



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:01 AM UTC

PDB ID : 9ESU / pdb_00009esu
Title : CDK2-cyclin A in complex with FragLite 20
Authors : Hope, I.; Martin, M.P.; Waring, M.J.; Noble, M.E.M.; Endicott, J.A.; Tatum, N.J.
Deposited on : 2024-03-26
Resolution : 2.40 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

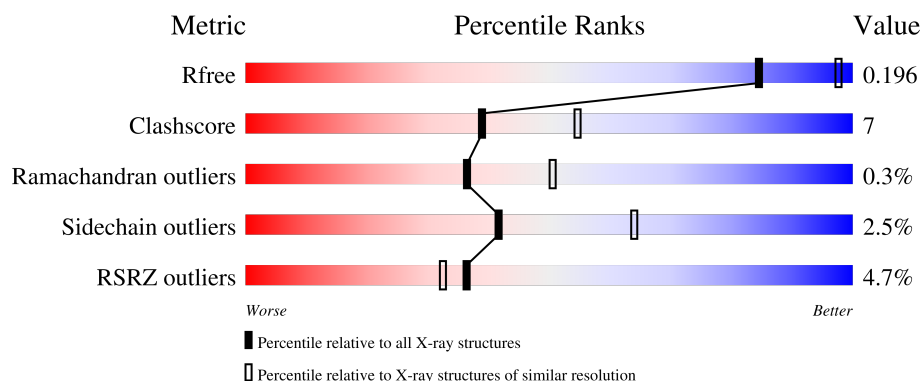
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	302	9% 77% 20% .
1	C	302	6% 79% 18% ..
2	B	268	88% 10% .
2	D	268	3% 87% 9% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9585 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	P	S	0	1	0
			2432	1577	415	431	1	8			
1	C	298	Total	C	N	O	P	S	0	2	0
			2411	1563	409	430	1	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-3	GLY	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	0	0
			2110	1366	344	390	10			
2	D	262	Total	C	N	O	S	0	1	0
			2118	1370	346	392	10			

There are 14 discrepancies between the modelled and reference sequences:

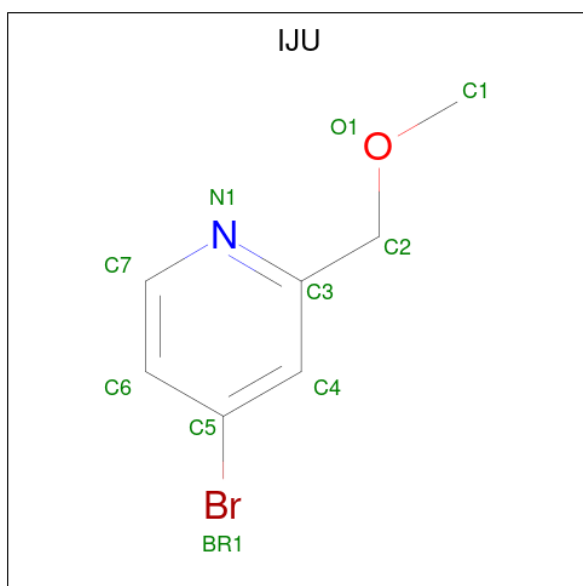
Chain	Residue	Modelled	Actual	Comment	Reference
B	171	GLY	-	expression tag	UNP P30274
B	433	HIS	-	expression tag	UNP P30274
B	434	HIS	-	expression tag	UNP P30274
B	435	HIS	-	expression tag	UNP P30274

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Chain	Residue	Modelled	Actual	Comment	Reference
B	436	HIS	-	expression tag	UNP P30274
B	437	HIS	-	expression tag	UNP P30274
B	438	HIS	-	expression tag	UNP P30274
D	171	GLY	-	expression tag	UNP P30274
D	433	HIS	-	expression tag	UNP P30274
D	434	HIS	-	expression tag	UNP P30274
D	435	HIS	-	expression tag	UNP P30274
D	436	HIS	-	expression tag	UNP P30274
D	437	HIS	-	expression tag	UNP P30274
D	438	HIS	-	expression tag	UNP P30274

- Molecule 3 is 4-bromanyl-2-(methoxymethyl)pyridine (CCD ID: IJU) (formula: C₇H₈BrNO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	1
			20	2	14	2	2		
3	C	1	Total	Br	C	N	O	0	1
			30	3	21	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	131	Total	O	0	0
			131	131		
4	B	150	Total	O	0	0
			150	150		

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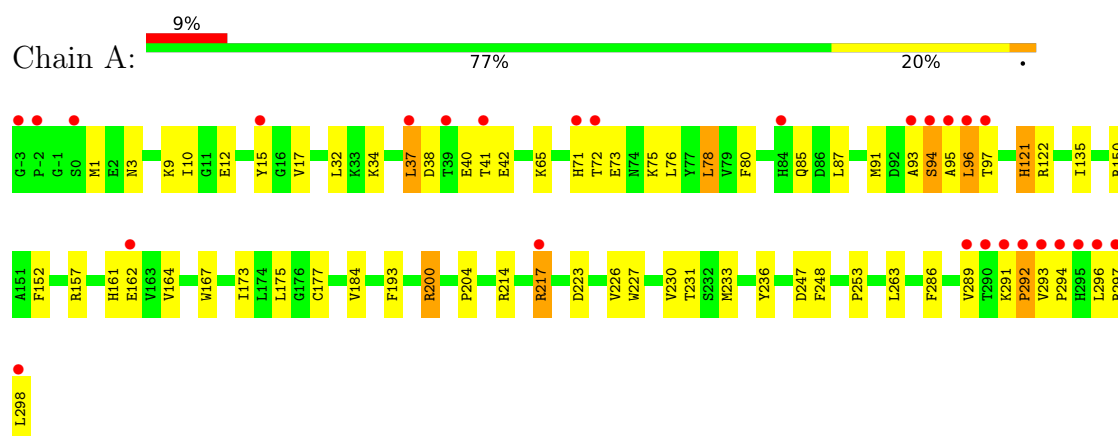
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	97	Total 97	O 97	0	0
4	D	86	Total 86	O 86	0	0

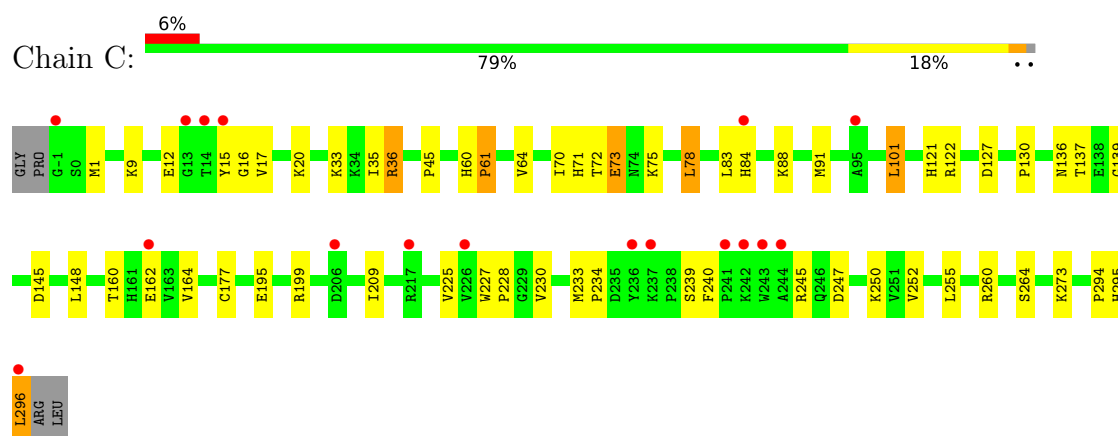
3 Residue-property plots [i](#)

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.

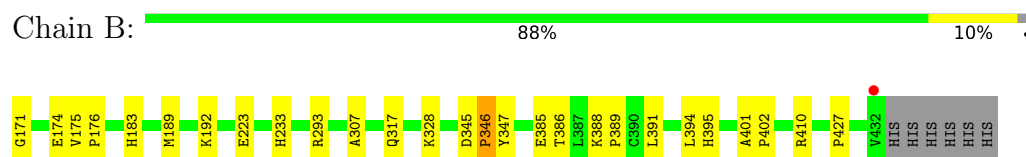
• Molecule 1: Cyclin-dependent kinase 2



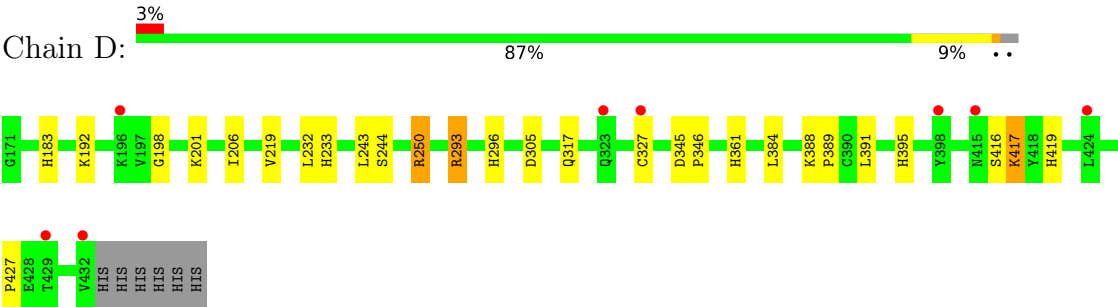
• Molecule 1: Cyclin-dependent kinase 2



• Molecule 2: Cyclin-A2



• Molecule 2: Cyclin-A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.13Å 133.74Å 147.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.32 – 2.40 99.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.0 (99.32-2.40) 91.0 (99.13-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.213 , 0.216 0.196 , 0.196	Depositor DCC
R_{free} test set	2787 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9585	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: IJU, TPO

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	0.67	0/2484	1.19	10/3370 (0.3%)
1	C	0.63	0/2462	1.11	2/3340 (0.1%)
2	B	0.62	0/2160	1.12	1/2937 (0.0%)
2	D	0.63	0/2168	1.13	0/2948
All	All	0.64	0/9274	1.14	13/12595 (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
1	A	0	3
2	B	0	2
2	D	0	2
All	All	0	7

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	SER	N-CA-C	-7.25	104.88	113.21
1	A	253	PRO	N-CA-C	5.78	117.75	110.70
2	B	328	LYS	CG-CD-CE	5.74	124.49	111.30
1	A	37	LEU	N-CA-C	-5.66	105.63	112.54
1	A	247	ASP	CB-CA-C	5.59	118.70	109.70
1	A	121	HIS	CA-CB-CG	-5.52	108.28	113.80
1	A	152	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	292	PRO	N-CA-CB	5.44	108.17	103.27
1	A	96	LEU	N-CA-C	-5.27	107.39	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	PHE	CA-CB-CG	5.14	118.94	113.80
1	C	61	PRO	N-CA-CB	5.10	108.58	103.48
1	C	225	VAL	N-CA-C	-5.09	107.78	111.90
1	A	80	PHE	CA-CB-CG	5.05	118.85	113.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ARG	Sidechain
1	A	200	ARG	Sidechain
1	A	217	ARG	Sidechain
2	B	293	ARG	Sidechain
2	B	410	ARG	Sidechain
2	D	250	ARG	Sidechain
2	D	293	ARG	Sidechain

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	2432	0	2473	51	0
1	C	2411	0	2444	48	0
2	B	2110	0	2128	15	0
2	D	2118	0	2133	17	0
3	A	20	0	0	1	0
3	C	30	0	0	1	0
4	A	131	0	0	3	0
4	B	150	0	0	4	0
4	C	97	0	0	3	0
4	D	86	0	0	2	0
All	All	9585	0	9178	125	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (125) 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:C:84[A]:HIS:CE1	1:C:296:LEU:HD23	2.03	0.92
1:A:177:CYS:SG	1:A:233:MET:HE3	2.18	0.82
1:C:45:PRO:HG3	4:C:448:HOH:O	1.82	0.79
1:C:296:LEU:H	1:C:296:LEU:HD13	1.49	0.77
1:C:177:CYS:HB2	4:C:424:HOH:O	1.87	0.74
1:C:296:LEU:CD1	1:C:296:LEU:N	2.53	0.72
2:B:223:GLU:HG2	4:B:610:HOH:O	1.89	0.71
1:A:177:CYS:SG	1:A:233:MET:HG2	2.31	0.70
1:C:15:TYR:CD2	1:C:33:LYS:HD3	2.28	0.69
1:A:298:LEU:HD13	2:D:243:LEU:O	1.94	0.67
1:C:296:LEU:HD13	1:C:296:LEU:N	2.08	0.66
1:C:12:GLU:HG3	1:C:16:GLY:O	1.95	0.65
1:A:121:HIS:O	1:A:122:ARG:HG3	1.98	0.64
1:C:71:HIS:HD2	2:D:296:HIS:NE2	1.95	0.64
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.80	0.62
1:A:93:ALA:C	1:A:95:ALA:H	2.09	0.61
1:A:291:LYS:HB3	4:A:502:HOH:O	2.00	0.60
1:C:9:LYS:HG3	1:C:17:VAL:HG23	1.83	0.59
1:A:96:LEU:O	1:A:97:THR:C	2.46	0.59
1:A:175:LEU:HD13	1:A:233:MET:HE2	1.84	0.57
2:D:395:HIS:HE1	2:D:427:PRO:O	1.88	0.57
1:C:137:THR:HG22	1:C:296:LEU:HD21	1.86	0.57
1:A:286:PHE:O	1:A:289:VAL:HG22	2.04	0.56
2:B:395:HIS:HE1	2:B:427:PRO:O	1.88	0.56
1:A:161:HIS:CD2	1:A:162:GLU:HG3	2.41	0.56
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.41	0.55
1:A:231:THR:HA	1:A:236:TYR:CD2	2.43	0.54
1:A:72:THR:HG22	1:A:73:GLU:N	2.22	0.54
1:A:121:HIS:C	1:A:122:ARG:HG3	2.33	0.54
1:C:84[B]:HIS:HD2	1:C:136:ASN:HA	1.71	0.53
1:C:127:ASP:CG	1:C:148:LEU:HD12	2.33	0.53
1:A:292:PRO:O	1:A:293:VAL:C	2.49	0.53
1:A:10:ILE:HD12	3:A:301[B]:IJU:C2	2.39	0.53
1:A:227:TRP:CH2	1:A:233:MET:HE1	2.43	0.52
1:A:294:PRO:HB2	4:A:456:HOH:O	2.09	0.52
1:C:247:ASP:H	1:C:250:LYS:HE2	1.73	0.52
1:C:64:VAL:HG11	3:C:301[B]:IJU:C2	2.40	0.52
1:C:294:PRO:O	1:C:296:LEU:HD12	2.10	0.52
1:C:252:VAL:HG23	1:C:252:VAL:O	2.10	0.51
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.76	0.51
1:C:72:THR:HG22	1:C:73:GLU:H	1.74	0.51
1:C:247:ASP:HB2	1:C:250:LYS:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:CD1	1:A:233:MET:HE2	2.40	0.51
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.47	0.50
2:B:233:HIS:HD2	4:B:585:HOH:O	1.94	0.50
1:A:214:ARG:HG3	1:A:217:ARG:HH11	1.76	0.50
1:A:37:LEU:O	1:A:38:ASP:C	2.55	0.50
1:A:230:VAL:HA	1:A:233:MET:SD	2.51	0.50
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.94	0.50
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.77	0.50
1:A:298:LEU:CD1	2:D:243:LEU:O	2.60	0.49
1:C:127:ASP:HB2	1:C:148:LEU:HD12	1.93	0.49
1:C:121:HIS:C	1:C:122:ARG:HG3	2.37	0.49
1:A:161:HIS:HE1	1:A:173:ILE:O	1.95	0.49
1:A:177:CYS:SG	1:A:233:MET:CE	2.95	0.49
1:C:296:LEU:C	1:C:296:LEU:HD22	2.37	0.49
1:C:230:VAL:HA	1:C:233:MET:SD	2.52	0.49
1:A:40:GLU:O	1:A:41:THR:C	2.53	0.49
1:C:91:MET:HE2	1:C:130:PRO:HB3	1.94	0.49
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.49	0.48
1:C:245:ARG:HH12	1:C:264:SER:HB2	1.79	0.47
1:A:72:THR:HG22	1:A:73:GLU:H	1.79	0.47
2:D:361:HIS:ND1	2:D:384:LEU:HD21	2.30	0.47
1:A:40:GLU:C	1:A:42:GLU:N	2.71	0.47
1:A:1:MET:HE1	1:A:32:LEU:HD13	1.97	0.47
1:C:195:GLU:O	1:C:199:ARG:N	2.45	0.46
1:A:78:LEU:N	1:A:78:LEU:HD23	2.31	0.46
2:B:386:THR:HB	4:B:555:HOH:O	2.16	0.46
1:C:15:TYR:HD2	1:C:33:LYS:HD3	1.79	0.46
1:A:37:LEU:O	1:A:40:GLU:HB3	2.15	0.46
1:C:239:SER:O	1:C:240:PHE:C	2.57	0.46
1:C:78:LEU:HD23	1:C:78:LEU:N	2.31	0.45
1:C:84[B]:HIS:CD2	1:C:137:THR:HG23	2.51	0.45
1:C:121:HIS:O	1:C:122:ARG:HG3	2.15	0.45
1:A:93:ALA:C	1:A:95:ALA:N	2.73	0.45
1:A:9:LYS:HE3	1:A:17:VAL:HG23	1.99	0.45
1:A:37:LEU:HD11	1:A:76:LEU:HB2	1.99	0.45
2:B:171:GLY:O	2:B:176:PRO:HD3	2.17	0.45
1:C:127:ASP:CB	1:C:148:LEU:HD12	2.46	0.45
1:A:177:CYS:HB2	4:A:443:HOH:O	2.17	0.45
1:A:177:CYS:SG	1:A:233:MET:SD	3.14	0.45
2:D:219:VAL:HG22	2:D:232:LEU:HD21	1.99	0.45
2:D:233:HIS:HD2	4:D:533:HOH:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:HD22	2:D:244:SER:O	2.17	0.45
1:C:177:CYS:SG	1:C:233:MET:HG2	2.56	0.45
1:A:65:LYS:HD3	1:A:297:ARG:HB2	1.99	0.44
2:D:327:CYS:HB3	2:D:419:HIS:CE1	2.52	0.44
1:A:87:LEU:HG	1:A:91:MET:HE2	1.99	0.44
1:A:122:ARG:NH2	2:B:307:ALA:HB1	2.33	0.44
1:A:291:LYS:HD2	1:A:292:PRO:HD2	1.99	0.44
1:C:1:MET:HB3	1:C:1:MET:HE3	1.86	0.44
1:C:15:TYR:HB3	1:C:35:ILE:HG12	1.99	0.44
2:D:345:ASP:HA	2:D:346:PRO:HA	1.80	0.44
1:A:3:ASN:OD1	2:D:293:ARG:NH2	2.50	0.43
1:C:227:TRP:O	1:C:228:PRO:C	2.62	0.43
2:B:174:GLU:O	2:B:175:VAL:C	2.62	0.43
2:B:189:MET:HE3	2:B:192:LYS:HD2	2.00	0.42
1:C:162[B]:GLU:H	1:C:162[B]:GLU:CD	2.28	0.42
1:A:223:ASP:H	1:A:226:VAL:HG12	1.84	0.42
1:C:12:GLU:HG3	1:C:16:GLY:C	2.43	0.42
1:C:255:LEU:O	1:C:260:ARG:NH1	2.53	0.42
1:C:84[A]:HIS:ND1	1:C:296:LEU:HD23	2.32	0.42
2:B:345:ASP:HA	2:B:346:PRO:HA	1.82	0.41
1:C:296:LEU:H	1:C:296:LEU:CD1	2.15	0.41
2:D:388:LYS:HB3	2:D:389:PRO:HD3	2.01	0.41
1:C:36:ARG:HA	1:C:75:LYS:HD3	2.03	0.41
1:A:9:LYS:NZ	1:A:12:GLU:OE1	2.49	0.41
1:A:34:LYS:HD2	1:A:75:LYS:HD3	2.03	0.41
1:A:94:SER:O	1:A:95:ALA:C	2.63	0.41
1:A:175:LEU:CD1	1:A:233:MET:CE	2.99	0.41
1:A:248:PHE:HE2	1:A:263:LEU:HD23	1.85	0.41
2:B:189:MET:CE	2:B:192:LYS:HD2	2.50	0.41
1:A:72:THR:CG2	1:A:73:GLU:N	2.84	0.40
2:B:233:HIS:HE1	4:B:511:HOH:O	2.02	0.40
2:B:401:ALA:N	2:B:402:PRO:CD	2.84	0.40
1:C:101:LEU:HD22	1:C:101:LEU:HA	1.94	0.40
2:D:416:SER:O	2:D:417:LYS:C	2.64	0.40
1:C:12:GLU:HA	1:C:16:GLY:O	2.22	0.40
1:C:20:LYS:NZ	4:C:403:HOH:O	2.45	0.40
2:B:347:TYR:OH	2:B:394:LEU:HA	2.22	0.40
2:B:388:LYS:HB3	2:B:389:PRO:HD3	2.03	0.40
2:D:206:ILE:HD13	2:D:206:ILE:HG21	1.88	0.40
1:A:85:GLN:HE21	1:A:135:ILE:HD11	1.85	0.40
2:D:198:GLY:O	2:D:201:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:HIS:HE1	4:D:551:HOH:O	2.03	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	300/302 (99%)	285 (95%)	14 (5%)	1 (0%)	36	50
1	C	297/302 (98%)	285 (96%)	10 (3%)	2 (1%)	18	28
2	B	260/268 (97%)	255 (98%)	5 (2%)	0	100	100
2	D	261/268 (97%)	257 (98%)	4 (2%)	0	100	100
All	All	1118/1140 (98%)	1082 (97%)	33 (3%)	3 (0%)	36	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	164	VAL
1	C	145	ASP

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	265/264 (100%)	259 (98%)	6 (2%)	44	66
1	C	263/264 (100%)	252 (96%)	11 (4%)	26	45
2	B	234/240 (98%)	231 (99%)	3 (1%)	61	80
2	D	235/240 (98%)	230 (98%)	5 (2%)	47	69
All	All	997/1008 (99%)	972 (98%)	25 (2%)	42	64

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	TYR
1	A	78	LEU
1	A	150	ARG
1	A	184	VAL
1	A	200	ARG
1	A	296	LEU
2	B	346	PRO
2	B	385	GLU
2	B	391	LEU
1	C	36	ARG
1	C	70	ILE
1	C	73	GLU
1	C	78	LEU
1	C	83	LEU
1	C	101	LEU
1	C	209	ILE
1	C	234	PRO
1	C	273	LYS
1	C	295	HIS
1	C	296	LEU
2	D	192	LYS
2	D	250	ARG
2	D	305	ASP
2	D	391	LEU
2	D	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	85	GLN

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Mol	Chain	Res	Type
1	A	265	GLN
1	A	295	HIS
2	B	179	HIS
2	B	228	GLN
2	B	254	GLN
2	B	312	ASN
2	B	317	GLN
2	B	378	GLN
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN
1	C	59	ASN
1	C	71	HIS
1	C	161	HIS
1	C	287	GLN
2	D	233	HIS
2	D	254	GLN
2	D	317	GLN
2	D	395	HIS
2	D	396	GLN
2	D	425	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	160	1	8,10,11	0.66	0	10,14,16	0.88	0
1	TPO	C	160	1	8,10,11	1.01	1 (12%)	10,14,16	0.97	1 (10%)

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
1	TPO	A	160	1	-	1/9/11/13	-
1	TPO	C	160	1	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	2.27	1.63	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O-C-CA	-2.07	119.45	124.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	O-C-CA-CB
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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	IJU	C	301[B]	-	10,10,10	0.19	0	10,12,12	0.71	0
3	IJU	C	301[D]	-	10,10,10	0.37	0	10,12,12	0.70	0
3	IJU	A	301[B]	-	10,10,10	0.38	0	10,12,12	0.91	0
3	IJU	C	301[C]	-	10,10,10	0.26	0	10,12,12	0.51	0
3	IJU	A	301[A]	-	10,10,10	0.36	0	10,12,12	0.86	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	IJU	C	301[B]	-	-	2/3/3/3	0/1/1/1
3	IJU	C	301[D]	-	-	1/3/3/3	0/1/1/1
3	IJU	A	301[B]	-	-	1/3/3/3	0/1/1/1
3	IJU	C	301[C]	-	-	0/3/3/3	0/1/1/1
3	IJU	A	301[A]	-	-	0/3/3/3	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301[B]	IJU	C3-C2-O1-C1
3	C	301[D]	IJU	C3-C2-O1-C1
3	C	301[B]	IJU	O1-C2-C3-N1
3	C	301[B]	IJU	O1-C2-C3-C4

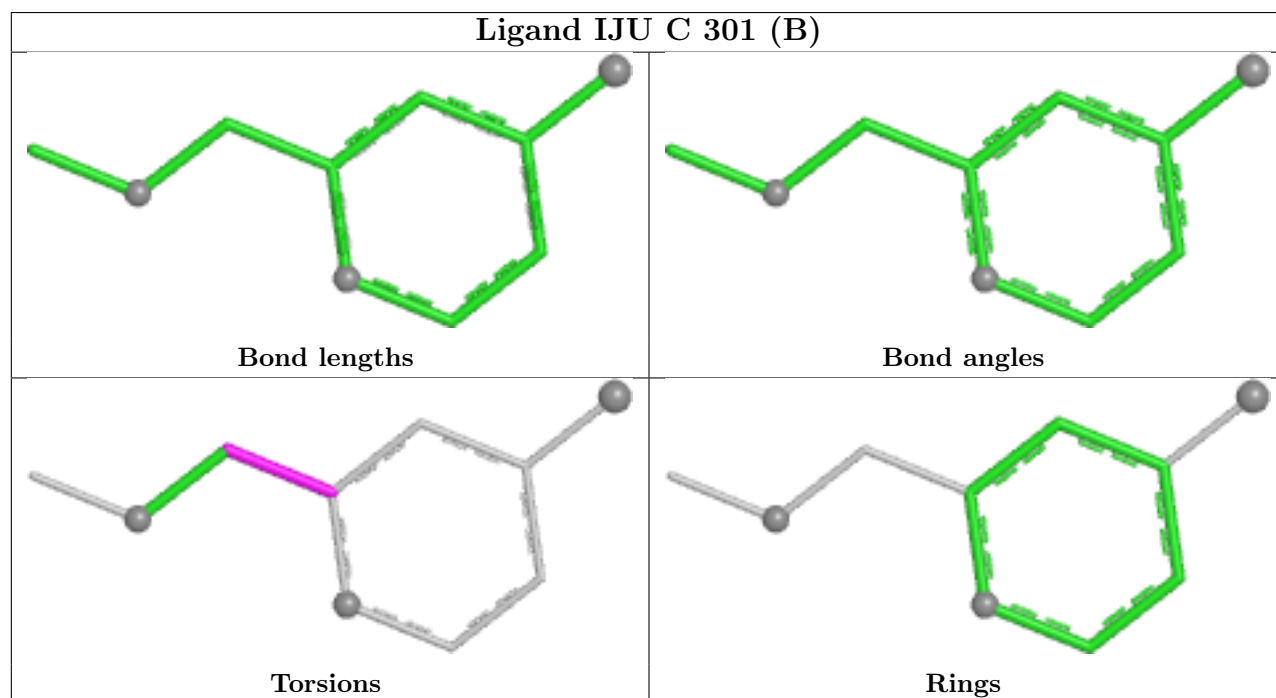
There are no ring outliers.

2 monomers are involved in 2 short contacts:

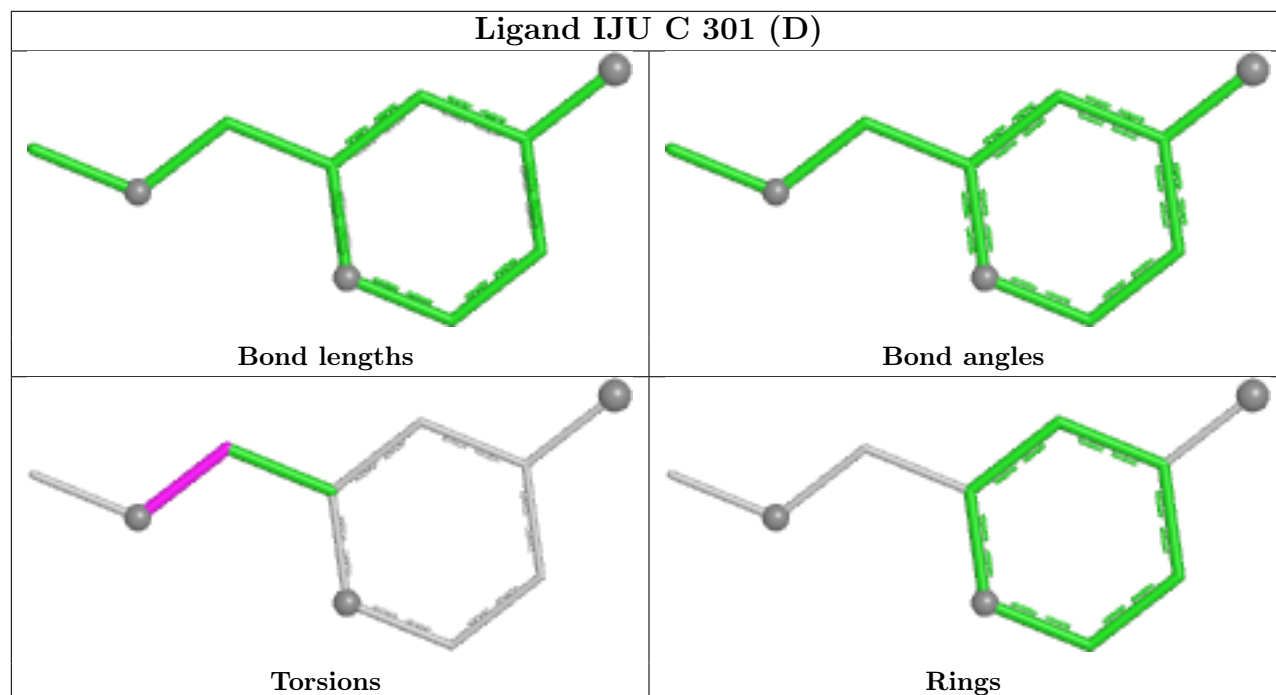
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301[B]	IJU	1	0
3	A	301[B]	IJU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

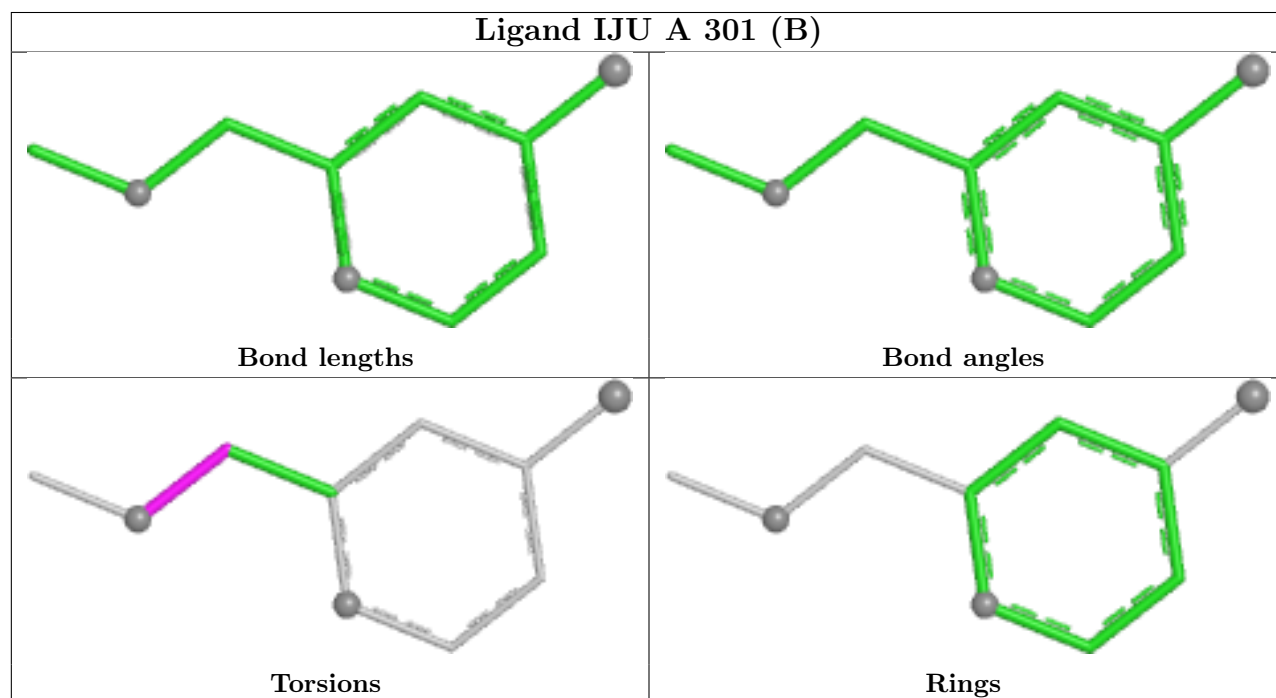
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

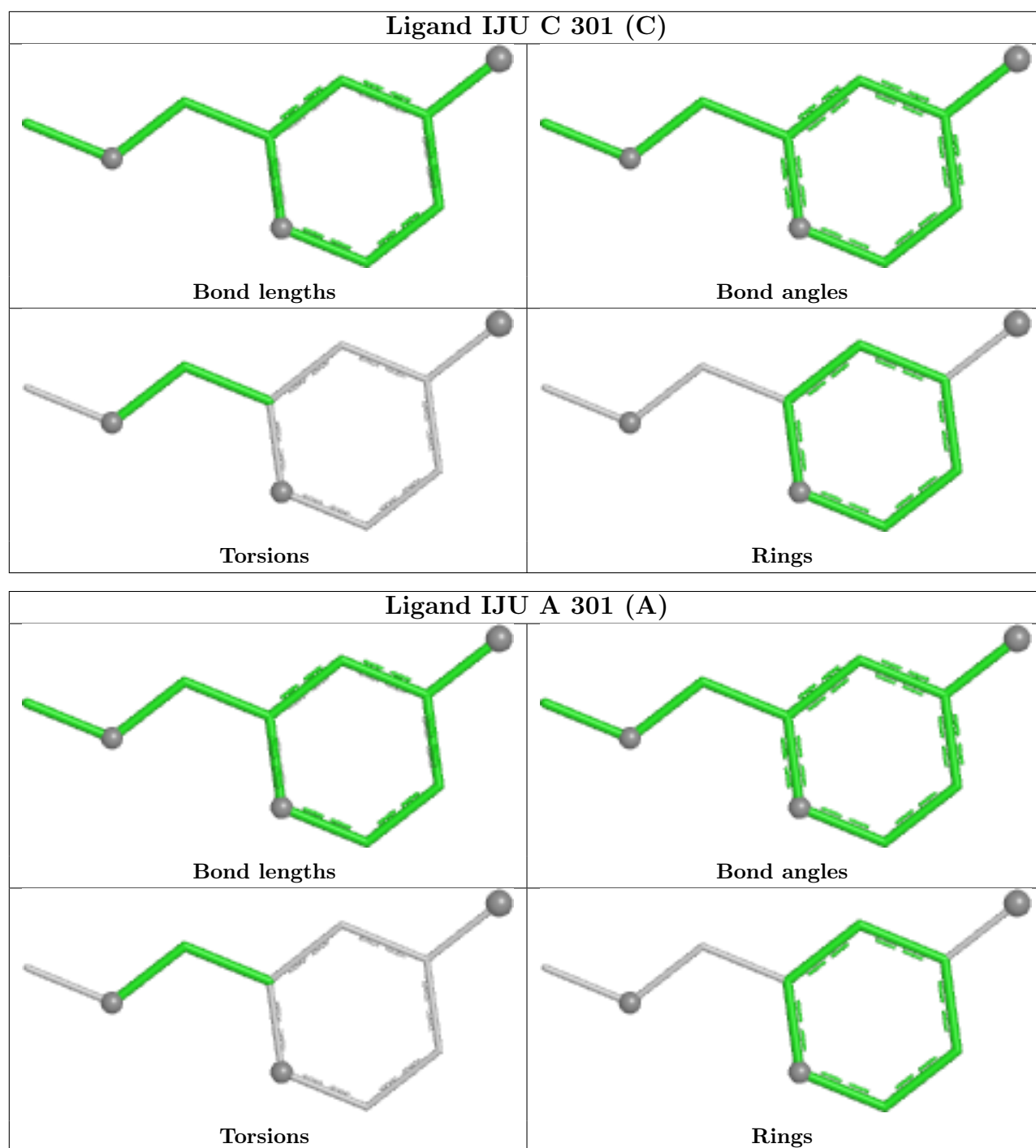


Ligand IJU C 301 (D)



Ligand IJU A 301 (B)





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	301/302 (99%)	0.11	27 (8%)	15 12	25, 46, 106, 166	1 (0%)
1	C	297/302 (98%)	0.27	17 (5%)	29 25	33, 58, 99, 144	2 (0%)
2	B	262/268 (97%)	-0.25	1 (0%)	88 86	35, 48, 75, 107	0
2	D	262/268 (97%)	0.29	8 (3%)	51 47	35, 60, 93, 127	1 (0%)
All	All	1122/1140 (98%)	0.11	53 (4%)	36 32	25, 52, 99, 166	4 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	LEU	5.4
1	A	290	THR	4.9
2	D	432	VAL	4.6
1	A	15	TYR	4.5
1	A	291	LYS	4.5
1	A	-2	PRO	4.4
1	A	296	LEU	4.3
1	A	-3	GLY	4.3
1	A	292	PRO	3.7
1	C	162[A]	GLU	3.6
1	A	37	LEU	3.5
1	C	241	PRO	3.5
2	D	415[A]	ASN	3.5
1	A	298	LEU	3.4
1	A	97	THR	3.4
1	C	296	LEU	3.3
1	A	71	HIS	3.3
1	A	84[A]	HIS	3.3
1	C	237	LYS	3.1
1	A	294	PRO	3.1
1	A	95	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	295	HIS	3.0
1	A	39	THR	3.0
2	D	323	GLN	2.8
1	A	297	ARG	2.8
1	A	0	SER	2.8
1	C	242	LYS	2.8
1	A	94	SER	2.8
1	C	15	TYR	2.8
1	C	217	ARG	2.7
1	A	293	VAL	2.6
1	A	93	ALA	2.6
1	C	14	THR	2.6
2	D	398	TYR	2.6
1	A	41	THR	2.4
1	A	217	ARG	2.4
2	B	432	VAL	2.4
1	C	206	ASP	2.4
2	D	429	THR	2.3
1	C	84[A]	HIS	2.3
1	C	236	TYR	2.3
1	C	95	ALA	2.3
1	C	-1	GLY	2.2
1	C	243	TRP	2.2
1	C	226	VAL	2.2
2	D	424	LEU	2.2
1	A	289	VAL	2.2
2	D	196	LYS	2.2
1	A	162	GLU	2.1
1	A	72	THR	2.1
2	D	327	CYS	2.1
1	C	244	ALA	2.1
1	C	13	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	A	160	11/12	0.98	0.05	38,43,45,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TPO	C	160	11/12	0.98	0.05	45,49,55,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

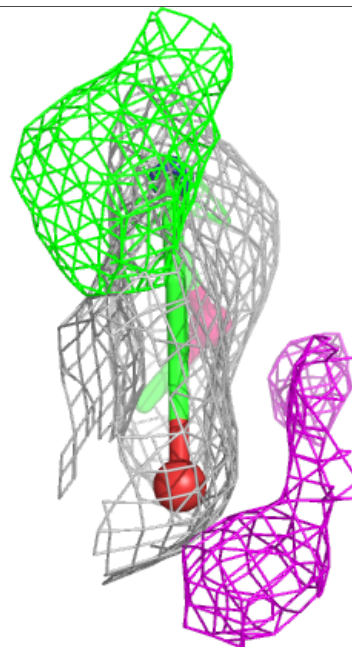
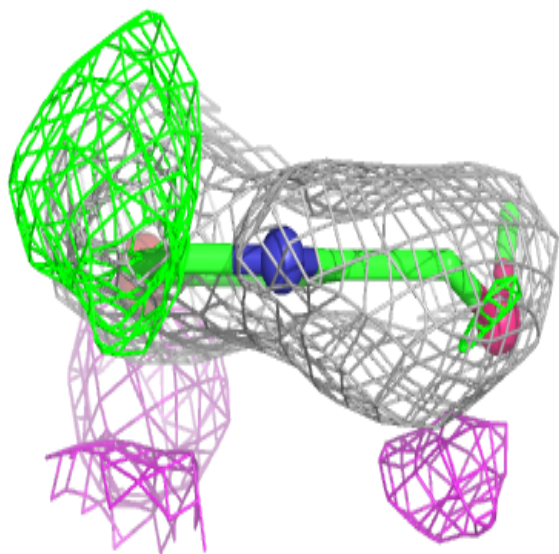
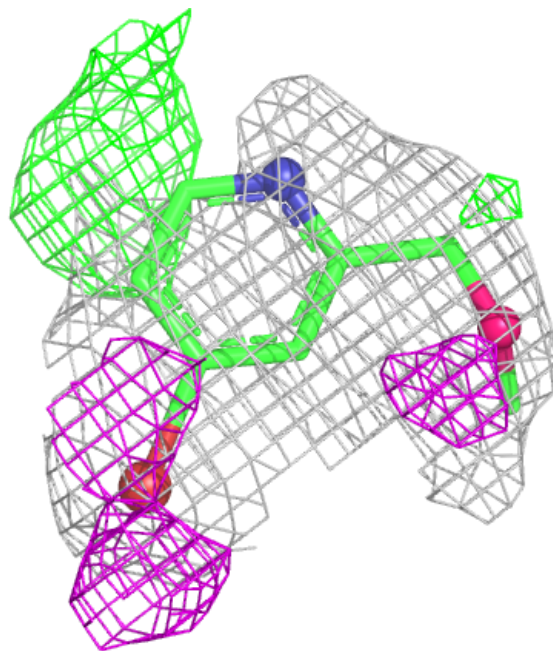
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IJU	A	301[A]	10/10	0.81	0.31	58,94,119,181	10
3	IJU	A	301[B]	10/10	0.81	0.31	59,74,82,116	10
3	IJU	C	301[B]	10/10	0.89	0.35	29,34,35,38	10
3	IJU	C	301[C]	10/10	0.89	0.35	40,43,56,62	10
3	IJU	C	301[D]	10/10	0.89	0.35	78,82,88,97	10

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.

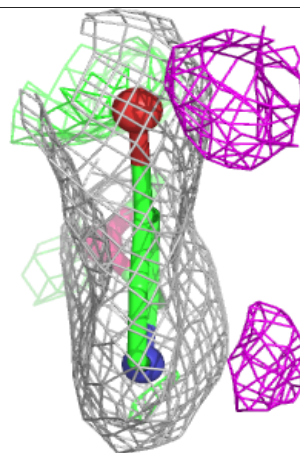
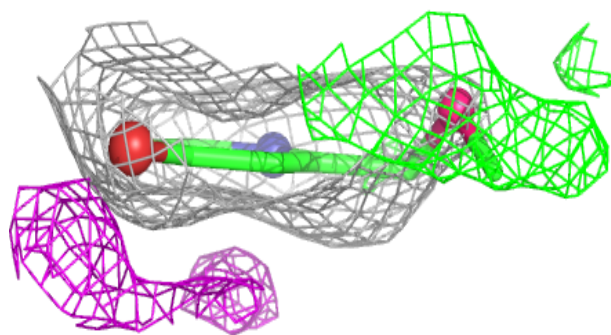
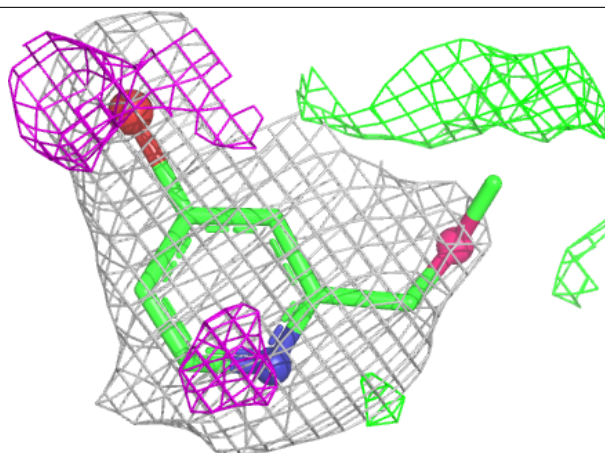
Electron density around IJU A 301 (A):

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

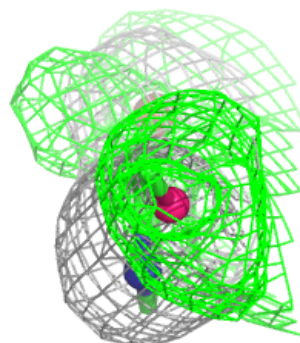
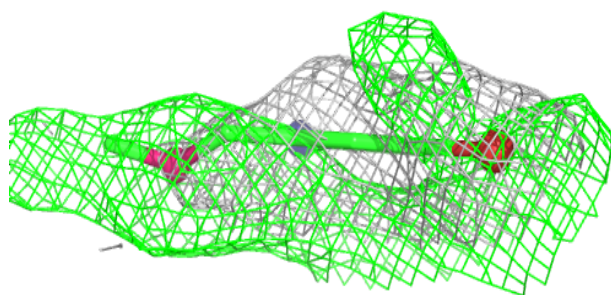
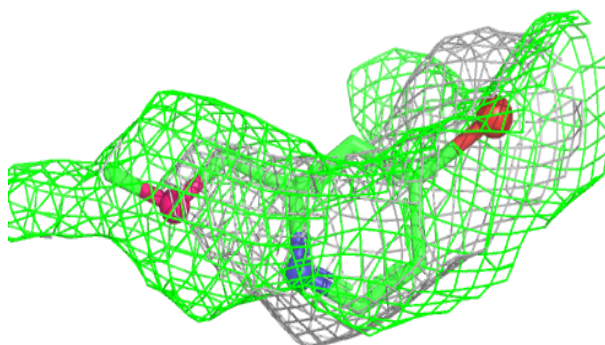


Electron density around IJU A 301 (B):

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

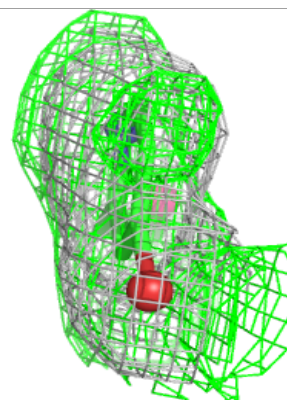
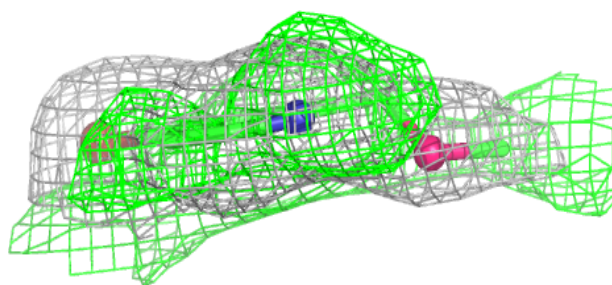
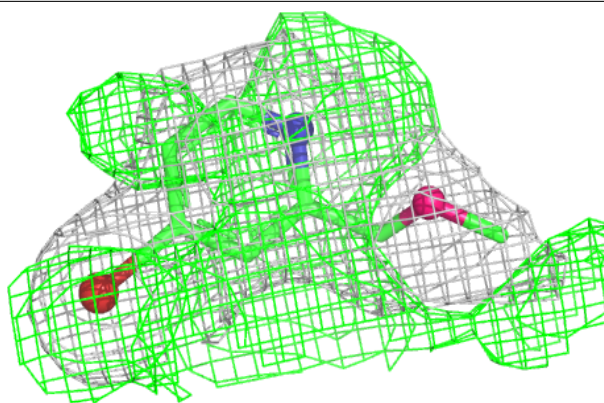
**Electron density around IJU C 301 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

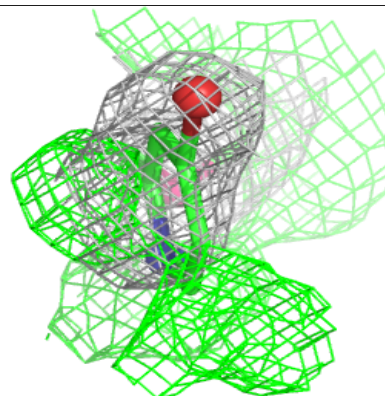
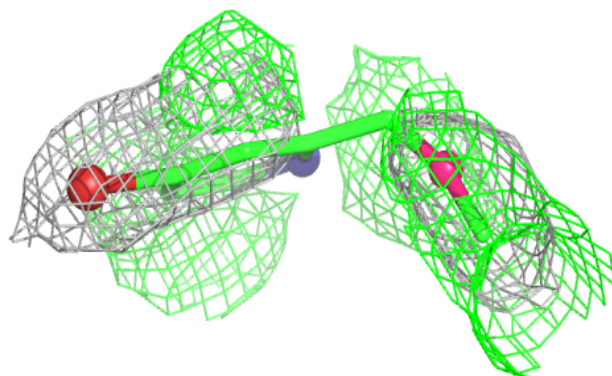
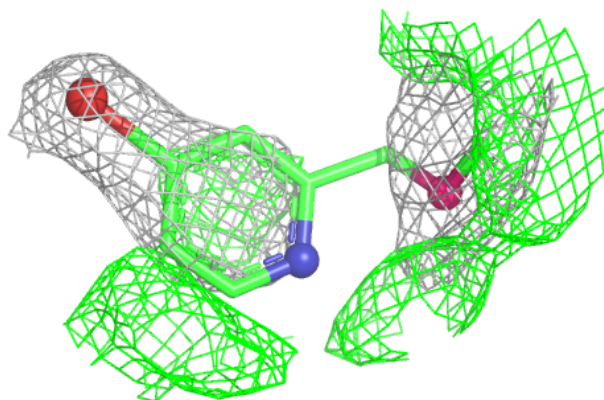


Electron density around IJU C 301 (C):

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

**Electron density around IJU C 301 (D):**

$2mF_o-DF_c$ (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.