



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 07:53 AM EDT

PDB ID : 5DHR
Title : Crystal structure of NAD kinase 1 from *Listeria monocytogenes* in complex with a novel inhibitor
Authors : Gelin, M.; Paoletti, J.; Assairi, L.; Huteau, V.; Pochet, S.; Labesse, G.
Deposited on : 2015-08-31
Resolution : 2.31 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

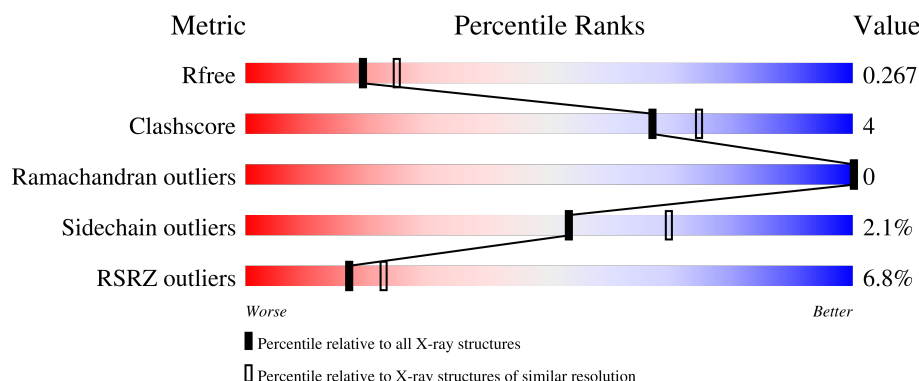
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	272	<div> <div>100%</div> <div> <div>86%</div> <div>10%</div> <div>•</div> </div> </div>
1	B	272	<div> <div>11%</div> <div> <div>84%</div> <div>12%</div> <div>•</div> </div> </div>
1	C	272	<div> <div>4%</div> <div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
1	D	272	<div> <div>10%</div> <div> <div>83%</div> <div>11%</div> <div>5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	A	301	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8587 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 NAD kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2071	1326	348	388	9			
1	B	262	Total	C	N	O	S	0	1	0
			2096	1345	351	391	9			
1	C	259	Total	C	N	O	S	0	0	0
			2010	1289	338	374	9			
1	D	259	Total	C	N	O	S	0	0	0
			2024	1298	342	375	9			

There are 32 discrepancies between the modelled and reference sequences:

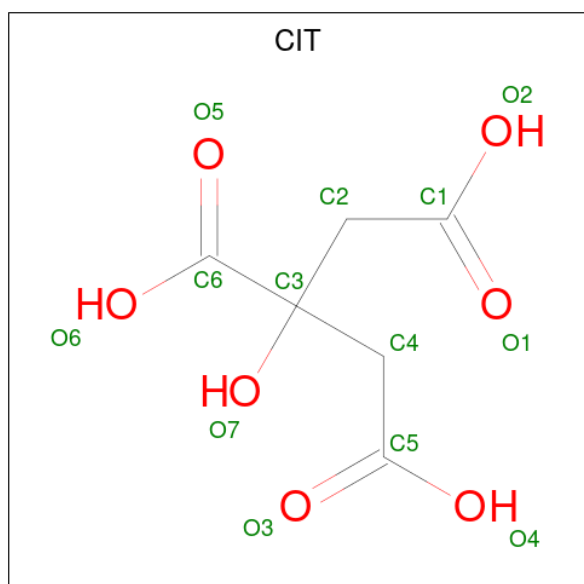
Chain	Residue	Modelled	Actual	Comment	Reference
A	265	LEU	-	expression tag	UNP Q8Y8D7
A	266	GLU	-	expression tag	UNP Q8Y8D7
A	267	HIS	-	expression tag	UNP Q8Y8D7
A	268	HIS	-	expression tag	UNP Q8Y8D7
A	269	HIS	-	expression tag	UNP Q8Y8D7
A	270	HIS	-	expression tag	UNP Q8Y8D7
A	271	HIS	-	expression tag	UNP Q8Y8D7
A	272	HIS	-	expression tag	UNP Q8Y8D7
B	265	LEU	-	expression tag	UNP Q8Y8D7
B	266	GLU	-	expression tag	UNP Q8Y8D7
B	267	HIS	-	expression tag	UNP Q8Y8D7
B	268	HIS	-	expression tag	UNP Q8Y8D7
B	269	HIS	-	expression tag	UNP Q8Y8D7
B	270	HIS	-	expression tag	UNP Q8Y8D7
B	271	HIS	-	expression tag	UNP Q8Y8D7
B	272	HIS	-	expression tag	UNP Q8Y8D7
C	265	LEU	-	expression tag	UNP Q8Y8D7
C	266	GLU	-	expression tag	UNP Q8Y8D7
C	267	HIS	-	expression tag	UNP Q8Y8D7
C	268	HIS	-	expression tag	UNP Q8Y8D7
C	269	HIS	-	expression tag	UNP Q8Y8D7

Continued on next page...

Continued from previous page...

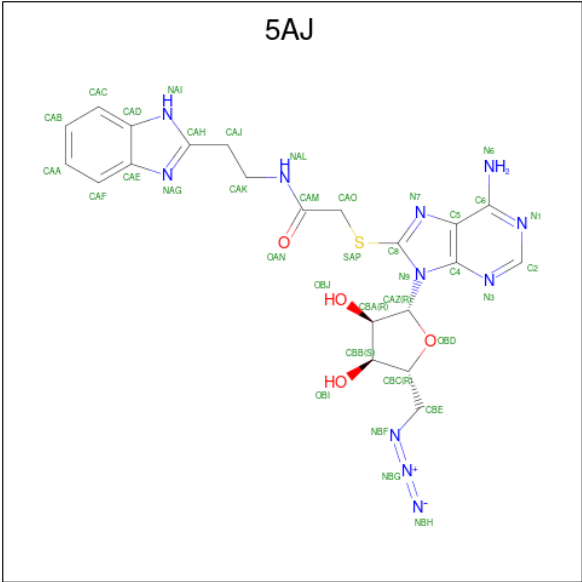
Chain	Residue	Modelled	Actual	Comment	Reference
C	270	HIS	-	expression tag	UNP Q8Y8D7
C	271	HIS	-	expression tag	UNP Q8Y8D7
C	272	HIS	-	expression tag	UNP Q8Y8D7
D	265	LEU	-	expression tag	UNP Q8Y8D7
D	266	GLU	-	expression tag	UNP Q8Y8D7
D	267	HIS	-	expression tag	UNP Q8Y8D7
D	268	HIS	-	expression tag	UNP Q8Y8D7
D	269	HIS	-	expression tag	UNP Q8Y8D7
D	270	HIS	-	expression tag	UNP Q8Y8D7
D	271	HIS	-	expression tag	UNP Q8Y8D7
D	272	HIS	-	expression tag	UNP Q8Y8D7

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



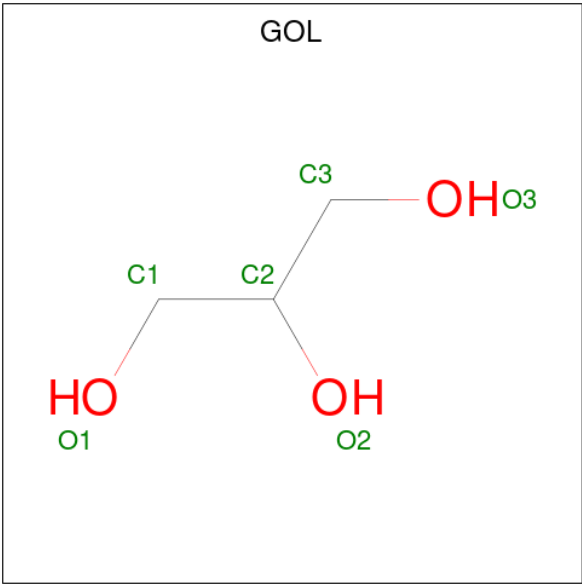
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 5'-azido-8-[(2-{[2-(1H-benzimidazol-2-yl)ethyl]amino}-2-oxoethyl)sulfanyl]-5'-deoxyadenosine (three-letter code: 5AJ) (formula: $C_{21}H_{23}N_{11}O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			37	21	11	4	1		
3	B	1	Total	C	N	O	S	0	0
			37	21	11	4	1		
3	C	1	Total	C	N	O	S	0	0
			37	21	11	4	1		
3	D	1	Total	C	N	O	S	0	0
			37	21	11	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

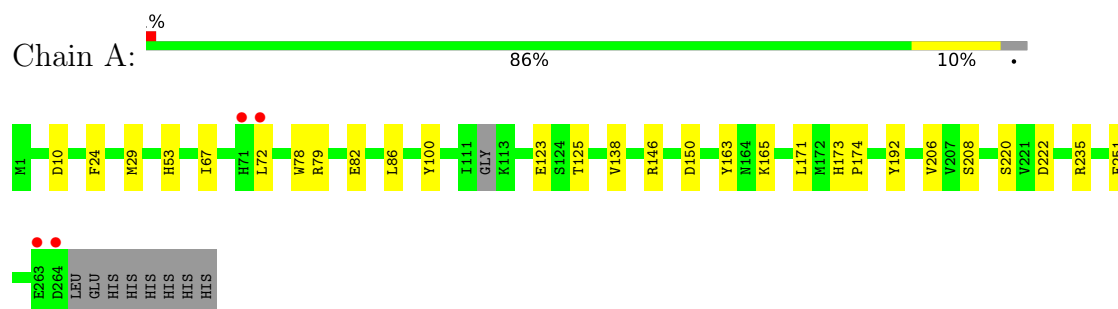
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total	O	0	0
			86	86		
5	B	30	Total	O	0	0
			30	30		
5	C	51	Total	O	0	0
			51	51		
5	D	39	Total	O	0	0
			39	39		

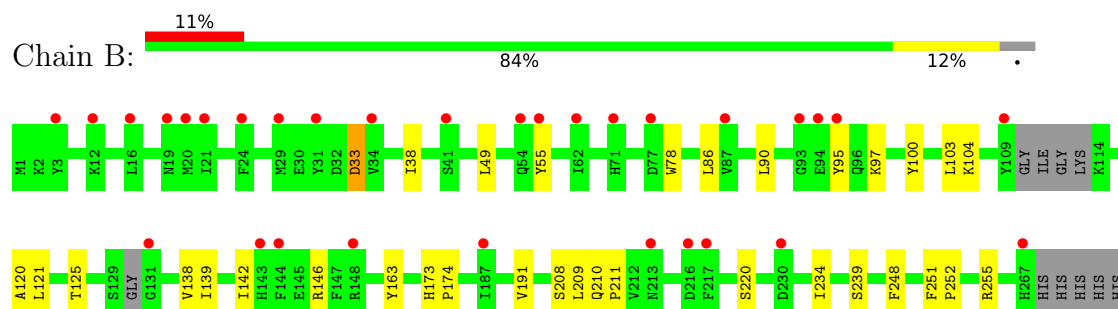
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

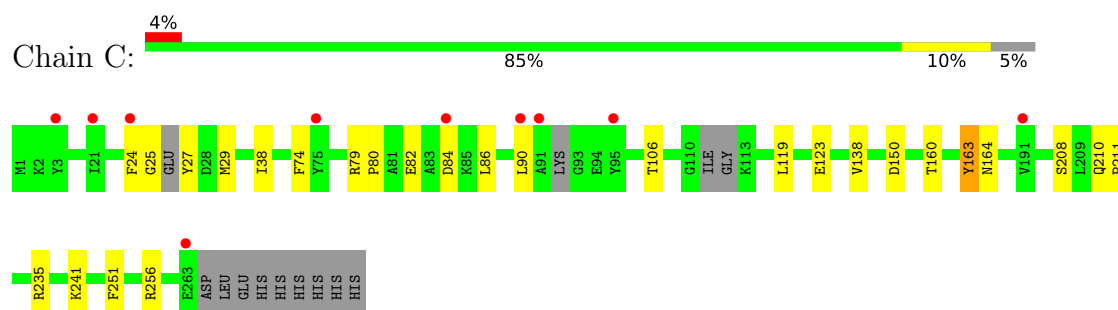
• Molecule 1: NAD kinase 1



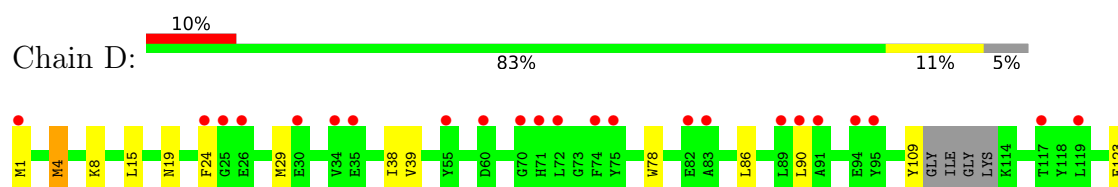
• Molecule 1: NAD kinase 1



• Molecule 1: NAD kinase 1



• Molecule 1: NAD kinase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.53Å 118.71Å 66.60Å 90.00° 100.43° 90.00°	Depositor
Resolution (Å)	57.30 – 2.31 59.35 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.4 (57.30-2.31) 99.4 (59.35-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.224 , 0.266 0.228 , 0.267	Depositor DCC
R_{free} test set	1379 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8587	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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: CIT, 5AJ, GOL

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	0.21	0/2121	0.35	0/2871
1	B	0.21	0/2147	0.34	0/2902
1	C	0.20	0/2058	0.35	0/2785
1	D	0.21	0/2074	0.35	0/2809
All	All	0.21	0/8400	0.35	0/11367

There are no bond length outliers.

There are no bond angle outliers.

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	2071	0	1994	15	0
1	B	2096	0	2033	19	0
1	C	2010	0	1913	14	0
1	D	2024	0	1939	15	0
2	A	13	0	5	1	0
2	B	13	0	5	2	0
3	A	37	0	0	1	0
3	B	37	0	0	1	0
3	C	37	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	37	0	0	1	0
4	C	6	0	8	0	0
5	A	86	0	0	1	0
5	B	30	0	0	1	0
5	C	51	0	0	0	0
5	D	39	0	0	1	0
All	All	8587	0	7897	64	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 (64) 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:125:THR:HG1	1:A:220:SER:HG	1.34	0.72
1:D:38:ILE:HG21	1:D:90:LEU:HD21	1.74	0.70
1:B:125:THR:HG1	1:B:220:SER:HG	1.38	0.64
1:D:160:THR:HG21	1:D:172:MET:HG2	1.79	0.63
1:C:24:PHE:HB3	1:C:29:MET:HB2	1.84	0.59
1:A:165:LYS:NZ	5:A:404:HOH:O	2.37	0.57
1:B:103:LEU:HB3	1:B:120:ALA:HB3	1.87	0.56
1:C:25:GLY:O	1:C:27:TYR:N	2.38	0.56
1:B:138:VAL:HB	1:B:208:SER:HB3	1.88	0.56
1:B:38:ILE:HD13	1:B:90:LEU:HD22	1.87	0.55
1:B:100:TYR:OH	2:B:301:CIT:O6	2.25	0.54
1:A:100:TYR:OH	2:A:301:CIT:O5	2.25	0.53
1:B:252:PRO:HD2	1:B:255:ARG:HD3	1.90	0.53
1:B:173:HIS:CE1	2:B:301:CIT:H42	2.44	0.53
1:A:165:LYS:HD2	1:A:171:LEU:HD21	1.91	0.53
1:B:146:ARG:NH2	1:B:191:VAL:O	2.41	0.52
1:C:38:ILE:HG21	1:C:90:LEU:HD21	1.92	0.52
1:B:104:LYS:HB2	1:B:239:SER:HB2	1.92	0.52
1:B:209:LEU:HB2	1:B:234:ILE:HB	1.91	0.52
1:D:78:TRP:HZ2	1:D:248:PHE:HB2	1.76	0.51
1:A:24:PHE:HD1	1:A:29:MET:HG3	1.76	0.50
1:B:49:LEU:HD23	1:B:121:LEU:HD23	1.93	0.50
1:C:74:PHE:HA	1:C:256:ARG:HD2	1.95	0.49
1:D:15:LEU:O	1:D:19:ASN:ND2	2.32	0.49
1:C:119:LEU:HD11	1:C:241:LYS:HD2	1.95	0.48
3:B:302:5AJ:NAG	3:B:302:5AJ:NAL	2.61	0.48
3:D:301:5AJ:OBD	3:D:301:5AJ:SAP	2.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLN:HA	1:C:211:PRO:HD3	1.83	0.46
1:C:79:ARG:HG3	1:C:80:PRO:HD2	1.98	0.45
1:D:1:MET:N	1:D:29:MET:SD	2.86	0.45
1:D:173:HIS:HA	1:D:174:PRO:HD3	1.86	0.45
1:A:53:HIS:NE2	1:A:222:ASP:OD2	2.43	0.45
1:C:38:ILE:HD13	1:C:90:LEU:HD11	1.98	0.45
1:A:150:ASP:OD2	1:C:163:TYR:OH	2.20	0.44
3:A:302:5AJ:N6	1:C:150:ASP:OD1	2.50	0.44
1:B:139:ILE:O	1:B:142:ILE:HG22	2.18	0.44
1:C:106:THR:HB	1:C:235:ARG:HB2	1.99	0.43
1:D:211:PRO:HG3	1:D:217:PHE:HE2	1.83	0.43
1:C:138:VAL:HB	1:C:208:SER:HB3	2.00	0.43
1:D:160:THR:HA	1:D:164:ASN:HB3	1.99	0.43
1:B:97:LYS:NZ	5:B:404:HOH:O	2.46	0.43
1:B:173:HIS:HA	1:B:174:PRO:HD3	1.84	0.43
1:D:210:GLN:HA	1:D:211:PRO:HD3	1.85	0.43
1:A:206:VAL:HG11	1:A:235:ARG:NH2	2.34	0.42
1:D:133:PHE:CD2	1:D:151:GLY:HA2	2.55	0.42
1:A:67:ILE:HG12	1:A:78:TRP:HB2	2.00	0.42
1:A:79:ARG:NH2	1:A:82:GLU:OE2	2.52	0.42
1:D:4:MET:HG2	1:D:39:VAL:HG22	2.01	0.42
1:C:160:THR:HA	1:C:164:ASN:HB3	2.00	0.42
1:C:82:GLU:O	1:C:86:LEU:HG	2.19	0.42
1:A:146:ARG:HG2	1:A:192:TYR:HD1	1.84	0.42
1:B:78:TRP:CE2	1:B:86:LEU:HD21	2.54	0.42
1:D:191:VAL:HG23	1:D:192:TYR:CD2	2.55	0.42
1:A:173:HIS:HA	1:A:174:PRO:HD3	1.84	0.41
1:B:33:ASP:O	1:B:55:TYR:OH	2.38	0.41
1:B:95:TYR:HB3	1:B:248:PHE:CE2	2.55	0.41
1:D:206:VAL:HG11	1:D:235:ARG:NH2	2.35	0.41
1:D:220:SER:HA	1:D:225:SER:HA	2.02	0.41
1:D:8:LYS:NZ	5:D:407:HOH:O	2.50	0.41
1:B:142:ILE:HD12	1:B:142:ILE:HA	1.96	0.41
1:A:10:ASP:OD1	1:A:10:ASP:N	2.54	0.41
1:B:210:GLN:HA	1:B:211:PRO:HD3	1.87	0.41
1:A:138:VAL:HB	1:A:208:SER:HB3	2.03	0.40
1:A:146:ARG:HG2	1:A:192:TYR:CD1	2.57	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	259/272 (95%)	246 (95%)	13 (5%)	0	100	100
1	B	257/272 (94%)	246 (96%)	11 (4%)	0	100	100
1	C	251/272 (92%)	235 (94%)	16 (6%)	0	100	100
1	D	255/272 (94%)	241 (94%)	14 (6%)	0	100	100
All	All	1022/1088 (94%)	968 (95%)	54 (5%)	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	220/237 (93%)	215 (98%)	5 (2%)	50	66
1	B	226/237 (95%)	223 (99%)	3 (1%)	69	81
1	C	210/237 (89%)	206 (98%)	4 (2%)	57	73
1	D	212/237 (90%)	206 (97%)	6 (3%)	43	59
All	All	868/948 (92%)	850 (98%)	18 (2%)	53	70

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	86	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	123	GLU
1	A	163	TYR
1	A	251	PHE
1	B	33	ASP
1	B	163	TYR
1	B	251	PHE
1	C	84	ASP
1	C	123	GLU
1	C	163	TYR
1	C	251	PHE
1	D	4	MET
1	D	24	PHE
1	D	86	LEU
1	D	109	TYR
1	D	123	GLU
1	D	251	PHE

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

Mol	Chain	Res	Type
1	C	205	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	5AJ	A	302	-	36,41,41	1.93	12 (33%)	34,58,58	1.51	5 (14%)
3	5AJ	B	302	-	36,41,41	1.53	5 (13%)	34,58,58	1.55	7 (20%)
2	CIT	A	301	-	12,12,12	1.04	0	17,17,17	1.64	1 (5%)
3	5AJ	D	301	-	36,41,41	1.62	7 (19%)	34,58,58	1.60	7 (20%)
2	CIT	B	301	-	12,12,12	1.03	0	17,17,17	1.45	2 (11%)
3	5AJ	C	302	-	36,41,41	1.81	10 (27%)	34,58,58	1.45	5 (14%)
4	GOL	C	301	-	5,5,5	0.37	0	5,5,5	0.27	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	5AJ	A	302	-	-	1/13/35/35	0/5/5/5
3	5AJ	B	302	-	-	4/13/35/35	0/5/5/5
2	CIT	A	301	-	-	0/16/16/16	-
3	5AJ	D	301	-	-	6/13/35/35	0/5/5/5
2	CIT	B	301	-	-	6/16/16/16	-
3	5AJ	C	302	-	-	4/13/35/35	0/5/5/5
4	GOL	C	301	-	-	2/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	5AJ	C8-N9	-5.94	1.30	1.36
3	D	301	5AJ	C8-N9	-4.92	1.31	1.36
3	B	302	5AJ	C8-N9	-4.90	1.31	1.36
3	C	302	5AJ	C8-N9	-4.65	1.31	1.36
3	C	302	5AJ	C4-N3	-3.41	1.30	1.35
3	A	302	5AJ	C4-N3	-3.36	1.31	1.35
3	A	302	5AJ	NBG-NBF	2.91	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	5AJ	CAF-CAE	-2.72	1.37	1.41
3	C	302	5AJ	C2-N1	-2.68	1.28	1.33
3	C	302	5AJ	CAF-CAE	-2.66	1.37	1.41
3	C	302	5AJ	CAE-NAG	-2.63	1.30	1.38
3	A	302	5AJ	C8-SAP	-2.60	1.68	1.75
3	C	302	5AJ	NBG-NBF	2.59	1.30	1.23
3	D	301	5AJ	NBG-NBF	2.57	1.30	1.23
3	C	302	5AJ	OBD-CBC	-2.57	1.39	1.45
3	B	302	5AJ	CAF-CAE	-2.55	1.37	1.41
3	A	302	5AJ	CAE-NAG	-2.51	1.30	1.38
3	A	302	5AJ	CAC-CAD	-2.50	1.37	1.41
3	A	302	5AJ	CAD-NAI	-2.48	1.30	1.38
3	A	302	5AJ	CAZ-N9	-2.47	1.42	1.49
3	B	302	5AJ	CAC-CAD	-2.43	1.37	1.41
3	C	302	5AJ	CAD-NAI	-2.39	1.31	1.38
3	D	301	5AJ	C4-N3	-2.38	1.32	1.35
3	B	302	5AJ	CAE-NAG	-2.33	1.31	1.38
3	D	301	5AJ	OBD-CBC	-2.29	1.39	1.45
3	A	302	5AJ	OBD-CBC	-2.28	1.39	1.45
3	C	302	5AJ	CAC-CAD	-2.26	1.37	1.41
3	B	302	5AJ	CAD-NAI	-2.25	1.31	1.38
3	D	301	5AJ	CAC-CAD	-2.17	1.38	1.41
3	D	301	5AJ	CAD-NAI	-2.12	1.32	1.38
3	C	302	5AJ	C5-C4	-2.09	1.35	1.40
3	D	301	5AJ	CAF-CAE	-2.07	1.38	1.41
3	A	302	5AJ	OBD-CAZ	-2.03	1.38	1.41
3	A	302	5AJ	C5-C4	-2.01	1.35	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	5AJ	N3-C2-N1	-4.51	121.62	128.68
2	A	301	CIT	O6-C6-C3	4.50	120.86	113.05
3	A	302	5AJ	N3-C2-N1	-4.42	121.78	128.68
3	D	301	5AJ	N3-C2-N1	-4.41	121.79	128.68
3	C	302	5AJ	N3-C2-N1	-4.25	122.03	128.68
2	B	301	CIT	O6-C6-C3	3.65	119.38	113.05
3	C	302	5AJ	CAZ-N9-C4	-3.26	121.01	126.71
3	D	301	5AJ	CAO-SAP-C8	-3.18	97.78	101.86
3	D	301	5AJ	OBD-CAZ-CBA	-3.05	102.46	106.93
3	A	302	5AJ	CBE-NBF-NBG	2.96	122.04	115.60
3	C	302	5AJ	CBE-NBF-NBG	2.96	122.03	115.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	5AJ	OBD-CBC-CBB	-2.89	99.40	105.11
3	B	302	5AJ	CAK-NAL-CAM	-2.87	117.52	122.84
3	B	302	5AJ	CBE-NBF-NBG	2.74	121.55	115.60
3	D	301	5AJ	CBE-NBF-NBG	2.71	121.50	115.60
3	A	302	5AJ	C4-C5-N7	-2.70	106.73	109.47
3	D	301	5AJ	NAI-CAH-NAG	-2.45	108.40	115.89
3	C	302	5AJ	NAI-CAH-NAG	-2.42	108.51	115.89
3	C	302	5AJ	C4-C5-N7	-2.35	107.08	109.47
3	A	302	5AJ	OBD-CBC-CBB	-2.32	100.52	105.11
3	B	302	5AJ	CBB-CBA-CAZ	2.31	104.45	100.98
3	A	302	5AJ	NAI-CAH-NAG	-2.26	108.98	115.89
3	B	302	5AJ	NAI-CAH-NAG	-2.24	109.06	115.89
3	B	302	5AJ	CAZ-N9-C4	-2.21	122.84	126.71
3	B	302	5AJ	C4-C5-N7	-2.21	107.23	109.47
2	B	301	CIT	O2-C1-C2	2.18	121.35	114.35
3	D	301	5AJ	C4-C5-N7	-2.12	107.32	109.47

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	CIT	O7-C3-C4-C5
3	B	302	5AJ	CBC-CBE-NBF-NBG
3	B	302	5AJ	CAH-CAJ-CAK-NAL
3	B	302	5AJ	NAI-CAH-CAJ-CAK
3	C	302	5AJ	CAH-CAJ-CAK-NAL
3	D	301	5AJ	OBD-CBC-CBE-NBF
3	D	301	5AJ	CAH-CAJ-CAK-NAL
3	D	301	5AJ	NAI-CAH-CAJ-CAK
2	B	301	CIT	C2-C3-C4-C5
3	A	302	5AJ	CAH-CAJ-CAK-NAL
2	B	301	CIT	C6-C3-C4-C5
4	C	301	GOL	O1-C1-C2-C3
3	C	302	5AJ	CBC-CBE-NBF-NBG
3	D	301	5AJ	CBC-CBE-NBF-NBG
4	C	301	GOL	O1-C1-C2-O2
3	C	302	5AJ	CBE-NBF-NBG-NBH
2	B	301	CIT	C1-C2-C3-O7
2	B	301	CIT	C2-C3-C6-O5
2	B	301	CIT	C2-C3-C6-O6
3	C	302	5AJ	CAM-CAO-SAP-C8
3	B	302	5AJ	CBE-NBF-NBG-NBH

Continued on next page...

Continued from previous page...

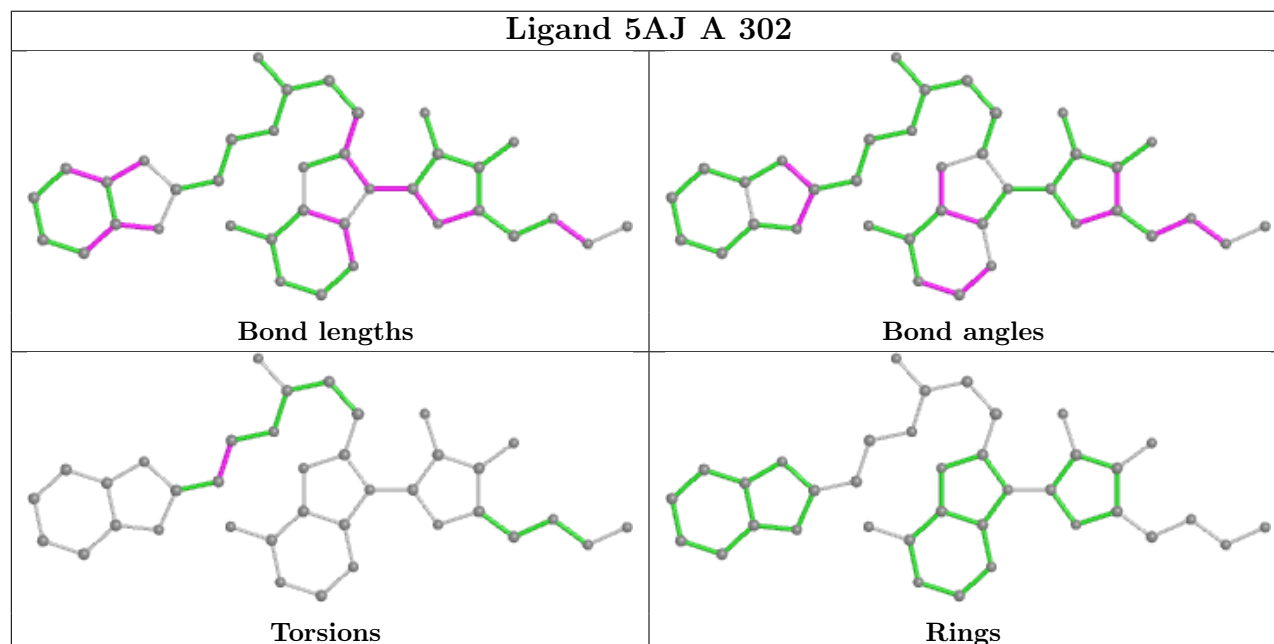
Mol	Chain	Res	Type	Atoms
3	D	301	5AJ	CAM-CAO-SAP-C8
3	D	301	5AJ	CBE-NBF-NBG-NBH

There are no ring outliers.

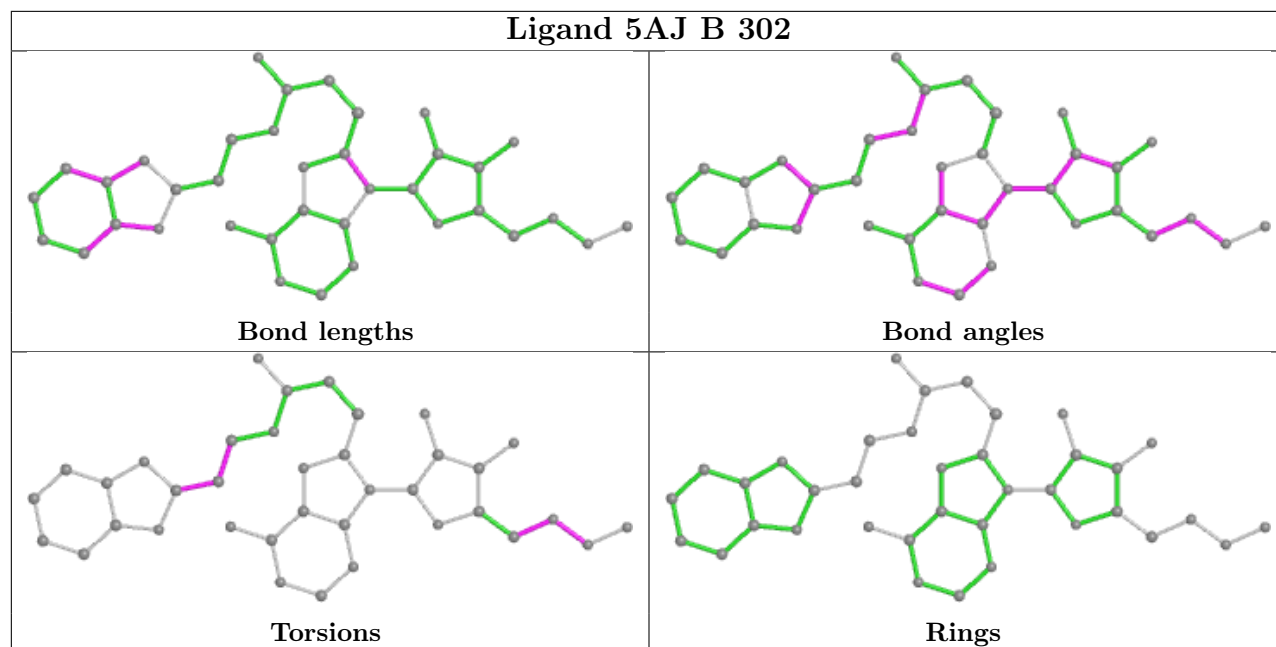
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	5AJ	1	0
3	B	302	5AJ	1	0
2	A	301	CIT	1	0
3	D	301	5AJ	1	0
2	B	301	CIT	2	0

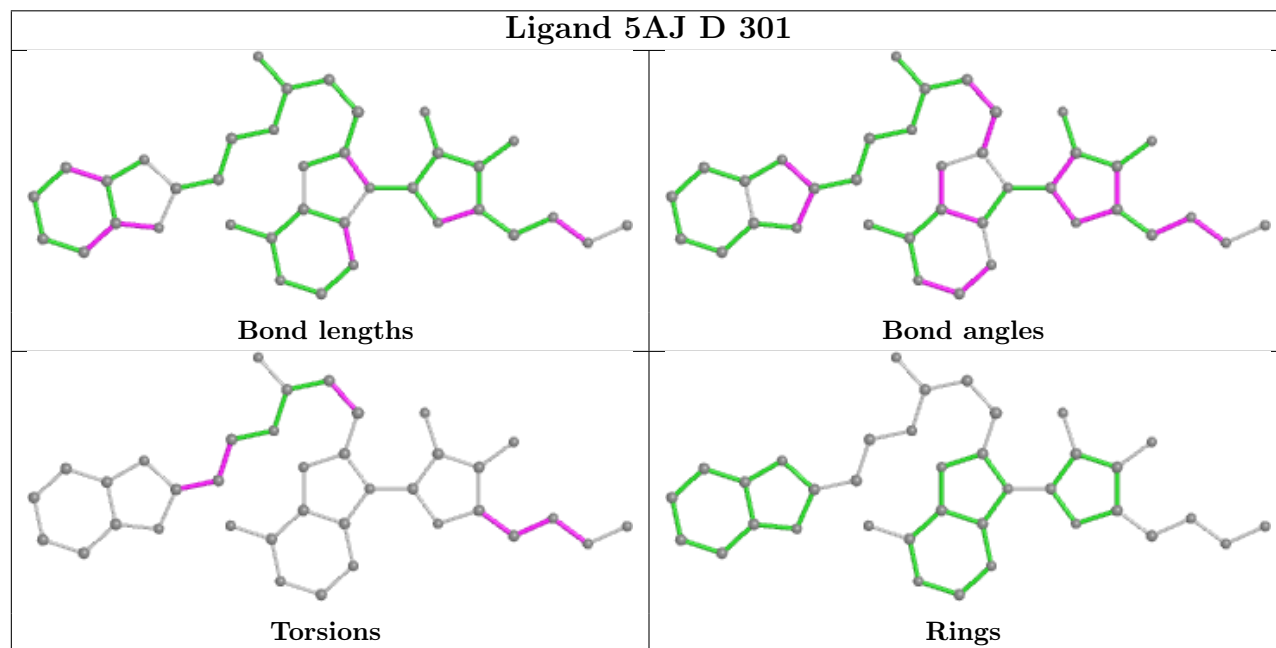
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

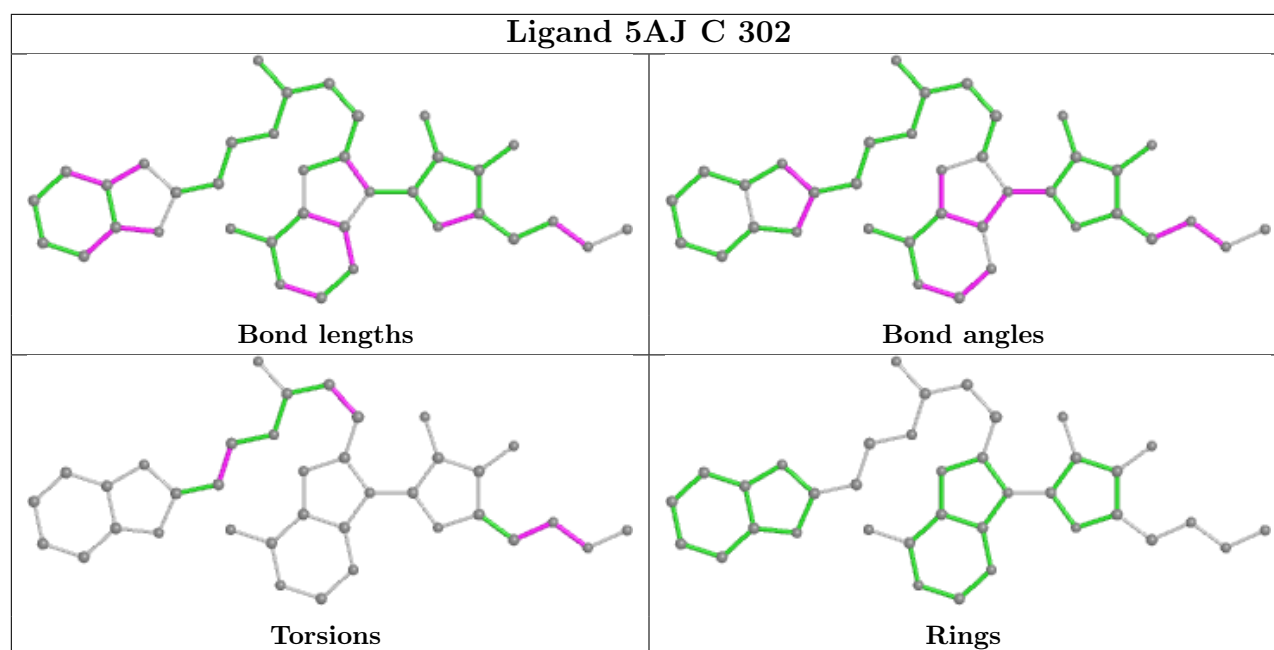


Ligand 5AJ B 302



Ligand 5AJ D 301





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	263/272 (96%)	0.22	4 (1%) 73 79	23, 47, 86, 134	53 (20%)
1	B	262/272 (96%)	0.89	31 (11%) 4 6	31, 76, 116, 139	46 (17%)
1	C	259/272 (95%)	0.43	10 (3%) 39 46	26, 57, 110, 124	41 (15%)
1	D	259/272 (95%)	0.75	26 (10%) 7 10	33, 72, 119, 146	36 (13%)
All	All	1043/1088 (95%)	0.57	71 (6%) 17 23	23, 62, 111, 146	176 (16%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	MET	6.0
1	D	91	ALA	5.2
1	B	87	VAL	5.1
1	B	31	TYR	4.4
1	D	70	GLY	4.4
1	D	24	PHE	4.3
1	B	217	PHE	4.1
1	B	29	MET	4.0
1	D	119	LEU	4.0
1	D	34	VAL	3.9
1	B	187	ILE	3.8
1	B	267	HIS	3.8
1	A	71	HIS	3.7
1	C	24	PHE	3.7
1	C	91	ALA	3.7
1	D	1	MET	3.6
1	B	71	HIS	3.4
1	A	72	LEU	3.3
1	D	248	PHE	3.2
1	D	94	GLU	3.2
1	B	109	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	95	TYR	3.0
1	B	16	LEU	3.0
1	D	117	THR	3.0
1	B	230	ASP	3.0
1	B	62	ILE	2.9
1	D	226	ILE	2.9
1	C	21	ILE	2.9
1	B	143	HIS	2.9
1	D	55	TYR	2.8
1	D	90	LEU	2.8
1	B	216	ASP	2.7
1	B	95	TYR	2.7
1	B	144	PHE	2.7
1	C	75	TYR	2.7
1	D	95	TYR	2.6
1	D	71	HIS	2.6
1	C	3	TYR	2.6
1	B	3	TYR	2.5
1	B	213	ASN	2.5
1	B	34	VAL	2.4
1	D	26	GLU	2.4
1	D	75	TYR	2.4
1	D	89	LEU	2.4
1	A	263	GLU	2.4
1	C	191	VAL	2.4
1	B	131	GLY	2.4
1	B	21	ILE	2.3
1	D	74	PHE	2.3
1	C	90	LEU	2.3
1	B	77	ASP	2.3
1	D	83	ALA	2.3
1	D	60	ASP	2.3
1	B	55	TYR	2.2
1	B	12	LYS	2.2
1	B	54	GLN	2.2
1	D	72	LEU	2.2
1	B	24	PHE	2.2
1	D	82	GLU	2.2
1	D	25	GLY	2.2
1	B	148	ARG	2.2
1	B	93	GLY	2.1
1	B	19	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	30	GLU	2.1
1	C	263	GLU	2.1
1	D	262	ILE	2.1
1	C	84	ASP	2.1
1	D	35	GLU	2.0
1	B	94	GLU	2.0
1	B	41	SER	2.0
1	A	264	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

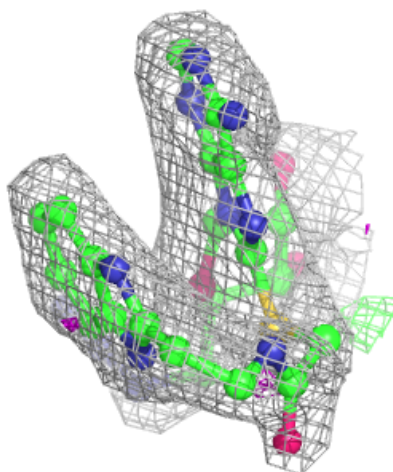
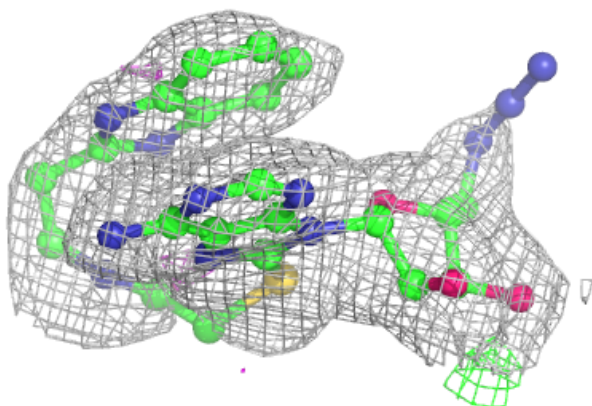
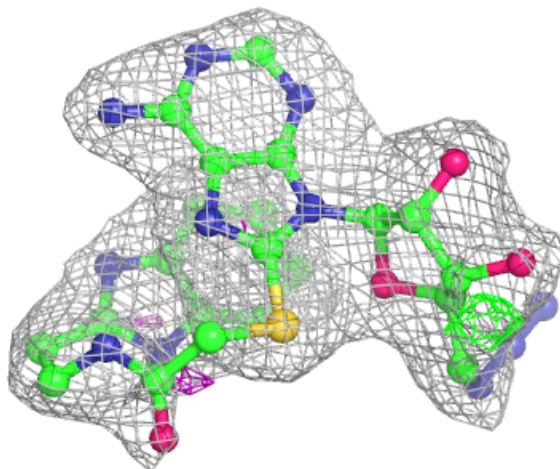
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CIT	A	301	13/13	0.68	0.42	62,65,74,74	13
2	CIT	B	301	13/13	0.74	0.29	65,75,81,89	13
3	5AJ	D	301	37/37	0.87	0.20	55,70,90,91	3
4	GOL	C	301	6/6	0.87	0.24	64,70,71,73	0
3	5AJ	B	302	37/37	0.92	0.14	48,60,81,86	3
3	5AJ	A	302	37/37	0.94	0.15	30,41,63,64	4
3	5AJ	C	302	37/37	0.95	0.12	23,35,62,67	4

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.

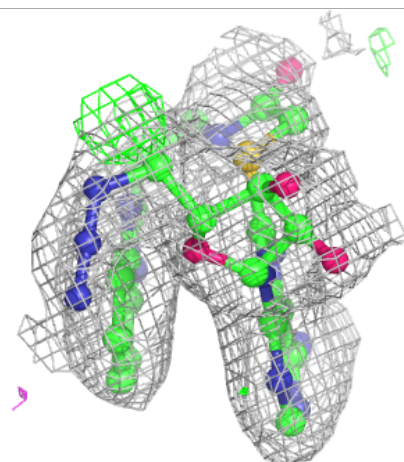
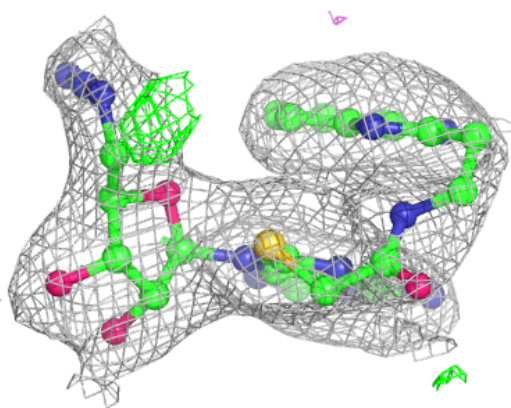
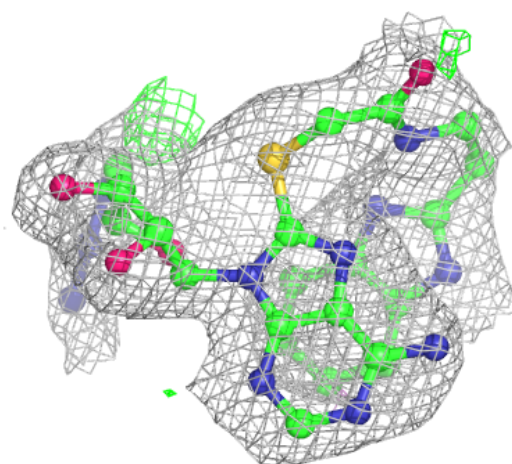
Electron density around 5AJ D 301:

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



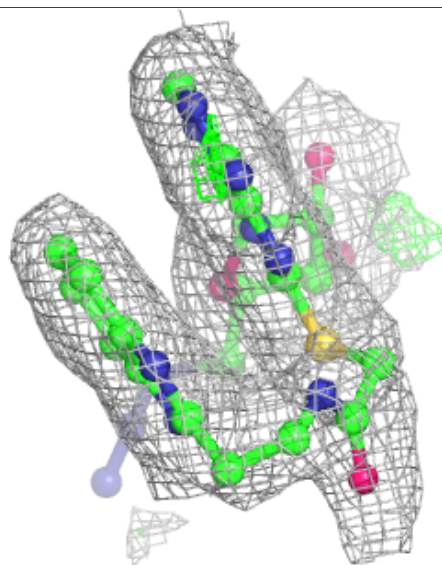
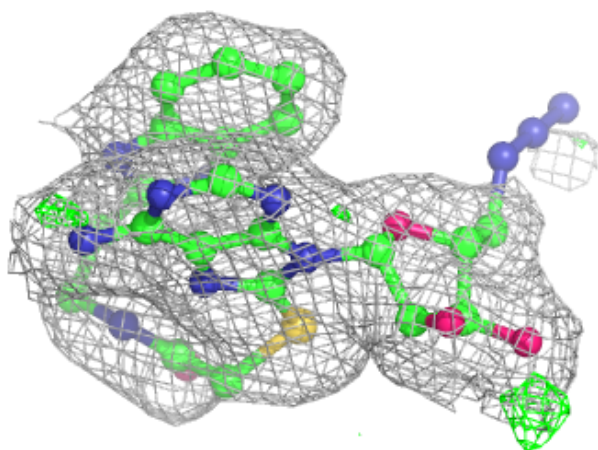
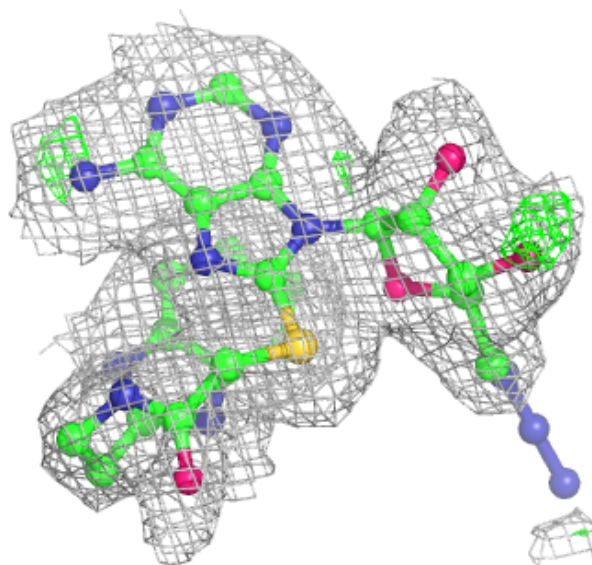
Electron density around 5AJ B 302:

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



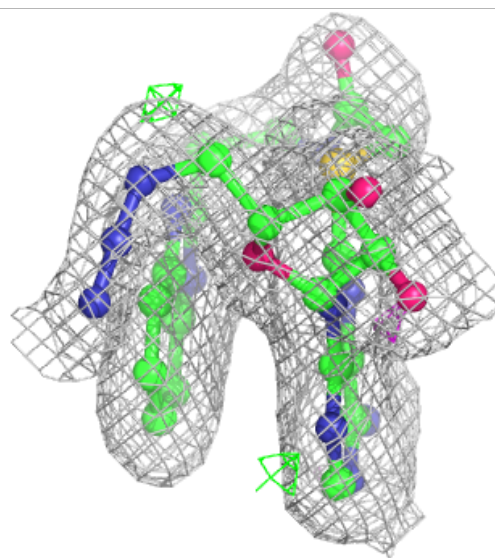
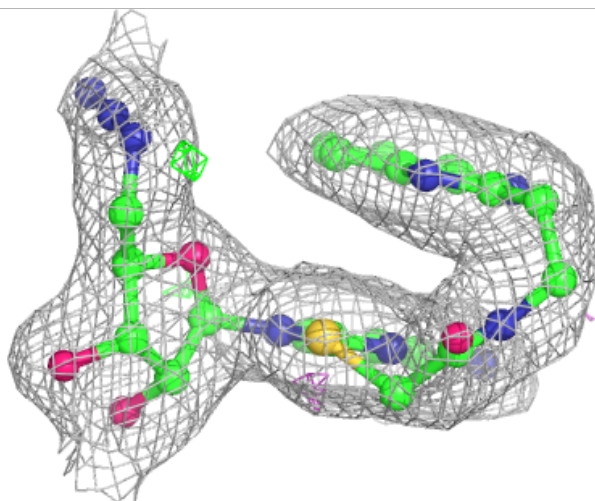
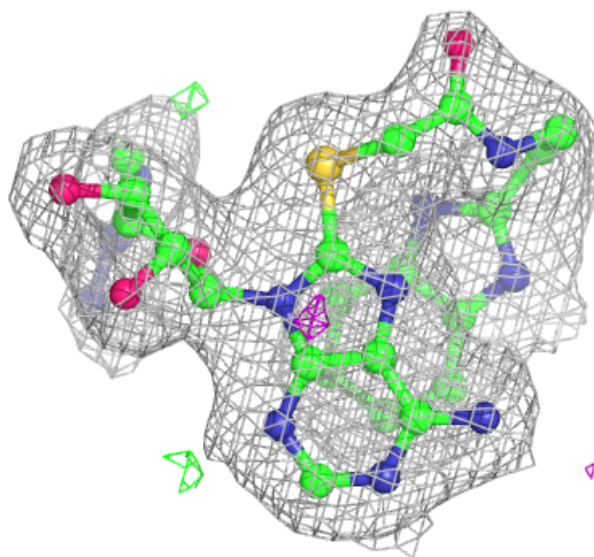
Electron density around 5AJ A 302:

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



Electron density around 5AJ C 302:

$2mF_o-DF_c$ (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.