



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:39 PM UTC

PDB ID : 4WNP / pdb_00004wnp
Title : Structure of ULK1 bound to a potent inhibitor
Authors : Lazarus, M.B.; Novotny, C.J.; Shokat, K.M.
Deposited on : 2014-10-14
Resolution : 1.88 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

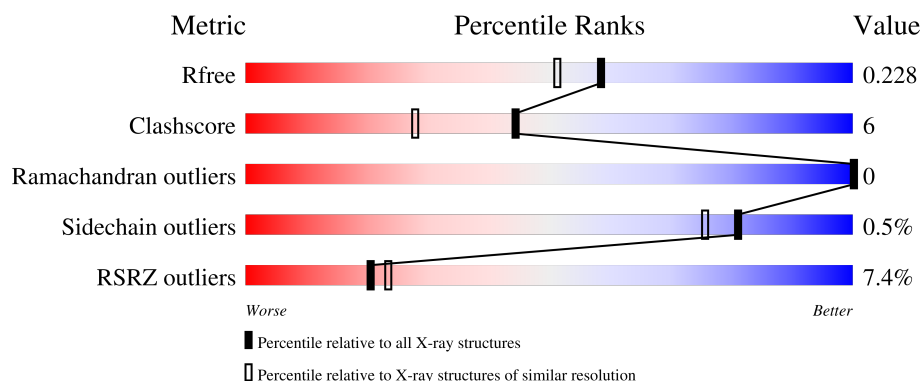
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	287	2% 89% 7% 5%
1	B	287	10% 79% 16% 5%
1	C	287	8% 79% 16% 5%
1	D	287	7% 83% 13% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9310 atoms, of which 96 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Serine/threonine-protein kinase ULK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	P	S	0	3	0
			2208	1406	391	394	1	16			
1	B	273	Total	C	N	O	P	S	0	4	0
			2212	1410	391	394	1	16			
1	C	272	Total	C	N	O	P	S	0	4	0
			2207	1407	390	393	1	16			
1	D	273	Total	C	N	O	P	S	0	4	0
			2212	1410	391	394	1	16			

There are 24 discrepancies between the modelled and reference sequences:

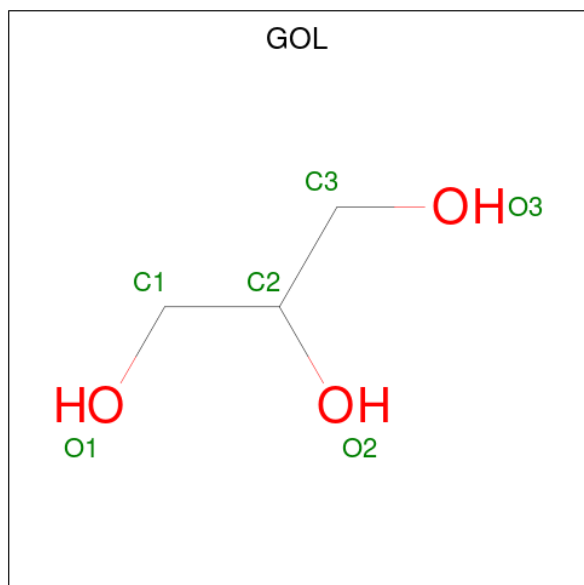
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP O75385
A	-2	GLY	-	expression tag	UNP O75385
A	-1	GLY	-	expression tag	UNP O75385
A	0	SER	-	expression tag	UNP O75385
A	37	ALA	GLU	engineered mutation	UNP O75385
A	38	ALA	LYS	engineered mutation	UNP O75385
B	-3	GLY	-	expression tag	UNP O75385
B	-2	GLY	-	expression tag	UNP O75385
B	-1	GLY	-	expression tag	UNP O75385
B	0	SER	-	expression tag	UNP O75385
B	37	ALA	GLU	engineered mutation	UNP O75385
B	38	ALA	LYS	engineered mutation	UNP O75385
C	-3	GLY	-	expression tag	UNP O75385
C	-2	GLY	-	expression tag	UNP O75385
C	-1	GLY	-	expression tag	UNP O75385
C	0	SER	-	expression tag	UNP O75385
C	37	ALA	GLU	engineered mutation	UNP O75385
C	38	ALA	LYS	engineered mutation	UNP O75385
D	-3	GLY	-	expression tag	UNP O75385
D	-2	GLY	-	expression tag	UNP O75385
D	-1	GLY	-	expression tag	UNP O75385

Continued on next page...

Continued from previous page...

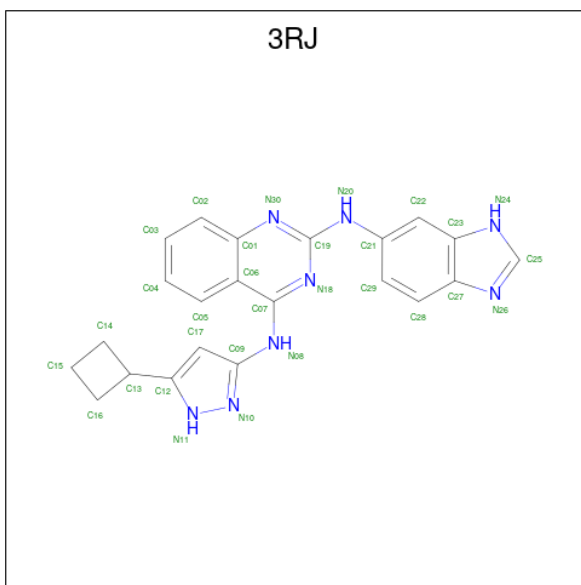
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP O75385
D	37	ALA	GLU	engineered mutation	UNP O75385
D	38	ALA	LYS	engineered mutation	UNP O75385

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is N 2 -(1H-benzimidazol-6-yl)-N 4 -(5-cyclobutyl-1H-pyrazol-3-yl)quinazoline-2, 4-diamine (CCD ID: 3RJ) (formula: $C_{22}H_{20}N_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			50	22	20	8		
3	B	1	Total	C	H	N	0	0
			50	22	20	8		
3	C	1	Total	C	H	N	0	0
			50	22	20	8		
3	D	1	Total	C	H	N	0	0
			50	22	20	8		

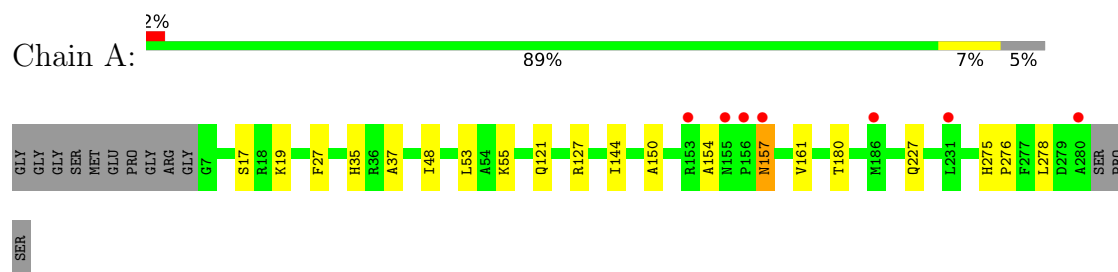
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total	O	0	0
			98	98		
4	B	42	Total	O	0	0
			42	42		
4	C	35	Total	O	0	0
			35	35		
4	D	68	Total	O	0	0
			68	68		

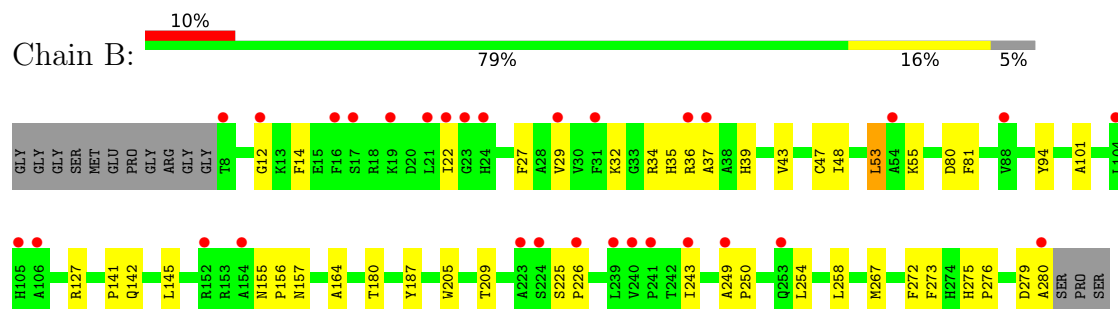
3 Residue-property plots [i](#)

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.

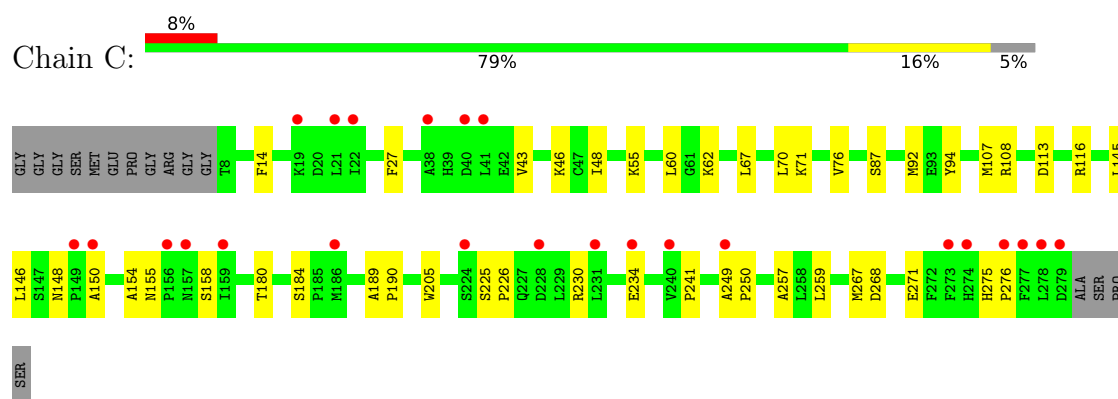
- Molecule 1: Serine/threonine-protein kinase ULK1



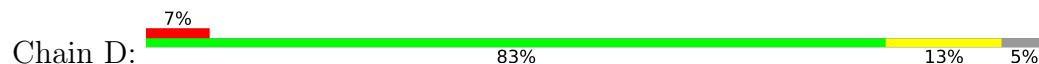
- Molecule 1: Serine/threonine-protein kinase ULK1

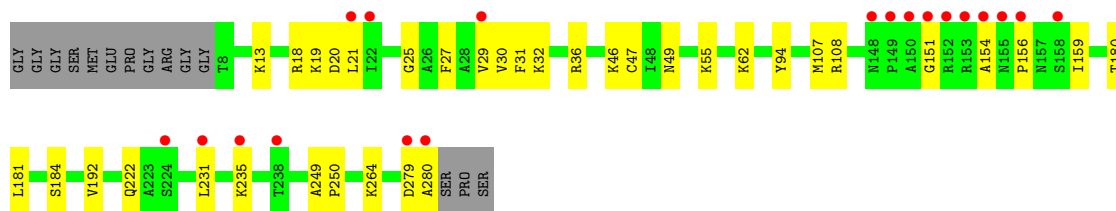


- Molecule 1: Serine/threonine-protein kinase ULK1



- Molecule 1: Serine/threonine-protein kinase ULK1





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	100.41Å 113.80Å 100.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.02 – 1.88 46.02 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.02-1.88) 99.8 (46.02-1.88)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.192 , 0.226 0.196 , 0.228	Depositor DCC
R_{free} test set	4722 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.049 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9310	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.17% 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: TPO, GOL, 3RJ

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	0.55	0/2242	0.74	0/3018
1	B	0.38	0/2246	0.73	2/3024 (0.1%)
1	C	0.44	0/2241	0.75	4/3017 (0.1%)
1	D	0.49	0/2246	0.76	2/3024 (0.1%)
All	All	0.47	0/8975	0.74	8/12083 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	SER	CA-C-N	7.15	128.78	119.84
1	D	184	SER	C-N-CA	7.15	128.78	119.84
1	C	184	SER	CA-C-N	5.78	127.07	119.84
1	C	184	SER	C-N-CA	5.78	127.07	119.84
1	C	148	ASN	CA-C-N	5.25	124.88	119.05
1	C	148	ASN	C-N-CA	5.25	124.88	119.05
1	B	243	ILE	CA-C-N	5.21	125.21	119.89
1	B	243	ILE	C-N-CA	5.21	125.21	119.89

There are no chirality outliers.

There are no planarity outliers.

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	2208	0	2232	15	0
1	B	2212	0	2239	38	0
1	C	2207	0	2234	33	0
1	D	2212	0	2239	22	0
2	A	12	16	16	0	0
3	A	30	20	20	0	0
3	B	30	20	20	0	0
3	C	30	20	20	3	0
3	D	30	20	20	0	0
4	A	98	0	0	0	0
4	B	42	0	0	0	0
4	C	35	0	0	3	0
4	D	68	0	0	1	0
All	All	9214	96	9040	108	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 6.

All (108) 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:B:279:ASP:HA	1:B:280:ALA:HB3	1.31	1.10
1:D:279:ASP:HA	1:D:280:ALA:HB3	1.25	1.10
1:C:150:ALA:HB3	1:C:154:ALA:HB2	1.39	1.01
1:D:156:PRO:HA	1:D:159:ILE:HD12	1.48	0.95
1:A:150:ALA:HB3	1:A:154:ALA:HB2	1.50	0.93
1:B:267:MET:HE3	1:B:272:PHE:HB2	1.49	0.92
1:D:279:ASP:HA	1:D:280:ALA:CB	2.06	0.85
1:B:258:LEU:HD21	1:B:267:MET:HE2	1.58	0.85
1:B:225:SER:HB2	1:B:226:PRO:HD2	1.64	0.78
1:B:258:LEU:CD2	1:B:267:MET:HE2	2.13	0.78
1:B:279:ASP:HA	1:B:280:ALA:CB	2.10	0.74
1:A:27:PHE:CE1	1:A:55:LYS:HD3	2.25	0.72
1:B:267:MET:HE3	1:B:272:PHE:CB	2.19	0.72
1:B:29[B]:VAL:HG13	1:B:47:CYS:HB2	1.73	0.71
1:D:19:LYS:HE3	1:D:20:ASP:OD1	1.92	0.69
1:C:107:MET:HE2	1:C:107:MET:HA	1.79	0.65
1:C:27:PHE:CE1	1:C:55:LYS:HD3	2.32	0.64
1:B:279:ASP:CA	1:B:280:ALA:HB3	2.20	0.64
1:C:150:ALA:HB3	1:C:154:ALA:CB	2.23	0.62
1:A:150:ALA:HB3	1:A:154:ALA:CB	2.28	0.62
1:B:27:PHE:CZ	1:B:55:LYS:HD3	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:HIS:CE1	1:B:37:ALA:HB3	2.36	0.61
1:D:27:PHE:CE1	1:D:55:LYS:HD3	2.36	0.60
1:B:32:LYS:HE3	1:B:94:TYR:CZ	2.36	0.60
1:D:30:VAL:HG22	1:D:46:LYS:HG2	1.82	0.60
1:D:156:PRO:HA	1:D:159:ILE:CD1	2.30	0.57
1:B:27:PHE:CE1	1:B:55:LYS:HD3	2.42	0.55
1:B:29[B]:VAL:CG1	1:B:47:CYS:HB2	2.35	0.55
1:B:249:ALA:N	1:B:250:PRO:HD2	2.22	0.54
1:B:22:ILE:HD11	1:B:32:LYS:CA	2.38	0.54
1:A:227:GLN:H	1:A:227:GLN:CD	2.16	0.54
1:A:121:GLN:HB2	1:A:161:VAL:CG1	2.37	0.53
1:D:27:PHE:CZ	1:D:55:LYS:HD3	2.44	0.53
1:B:254:LEU:HD11	1:B:267:MET:HE1	1.90	0.53
1:B:155:ASN:OD1	1:B:156:PRO:HD2	2.10	0.52
1:B:205:TRP:O	1:B:209:THR:HG23	2.09	0.52
1:C:145:LEU:HD11	3:C:401:3RJ:H162	1.91	0.52
1:B:14:PHE:CE2	1:B:43:VAL:HG11	2.44	0.52
1:C:150:ALA:CB	1:C:154:ALA:HB2	2.28	0.52
1:C:70:LEU:O	1:C:71:LYS:HD3	2.09	0.52
1:A:144:ILE:CG2	1:A:161:VAL:HG23	2.40	0.52
1:D:32:LYS:HE3	1:D:94:TYR:CZ	2.44	0.52
1:C:92:MET:HE1	4:C:529:HOH:O	2.10	0.51
1:A:144:ILE:CG2	1:A:161:VAL:CG2	2.89	0.51
1:D:231:LEU:HB3	1:D:235:LYS:HE3	1.92	0.50
1:B:22:ILE:HD11	1:B:32:LYS:HA	1.92	0.50
1:C:76:VAL:HB	4:C:522:HOH:O	2.11	0.50
1:B:12:GLY:O	1:B:36:ARG:NH1	2.44	0.50
1:B:145:LEU:HD12	1:B:164:ALA:HB2	1.94	0.49
1:A:27:PHE:CZ	1:A:55:LYS:HD3	2.47	0.49
1:B:258:LEU:HD21	1:B:267:MET:CE	2.37	0.48
1:C:230:ARG:NH1	1:C:234:GLU:OE2	2.46	0.48
1:B:155:ASN:ND2	1:B:157:ASN:HB2	2.28	0.48
1:C:46:LYS:HE2	1:C:60:LEU:HD21	1.95	0.48
1:D:18:ARG:HA	1:D:31:PHE:CD1	2.49	0.48
1:D:62:LYS:NZ	4:D:501:HOH:O	2.41	0.47
1:B:48:ILE:HG21	1:B:53:LEU:CD1	2.44	0.47
1:B:22:ILE:HD11	1:B:32:LYS:CB	2.45	0.47
1:C:225:SER:HB2	1:C:226:PRO:HD2	1.97	0.47
1:A:48:ILE:HG21	1:A:53:LEU:HD12	1.97	0.47
1:C:249:ALA:HB3	1:C:250:PRO:HD3	1.97	0.47
1:C:275:HIS:CG	1:C:276:PRO:HD2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LEU:CG	1:B:267:MET:HE2	2.45	0.46
1:C:145:LEU:HD11	3:C:401:3RJ:C16	2.46	0.46
1:A:275:HIS:CG	1:A:276:PRO:HD2	2.51	0.46
1:B:275:HIS:CG	1:B:276:PRO:HD2	2.51	0.45
1:C:113:ASP:HA	1:C:116:ARG:HH12	1.80	0.45
1:C:48:ILE:HD12	1:C:87:SER:HA	1.99	0.45
1:C:62:LYS:NZ	4:C:502:HOH:O	2.49	0.45
1:B:127:ARG:HA	1:B:273:PHE:CZ	2.52	0.45
1:C:107:MET:O	1:C:108:ARG:HB2	2.15	0.45
1:D:249:ALA:HB3	1:D:250:PRO:HD3	1.99	0.45
1:C:107:MET:HE2	1:C:107:MET:CA	2.46	0.45
1:D:13:LYS:C	1:D:36:ARG:HD3	2.42	0.44
1:C:189:ALA:HA	1:C:205:TRP:CD1	2.52	0.44
1:C:268:ASP:OD1	1:C:271:GLU:HG3	2.17	0.44
1:B:101:ALA:CB	1:B:142:GLN:HG3	2.48	0.44
1:C:241:PRO:HG3	1:C:259:LEU:HD12	1.99	0.44
1:D:21:LEU:HD11	1:D:29[A]:VAL:HG13	1.99	0.44
1:D:25:GLY:O	1:D:49:ASN:ND2	2.47	0.44
1:B:34:ARG:HD2	1:B:39:HIS:ND1	2.33	0.44
1:A:150:ALA:CB	1:A:154:ALA:HB2	2.35	0.44
1:B:80:ASP:OD1	1:B:81:PHE:N	2.46	0.44
1:C:14:PHE:CE2	1:C:43:VAL:HG11	2.53	0.43
1:A:35:HIS:CE1	1:A:37:ALA:HB3	2.54	0.42
1:D:107:MET:O	1:D:108:ARG:HB2	2.19	0.42
1:C:190:PRO:HD3	1:C:205:TRP:CE2	2.54	0.42
1:D:181:LEU:HD13	1:D:192:VAL:O	2.19	0.42
1:D:29[B]:VAL:HG23	1:D:47:CYS:HB2	2.02	0.42
1:C:46:LYS:HE2	1:C:60:LEU:CD2	2.50	0.42
1:D:151:GLY:O	1:D:154:ALA:HB2	2.20	0.42
1:B:225:SER:HB2	1:B:226:PRO:CD	2.45	0.42
1:C:70:LEU:C	1:C:71:LYS:HD3	2.45	0.42
1:C:267:MET:HG3	1:C:271:GLU:HB2	2.01	0.42
1:B:141:PRO:HD3	1:B:187:TYR:CE1	2.54	0.41
1:B:254:LEU:HB2	1:B:275:HIS:CE1	2.55	0.41
1:C:257:ALA:HB3	1:C:267:MET:HE3	2.01	0.41
1:C:155:ASN:O	1:C:158:SER:HB2	2.21	0.41
1:A:278:LEU:HA	1:A:278:LEU:HD23	1.84	0.41
1:B:48:ILE:HG21	1:B:53:LEU:HD13	2.02	0.41
1:B:258:LEU:HG	1:B:267:MET:HE2	2.02	0.41
1:D:231:LEU:O	1:D:235:LYS:HG3	2.21	0.41
1:A:17:SER:OG	1:A:19:LYS:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:TYR:HA	3:C:401:3RJ:N10	2.37	0.40
1:A:157:ASN:OD1	1:A:157:ASN:N	2.53	0.40
1:C:190:PRO:HD3	1:C:205:TRP:CD2	2.57	0.40
1:C:67:LEU:HD23	1:C:67:LEU:HA	1.94	0.40
1:D:264:LYS:HD2	1:D:264:LYS:O	2.21	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	274/287 (96%)	265 (97%)	9 (3%)	0	100	100
1	B	274/287 (96%)	262 (96%)	12 (4%)	0	100	100
1	C	273/287 (95%)	263 (96%)	10 (4%)	0	100	100
1	D	274/287 (96%)	267 (97%)	7 (3%)	0	100	100
All	All	1095/1148 (95%)	1057 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	235/240 (98%)	233 (99%)	2 (1%)	70	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	236/240 (98%)	235 (100%)	1 (0%)	84	79
1	C	236/240 (98%)	235 (100%)	1 (0%)	84	79
1	D	236/240 (98%)	235 (100%)	1 (0%)	84	79
All	All	943/960 (98%)	938 (100%)	5 (0%)	81	76

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ARG
1	A	157	ASN
1	B	53	LEU
1	C	146	LEU
1	D	222	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	260	GLN
1	A	263	HIS
1	B	130	HIS
1	C	24	HIS
1	C	130	HIS
1	C	173	GLN
1	D	130	HIS
1	D	263	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	C	180	1	8,10,11	1.06	0	10,14,16	1.42	1 (10%)
1	TPO	D	180	1	8,10,11	1.47	1 (12%)	10,14,16	1.51	2 (20%)
1	TPO	B	180	1	8,10,11	1.56	1 (12%)	10,14,16	1.42	2 (20%)
1	TPO	A	180	1	8,10,11	1.58	1 (12%)	10,14,16	1.61	2 (20%)

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	C	180	1	-	0/9/11/13	-
1	TPO	D	180	1	-	0/9/11/13	-
1	TPO	B	180	1	-	0/9/11/13	-
1	TPO	A	180	1	-	0/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	TPO	P-O1P	3.63	1.61	1.50
1	B	180	TPO	P-O1P	3.34	1.60	1.50
1	D	180	TPO	P-O1P	2.78	1.59	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	TPO	P-OG1-CB	-3.79	113.02	123.33
1	A	180	TPO	P-OG1-CB	-3.50	113.82	123.33
1	D	180	TPO	P-OG1-CB	-3.30	114.37	123.33
1	B	180	TPO	P-OG1-CB	-2.72	115.94	123.33
1	B	180	TPO	CG2-CB-CA	-2.71	107.98	113.26
1	A	180	TPO	CG2-CB-CA	-2.37	108.64	113.26
1	D	180	TPO	CG2-CB-CA	-2.27	108.84	113.26

There are no chirality outliers.

There are no torsion outliers.

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](#)

6 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	3RJ	B	401	-	34,35,35	1.84	9 (26%)	48,50,50	2.29	10 (20%)
3	3RJ	D	401	-	34,35,35	1.77	6 (17%)	48,50,50	2.18	11 (22%)
3	3RJ	C	401	-	34,35,35	1.74	7 (20%)	48,50,50	2.04	10 (20%)
2	GOL	A	302	-	5,5,5	0.38	0	5,5,5	0.09	0
2	GOL	A	301	-	5,5,5	0.38	0	5,5,5	0.24	0
3	3RJ	A	303	-	34,35,35	1.51	5 (14%)	48,50,50	1.90	10 (20%)

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	3RJ	B	401	-	-	4/10/18/18	0/6/6/6
3	3RJ	D	401	-	-	4/10/18/18	0/6/6/6
3	3RJ	C	401	-	-	4/10/18/18	0/6/6/6
2	GOL	A	302	-	-	2/4/4/4	-
2	GOL	A	301	-	-	4/4/4/4	-
3	3RJ	A	303	-	-	4/10/18/18	0/6/6/6

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	3RJ	C09-N08	5.96	1.47	1.37
3	B	401	3RJ	C09-N08	5.81	1.46	1.37
3	D	401	3RJ	C09-N08	5.69	1.46	1.37
3	A	303	3RJ	C09-N08	4.33	1.44	1.37
3	D	401	3RJ	C06-C01	-3.89	1.36	1.42
3	B	401	3RJ	C19-N20	3.79	1.44	1.36
3	C	401	3RJ	C06-C01	-3.73	1.36	1.42
3	B	401	3RJ	C06-C01	-3.34	1.37	1.42
3	D	401	3RJ	C19-N20	3.18	1.43	1.36
3	C	401	3RJ	C19-N20	3.11	1.43	1.36
3	A	303	3RJ	C06-C01	-3.09	1.37	1.42
3	A	303	3RJ	C16-C13	-2.71	1.49	1.54
3	A	303	3RJ	C17-C12	2.52	1.41	1.37
3	B	401	3RJ	C14-C13	-2.42	1.49	1.54
3	B	401	3RJ	C09-N10	2.39	1.36	1.33
3	A	303	3RJ	C19-N20	2.38	1.41	1.36
3	D	401	3RJ	C16-C13	-2.32	1.49	1.54
3	B	401	3RJ	C23-C27	-2.30	1.36	1.40
3	D	401	3RJ	C14-C13	-2.29	1.50	1.54
3	C	401	3RJ	C16-C13	-2.28	1.50	1.54
3	B	401	3RJ	C07-N18	2.27	1.36	1.33
3	D	401	3RJ	C23-C27	-2.23	1.37	1.40
3	C	401	3RJ	C22-C23	2.20	1.43	1.39
3	B	401	3RJ	C16-C13	-2.19	1.50	1.54
3	C	401	3RJ	C09-N10	2.14	1.36	1.33
3	B	401	3RJ	C17-C12	2.11	1.41	1.37
3	C	401	3RJ	C14-C13	-2.08	1.50	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	3RJ	C17-C09-N10	-7.12	107.05	112.14
3	B	401	3RJ	C07-C06-C01	6.61	119.77	115.86
3	D	401	3RJ	C17-C09-N10	-6.52	107.48	112.14
3	C	401	3RJ	C17-C09-N10	-6.50	107.50	112.14
3	D	401	3RJ	C09-N10-N11	6.31	108.30	103.71
3	B	401	3RJ	C09-N10-N11	5.86	107.97	103.71
3	D	401	3RJ	C07-C06-C01	5.84	119.31	115.86
3	C	401	3RJ	C09-N10-N11	5.50	107.71	103.71
3	C	401	3RJ	C07-C06-C01	5.27	118.97	115.86
3	A	303	3RJ	C09-N10-N11	5.21	107.50	103.71
3	B	401	3RJ	C16-C13-C12	-4.91	109.80	118.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	3RJ	C17-C09-N10	-4.74	108.75	112.14
3	D	401	3RJ	C16-C13-C12	-4.71	110.15	118.16
3	A	303	3RJ	C16-C13-C12	-4.20	111.00	118.16
3	A	303	3RJ	C07-C06-C01	4.07	118.26	115.86
3	C	401	3RJ	C16-C13-C12	-3.98	111.38	118.16
3	D	401	3RJ	N24-C25-N26	-3.84	108.03	113.87
3	A	303	3RJ	C06-C01-N30	-3.77	118.81	122.80
3	A	303	3RJ	N24-C25-N26	-3.73	108.19	113.87
3	B	401	3RJ	N24-C25-N26	-3.68	108.27	113.87
3	D	401	3RJ	C06-C01-N30	-3.61	118.98	122.80
3	B	401	3RJ	C21-N20-C19	-3.58	119.74	129.38
3	C	401	3RJ	N24-C25-N26	-3.41	108.68	113.87
3	B	401	3RJ	C12-C17-C09	3.28	107.07	104.78
3	B	401	3RJ	C06-C01-N30	-3.22	119.39	122.80
3	D	401	3RJ	N30-C19-N18	-3.11	121.17	126.25
3	C	401	3RJ	C06-C01-N30	-3.10	119.51	122.80
3	A	303	3RJ	C19-N30-C01	3.06	120.40	115.54
3	D	401	3RJ	C19-N30-C01	3.01	120.32	115.54
3	C	401	3RJ	C21-N20-C19	-2.94	121.47	129.38
3	C	401	3RJ	C19-N30-C01	2.78	119.95	115.54
3	B	401	3RJ	N30-C19-N18	-2.78	121.70	126.25
3	D	401	3RJ	C21-N20-C19	-2.75	121.95	129.38
3	A	303	3RJ	C21-N20-C19	-2.74	121.99	129.38
3	B	401	3RJ	C19-N30-C01	2.68	119.80	115.54
3	C	401	3RJ	N30-C19-N18	-2.62	121.96	126.25
3	C	401	3RJ	C12-C17-C09	2.58	106.59	104.78
3	A	303	3RJ	N30-C19-N18	-2.32	122.45	126.25
3	A	303	3RJ	C02-C01-C06	2.29	121.61	119.13
3	D	401	3RJ	C28-C27-N26	2.08	133.45	129.62
3	D	401	3RJ	C12-C17-C09	2.06	106.22	104.78

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	GOL	C1-C2-C3-O3
2	A	302	GOL	O2-C2-C3-O3
3	A	303	3RJ	C17-C12-C13-C14
3	A	303	3RJ	C17-C12-C13-C16
3	B	401	3RJ	C17-C12-C13-C14
3	B	401	3RJ	C17-C12-C13-C16
3	C	401	3RJ	C17-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	401	3RJ	C17-C12-C13-C16
3	D	401	3RJ	C17-C12-C13-C14
3	D	401	3RJ	C17-C12-C13-C16
3	D	401	3RJ	C22-C21-N20-C19
3	A	303	3RJ	C29-C21-N20-C19
3	D	401	3RJ	C29-C21-N20-C19
3	A	303	3RJ	C22-C21-N20-C19
3	C	401	3RJ	C22-C21-N20-C19
2	A	301	GOL	O1-C1-C2-O2
3	C	401	3RJ	C29-C21-N20-C19
2	A	301	GOL	O2-C2-C3-O3
2	A	301	GOL	O1-C1-C2-C3
3	B	401	3RJ	C22-C21-N20-C19
2	A	301	GOL	C1-C2-C3-O3
3	B	401	3RJ	C29-C21-N20-C19

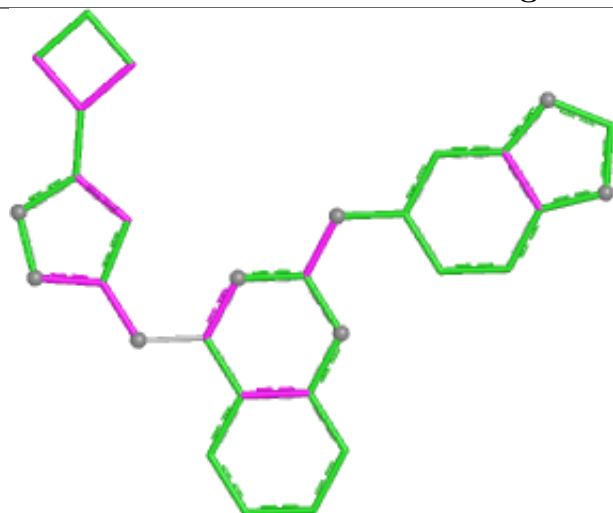
There are no ring outliers.

1 monomer is involved in 3 short contacts:

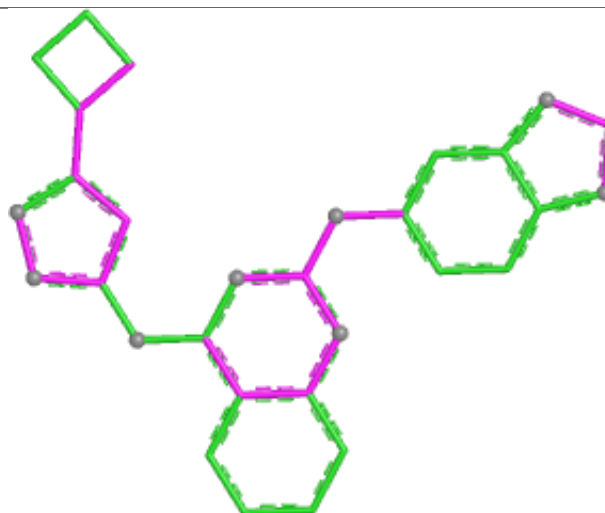
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	3RJ	3	0

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.

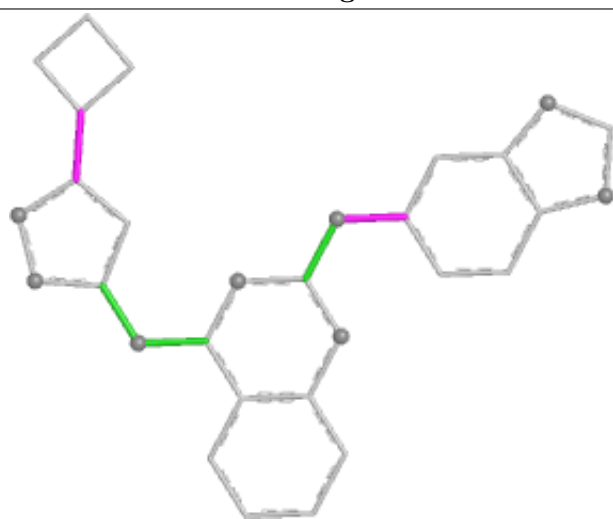
Ligand 3RJ B 401



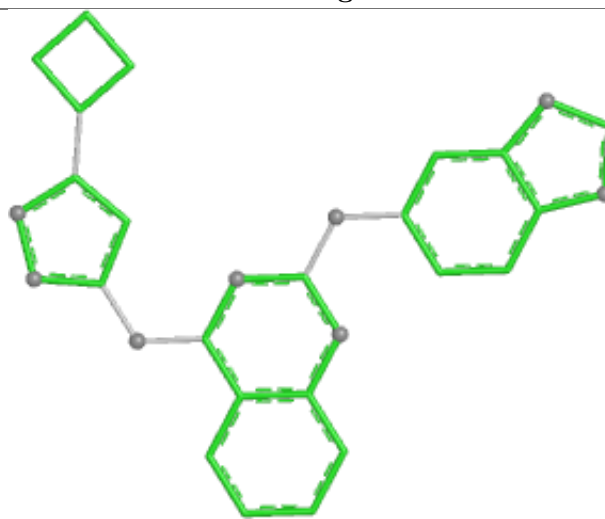
Bond lengths



Bond angles

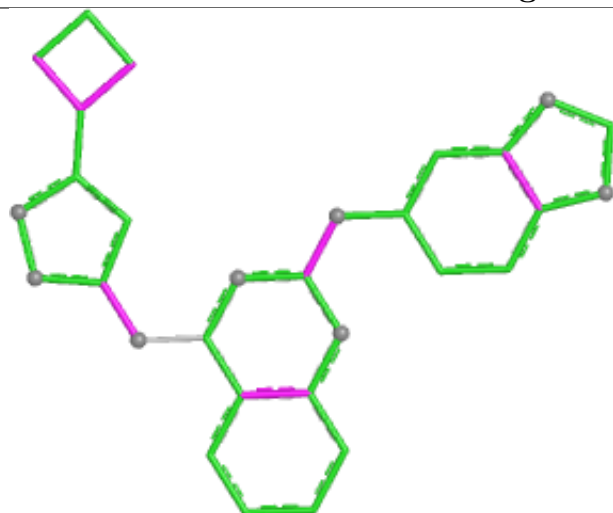


Torsions

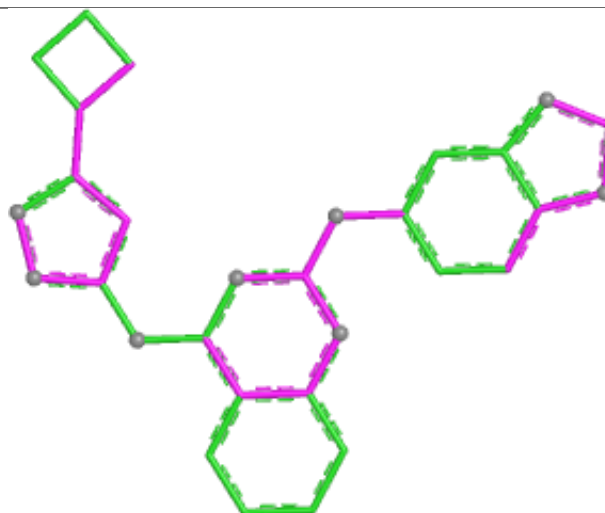


Rings

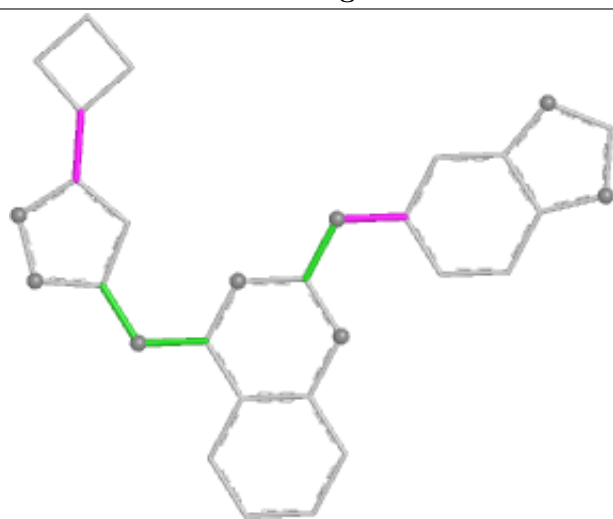
Ligand 3RJ D 401



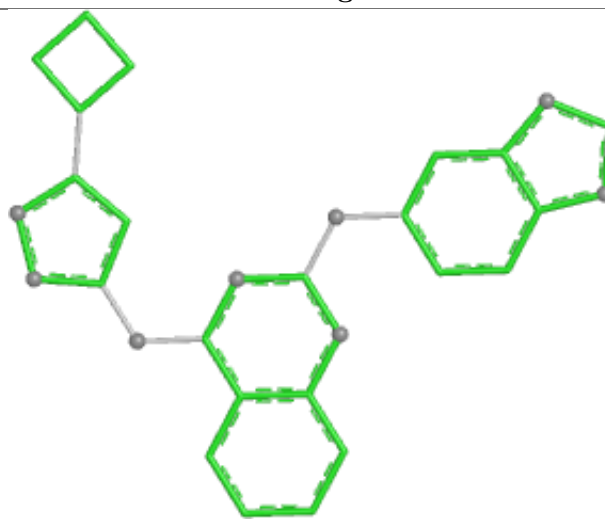
Bond lengths



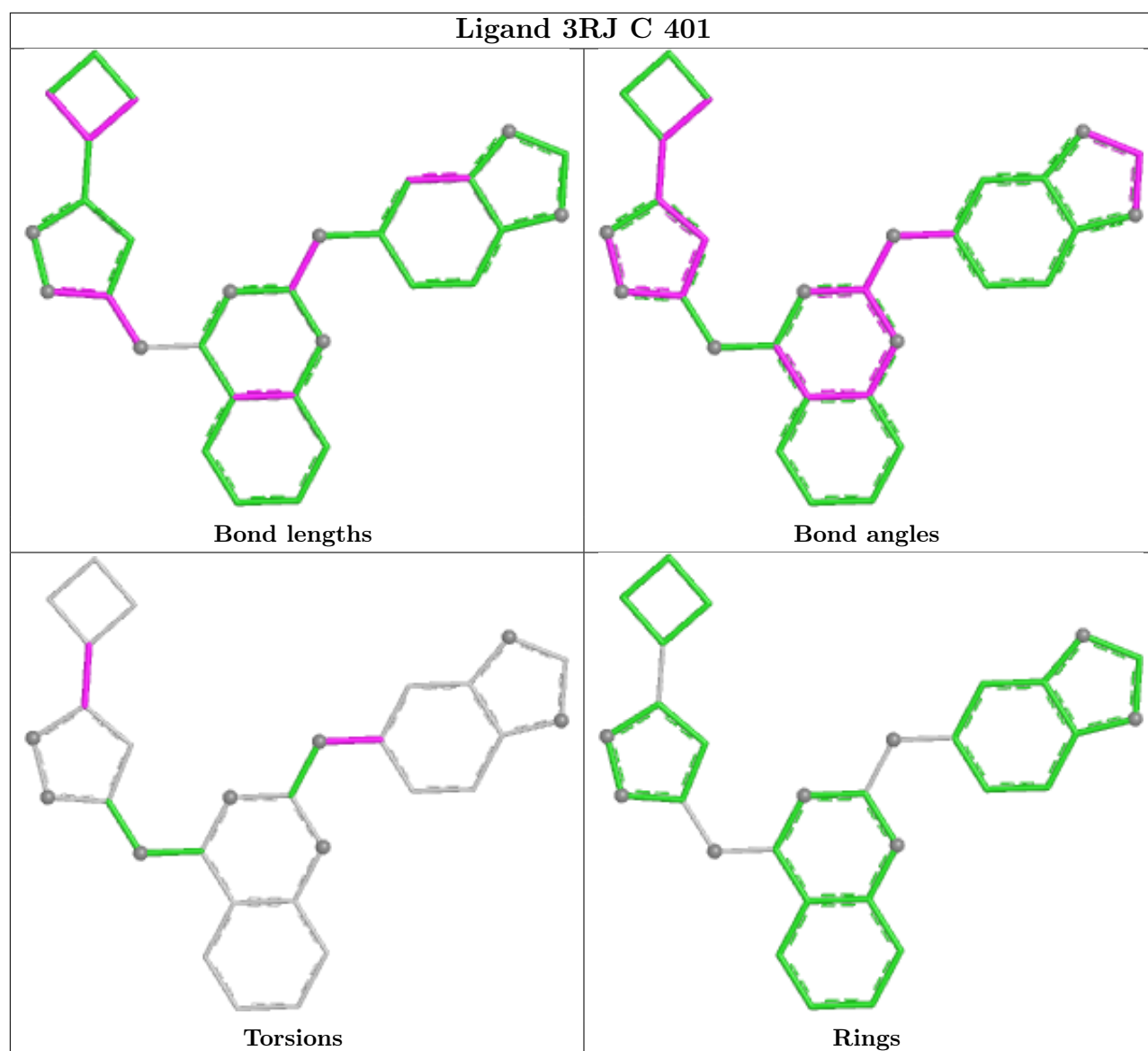
Bond angles

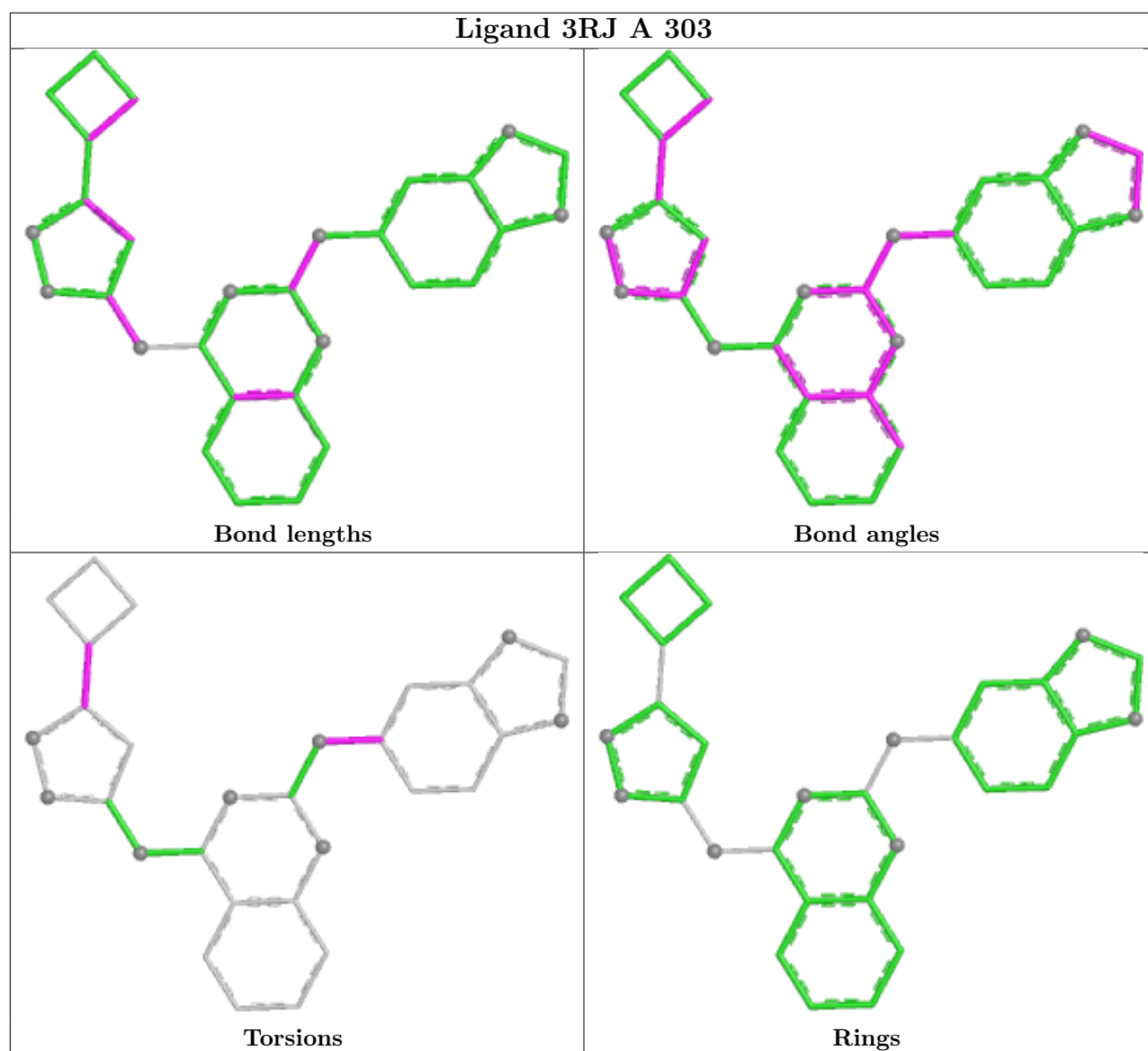


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/287 (95%)	-0.05	7 (2%) 57 62	12, 28, 54, 76	3 (1%)
1	B	272/287 (94%)	0.80	30 (11%) 10 12	12, 52, 83, 90	4 (1%)
1	C	271/287 (94%)	0.79	24 (8%) 15 17	15, 47, 73, 92	4 (1%)
1	D	272/287 (94%)	0.25	19 (6%) 22 25	9, 34, 67, 103	4 (1%)
All	All	1088/1148 (94%)	0.45	80 (7%) 20 23	9, 40, 77, 103	15 (1%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	150	ALA	6.6
1	D	149	PRO	4.9
1	B	105	HIS	4.5
1	B	280	ALA	4.4
1	A	156	PRO	4.1
1	B	104	LEU	3.8
1	D	148	ASN	3.8
1	B	29[A]	VAL	3.7
1	C	231	LEU	3.6
1	D	151	GLY	3.4
1	D	152	ARG	3.3
1	B	31	PHE	3.1
1	B	106	ALA	3.1
1	C	249	ALA	3.1
1	B	154	ALA	3.1
1	B	223	ALA	3.0
1	B	22	ILE	3.0
1	B	16	PHE	2.9
1	A	155	ASN	2.9
1	A	280	ALA	2.9
1	C	156	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	226	PRO	2.8
1	C	186	MET	2.8
1	D	154	ALA	2.8
1	D	158	SER	2.8
1	B	21	LEU	2.8
1	C	159	ILE	2.8
1	B	224	SER	2.8
1	C	38	ALA	2.8
1	C	150	ALA	2.8
1	B	37	ALA	2.7
1	C	41	LEU	2.7
1	C	149	PRO	2.7
1	D	22	ILE	2.7
1	C	278	LEU	2.7
1	C	22	ILE	2.7
1	D	155	ASN	2.7
1	D	231	LEU	2.6
1	B	240	VAL	2.6
1	D	153	ARG	2.5
1	C	240	VAL	2.5
1	D	21	LEU	2.5
1	B	17	SER	2.5
1	B	152	ARG	2.5
1	B	8	THR	2.5
1	D	29[A]	VAL	2.5
1	C	276	PRO	2.5
1	A	186	MET	2.4
1	D	280	ALA	2.4
1	D	279	ASP	2.4
1	D	156	PRO	2.4
1	C	234	GLU	2.4
1	B	12	GLY	2.4
1	D	224	SER	2.4
1	C	19	LYS	2.4
1	B	24	HIS	2.3
1	C	157	ASN	2.3
1	B	19	LYS	2.3
1	B	36	ARG	2.3
1	B	241	PRO	2.3
1	C	21	LEU	2.3
1	D	238	THR	2.3
1	B	54	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	243	ILE	2.3
1	C	40	ASP	2.3
1	B	239	LEU	2.3
1	B	249	ALA	2.2
1	D	235	LYS	2.2
1	A	153	ARG	2.2
1	C	277	PHE	2.1
1	A	231	LEU	2.1
1	C	274	HIS	2.1
1	C	273	PHE	2.1
1	C	224	SER	2.1
1	A	157	ASN	2.1
1	B	253	GLN	2.1
1	C	228	ASP	2.0
1	C	279	ASP	2.0
1	B	23	GLY	2.0
1	B	88	VAL	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	B	180	11/12	0.98	0.06	28,31,34,35	0
1	TPO	C	180	11/12	0.98	0.05	23,26,30,30	0
1	TPO	D	180	11/12	0.98	0.05	19,21,23,24	0
1	TPO	A	180	11/12	0.99	0.04	22,24,26,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

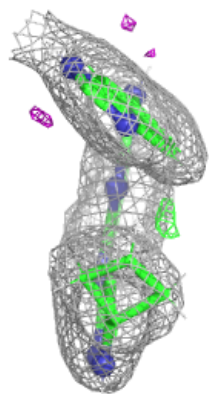
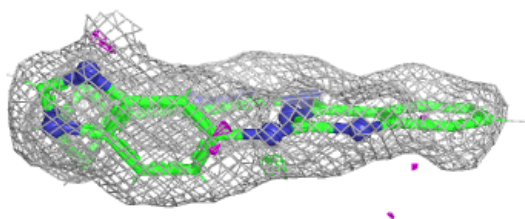
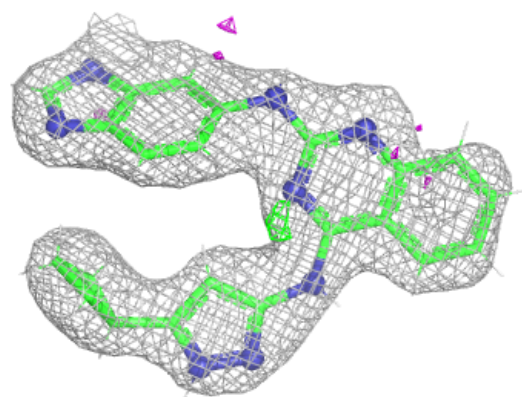
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	GOL	A	302	6/6	0.84	0.12	48,57,65,67	0
2	GOL	A	301	6/6	0.85	0.11	48,57,62,63	0
3	3RJ	B	401	30/30	0.89	0.10	35,52,67,68	0
3	3RJ	C	401	30/30	0.91	0.09	33,35,43,46	0
3	3RJ	D	401	30/30	0.95	0.07	27,33,40,42	0
3	3RJ	A	303	30/30	0.96	0.06	15,22,26,31	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.

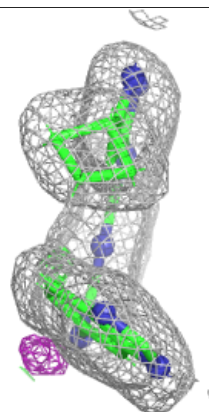
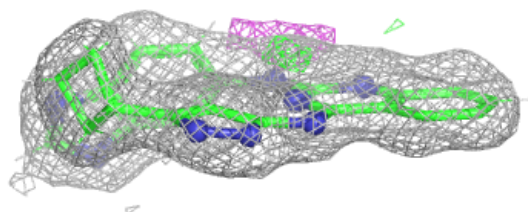
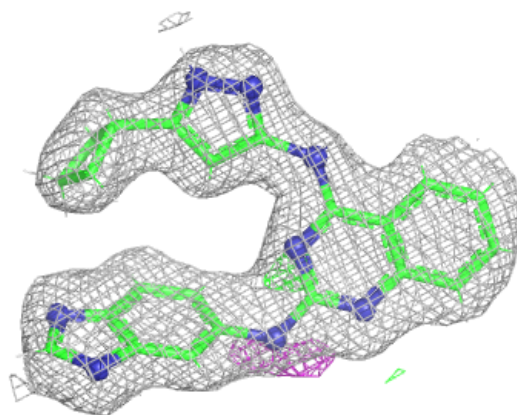
Electron density around 3RJ B 401:

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

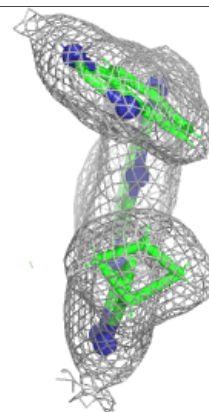
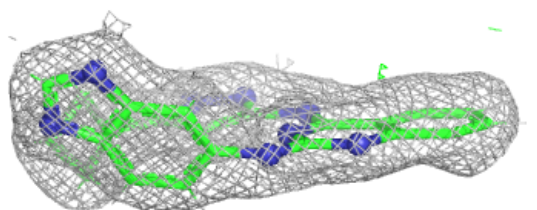
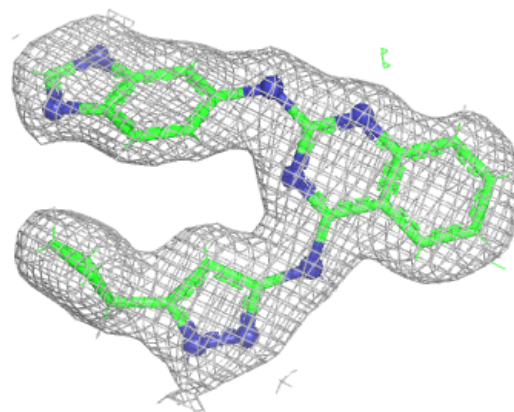


Electron density around 3RJ C 401:

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

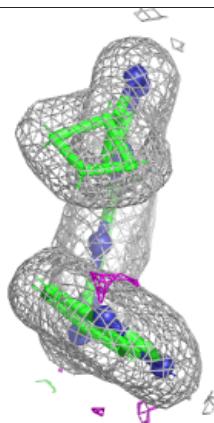
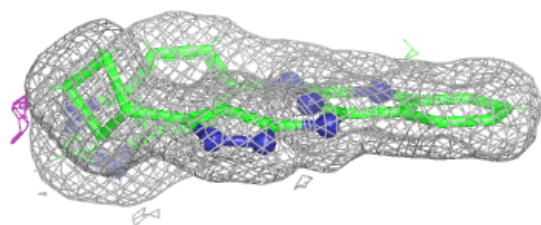
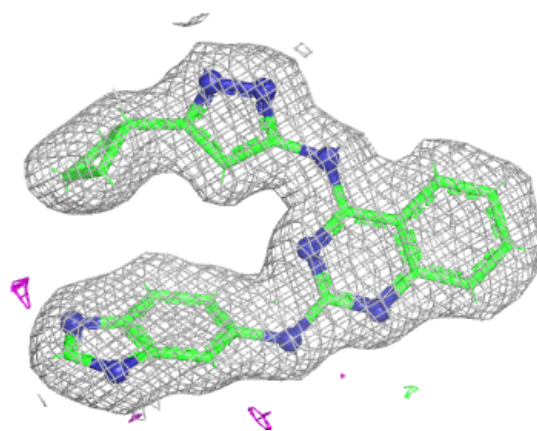
**Electron density around 3RJ D 401:**

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



Electron density around 3RJ A 303:

$2mF_o-DF_c$ (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.