



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:08 AM UTC

PDB ID : 5ORH / pdb_00005orh
Title : The crystal structure of CK2alpha in complex with compound 2
Authors : Brear, P.; De Fusco, C.; Iegre, J.; Yoshida, M.; Mitchell, S.; Rossmann, M.; Carro, L.; Sore, H.; Hyvonen, M.; Spring, D.
Deposited on : 2017-08-16
Resolution : 1.75 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

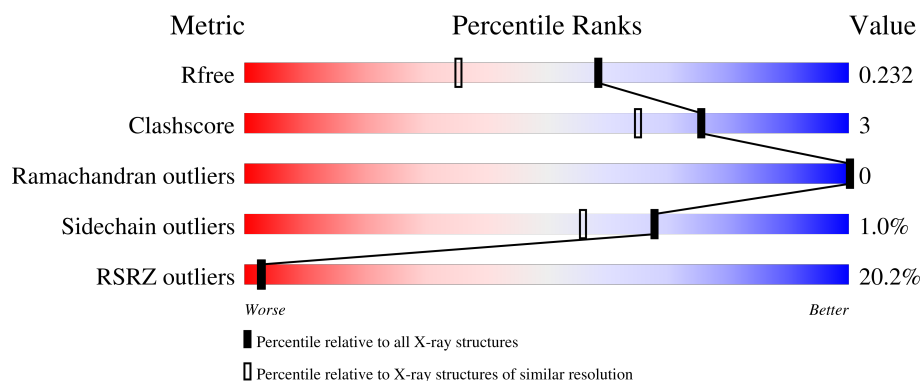
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	352	30% 82% 9% 8%
1	B	352	8% 84% 8% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A4N	B	402	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5902 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	2	0
			2754	1766	481	495	12			
1	B	325	Total	C	N	O	S	0	2	0
			2758	1768	482	496	12			

There are 50 discrepancies between the modelled and reference sequences:

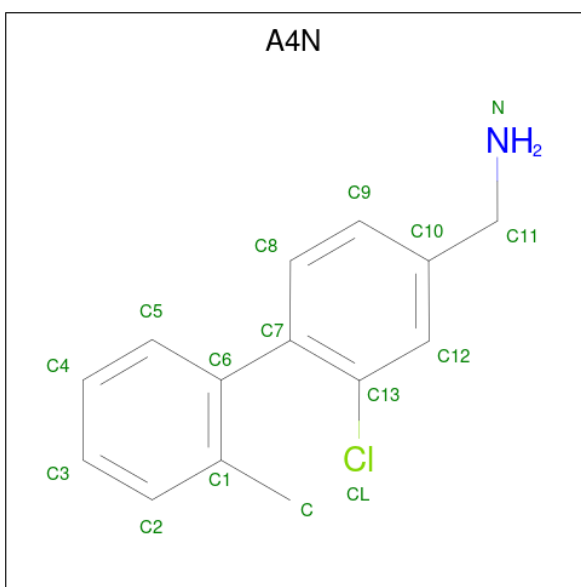
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	UNP P68400
A	-15	ASP	-	expression tag	UNP P68400
A	-14	ASP	-	expression tag	UNP P68400
A	-13	ASP	-	expression tag	UNP P68400
A	-12	ALA	-	expression tag	UNP P68400
A	-11	ASP	-	expression tag	UNP P68400
A	-10	ASP	-	expression tag	UNP P68400
A	-9	ASP	-	expression tag	UNP P68400
A	-8	GLY	-	expression tag	UNP P68400
A	-7	SER	-	expression tag	UNP P68400
A	-6	GLY	-	expression tag	UNP P68400
A	-5	SER	-	expression tag	UNP P68400
A	-4	GLY	-	expression tag	UNP P68400
A	-3	SER	-	expression tag	UNP P68400
A	-2	GLY	-	expression tag	UNP P68400
A	-1	SER	-	expression tag	UNP P68400
A	0	GLY	-	expression tag	UNP P68400
A	1	SER	-	expression tag	UNP P68400
A	21	SER	ARG	engineered mutation	UNP P68400

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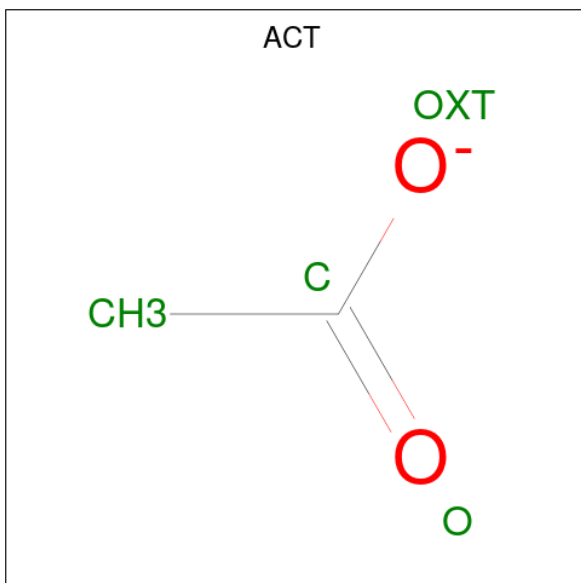
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P68400
B	-21	SER	-	expression tag	UNP P68400
B	-20	MET	-	expression tag	UNP P68400
B	-19	ASP	-	expression tag	UNP P68400
B	-18	ILE	-	expression tag	UNP P68400
B	-17	GLU	-	expression tag	UNP P68400
B	-16	PHE	-	expression tag	UNP P68400
B	-15	ASP	-	expression tag	UNP P68400
B	-14	ASP	-	expression tag	UNP P68400
B	-13	ASP	-	expression tag	UNP P68400
B	-12	ALA	-	expression tag	UNP P68400
B	-11	ASP	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	ASP	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	SER	-	expression tag	UNP P68400
B	-6	GLY	-	expression tag	UNP P68400
B	-5	SER	-	expression tag	UNP P68400
B	-4	GLY	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLY	-	expression tag	UNP P68400
B	-1	SER	-	expression tag	UNP P68400
B	0	GLY	-	expression tag	UNP P68400
B	1	SER	-	expression tag	UNP P68400
B	21	SER	ARG	engineered mutation	UNP P68400

- Molecule 2 is [3-chloranyl-4-(2-methylphenyl)phenyl]methanamine (CCD ID: A4N) (formula: C₁₄H₁₄ClN) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			16	14	1	1		
2	A	1	Total	C	Cl	N	0	0
			16	14	1	1		
2	B	1	Total	C	Cl	N	0	0
			16	14	1	1		
2	B	1	Total	C	Cl	N	0	0
			16	14	1	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	105	Total O 105 105	0	0
4	B	209	Total O 209 209	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.52Å 67.97Å 333.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.33 – 1.75 83.33 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (83.33-1.75) 99.9 (83.33-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.75Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.208 , 0.227 0.210 , 0.232	Depositor DCC
R_{free} test set	3793 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.054 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5902	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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: ACT, A4N

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	0.78	0/2829	1.05	9/3826 (0.2%)
1	B	0.98	5/2833 (0.2%)	1.04	6/3832 (0.2%)
All	All	0.88	5/5662 (0.1%)	1.05	15/7658 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	ILE	C-O	-5.66	1.18	1.24
1	B	85	LEU	C-O	-5.55	1.17	1.24
1	B	21	SER	C-O	-5.49	1.17	1.24
1	B	82	ILE	C-O	-5.17	1.18	1.24
1	B	99	ASP	C-O	-5.16	1.17	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	MET	N-CA-C	7.34	119.36	111.36
1	A	51	SER	N-CA-C	7.01	118.83	108.60
1	A	105	VAL	N-CA-C	6.80	117.56	110.62
1	B	180	GLU	CB-CG-CD	6.18	123.10	112.60
1	B	51	SER	N-CA-C	6.04	117.96	108.96
1	A	127	THR	N-CA-C	6.04	120.81	113.38
1	A	126	GLN	N-CA-C	5.95	117.84	111.36
1	A	314	THR	N-CA-C	-5.67	103.22	110.53
1	A	118	ASN	N-CA-C	5.37	117.49	109.59
1	A	55	GLU	N-CA-C	-5.34	101.76	110.20
1	B	55	GLU	N-CA-C	-5.32	101.79	110.20
1	A	24	TRP	N-CA-C	5.28	120.58	113.72
1	B	24	TRP	N-CA-C	5.21	120.50	113.72
1	B	216	TRP	N-CA-C	-5.17	105.56	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	THR	N-CA-C	-5.11	103.94	110.53

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	2754	0	2693	18	0
1	B	2758	0	2695	15	1
2	A	32	0	0	2	0
2	B	32	0	0	8	0
3	B	12	0	9	0	0
4	A	105	0	0	0	0
4	B	209	0	0	2	0
All	All	5902	0	5397	33	1

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 3.

All (33) 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:225:MET:HG3	2:B:402:A4N:C2	2.02	0.90
1:A:116:VAL:HB	1:A:163[B]:MET:HE2	1.63	0.79
1:A:116:VAL:HB	1:A:163[B]:MET:CE	2.25	0.66
1:B:124:LEU:HA	1:B:127:THR:HG22	1.79	0.63
1:B:221:MET:HE1	2:B:402:A4N:CL	2.36	0.63
1:B:225:MET:HG3	2:B:402:A4N:C1	2.29	0.62
1:A:133:ILE:HG12	1:A:225:MET:HE3	1.84	0.60
1:A:128:LEU:HD22	1:A:132:ASP:HB3	1.84	0.59
1:B:39:TYR:O	2:B:401:A4N:N	2.39	0.56
1:A:105:VAL:HG21	1:B:20:PRO:HG2	1.89	0.54
1:B:5:VAL:HB	1:B:261:TYR:HA	1.90	0.53
1:B:225:MET:CG	2:B:402:A4N:C2	2.84	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163[A]:MET:HA	1:A:163[A]:MET:HE2	1.91	0.52
1:A:5:VAL:HB	1:A:261:TYR:HA	1.91	0.52
1:B:129:THR:HG22	1:B:132:ASP:CG	2.35	0.51
1:B:17:THR:HG22	4:B:602:HOH:O	2.13	0.49
1:A:49:LYS:HD3	1:A:50:TYR:CE1	2.49	0.48
2:B:402:A4N:N	4:B:502:HOH:O	2.36	0.47
1:B:129:THR:HG23	1:B:132:ASP:H	1.81	0.46
1:B:162:VAL:HG11	2:B:402:A4N:CL	2.53	0.45
1:A:47:ARG:HG3	1:A:52:GLU:HG2	1.99	0.45
1:A:33:TRP:CZ3	1:A:100:ILE:HG22	2.52	0.45
1:A:26:TYR:HE1	1:A:76:LYS:HG2	1.83	0.43
1:A:128:LEU:HD22	1:A:132:ASP:CB	2.48	0.43
1:B:124:LEU:O	1:B:128:LEU:HG	2.19	0.42
1:A:121:PHE:HZ	1:A:230:GLU:HG3	1.85	0.42
1:B:265:LEU:HD22	1:B:269:PHE:CD2	2.56	0.41
1:A:140:ILE:HD11	2:A:402:A4N:CL	2.58	0.41
1:A:128:LEU:HD12	1:A:225:MET:CE	2.50	0.41
1:A:225:MET:HG3	2:A:402:A4N:C1	2.51	0.41
1:A:303:LYS:HB3	1:A:313:LEU:HG	2.02	0.41
1:A:103:ASP:HA	1:A:104:PRO:HD2	1.91	0.40
1:B:225:MET:CG	2:B:402:A4N:C1	2.98	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:GLU:OE2	1:B:280:ARG:NH2[8_597]	1.74	0.46

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	324/352 (92%)	314 (97%)	10 (3%)	0	100	100
1	B	325/352 (92%)	319 (98%)	6 (2%)	0	100	100
All	All	649/704 (92%)	633 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	301/319 (94%)	297 (99%)	4 (1%)	61	46
1	B	301/319 (94%)	299 (99%)	2 (1%)	76	67
All	All	602/638 (94%)	596 (99%)	6 (1%)	68	56

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	73	VAL
1	A	205	ASP
1	A	230	GLU
1	B	124	LEU
1	B	282	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	118	ASN
1	A	168	HIS
1	A	207	GLN
1	A	262	ASN
1	A	270	ASN
1	B	18	HIS

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Mol	Chain	Res	Type
1	B	118	ASN
1	B	123	GLN
1	B	168	HIS
1	B	186	GLN
1	B	262	ASN
1	B	270	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	B	403	-	3,3,3	1.24	0	3,3,3	1.18	0
3	ACT	B	405	-	3,3,3	1.31	0	3,3,3	0.90	0
2	A4N	A	402	-	17,17,17	0.19	0	23,23,23	0.41	0
3	ACT	B	404	-	3,3,3	1.76	1 (33%)	3,3,3	0.73	0
2	A4N	B	402	-	17,17,17	0.17	0	23,23,23	0.22	0
2	A4N	B	401	-	17,17,17	0.16	0	23,23,23	0.22	0
2	A4N	A	401	-	17,17,17	0.15	0	23,23,23	0.22	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
2	A4N	B	402	-	-	0/6/6/6	0/2/2/2
2	A4N	B	401	-	-	0/6/6/6	0/2/2/2
2	A4N	A	402	-	-	0/6/6/6	0/2/2/2
2	A4N	A	401	-	-	0/6/6/6	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	ACT	OXT-C	-2.29	1.20	1.30

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

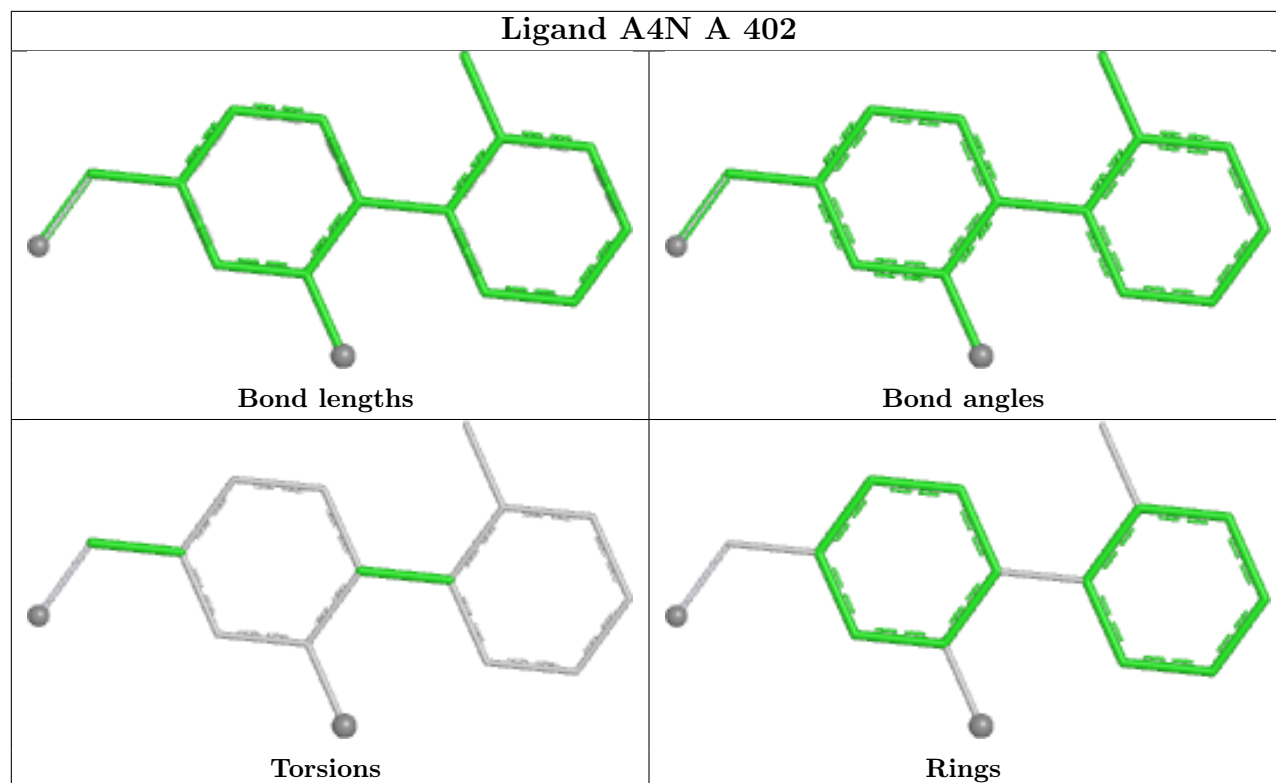
There are no ring outliers.

3 monomers are involved in 10 short contacts:

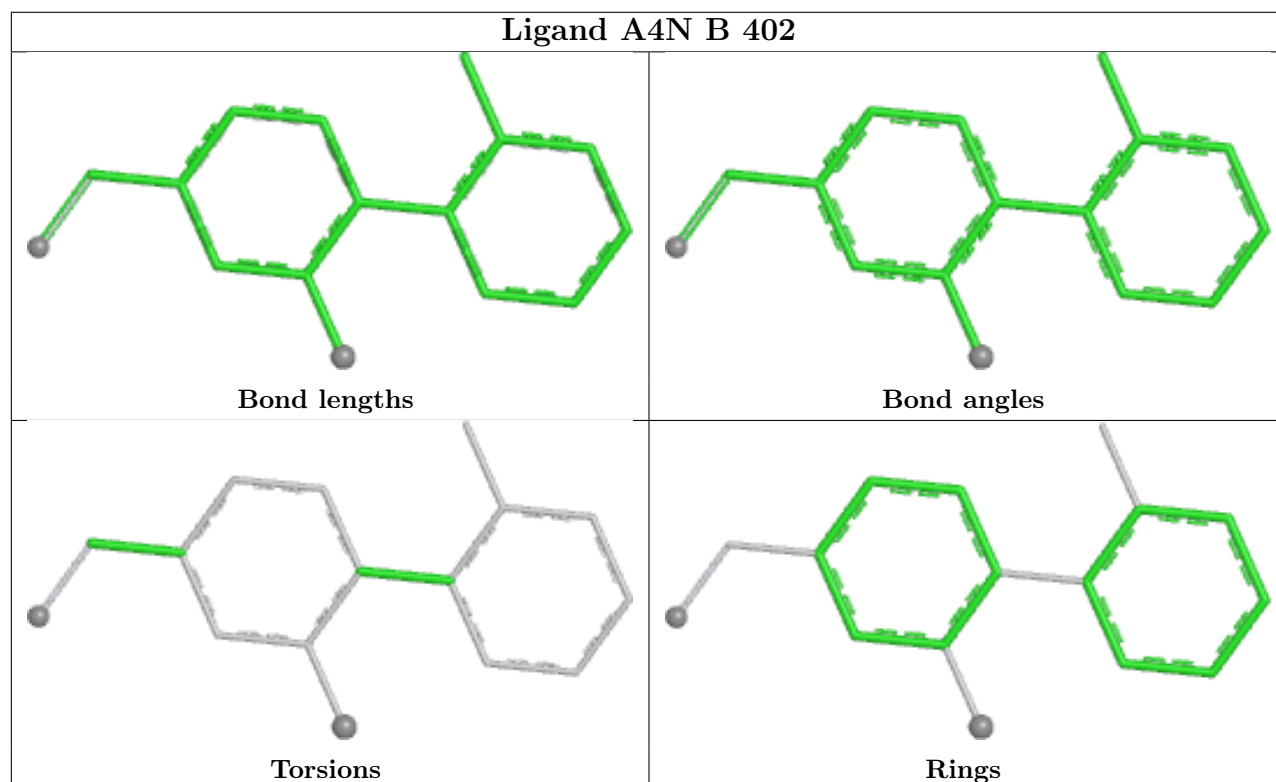
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	A4N	2	0
2	B	402	A4N	7	0
2	B	401	A4N	1	0

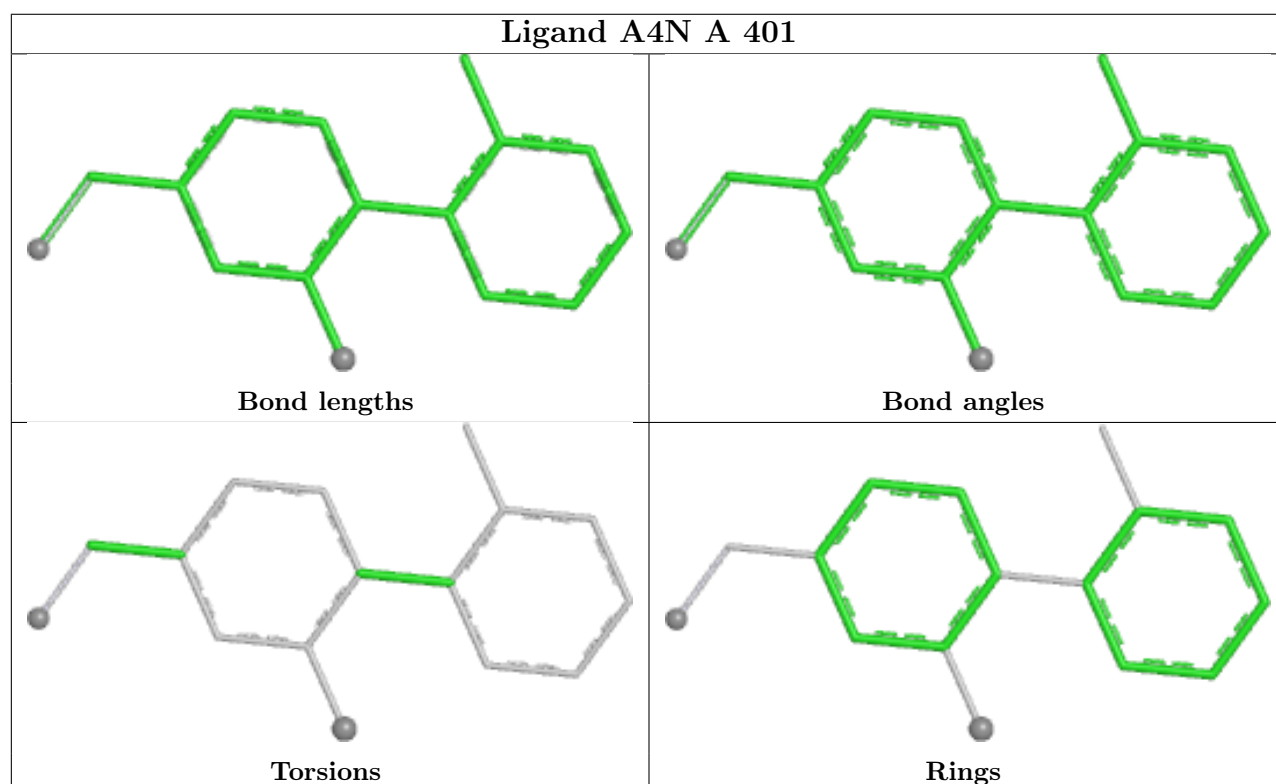
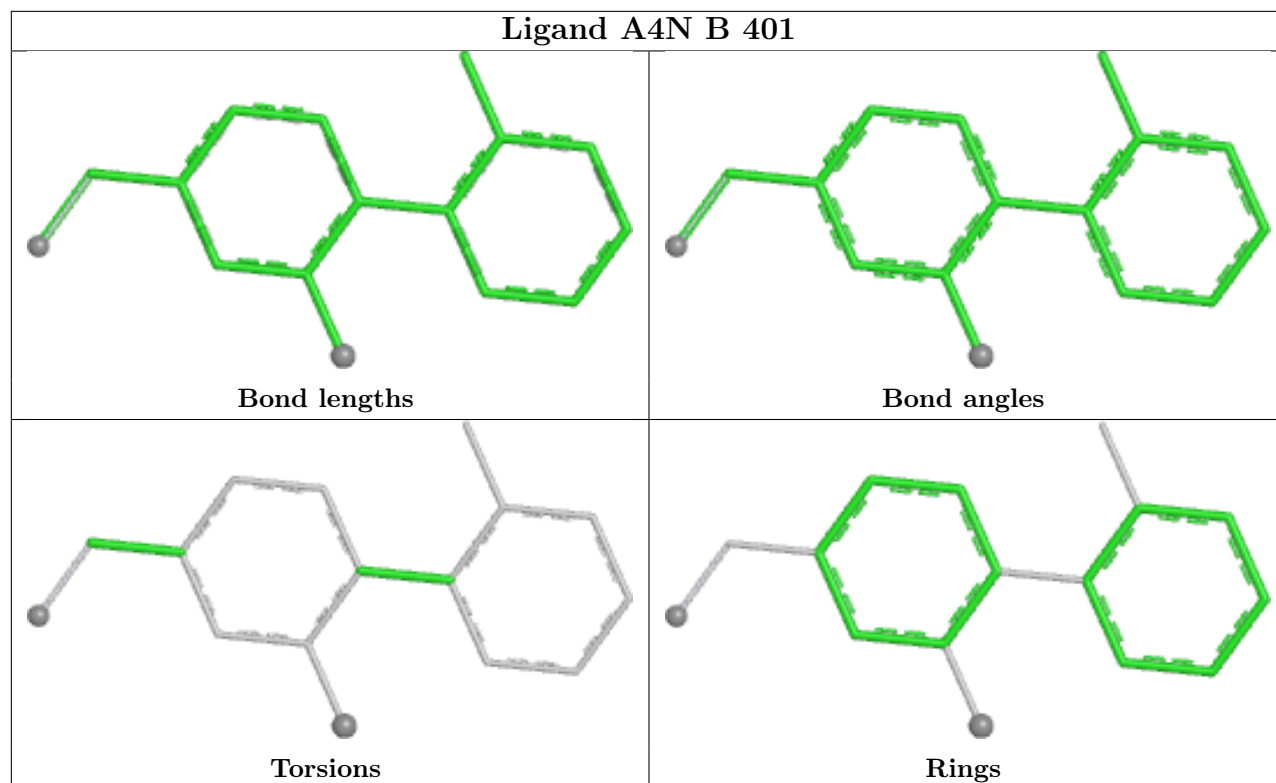
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A4N A 402



Ligand A4N B 402





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	324/352 (92%)	1.48	104 (32%) 1 1	16, 42, 72, 91	2 (0%)
1	B	325/352 (92%)	0.56	27 (8%) 17 20	12, 28, 58, 90	2 (0%)
All	All	649/704 (92%)	1.02	131 (20%) 3 3	12, 35, 69, 91	4 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	LEU	7.7
1	B	50	TYR	7.1
1	B	121	PHE	6.4
1	B	73	VAL	6.0
1	A	125	TYR	5.9
1	B	125	TYR	5.8
1	A	327	VAL	5.4
1	A	104	PRO	4.7
1	B	107	ARG	4.6
1	A	50	TYR	4.5
1	B	72	PRO	4.4
1	A	73	VAL	4.4
1	A	255	TYR	4.2
1	A	121	PHE	4.1
1	B	327	VAL	4.1
1	A	254	LEU	3.9
1	B	128	LEU	3.9
1	A	272	ILE	3.8
1	A	105	VAL	3.8
1	A	257	TYR	3.8
1	A	325	TYR	3.8
1	B	71	LYS	3.7
1	A	267	PRO	3.7
1	A	258	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	270	ASN	3.6
1	A	124	LEU	3.5
1	A	249	LEU	3.5
1	A	72	PRO	3.5
1	A	33	TRP	3.5
1	A	292	LEU	3.5
1	A	307	TYR	3.5
1	B	104	PRO	3.5
1	A	122	LYS	3.4
1	B	105	VAL	3.4
1	A	286	HIS	3.4
1	A	251	THR	3.4
1	A	46	GLY	3.3
1	A	273	LEU	3.3
1	A	45	LEU	3.3
1	A	107	ARG	3.3
1	A	278	ARG	3.3
1	A	227	PHE	3.2
1	A	269	PHE	3.2
1	B	325	TYR	3.1
1	A	263	ILE	3.1
1	A	248	VAL	3.1
1	A	57	ILE	3.1
1	A	102	LYS	3.1
1	A	265	LEU	3.1
1	B	49	LYS	3.0
1	A	117	ASN	3.0
1	A	225	MET	2.9
1	A	226	ILE	2.9
1	A	290	GLN	2.9
1	A	285	VAL	2.9
1	A	246	ALA	2.9
1	A	237	ASP	2.8
1	A	5	VAL	2.8
1	A	206	TYR	2.8
1	A	64	LYS	2.8
1	A	71	LYS	2.8
1	A	75	LYS	2.8
1	A	131	TYR	2.8
1	A	268	ARG	2.7
1	A	281	TRP	2.7
1	B	33	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	287	SER	2.7
1	B	122	LYS	2.7
1	A	326	THR	2.6
1	A	101	VAL	2.6
1	B	258	ILE	2.6
1	A	70	LEU	2.6
1	B	89	ARG	2.6
1	A	35	ASN	2.6
1	A	239	TYR	2.5
1	A	260	LYS	2.5
1	A	100	ILE	2.5
1	A	48	GLY	2.5
1	A	253	ASP	2.5
1	A	271	ASP	2.5
1	A	293	VAL	2.5
1	A	128	LEU	2.4
1	A	127	THR	2.4
1	A	301	LEU	2.4
1	A	74	LYS	2.4
1	A	106	SER	2.4
1	A	305	LEU	2.4
1	A	302	ASP	2.4
1	A	49	LYS	2.4
1	A	103	ASP	2.3
1	A	203	LEU	2.3
1	B	316	ARG	2.3
1	A	40	GLN	2.3
1	B	191	ARG	2.3
1	A	6	PRO	2.3
1	A	276	HIS	2.3
1	A	216	TRP	2.2
1	A	41	LEU	2.2
1	B	271	ASP	2.2
1	B	123	GLN	2.2
1	A	277	SER	2.2
1	A	59	ILE	2.2
1	A	245	ILE	2.2
1	A	256	ASP	2.2
1	A	297	ALA	2.2
1	B	120	ASP	2.2
1	A	252	GLU	2.2
1	A	250	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	47	ARG	2.2
1	A	228	ARG	2.2
1	A	289	ASN	2.2
1	A	261	TYR	2.2
1	A	42	VAL	2.1
1	B	126	GLN	2.1
1	A	232	PHE	2.1
1	A	78	ILE	2.1
1	A	17	THR	2.1
1	A	306	ARG	2.1
1	A	69	ILE	2.1
1	A	298	LEU	2.1
1	A	233	PHE	2.1
1	A	284	PHE	2.1
1	A	323	TYR	2.1
1	A	186	GLN	2.0
1	A	30	VAL	2.0
1	B	127	THR	2.0
1	B	129	THR	2.0
1	A	4	PRO	2.0
1	A	230	GLU	2.0
1	A	8	ARG	2.0
1	B	283	ARG	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.

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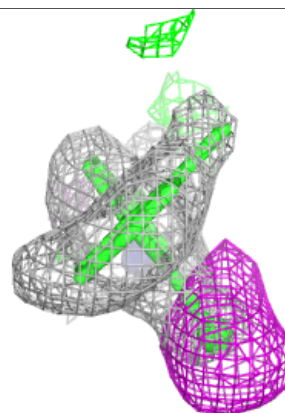
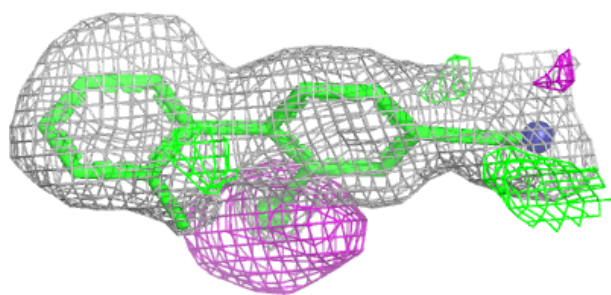
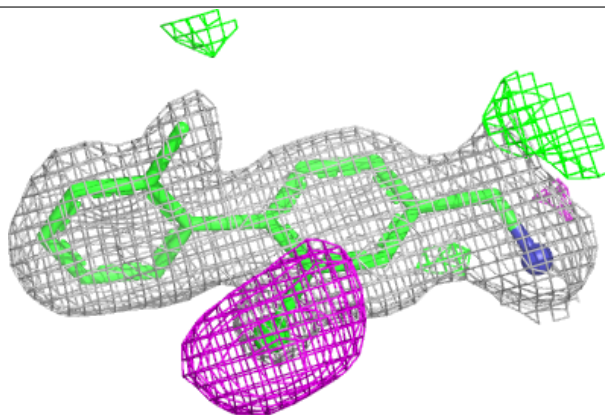
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	B	405	4/4	0.65	0.22	59,61,61,62	0
2	A4N	B	402	16/16	0.73	0.18	33,38,42,54	0
2	A4N	A	401	16/16	0.78	0.17	45,53,59,61	0
2	A4N	A	402	16/16	0.81	0.17	32,47,49,56	0
3	ACT	B	404	4/4	0.87	0.12	29,30,31,38	0
2	A4N	B	401	16/16	0.87	0.13	34,37,46,47	0
3	ACT	B	403	4/4	0.95	0.09	36,41,42,42	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.

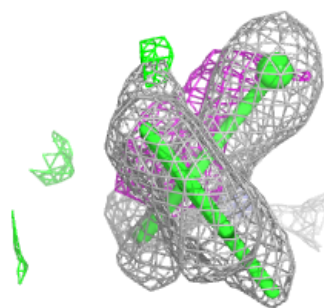
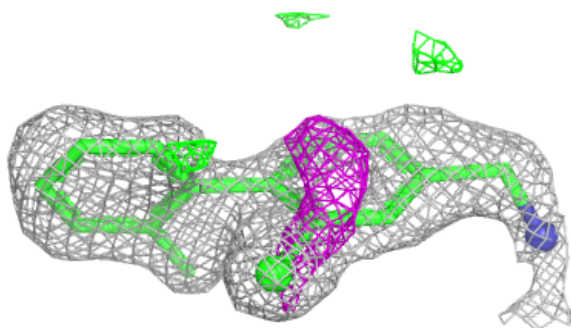
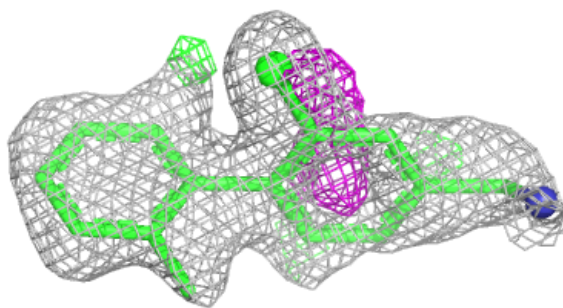
Electron density around A4N B 402:

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

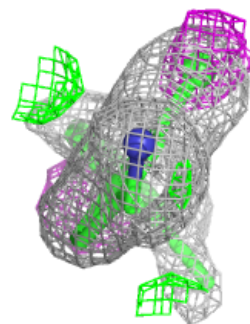
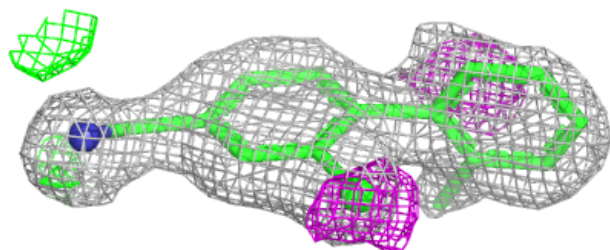
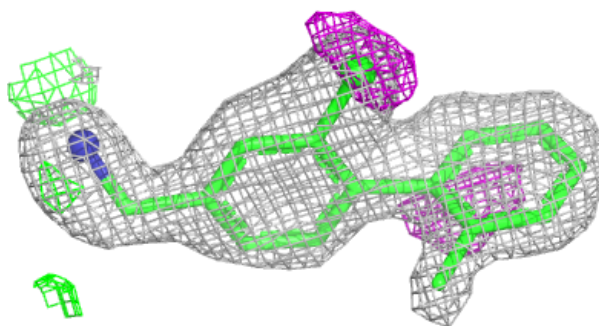


Electron density around A4N A 401:

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

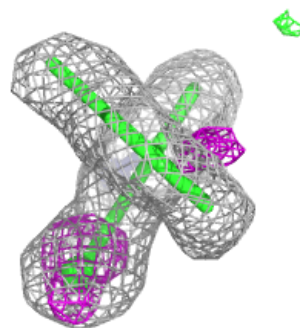
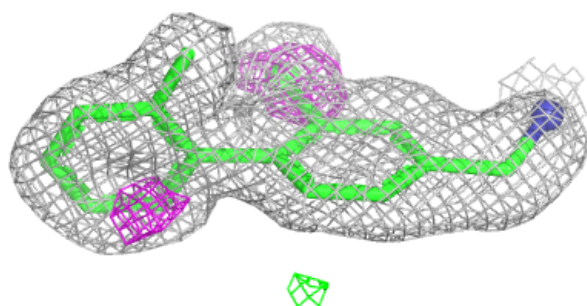
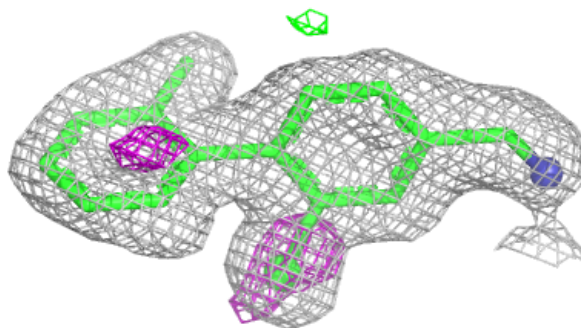
**Electron density around A4N A 402:**

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



Electron density around A4N B 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.