



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:13 PM EDT

PDB ID : 6YQ1 / pdb_00006yq1
Title : FOCAL ADHESION KINASE CATALYTIC DOMAIN IN COMPLEX WITH
N-Methyl-N-(3-{[2-(2-oxo-1,2,3,4-tetrahydro-quinolin-6-ylamino)-5-trifluoromethyl-pyrimidin-4-ylamino]-methyl}-pyridin-2-yl)-methanesulfonamide
Authors : Musil, D.; Heinrich, T.; Amaral, M.
Deposited on : 2020-04-16
Resolution : 1.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

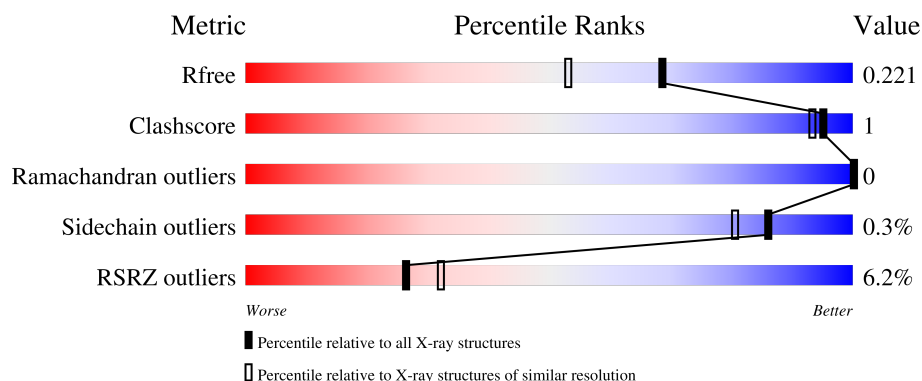
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	282	5% 93% 5%
1	B	282	5% 92% 5%
1	C	282	5% 90% 6%
1	D	282	9% 87% 5% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9732 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.

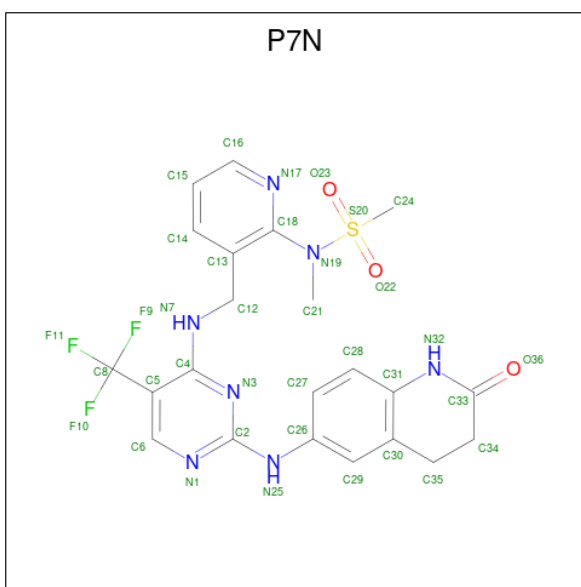
- Molecule 1 is a protein called Focal adhesion kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	7	0
			2225	1416	383	408	18			
1	B	274	Total	C	N	O	S	0	4	0
			2228	1419	384	407	18			
1	C	264	Total	C	N	O	S	0	1	0
			2134	1361	371	384	18			
1	D	258	Total	C	N	O	S	0	0	0
			2073	1324	360	372	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	GLY	-	expression tag	UNP Q05397
A	409	SER	-	expression tag	UNP Q05397
A	410	GLY	-	expression tag	UNP Q05397
B	408	GLY	-	expression tag	UNP Q05397
B	409	SER	-	expression tag	UNP Q05397
B	410	GLY	-	expression tag	UNP Q05397
C	408	GLY	-	expression tag	UNP Q05397
C	409	SER	-	expression tag	UNP Q05397
C	410	GLY	-	expression tag	UNP Q05397
D	408	GLY	-	expression tag	UNP Q05397
D	409	SER	-	expression tag	UNP Q05397
D	410	GLY	-	expression tag	UNP Q05397

- Molecule 2 is {N}-methyl- {N}-[3-[[[2-[(2-oxidanylidene-3,4-dihydro-1 {H}-quinolin-6-yl) amino]-5-(trifluoromethyl)pyrimidin-4-yl]amino]methyl]pyridin-2-yl]methanesulfonamide (CCD ID: P7N) (formula: C₂₂H₂₂F₃N₇O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			36	22	3	7	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			36	22	3	7	3	1		
2	C	1	Total	C	F	N	O	S	0	0
			36	22	3	7	3	1		
2	D	1	Total	C	F	N	O	S	0	0
			36	22	3	7	3	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

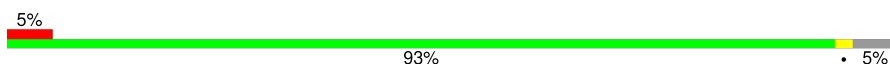
- Molecule 5 is water.

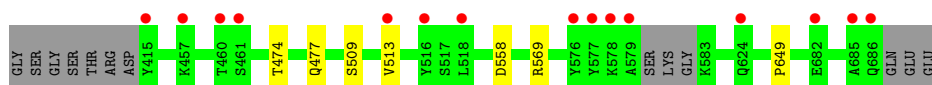
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	260	Total	O	0	0
			260	260		
5	B	245	Total	O	0	0
			245	245		
5	C	261	Total	O	0	0
			261	261		
5	D	156	Total	O	0	0
			156	156		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Focal adhesion kinase 1

Chain A: 

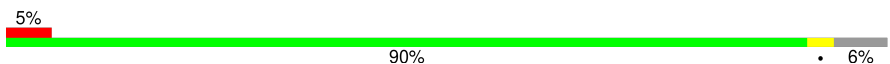


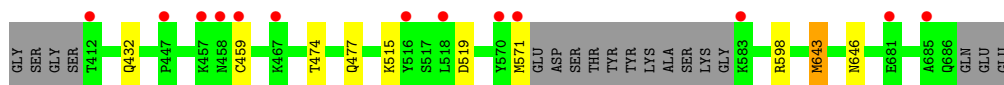
- Molecule 1: Focal adhesion kinase 1

Chain B: 



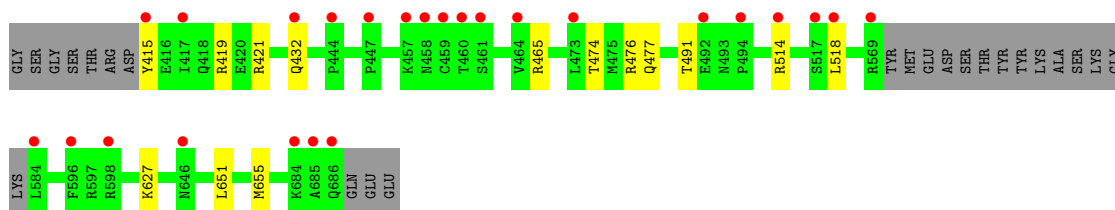
- Molecule 1: Focal adhesion kinase 1

Chain C: 



- Molecule 1: Focal adhesion kinase 1

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.53Å 75.75Å 173.26Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	169.25 – 1.78 169.24 – 1.78	Depositor EDS
% Data completeness (in resolution range)	60.9 (169.25-1.78) 60.9 (169.24-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.78Å)	Xtriage
Refinement program	BUSTER 2.11.7 (19-MAR-2020)	Depositor
R, R_{free}	0.183 , 0.214 0.193 , 0.221	Depositor DCC
R_{free} test set	4085 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9732	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: P7N, NA, SO4

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	0.74	0/2274	0.99	1/3073 (0.0%)
1	B	0.77	0/2280	1.02	3/3080 (0.1%)
1	C	0.79	1/2181 (0.0%)	1.02	2/2948 (0.1%)
1	D	0.69	0/2119	1.00	0/2865
All	All	0.75	1/8854 (0.0%)	1.01	6/11966 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	643	MET	SD-CE	-8.81	1.57	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	582	GLY	CA-C-N	7.32	131.22	120.90
1	B	582	GLY	C-N-CA	7.32	131.22	120.90
1	C	646	ASN	CA-CB-CG	-6.04	106.56	112.60
1	B	569	ARG	N-CA-C	6.03	117.86	111.28
1	A	569	ARG	N-CA-C	5.79	119.17	111.75
1	C	519	ASP	CA-CB-CG	5.14	117.74	112.60

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	2225	0	2213	5	0
1	B	2228	0	2228	8	0
1	C	2134	0	2146	4	0
1	D	2073	0	2086	8	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
2	C	36	0	0	0	0
2	D	36	0	0	0	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	260	0	0	0	0
5	B	245	0	0	1	0
5	C	261	0	0	1	0
5	D	156	0	0	1	0
All	All	9732	0	8673	21	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 1.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:TYR:HB2	1:D:419:ARG:HD3	1.68	0.74
1:B:654:LEU:HA	1:B:657:LYS:HE3	1.77	0.65
1:A:509:SER:O	1:A:513:VAL:HG23	2.02	0.58
1:B:412:THR:HG21	1:B:491:THR:HG21	1.87	0.56
1:D:651:LEU:HG	1:D:655:MET:HE3	1.93	0.51
1:D:514:ARG:HE	1:D:518:LEU:HD21	1.77	0.50
1:B:545:ARG:HD2	5:B:822:HOH:O	2.12	0.49
1:B:479:ASP:HA	1:B:485:LYS:NZ	2.29	0.47
1:D:432:GLN:HG3	5:D:900:HOH:O	2.14	0.47
1:A:474:THR:O	1:A:477:GLN:HG2	2.15	0.46
1:C:432:GLN:HB2	1:C:571:MET:HE3	1.97	0.46
1:D:415:TYR:CE2	1:D:476:ARG:NE	2.81	0.45
1:A:513:VAL:HG11	1:B:512:GLN:HG3	1.99	0.45
1:D:474:THR:O	1:D:477:GLN:HG2	2.17	0.45
1:A:649:PRO:HB3	1:C:643:MET:CE	2.49	0.43
1:B:474:THR:O	1:B:477:GLN:HG2	2.18	0.43
1:D:465:ARG:NH1	1:D:491:THR:O	2.52	0.43
1:C:474:THR:O	1:C:477:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:GLU:HG2	1:B:675:GLN:HE21	1.84	0.42
1:C:459:CYS:HB2	5:C:922:HOH:O	2.19	0.41
1:A:558:ASP:OD1	1:D:421:ARG:NH1	2.54	0.41

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	272/282 (96%)	268 (98%)	4 (2%)	0	100	100
1	B	274/282 (97%)	269 (98%)	5 (2%)	0	100	100
1	C	261/282 (93%)	256 (98%)	5 (2%)	0	100	100
1	D	254/282 (90%)	251 (99%)	3 (1%)	0	100	100
All	All	1061/1128 (94%)	1044 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/249 (99%)	246 (100%)	0	100	100
1	B	247/249 (99%)	247 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	236/249 (95%)	234 (99%)	2 (1%)	73	63
1	D	229/249 (92%)	228 (100%)	1 (0%)	84	78
All	All	958/996 (96%)	955 (100%)	3 (0%)	86	80

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	515	LYS
1	C	598	ARG
1	D	627	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	557	ASN
1	A	618	HIS
1	B	470	GLN
1	B	675	GLN
1	C	432	GLN
1	D	493	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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$
4	SO4	A	703	-	4,4,4	0.31	0	6,6,6	0.23	0
2	P7N	C	701	-	39,39,39	1.51	4 (10%)	52,58,58	1.97	13 (25%)
2	P7N	D	701	-	39,39,39	1.55	4 (10%)	52,58,58	1.94	15 (28%)
2	P7N	A	701	-	39,39,39	1.55	5 (12%)	52,58,58	2.10	17 (32%)
2	P7N	B	701	-	39,39,39	1.27	6 (15%)	52,58,58	2.05	16 (30%)

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	P7N	C	701	-	-	0/25/34/34	0/4/4/4
2	P7N	A	701	-	-	0/25/34/34	0/4/4/4
2	P7N	B	701	-	-	0/25/34/34	0/4/4/4
2	P7N	D	701	-	-	0/25/34/34	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	P7N	C18-N19	-7.21	1.40	1.44
2	A	701	P7N	C18-N19	-7.02	1.40	1.44
2	C	701	P7N	C18-N19	-6.71	1.40	1.44
2	B	701	P7N	C18-N19	-4.06	1.42	1.44
2	B	701	P7N	C4-N7	3.30	1.39	1.34
2	D	701	P7N	C4-N7	3.11	1.39	1.34
2	C	701	P7N	C4-N7	3.07	1.39	1.34
2	A	701	P7N	C4-N7	3.01	1.39	1.34
2	C	701	P7N	S20-N19	2.65	1.68	1.64
2	A	701	P7N	C24-S20	2.55	1.81	1.75
2	B	701	P7N	S20-N19	2.47	1.68	1.64
2	B	701	P7N	C24-S20	2.44	1.81	1.75
2	B	701	P7N	F10-C8	2.17	1.40	1.33
2	C	701	P7N	C24-S20	2.15	1.80	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	P7N	S20-N19	2.14	1.67	1.64
2	D	701	P7N	C24-S20	2.06	1.80	1.75
2	B	701	P7N	F11-C8	2.06	1.40	1.33
2	A	701	P7N	F10-C8	2.04	1.40	1.33
2	D	701	P7N	F11-C8	2.01	1.40	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	P7N	O23-S20-O22	5.47	126.63	118.46
2	D	701	P7N	C34-C33-N32	5.41	122.39	116.31
2	B	701	P7N	C34-C33-N32	5.35	122.32	116.31
2	C	701	P7N	C34-C33-N32	5.26	122.22	116.31
2	D	701	P7N	N1-C2-N3	-5.16	121.43	126.42
2	A	701	P7N	C34-C33-N32	5.16	122.11	116.31
2	C	701	P7N	N1-C2-N3	-5.13	121.46	126.42
2	A	701	P7N	N1-C2-N3	-5.00	121.59	126.42
2	B	701	P7N	N1-C2-N3	-4.85	121.73	126.42
2	A	701	P7N	C31-N32-C33	-4.60	118.94	124.45
2	B	701	P7N	C24-S20-N19	-4.15	101.75	106.82
2	B	701	P7N	C6-N1-C2	4.06	121.37	115.81
2	C	701	P7N	C24-S20-N19	-3.96	101.99	106.82
2	D	701	P7N	C16-N17-C18	3.84	123.75	115.05
2	D	701	P7N	C31-N32-C33	-3.81	119.89	124.45
2	A	701	P7N	C24-S20-N19	-3.77	102.21	106.82
2	C	701	P7N	C31-N32-C33	-3.77	119.94	124.45
2	B	701	P7N	C5-C6-N1	-3.72	119.17	124.18
2	D	701	P7N	C6-N1-C2	3.65	120.81	115.81
2	B	701	P7N	C31-N32-C33	-3.64	120.09	124.45
2	B	701	P7N	O23-S20-O22	3.56	123.78	118.46
2	A	701	P7N	C6-N1-C2	3.52	120.64	115.81
2	C	701	P7N	C35-C30-C31	3.42	122.09	118.54
2	B	701	P7N	C35-C30-C31	3.39	122.06	118.54
2	C	701	P7N	C6-N1-C2	3.35	120.40	115.81
2	A	701	P7N	C5-C6-N1	-3.32	119.70	124.18
2	D	701	P7N	C12-N7-C4	-3.18	118.97	123.08
2	C	701	P7N	C16-N17-C18	3.17	122.24	115.05
2	C	701	P7N	C5-C6-N1	-3.08	120.03	124.18
2	B	701	P7N	C12-N7-C4	-3.08	119.11	123.08
2	D	701	P7N	C5-C6-N1	-3.05	120.07	124.18
2	C	701	P7N	O23-S20-O22	3.04	123.00	118.46
2	A	701	P7N	C16-N17-C18	2.97	121.78	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	P7N	C35-C30-C31	2.88	121.52	118.54
2	A	701	P7N	C5-C4-N3	-2.87	117.71	122.02
2	B	701	P7N	C16-N17-C18	2.87	121.54	115.05
2	B	701	P7N	O23-S20-N19	-2.84	103.89	107.14
2	D	701	P7N	C24-S20-N19	-2.84	103.35	106.82
2	A	701	P7N	C35-C30-C31	2.74	121.38	118.54
2	C	701	P7N	C5-C4-N3	-2.69	117.98	122.02
2	D	701	P7N	C5-C4-N3	-2.60	118.12	122.02
2	B	701	P7N	C21-N19-C18	2.59	118.91	115.72
2	A	701	P7N	F11-C8-C5	-2.55	108.12	112.65
2	C	701	P7N	C12-N7-C4	-2.54	119.80	123.08
2	A	701	P7N	C34-C35-C30	-2.41	107.17	111.97
2	D	701	P7N	C21-N19-C18	2.40	118.67	115.72
2	B	701	P7N	C5-C4-N3	-2.33	118.53	122.02
2	C	701	P7N	C2-N3-C4	2.33	122.08	116.36
2	B	701	P7N	O36-C33-N32	-2.28	118.98	121.39
2	A	701	P7N	C21-N19-C18	2.18	118.40	115.72
2	D	701	P7N	C15-C16-N17	-2.18	119.97	123.42
2	A	701	P7N	C2-N3-C4	2.17	121.69	116.36
2	D	701	P7N	C2-N3-C4	2.14	121.62	116.36
2	A	701	P7N	O36-C33-C34	-2.10	117.90	122.20
2	D	701	P7N	O36-C33-C34	-2.10	117.91	122.20
2	A	701	P7N	C35-C34-C33	-2.07	109.16	113.77
2	A	701	P7N	F9-C8-C5	-2.07	108.97	112.65
2	B	701	P7N	C8-C5-C4	2.07	122.71	120.06
2	D	701	P7N	O23-S20-O22	2.07	121.55	118.46
2	C	701	P7N	C21-N19-C18	2.04	118.24	115.72
2	B	701	P7N	C15-C14-C13	-2.01	117.94	120.88

There are no chirality outliers.

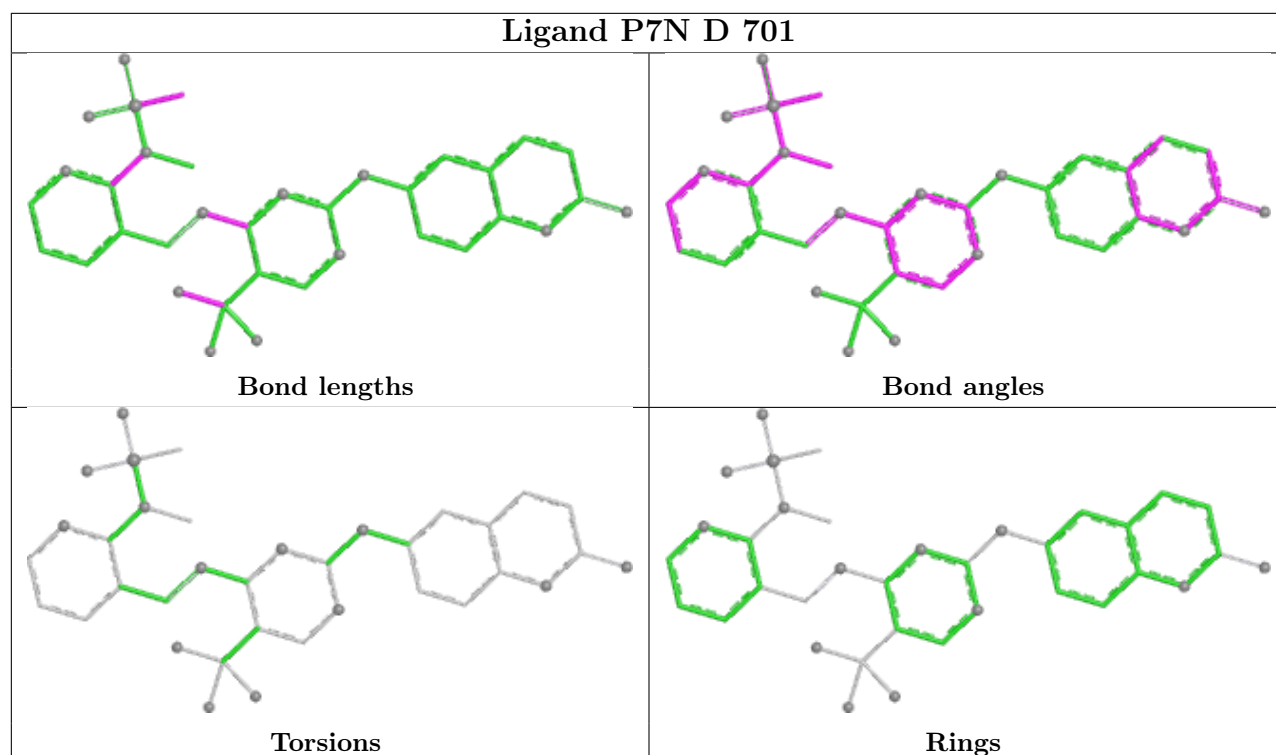
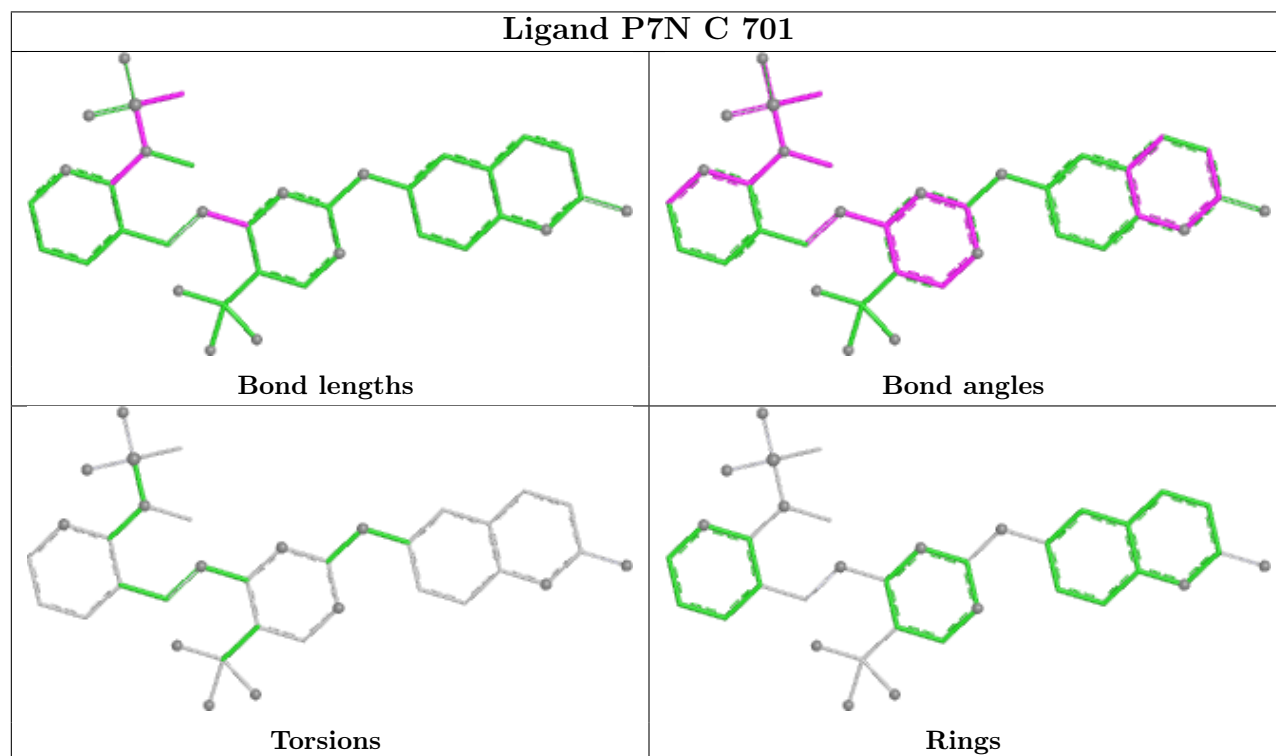
There are no torsion outliers.

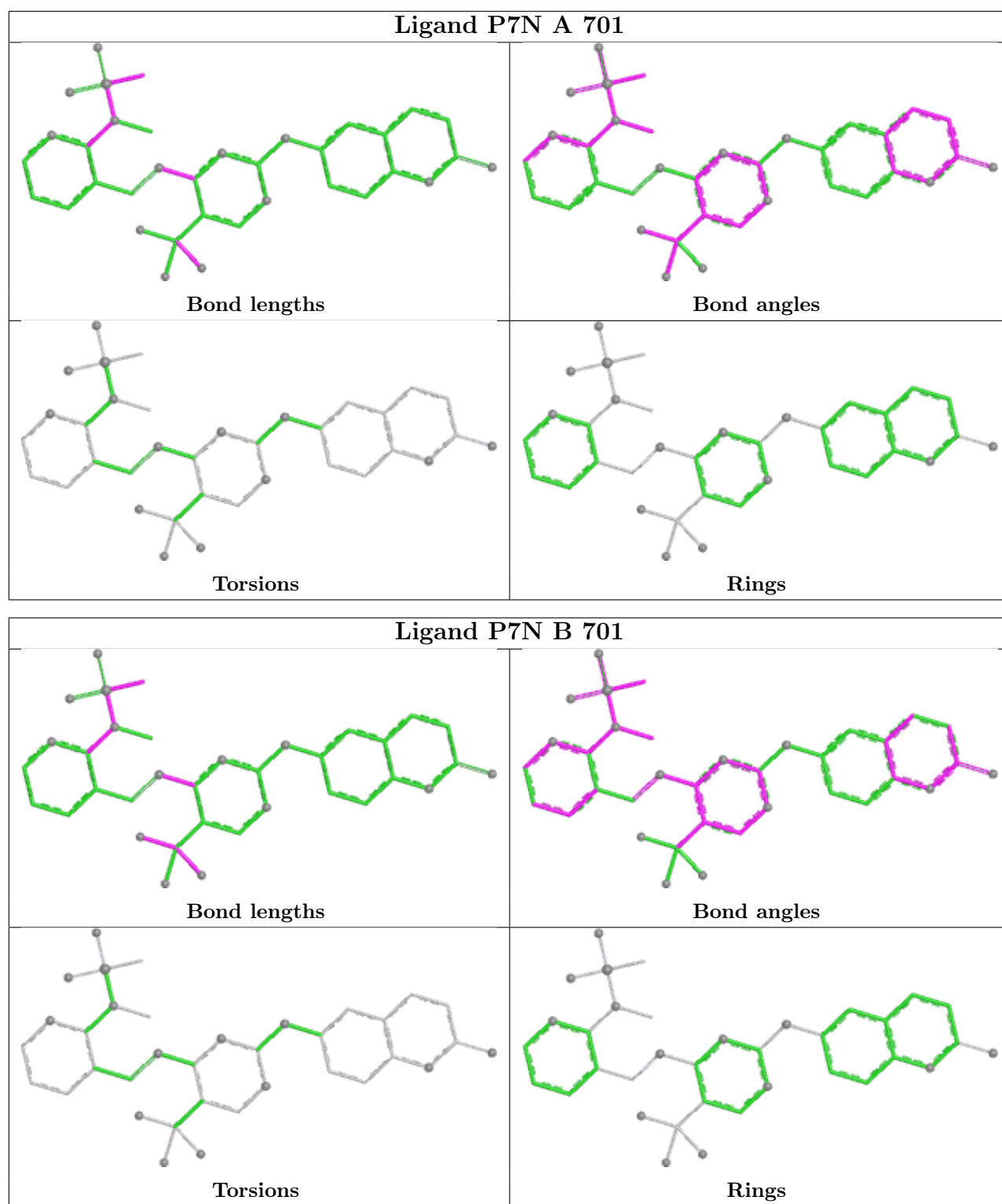
There are no ring outliers.

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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	269/282 (95%)	0.36	15 (5%) 30 36	9, 26, 51, 66	7 (2%)
1	B	274/282 (97%)	0.23	13 (4%) 36 42	9, 25, 46, 67	4 (1%)
1	C	264/282 (93%)	0.23	13 (4%) 35 41	13, 24, 48, 70	1 (0%)
1	D	258/282 (91%)	0.70	25 (9%) 13 15	18, 34, 62, 78	0
All	All	1065/1128 (94%)	0.38	66 (6%) 26 32	9, 28, 52, 78	12 (1%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	TYR	5.4
1	C	516	TYR	5.1
1	B	576	TYR	4.8
1	D	415	TYR	4.5
1	B	410	GLY	4.5
1	D	461	SER	4.1
1	B	411	SER	3.7
1	A	579	ALA	3.7
1	C	570	TYR	3.5
1	A	576	TYR	3.5
1	D	458	ASN	3.4
1	D	464	VAL	3.4
1	D	518	LEU	3.3
1	D	569	ARG	3.3
1	C	412	THR	3.2
1	D	459	CYS	3.2
1	A	624	GLN	3.1
1	B	665	ARG	3.0
1	A	461[A]	SER	2.9
1	D	417	ILE	2.9
1	C	571	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	686	GLN	2.9
1	D	685	ALA	2.8
1	B	581	LYS	2.8
1	D	596	PHE	2.7
1	A	518	LEU	2.7
1	C	459	CYS	2.7
1	C	458	ASN	2.7
1	C	583	LYS	2.7
1	B	577	TYR	2.7
1	A	457	LYS	2.7
1	A	686	GLN	2.6
1	B	686	GLN	2.6
1	D	584	LEU	2.6
1	C	518	LEU	2.6
1	C	685	ALA	2.5
1	B	597	ARG	2.5
1	C	681	GLU	2.5
1	A	685	ALA	2.5
1	D	598	ARG	2.4
1	A	516	TYR	2.4
1	D	447	PRO	2.4
1	A	577	TYR	2.4
1	D	460	THR	2.3
1	D	514	ARG	2.3
1	B	447	PRO	2.3
1	D	457	LYS	2.3
1	D	444	PRO	2.2
1	D	646	ASN	2.2
1	B	444	PRO	2.2
1	D	494	PRO	2.2
1	A	578	LYS	2.2
1	D	492	GLU	2.2
1	D	432	GLN	2.1
1	A	513	VAL	2.1
1	D	473	LEU	2.1
1	D	684	LYS	2.1
1	A	460	THR	2.1
1	B	618	HIS	2.1
1	C	467	LYS	2.1
1	B	462	ASP	2.0
1	D	517	SER	2.0
1	C	447	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	682	GLU	2.0
1	B	446	ASN	2.0
1	C	457	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

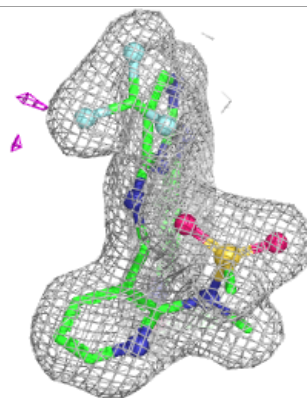
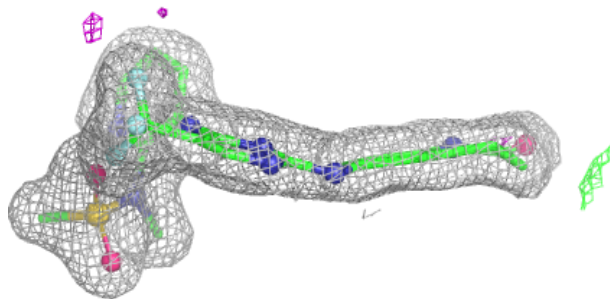
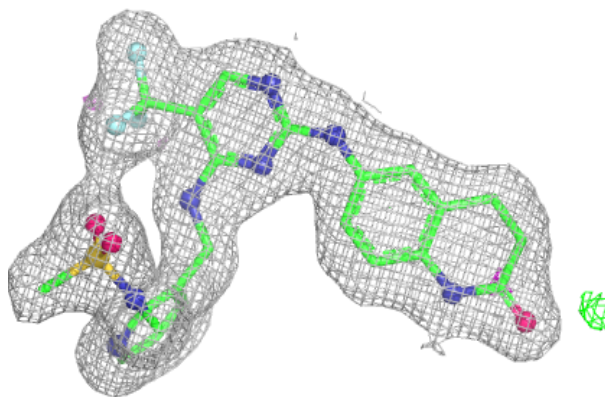
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	A	702	1/1	0.87	0.18	60,60,60,60	0
4	SO4	A	703	5/5	0.95	0.12	33,33,33,33	0
2	P7N	B	701	36/36	0.97	0.06	13,17,21,23	0
2	P7N	D	701	36/36	0.97	0.06	21,25,29,31	0
2	P7N	C	701	36/36	0.98	0.05	17,20,26,28	0
2	P7N	A	701	36/36	0.98	0.06	17,19,26,29	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.

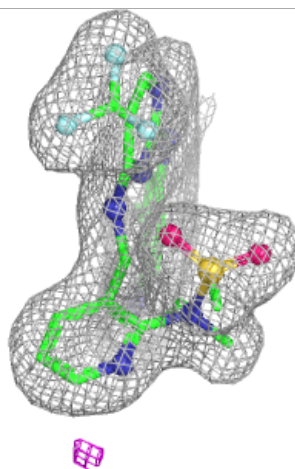
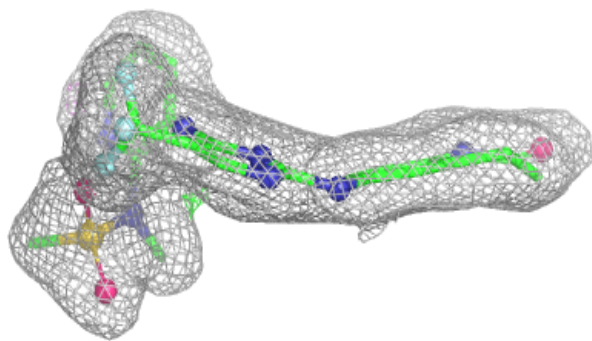
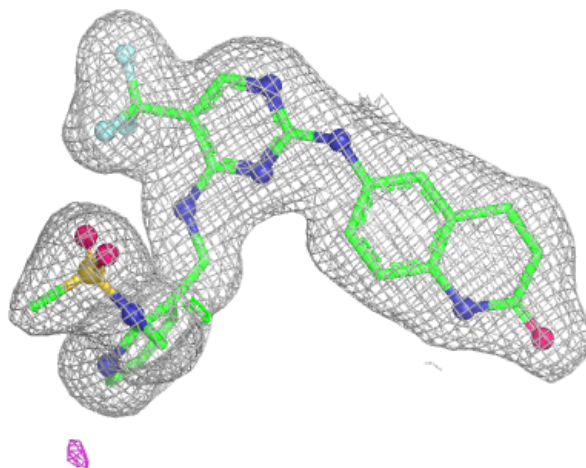
Electron density around P7N B 701:

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



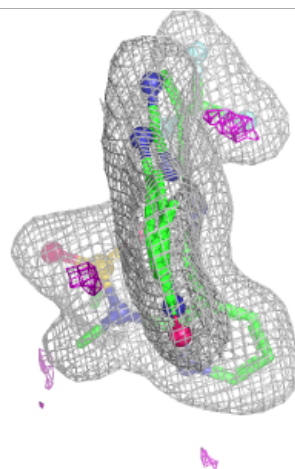
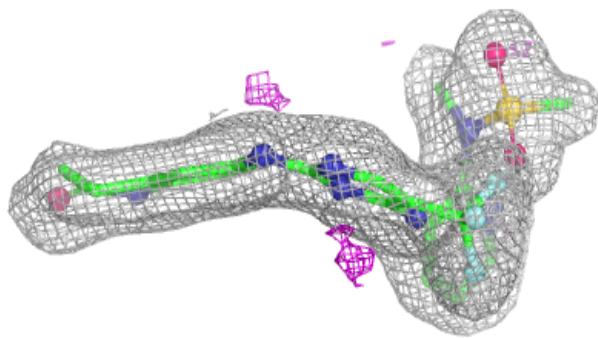
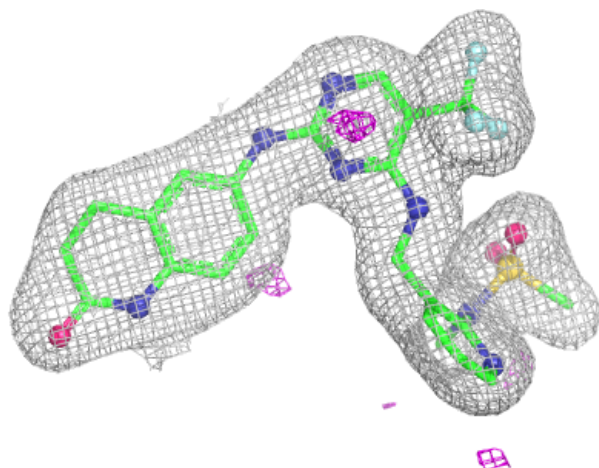
Electron density around P7N D 701:

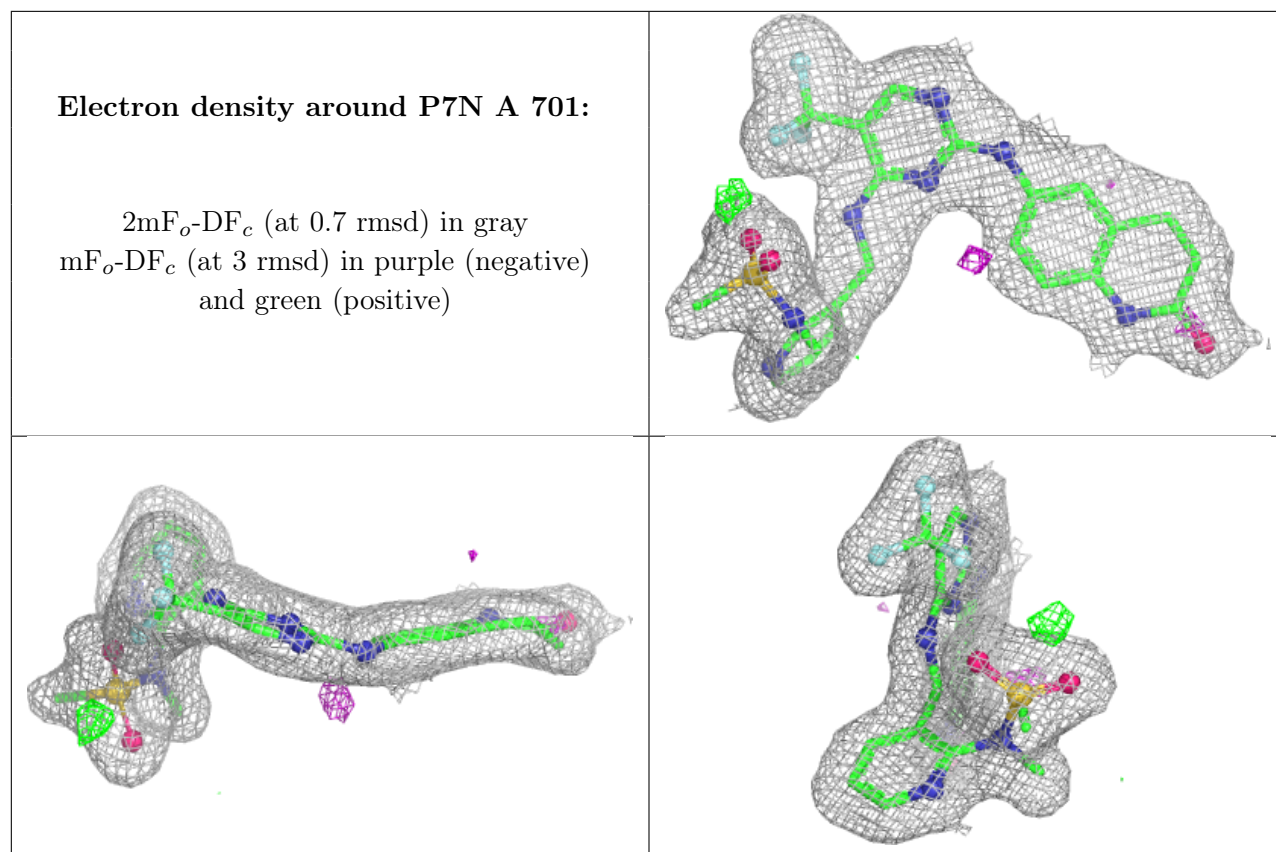
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P7N C 701:

$2mF_o-DF_c$ (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.