



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:23 AM UTC

PDB ID : 9LFV / pdb_00009lfv
Title : Crystal structure of mouse RIP3 kinase domain complexed with LK01004
Authors : Xie, H.; Su, H.X.; Li, M.J.; Xu, Y.C.
Deposited on : 2025-01-09
Resolution : 2.78 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

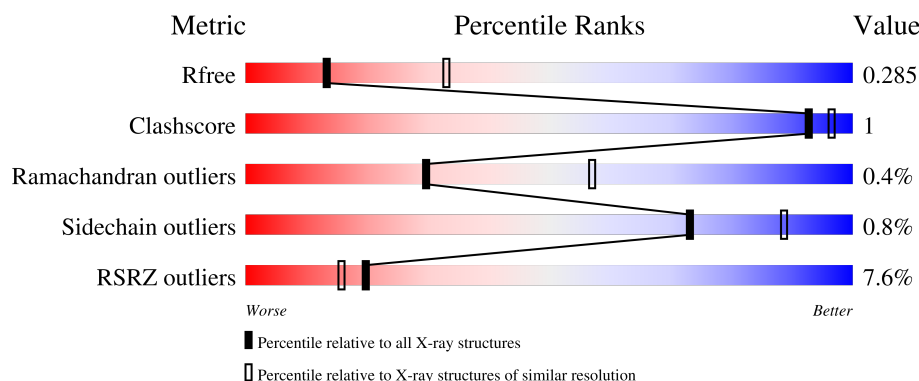
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	2% 75% 20%
1	B	325	3% 76% 21%
1	C	325	8% 74% 23%
1	D	325	11% 73% 6% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7545 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 Receptor-interacting serine/threonine-protein kinase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1955	1261	329	357	8			
1	B	256	Total	C	N	O	S	0	0	0
			1916	1232	331	345	8			
1	C	250	Total	C	N	O	S	0	0	0
			1753	1123	302	320	8			
1	D	255	Total	C	N	O	S	0	0	0
			1772	1138	305	323	6			

There are 60 discrepancies between the modelled and reference sequences:

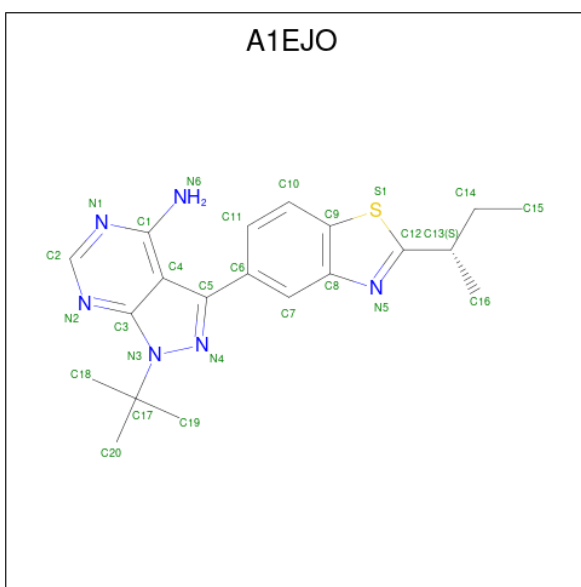
Chain	Residue	Modelled	Actual	Comment	Reference
A	111	ALA	CYS	conflict	UNP Q9QZL0
A	136	ASP	ASN	conflict	UNP Q9QZL0
A	194	LYS	ASP	conflict	UNP Q9QZL0
A	310	LEU	-	expression tag	UNP Q9QZL0
A	311	GLU	-	expression tag	UNP Q9QZL0
A	312	HIS	-	expression tag	UNP Q9QZL0
A	313	HIS	-	expression tag	UNP Q9QZL0
A	314	HIS	-	expression tag	UNP Q9QZL0
A	315	HIS	-	expression tag	UNP Q9QZL0
A	316	HIS	-	expression tag	UNP Q9QZL0
A	317	HIS	-	expression tag	UNP Q9QZL0
A	318	HIS	-	expression tag	UNP Q9QZL0
A	319	HIS	-	expression tag	UNP Q9QZL0
A	320	HIS	-	expression tag	UNP Q9QZL0
A	321	HIS	-	expression tag	UNP Q9QZL0
B	111	ALA	CYS	conflict	UNP Q9QZL0
B	136	ASP	ASN	conflict	UNP Q9QZL0
B	194	LYS	ASP	conflict	UNP Q9QZL0
B	310	LEU	-	expression tag	UNP Q9QZL0
B	311	GLU	-	expression tag	UNP Q9QZL0
B	312	HIS	-	expression tag	UNP Q9QZL0

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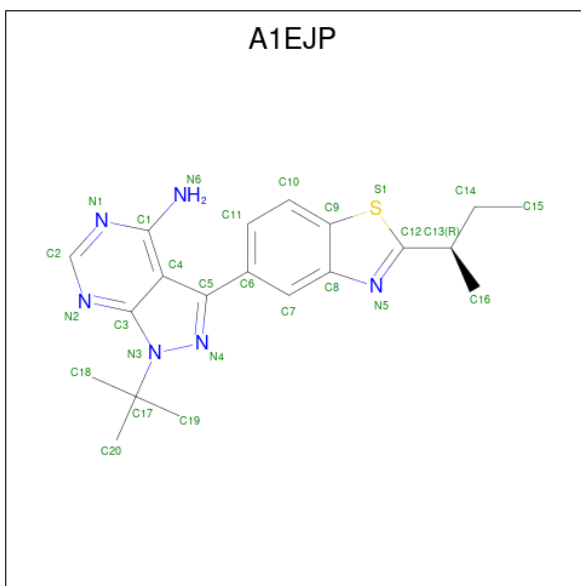
Chain	Residue	Modelled	Actual	Comment	Reference
B	313	HIS	-	expression tag	UNP Q9QZL0
B	314	HIS	-	expression tag	UNP Q9QZL0
B	315	HIS	-	expression tag	UNP Q9QZL0
B	316	HIS	-	expression tag	UNP Q9QZL0
B	317	HIS	-	expression tag	UNP Q9QZL0
B	318	HIS	-	expression tag	UNP Q9QZL0
B	319	HIS	-	expression tag	UNP Q9QZL0
B	320	HIS	-	expression tag	UNP Q9QZL0
B	321	HIS	-	expression tag	UNP Q9QZL0
C	111	ALA	CYS	conflict	UNP Q9QZL0
C	136	ASP	ASN	conflict	UNP Q9QZL0
C	194	LYS	ASP	conflict	UNP Q9QZL0
C	310	LEU	-	expression tag	UNP Q9QZL0
C	311	GLU	-	expression tag	UNP Q9QZL0
C	312	HIS	-	expression tag	UNP Q9QZL0
C	313	HIS	-	expression tag	UNP Q9QZL0
C	314	HIS	-	expression tag	UNP Q9QZL0
C	315	HIS	-	expression tag	UNP Q9QZL0
C	316	HIS	-	expression tag	UNP Q9QZL0
C	317	HIS	-	expression tag	UNP Q9QZL0
C	318	HIS	-	expression tag	UNP Q9QZL0
C	319	HIS	-	expression tag	UNP Q9QZL0
C	320	HIS	-	expression tag	UNP Q9QZL0
C	321	HIS	-	expression tag	UNP Q9QZL0
D	111	ALA	CYS	conflict	UNP Q9QZL0
D	136	ASP	ASN	conflict	UNP Q9QZL0
D	194	LYS	ASP	conflict	UNP Q9QZL0
D	310	LEU	-	expression tag	UNP Q9QZL0
D	311	GLU	-	expression tag	UNP Q9QZL0
D	312	HIS	-	expression tag	UNP Q9QZL0
D	313	HIS	-	expression tag	UNP Q9QZL0
D	314	HIS	-	expression tag	UNP Q9QZL0
D	315	HIS	-	expression tag	UNP Q9QZL0
D	316	HIS	-	expression tag	UNP Q9QZL0
D	317	HIS	-	expression tag	UNP Q9QZL0
D	318	HIS	-	expression tag	UNP Q9QZL0
D	319	HIS	-	expression tag	UNP Q9QZL0
D	320	HIS	-	expression tag	UNP Q9QZL0
D	321	HIS	-	expression tag	UNP Q9QZL0

- Molecule 2 is 3-[2-[(2 {S})-butan-2-yl]-1,3-benzothiazol-5-yl]-1- {tert}-butyl-pyrazolo[3,4-d]pyrimidin-4-amine (CCD ID: A1EJO) (formula: C₂₀H₂₄N₆S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	1
			27	20	6	1		

- Molecule 3 is 3-[2-[(2 {R})-butan-2-yl]-1,3-benzothiazol-5-yl]-1- {tert}-butyl-pyrazolo[3,4-d]pyrimidin-4-amine (CCD ID: A1EJP) (formula: C₂₀H₂₄N₆S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	1
			27	20	6	1		
3	B	1	Total	C	N	S	0	0
			27	20	6	1		

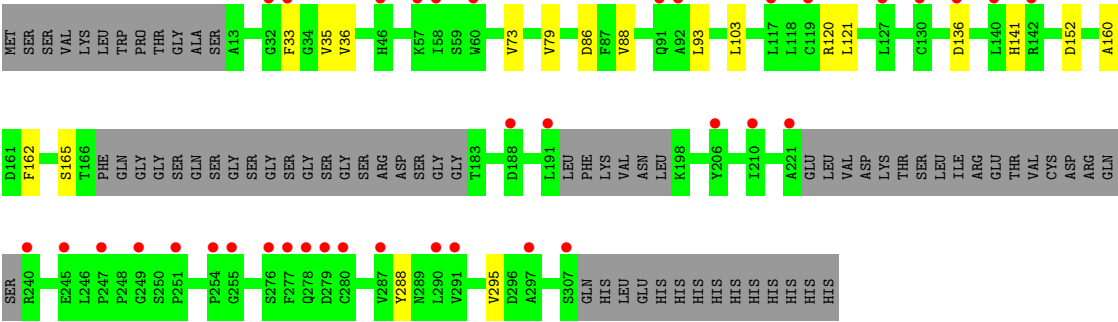
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	S	0	0
			27	20	6	1		
3	D	1	Total	C	N	S	0	0
			27	20	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	5	Total	O	0	0
			5	5		
4	D	2	Total	O	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.66Å 94.66Å 122.21Å 90.00° 90.98° 90.00°	Depositor
Resolution (Å)	61.10 – 2.78 61.10 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.0 (61.10-2.78) 99.0 (61.10-2.78)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.247 , 0.280 0.248 , 0.285	Depositor DCC
R_{free} test set	1523 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	69.9	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7545	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.47% 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: A1EJO, A1EJP

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	0.33	0/2002	0.61	0/2733
1	B	0.32	1/1960 (0.1%)	0.57	0/2676
1	C	0.29	0/1794	0.55	0/2465
1	D	0.28	0/1816	0.55	0/2501
All	All	0.31	1/7572 (0.0%)	0.57	0/10375

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	ASP	C-N	5.33	1.39	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	136	ASP	Peptide
1	C	136	ASP	Peptide
1	D	136	ASP	Peptide

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	1955	0	1892	6	0
1	B	1916	0	1857	4	0
1	C	1753	0	1567	4	0
1	D	1772	0	1569	9	0
2	A	27	0	0	0	0
3	A	27	0	0	0	0
3	B	27	0	0	0	0
3	C	27	0	0	0	0
3	D	27	0	0	1	0
4	A	7	0	0	0	0
4	B	5	0	0	0	0
4	D	2	0	0	0	0
All	All	7545	0	6885	21	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 1.

All (21) 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:D:120:ARG:HD3	1:D:295:VAL:HG11	1.87	0.57
1:C:120:ARG:HD3	1:C:295:VAL:HG11	1.86	0.56
1:A:113:ARG:HB3	1:A:118:LEU:HD11	1.88	0.54
1:C:116:PRO:HB2	1:C:295:VAL:HG22	1.89	0.54
1:D:35:VAL:HG21	1:D:88:VAL:HG11	1.95	0.47
1:C:73:VAL:HG13	1:C:162:PHE:HZ	1.79	0.47
1:A:154:GLU:HG3	1:B:154:GLU:HG3	1.96	0.47
1:A:102:SER:HA	1:A:150:LEU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:PHE:H	1:D:165:SER:HB3	1.81	0.45
1:D:73:VAL:HG13	1:D:162:PHE:HZ	1.81	0.45
1:D:141:HIS:NE2	1:D:160:ALA:O	2.41	0.45
1:C:202:ALA:HB1	1:C:274:ARG:HD2	1.98	0.44
1:D:36:VAL:HG21	3:D:401:A1EJP:N4	2.32	0.44
1:A:156:HIS:NE2	1:B:154:GLU:OE2	2.34	0.44
1:D:79:VAL:HG12	1:D:93:LEU:HD23	1.99	0.44
1:D:103:LEU:HD13	1:D:121:LEU:HD13	1.99	0.43
1:A:28:VAL:HG21	1:A:97:PHE:HE1	1.84	0.43
1:D:288:TYR:HE1	1:D:295:VAL:HG21	1.84	0.42
1:A:103:LEU:HD13	1:A:121:LEU:HD13	2.04	0.40
1:B:124:GLU:OE2	1:B:156:HIS:ND1	2.54	0.40
1:B:212:VAL:O	1:B:216:LEU:HG	2.22	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	251/325 (77%)	238 (95%)	12 (5%)	1 (0%)	30	57
1	B	248/325 (76%)	237 (96%)	10 (4%)	1 (0%)	30	57
1	C	240/325 (74%)	229 (95%)	10 (4%)	1 (0%)	30	57
1	D	247/325 (76%)	238 (96%)	8 (3%)	1 (0%)	30	57
All	All	986/1300 (76%)	942 (96%)	40 (4%)	4 (0%)	30	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
1	B	86	ASP

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Mol	Chain	Res	Type
1	D	86	ASP
1	C	86	ASP

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	204/283 (72%)	202 (99%)	2 (1%)	68	86
1	B	198/283 (70%)	197 (100%)	1 (0%)	81	92
1	C	162/283 (57%)	160 (99%)	2 (1%)	63	84
1	D	160/283 (56%)	159 (99%)	1 (1%)	78	91
All	All	724/1132 (64%)	718 (99%)	6 (1%)	73	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	152	ASP
1	B	152	ASP
1	C	35	VAL
1	C	152	ASP
1	D	152	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN

5.3.3 RNA ⓘ

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](#)

5 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	$\# Z > 2$
3	A1EJP	D	401	-	30,30,30	0.65	1 (3%)	40,46,46	1.40	9 (22%)
3	A1EJP	A	402[B]	-	30,30,30	0.73	1 (3%)	40,46,46	1.75	11 (27%)
3	A1EJP	B	401	-	30,30,30	0.69	1 (3%)	40,46,46	1.68	10 (25%)
3	A1EJP	C	401	-	30,30,30	0.63	1 (3%)	40,46,46	1.35	8 (20%)
2	A1EJO	A	401[A]	-	30,30,30	0.63	1 (3%)	40,46,46	1.31	7 (17%)

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	A1EJP	D	401	-	-	4/16/16/16	0/4/4/4
3	A1EJP	A	402[B]	-	-	5/16/16/16	0/4/4/4
3	A1EJP	B	401	-	-	4/16/16/16	0/4/4/4
3	A1EJP	C	401	-	-	5/16/16/16	0/4/4/4
2	A1EJO	A	401[A]	-	-	6/16/16/16	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[B]	A1EJP	C4-C5	-2.54	1.37	1.44
2	A	401[A]	A1EJO	C4-C5	-2.32	1.38	1.44
3	D	401	A1EJP	C4-C5	-2.19	1.38	1.44
3	C	401	A1EJP	C4-C5	-2.18	1.38	1.44
3	B	401	A1EJP	C4-C5	-2.13	1.38	1.44

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	A1EJP	C6-C5-N4	4.28	124.47	118.91
3	A	402[B]	A1EJP	C6-C5-N4	4.01	124.13	118.91
3	B	401	A1EJP	C4-C5-C6	-3.63	126.97	131.28
3	A	402[B]	A1EJP	C4-C5-C6	-3.61	126.99	131.28
3	A	402[B]	A1EJP	C11-C6-C5	-3.53	116.27	120.64
3	A	402[B]	A1EJP	C1-C4-C5	-3.50	135.52	139.07
3	A	402[B]	A1EJP	C4-C3-N2	-3.32	123.45	126.97
3	A	402[B]	A1EJP	C3-C4-C5	3.24	106.99	104.74
3	D	401	A1EJP	C6-C5-N4	3.12	122.97	118.91
2	A	401[A]	A1EJO	C4-C3-N2	-3.02	123.76	126.97
3	B	401	A1EJP	C11-C6-C5	-3.00	116.93	120.64
3	B	401	A1EJP	C3-C4-C5	2.97	106.81	104.74
3	B	401	A1EJP	C1-C4-C5	-2.92	136.11	139.07
3	B	401	A1EJP	C17-N3-N4	2.91	123.11	117.90
3	A	402[B]	A1EJP	N2-C3-N3	2.91	130.07	125.48
3	C	401	A1EJP	C6-C5-N4	2.89	122.67	118.91
3	C	401	A1EJP	C4-C3-N2	-2.85	123.95	126.97
3	B	401	A1EJP	C4-C3-N2	-2.83	123.96	126.97
3	D	401	A1EJP	C11-C6-C5	-2.74	117.24	120.64
2	A	401[A]	A1EJO	N2-C3-N3	2.73	129.79	125.48
3	D	401	A1EJP	C4-C3-N2	-2.73	124.07	126.97
3	A	402[B]	A1EJP	C7-C6-C5	2.73	124.67	120.34
3	D	401	A1EJP	C4-C5-C6	-2.66	128.13	131.28
3	D	401	A1EJP	C17-N3-N4	2.62	122.57	117.90
3	C	401	A1EJP	C4-C5-C6	-2.59	128.21	131.28
2	A	401[A]	A1EJO	C6-C5-N4	2.56	122.24	118.91
3	B	401	A1EJP	C7-C6-C5	2.56	124.40	120.34
3	C	401	A1EJP	N2-C3-N3	2.52	129.46	125.48
3	B	401	A1EJP	C4-C5-N4	-2.51	108.46	110.19
3	C	401	A1EJP	C11-C6-C5	-2.51	117.53	120.64
3	D	401	A1EJP	C3-C4-C5	2.51	106.48	104.74
3	C	401	A1EJP	C1-C4-C5	-2.50	136.54	139.07
3	B	401	A1EJP	N2-C3-N3	2.50	129.43	125.48
3	D	401	A1EJP	C1-C4-C5	-2.47	136.57	139.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[A]	A1EJO	C1-C4-C5	-2.47	136.57	139.07
3	D	401	A1EJP	N2-C3-N3	2.43	129.32	125.48
2	A	401[A]	A1EJO	C3-C4-C5	2.34	106.36	104.74
3	A	402[B]	A1EJP	C1-C4-C3	2.32	117.48	115.74
2	A	401[A]	A1EJO	C4-C5-C6	-2.31	128.54	131.28
3	C	401	A1EJP	C17-N3-N4	2.30	122.01	117.90
3	C	401	A1EJP	C3-C4-C5	2.29	106.33	104.74
3	A	402[B]	A1EJP	C4-C5-N4	-2.28	108.63	110.19
3	A	402[B]	A1EJP	C18-C17-N3	2.18	111.98	108.87
2	A	401[A]	A1EJO	C11-C6-C5	-2.16	117.97	120.64
3	D	401	A1EJP	C7-C6-C5	2.02	123.54	120.34

There are no chirality outliers.

All (24) torsion outliers are listed below:

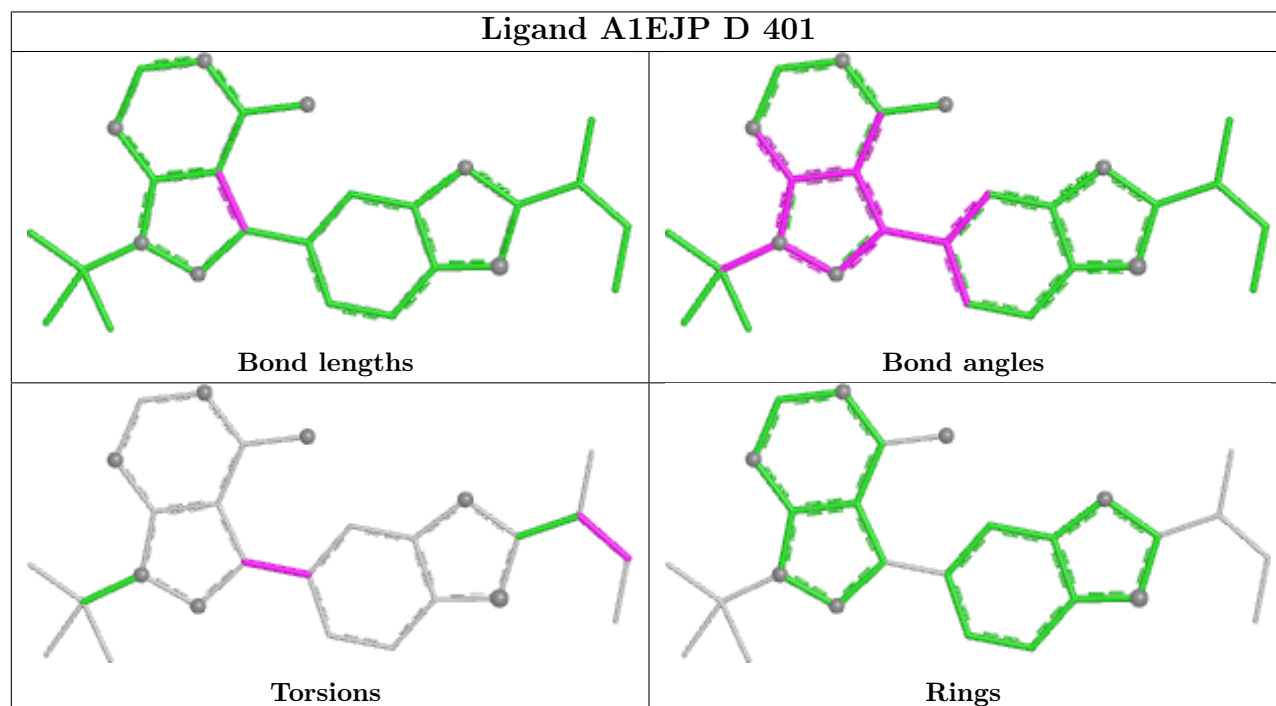
Mol	Chain	Res	Type	Atoms
3	B	401	A1EJP	C16-C13-C14-C15
3	D	401	A1EJP	C16-C13-C14-C15
3	A	402[B]	A1EJP	N4-C5-C6-C7
3	C	401	A1EJP	N4-C5-C6-C7
3	B	401	A1EJP	N4-C5-C6-C7
3	C	401	A1EJP	C4-C5-C6-C7
2	A	401[A]	A1EJO	N5-C12-C13-C14
2	A	401[A]	A1EJO	S1-C12-C13-C14
3	A	402[B]	A1EJP	C4-C5-C6-C7
2	A	401[A]	A1EJO	N4-C5-C6-C7
3	A	402[B]	A1EJP	N4-C5-C6-C11
3	C	401	A1EJP	N4-C5-C6-C11
2	A	401[A]	A1EJO	C4-C5-C6-C7
3	D	401	A1EJP	N4-C5-C6-C7
3	B	401	A1EJP	C4-C5-C6-C7
3	C	401	A1EJP	S1-C12-C13-C16
3	A	402[B]	A1EJP	C16-C13-C14-C15
3	C	401	A1EJP	C4-C5-C6-C11
2	A	401[A]	A1EJO	C4-C5-C6-C11
2	A	401[A]	A1EJO	N4-C5-C6-C11
3	B	401	A1EJP	N4-C5-C6-C11
3	D	401	A1EJP	N4-C5-C6-C11
3	A	402[B]	A1EJP	C4-C5-C6-C11
3	D	401	A1EJP	C4-C5-C6-C7

There are no ring outliers.

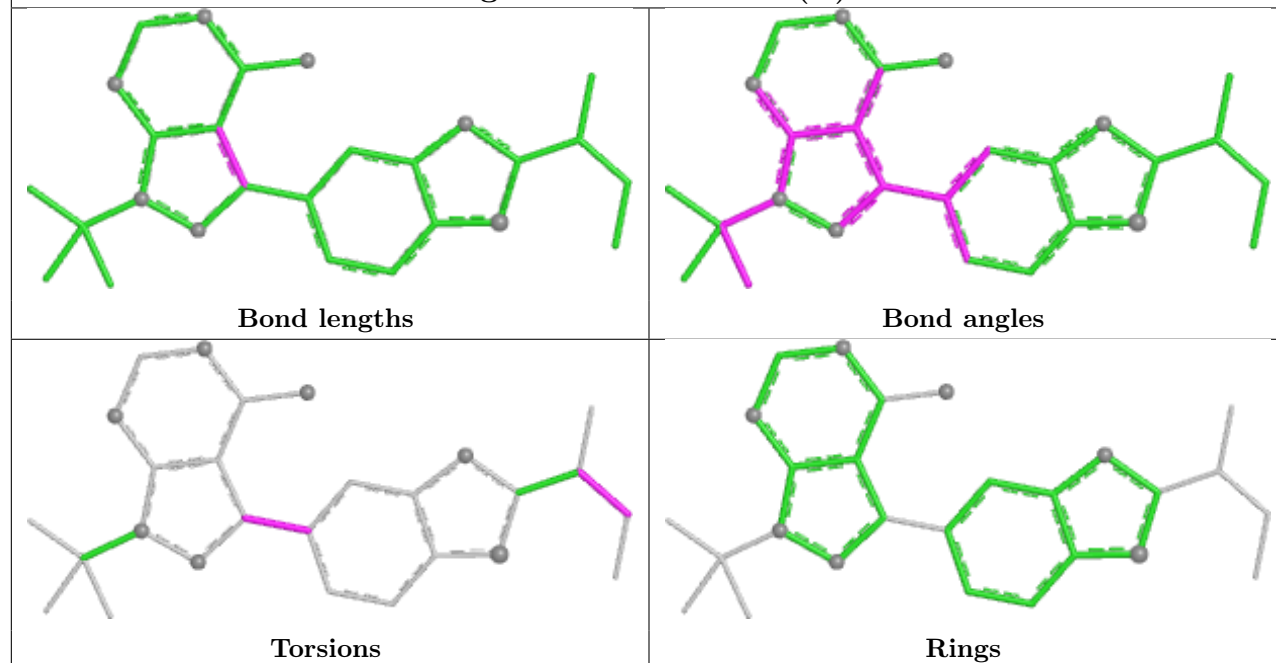
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	A1EJP	1	0

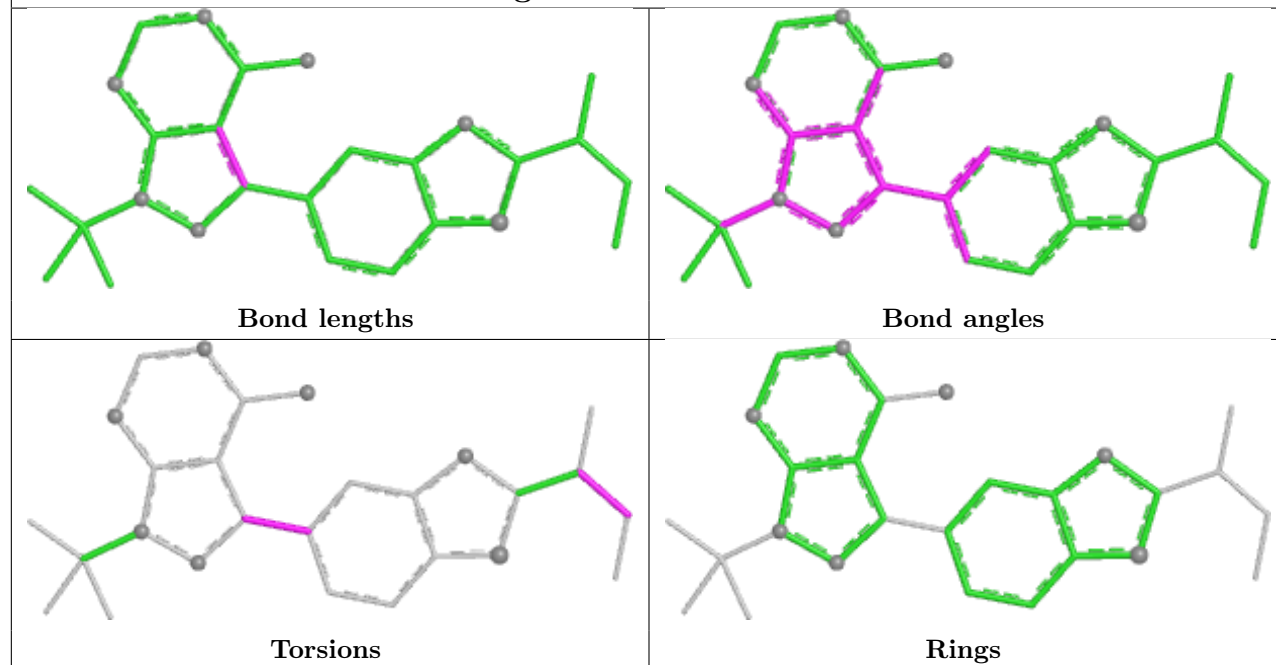
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

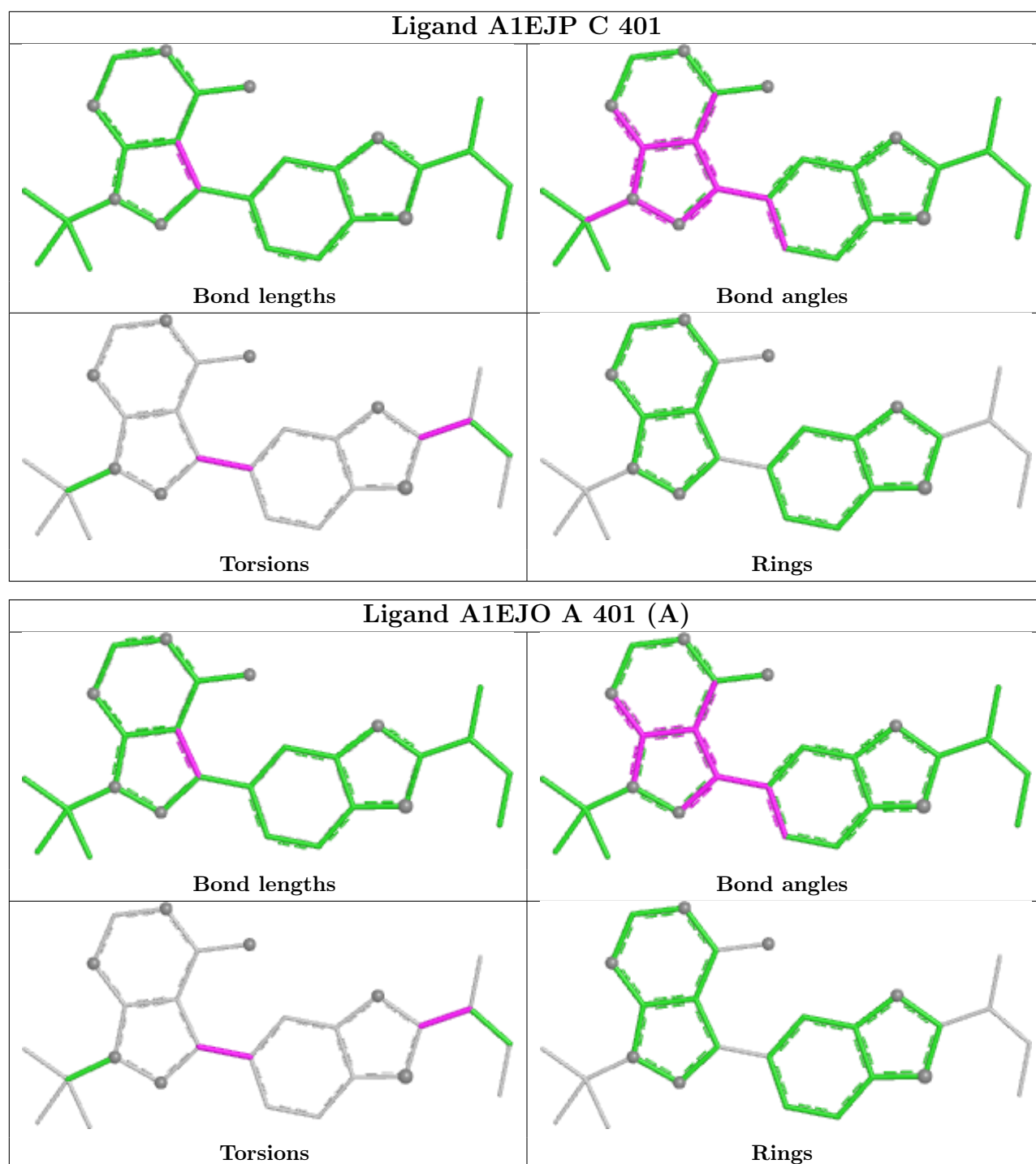


Ligand A1EJP A 402 (B)



Ligand A1EJP B 401





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	259/325 (79%)	0.36	7 (2%) 56 48	33, 59, 88, 112	0
1	B	256/325 (78%)	0.53	9 (3%) 47 40	37, 64, 93, 109	0
1	C	250/325 (76%)	1.02	25 (10%) 12 10	52, 84, 113, 129	0
1	D	255/325 (78%)	1.19	37 (14%) 6 5	51, 89, 118, 137	0
All	All	1020/1300 (78%)	0.77	78 (7%) 20 16	33, 72, 110, 137	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	HIS	4.4
1	D	251	PRO	4.3
1	D	254	PRO	3.7
1	D	290	LEU	3.6
1	C	221	ALA	3.6
1	D	58	ILE	3.4
1	C	273	ASN	3.4
1	D	206	TYR	3.3
1	A	182	GLY	3.3
1	D	210	ILE	3.3
1	B	32	GLY	3.2
1	C	295	VAL	3.2
1	D	255	GLY	3.1
1	D	297	ALA	3.1
1	D	307	SER	3.1
1	C	189	PRO	3.1
1	C	184	LEU	3.0
1	D	91	GLN	3.0
1	D	245	GLU	3.0
1	B	255	GLY	3.0
1	D	140	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	142	ARG	2.9
1	C	241	PRO	2.9
1	D	127	LEU	2.9
1	D	280	CYS	2.8
1	D	33	PHE	2.8
1	A	183	THR	2.8
1	D	130	CYS	2.8
1	B	165	SER	2.8
1	D	191	LEU	2.8
1	D	247	PRO	2.7
1	D	249	GLY	2.7
1	C	255	GLY	2.7
1	B	167	PHE	2.7
1	C	142	ARG	2.6
1	C	61	GLU	2.6
1	D	291	VAL	2.6
1	C	136	ASP	2.6
1	D	221	ALA	2.6
1	D	240	ARG	2.6
1	C	249	GLY	2.5
1	D	277	PHE	2.5
1	B	184	LEU	2.5
1	B	307	SER	2.4
1	C	245	GLU	2.4
1	D	278	GLN	2.4
1	D	32	GLY	2.4
1	A	273	ASN	2.4
1	C	265	HIS	2.4
1	C	307	SER	2.4
1	D	276	SER	2.4
1	C	162	PHE	2.4
1	D	92	ALA	2.4
1	D	136	ASP	2.4
1	C	244	THR	2.3
1	D	119	CYS	2.3
1	C	87	PHE	2.3
1	C	186	TYR	2.3
1	C	53	VAL	2.2
1	A	31	GLY	2.2
1	C	247	PRO	2.2
1	B	136	ASP	2.2
1	B	243	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	222	GLU	2.1
1	A	305	TYR	2.1
1	C	117	LEU	2.1
1	D	279	ASP	2.1
1	C	81	GLU	2.1
1	D	60	TRP	2.1
1	B	305	TYR	2.1
1	A	167	PHE	2.1
1	C	34	GLY	2.1
1	D	287	VAL	2.1
1	D	188	ASP	2.0
1	D	57	LYS	2.0
1	C	60	TRP	2.0
1	D	117	LEU	2.0
1	C	294	LYS	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.

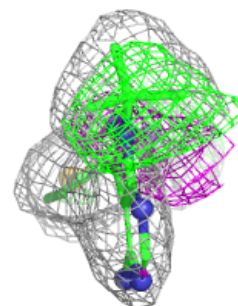
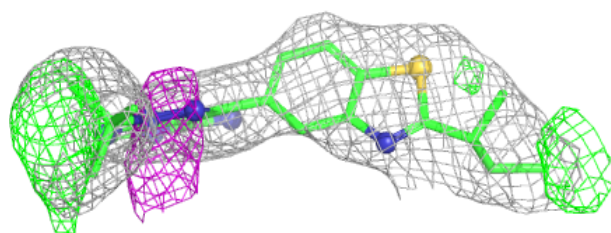
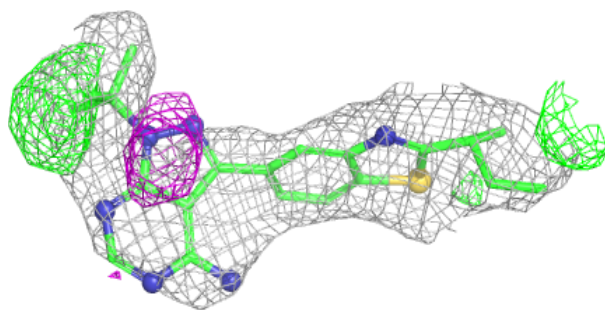
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1EJP	D	401	27/27	0.73	0.23	41,70,83,92	0
2	A1EJO	A	401[A]	27/27	0.78	0.27	44,51,55,57	27
3	A1EJP	B	401	27/27	0.79	0.19	26,55,66,73	0
3	A1EJP	A	402[B]	27/27	0.79	0.21	43,51,56,58	27
3	A1EJP	C	401	27/27	0.81	0.20	55,73,83,88	0

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.

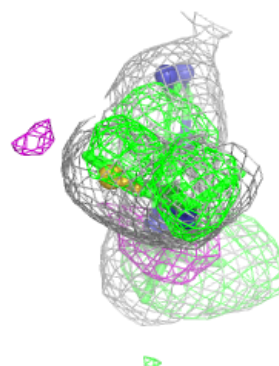
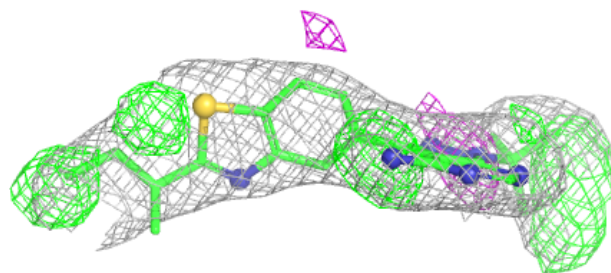
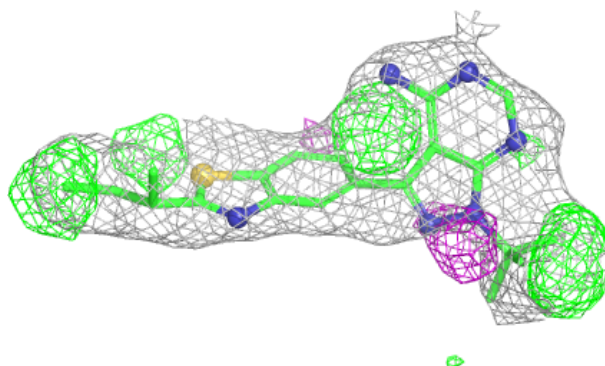
Electron density around A1EJP D 401:

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



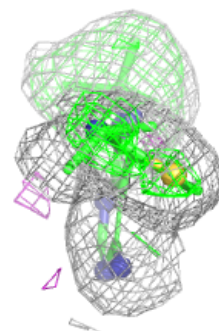
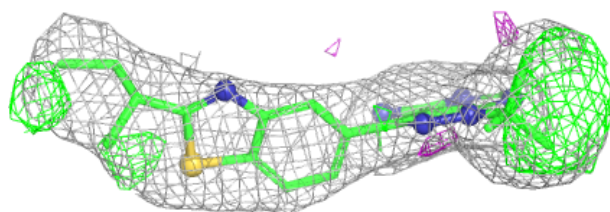
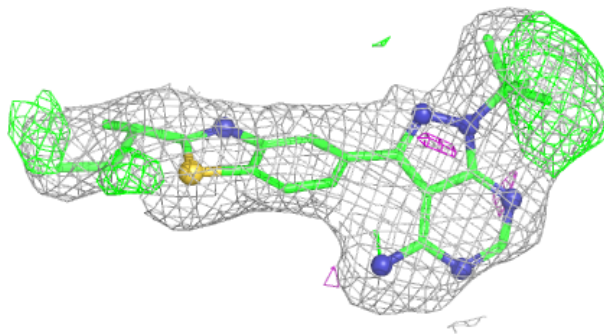
Electron density around A1EJO A 401 (A):

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

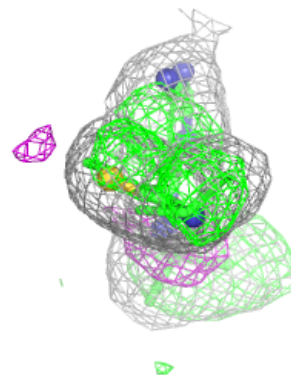
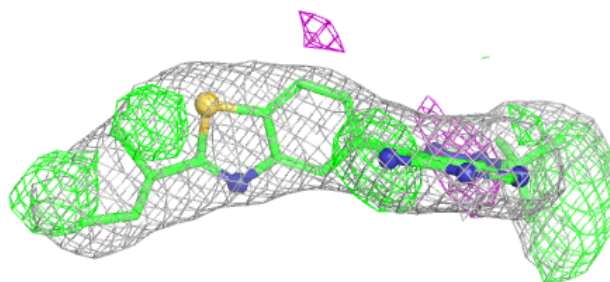
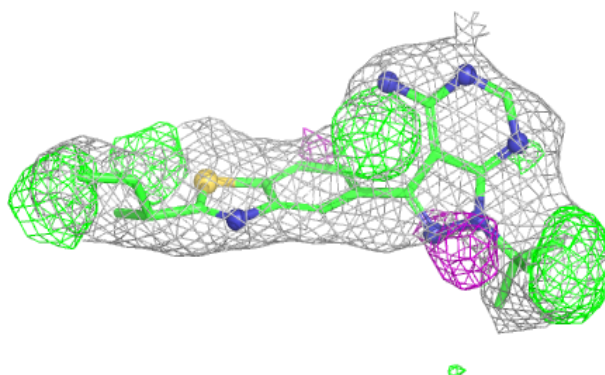


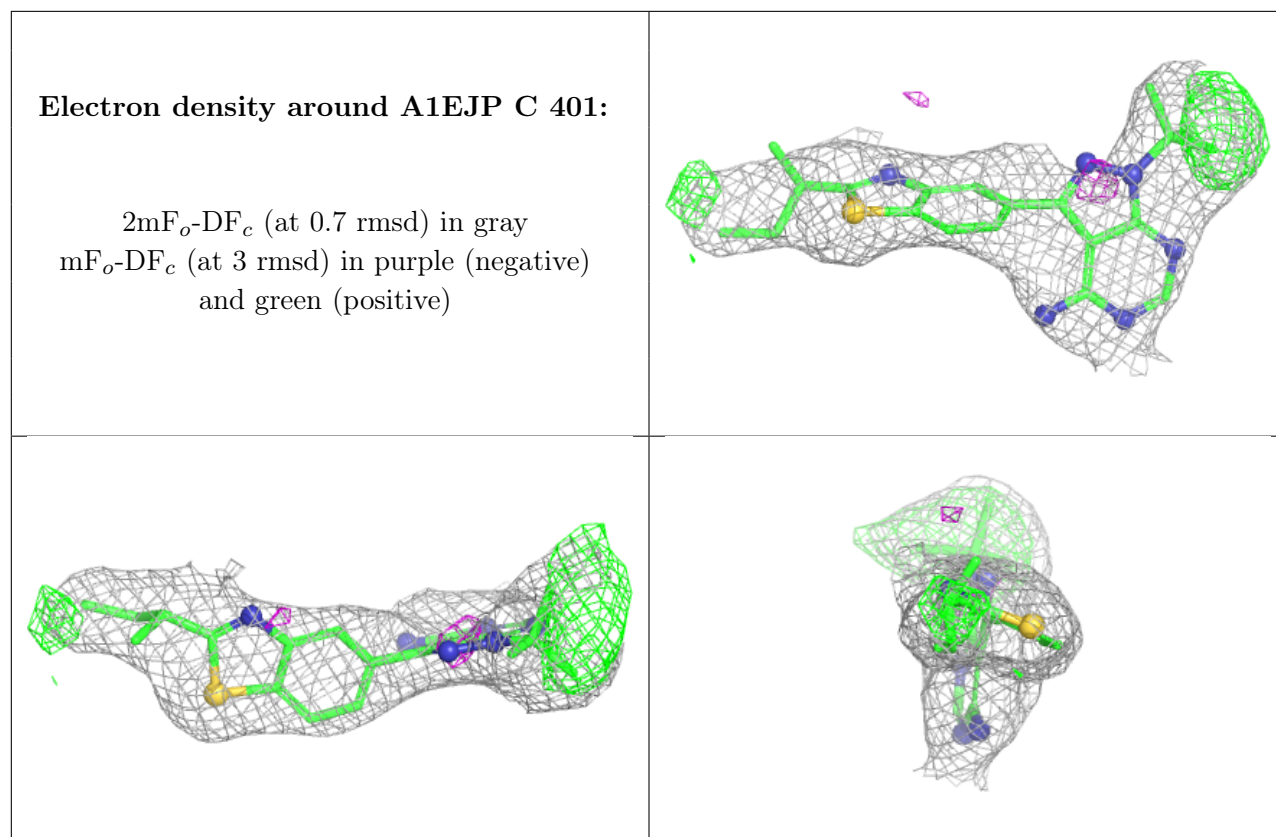
Electron density around A1EJP B 401:

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

**Electron density around A1EJP A 402 (B):**

$2mF_o-DF_c$ (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.