



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:42 PM UTC

PDB ID : 6EIS / pdb_00006eis
Title : DYRK1A in complex with JWC-055
Authors : Rothweiler, U.
Deposited on : 2017-09-19
Resolution : 2.36 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

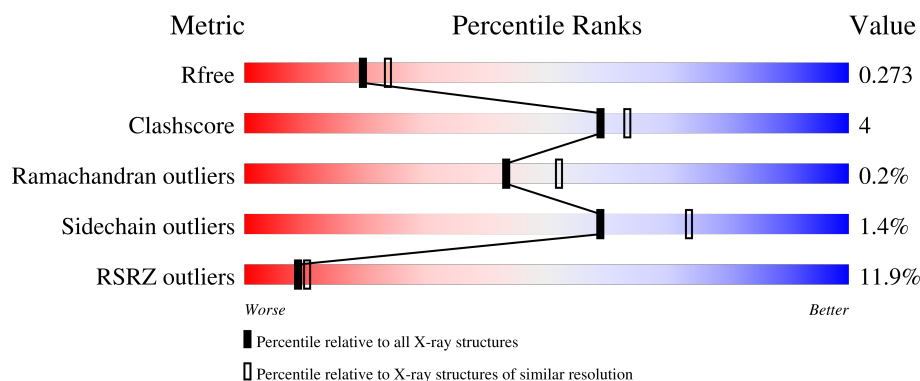
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	368	
1	B	368	
1	C	368	
1	D	368	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11510 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.

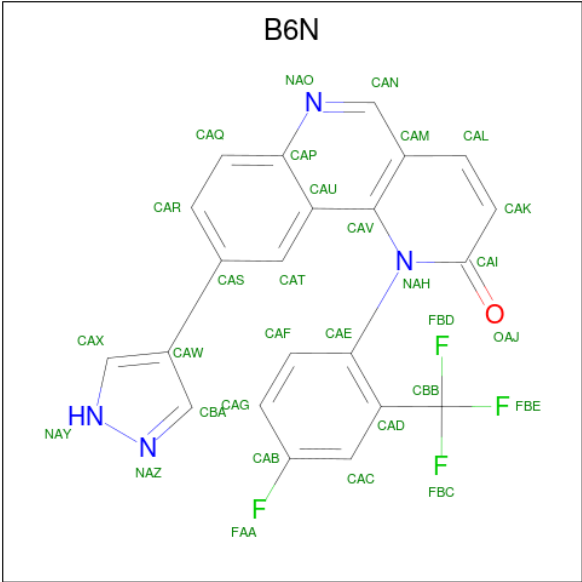
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	P	S	0	0	0
			2795	1799	476	502	1	17			
1	B	340	Total	C	N	O	P	S	0	1	0
			2759	1775	470	495	1	18			
1	C	341	Total	C	N	O	P	S	0	0	0
			2736	1759	463	496	1	17			
1	D	339	Total	C	N	O	P	S	0	0	0
			2757	1777	467	495	1	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLY	-	expression tag	UNP Q13627
A	124	ALA	-	expression tag	UNP Q13627
A	125	SER	-	expression tag	UNP Q13627
B	123	GLY	-	expression tag	UNP Q13627
B	124	ALA	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
C	123	GLY	-	expression tag	UNP Q13627
C	124	ALA	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
D	123	GLY	-	expression tag	UNP Q13627
D	124	ALA	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627

- Molecule 2 is 1-[4-fluoranyl-2-(trifluoromethyl)phenyl]-9-(1 {H}-pyrazol-4-yl)benzo[h][1,6]naphthyridin-2-one (CCD ID: B6N) (formula: C₂₂H₁₂F₄N₄O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			31	22	4	4	1		
2	B	1	Total	C	F	N	O	0	0
			31	22	4	4	1		
2	C	1	Total	C	F	N	O	0	0
			31	22	4	4	1		
2	D	1	Total	C	F	N	O	0	0
			31	22	4	4	1		

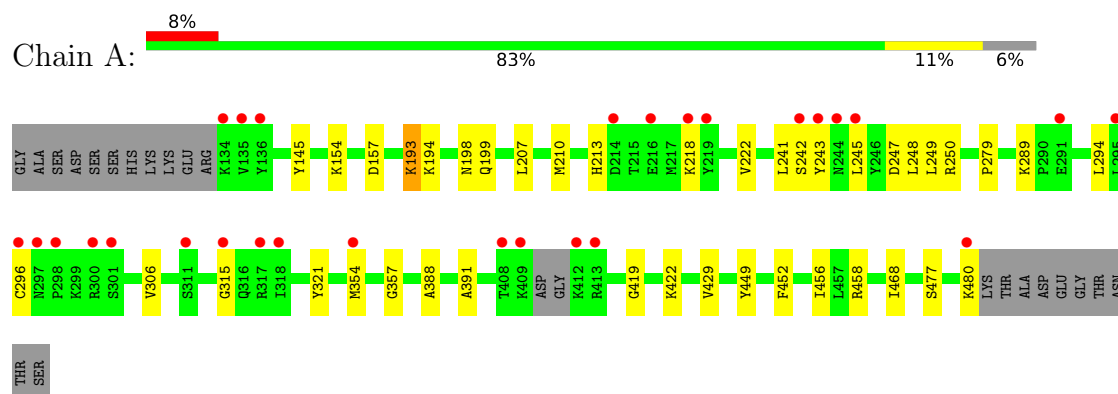
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total	O	0	0
			130	130		
3	B	61	Total	O	0	0
			61	61		
3	C	59	Total	O	0	0
			59	59		
3	D	89	Total	O	0	0
			89	89		

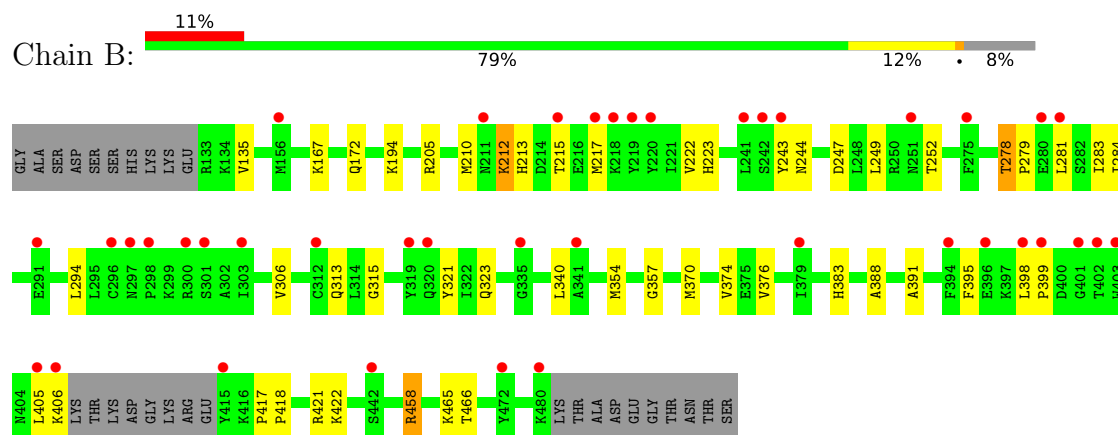
3 Residue-property plots

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.

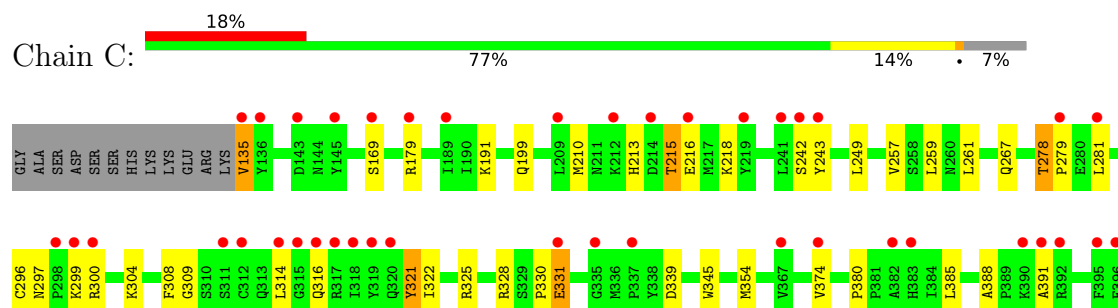
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

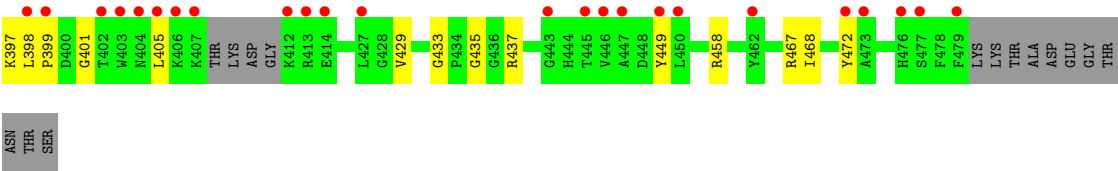


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

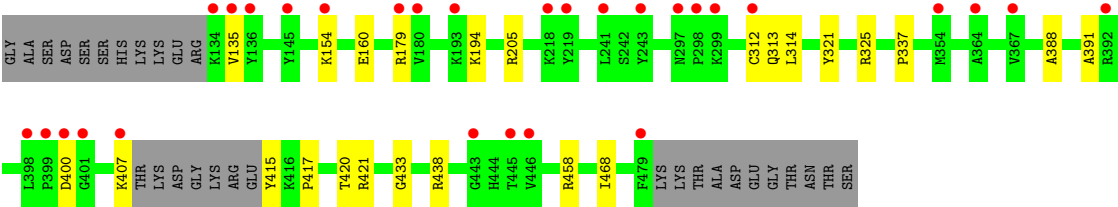
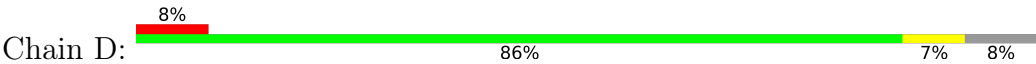


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.48Å 89.05Å 230.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.37 – 2.36 48.37 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.37-2.36) 99.8 (48.37-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.221 , 0.262 (Not available) , 0.273	Depositor DCC
R_{free} test set	3757 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11510	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: PTR, B6N

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	0.25	0/2843	0.70	0/3838
1	B	0.26	0/2806	0.71	2/3788 (0.1%)
1	C	0.27	0/2783	0.72	5/3765 (0.1%)
1	D	0.25	0/2805	0.68	0/3786
All	All	0.26	0/11237	0.70	7/15177 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	THR	N-CA-C	5.92	117.97	110.33
1	C	398	LEU	CA-C-N	5.52	126.74	119.84
1	C	398	LEU	C-N-CA	5.52	126.74	119.84
1	C	278	THR	CA-C-N	5.12	124.56	119.24
1	C	278	THR	C-N-CA	5.12	124.56	119.24
1	B	278	THR	CA-C-N	5.12	126.23	119.84
1	B	278	THR	C-N-CA	5.12	126.23	119.84

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	2795	0	2767	25	0
1	B	2759	0	2732	26	0
1	C	2736	0	2670	36	0
1	D	2757	0	2739	13	0
2	A	31	0	0	1	0
2	B	31	0	0	1	0
2	C	31	0	0	1	0
2	D	31	0	0	1	0
3	A	130	0	0	1	0
3	B	61	0	0	0	0
3	C	59	0	0	1	0
3	D	89	0	0	2	0
All	All	11510	0	10908	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ASN:HB3	1:C:300:ARG:HB3	1.58	0.85
1:B:222:VAL:HG21	1:B:306:VAL:HG12	1.66	0.77
1:C:374:VAL:HG21	1:C:405:LEU:HD12	1.71	0.72
1:A:279:PRO:HG3	1:D:337:PRO:HG3	1.71	0.70
1:C:199:GLN:HE22	1:D:194:LYS:HD3	1.61	0.66
1:C:296:CYS:SG	1:C:304:LYS:NZ	2.70	0.64
1:C:429:VAL:HA	1:C:449:TYR:HD2	1.61	0.64
1:A:419:GLY:O	1:A:422:LYS:NZ	2.29	0.64
1:B:388:ALA:HB3	1:B:391:ALA:HB2	1.80	0.63
1:B:217:MET:HG3	1:B:223:HIS:HB2	1.81	0.63
1:C:278:THR:HB	1:C:281:LEU:HD12	1.81	0.62
1:C:322:ILE:O	1:C:328:ARG:NH1	2.32	0.61
1:B:458:ARG:NH2	1:B:466:THR:O	2.32	0.61
1:B:205:ARG:NH2	1:B:313:GLN:OE1	2.30	0.61
1:D:154:LYS:HZ2	1:D:160:GLU:HB2	1.65	0.60
1:C:199:GLN:NE2	1:C:309:GLY:O	2.35	0.60
1:C:213:HIS:O	1:C:218:LYS:NZ	2.35	0.59
1:B:281:LEU:O	1:C:316:GLN:NE2	2.36	0.58
1:A:222:VAL:HG11	1:A:306:VAL:HG12	1.85	0.58
1:A:207:LEU:HA	1:A:210:MET:HE3	1.86	0.57
1:A:241:LEU:HD22	1:A:296:CYS:HA	1.86	0.57
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:GLU:OE2	1:C:467:ARG:NH1	2.36	0.57
1:D:388:ALA:HB3	1:D:391:ALA:HB2	1.87	0.56
1:B:398:LEU:HB3	1:B:399:PRO:HD2	1.88	0.55
1:C:380:PRO:HB2	1:C:385:LEU:HD11	1.89	0.55
1:C:242:SER:OG	1:C:243:TYR:N	2.40	0.54
1:B:406:LYS:C	1:B:406:LYS:HD2	2.33	0.53
1:A:247:ASP:OD1	1:A:250:ARG:NH2	2.42	0.53
1:B:167:LYS:HG2	1:B:172:GLN:HG2	1.90	0.53
1:B:249:LEU:HD21	1:B:354:MET:HA	1.90	0.53
1:C:458:ARG:HB3	1:C:468:ILE:HB	1.92	0.51
2:C:501:B6N:CAT	2:C:501:B6N:CAE	2.89	0.50
2:D:501:B6N:CAT	2:D:501:B6N:CAE	2.89	0.50
1:A:388:ALA:HB3	1:A:391:ALA:HB2	1.93	0.50
1:A:289:LYS:NZ	3:A:608:HOH:O	2.43	0.49
2:B:501:B6N:CAE	2:B:501:B6N:CAT	2.90	0.49
1:B:212:LYS:HG2	1:B:213:HIS:ND1	2.27	0.49
1:C:429:VAL:HA	1:C:449:TYR:CD2	2.46	0.49
1:C:135:VAL:O	1:D:325:ARG:NH2	2.46	0.49
1:C:429:VAL:HG22	1:C:449:TYR:HB3	1.94	0.48
1:B:374:VAL:HG21	1:B:405:LEU:HD21	1.95	0.48
1:C:435:GLY:HA3	1:C:437:ARG:NH1	2.28	0.48
1:A:477:SER:HA	1:A:480:LYS:HD2	1.95	0.48
2:A:501:B6N:CAT	2:A:501:B6N:CAE	2.91	0.48
1:C:433:GLY:HA2	1:C:449:TYR:HE2	1.77	0.48
1:B:370:MET:HE2	1:B:395:PHE:HZ	1.78	0.47
1:B:284:ILE:HG12	1:B:340:LEU:HG	1.97	0.46
1:D:415:TYR:N	3:D:604:HOH:O	2.49	0.46
1:B:167:LYS:HE2	1:B:172:GLN:HG2	1.98	0.46
1:C:257:VAL:HB	1:C:261:LEU:HD23	1.98	0.45
1:A:429:VAL:HG22	1:A:449:TYR:HB3	1.99	0.45
1:C:135:VAL:N	3:C:607:HOH:O	2.48	0.45
1:C:215:THR:OG1	1:C:216:GLU:N	2.50	0.45
1:A:452:PHE:O	1:A:456:ILE:HG12	2.17	0.45
1:A:241:LEU:HD12	1:A:294:LEU:HD12	1.97	0.45
1:A:245:LEU:HD21	1:A:354:MET:SD	2.57	0.44
1:D:433:GLY:HA3	1:D:438:ARG:HB2	1.98	0.44
1:A:243:TYR:HD1	1:A:247:ASP:HB2	1.82	0.44
1:B:376:VAL:HA	1:B:421:ARG:O	2.18	0.44
1:C:249:LEU:HD21	1:C:354:MET:HA	1.99	0.44
1:B:383:HIS:O	1:C:472:TYR:OH	2.36	0.44
1:D:179:ARG:HE	1:D:179:ARG:HB2	1.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:PRO:HA	1:B:418:PRO:HD3	1.80	0.43
1:A:243:TYR:HE1	1:A:248:LEU:HB2	1.82	0.43
1:C:330:PRO:HD3	1:C:345:TRP:CE2	2.53	0.43
1:A:145:TYR:CZ	1:A:193:LYS:HE3	2.54	0.43
1:A:249:LEU:HD22	1:A:357:GLY:HA2	2.01	0.43
1:B:278:THR:HA	1:B:279:PRO:HD2	1.86	0.43
1:C:397:LYS:HE3	1:C:401:GLY:HA2	2.00	0.43
1:C:210:MET:HE1	1:C:308:PHE:CE2	2.54	0.43
1:D:421:ARG:NH1	3:D:607:HOH:O	2.51	0.43
1:A:218:LYS:HB3	1:A:218:LYS:HE3	1.81	0.42
1:A:315:GLY:HA2	1:D:314:LEU:O	2.19	0.42
1:C:259:LEU:HD22	1:C:449:TYR:CE1	2.54	0.42
1:A:154:LYS:NZ	1:A:157:ASP:HA	2.35	0.42
1:C:321:PTR:O3P	1:C:325:ARG:NH1	2.52	0.42
1:A:194:LYS:HG3	1:A:198:ASN:ND2	2.35	0.42
1:B:243:TYR:HB3	1:B:247:ASP:HB2	2.00	0.42
1:B:249:LEU:O	1:B:252:THR:OG1	2.33	0.42
1:D:205:ARG:NH2	1:D:313:GLN:OE1	2.52	0.42
1:C:169:SER:O	1:C:191:LYS:HE2	2.20	0.42
1:C:405:LEU:HA	1:C:405:LEU:HD23	1.78	0.41
1:D:417:PRO:HD2	1:D:420:THR:HG21	2.02	0.41
1:A:213:HIS:O	1:A:218:LYS:HE2	2.19	0.41
1:B:244:ASN:HA	1:B:294:LEU:HA	2.03	0.41
1:A:458:ARG:HB3	1:A:468:ILE:HB	2.01	0.41
1:B:315:GLY:HA2	1:C:314:LEU:O	2.19	0.41
1:C:374:VAL:HG21	1:C:405:LEU:CD1	2.45	0.41
1:A:199:GLN:HE22	1:B:194:LYS:HE2	1.85	0.41
1:C:339:ASP:N	1:C:339:ASP:OD1	2.54	0.41
1:C:278:THR:HA	1:C:279:PRO:HD3	1.97	0.41
1:A:243:TYR:CD1	1:A:247:ASP:HB2	2.55	0.41
1:D:458:ARG:HB3	1:D:468:ILE:HB	2.02	0.41
1:B:210:MET:HE2	1:B:283:ILE:HD13	2.02	0.40
1:B:249:LEU:HD22	1:B:357:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/368 (92%)	328 (96%)	11 (3%)	1 (0%)	36	43
1	B	336/368 (91%)	320 (95%)	15 (4%)	1 (0%)	36	43
1	C	336/368 (91%)	313 (93%)	22 (6%)	1 (0%)	36	43
1	D	334/368 (91%)	320 (96%)	14 (4%)	0	100	100
All	All	1346/1472 (91%)	1281 (95%)	62 (5%)	3 (0%)	43	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	SER
1	C	399	PRO
1	B	323	GLN

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	298/324 (92%)	297 (100%)	1 (0%)	86	92
1	B	295/324 (91%)	289 (98%)	6 (2%)	48	63
1	C	289/324 (89%)	284 (98%)	5 (2%)	53	68
1	D	296/324 (91%)	292 (99%)	4 (1%)	59	73
All	All	1178/1296 (91%)	1162 (99%)	16 (1%)	59	73

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	LYS
1	B	135	VAL
1	B	212	LYS
1	B	215	THR
1	B	422	LYS
1	B	458	ARG
1	B	465	LYS
1	C	135	VAL
1	C	179	ARG
1	C	267	GLN
1	C	299	LYS
1	C	331	GLU
1	D	135	VAL
1	D	312	CYS
1	D	400	ASP
1	D	407	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	C	199	GLN
1	D	223	HIS
1	D	323	GLN
1	D	371	ASN
1	D	387	GLN

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	PTR	C	321	1	15,16,17	1.33	1 (6%)	17,22,24	0.50	0
1	PTR	D	321	1	15,16,17	1.34	1 (6%)	17,22,24	0.43	0
1	PTR	B	321	1	15,16,17	1.34	1 (6%)	17,22,24	0.50	0
1	PTR	A	321	1	15,16,17	1.31	1 (6%)	17,22,24	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	C	321	1	-	0/10/11/13	0/1/1/1
1	PTR	D	321	1	-	1/10/11/13	0/1/1/1
1	PTR	B	321	1	-	0/10/11/13	0/1/1/1
1	PTR	A	321	1	-	1/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	321	PTR	OH-CZ	-4.47	1.30	1.40
1	B	321	PTR	OH-CZ	-4.47	1.30	1.40
1	C	321	PTR	OH-CZ	-4.42	1.30	1.40
1	A	321	PTR	OH-CZ	-4.32	1.31	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	321	PTR	CZ-OH-P-O1P
1	D	321	PTR	CZ-OH-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	321	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	B6N	A	501	-	34,35,35	2.77	12 (35%)	47,53,53	2.02	16 (34%)
2	B6N	D	501	-	34,35,35	2.79	12 (35%)	47,53,53	2.11	18 (38%)
2	B6N	B	501	-	34,35,35	2.78	12 (35%)	47,53,53	2.02	18 (38%)
2	B6N	C	501	-	34,35,35	2.76	11 (32%)	47,53,53	2.10	18 (38%)

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	B6N	A	501	-	-	0/14/14/14	0/5/5/5
2	B6N	D	501	-	-	0/14/14/14	0/5/5/5
2	B6N	B	501	-	-	0/14/14/14	0/5/5/5
2	B6N	C	501	-	-	0/14/14/14	0/5/5/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	B6N	CAE-NAH	-9.00	1.35	1.44
2	A	501	B6N	CAE-NAH	-8.94	1.35	1.44
2	C	501	B6N	CAE-NAH	-8.88	1.35	1.44
2	B	501	B6N	CAE-NAH	-8.82	1.35	1.44
2	D	501	B6N	CAS-CAW	-7.73	1.33	1.48
2	B	501	B6N	CAS-CAW	-7.69	1.33	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	B6N	CAS-CAW	-7.64	1.33	1.48
2	C	501	B6N	CAS-CAW	-7.61	1.33	1.48
2	B	501	B6N	CBB-CAD	-4.77	1.40	1.50
2	C	501	B6N	CBB-CAD	-4.65	1.40	1.50
2	A	501	B6N	CBB-CAD	-4.65	1.40	1.50
2	D	501	B6N	CBB-CAD	-4.62	1.40	1.50
2	D	501	B6N	NAY-NAZ	-4.38	1.24	1.35
2	B	501	B6N	CAN-NAO	4.30	1.39	1.31
2	C	501	B6N	CAN-NAO	4.26	1.39	1.31
2	D	501	B6N	CAN-NAO	4.21	1.38	1.31
2	A	501	B6N	CAN-NAO	4.20	1.38	1.31
2	B	501	B6N	NAY-NAZ	-4.18	1.24	1.35
2	C	501	B6N	NAY-NAZ	-4.14	1.25	1.35
2	A	501	B6N	NAY-NAZ	-4.06	1.25	1.35
2	B	501	B6N	CBA-CAW	-3.63	1.32	1.40
2	D	501	B6N	CBA-CAW	-3.63	1.32	1.40
2	C	501	B6N	CBA-CAW	-3.59	1.32	1.40
2	A	501	B6N	CBA-CAW	-3.58	1.32	1.40
2	A	501	B6N	CAV-NAH	-3.55	1.38	1.41
2	B	501	B6N	CAV-NAH	-3.55	1.38	1.41
2	D	501	B6N	CAV-NAH	-3.45	1.38	1.41
2	C	501	B6N	CAV-NAH	-3.45	1.38	1.41
2	B	501	B6N	CAX-CAW	-3.36	1.32	1.38
2	A	501	B6N	CAX-CAW	-3.31	1.32	1.38
2	D	501	B6N	CAX-CAW	-3.30	1.32	1.38
2	C	501	B6N	CAX-CAW	-3.25	1.32	1.38
2	D	501	B6N	CAM-CAL	-2.63	1.39	1.44
2	C	501	B6N	CAM-CAL	-2.62	1.39	1.44
2	B	501	B6N	CAM-CAL	-2.59	1.39	1.44
2	A	501	B6N	CAM-CAL	-2.59	1.39	1.44
2	C	501	B6N	CAK-CAL	2.20	1.38	1.34
2	A	501	B6N	CAP-NAO	-2.16	1.33	1.37
2	B	501	B6N	CAP-NAO	-2.15	1.33	1.37
2	D	501	B6N	CAK-CAL	2.12	1.38	1.34
2	D	501	B6N	CAP-NAO	-2.11	1.33	1.37
2	A	501	B6N	CAK-CAL	2.10	1.38	1.34
2	B	501	B6N	CAK-CAL	2.07	1.38	1.34
2	D	501	B6N	CAK-CAI	-2.06	1.38	1.43
2	A	501	B6N	CAK-CAI	-2.06	1.38	1.43
2	C	501	B6N	CAP-NAO	-2.02	1.34	1.37
2	B	501	B6N	CAK-CAI	-2.01	1.38	1.43

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	B6N	CAD-CAE-NAH	-6.35	119.82	123.34
2	C	501	B6N	CAD-CAE-NAH	-6.08	119.97	123.34
2	A	501	B6N	CAD-CAE-NAH	-4.67	120.75	123.34
2	D	501	B6N	CAM-CAV-CAU	-4.50	116.23	121.06
2	B	501	B6N	CAM-CAV-CAU	-4.42	116.31	121.06
2	A	501	B6N	CAM-CAV-CAU	-4.38	116.36	121.06
2	C	501	B6N	CAM-CAV-CAU	-4.35	116.39	121.06
2	B	501	B6N	CAD-CAE-NAH	-4.34	120.94	123.34
2	A	501	B6N	CAK-CAI-NAH	4.27	122.34	114.02
2	B	501	B6N	CAK-CAI-NAH	4.25	122.29	114.02
2	C	501	B6N	CAK-CAI-NAH	4.19	122.19	114.02
2	D	501	B6N	CAK-CAI-NAH	4.19	122.19	114.02
2	A	501	B6N	CAN-CAM-CAL	-4.03	116.41	122.91
2	B	501	B6N	CAN-CAM-CAL	-3.93	116.57	122.91
2	D	501	B6N	CAN-CAM-CAL	-3.89	116.64	122.91
2	C	501	B6N	CAN-CAM-CAL	-3.78	116.82	122.91
2	A	501	B6N	CAM-CAN-NAO	-3.05	120.17	124.14
2	B	501	B6N	CAM-CAN-NAO	-3.05	120.18	124.14
2	D	501	B6N	CAU-CAV-NAH	3.01	126.77	120.73
2	C	501	B6N	CAT-CAU-CAP	-2.99	115.47	118.99
2	A	501	B6N	CAU-CAV-NAH	2.99	126.72	120.73
2	D	501	B6N	CAT-CAU-CAP	-2.96	115.50	118.99
2	B	501	B6N	CAU-CAV-NAH	2.95	126.65	120.73
2	C	501	B6N	CAM-CAN-NAO	-2.94	120.32	124.14
2	B	501	B6N	CAT-CAU-CAP	-2.90	115.58	118.99
2	D	501	B6N	CAM-CAN-NAO	-2.89	120.38	124.14
2	A	501	B6N	CAT-CAU-CAP	-2.89	115.58	118.99
2	C	501	B6N	CAU-CAV-NAH	2.88	126.51	120.73
2	C	501	B6N	CAN-NAO-CAP	2.70	120.08	116.96
2	B	501	B6N	CAN-NAO-CAP	2.68	120.06	116.96
2	A	501	B6N	CAN-NAO-CAP	2.67	120.05	116.96
2	B	501	B6N	CAW-CBA-NAZ	-2.66	105.70	110.83
2	D	501	B6N	CAW-CBA-NAZ	-2.65	105.71	110.83
2	C	501	B6N	CAW-CBA-NAZ	-2.65	105.72	110.83
2	A	501	B6N	CAW-CBA-NAZ	-2.58	105.84	110.83
2	B	501	B6N	CAG-CAB-CAC	-2.58	119.83	123.23
2	C	501	B6N	CAG-CAB-CAC	-2.52	119.91	123.23
2	D	501	B6N	CAN-NAO-CAP	2.51	119.87	116.96
2	A	501	B6N	CAG-CAB-CAC	-2.50	119.94	123.23
2	D	501	B6N	CAG-CAB-CAC	-2.47	119.97	123.23
2	D	501	B6N	CAV-CAU-CAP	2.44	120.29	115.74
2	C	501	B6N	CAV-CAU-CAP	2.42	120.25	115.74
2	B	501	B6N	CAV-CAU-CAP	2.39	120.20	115.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	B6N	CAX-CAW-CBA	2.38	108.81	104.00
2	C	501	B6N	CAS-CAT-CAU	2.36	123.80	121.15
2	C	501	B6N	CAX-CAW-CBA	2.35	108.76	104.00
2	A	501	B6N	CAX-CAW-CBA	2.35	108.75	104.00
2	D	501	B6N	CAX-CAW-CBA	2.31	108.67	104.00
2	B	501	B6N	CAD-CAC-CAB	2.30	120.48	117.50
2	A	501	B6N	CAD-CAC-CAB	2.28	120.45	117.50
2	D	501	B6N	CAS-CAT-CAU	2.25	123.68	121.15
2	A	501	B6N	CAV-CAU-CAP	2.24	119.92	115.74
2	C	501	B6N	CAD-CAC-CAB	2.20	120.35	117.50
2	D	501	B6N	CBA-NAZ-NAY	2.19	110.03	105.75
2	B	501	B6N	CAS-CAT-CAU	2.18	123.61	121.15
2	D	501	B6N	CAD-CAC-CAB	2.18	120.33	117.50
2	A	501	B6N	CAQ-CAP-CAU	2.17	121.47	119.13
2	C	501	B6N	CBA-NAZ-NAY	2.16	109.97	105.75
2	B	501	B6N	CBA-NAZ-NAY	2.11	109.88	105.75
2	B	501	B6N	FBD-CBB-CAD	-2.11	108.91	112.65
2	D	501	B6N	CAQ-CAP-CAU	2.09	121.38	119.13
2	C	501	B6N	CAQ-CAR-CAS	-2.06	118.33	120.78
2	A	501	B6N	CBA-NAZ-NAY	2.06	109.78	105.75
2	C	501	B6N	CAQ-CAP-CAU	2.06	121.35	119.13
2	B	501	B6N	OAJ-CAI-CAK	-2.05	118.53	124.35
2	D	501	B6N	CAQ-CAR-CAS	-2.04	118.36	120.78
2	B	501	B6N	CAQ-CAP-CAU	2.03	121.32	119.13
2	A	501	B6N	FBD-CBB-CAD	-2.03	109.05	112.65
2	C	501	B6N	FBE-CBB-CAD	-2.03	109.06	112.65
2	D	501	B6N	FBD-CBB-CAD	-2.03	109.06	112.65

There are no chirality outliers.

There are no torsion outliers.

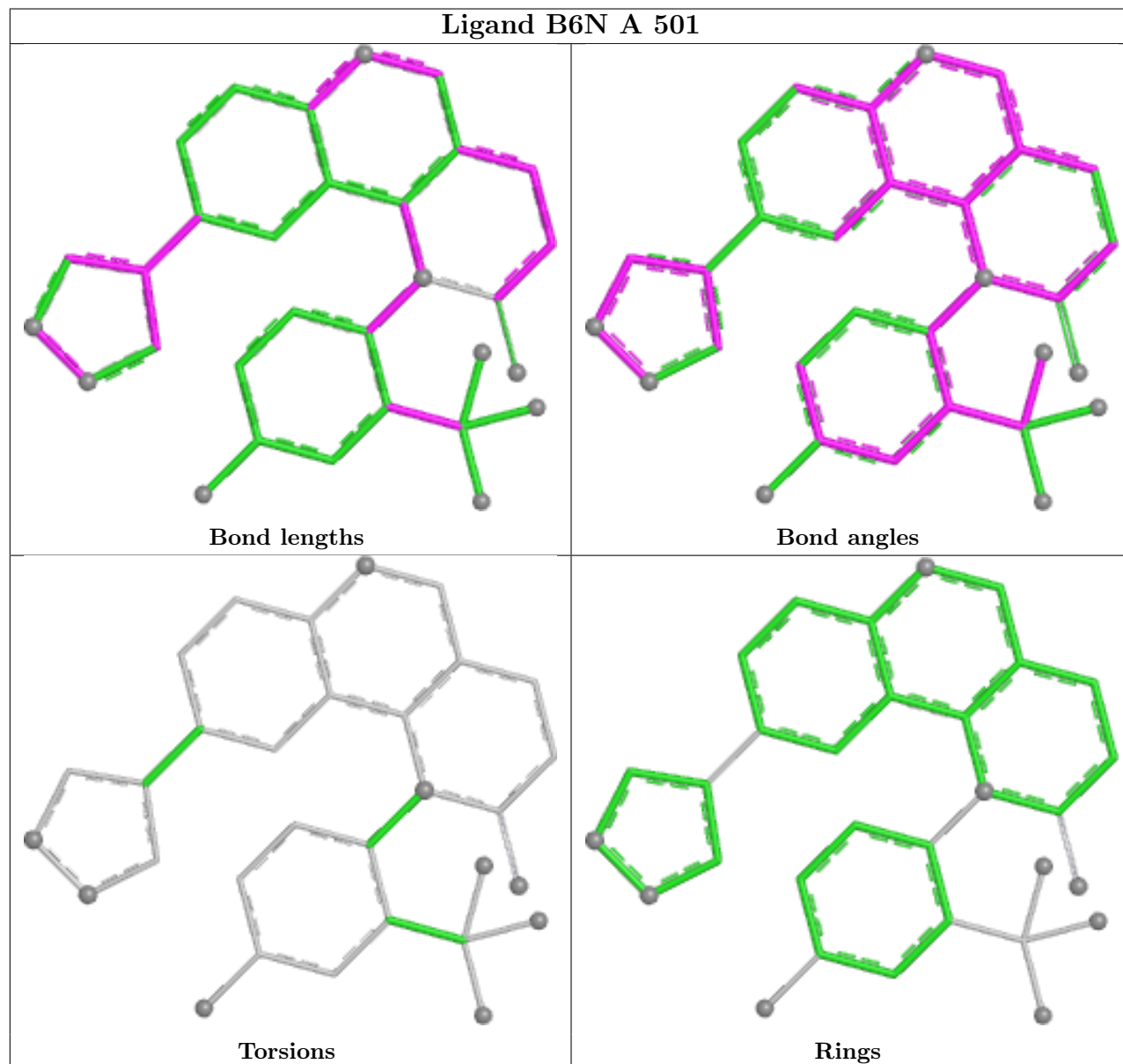
There are no ring outliers.

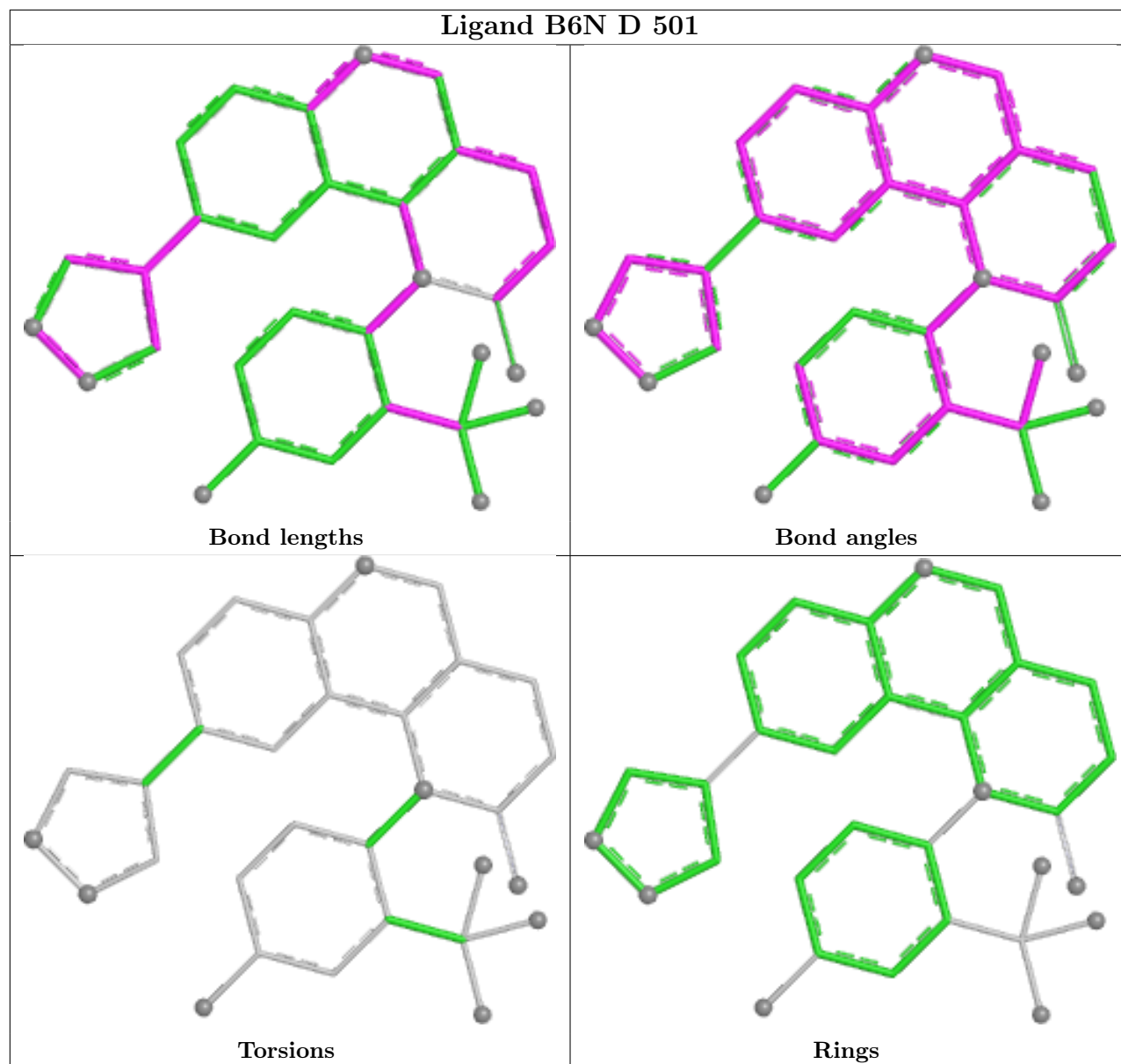
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	B6N	1	0
2	D	501	B6N	1	0
2	B	501	B6N	1	0
2	C	501	B6N	1	0

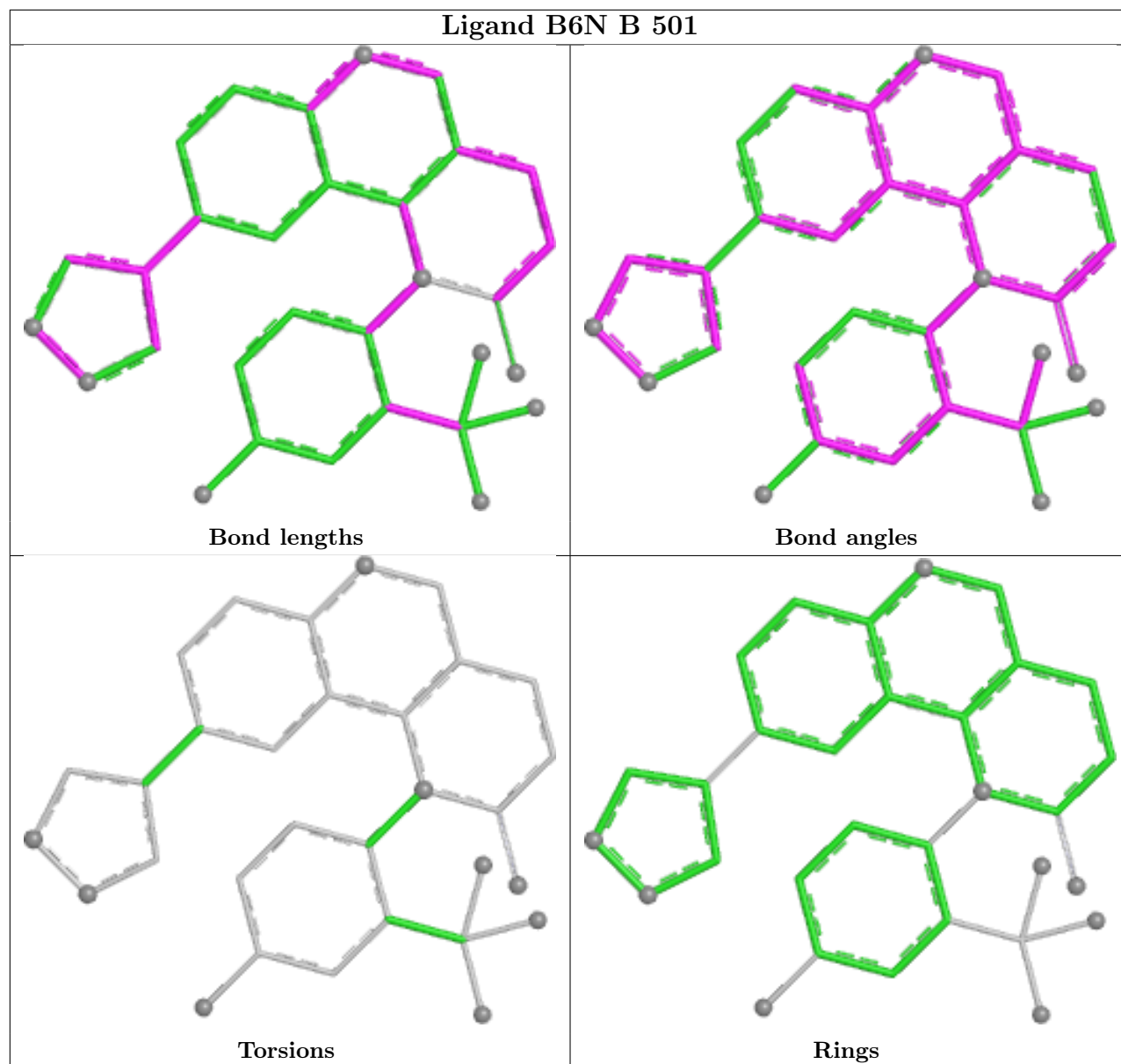
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

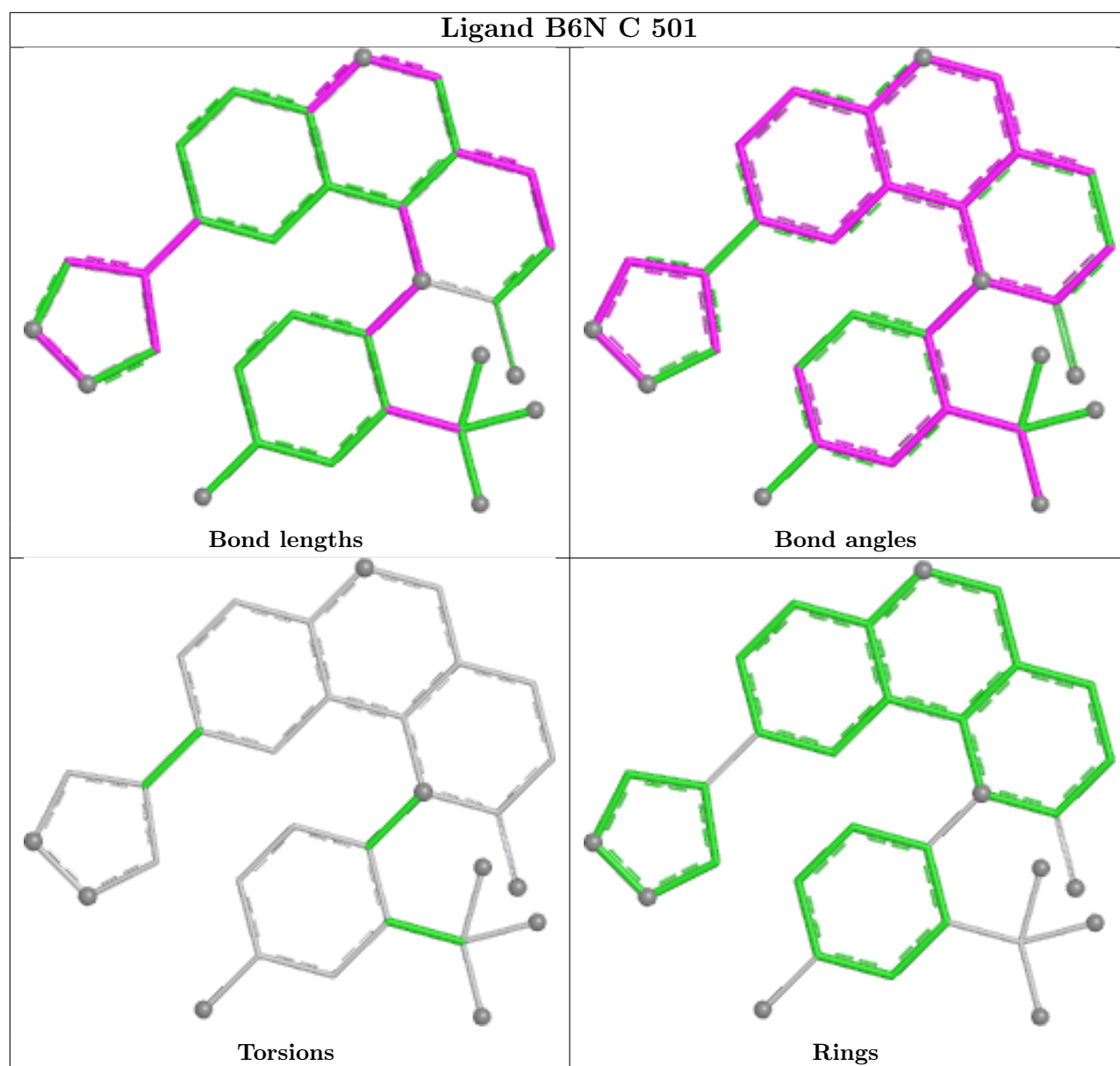
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand B6N 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	344/368 (93%)	0.53	28 (8%) 18 20	29, 44, 72, 94	0
1	B	339/368 (92%)	0.97	40 (11%) 9 10	31, 61, 88, 105	1 (0%)
1	C	340/368 (92%)	1.22	65 (19%) 3 3	39, 64, 94, 103	0
1	D	338/368 (91%)	0.70	29 (8%) 16 18	32, 54, 81, 92	0
All	All	1361/1472 (92%)	0.85	162 (11%) 9 10	29, 55, 88, 105	1 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	TYR	6.5
1	C	135	VAL	5.3
1	A	219	TYR	5.2
1	B	243	TYR	5.1
1	B	415	TYR	5.0
1	C	405	LEU	4.8
1	A	409	LYS	4.8
1	B	406	LYS	4.8
1	C	407	LYS	4.7
1	C	243	TYR	4.5
1	B	312[A]	CYS	4.3
1	C	320	GLN	4.3
1	A	296	CYS	4.2
1	A	300	ARG	4.2
1	B	219	TYR	4.1
1	B	472	TYR	4.1
1	C	445	THR	4.1
1	C	412	LYS	4.1
1	D	135	VAL	4.1
1	D	243	TYR	4.0
1	B	398	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	449	TYR	4.0
1	C	316	GLN	3.9
1	A	297	ASN	3.9
1	B	217	MET	3.9
1	C	398	LEU	3.8
1	D	398	LEU	3.8
1	A	408	THR	3.7
1	C	136	TYR	3.7
1	C	145	TYR	3.6
1	C	242	SER	3.6
1	A	412	LYS	3.6
1	D	399	PRO	3.5
1	B	215	THR	3.5
1	C	404	ASN	3.5
1	C	472	TYR	3.4
1	D	145	TYR	3.4
1	D	154	LYS	3.3
1	A	295	LEU	3.3
1	C	318	ILE	3.3
1	B	319	TYR	3.3
1	B	405	LEU	3.2
1	C	406	LYS	3.2
1	A	354	MET	3.2
1	C	143	ASP	3.2
1	D	136	TYR	3.2
1	D	134	LYS	3.1
1	A	318	ILE	3.1
1	C	317	ARG	3.1
1	B	218	LYS	3.1
1	C	298	PRO	3.1
1	A	135	VAL	3.1
1	B	399	PRO	3.1
1	A	136	TYR	3.0
1	A	214	ASP	3.0
1	B	241	LEU	3.0
1	B	401	GLY	3.0
1	C	216	GLU	3.0
1	D	407	LYS	2.9
1	C	447	ALA	2.9
1	C	392	ARG	2.9
1	B	301	SER	2.9
1	C	413	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	476	HIS	2.9
1	C	395	PHE	2.9
1	A	242	SER	2.8
1	C	367	VAL	2.8
1	B	403	TRP	2.8
1	C	314	LEU	2.8
1	C	179	ARG	2.8
1	D	312	CYS	2.8
1	A	480	LYS	2.8
1	C	299	LYS	2.8
1	D	479	PHE	2.8
1	A	291	GLU	2.7
1	A	245	LEU	2.7
1	C	209	LEU	2.7
1	D	179	ARG	2.7
1	B	251	ASN	2.7
1	A	216	GLU	2.7
1	D	445	THR	2.7
1	B	280	GLU	2.7
1	C	279	PRO	2.7
1	C	414	GLU	2.7
1	B	480	LYS	2.7
1	C	189	ILE	2.7
1	C	281	LEU	2.7
1	C	396	GLU	2.6
1	C	214	ASP	2.6
1	A	298	PRO	2.6
1	B	281	LEU	2.6
1	D	241	LEU	2.6
1	A	315	GLY	2.6
1	B	242	SER	2.6
1	C	311	SER	2.6
1	C	315	GLY	2.5
1	D	193	LYS	2.5
1	A	301	SER	2.5
1	D	219	TYR	2.5
1	C	450	LEU	2.5
1	B	296	CYS	2.5
1	D	392	ARG	2.5
1	D	354	MET	2.5
1	A	317	ARG	2.4
1	C	402	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	394	PHE	2.4
1	C	399	PRO	2.4
1	D	298	PRO	2.4
1	B	211	ASN	2.3
1	C	319	TYR	2.3
1	B	335	GLY	2.3
1	C	446	VAL	2.3
1	B	396	GLU	2.3
1	A	244	ASN	2.3
1	D	443	GLY	2.3
1	C	443	GLY	2.3
1	B	300	ARG	2.3
1	B	303	ILE	2.3
1	B	379	ILE	2.3
1	C	374	VAL	2.3
1	A	134	LYS	2.3
1	C	312	CYS	2.3
1	B	156	MET	2.3
1	A	311	SER	2.3
1	C	477	SER	2.3
1	C	331	GLU	2.3
1	D	299	LYS	2.3
1	B	341	ALA	2.2
1	D	364	ALA	2.2
1	B	402	THR	2.2
1	C	169	SER	2.2
1	D	297	ASN	2.2
1	C	382	ALA	2.2
1	C	462	TYR	2.2
1	B	275	PHE	2.2
1	C	391	ALA	2.2
1	C	403	TRP	2.2
1	C	241	LEU	2.2
1	B	291	GLU	2.2
1	A	413	ARG	2.1
1	B	297	ASN	2.1
1	D	400	ASP	2.1
1	C	337	PRO	2.1
1	C	479	PHE	2.1
1	C	473	ALA	2.1
1	C	300	ARG	2.1
1	C	219	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	218	LYS	2.1
1	C	383	HIS	2.1
1	B	442	SER	2.1
1	D	218	LYS	2.1
1	C	427	LEU	2.1
1	B	298	PRO	2.1
1	D	401	GLY	2.1
1	C	212	LYS	2.1
1	C	390	LYS	2.1
1	B	320	GLN	2.1
1	D	180	VAL	2.1
1	B	220	TYR	2.0
1	D	367	VAL	2.0
1	D	446	VAL	2.0
1	C	335	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PTR	C	321	16/17	0.92	0.12	50,56,65,67	0
1	PTR	B	321	16/17	0.95	0.09	46,51,58,62	0
1	PTR	A	321	16/17	0.95	0.09	34,37,45,51	0
1	PTR	D	321	16/17	0.96	0.07	32,37,58,62	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

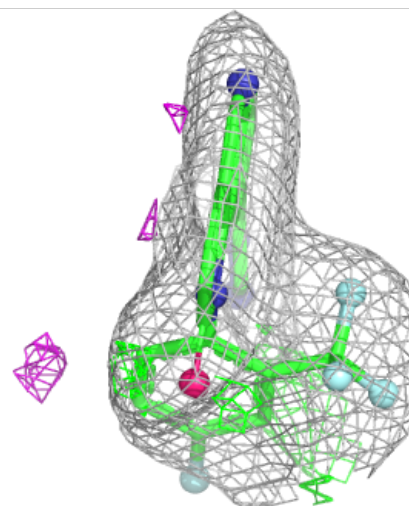
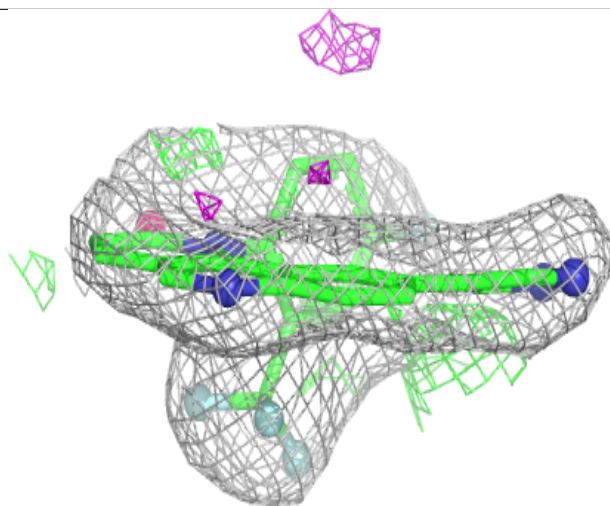
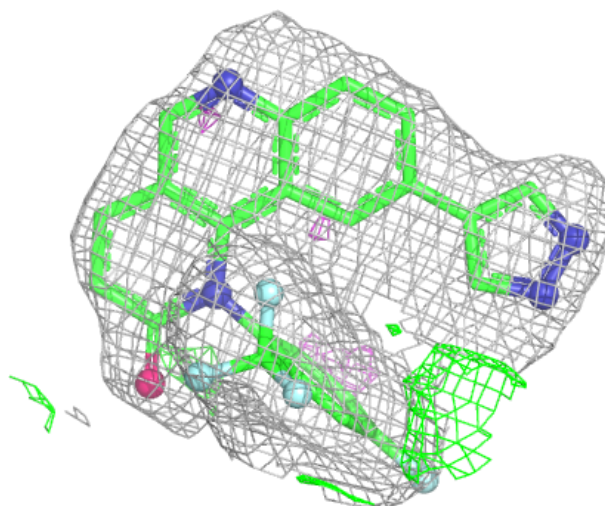
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B6N	B	501	31/31	0.82	0.16	60,73,79,91	0
2	B6N	C	501	31/31	0.89	0.12	43,52,63,68	0
2	B6N	A	501	31/31	0.90	0.11	42,49,55,59	0
2	B6N	D	501	31/31	0.93	0.10	42,55,64,66	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.

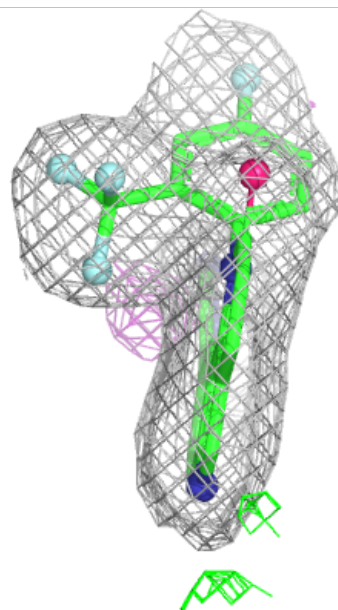
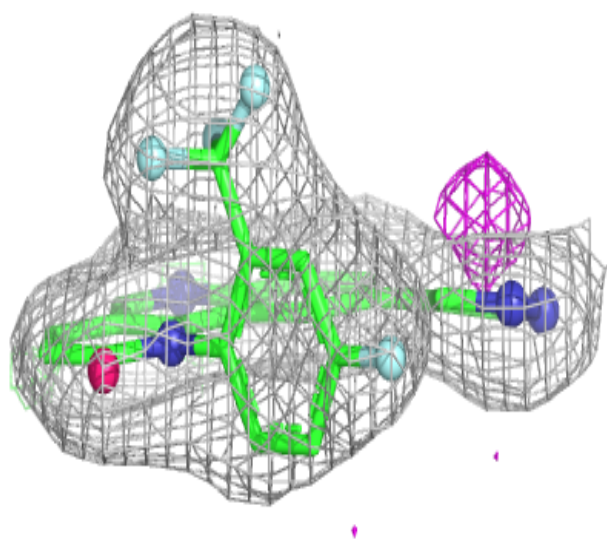
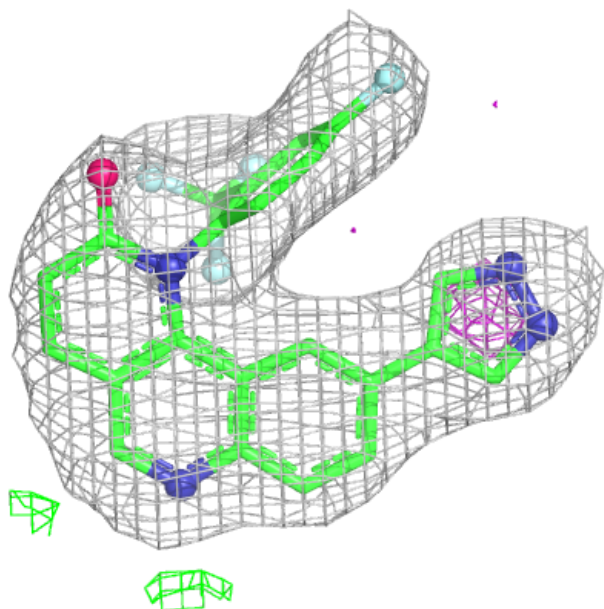
Electron density around B6N B 501:

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



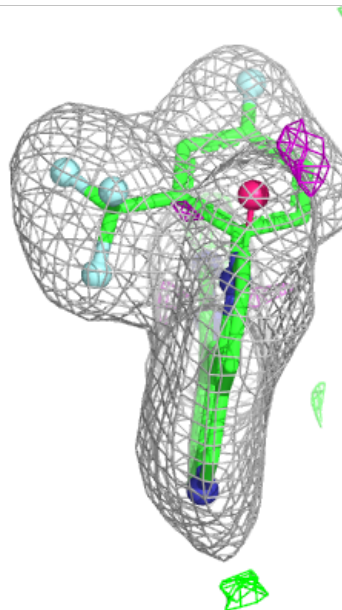
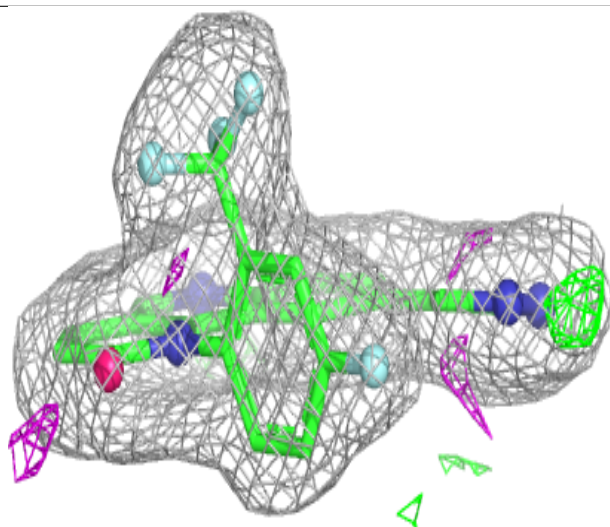
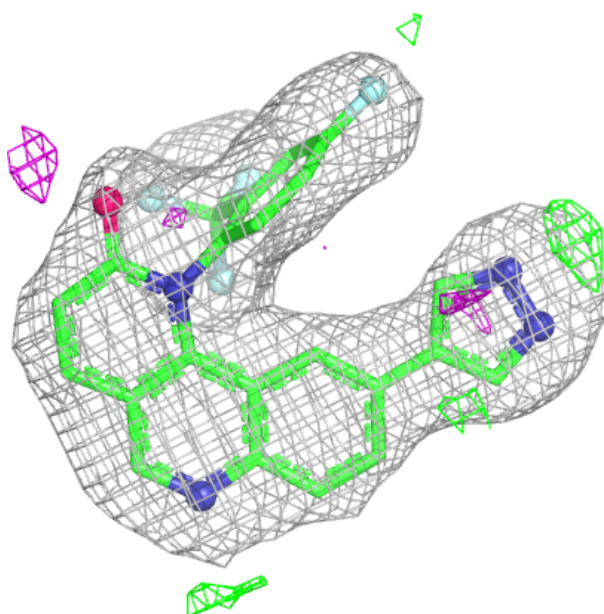
Electron density around B6N C 501:

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



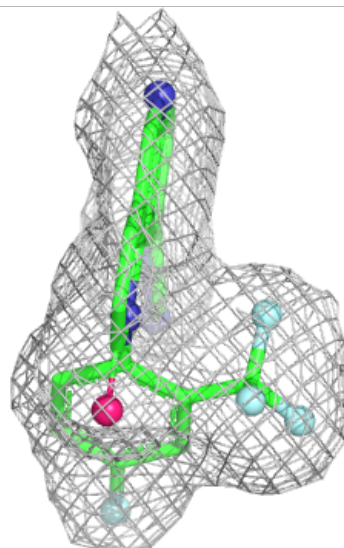
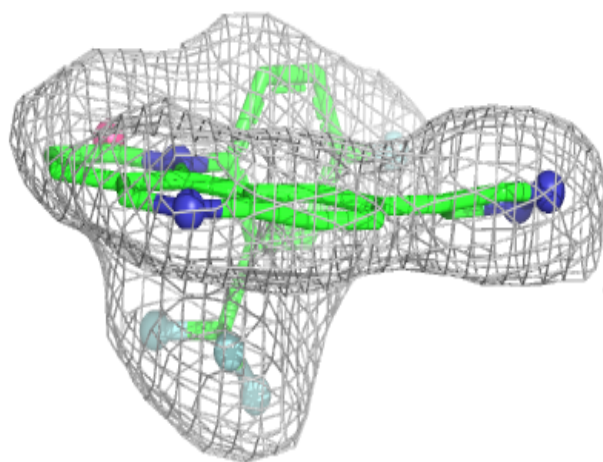
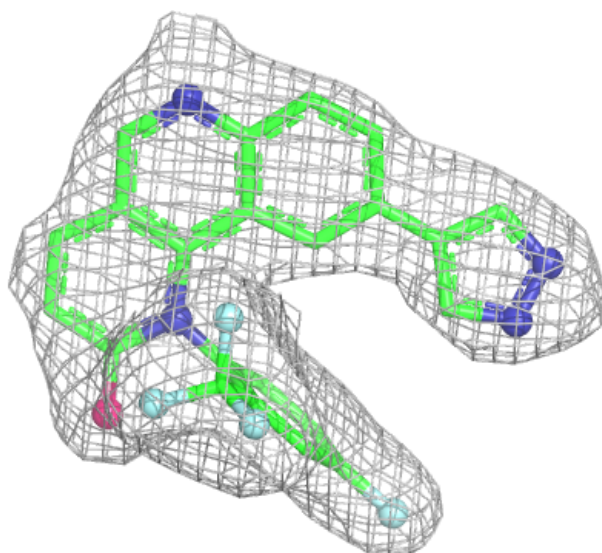
Electron density around B6N A 501:

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



Electron density around B6N D 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.