



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:56 PM UTC

PDB ID : 6UIP / pdb_00006uip
Title : DYRK1A Kinase Domain in Complex with a 6-azaindole Derivative, GNF2133.
Authors : DiDonato, M.; Spraggon, G.
Deposited on : 2019-10-01
Resolution : 3.70 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

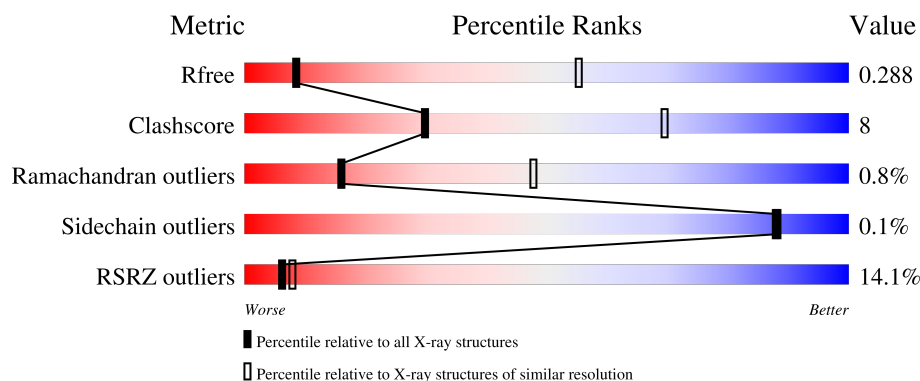
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	361	8% 73% 22% .
1	B	361	9% 73% 20% 6%
1	C	361	21% 65% 20% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8203 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.

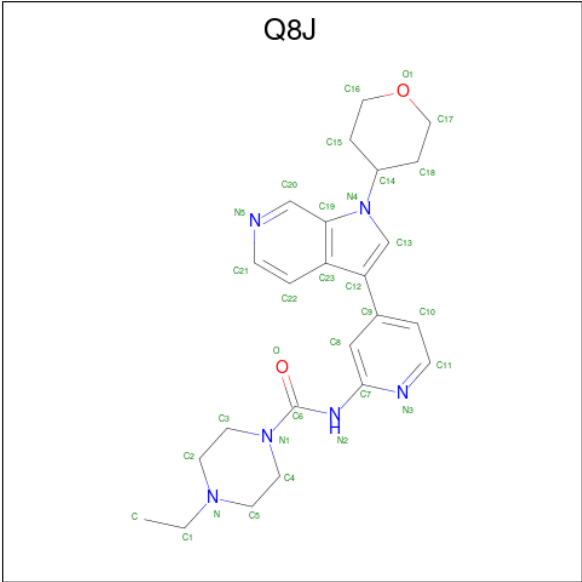
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	P	S	0	0	0
			2833	1821	488	506	1	17			
1	B	338	Total	C	N	O	P	S	0	0	0
			2766	1778	473	497	1	17			
1	C	306	Total	C	N	O	P	S	0	0	0
			2508	1619	432	442	1	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
B	126	MET	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
C	126	MET	-	expression tag	UNP Q13627

- Molecule 2 is 4-ethyl-N-{4-[1-(oxan-4-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]pyridin-2-yl}piperazine-1-carboxamide (CCD ID: Q8J) (formula: C₂₄H₃₀N₆O₂) (labeled as "Ligand of Interest" by depositor).

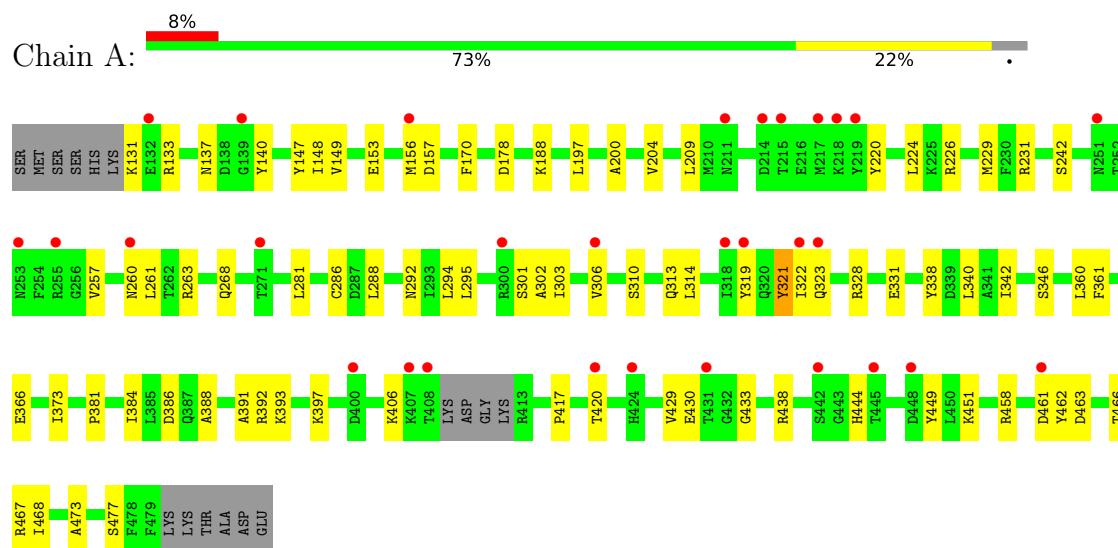


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	24	6	2		
2	B	1	Total	C	N	O	0	0
			32	24	6	2		
2	C	1	Total	C	N	O	0	0
			32	24	6	2		

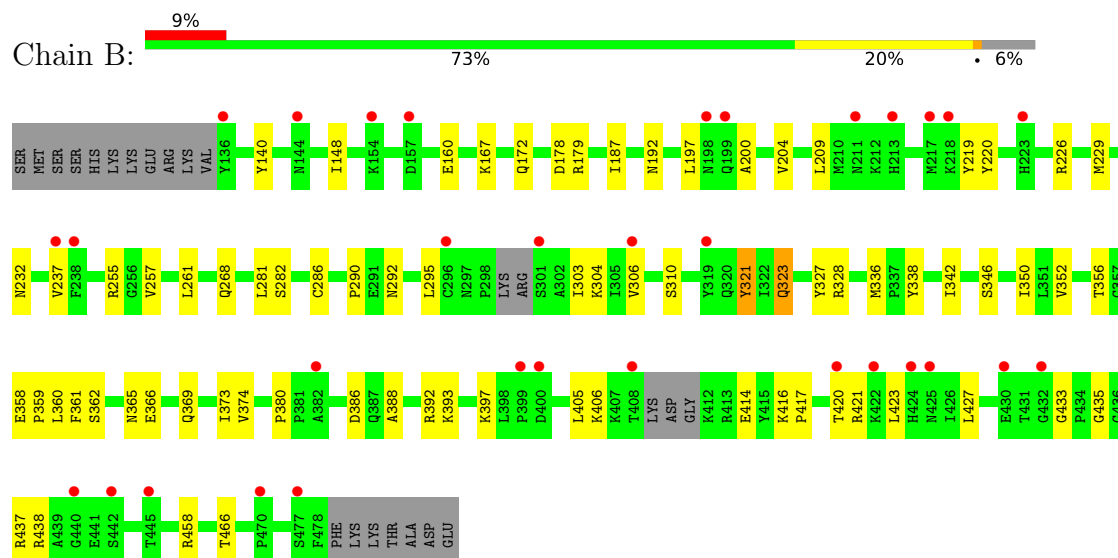
3 Residue-property plots

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: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	112.88Å 112.88Å 304.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.26 – 3.70 48.26 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.26-3.70) 98.5 (48.26-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.81 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.271 , 0.290 0.272 , 0.288	Depositor DCC
R_{free} test set	1163 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 15.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	8203	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Q8J, PTR

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	0.14	0/2881	0.39	0/3881
1	B	0.13	0/2812	0.34	0/3790
1	C	0.14	0/2542	0.37	0/3416
All	All	0.14	0/8235	0.37	0/11087

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2833	0	2841	50	0
1	B	2766	0	2764	43	0
1	C	2508	0	2530	48	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
All	All	8203	0	8135	138	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 8.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:HB3	1:A:133:ARG:HH12	1.35	0.89
1:C:458:ARG:HG3	1:C:468:ILE:HB	1.58	0.86
1:A:294:LEU:HD12	1:A:306:VAL:HG11	1.61	0.80
1:A:438:ARG:HB3	1:A:444:HIS:HD1	1.53	0.73
1:B:178:ASP:OD2	1:B:226:ARG:NH1	2.22	0.73
1:B:192:ASN:ND2	1:B:232:ASN:O	2.25	0.69
1:A:131:LYS:HB3	1:A:133:ARG:NH1	2.08	0.68
1:B:386:ASP:OD1	1:B:397:LYS:NZ	2.21	0.68
1:A:321:PTR:O3P	1:A:328:ARG:NH2	2.25	0.68
1:C:422:LYS:HG3	1:C:424:HIS:H	1.58	0.68
1:B:356:THR:HG23	1:B:358:GLU:H	1.59	0.68
1:B:392:ARG:O	1:B:406:LYS:NZ	2.26	0.67
1:B:255:ARG:O	1:B:437:ARG:NH1	2.29	0.65
1:C:352:VAL:HG11	1:C:360:LEU:HD12	1.79	0.65
1:B:359:PRO:HG2	1:B:362:SER:HB3	1.78	0.64
1:C:452:PHE:HB3	1:C:453:LYS:NZ	2.12	0.63
1:A:197:LEU:HD11	1:A:229:MET:HE1	1.81	0.63
1:C:375:GLU:HG2	1:C:416:LYS:HB2	1.81	0.62
1:A:388:ALA:HB3	1:A:391:ALA:HB2	1.80	0.62
1:C:323:GLN:HB2	1:C:328:ARG:HG3	1.82	0.61
1:B:295:LEU:HD23	1:B:303:ILE:HG22	1.81	0.61
1:C:295:LEU:HD23	1:C:303:ILE:HG22	1.85	0.59
1:B:257:VAL:HB	1:B:261:LEU:HD23	1.85	0.59
1:C:452:PHE:HB3	1:C:453:LYS:HZ2	1.68	0.59
1:A:281:LEU:O	1:A:313:GLN:NE2	2.36	0.58
1:A:295:LEU:HD23	1:A:303:ILE:HG22	1.86	0.58
1:C:142:ASP:OD1	1:C:143:ASP:N	2.37	0.58
1:A:220:TYR:HE1	1:A:268:GLN:HG2	1.69	0.56
1:A:461:ASP:OD2	1:A:466:THR:OG1	2.24	0.56
1:B:160:GLU:OE2	1:B:179:ARG:NE	2.40	0.55
1:B:167:LYS:NZ	1:B:172:GLN:HE21	2.05	0.55
1:C:374:VAL:HG21	1:C:405:LEU:HD11	1.88	0.55
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.89	0.55
1:A:429:VAL:HG23	1:A:449:TYR:HB2	1.89	0.54
1:B:220:TYR:HE1	1:B:268:GLN:HG2	1.72	0.54
1:A:458:ARG:HG3	1:A:468:ILE:HB	1.89	0.54
1:C:204:VAL:HG11	1:C:227:HIS:CD2	2.42	0.54
1:A:140:TYR:O	1:A:148:ILE:HG22	2.08	0.54
1:B:197:LEU:HD11	1:B:229:MET:HE1	1.89	0.53
1:A:381:PRO:HD2	1:A:384:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ILE:HD11	1:C:173:VAL:HG12	1.89	0.53
1:B:327:TYR:OH	1:C:413:ARG:NH2	2.42	0.52
1:C:447:ALA:HA	1:C:450:LEU:HD12	1.91	0.52
1:C:287:ASP:O	1:C:292:ASN:ND2	2.43	0.52
1:A:147:TYR:OH	1:A:231:ARG:NH1	2.42	0.51
1:A:461:ASP:O	1:A:463:ASP:N	2.42	0.51
1:A:328:ARG:NH1	1:A:366:GLU:OE2	2.44	0.51
1:C:203:GLU:HG3	1:C:308:PHE:HB2	1.91	0.51
1:A:200:ALA:O	1:A:204:VAL:HG23	2.11	0.50
1:C:286:CYS:O	1:C:323:GLN:HA	2.12	0.50
1:A:260:ASN:HA	1:A:263:ARG:NH1	2.27	0.50
1:C:458:ARG:HH12	1:C:466:THR:HG22	1.75	0.50
1:A:153:GLU:OE2	1:A:231:ARG:NH1	2.42	0.50
1:B:352:VAL:O	1:B:356:THR:HG22	2.11	0.50
1:C:429:VAL:HG22	1:C:453:LYS:HE2	1.94	0.49
1:C:257:VAL:O	1:C:261:LEU:HB3	2.11	0.49
1:A:417:PRO:HG2	1:A:420:THR:HG21	1.94	0.49
1:B:286:CYS:HB2	1:B:310:SER:O	2.12	0.49
1:C:193:LYS:O	1:C:195:ALA:N	2.41	0.49
1:A:386:ASP:OD1	1:A:397:LYS:NZ	2.37	0.49
1:A:392:ARG:O	1:A:406:LYS:NZ	2.46	0.49
1:A:461:ASP:C	1:A:463:ASP:H	2.20	0.49
1:C:198:ASN:OD1	1:C:199:GLN:N	2.46	0.49
1:A:451:LYS:NZ	1:A:477:SER:O	2.40	0.48
1:A:242:SER:O	1:A:294:LEU:HD22	2.13	0.48
1:B:140:TYR:O	1:B:148:ILE:HG22	2.13	0.48
1:A:429:VAL:HG13	1:A:430:GLU:H	1.78	0.48
1:A:323:GLN:NE2	1:A:346:SER:OG	2.45	0.48
1:B:458:ARG:NH2	1:B:466:THR:O	2.47	0.48
1:C:257:VAL:HB	1:C:261:LEU:HD23	1.96	0.48
1:A:323:GLN:OE1	1:A:342:ILE:HB	2.14	0.48
1:A:433:GLY:HA3	1:A:438:ARG:HB2	1.96	0.47
1:A:393:LYS:C	1:A:406:LYS:HZ1	2.20	0.47
1:B:323:GLN:NE2	1:B:346:SER:OG	2.48	0.47
1:C:361:PHE:CE1	1:C:373:ILE:HA	2.49	0.47
1:B:200:ALA:O	1:B:204:VAL:HG23	2.15	0.47
1:B:209:LEU:HD22	1:B:281:LEU:HB3	1.96	0.47
1:A:319:TYR:O	1:A:338:TYR:OH	2.31	0.47
1:B:338:TYR:HB2	1:B:342:ILE:HG21	1.96	0.47
1:C:146:ASP:OD1	1:C:191:LYS:NZ	2.48	0.47
1:A:257:VAL:HB	1:A:261:LEU:HD23	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLU:OE1	1:A:467:ARG:NH1	2.48	0.46
1:B:435:GLY:HA2	1:C:435:GLY:HA2	1.96	0.46
1:C:192:ASN:OD1	1:C:232:ASN:HB3	2.14	0.46
1:C:268:GLN:OE1	1:C:303:ILE:HG12	2.14	0.46
1:C:429:VAL:HG12	1:C:446:VAL:HG13	1.96	0.46
1:C:359:PRO:O	1:C:361:PHE:N	2.45	0.46
1:C:458:ARG:NH1	1:C:466:THR:O	2.49	0.46
1:B:366:GLU:OE1	1:B:393:LYS:NZ	2.46	0.46
1:B:290:PRO:HD3	1:B:350:ILE:HG12	1.99	0.45
1:B:416:LYS:HD2	1:B:421:ARG:HB2	1.98	0.45
1:A:268:GLN:HE22	1:A:302:ALA:HA	1.82	0.45
1:B:374:VAL:HG21	1:B:405:LEU:HD11	1.99	0.45
1:B:361:PHE:CE1	1:B:373:ILE:HA	2.52	0.45
1:A:292:ASN:O	1:A:306:VAL:HG22	2.18	0.44
1:A:314:LEU:HD12	1:A:340:LEU:HD13	2.00	0.44
1:C:170:PHE:CD1	1:C:188:LYS:HE3	2.52	0.44
1:C:290:PRO:HD2	1:C:327:TYR:CE2	2.52	0.44
1:C:461:ASP:O	1:C:467:ARG:NH2	2.48	0.44
1:B:219:TYR:O	1:B:304:LYS:HE2	2.18	0.44
1:B:365:ASN:O	1:B:369:GLN:N	2.47	0.44
1:A:286:CYS:HB2	1:A:310:SER:O	2.18	0.44
1:C:268:GLN:OE1	1:C:303:ILE:N	2.45	0.43
1:C:285:HIS:HD2	1:C:305:ILE:HG21	1.82	0.43
1:C:438:ARG:HG3	1:C:449:TYR:OH	2.18	0.43
1:A:178:ASP:OD2	1:A:226:ARG:NH2	2.51	0.43
1:A:429:VAL:HG13	1:A:430:GLU:N	2.32	0.43
1:C:338:TYR:HB2	1:C:342:ILE:HG21	2.01	0.43
1:A:170:PHE:CD1	1:A:188:LYS:HE3	2.53	0.43
1:A:468:ILE:HD11	1:A:473:ALA:HA	2.00	0.43
1:B:417:PRO:HG2	1:B:420:THR:HG21	2.00	0.43
1:B:336:MET:HG2	1:B:388:ALA:HA	2.00	0.43
1:C:449:TYR:O	1:C:453:LYS:NZ	2.44	0.43
1:B:423:LEU:HD22	1:B:427:LEU:HG	2.01	0.42
1:A:204:VAL:HG13	1:A:224:LEU:HD21	2.01	0.42
1:B:433:GLY:HA3	1:B:438:ARG:HB2	2.01	0.42
1:C:192:ASN:O	1:C:192:ASN:ND2	2.52	0.42
1:C:200:ALA:O	1:C:204:VAL:HG23	2.19	0.42
1:C:427:LEU:HA	1:C:427:LEU:HD23	1.78	0.42
1:B:148:ILE:O	1:B:148:ILE:HG23	2.20	0.42
1:B:414:GLU:CD	1:C:325:ARG:HH22	2.27	0.42
1:C:449:TYR:C	1:C:453:LYS:HZ3	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:HD22	1:A:281:LEU:HD23	2.02	0.42
1:A:360:LEU:HD22	1:A:361:PHE:CZ	2.54	0.42
1:B:292:ASN:O	1:B:306:VAL:HG22	2.20	0.41
1:C:381:PRO:HD2	1:C:384:ILE:HD12	2.01	0.41
1:B:187:ILE:HG12	1:B:237:VAL:HG22	2.01	0.41
1:B:321:PTR:P	1:B:328:ARG:HH22	2.43	0.41
1:B:374:VAL:HG12	1:B:380:PRO:HD3	2.01	0.41
1:C:285:HIS:NE2	1:C:307:ASP:O	2.54	0.41
1:A:137:ASN:C	1:A:137:ASN:HD22	2.29	0.41
1:A:322:ILE:HD13	1:A:338:TYR:CZ	2.56	0.41
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.84	0.40
1:A:361:PHE:CE1	1:A:373:ILE:HA	2.56	0.40
1:B:179:ARG:HA	1:B:179:ARG:HD3	1.81	0.40
1:B:323:GLN:OE1	1:B:342:ILE:HB	2.22	0.40
1:C:208:GLU:O	1:C:212:LYS:HG2	2.21	0.40
1:B:352:VAL:HB	1:B:360:LEU:HD12	2.04	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	340/361 (94%)	308 (91%)	28 (8%)	4 (1%)	10	40
1	B	331/361 (92%)	307 (93%)	22 (7%)	2 (1%)	21	52
1	C	287/361 (80%)	263 (92%)	22 (8%)	2 (1%)	18	50
All	All	958/1083 (88%)	878 (92%)	72 (8%)	8 (1%)	16	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	282	SER

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Mol	Chain	Res	Type
1	A	462	TYR
1	C	194	LYS
1	C	195	ALA
1	A	156	MET
1	B	323	GLN
1	A	157	ASP
1	A	301	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/320 (96%)	305 (100%)	1 (0%)	86	83
1	B	299/320 (93%)	299 (100%)	0	100	100
1	C	271/320 (85%)	271 (100%)	0	100	100
All	All	876/960 (91%)	875 (100%)	1 (0%)	88	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	151	ASN
1	A	192	ASN
1	A	260	ASN
1	A	268	GLN
1	A	285	HIS
1	A	371	ASN
1	A	475	GLN
1	B	172	GLN

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Mol	Chain	Res	Type
1	B	192	ASN
1	B	260	ASN
1	B	316	GLN
1	B	371	ASN
1	C	424	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	PTR	B	321	1	15,16,17	1.30	1 (6%)	17,22,24	0.56	0
1	PTR	C	321	1	15,16,17	1.34	1 (6%)	17,22,24	0.54	0
1	PTR	A	321	1	15,16,17	1.29	1 (6%)	17,22,24	0.64	1 (5%)

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	PTR	B	321	1	-	1/10/11/13	0/1/1/1
1	PTR	C	321	1	-	0/10/11/13	0/1/1/1
1	PTR	A	321	1	-	0/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	321	PTR	OH-CZ	-4.38	1.30	1.40
1	B	321	PTR	OH-CZ	-4.21	1.31	1.40
1	A	321	PTR	OH-CZ	-4.12	1.31	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	PTR	O3P-P-OH	2.20	111.81	105.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	321	PTR	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	321	PTR	1	0
1	A	321	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	Q8J	A	501	-	36,36,36	0.21	0	44,50,50	1.09	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Q8J	B	501	-	36,36,36	0.16	0	44,50,50	1.08	4 (9%)
2	Q8J	C	501	-	36,36,36	0.21	0	44,50,50	0.98	2 (4%)

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	Q8J	A	501	-	-	7/18/36/36	1/5/5/5
2	Q8J	B	501	-	-	7/18/36/36	0/5/5/5
2	Q8J	C	501	-	-	5/18/36/36	1/5/5/5

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	Q8J	C20-C19-C23	-3.84	117.24	120.68
2	B	501	Q8J	C20-C19-C23	-3.80	117.27	120.68
2	A	501	Q8J	C20-C19-C23	-3.63	117.42	120.68
2	A	501	Q8J	C23-C12-C13	-3.62	104.13	106.02
2	B	501	Q8J	C23-C12-C13	-3.32	104.29	106.02
2	A	501	Q8J	C12-C13-N4	2.99	111.79	110.54
2	B	501	Q8J	C12-C13-N4	2.96	111.78	110.54
2	C	501	Q8J	C23-C12-C13	-2.72	104.61	106.02
2	B	501	Q8J	C23-C12-C9	2.54	131.21	126.62
2	A	501	Q8J	C19-C23-C12	2.19	108.09	106.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	Q8J	O-C6-N1-C4
2	B	501	Q8J	N2-C6-N1-C4
2	A	501	Q8J	C15-C14-N4-C13
2	A	501	Q8J	C18-C14-N4-C13
2	C	501	Q8J	C15-C14-N4-C13
2	C	501	Q8J	C18-C14-N4-C13
2	A	501	Q8J	C18-C14-N4-C19
2	B	501	Q8J	C18-C14-N4-C19

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Mol	Chain	Res	Type	Atoms
2	C	501	Q8J	C18-C14-N4-C19
2	B	501	Q8J	C15-C14-N4-C13
2	B	501	Q8J	C18-C14-N4-C13
2	C	501	Q8J	C23-C12-C9-C10
2	C	501	Q8J	C23-C12-C9-C8
2	B	501	Q8J	C23-C12-C9-C8
2	A	501	Q8J	N2-C6-N1-C4
2	A	501	Q8J	C23-C12-C9-C10
2	A	501	Q8J	C23-C12-C9-C8
2	B	501	Q8J	C23-C12-C9-C10
2	A	501	Q8J	N3-C7-N2-C6

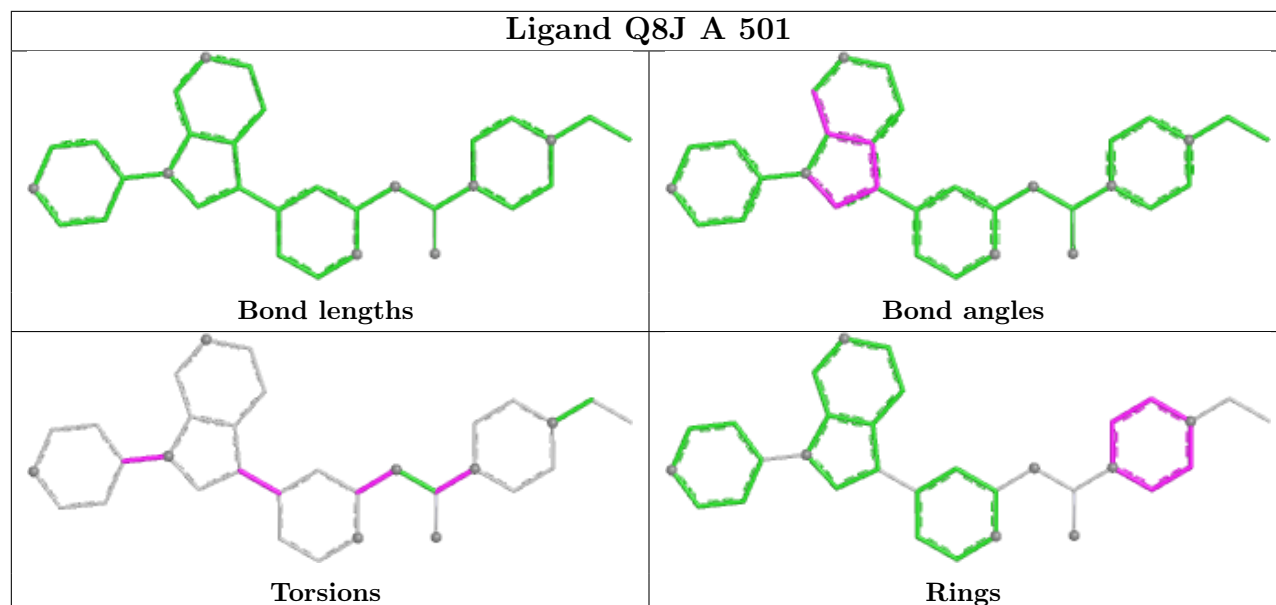
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	Q8J	C2-C3-C4-C5-N-N1
2	A	501	Q8J	C2-C3-C4-C5-N-N1

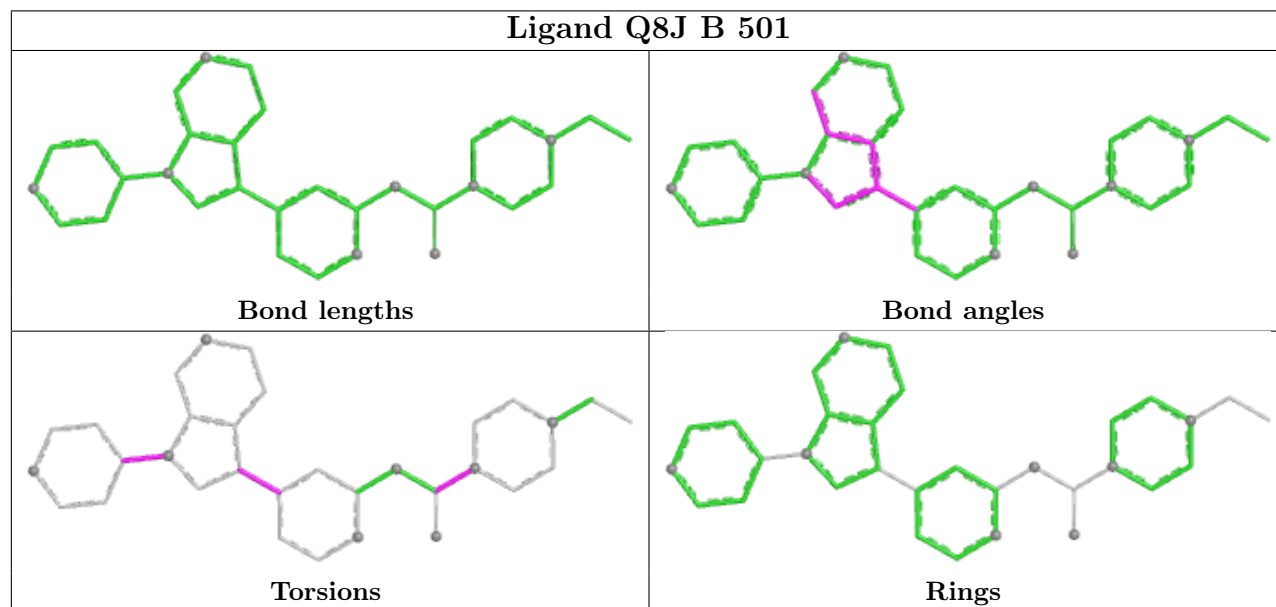
No monomer is involved in short contacts.

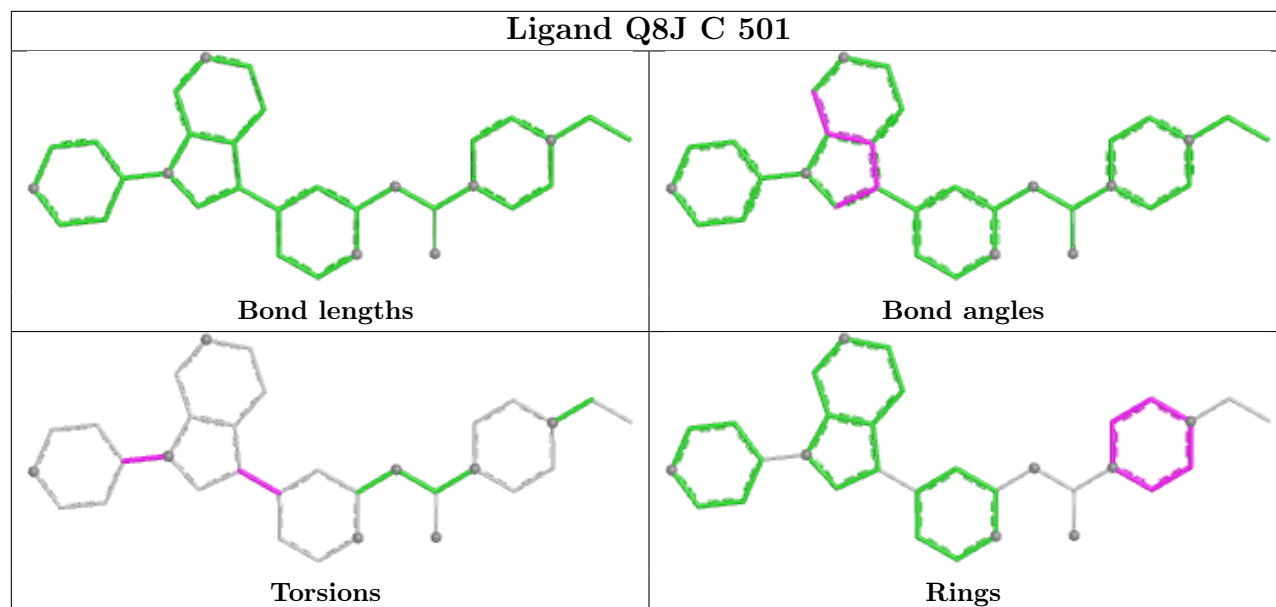
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 Q8J A 501



Ligand Q8J B 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

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	344/361 (95%)	0.78	30 (8%)	16 14	12, 30, 43, 61	0
1	B	337/361 (93%)	0.99	32 (9%)	14 13	34, 46, 60, 76	0
1	C	305/361 (84%)	1.59	77 (25%)	1 2	51, 70, 81, 87	0
All	All	986/1083 (91%)	1.10	139 (14%)	6 8	12, 45, 76, 87	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	TYR	6.7
1	C	309	GLY	5.6
1	C	132	GLU	5.2
1	C	408	THR	4.9
1	C	194	LYS	4.7
1	A	132	GLU	4.6
1	C	223	HIS	4.5
1	A	214	ASP	4.4
1	C	213	HIS	4.3
1	C	430	GLU	4.1
1	C	142	ASP	4.0
1	C	320	GLN	4.0
1	B	223	HIS	3.9
1	C	453	LYS	3.9
1	C	448	ASP	3.8
1	A	408	THR	3.8
1	B	470	PRO	3.7
1	C	283	ILE	3.7
1	B	422	LYS	3.7
1	B	430	GLU	3.6
1	C	471	TYR	3.6
1	B	424	HIS	3.5
1	C	260	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	213	HIS	3.4
1	B	432	GLY	3.3
1	B	399	PRO	3.3
1	B	211	ASN	3.3
1	A	448	ASP	3.2
1	C	406	LYS	3.2
1	C	277	ALA	3.1
1	A	217	MET	3.0
1	A	445	THR	3.0
1	B	420	THR	3.0
1	C	305	ILE	3.0
1	A	461	ASP	3.0
1	C	286	CYS	3.0
1	C	413	ARG	3.0
1	A	407	LYS	2.9
1	C	133	ARG	2.9
1	A	322	ILE	2.9
1	B	408	THR	2.9
1	C	264	LYS	2.9
1	C	358	GLU	2.9
1	B	440	GLY	2.8
1	C	197	LEU	2.8
1	C	322	ILE	2.8
1	C	472	TYR	2.8
1	C	451	LYS	2.8
1	B	301	SER	2.8
1	C	261	LEU	2.8
1	C	424	HIS	2.8
1	C	195	ALA	2.8
1	B	157	ASP	2.7
1	B	477	SER	2.7
1	C	267	GLN	2.7
1	B	136	TYR	2.7
1	C	337	PRO	2.6
1	C	454	ASP	2.6
1	A	306	VAL	2.6
1	C	455	LEU	2.6
1	A	271	THR	2.6
1	C	184	TRP	2.6
1	C	362	SER	2.6
1	C	226	ARG	2.6
1	B	238	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	138	ASP	2.5
1	C	131	LYS	2.5
1	C	383	HIS	2.5
1	C	324	SER	2.5
1	B	442	SER	2.5
1	A	215	THR	2.5
1	C	349	CYS	2.4
1	C	397	LYS	2.4
1	B	382	ALA	2.4
1	B	445	THR	2.4
1	C	262	THR	2.4
1	A	424	HIS	2.4
1	C	336	MET	2.4
1	C	276	LEU	2.4
1	C	419	GLY	2.4
1	C	402	THR	2.4
1	C	466	THR	2.4
1	C	386	ASP	2.4
1	A	420	THR	2.3
1	C	289	LYS	2.3
1	C	464	PRO	2.3
1	C	437	ARG	2.3
1	C	452	PHE	2.3
1	A	442	SER	2.3
1	B	144	ASN	2.3
1	C	169	SER	2.3
1	C	279	PRO	2.3
1	C	420	THR	2.2
1	B	199	GLN	2.2
1	B	198	ASN	2.2
1	C	381	PRO	2.2
1	A	319	TYR	2.2
1	C	139	GLY	2.2
1	C	470	PRO	2.2
1	A	251	ASN	2.2
1	A	219	TYR	2.2
1	B	319	TYR	2.2
1	A	255	ARG	2.1
1	B	296	CYS	2.1
1	C	477	SER	2.1
1	B	237	VAL	2.1
1	C	212	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	156	MET	2.1
1	A	400	ASP	2.1
1	B	400	ASP	2.1
1	C	364	ALA	2.1
1	C	434	PRO	2.1
1	C	210	MET	2.1
1	C	447	ALA	2.1
1	A	253	ASN	2.1
1	A	318	ILE	2.1
1	B	306	VAL	2.1
1	A	431	THR	2.1
1	A	323	GLN	2.1
1	C	365	ASN	2.1
1	C	446	VAL	2.1
1	B	217	MET	2.1
1	C	270	CYS	2.1
1	A	260	ASN	2.1
1	C	344	MET	2.1
1	A	300	ARG	2.0
1	C	263	ARG	2.0
1	A	218	LYS	2.0
1	C	414	GLU	2.0
1	C	204	VAL	2.0
1	C	429	VAL	2.0
1	A	139	GLY	2.0
1	B	154	LYS	2.0
1	C	278	THR	2.0
1	A	211	ASN	2.0
1	B	425	ASN	2.0
1	C	296	CYS	2.0
1	B	218	LYS	2.0
1	C	167	LYS	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	PTR	C	321	16/17	0.85	0.17	61,64,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PTR	B	321	16/17	0.93	0.14	34,34,35,36	0
1	PTR	A	321	16/17	0.93	0.14	19,21,25,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

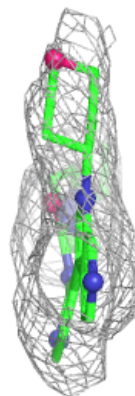
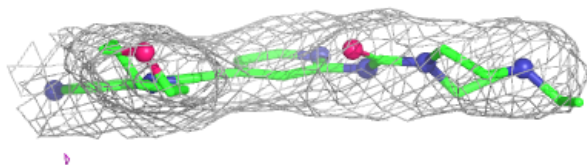
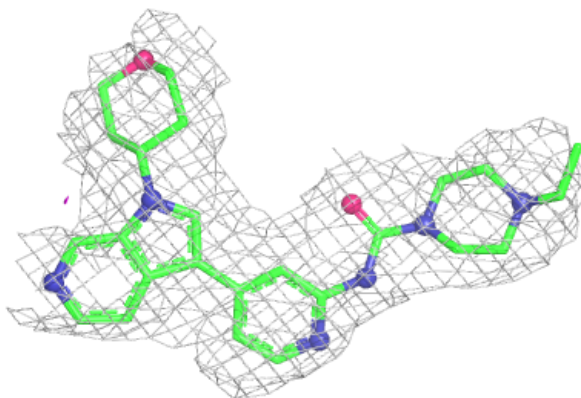
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	Q8J	C	501	32/32	0.91	0.16	64,67,70,70	0
2	Q8J	B	501	32/32	0.92	0.16	39,42,43,44	0
2	Q8J	A	501	32/32	0.95	0.14	20,25,27,27	0

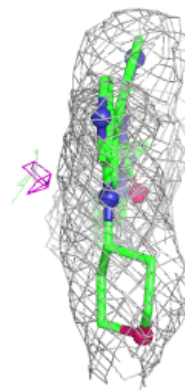
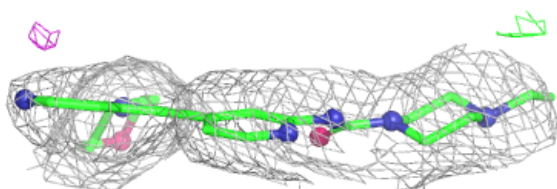
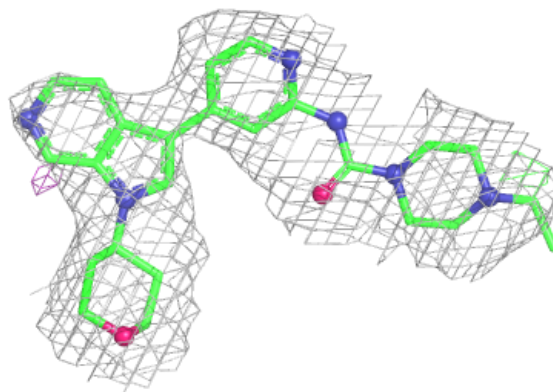
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Q8J C 501:

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

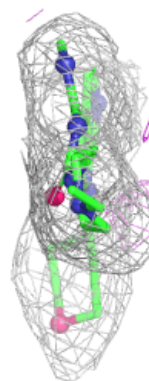
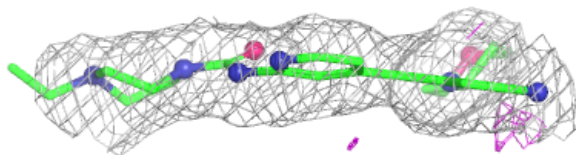
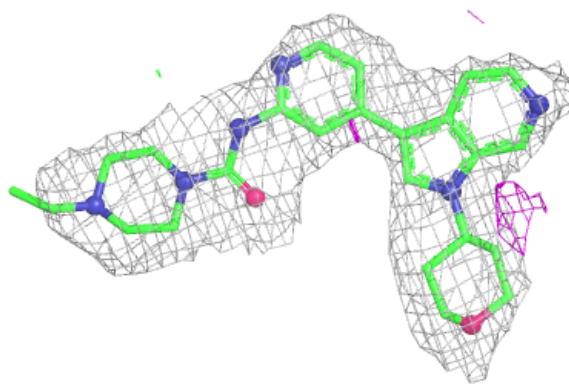
**Electron density around Q8J B 501:**

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



Electron density around Q8J A 501:

$2mF_o-DF_c$ (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.