



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:18 pm BST

PDB ID : 5PGU
Title : CRYSTAL STRUCTURE OF 11BETA-HSD1 DOUBLE MUTANT (L262R, F278E) COMPLEXED WITH 2-[2-(4-fluorophenyl)-2-adamantyl]-1-(3-methoxyazetidyl)ethanone
Authors : Sheriff, S.
Deposited on : 2017-02-06
Resolution : 2.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

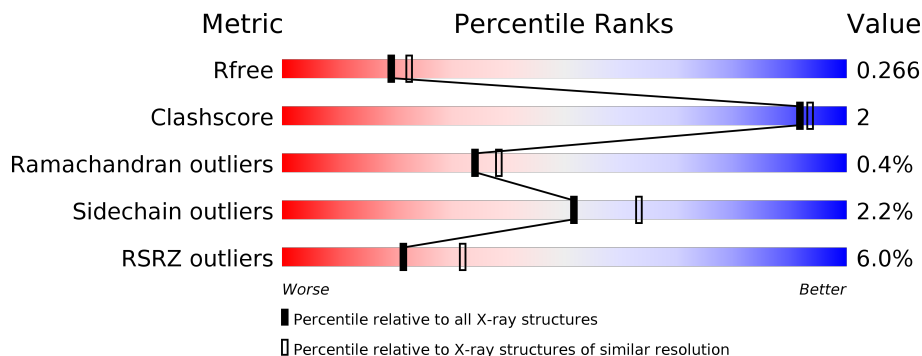
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	286	
1	B	286	
1	D	286	
1	E	286	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8673 atoms, of which 224 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	1998	1270	338	373	17	0	0	0
1	B	273	2070	1311	355	386	18	0	0	0
1	D	266	2011	1276	343	376	16	0	0	0
1	E	263	1986	1261	337	372	16	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLY	-	expression tag	UNP P28845
A	8	SER	-	expression tag	UNP P28845
A	9	HIS	-	expression tag	UNP P28845
A	10	MET	-	expression tag	UNP P28845
A	11	ALA	-	expression tag	UNP P28845
A	12	SER	-	expression tag	UNP P28845
A	13	MET	-	expression tag	UNP P28845
A	14	THR	-	expression tag	UNP P28845
A	15	GLY	-	expression tag	UNP P28845
A	16	GLY	-	expression tag	UNP P28845
A	17	GLN	-	expression tag	UNP P28845
A	18	GLN	-	expression tag	UNP P28845
A	19	MET	-	expression tag	UNP P28845
A	20	GLY	-	expression tag	UNP P28845
A	21	ARG	-	expression tag	UNP P28845
A	22	GLY	-	expression tag	UNP P28845
A	23	SER	-	expression tag	UNP P28845
A	262	ARG	LEU	engineered mutation	UNP P28845
A	278	GLU	PHE	engineered mutation	UNP P28845
B	7	GLY	-	expression tag	UNP P28845
B	8	SER	-	expression tag	UNP P28845

Continued on next page...

Continued from previous page...

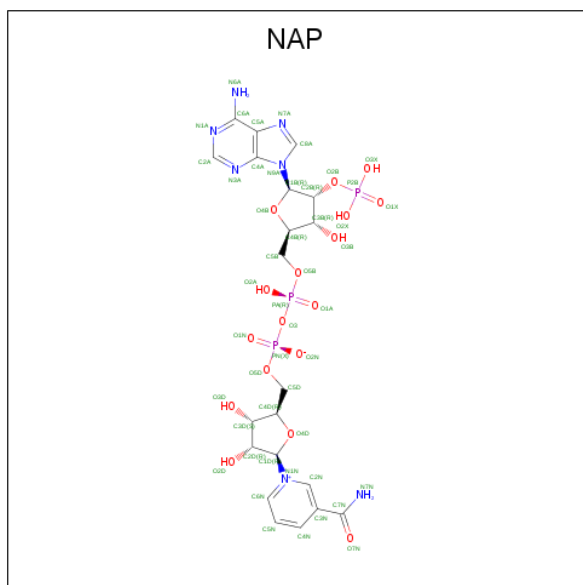
Chain	Residue	Modelled	Actual	Comment	Reference
B	9	HIS	-	expression tag	UNP P28845
B	10	MET	-	expression tag	UNP P28845
B	11	ALA	-	expression tag	UNP P28845
B	12	SER	-	expression tag	UNP P28845
B	13	MET	-	expression tag	UNP P28845
B	14	THR	-	expression tag	UNP P28845
B	15	GLY	-	expression tag	UNP P28845
B	16	GLY	-	expression tag	UNP P28845
B	17	GLN	-	expression tag	UNP P28845
B	18	GLN	-	expression tag	UNP P28845
B	19	MET	-	expression tag	UNP P28845
B	20	GLY	-	expression tag	UNP P28845
B	21	ARG	-	expression tag	UNP P28845
B	22	GLY	-	expression tag	UNP P28845
B	23	SER	-	expression tag	UNP P28845
B	262	ARG	LEU	engineered mutation	UNP P28845
B	278	GLU	PHE	engineered mutation	UNP P28845
D	7	GLY	-	expression tag	UNP P28845
D	8	SER	-	expression tag	UNP P28845
D	9	HIS	-	expression tag	UNP P28845
D	10	MET	-	expression tag	UNP P28845
D	11	ALA	-	expression tag	UNP P28845
D	12	SER	-	expression tag	UNP P28845
D	13	MET	-	expression tag	UNP P28845
D	14	THR	-	expression tag	UNP P28845
D	15	GLY	-	expression tag	UNP P28845
D	16	GLY	-	expression tag	UNP P28845
D	17	GLN	-	expression tag	UNP P28845
D	18	GLN	-	expression tag	UNP P28845
D	19	MET	-	expression tag	UNP P28845
D	20	GLY	-	expression tag	UNP P28845
D	21	ARG	-	expression tag	UNP P28845
D	22	GLY	-	expression tag	UNP P28845
D	23	SER	-	expression tag	UNP P28845
D	262	ARG	LEU	engineered mutation	UNP P28845
D	278	GLU	PHE	engineered mutation	UNP P28845
E	7	GLY	-	expression tag	UNP P28845
E	8	SER	-	expression tag	UNP P28845
E	9	HIS	-	expression tag	UNP P28845
E	10	MET	-	expression tag	UNP P28845
E	11	ALA	-	expression tag	UNP P28845
E	12	SER	-	expression tag	UNP P28845

Continued on next page...

Continued from previous page...

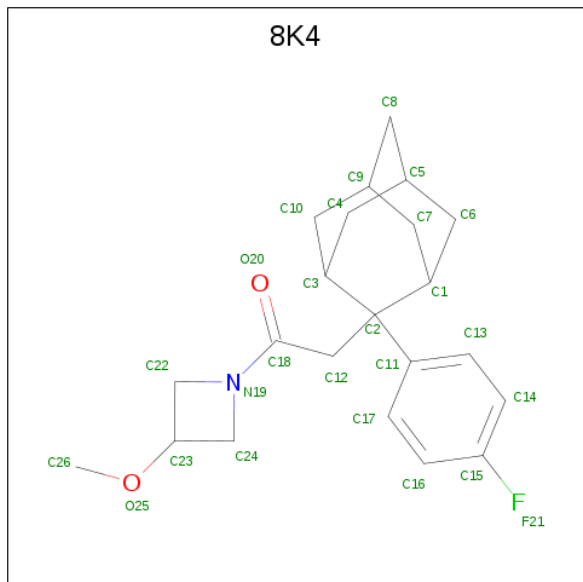
Chain	Residue	Modelled	Actual	Comment	Reference
E	13	MET	-	expression tag	UNP P28845
E	14	THR	-	expression tag	UNP P28845
E	15	GLY	-	expression tag	UNP P28845
E	16	GLY	-	expression tag	UNP P28845
E	17	GLN	-	expression tag	UNP P28845
E	18	GLN	-	expression tag	UNP P28845
E	19	MET	-	expression tag	UNP P28845
E	20	GLY	-	expression tag	UNP P28845
E	21	ARG	-	expression tag	UNP P28845
E	22	GLY	-	expression tag	UNP P28845
E	23	SER	-	expression tag	UNP P28845
E	262	ARG	LEU	engineered mutation	UNP P28845
E	278	GLU	PHE	engineered mutation	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	Total	C	H	N	O	P	28	0
			76	21	28	7	17	3		
2	B	1	Total	C	H	N	O	P	28	0
			76	21	28	7	17	3		
2	D	1	Total	C	H	N	O	P	28	0
			76	21	28	7	17	3		
2	E	1	Total	C	H	N	O	P	28	0
			76	21	28	7	17	3		

- Molecule 3 is 2-[2-(4-fluorophenyl)-2-adamantyl]-1-(3-methoxyazetid-1-yl)ethanone (three-letter code: 8K4) (formula: C₂₂H₂₈FNO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	H	N			O
3	A	1	Total	C	F	H	N	O	28	0
			54	22	1	28	1	2		
3	B	1	Total	C	F	H	N	O	28	0
			54	22	1	28	1	2		
3	D	1	Total	C	F	H	N	O	28	0
			54	22	1	28	1	2		
3	E	1	Total	C	F	H	N	O	28	0
			54	22	1	28	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	38	Total	O	0	0
			38	38		
4	D	17	Total	O	0	0
			17	17		
4	E	4	Total	O	0	0
			4	4		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.30Å 93.80Å 168.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.68 – 2.35 26.68 – 2.35	Depositor EDS
% Data completeness (in resolution range)	74.3 (26.68-2.35) 74.2 (26.68-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 2.34Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.230 , 0.254 0.239 , 0.266	Depositor DCC
R_{free} test set	1047 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtrriage
Anisotropy	0.562	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8673	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: NAP, 8K4

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	0.49	0/2030	0.64	0/2742
1	B	0.54	1/2103 (0.0%)	0.68	0/2836
1	D	0.44	0/2043	0.64	0/2758
1	E	0.43	0/2019	0.63	0/2729
All	All	0.48	1/8195 (0.0%)	0.65	0/11065

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	ASP	CG-OD2	6.42	1.40	1.25

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	1998	0	2026	7	0
1	B	2070	0	2098	10	1
1	D	2011	0	2040	8	0
1	E	1986	0	1987	8	0
2	A	48	28	25	1	0
2	B	48	28	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	28	25	0	0
2	E	48	28	25	0	0
3	A	26	28	0	0	0
3	B	26	28	0	1	0
3	D	26	28	0	1	0
3	E	26	28	0	0	0
4	A	29	0	0	0	0
4	B	38	0	0	1	0
4	D	17	0	0	0	0
4	E	4	0	0	0	0
All	All	8449	224	8251	27	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 2.

All (27) 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:D:145:LEU:HD12	1:E:133:ILE:HD11	1.64	0.80
1:D:145:LEU:HD21	1:E:137:ARG:NH2	2.12	0.65
1:D:145:LEU:CD1	1:E:133:ILE:HD11	2.28	0.61
1:B:130:HIS:NE2	1:B:132:ASP:OD2	2.35	0.60
1:B:67:SER:HB2	4:B:419:HOH:O	2.05	0.56
1:E:25:GLU:HG2	1:E:26:GLU:H	1.69	0.56
1:D:264:THR:HA	1:E:276:LEU:HD21	1.89	0.55
1:D:101:GLN:O	1:D:105:GLN:HG2	2.06	0.55
1:B:101:GLN:O	1:B:105:GLN:HG2	2.08	0.52
1:B:264:THR:O	1:B:268:ILE:HG13	2.10	0.51
1:A:203:VAL:HG21	1:A:286:MET:SD	2.57	0.45
3:B:302:8K4:C17	3:B:302:8K4:C18	2.96	0.44
1:D:36:LYS:HG2	1:D:110:MET:HB3	2.00	0.44
1:A:264:THR:HA	1:B:276:LEU:HD21	2.00	0.43
1:A:275:ILE:HD13	1:E:272:CYS:SG	2.58	0.43
1:D:141:GLU:HA	1:D:145:LEU:HB3	2.01	0.43
1:D:137:ARG:HH22	1:E:96:MET:HG3	1.84	0.43
1:B:257:TYR:CE2	1:B:269:ARG:HD3	2.55	0.42
1:A:169:SER:O	2:A:301:NAP:H6N	2.20	0.42
1:B:36:LYS:HG2	1:B:110:MET:HB3	2.01	0.42
3:D:302:8K4:C17	3:D:302:8K4:C18	2.98	0.41
1:A:276:LEU:HD21	1:B:264:THR:HA	2.03	0.41
1:B:175:VAL:HG23	1:B:177:TYR:CE2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:VAL:HB	1:B:231:VAL:HB	2.02	0.41
1:A:36:LYS:HG2	1:A:110:MET:HB3	2.01	0.40
1:A:175:VAL:HG23	1:A:177:TYR:CE1	2.56	0.40
1:E:36:LYS:HG2	1:E:110:MET:HB3	2.03	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:80:GLU:OE2	1:B:132:ASP:OD2[4_456]	2.17	0.03

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	260/286 (91%)	251 (96%)	8 (3%)	1 (0%)	34	38
1	B	271/286 (95%)	258 (95%)	12 (4%)	1 (0%)	34	38
1	D	264/286 (92%)	253 (96%)	10 (4%)	1 (0%)	34	38
1	E	261/286 (91%)	250 (96%)	10 (4%)	1 (0%)	34	38
All	All	1056/1144 (92%)	1012 (96%)	40 (4%)	4 (0%)	34	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	ASP
1	B	219	ASP
1	E	219	ASP
1	D	219	ASP

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	215/237 (91%)	209 (97%)	6 (3%)	43	53
1	B	222/237 (94%)	217 (98%)	5 (2%)	50	61
1	D	216/237 (91%)	213 (99%)	3 (1%)	67	78
1	E	210/237 (89%)	205 (98%)	5 (2%)	49	59
All	All	863/948 (91%)	844 (98%)	19 (2%)	52	63

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	105	GLN
1	A	199	LYS
1	A	262	ARG
1	A	284	TYR
1	A	285	ASN
1	B	24	ASN
1	B	28	ARG
1	B	199	LYS
1	B	269	ARG
1	B	284	TYR
1	D	68	LYS
1	D	77	HIS
1	D	199	LYS
1	E	25	GLU
1	E	68	LYS
1	E	105	GLN
1	E	199	LYS
1	E	284	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	77	HIS
1	B	134	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	8K4	E	302	-	26,30,30	0.59	1 (3%)	32,46,46	0.38	0
2	NAP	A	301	-	45,52,52	0.82	1 (2%)	56,80,80	0.89	2 (3%)
3	8K4	A	302	-	26,30,30	0.59	1 (3%)	32,46,46	0.71	1 (3%)
2	NAP	E	301	-	45,52,52	0.83	1 (2%)	56,80,80	0.89	2 (3%)
3	8K4	D	302	-	26,30,30	0.59	1 (3%)	32,46,46	0.79	1 (3%)
3	8K4	B	302	-	26,30,30	0.59	1 (3%)	32,46,46	0.79	1 (3%)
2	NAP	B	301	-	45,52,52	1.13	2 (4%)	56,80,80	0.88	2 (3%)
2	NAP	D	301	-	45,52,52	0.85	2 (4%)	56,80,80	0.81	2 (3%)

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
3	8K4	E	302	-	-	6/13/57/57	0/6/5/5
2	NAP	A	301	-	-	3/31/67/67	0/5/5/5
3	8K4	A	302	-	-	6/13/57/57	0/6/5/5
2	NAP	E	301	-	-	6/31/67/67	0/5/5/5
3	8K4	D	302	-	-	6/13/57/57	0/6/5/5
3	8K4	B	302	-	-	6/13/57/57	0/6/5/5
2	NAP	B	301	-	-	5/31/67/67	0/5/5/5
2	NAP	D	301	-	-	4/31/67/67	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C2N-N1N	5.82	1.42	1.35
2	E	301	NAP	C2N-N1N	4.21	1.40	1.35
2	D	301	NAP	C2N-N1N	3.91	1.39	1.35
2	A	301	NAP	C2N-N1N	3.44	1.39	1.35
3	D	302	8K4	C2-C11	2.50	1.58	1.51
3	E	302	8K4	C2-C11	2.37	1.57	1.51
3	A	302	8K4	C2-C11	2.35	1.57	1.51
2	D	301	NAP	P2B-O1X	-2.28	1.43	1.50
2	B	301	NAP	P2B-O1X	-2.27	1.43	1.50
3	B	302	8K4	C2-C11	2.24	1.57	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	8K4	O25-C23-C22	-4.17	103.85	113.99
3	B	302	8K4	O25-C23-C22	-4.15	103.90	113.99
2	E	301	NAP	O4D-C1D-C2D	-4.13	100.90	106.93
2	A	301	NAP	O4D-C1D-C2D	-3.60	101.67	106.93
3	A	302	8K4	O25-C23-C22	-3.48	105.51	113.99
2	B	301	NAP	O4D-C1D-C2D	-3.01	102.52	106.93
2	D	301	NAP	O4D-C1D-C2D	-2.94	102.64	106.93
2	A	301	NAP	C5A-C6A-N6A	2.60	124.30	120.35
2	B	301	NAP	C5A-C6A-N6A	2.60	124.30	120.35
2	E	301	NAP	C5A-C6A-N6A	2.44	124.05	120.35
2	D	301	NAP	C5A-C6A-N6A	2.43	124.04	120.35

There are no chirality outliers.

All (42) torsion outliers are listed below:

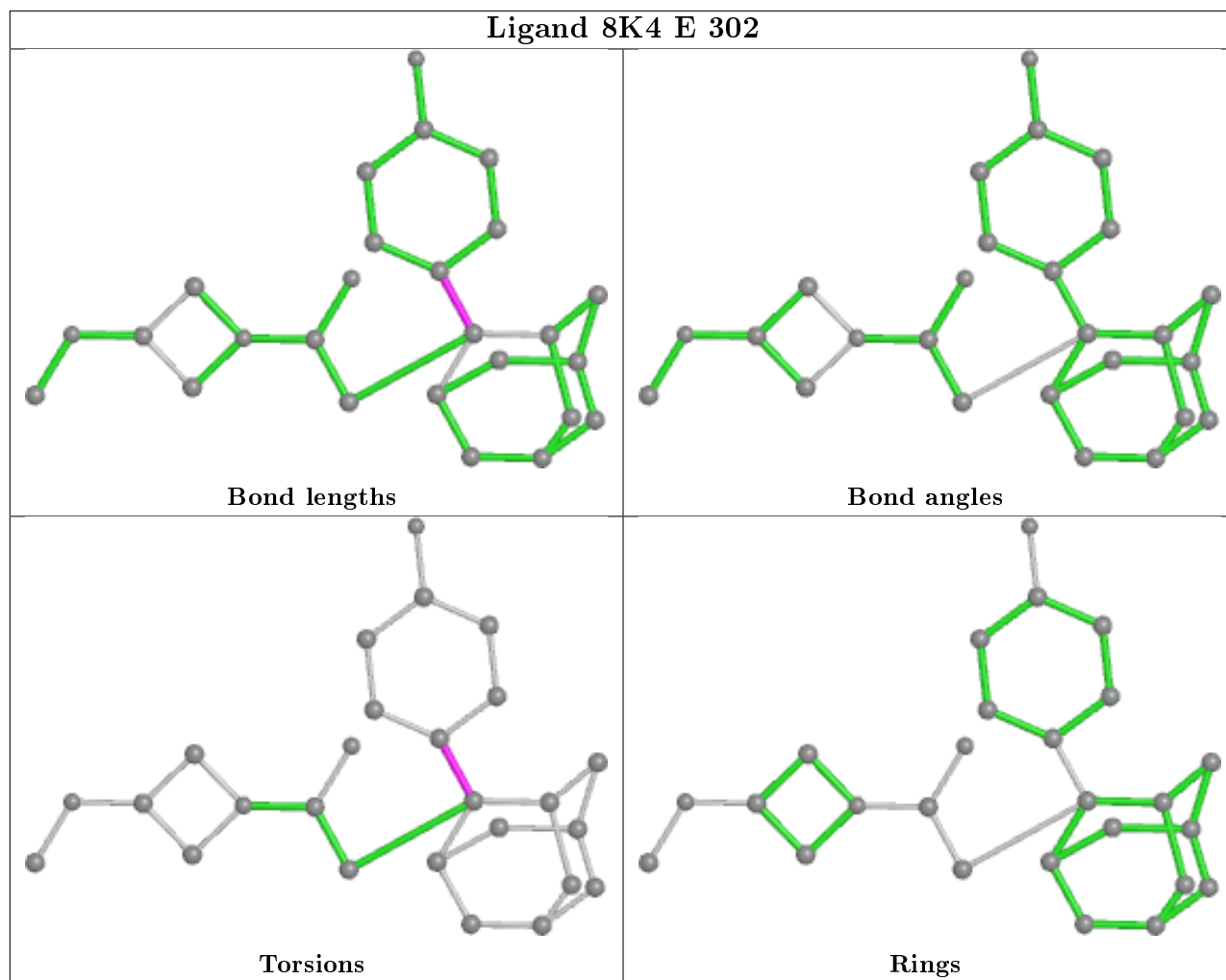
Mol	Chain	Res	Type	Atoms
3	E	302	8K4	C13-C11-C2-C3
3	E	302	8K4	C17-C11-C2-C3
3	A	302	8K4	C13-C11-C2-C3
3	A	302	8K4	C17-C11-C2-C3
2	E	301	NAP	C5D-O5D-PN-O1N
2	E	301	NAP	C5D-O5D-PN-O2N
3	D	302	8K4	C13-C11-C2-C3
3	D	302	8K4	C17-C11-C2-C3
3	B	302	8K4	C17-C11-C2-C3
3	E	302	8K4	C13-C11-C2-C12
3	E	302	8K4	C17-C11-C2-C12
3	A	302	8K4	C13-C11-C2-C12
3	A	302	8K4	C17-C11-C2-C12
3	D	302	8K4	C13-C11-C2-C12
3	D	302	8K4	C17-C11-C2-C12
3	B	302	8K4	C13-C11-C2-C12
3	B	302	8K4	C17-C11-C2-C12
2	B	301	NAP	C3B-C2B-O2B-P2B
3	E	302	8K4	C13-C11-C2-C1
3	E	302	8K4	C17-C11-C2-C1
3	A	302	8K4	C13-C11-C2-C1
3	A	302	8K4	C17-C11-C2-C1
3	D	302	8K4	C13-C11-C2-C1
3	D	302	8K4	C17-C11-C2-C1
3	B	302	8K4	C13-C11-C2-C1
3	B	302	8K4	C13-C11-C2-C3
3	B	302	8K4	C17-C11-C2-C1
2	B	301	NAP	C1B-C2B-O2B-P2B
2	D	301	NAP	PN-O3-PA-O1A
2	A	301	NAP	O4B-C4B-C5B-O5B
2	A	301	NAP	PN-O3-PA-O1A
2	E	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	O4B-C4B-C5B-O5B
2	A	301	NAP	C5D-O5D-PN-O3
2	E	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5D-O5D-PN-O3
2	D	301	NAP	O4B-C4B-C5B-O5B
2	E	301	NAP	PA-O3-PN-O1N
2	E	301	NAP	PA-O3-PN-O2N
2	D	301	NAP	PN-O3-PA-O2A
2	B	301	NAP	C5D-O5D-PN-O1N
2	D	301	NAP	C1B-C2B-O2B-P2B

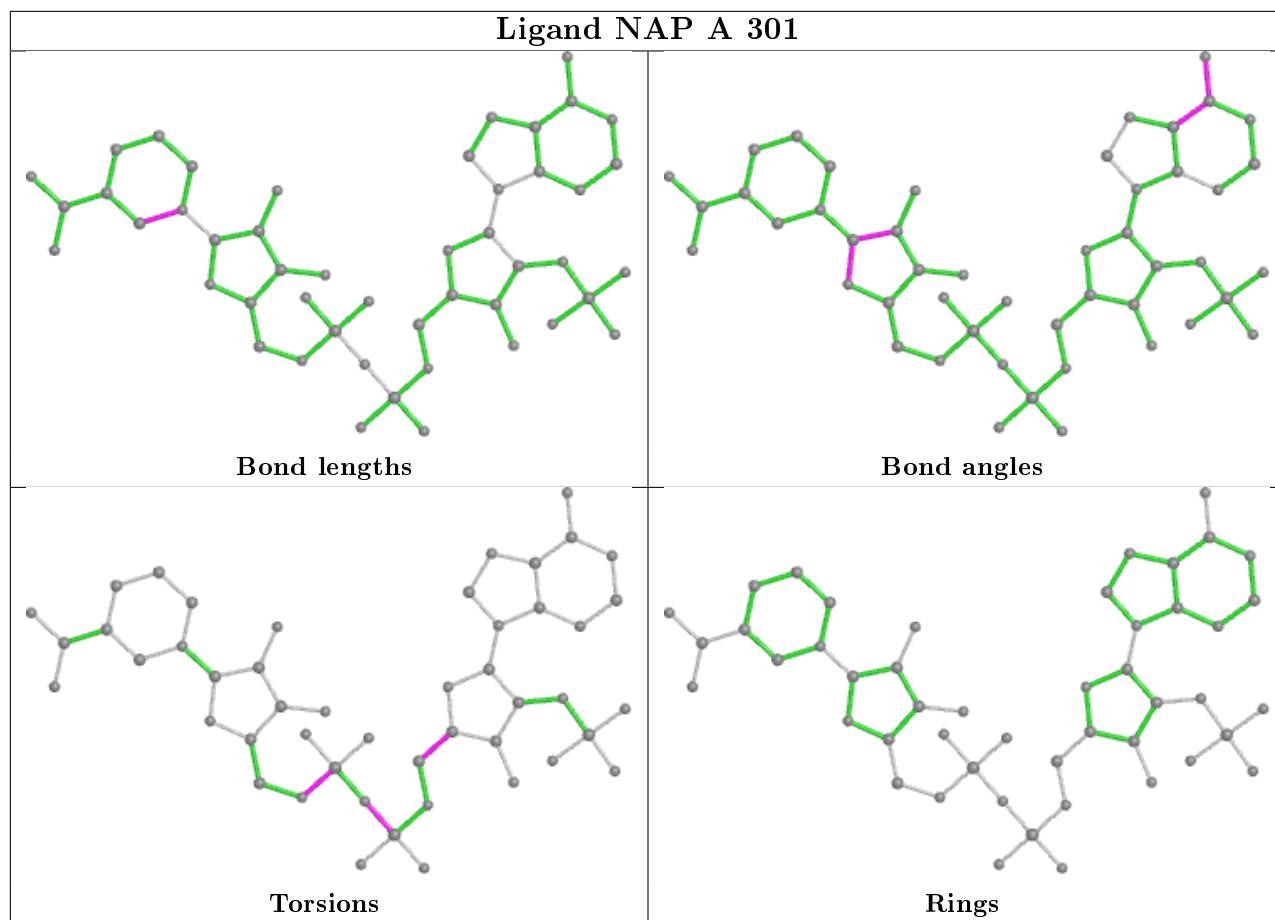
There are no ring outliers.

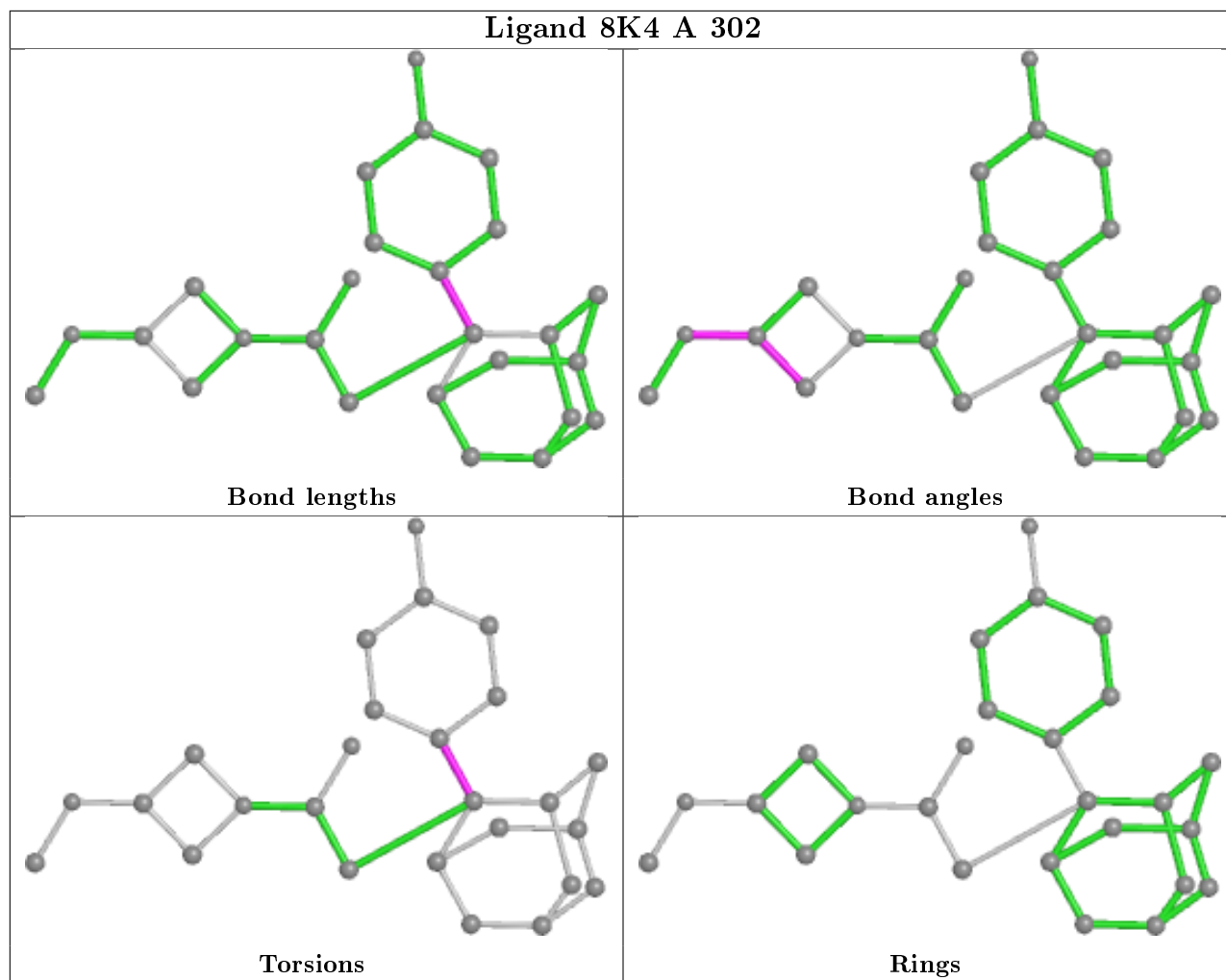
3 monomers are involved in 3 short contacts:

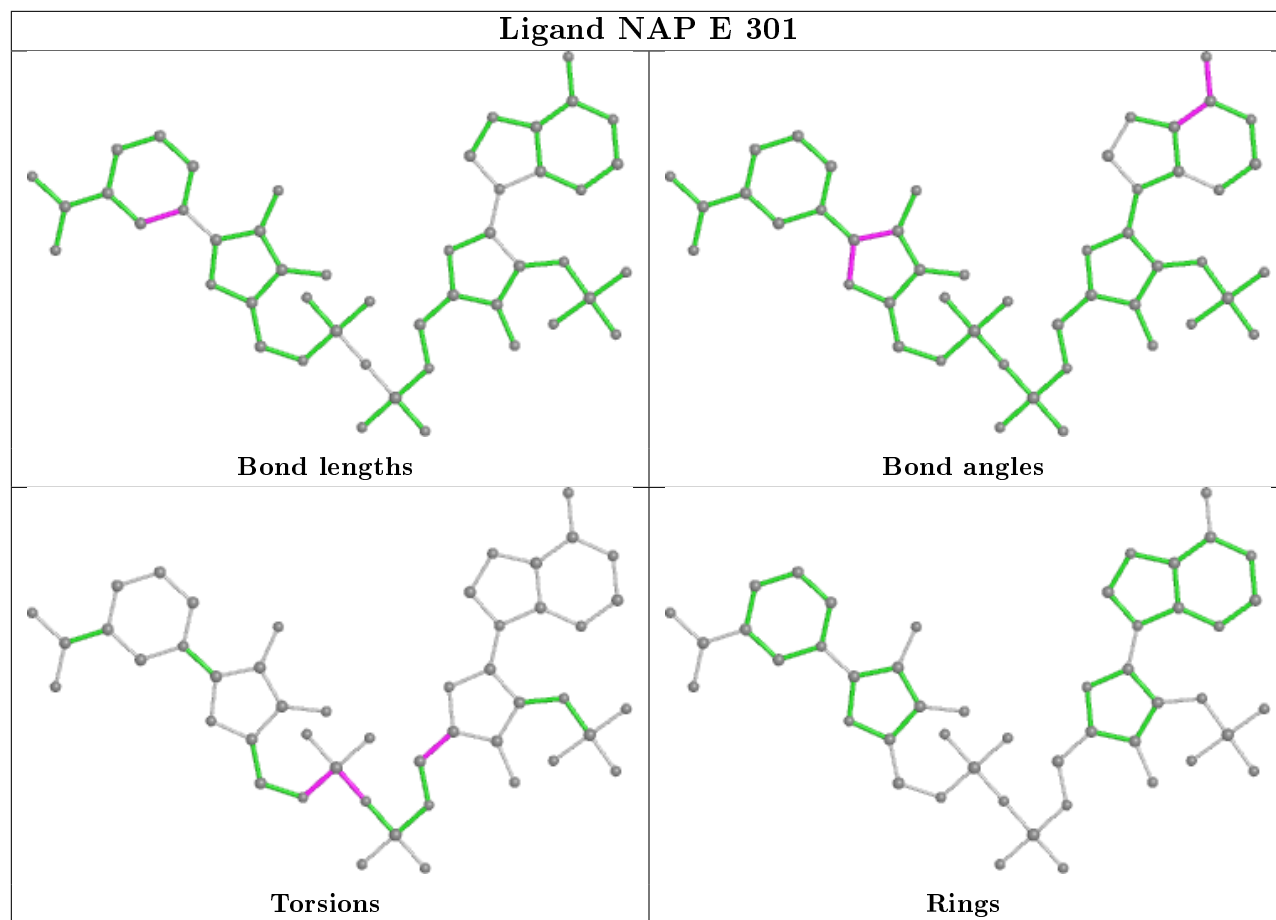
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAP	1	0
3	D	302	8K4	1	0
3	B	302	8K4	1	0

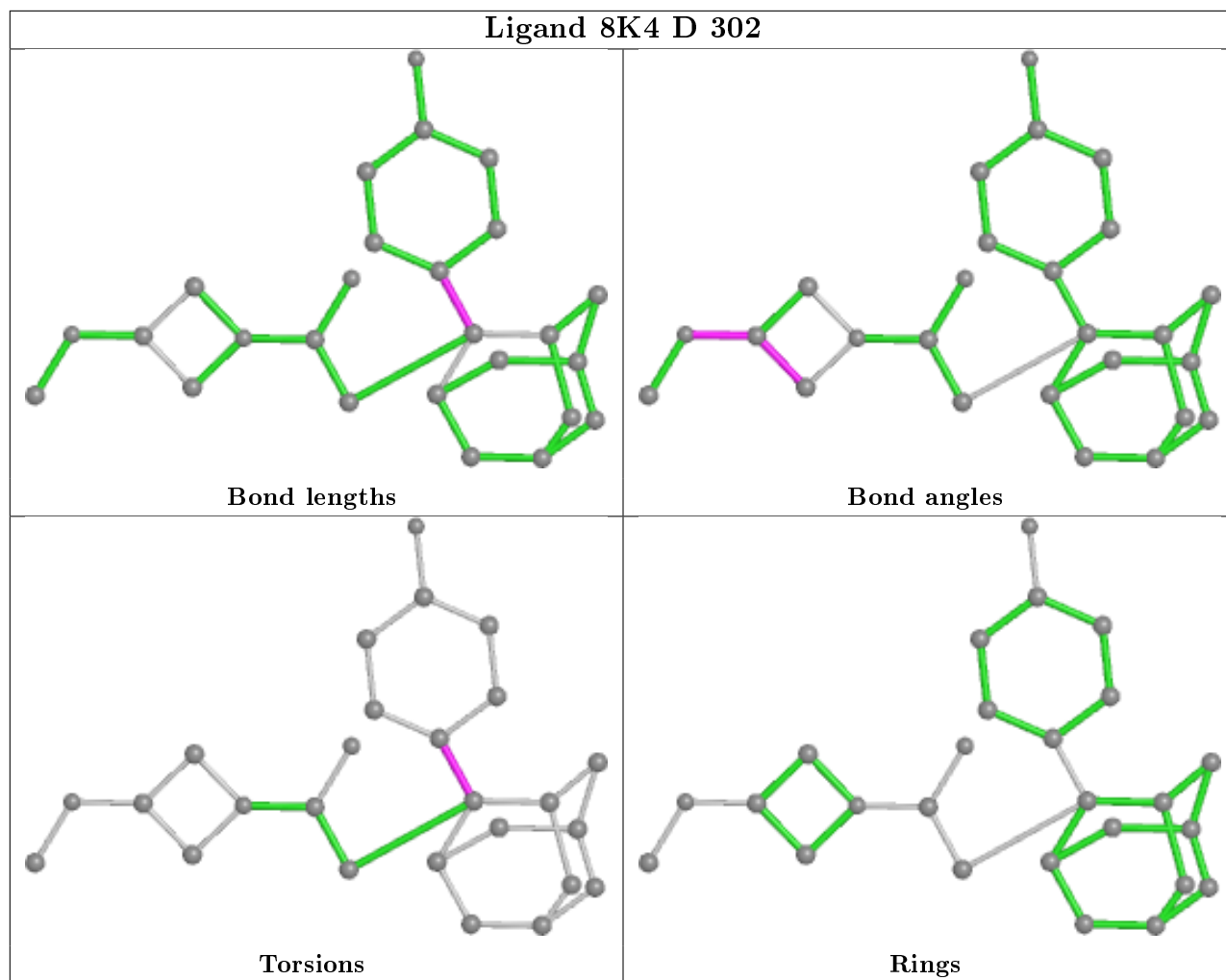
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

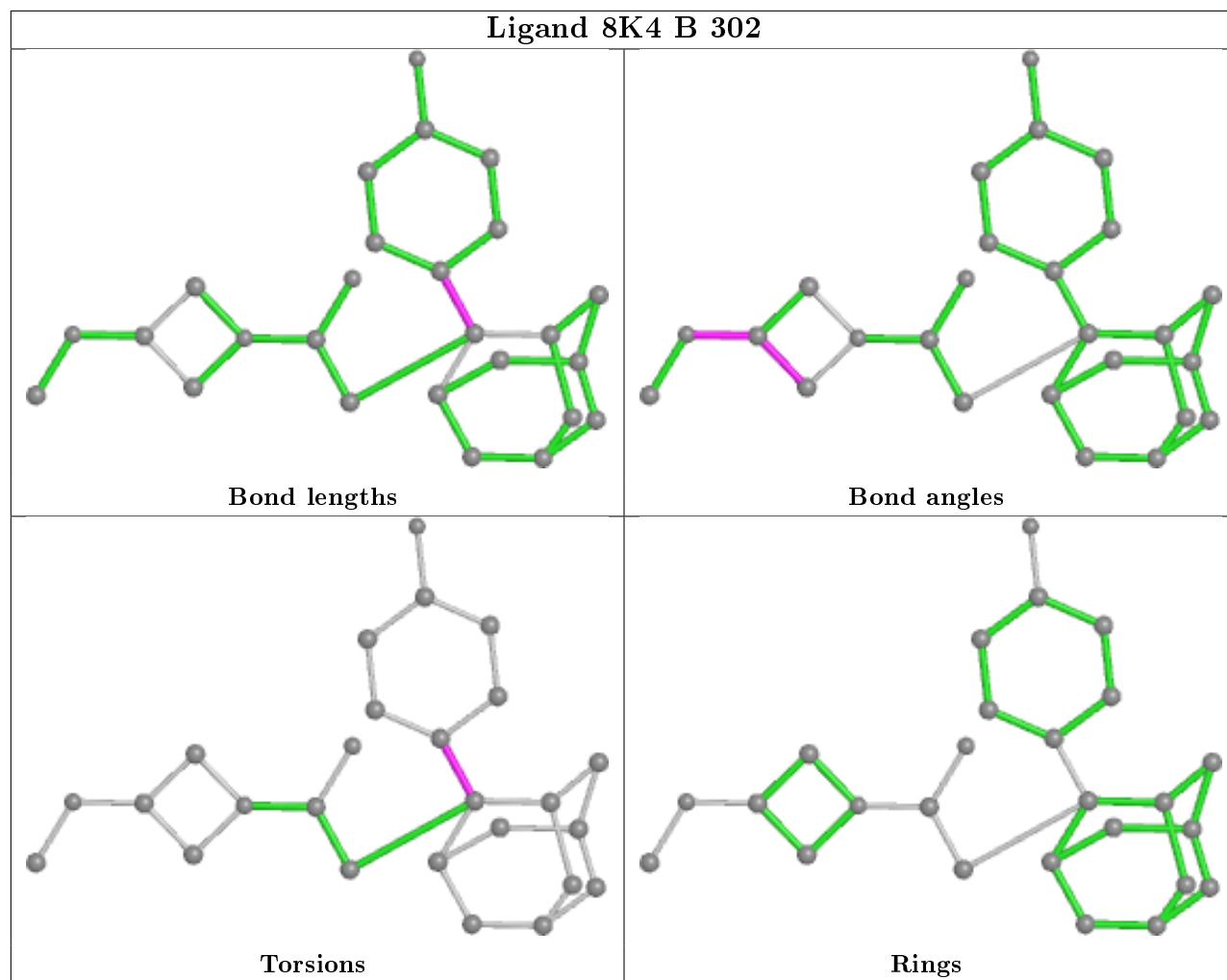


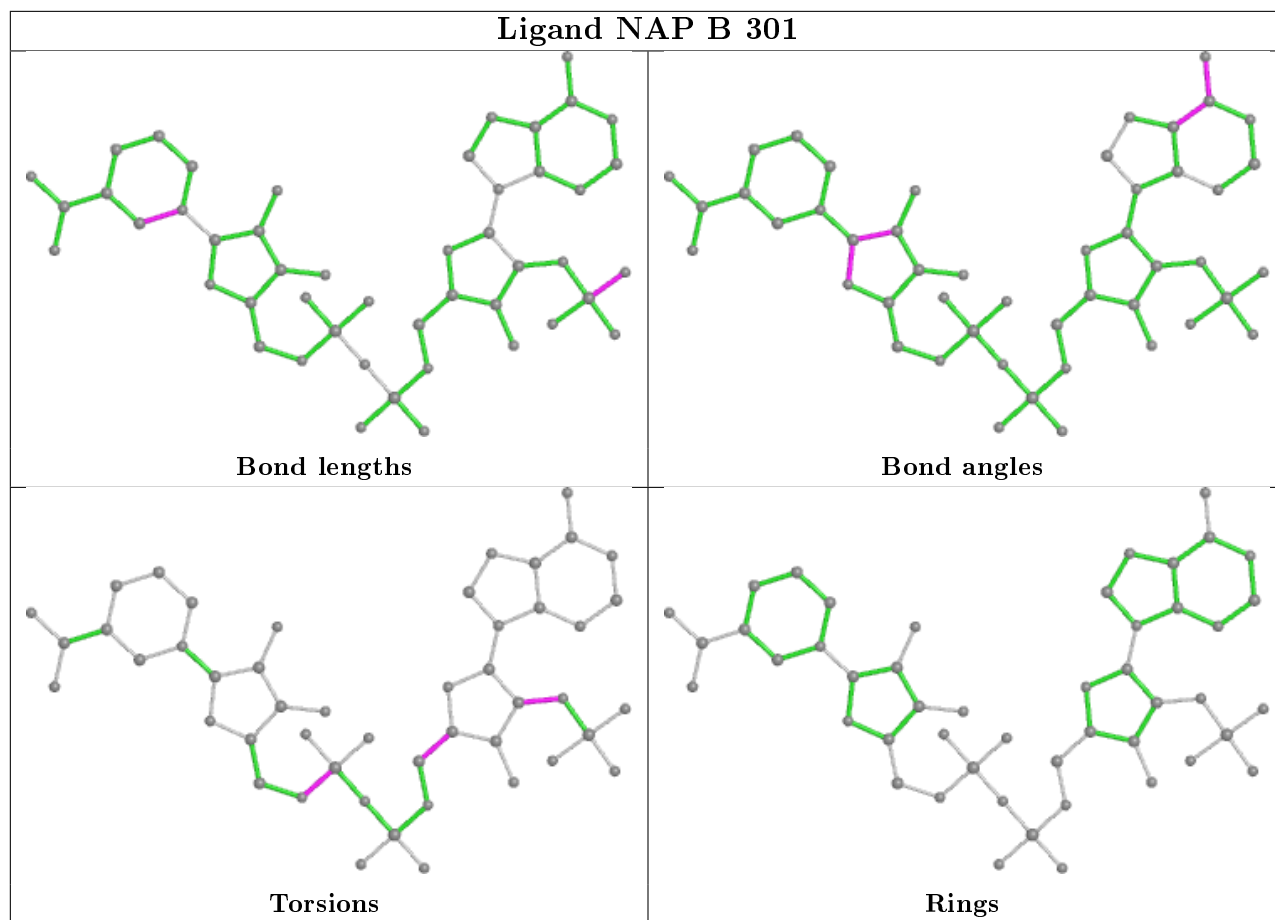


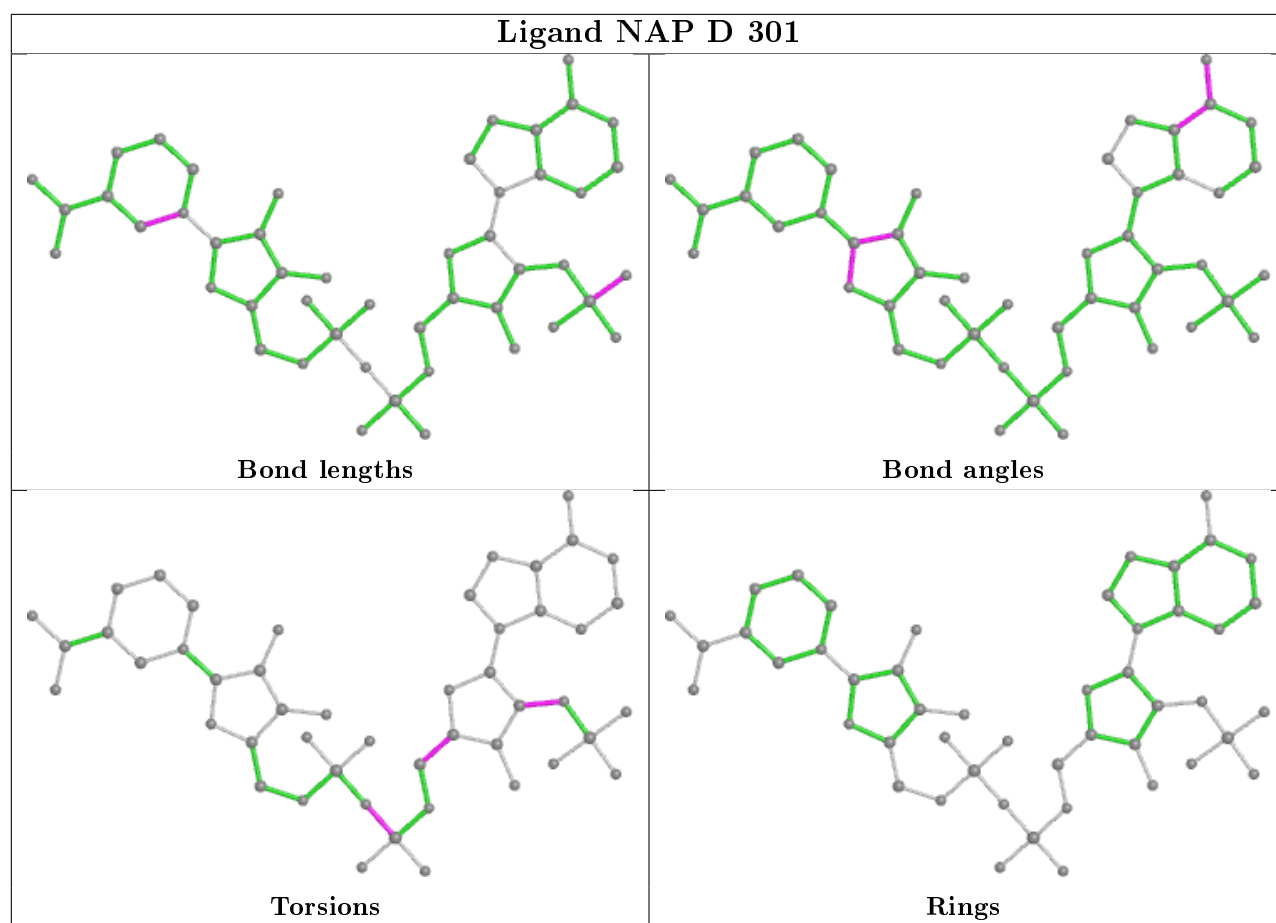












5.7 Other polymers [\(i\)](#)

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	262/286 (91%)	-0.05	5 (1%) 66 76	21, 34, 71, 128	0
1	B	273/286 (95%)	-0.21	11 (4%) 38 51	20, 29, 64, 129	0
1	D	266/286 (93%)	0.18	16 (6%) 21 32	25, 40, 83, 110	0
1	E	263/286 (91%)	0.54	32 (12%) 4 7	32, 55, 86, 146	0
All	All	1064/1144 (93%)	0.11	64 (6%) 21 32	20, 39, 79, 146	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	ILE	8.3
1	D	24	ASN	7.2
1	D	22	GLY	6.9
1	B	12	SER	6.5
1	D	19	MET	5.9
1	E	25	GLU	5.7
1	B	284	TYR	5.4
1	E	284	TYR	5.3
1	E	287	ASP	4.8
1	A	231	VAL	4.7
1	D	18	GLN	4.3
1	D	23	SER	4.2
1	E	229	GLY	3.9
1	B	13	MET	3.7
1	E	263	TRP	3.6
1	E	232	HIS	3.6
1	D	262	ARG	3.6
1	B	283	SER	3.5
1	E	286	MET	3.5
1	D	282	THR	3.5
1	E	41	GLY	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	262	ARG	3.5
1	E	40	THR	3.4
1	A	287	ASP	3.3
1	D	20	GLY	3.3
1	E	27	PHE	3.2
1	E	230	ILE	3.1
1	D	280	TYR	3.1
1	E	39	VAL	3.1
1	E	282	THR	3.1
1	D	25	GLU	2.8
1	E	283	SER	2.8
1	E	69	GLU	2.8
1	E	33	GLN	2.8
1	E	68	LYS	2.8
1	E	117	ILE	2.7
1	E	203	VAL	2.7
1	D	279	LEU	2.7
1	E	285	ASN	2.7
1	E	234	GLN	2.7
1	B	262	ARG	2.7
1	E	28	ARG	2.7
1	E	280	TYR	2.7
1	B	118	LEU	2.7
1	A	286	MET	2.7
1	E	26	GLU	2.6
1	D	263	TRP	2.6
1	E	119	ASN	2.4
1	E	118	LEU	2.4
1	B	279	LEU	2.4
1	E	160	GLN	2.4
1	B	117	ILE	2.3
1	E	231	VAL	2.3
1	D	130	HIS	2.3
1	D	21	ARG	2.3
1	B	278	GLU	2.2
1	B	280	TYR	2.2
1	E	168	VAL	2.2
1	D	118	LEU	2.1
1	E	64	THR	2.1
1	D	117	ILE	2.1
1	B	282	THR	2.0
1	A	263	TRP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	235	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

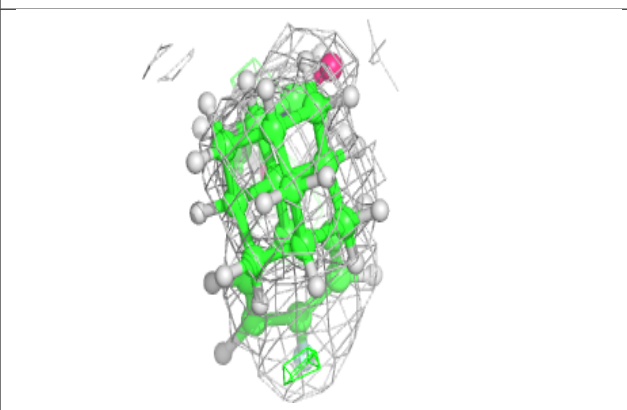
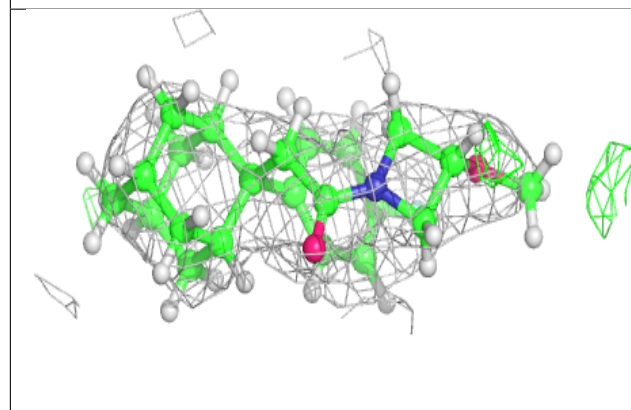
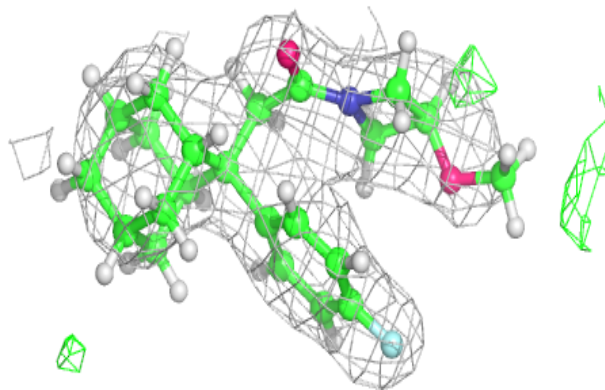
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	8K4	D	302	26/26	0.93	0.16	44,50,54,54	28
3	8K4	E	302	26/26	0.94	0.11	34,40,59,59	28
3	8K4	A	302	26/26	0.95	0.12	25,29,45,45	28
3	8K4	B	302	26/26	0.95	0.12	24,27,53,53	28
2	NAP	E	301	48/48	0.96	0.13	37,45,53,56	28
2	NAP	D	301	48/48	0.97	0.09	21,33,37,39	28
2	NAP	B	301	48/48	0.98	0.10	10,21,32,35	28
2	NAP	A	301	48/48	0.98	0.10	22,28,32,38	28

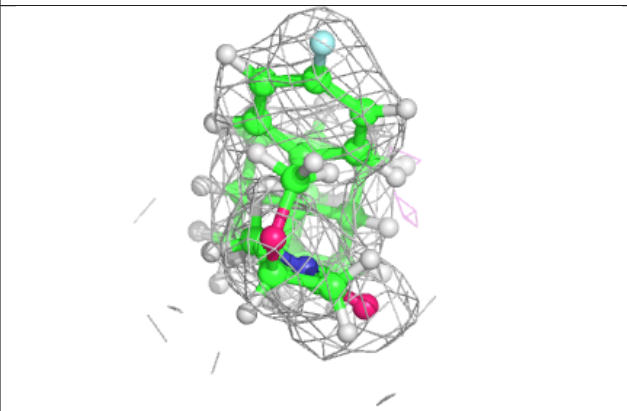
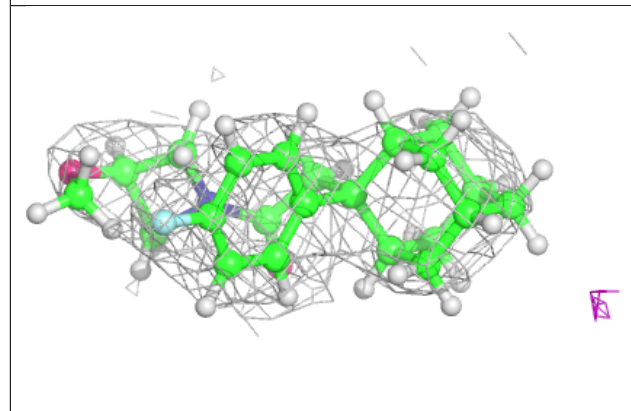
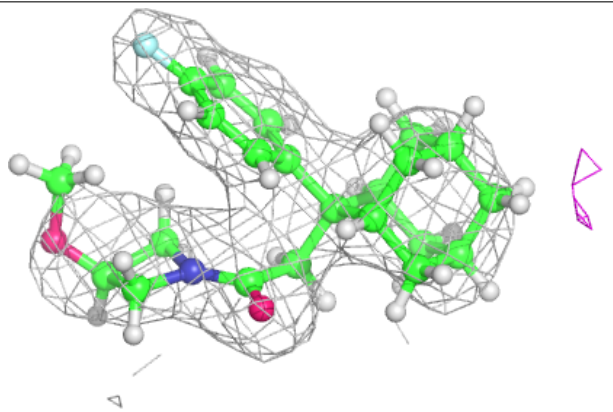
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8K4 D 302:

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

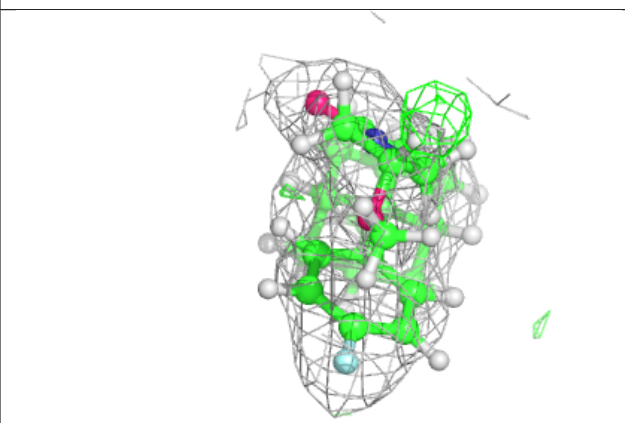
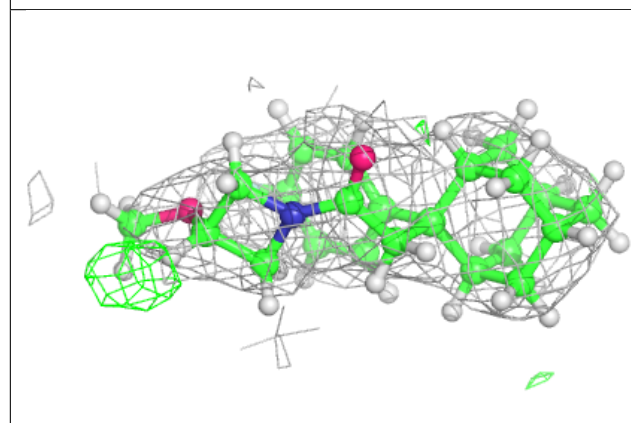
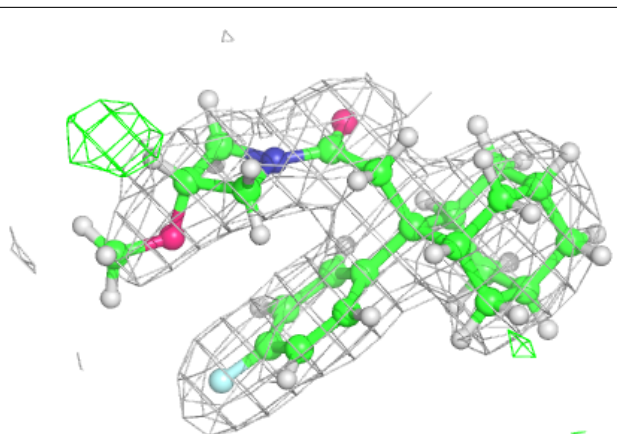
**Electron density around 8K4 E 302:**

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

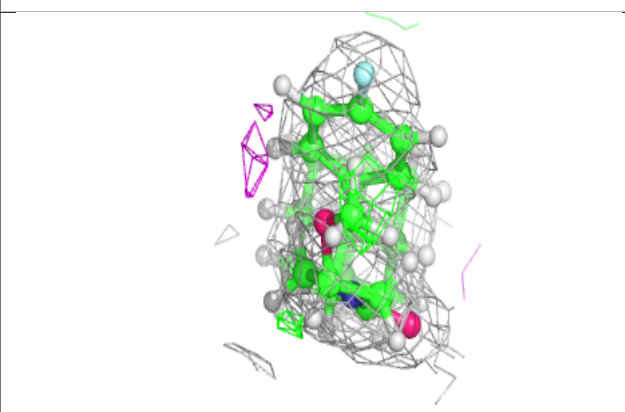
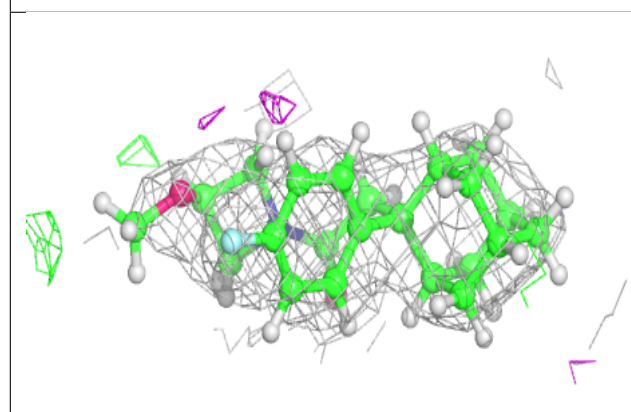
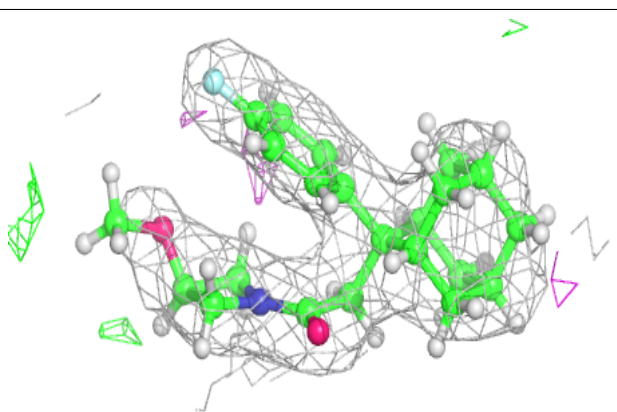


Electron density around 8K4 A 302:

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

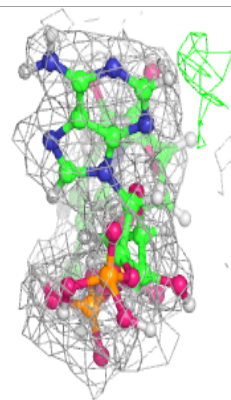
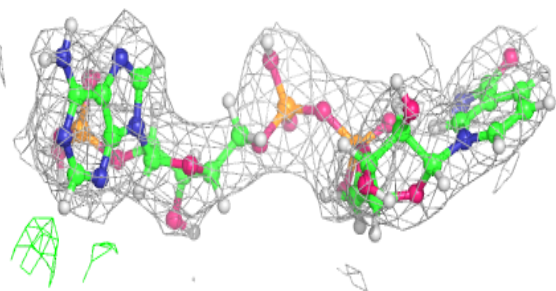
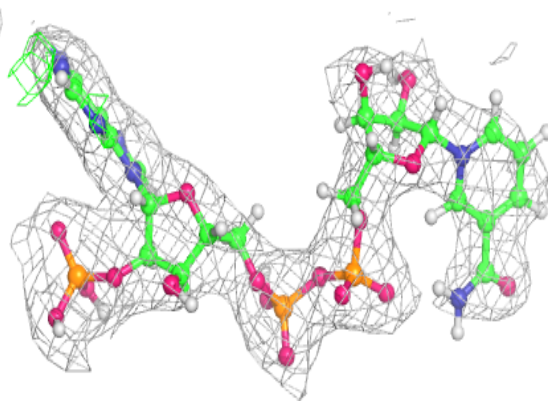
**Electron density around 8K4 B 302:**

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

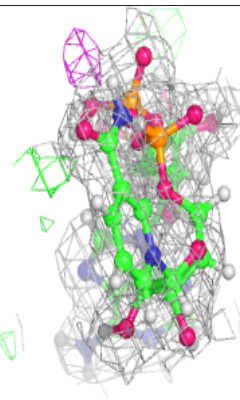
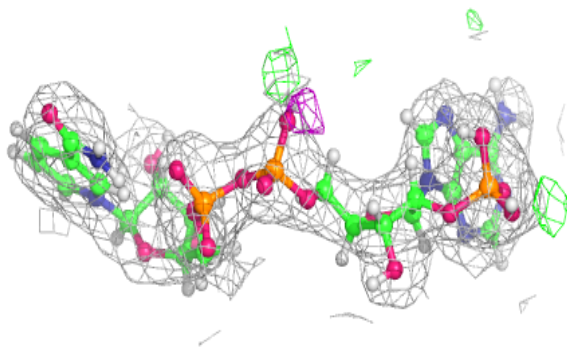
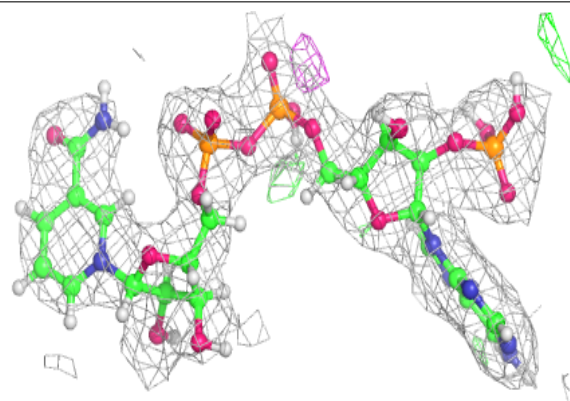


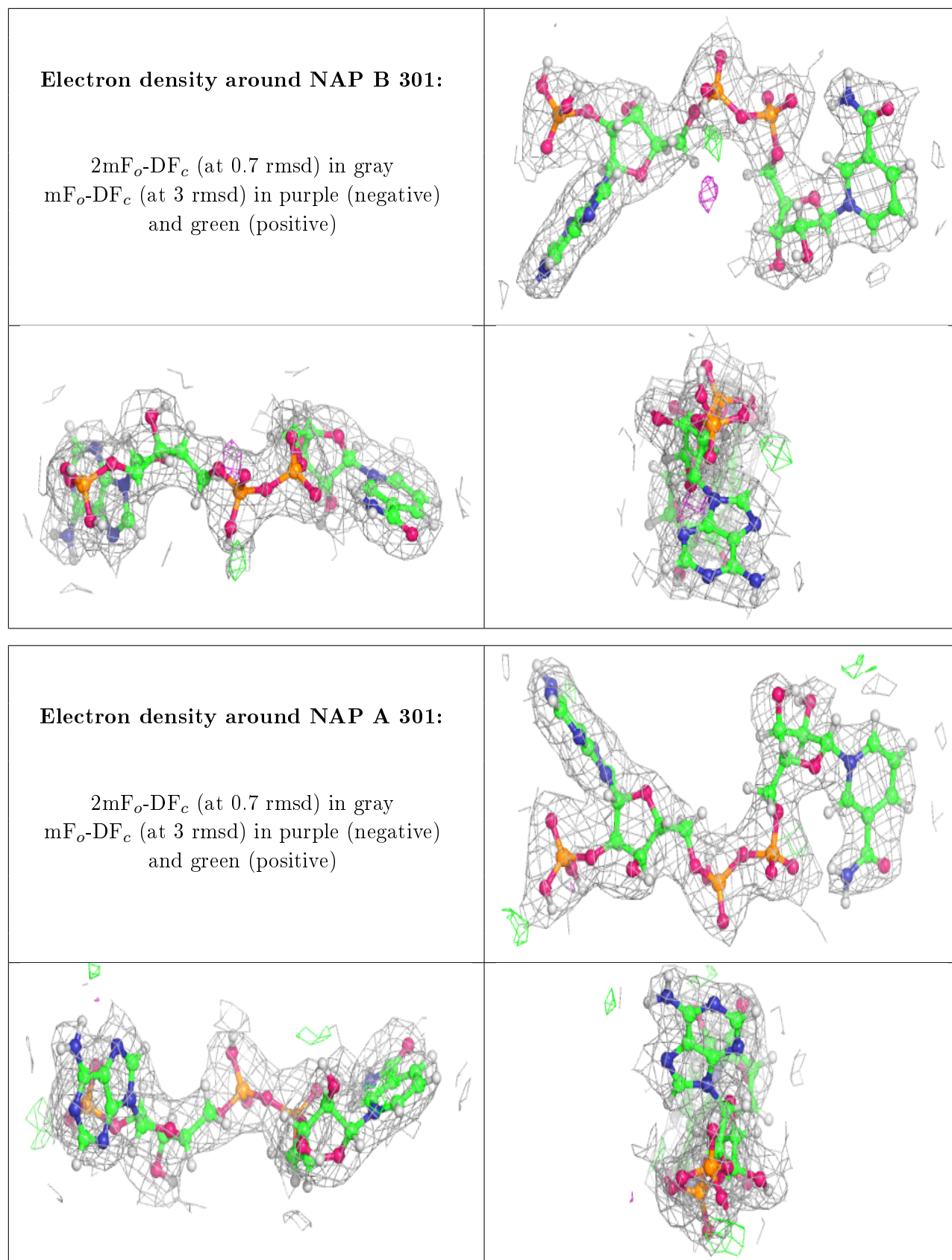
Electron density around NAP E 301:

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

**Electron density around NAP D 301:**

$2mF_o-DF_c$ (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.