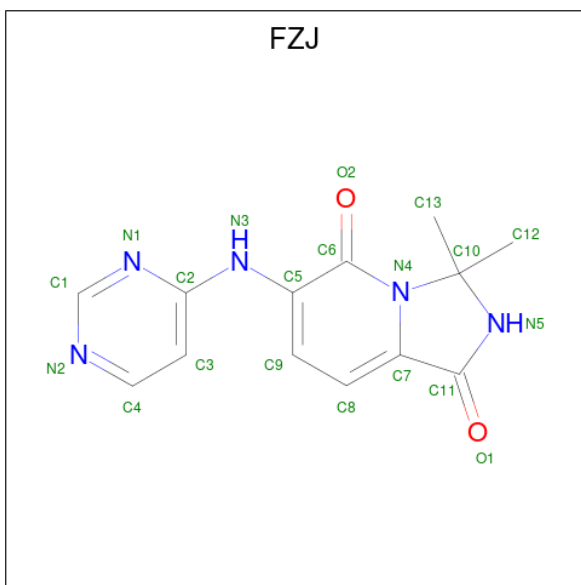
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLY	-	expression tag	UNP Q9HBH9
A	71	SER	-	expression tag	UNP Q9HBH9
A	228	GLY	ASP	engineered mutation	UNP Q9HBH9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 3,3-dimethyl-6-[(pyrimidin-4-yl)amino]-2,3-dihydroimidazo[1,5-a]pyridine-1,5-dione (CCD ID: FZJ) (formula: C₁₃H₁₃N₅O₂).



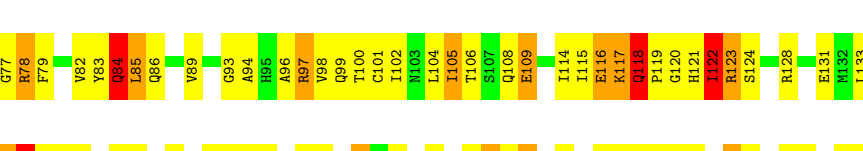
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	13	5	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		

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.

- Chain A: 



Position	Residue	Conservation Category
1	ILE	Grey
2	C311	Green
3	P312	Green
4	LYS	Green
5	A313	Green
6	C314	Green
7	ASN	Green
8	GLY	Green
9	ASP	Green
10	N316	Green
11	N317	Green
12	E320	Green
13	Q323	Green
14	Y327	Green
15	E328	Green
16	F329	Green
17	P330	Green
18	D331	Green
19	K332	Green
20	D335	Green
21	W334	Green
22	I337	Green
23	S338	Green
24	C339	Green
25	A340	Green
26	A341	Green
27	K342	Green
28	I345	Green
29	S346	Green
30	K347	Green
31	L348	Green
32	D352	Green
33	Q355	Green
34	K356	Green
35	L357	Green
36	H365	Green
37	P366	Green
38	W367	Green
39	V368	Green
40	Q369	Green
41	G370	Green
42	C371	Green
43	ALA	Green
44	PRO	Green
45	GLU	Green
46	ASN	Green
47	THR	Green
48	LEU	Green
49	PRO	Green
50	THR	Green
51	PRO	Green
52	MET	Green
53	VAL	Green
54	LEU	Green
55	GLN	Green
56	ARG	Green
57	ASP	Green
58	THR	Green
59	G384	Green
60	C303	Green
61	ASP	Green
62	GLY	Green
63	ARG	Green
64	G228	Green
65	F227	Green
66	K223	Green
67	V222	Green
68	GLY	Green
69	V219	Green
70	Q218	Green
71	C213	Green
72	L212	Green
73	E209	Green
74	G120	Green
75	P119	Green
76	Q118	Green
77	L206	Green
78	D205	Green
79	R204	Green
80	I115	Green
81	I114	Green
82	E109	Green
83	Q108	Green
84	S107	Green
85	F195	Green
86	S191	Green
87	L186	Green
88	V184	Green
89	Q185	Green
90	F177	Green
91	H176	Green
92	R175	Green
93	R174	Green
94	V167	Green
95	M162	Green
96	K161	Green
97	Y156	Green
98	F155	Green
99	R154	Green
100	D153	Green
101	E152	Green
102	N151	Green
103	E150	Green
104	F149	Green
105	A148	Green
106	S147	Green
107	S146	Green
108	G145	Green
109	S144	Green
110	S143	Green
111	S142	Green
112	S141	Green
113	S140	Green
114	S139	Green
115	S138	Green
116	S137	Green
117	S136	Green
118	S135	Green
119	S134	Green
120	S133	Green
121	S132	Green
122	S131	Green
123	S130	Green
124	S129	Green
125	S128	Green
126	S127	Green
127	S126	Green
128	S125	Green
129	S124	Green
130	S123	Green
131	S122	Green
132	S121	Green
133	S120	Green
134	S119	Green
135	S118	Green
136	S117	Green
137	S116	Green
138	S115	Green
139	S114	Green
140	S113	Green
141	S112	Green
142	S111	Green
143	S110	Green
144	S109	Green
145	S108	Green
146	S107	Green
147	S106	Green
148	S105	Green
149	S	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.28 Å 104.28 Å 71.36 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.95 40.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.95) 99.6 (40.00-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.95 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.190 , 0.257 0.186 , 0.256	Depositor DCC
R_{free} test set	462 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	95.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2182	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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: ZN, FZJ

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	1.01	3/2199 (0.1%)	1.18	12/2964 (0.4%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ILE	CA-C	5.61	1.59	1.52
1	A	84	GLN	N-CA	-5.13	1.40	1.46
1	A	176	HIS	CG-CD2	5.06	1.41	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ARG	N-CA-C	10.16	121.29	108.19
1	A	312	PRO	N-CA-C	8.06	129.09	112.47
1	A	118	GLN	N-CA-C	6.73	124.69	109.81
1	A	198	ASN	N-CA-C	6.07	117.90	111.28
1	A	147	GLU	N-CA-C	6.06	117.10	108.74
1	A	123	ARG	N-CA-C	5.86	123.28	110.80
1	A	122	ILE	N-CA-C	5.74	121.28	109.34
1	A	124	SER	N-CA-C	-5.64	106.24	113.01
1	A	311	CYS	N-CA-C	5.58	116.43	109.57
1	A	227	PHE	N-CA-C	5.46	118.16	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	SER	N-CA-C	5.20	115.40	108.38
1	A	184	VAL	CB-CA-C	-5.13	105.30	112.02

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ILE	Peptide
1	A	312	PRO	Peptide
1	A	328	GLU	Peptide

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	2154	0	2087	93	0
2	A	1	0	0	0	0
3	A	20	0	0	1	0
4	A	7	0	0	0	0
All	All	2182	0	2087	94	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 22.

All (94) 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:263:GLU:HA	1:A:263:GLU:OE1	1.53	1.09
1:A:369:GLN:HE21	1:A:369:GLN:HA	1.18	1.07
1:A:365:HIS:HD2	1:A:367:TRP:H	1.08	1.00
1:A:97:ARG:HH21	1:A:97:ARG:HG3	1.27	0.97
1:A:108:GLN:HE21	1:A:109:GLU:H	1.13	0.91
1:A:328:GLU:CB	1:A:330:PRO:HD3	2.00	0.90
1:A:328:GLU:HB3	1:A:330:PRO:HD3	1.54	0.89
1:A:365:HIS:CD2	1:A:367:TRP:H	1.91	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:HE21	1:A:369:GLN:CA	1.90	0.84
1:A:312:PRO:N	1:A:313:ALA:HB3	1.97	0.79
1:A:97:ARG:HH21	1:A:97:ARG:CG	1.96	0.78
1:A:108:GLN:HE21	1:A:109:GLU:N	1.80	0.78
1:A:116:GLU:OE2	1:A:154:ARG:HD3	1.84	0.78
1:A:263:GLU:O	1:A:266:SER:HB3	1.84	0.77
1:A:139:HIS:HD2	1:A:141:ASN:H	1.32	0.75
1:A:334:TRP:O	1:A:342:LYS:NZ	2.18	0.74
1:A:263:GLU:OE1	1:A:263:GLU:CA	2.35	0.72
1:A:328:GLU:HB2	1:A:330:PRO:HD3	1.73	0.69
1:A:285:LEU:HD12	1:A:285:LEU:O	1.93	0.68
1:A:275:ARG:HA	1:A:278:LEU:HD23	1.78	0.66
1:A:97:ARG:HG3	1:A:97:ARG:NH2	2.04	0.65
1:A:369:GLN:HA	1:A:369:GLN:NE2	2.03	0.64
1:A:84:GLN:HB2	1:A:104:LEU:HD21	1.79	0.63
1:A:365:HIS:HD2	1:A:367:TRP:N	1.90	0.62
1:A:79:PHE:CE1	1:A:83:TYR:HB2	2.37	0.60
1:A:174:ARG:NH2	1:A:181:GLU:OE2	2.34	0.59
1:A:115:ILE:HB	1:A:155:PHE:HB2	1.85	0.58
1:A:120:GLY:O	1:A:122:ILE:N	2.34	0.58
1:A:348:LEU:O	1:A:356:ARG:HG3	2.04	0.57
3:A:402:FZJ:C9	3:A:402:FZJ:C3	2.82	0.57
1:A:328:GLU:HB3	1:A:330:PRO:CD	2.33	0.56
1:A:285:LEU:HD12	1:A:285:LEU:C	2.31	0.55
1:A:152:GLU:O	1:A:153:ASP:OD2	2.25	0.55
1:A:260:GLU:C	1:A:263:GLU:HB2	2.32	0.54
1:A:120:GLY:C	1:A:122:ILE:H	2.15	0.54
1:A:139:HIS:HD2	1:A:141:ASN:N	2.04	0.54
1:A:298:ARG:HB3	1:A:298:ARG:CZ	2.37	0.53
1:A:315:GLN:O	1:A:316:ASN:C	2.51	0.53
1:A:118:GLN:N	1:A:119:PRO:HA	2.25	0.52
1:A:149:PHE:HB2	1:A:156:TYR:HB2	1.93	0.50
1:A:312:PRO:CD	1:A:313:ALA:HB3	2.41	0.50
1:A:347:LYS:O	1:A:357:LEU:HD13	2.12	0.50
1:A:260:GLU:HA	1:A:263:GLU:HB2	1.93	0.50
1:A:260:GLU:O	1:A:263:GLU:HB2	2.12	0.50
1:A:86:GLN:CD	1:A:102:ILE:HD12	2.38	0.49
1:A:320:GLU:O	1:A:323:GLN:HB2	2.13	0.49
1:A:278:LEU:HG	1:A:357:LEU:O	2.12	0.49
1:A:139:HIS:CD2	1:A:141:ASN:H	2.21	0.49
1:A:369:GLN:CA	1:A:369:GLN:NE2	2.64	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ASN:HB3	1:A:317:MET:HE2	1.95	0.47
1:A:327:TYR:OH	1:A:346:SER:HA	2.14	0.47
1:A:311:CYS:O	1:A:314:CYS:HB2	2.15	0.47
1:A:85:LEU:HD11	1:A:99:GLN:HE21	1.80	0.47
1:A:100:THR:HG22	1:A:101:CYS:N	2.30	0.46
1:A:296:VAL:HG12	1:A:297:GLY:N	2.30	0.46
1:A:312:PRO:HD2	1:A:313:ALA:CB	2.46	0.46
1:A:85:LEU:HD12	1:A:86:GLN:H	1.80	0.46
1:A:105:ILE:HG13	1:A:106:THR:HG23	1.97	0.46
1:A:195:PHE:CD2	1:A:196:LEU:HD23	2.51	0.46
1:A:197:HIS:HD2	1:A:201:ILE:O	1.98	0.46
1:A:117:LYS:HG3	1:A:153:ASP:C	2.41	0.46
1:A:195:PHE:HD2	1:A:196:LEU:HD23	1.80	0.45
1:A:263:GLU:O	1:A:269:ALA:CB	2.65	0.45
1:A:311:CYS:HA	1:A:312:PRO:HD3	1.78	0.45
1:A:121:HIS:O	1:A:122:ILE:O	2.35	0.45
1:A:97:ARG:CG	1:A:97:ARG:NH2	2.65	0.44
1:A:272:TYR:O	1:A:275:ARG:N	2.44	0.44
1:A:329:PHE:N	1:A:330:PRO:HD3	2.32	0.44
1:A:275:ARG:O	1:A:278:LEU:N	2.45	0.44
1:A:298:ARG:O	1:A:314:CYS:HA	2.18	0.44
1:A:207:LYS:HB2	1:A:208:PRO:CD	2.49	0.43
1:A:75:PHE:O	1:A:77:GLY:N	2.52	0.43
1:A:174:ARG:HG3	1:A:177:PHE:CE1	2.53	0.43
1:A:260:GLU:O	1:A:263:GLU:CB	2.67	0.43
1:A:285:LEU:HG	1:A:345:ILE:HD11	2.01	0.42
1:A:93:GLY:N	1:A:96:ALA:O	2.43	0.42
1:A:312:PRO:HA	1:A:315:GLN:H	1.85	0.42
1:A:86:GLN:OE1	1:A:102:ILE:HD12	2.19	0.42
1:A:260:GLU:CA	1:A:263:GLU:HB2	2.50	0.42
1:A:108:GLN:NE2	1:A:109:GLU:H	1.97	0.42
1:A:141:ASN:O	1:A:223:LYS:HA	2.20	0.42
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.75	0.42
1:A:365:HIS:HA	1:A:366:PRO:HD2	1.62	0.41
1:A:197:HIS:CD2	1:A:274:LYS:HG2	2.56	0.41
1:A:205:ASP:O	1:A:206:LEU:C	2.63	0.41
1:A:352:ASP:O	1:A:355:GLN:HB2	2.20	0.41
1:A:212:LEU:O	1:A:222:VAL:HA	2.21	0.41
1:A:117:LYS:HE3	1:A:153:ASP:H	1.86	0.41
1:A:167:ILE:HG22	1:A:208:PRO:O	2.21	0.41
1:A:186:VAL:HG21	1:A:285:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:MET:HE3	1:A:213:CYS:C	2.46	0.41
1:A:78:ARG:HH11	1:A:78:ARG:HB3	1.85	0.40
1:A:146:ILE:HG22	1:A:147:GLU:N	2.37	0.40
1:A:279:TRP:CD1	1:A:279:TRP:C	3.00	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	263/316 (83%)	219 (83%)	34 (13%)	10 (4%)	2 6

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ILE
1	A	123	ARG
1	A	312	PRO
1	A	366	PRO
1	A	76	SER
1	A	94	ALA
1	A	153	ASP
1	A	369	GLN
1	A	263	GLU
1	A	341	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	232/274 (85%)	184 (79%)	48 (21%)	1 3

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	SER
1	A	78	ARG
1	A	82	VAL
1	A	84	GLN
1	A	85	LEU
1	A	89	VAL
1	A	97	ARG
1	A	98	VAL
1	A	105	ILE
1	A	109	GLU
1	A	114	ILE
1	A	116	GLU
1	A	117	LYS
1	A	118	GLN
1	A	128	ARG
1	A	131	GLU
1	A	133	LEU
1	A	135	GLN
1	A	146	ILE
1	A	151	GLU
1	A	152	GLU
1	A	153	ASP
1	A	161	LYS
1	A	175	ARG
1	A	180	LEU
1	A	184	VAL
1	A	191	SER
1	A	196	LEU
1	A	198	ASN
1	A	204	ARG
1	A	209	GLU
1	A	212	LEU
1	A	218	GLN
1	A	219	VAL
1	A	255	GLU

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Mol	Chain	Res	Type
1	A	262	VAL
1	A	263	GLU
1	A	271	ILE
1	A	273	ASP
1	A	285	LEU
1	A	298	ARG
1	A	303	CYS
1	A	315	GLN
1	A	332	LYS
1	A	337	ILE
1	A	338	SER
1	A	339	CYS
1	A	369	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	103	ASN
1	A	108	GLN
1	A	139	HIS
1	A	172	HIS
1	A	187	GLN
1	A	197	HIS
1	A	218	GLN
1	A	315	GLN
1	A	316	ASN
1	A	364	GLN
1	A	365	HIS
1	A	369	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	FZJ	A	402	-	21,22,22	1.52	4 (19%)	24,33,33	2.78	12 (50%)

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	FZJ	A	402	-	-	0/4/19/19	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	FZJ	O1-C11	3.48	1.30	1.23
3	A	402	FZJ	C7-N4	-3.37	1.32	1.39
3	A	402	FZJ	C6-N4	-3.23	1.33	1.39
3	A	402	FZJ	C9-C5	2.01	1.41	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	FZJ	C6-C5-N3	7.14	118.72	112.05
3	A	402	FZJ	C7-C11-N5	5.38	113.79	105.34
3	A	402	FZJ	C9-C5-C6	-5.29	116.58	120.46
3	A	402	FZJ	N2-C1-N1	-3.94	120.64	127.33
3	A	402	FZJ	C3-C2-N1	-3.06	117.95	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	FZJ	C9-C8-C7	-2.58	118.10	122.18
3	A	402	FZJ	O1-C11-N5	-2.54	120.30	126.20
3	A	402	FZJ	C4-N2-C1	2.45	120.25	115.35
3	A	402	FZJ	C12-C10-C13	-2.26	107.65	111.32
3	A	402	FZJ	O2-C6-C5	-2.08	119.42	122.00
3	A	402	FZJ	C3-C4-N2	-2.07	120.06	123.60
3	A	402	FZJ	C1-N1-C2	2.05	121.94	115.25

There are no chirality outliers.

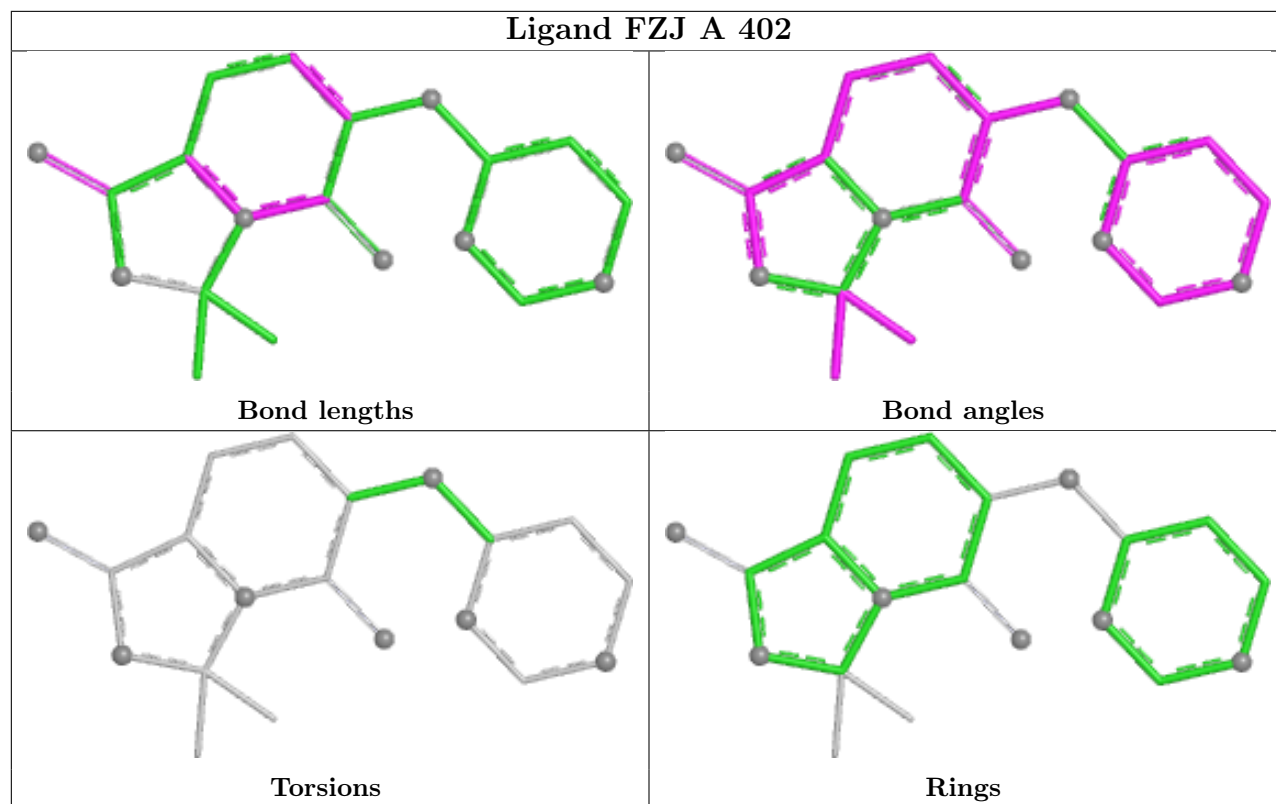
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	FZJ	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 [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	271/316 (85%)	-0.54	2 (0%) 84 80	70, 100, 150, 188	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	GLY	2.6
1	A	252	GLY	2.2

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.

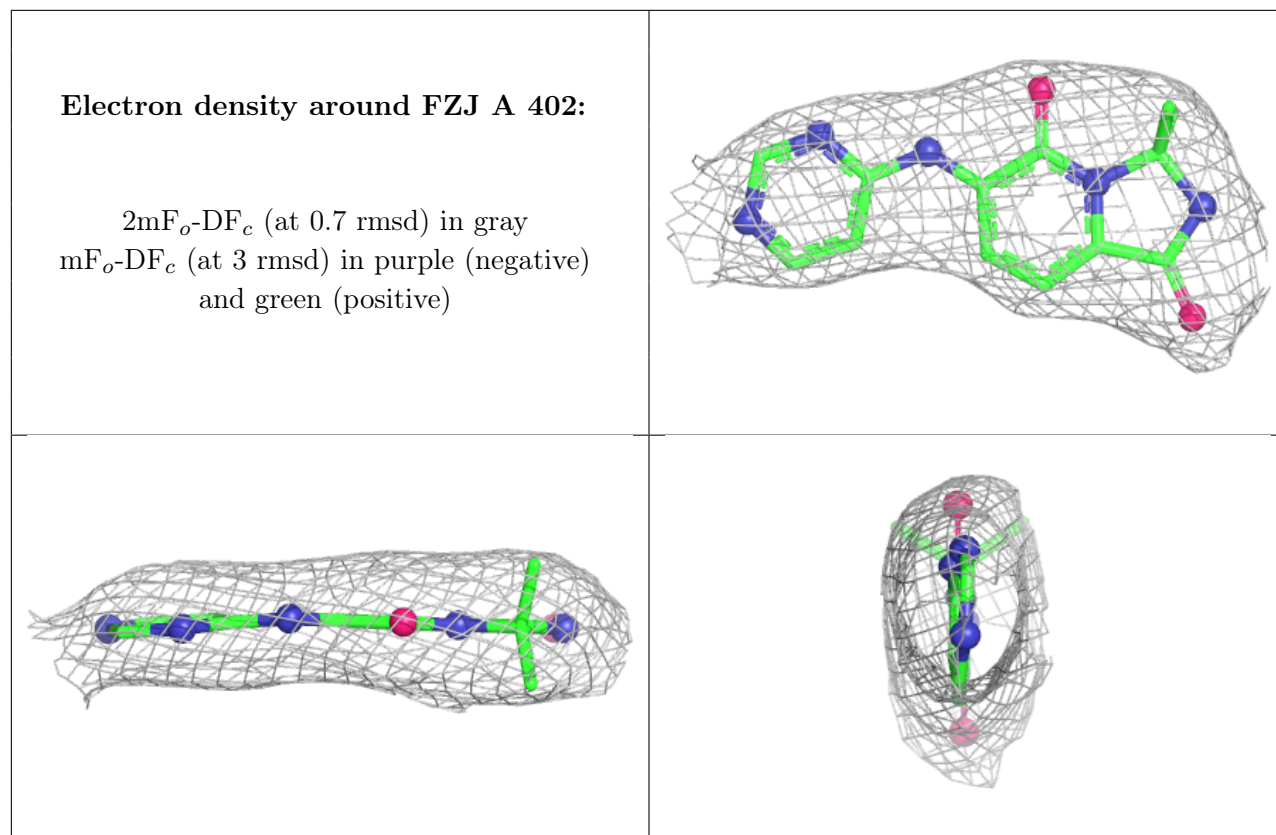
6.4 Ligands [i](#)

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	ZN	A	401	1/1	0.95	0.05	171,171,171,171	0
3	FZJ	A	402	20/20	0.99	0.05	66,77,87,88	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.