Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 08:08 am BST

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PDB ID	:	3W18
Title	:	Structure of Aurora kinase A complexed to benzoimidazole-indazole inhibitor XIII
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Deposited on	:	2012-11-09
Resolution	:	2.50 Å(reported)

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 2.50 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.
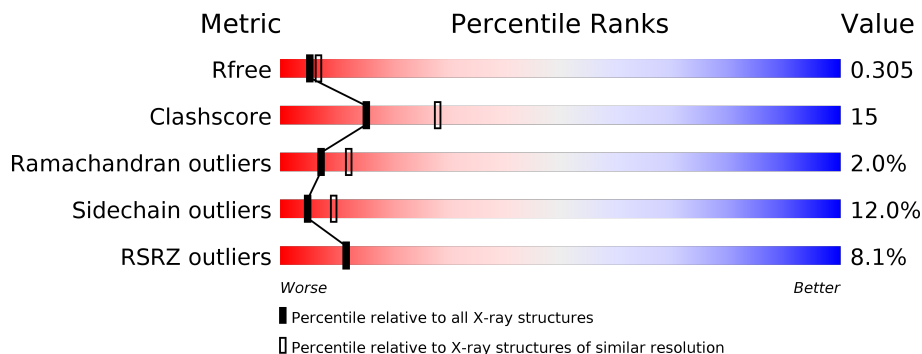
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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 <=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	278	5% / 58% 21% 6% 16%
1	B	278	9% / 59% 21% · · 15%

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	N13	A	501	-	-	X	-
2	N13	B	501	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3992 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 Aurora kinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1922	1240	332	346	4			
1	B	236	Total	C	N	O	S	0	0	0
			1921	1240	329	348	4			

- Molecule 2 is 2-{3-[3-(1H-benzimidazol-2-yl)-1H-indazol-6-yl]-1H-pyrazol-5-yl}-N-(3-fluorop henyl)acetamide (three-letter code: N13) (formula: $C_{25}H_{18}FN_7O$).
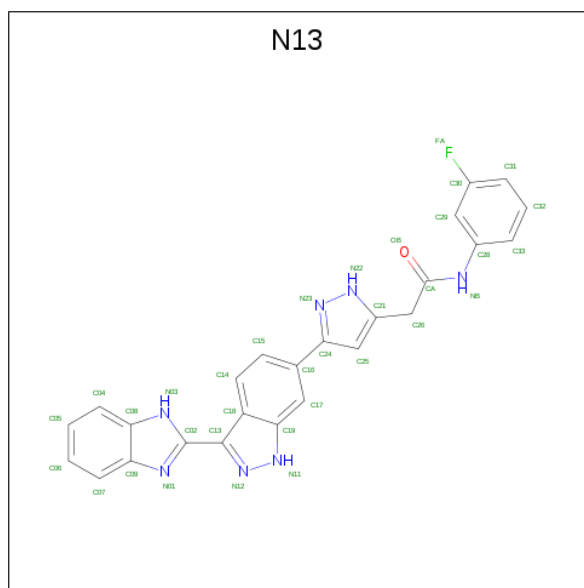
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			34	25	1	7	1		
2	B	1	Total	C	F	N	O	0	0
			34	25	1	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total 38	O 38	0	0
3	B	43	Total 43	O 43	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Aurora kinase A
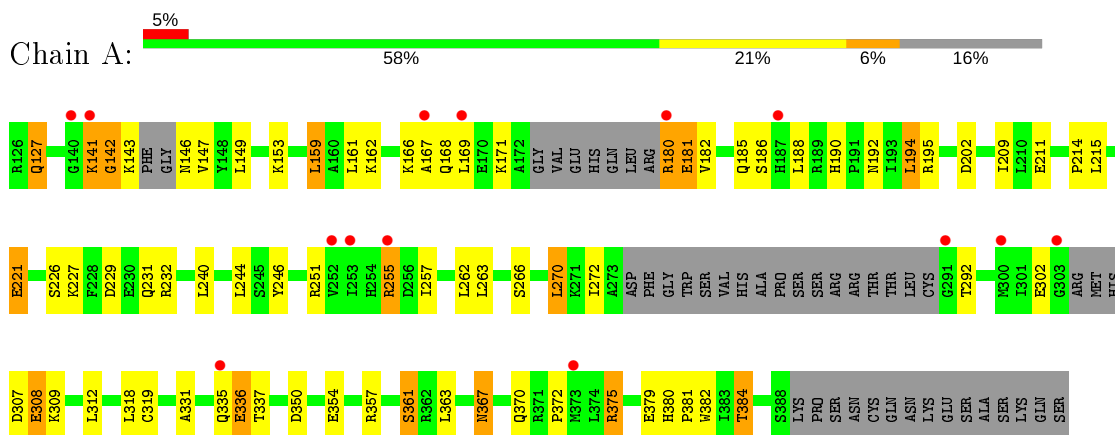
- Molecule 1: Aurora kinase A
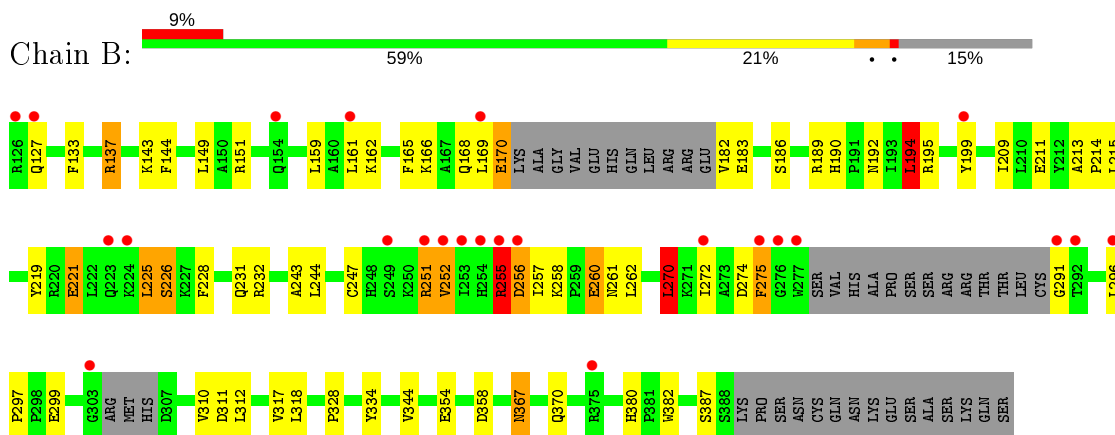
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.94Å 85.86Å 85.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.17 – 2.50 19.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.17-2.50) 99.8 (19.17-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 2.49Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.240 , 0.315 0.236 , 0.305	Depositor DCC
R_{free} test set	1013 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.3	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3992	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 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: N13

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	0.76	1/1964 (0.1%)	0.85	2/2649 (0.1%)
1	B	0.77	1/1965 (0.1%)	0.80	2/2655 (0.1%)
All	All	0.76	2/3929 (0.1%)	0.83	4/5304 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	GLU	CG-CD	6.31	1.61	1.51
1	B	260	GLU	CG-CD	5.12	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	270	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	263	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	B	194	LEU	CA-CB-CG	5.06	126.94	115.30

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	1922	0	1937	52	2
1	B	1921	0	1913	54	1
2	A	34	0	18	9	0
2	B	34	0	18	11	0
3	A	38	0	0	4	0
3	B	43	0	0	6	0
All	All	3992	0	3886	116	2

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 15.

All (116) 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)
2:B:501:N13:FA	2:B:501:N13:C30	1.71	1.28
1:B:354:GLU:HG3	3:B:619:HOH:O	1.32	1.27
1:B:162:LYS:NZ	2:B:501:N13:H6	1.62	1.15
1:B:162:LYS:HZ2	2:B:501:N13:H6	1.08	1.12
2:B:501:N13:OB	2:B:501:N13:H1	1.52	1.08
2:B:501:N13:OB	2:B:501:N13:C29	2.12	0.94
2:A:501:N13:H9	2:A:501:N13:H5	1.16	0.89
1:A:190:HIS:CD2	1:A:192:ASN:H	1.91	0.88
1:A:190:HIS:HD2	1:A:192:ASN:H	1.23	0.85
1:B:144:PHE:O	2:B:501:N13:H8	1.75	0.84
1:B:162:LYS:HZ2	2:B:501:N13:C26	1.88	0.84
1:A:292:THR:HG22	3:A:601:HOH:O	1.81	0.80
1:B:257:ILE:HG23	1:B:262:LEU:HD21	1.63	0.79
1:B:380:HIS:HD2	1:B:382:TRP:H	1.28	0.79
1:A:162:LYS:NZ	2:A:501:N13:H6	1.96	0.79
1:A:307:ASP:CG	1:A:308:GLU:H	1.84	0.78
1:A:141:LYS:O	1:A:142:GLY:O	2.02	0.77
1:B:380:HIS:CD2	1:B:382:TRP:H	2.02	0.76
1:B:257:ILE:CG2	1:B:262:LEU:HD21	2.17	0.74
1:B:162:LYS:NZ	2:B:501:N13:C26	2.48	0.74
1:A:380:HIS:HD2	1:A:382:TRP:H	1.33	0.73
1:B:367:ASN:HB2	3:B:603:HOH:O	1.87	0.73
1:B:190:HIS:HD2	1:B:192:ASN:H	1.36	0.72
1:A:292:THR:HG21	3:A:627:HOH:O	1.93	0.69
1:A:331:ALA:HB1	1:A:336:GLU:HB3	1.74	0.68
1:A:162:LYS:HZ3	2:A:501:N13:H6	1.59	0.68
2:A:501:N13:OB	2:A:501:N13:H4	1.91	0.68
2:B:501:N13:OB	2:B:501:N13:N22	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLN:HG2	2:A:501:N13:H2	1.74	0.68
1:A:357:ARG:O	1:A:361:SER:HB2	1.94	0.67
1:B:195:ARG:HD2	3:B:630:HOH:O	1.94	0.67
1:B:166:LYS:O	1:B:169:LEU:HD12	1.95	0.66
1:A:380:HIS:CD2	1:A:382:TRP:H	2.13	0.66
1:B:162:LYS:HZ3	2:B:501:N13:H6	1.57	0.66
1:B:291:GLY:O	3:B:639:HOH:O	2.14	0.65
1:A:180:ARG:HD3	1:A:181:GLU:HG2	1.79	0.64
1:B:168:GLN:O	1:B:169:LEU:HG	1.98	0.64
1:A:257:ILE:CG2	1:A:262:LEU:HD21	2.29	0.63
1:A:190:HIS:HD2	1:A:192:ASN:N	1.97	0.62
1:A:307:ASP:CG	1:A:308:GLU:N	2.55	0.59
1:B:367:ASN:HB3	1:B:370:GLN:HG3	1.84	0.59
1:A:188:LEU:HD22	1:A:246:TYR:HE2	1.67	0.59
1:A:162:LYS:HZ2	2:A:501:N13:H6	1.66	0.59
1:B:255:ARG:NH2	1:B:274:ASP:OD2	2.36	0.58
2:B:501:N13:H1	2:B:501:N13:H9	1.68	0.58
1:A:380:HIS:HD2	1:A:382:TRP:N	2.02	0.57
1:B:137:ARG:NH1	3:B:628:HOH:O	2.33	0.57
1:A:257:ILE:HG21	1:A:262:LEU:HD21	1.86	0.57
2:A:501:N13:OB	2:A:501:N13:C33	2.53	0.57
1:B:258:LYS:O	1:B:262:LEU:HG	2.05	0.56
1:B:256:ASP:N	1:B:256:ASP:OD2	2.39	0.56
1:A:380:HIS:O	1:A:384:THR:HG23	2.06	0.55
2:A:501:N13:N22	2:A:501:N13:NB	2.30	0.55
1:B:190:HIS:CD2	1:B:192:ASN:H	2.22	0.55
1:B:225:LEU:O	1:B:226:SER:HB3	2.05	0.55
1:B:143:LYS:O	1:B:162:LYS:NZ	2.40	0.55
1:B:244:LEU:HD13	1:B:311:ASP:HB3	1.89	0.54
1:A:331:ALA:HB3	1:A:337:THR:OG1	2.07	0.53
1:B:226:SER:HB2	3:B:623:HOH:O	2.09	0.53
1:A:127:GLN:HA	3:A:619:HOH:O	2.09	0.52
1:A:367:ASN:HB3	1:A:370:GLN:HG3	1.90	0.52
1:A:214:PRO:HG2	1:A:266:SER:HB3	1.92	0.52
1:A:194:LEU:HD22	1:A:211:GLU:HB3	1.92	0.51
1:A:167:ALA:C	1:A:169:LEU:H	2.13	0.51
1:B:251:ARG:O	1:B:252:VAL:HG23	2.11	0.51
1:B:274:ASP:O	1:B:275:PHE:C	2.49	0.50
1:A:180:ARG:HB2	1:A:181:GLU:OE1	2.11	0.50
1:B:219:TYR:CD1	1:B:260:GLU:HG2	2.46	0.50
1:B:159:LEU:HD13	1:B:209:ILE:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:VAL:HG13	1:B:328:PRO:HD2	1.93	0.50
1:A:312:LEU:HG	1:A:372:PRO:O	2.11	0.50
1:A:308:GLU:O	1:A:308:GLU:HG2	2.12	0.49
1:A:143:LYS:NZ	1:A:143:LYS:HB3	2.27	0.48
1:A:181:GLU:N	1:A:181:GLU:OE1	2.45	0.48
1:A:229:ASP:OD2	1:A:231:GLN:N	2.45	0.48
1:A:221:GLU:OE2	1:A:232:ARG:NH1	2.47	0.47
1:B:190:HIS:HD2	1:B:192:ASN:N	2.10	0.47
1:A:226:SER:O	3:A:609:HOH:O	2.20	0.47
1:B:194:LEU:HD22	1:B:211:GLU:HB3	1.97	0.47
1:A:166:LYS:NZ	1:A:202:ASP:O	2.45	0.47
1:B:221:GLU:OE2	1:B:232:ARG:NH1	2.48	0.47
2:A:501:N13:N01	2:A:501:N13:H12	2.30	0.47
1:B:380:HIS:HD2	1:B:382:TRP:N	2.05	0.46
1:A:240:LEU:HD23	1:A:272:ILE:HD11	1.97	0.46
1:A:375:ARG:HD2	1:A:379:GLU:OE2	2.16	0.46
1:B:247:CYS:HB3	1:B:252:VAL:O	2.16	0.46
1:A:255:ARG:HG2	1:A:255:ARG:H	1.54	0.46
1:A:159:LEU:HD13	1:A:209:ILE:HG23	1.99	0.45
1:B:228:PHE:CD1	1:B:232:ARG:HD2	2.52	0.44
1:A:309:LYS:HD3	1:A:312:LEU:HD23	1.97	0.44
1:B:296:LEU:HA	1:B:297:PRO:HD3	1.63	0.44
1:B:252:VAL:O	1:B:252:VAL:HG12	2.17	0.44
1:A:167:ALA:O	1:A:169:LEU:N	2.51	0.43
1:A:180:ARG:C	1:A:182:VAL:H	2.22	0.43
1:A:380:HIS:CD2	1:A:381:PRO:HD2	2.53	0.43
1:B:270:LEU:C	1:B:270:LEU:HD12	2.38	0.43
1:B:213:ALA:HA	1:B:214:PRO:HD3	1.76	0.43
1:A:380:HIS:HA	1:A:381:PRO:HD3	1.84	0.43
1:B:169:LEU:HB2	1:B:170:GLU:OE2	2.20	0.42
1:A:309:LYS:HA	1:A:312:LEU:HD23	2.01	0.42
1:B:297:PRO:HG2	1:B:310:VAL:HB	2.02	0.42
1:A:363:LEU:HD23	1:A:372:PRO:HD2	2.02	0.42
1:B:344:VAL:O	1:B:344:VAL:HG12	2.20	0.42
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.94	0.42
1:B:358:ASP:OD2	1:B:380:HIS:HE1	2.01	0.42
1:A:166:LYS:O	1:A:167:ALA:C	2.59	0.41
1:B:258:LYS:O	1:B:261:ASN:HB2	2.20	0.41
1:B:387:SER:OG	1:B:387:SER:O	2.36	0.41
1:A:188:LEU:HD22	1:A:246:TYR:CE2	2.51	0.41
1:A:166:LYS:O	1:A:169:LEU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:VAL:HG22	1:B:199:TYR:CE2	2.56	0.41
1:B:133:PHE:HA	1:B:151:ARG:O	2.21	0.41
1:B:258:LYS:HB2	1:B:258:LYS:HE3	1.88	0.41
1:A:142:GLY:O	1:A:143:LYS:C	2.59	0.41
1:B:228:PHE:CG	1:B:232:ARG:HD2	2.56	0.41
1:B:243:ALA:HB1	1:B:272:ILE:HD12	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:NZ	1:B:354:GLU:OE1[4_545]	2.04	0.16
1:A:153:LYS:NZ	1:A:350:ASP:OD2[3_545]	2.16	0.04

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	224/278 (81%)	208 (93%)	11 (5%)	5 (2%)	6	10
1	B	228/278 (82%)	210 (92%)	14 (6%)	4 (2%)	8	14
All	All	452/556 (81%)	418 (92%)	25 (6%)	9 (2%)	7	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	GLY
1	A	168	GLN
1	B	255	ARG
1	B	334	TYR
1	A	251	ARG
1	B	252	VAL

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Mol	Chain	Res	Type
1	B	275	PHE
1	A	302	GLU
1	A	255	ARG

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	206/246 (84%)	179 (87%)	27 (13%)	4	7
1	B	204/246 (83%)	182 (89%)	22 (11%)	6	12
All	All	410/492 (83%)	361 (88%)	49 (12%)	5	9

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	141	LYS
1	A	146	ASN
1	A	147	VAL
1	A	149	LEU
1	A	159	LEU
1	A	161	LEU
1	A	171	LYS
1	A	180	ARG
1	A	181	GLU
1	A	186	SER
1	A	194	LEU
1	A	195	ARG
1	A	215	LEU
1	A	221	GLU
1	A	227	LYS
1	A	244	LEU
1	A	270	LEU
1	A	308	GLU
1	A	318	LEU

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Mol	Chain	Res	Type
1	A	319	CYS
1	A	335	GLN
1	A	336	GLU
1	A	361	SER
1	A	367	ASN
1	A	375	ARG
1	A	384	THR
1	B	127	GLN
1	B	137	ARG
1	B	149	LEU
1	B	165	PHE
1	B	170	GLU
1	B	183	GLU
1	B	186	SER
1	B	189	ARG
1	B	194	LEU
1	B	215	LEU
1	B	221	GLU
1	B	225	LEU
1	B	226	SER
1	B	231	GLN
1	B	251	ARG
1	B	255	ARG
1	B	256	ASP
1	B	270	LEU
1	B	299	GLU
1	B	312	LEU
1	B	318	LEU
1	B	367	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	168	GLN
1	A	185	GLN
1	A	190	HIS
1	A	192	ASN
1	A	242	ASN
1	A	335	GLN
1	A	366	HIS
1	A	367	ASN

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Mol	Chain	Res	Type
1	A	380	HIS
1	B	168	GLN
1	B	190	HIS
1	B	201	HIS
1	B	231	GLN
1	B	242	ASN
1	B	367	ASN
1	B	380	HIS
1	B	386	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	$\#|Z| > 2$
2	N13	B	501	-	37,39,39	4.08	18 (48%)	38,56,56	2.51	14 (36%)
2	N13	A	501	-	37,39,39	3.51	17 (45%)	38,56,56	1.60	9 (23%)

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
2	N13	B	501	-	-	0/10/16/16	0/6/6/6
2	N13	A	501	-	-	2/10/16/16	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	N13	FA-C30	14.60	1.71	1.36
2	A	501	N13	N23-N22	-13.82	1.10	1.37
2	B	501	N13	N23-N22	-10.36	1.17	1.37
2	B	501	N13	C16-C24	-9.43	1.34	1.48
2	A	501	N13	C16-C24	-7.82	1.36	1.48
2	B	501	N13	C17-C19	-5.41	1.33	1.41
2	A	501	N13	FA-C30	5.19	1.48	1.36
2	A	501	N13	C04-C08	-4.98	1.33	1.41
2	A	501	N13	C13-C02	-4.85	1.34	1.48
2	B	501	N13	C25-C21	-4.75	1.32	1.39
2	B	501	N13	C13-C02	-4.31	1.36	1.48
2	A	501	N13	C28-NB	-4.23	1.33	1.41
2	B	501	N13	C28-NB	-4.21	1.33	1.41
2	A	501	N13	C14-C18	-4.08	1.33	1.42
2	B	501	N13	C04-C08	-3.96	1.35	1.41
2	A	501	N13	C07-C09	-3.64	1.35	1.41
2	A	501	N13	C17-C19	-3.54	1.36	1.41
2	B	501	N13	C14-C18	-3.43	1.35	1.42
2	B	501	N13	C26-C21	-3.32	1.48	1.51
2	B	501	N13	C25-C24	-3.24	1.34	1.40
2	A	501	N13	C25-C21	-3.16	1.34	1.39
2	B	501	N13	C18-C19	-2.95	1.34	1.42
2	A	501	N13	C18-C19	-2.83	1.35	1.42
2	A	501	N13	C25-C24	-2.80	1.35	1.40
2	B	501	N13	C07-C09	-2.79	1.37	1.41
2	B	501	N13	C02-N01	-2.72	1.32	1.35
2	B	501	N13	C09-C08	-2.59	1.33	1.42
2	B	501	N13	C31-C30	2.39	1.41	1.37
2	B	501	N13	C32-C31	2.25	1.43	1.38
2	B	501	N13	N11-N12	2.19	1.42	1.37
2	A	501	N13	C31-C30	2.16	1.41	1.37
2	A	501	N13	C05-C04	2.09	1.41	1.36
2	A	501	N13	C26-CA	2.08	1.56	1.51
2	A	501	N13	C06-C07	2.05	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	N13	C09-C08	-2.03	1.35	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	N13	C28-NB-CA	-8.72	112.23	127.50
2	B	501	N13	C28-C29-C30	6.32	123.59	117.95
2	B	501	N13	C31-C30-C29	-5.10	116.66	123.29
2	B	501	N13	FA-C30-C31	4.14	125.57	118.54
2	A	501	N13	C24-C25-C21	-4.00	99.99	105.29
2	A	501	N13	C28-NB-CA	-3.96	120.58	127.50
2	B	501	N13	C24-C25-C21	-3.61	100.50	105.29
2	A	501	N13	FA-C30-C31	2.68	123.10	118.54
2	A	501	N13	C13-C02-N03	2.65	127.54	122.27
2	B	501	N13	C14-C15-C16	-2.62	116.75	121.00
2	A	501	N13	C31-C30-C29	-2.60	119.92	123.29
2	A	501	N13	C28-C29-C30	2.54	120.22	117.95
2	B	501	N13	C02-N03-C08	2.54	108.81	103.78
2	B	501	N13	C32-C33-C28	-2.42	116.83	119.72
2	A	501	N13	C05-C06-C07	-2.32	117.19	120.44
2	B	501	N13	C13-C02-N01	2.17	126.59	122.27
2	B	501	N13	C26-CA-NB	2.17	119.24	114.77
2	A	501	N13	C02-N01-C09	2.16	108.07	103.78
2	A	501	N13	C25-C24-C16	2.14	132.41	129.44
2	B	501	N13	C05-C06-C07	-2.13	117.45	120.44
2	B	501	N13	C14-C18-C19	2.11	120.97	118.17
2	B	501	N13	OB-CA-C26	-2.06	117.35	122.03
2	B	501	N13	C02-N01-C09	2.01	107.77	103.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	N13	C21-C26-CA-OB
2	A	501	N13	C21-C26-CA-NB

There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	N13	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	N13	9	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 then 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 N13 B 501

Ligand N13 A 501
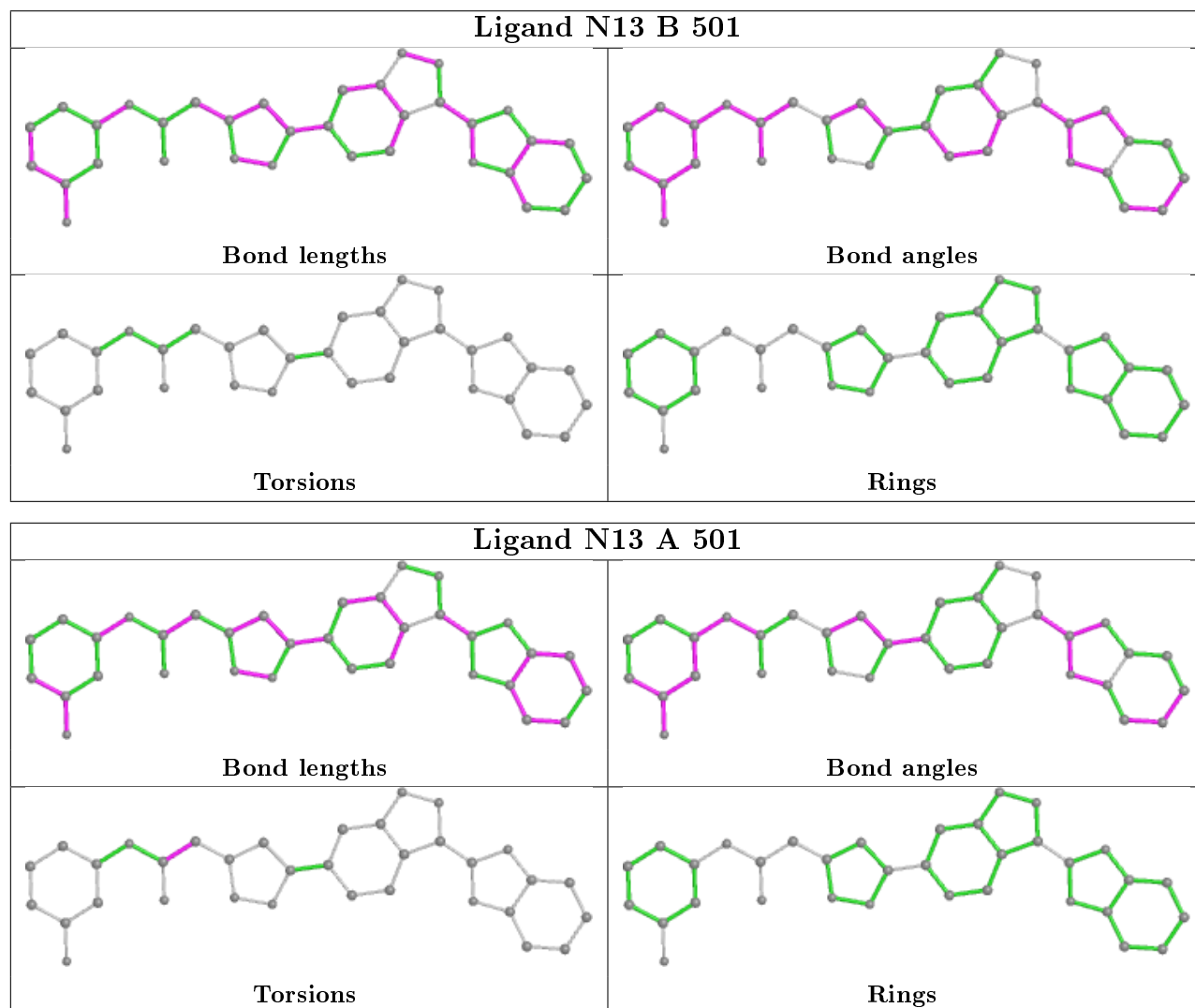
5.7 Other polymers (i)

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	234/278 (84%)	0.32	14 (5%)	21	22	23, 39, 73, 83	0
1	B	236/278 (84%)	0.46	24 (10%)	6	6	26, 41, 68, 81	0
All	All	470/556 (84%)	0.39	38 (8%)	12	12	23, 40, 72, 83	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	GLY	5.8
1	B	253	ILE	5.1
1	B	169	LEU	4.8
1	B	251	ARG	4.6
1	B	254	HIS	4.4
1	B	303	GLY	4.0
1	B	255	ARG	3.9
1	B	127	GLN	3.8
1	B	276	GLY	3.7
1	B	275	PHE	3.6
1	A	253	ILE	3.6
1	B	292	THR	3.5
1	A	291	GLY	3.3
1	A	141	LYS	3.1
1	B	199	TYR	2.9
1	B	252	VAL	2.8
1	A	252	VAL	2.8
1	A	140	GLY	2.8
1	B	249	SER	2.7
1	B	154	GLN	2.6
1	B	223	GLN	2.6
1	A	169	LEU	2.4
1	B	224	LYS	2.4
1	A	180	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	272	ILE	2.3
1	B	126	ARG	2.3
1	B	256	ASP	2.3
1	B	291	GLY	2.2
1	A	167	ALA	2.2
1	B	161	LEU	2.2
1	A	300	MET	2.2
1	B	277	TRP	2.2
1	A	187	HIS	2.2
1	A	335	GLN	2.2
1	A	255	ARG	2.2
1	A	373	MET	2.1
1	B	375	ARG	2.1
1	B	296	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

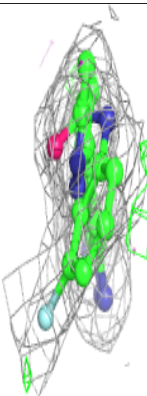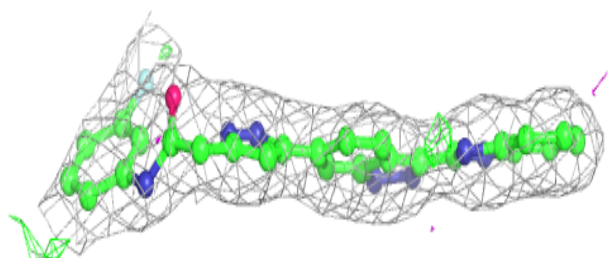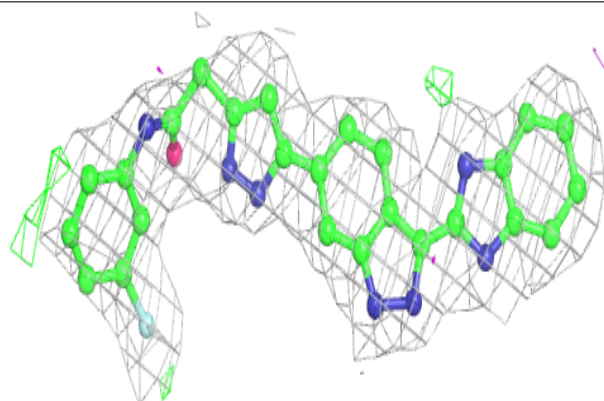| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	N13	A	501	34/34	0.94	0.14	18,26,49,50	0
2	N13	B	501	34/34	0.95	0.14	20,26,46,48	0

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 N13 A 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
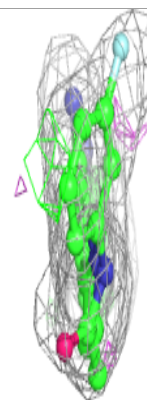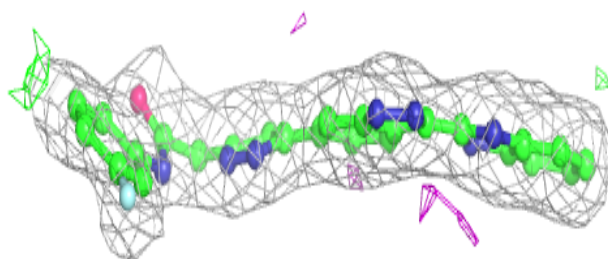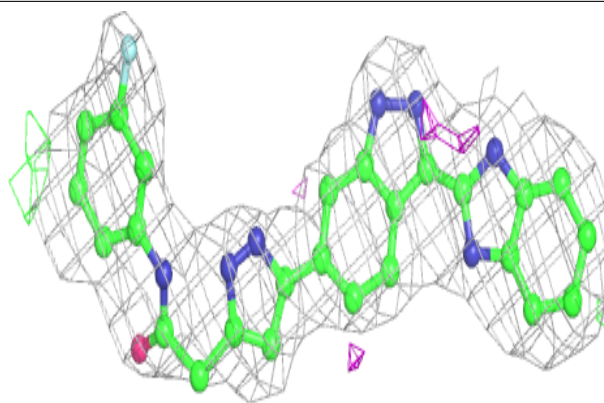
Electron density around N13 B 501:

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

6.5 Other polymers (i)

There are no such residues in this entry.