



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:42 PM UTC

PDB ID : 5QII / pdb_00005qii
Title : CRYSTAL STRUCTURE OF 11BETA-HSD1 DOUBLE MUTANT (L262R, F278E) COMPLEXED WITH 2-(3-(1-(4-CHLOROPHENYL)CYCLOPROPYL) -[1,2,4]TRIAZOLO[4,3-A]PYRIDIN-8-YL)PROPAN-2-OL
Authors : Sheriff, S.
Deposited on : 2018-07-03
Resolution : 2.45 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:

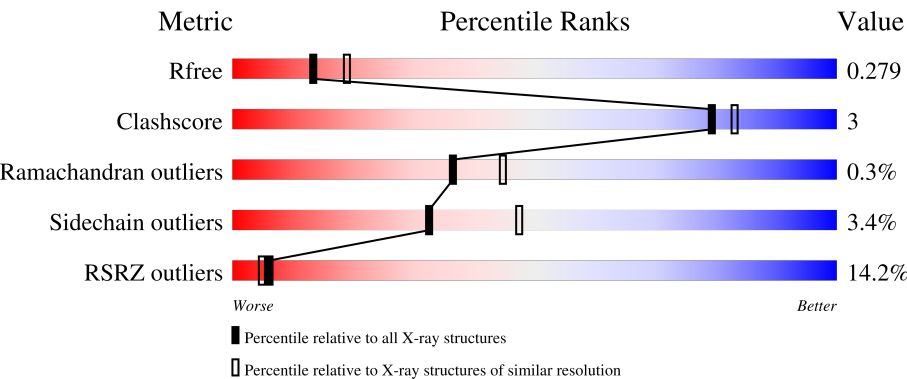
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	286	18% 80%10%8%
1	B	286	31% 83%8%7%
1	D	286	84%11%5%
1	E	286	3% 81%10%7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8728 atoms, of which 184 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
1	A	262	Total	C	N	O	S	0	1	0
			2007	1276	342	373	16			
1	B	265	Total	C	N	O	S	0	0	0
			2030	1291	347	375	17			
1	D	273	Total	C	N	O	S	0	0	0
			2070	1311	354	387	18			
1	E	265	Total	C	N	O	S	0	0	0
			2026	1286	344	379	17			

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

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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

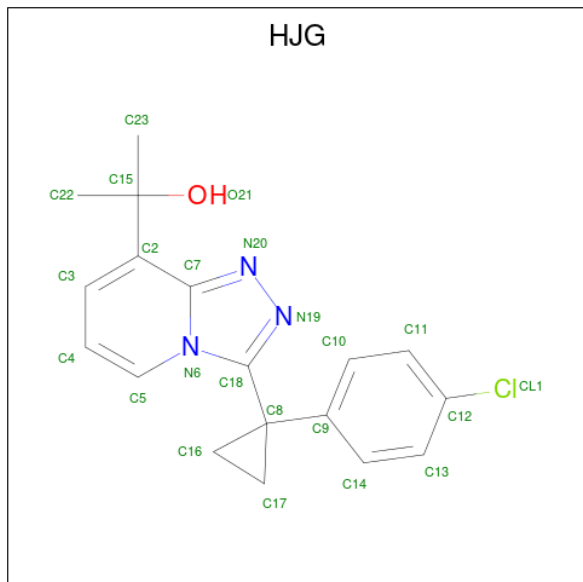
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Chain	Residue	Modelled	Actual	Comment	Reference
E	13	MET	-	expression tag	UNP P28845
E	14	THR	-	expression tag	UNP P28845
E	15	GLY	-	expression tag	UNP P28845
E	16	GLY	-	expression tag	UNP P28845
E	17	GLN	-	expression tag	UNP P28845
E	18	GLN	-	expression 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

- # NAP
-
- The image displays the chemical structure of Naproxen (NAP), a non-steroidal anti-inflammatory drug. The structure is shown with stereochemistry and atom numbering. The naphthalene ring system is colored blue, and the propionic acid side chain is colored red. The stereochemistry is indicated by wedges and dashes at the chiral centers C4 and C5. The carboxylic acid group is shown in red, and the naphthalene ring is shown in blue.
- Chemical structure of Naproxen (NAP) is shown, featuring a naphthalene ring system substituted with a propionic acid side chain. The structure includes stereochemistry (wedges and dashes) and atom numbering (1-15). The carboxylic acid group is highlighted in red, and the naphthalene ring is highlighted in blue.



- Molecule 3 is 2-{3-[1-(4-chlorophenyl)cyclopropyl][1,2,4]triazolo[4,3-a]pyridin-8-yl}propan-2-ol (CCD ID: HJG) (formula: C₁₈H₁₈ClN₃O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	N	O	18	0
			41	18	1	18	3	1		
3	B	1	Total	C	Cl	H	N	O	18	0
			41	18	1	18	3	1		
3	D	1	Total	C	Cl	H	N	O	18	0
			41	18	1	18	3	1		
3	E	1	Total	C	Cl	H	N	O	18	0
			41	18	1	18	3	1		

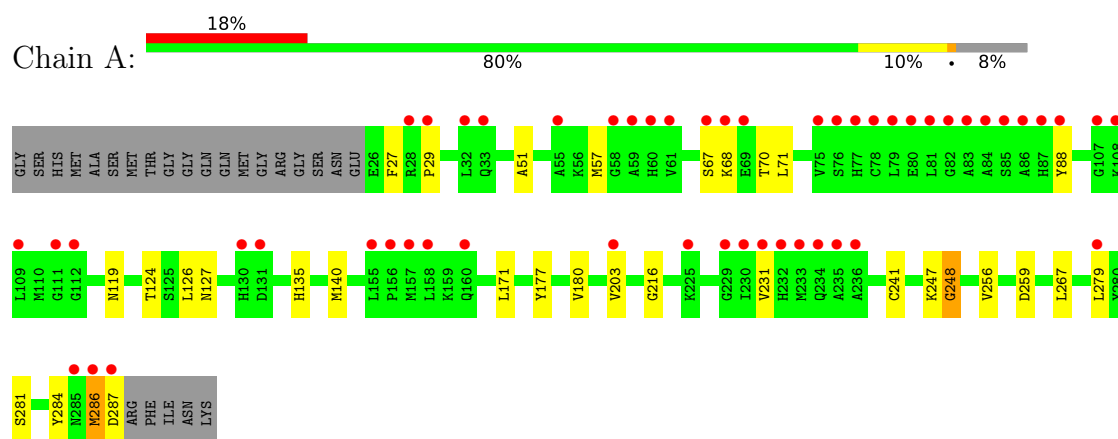
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	14	Total	O	0	0
			14	14		
4	D	58	Total	O	0	0
			58	58		
4	E	34	Total	O	0	0
			34	34		

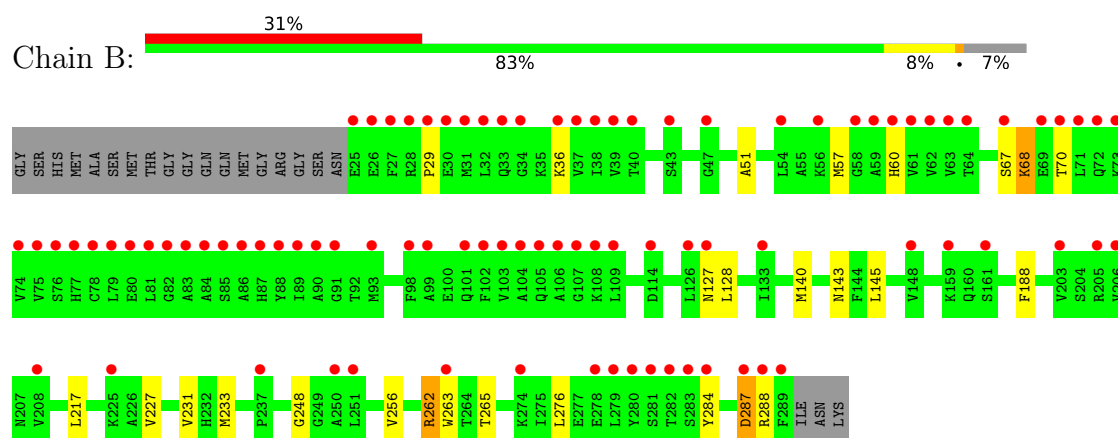
3 Residue-property plots [i](#)

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.

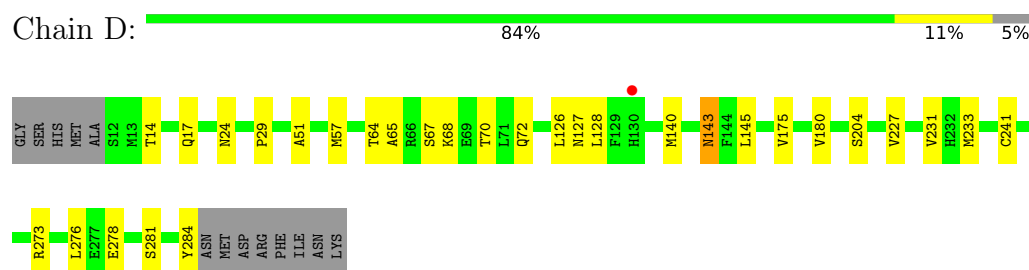
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



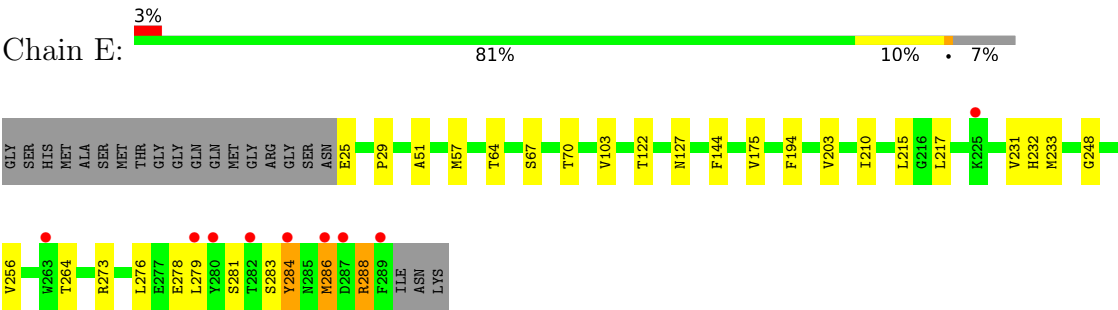
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



● Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.50Å 93.90Å 162.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 2.45 46.96 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.96-2.45) 98.7 (46.96-2.45)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.222 , 0.261 0.240 , 0.279	Depositor DCC
R_{free} test set	1073 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8728	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: HJG, NAP

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	0/2044	1.45	12/2761 (0.4%)
1	B	0.79	0/2064	1.44	12/2786 (0.4%)
1	D	0.85	0/2103	1.43	14/2837 (0.5%)
1	E	0.83	0/2058	1.45	10/2776 (0.4%)
All	All	0.81	0/8269	1.44	48/11160 (0.4%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	SER	CA-C-N	6.86	129.36	120.44
1	D	67	SER	C-N-CA	6.86	129.36	120.44
1	A	171	LEU	N-CA-C	-6.38	104.42	111.82
1	A	67	SER	CA-C-N	6.38	128.73	120.44
1	A	67	SER	C-N-CA	6.38	128.73	120.44
1	E	284	TYR	CA-C-N	6.23	130.94	122.84
1	E	284	TYR	C-N-CA	6.23	130.94	122.84
1	E	67	SER	CA-C-N	6.15	128.44	120.44
1	E	67	SER	C-N-CA	6.15	128.44	120.44
1	B	67	SER	CA-C-N	6.07	128.33	120.44
1	B	67	SER	C-N-CA	6.07	128.33	120.44
1	B	188	PHE	CA-C-N	5.87	128.14	120.28
1	B	188	PHE	C-N-CA	5.87	128.14	120.28
1	A	119	ASN	CA-CB-CG	5.64	118.24	112.60
1	A	51	ALA	CA-C-N	5.50	127.66	120.28
1	A	51	ALA	C-N-CA	5.50	127.66	120.28
1	A	248	GLY	CA-C-N	5.43	125.96	119.94
1	A	248	GLY	C-N-CA	5.43	125.96	119.94
1	D	64	THR	CA-C-N	5.39	131.84	121.54
1	D	64	THR	C-N-CA	5.39	131.84	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	ALA	CA-C-N	5.39	127.50	120.28
1	E	51	ALA	C-N-CA	5.39	127.50	120.28
1	D	241	CYS	CA-C-N	5.36	127.72	120.38
1	D	241	CYS	C-N-CA	5.36	127.72	120.38
1	E	64	THR	CA-C-N	5.30	131.67	121.54
1	E	64	THR	C-N-CA	5.30	131.67	121.54
1	B	287	ASP	CA-C-N	5.18	131.44	121.54
1	B	287	ASP	C-N-CA	5.18	131.44	121.54
1	D	143	ASN	CA-CB-CG	5.18	117.78	112.60
1	D	51	ALA	CA-C-N	5.17	127.21	120.28
1	D	51	ALA	C-N-CA	5.17	127.21	120.28
1	E	103	VAL	CA-C-N	5.14	127.12	120.44
1	E	103	VAL	C-N-CA	5.14	127.12	120.44
1	B	68	LYS	CA-C-N	5.12	127.14	120.28
1	B	68	LYS	C-N-CA	5.12	127.14	120.28
1	B	51	ALA	CA-C-N	5.07	127.08	120.28
1	B	51	ALA	C-N-CA	5.07	127.08	120.28
1	B	262	ARG	CA-C-N	5.07	127.07	120.28
1	B	262	ARG	C-N-CA	5.07	127.07	120.28
1	D	24	ASN	N-CA-C	-5.05	107.11	113.28
1	A	241	CYS	CA-C-N	5.05	127.30	120.38
1	A	241	CYS	C-N-CA	5.05	127.30	120.38
1	D	68	LYS	CA-C-N	5.03	127.02	120.28
1	D	68	LYS	C-N-CA	5.03	127.02	120.28
1	A	68	LYS	CA-C-N	5.01	126.99	120.28
1	A	68	LYS	C-N-CA	5.01	126.99	120.28
1	D	204	SER	CA-C-N	5.00	129.51	122.46
1	D	204	SER	C-N-CA	5.00	129.51	122.46

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	2007	0	2037	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2030	0	2063	15	0
1	D	2070	0	2096	13	0
1	E	2026	0	2061	17	0
2	A	48	28	25	0	0
2	B	48	28	25	0	0
2	D	48	28	25	0	0
2	E	48	28	25	0	0
3	A	23	18	0	0	0
3	B	23	18	0	0	0
3	D	23	18	0	0	0
3	E	23	18	0	0	0
4	A	21	0	0	0	0
4	B	14	0	0	0	0
4	D	58	0	0	0	0
4	E	34	0	0	0	0
All	All	8544	184	8357	45	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 3.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:MET:HE1	1:B:128:LEU:HD21	1.55	0.87
1:A:203:VAL:HG21	1:A:286:MET:SD	2.18	0.84
1:E:203:VAL:HG21	1:E:286:MET:HE2	1.69	0.73
1:D:140:MET:HE3	1:E:144:PHE:CE2	2.33	0.63
1:D:128:LEU:HD21	1:E:286:MET:HE3	1.83	0.59
1:A:140:MET:HE2	1:B:140:MET:HE2	1.85	0.58
1:E:217:LEU:HD22	1:E:233:MET:HG3	1.85	0.58
1:E:281:SER:HA	1:E:284:TYR:CZ	2.40	0.57
1:D:281:SER:HA	1:D:284:TYR:CZ	2.40	0.56
1:A:281:SER:HA	1:A:284:TYR:CZ	2.42	0.55
1:E:231:VAL:HG12	1:E:233:MET:HG2	1.89	0.54
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.89	0.53
1:D:248:GLY:HA3	1:D:256:VAL:HG21	1.90	0.53
1:B:263:TRP:HH2	1:E:279:LEU:HD21	1.73	0.53
1:A:216:GLY:HA3	1:A:259:ASP:OD1	2.09	0.53
1:D:227:VAL:HB	1:D:231:VAL:HB	1.90	0.52
1:B:217:LEU:HD22	1:B:233:MET:HG3	1.91	0.52
1:E:248:GLY:HA3	1:E:256:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:THR:HA	1:E:276:LEU:HD21	1.93	0.51
1:B:231:VAL:HG12	1:B:233:MET:HG2	1.91	0.50
1:A:177:TYR:HE2	1:B:284:TYR:HH	1.55	0.50
1:B:263:TRP:CH2	1:E:279:LEU:HD21	2.46	0.50
1:D:29:PRO:HB3	1:D:57:MET:HG2	1.94	0.49
1:A:177:TYR:HE2	1:B:284:TYR:OH	1.95	0.49
1:B:29:PRO:HB3	1:B:57:MET:HG2	1.96	0.48
1:A:286:MET:CE	1:B:128:LEU:HD21	2.37	0.47
1:E:29:PRO:HB3	1:E:57:MET:HG2	1.97	0.45
1:D:273:ARG:HG3	1:E:175:VAL:HG12	2.00	0.44
1:D:276:LEU:HD21	1:E:264:THR:HA	2.00	0.44
1:A:29:PRO:HB3	1:A:57:MET:HG2	2.00	0.43
1:B:36:LYS:HA	1:B:60:HIS:HB2	2.00	0.43
1:A:124:THR:HG23	1:A:135:HIS:NE2	2.33	0.43
1:B:248:GLY:HA3	1:B:256:VAL:HG21	2.01	0.43
1:A:27:PHE:CD2	1:A:247:LYS:HG2	2.53	0.43
1:B:227:VAL:HB	1:B:231:VAL:HB	2.00	0.43
1:D:175:VAL:HG12	1:E:273:ARG:HG3	2.00	0.42
1:D:231:VAL:HG12	1:D:233:MET:HG2	2.01	0.42
1:E:194:PHE:HB3	1:E:210:ILE:HG21	2.01	0.42
1:A:126:LEU:HD23	1:A:180:VAL:HG13	2.02	0.42
1:D:126:LEU:HD23	1:D:180:VAL:HG13	2.01	0.42
1:A:71:LEU:HD13	1:A:88:TYR:HB2	2.02	0.41
1:E:248:GLY:HA3	1:E:256:VAL:CG2	2.50	0.41
1:A:267:LEU:HB2	1:B:276:LEU:HG	2.03	0.41
1:D:233:MET:HE2	1:E:283:SER:CB	2.51	0.40
1:A:279:LEU:HD22	1:B:263:TRP:HZ3	1.86	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	261/286 (91%)	250 (96%)	11 (4%)	0	100	100
1	B	263/286 (92%)	251 (95%)	11 (4%)	1 (0%)	30	37
1	D	271/286 (95%)	259 (96%)	11 (4%)	1 (0%)	30	37
1	E	263/286 (92%)	251 (95%)	11 (4%)	1 (0%)	30	37
All	All	1058/1144 (92%)	1011 (96%)	44 (4%)	3 (0%)	36	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	288	ARG
1	E	288	ARG
1	D	65	ALA

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	217/237 (92%)	212 (98%)	5 (2%)	44	59
1	B	219/237 (92%)	211 (96%)	8 (4%)	30	44
1	D	222/237 (94%)	214 (96%)	8 (4%)	31	45
1	E	220/237 (93%)	211 (96%)	9 (4%)	27	40
All	All	878/948 (93%)	848 (97%)	30 (3%)	32	47

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	THR
1	A	127	ASN
1	A	231	VAL
1	A	286	MET
1	A	287	ASP
1	B	68	LYS
1	B	70	THR
1	B	127	ASN

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Mol	Chain	Res	Type
1	B	143	ASN
1	B	145	LEU
1	B	262	ARG
1	B	265	THR
1	B	287	ASP
1	D	14	THR
1	D	17	GLN
1	D	70	THR
1	D	72	GLN
1	D	127	ASN
1	D	143	ASN
1	D	145	LEU
1	D	278	GLU
1	E	25	GLU
1	E	70	THR
1	E	122	THR
1	E	127	ASN
1	E	215	LEU
1	E	232	HIS
1	E	278	GLU
1	E	286	MET
1	E	288	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	87	HIS
1	A	105	GLN
1	A	130	HIS
1	A	162	ASN
1	A	270	ASN
1	B	72	GLN
1	B	119	ASN
1	B	130	HIS
1	B	162	ASN
1	B	270	ASN
1	B	285	ASN
1	D	119	ASN
1	D	130	HIS
1	D	162	ASN
1	E	72	GLN

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Mol	Chain	Res	Type
1	E	87	HIS
1	E	105	GLN
1	E	119	ASN
1	E	130	HIS
1	E	162	ASN
1	E	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 ⓘ

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	$\# Z > 2$
2	NAP	B	301	-	50,52,52	0.96	1 (2%)	71,80,80	0.86	3 (4%)
3	HJG	D	302	-	23,26,26	0.28	0	34,41,41	0.91	1 (2%)
2	NAP	E	301	-	50,52,52	0.87	1 (2%)	71,80,80	0.73	3 (4%)
3	HJG	B	302	-	23,26,26	0.29	0	34,41,41	0.81	1 (2%)
2	NAP	A	301	-	50,52,52	0.69	1 (2%)	71,80,80	0.73	3 (4%)
3	HJG	A	302	-	23,26,26	0.30	0	34,41,41	0.85	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	D	301	-	50,52,52	0.84	1 (2%)	71,80,80	0.66	0
3	HJG	E	302	-	23,26,26	0.31	0	34,41,41	0.86	1 (2%)

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	NAP	B	301	-	-	6/35/67/67	0/5/5/5
3	HJG	D	302	-	-	3/11/22/22	0/4/4/4
2	NAP	E	301	-	-	4/35/67/67	0/5/5/5
3	HJG	B	302	-	-	0/11/22/22	0/4/4/4
2	NAP	A	301	-	-	5/35/67/67	0/5/5/5
3	HJG	A	302	-	-	4/11/22/22	0/4/4/4
2	NAP	D	301	-	-	0/35/67/67	0/5/5/5
3	HJG	E	302	-	-	4/11/22/22	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C2N-N1N	5.96	1.41	1.35
2	E	301	NAP	C2N-N1N	5.17	1.40	1.35
2	D	301	NAP	C2N-N1N	4.87	1.40	1.35
2	A	301	NAP	C2N-N1N	3.84	1.39	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAP	C2B-C1B-N9A	3.49	119.49	113.75
2	B	301	NAP	C4D-O4D-C1D	2.69	112.39	109.92
3	D	302	HJG	C8-C18-N6	-2.68	124.60	127.01
3	A	302	HJG	C8-C18-N6	-2.58	124.69	127.01
2	E	301	NAP	C6N-N1N-C2N	-2.34	119.89	121.88
2	A	301	NAP	O3-PA-O1A	2.32	117.68	110.70
3	B	302	HJG	C15-C2-C7	-2.30	118.85	122.15
2	A	301	NAP	O3X-P2B-O2B	-2.26	97.06	105.85
3	E	302	HJG	C8-C18-N6	-2.23	125.01	127.01
2	A	301	NAP	O2A-PA-O3	-2.22	101.27	107.27
2	E	301	NAP	O2X-P2B-O2B	2.17	114.29	105.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAP	C6N-N1N-C2N	-2.14	120.06	121.88
2	E	301	NAP	O3-PA-O1A	2.13	117.11	110.70
3	A	302	HJG	N6-C7-N20	-2.04	108.32	110.45

There are no chirality outliers.

All (26) torsion outliers are listed below:

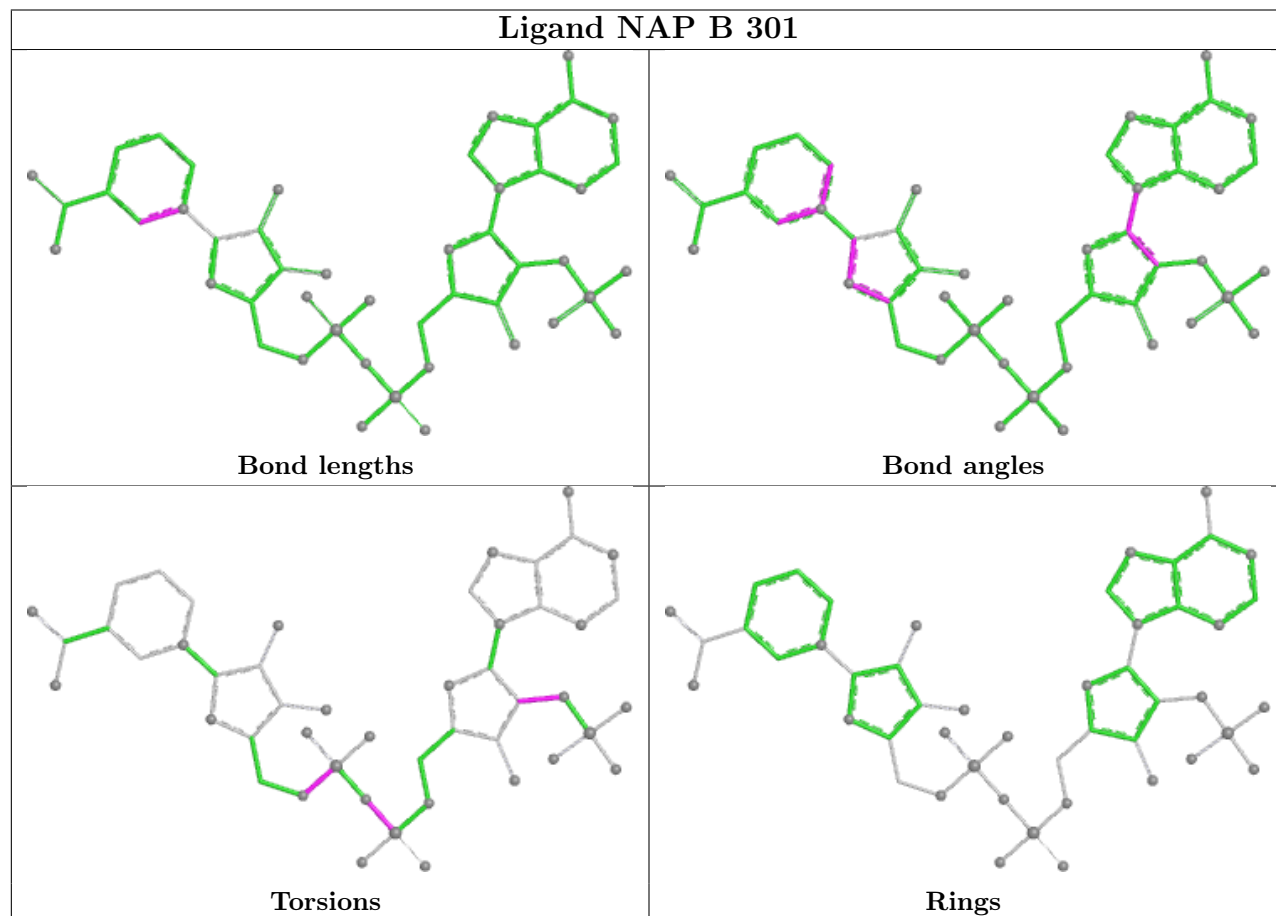
Mol	Chain	Res	Type	Atoms
2	B	301	NAP	C1B-C2B-O2B-P2B
2	B	301	NAP	C5D-O5D-PN-O2N
2	E	301	NAP	C5D-O5D-PN-O2N
3	A	302	HJG	C16-C8-C9-C10
3	D	302	HJG	C16-C8-C9-C10
2	B	301	NAP	C3B-C2B-O2B-P2B
2	B	301	NAP	PN-O3-PA-O1A
2	B	301	NAP	C5D-O5D-PN-O3
2	E	301	NAP	C5D-O5D-PN-O3
3	A	302	HJG	C18-C8-C9-C10
3	D	302	HJG	C18-C8-C9-C10
3	E	302	HJG	C18-C8-C9-C10
3	E	302	HJG	C18-C8-C9-C14
3	A	302	HJG	C16-C8-C9-C14
3	D	302	HJG	C16-C8-C9-C14
3	E	302	HJG	C16-C8-C9-C10
3	E	302	HJG	C16-C8-C9-C14
2	A	301	NAP	C3B-C2B-O2B-P2B
2	A	301	NAP	C1B-C2B-O2B-P2B
3	A	302	HJG	C17-C8-C9-C14
2	A	301	NAP	PN-O3-PA-O1A
2	B	301	NAP	PN-O3-PA-O2A
2	A	301	NAP	O4B-C4B-C5B-O5B
2	E	301	NAP	O4B-C4B-C5B-O5B
2	A	301	NAP	PN-O3-PA-O2A
2	E	301	NAP	PN-O3-PA-O2A

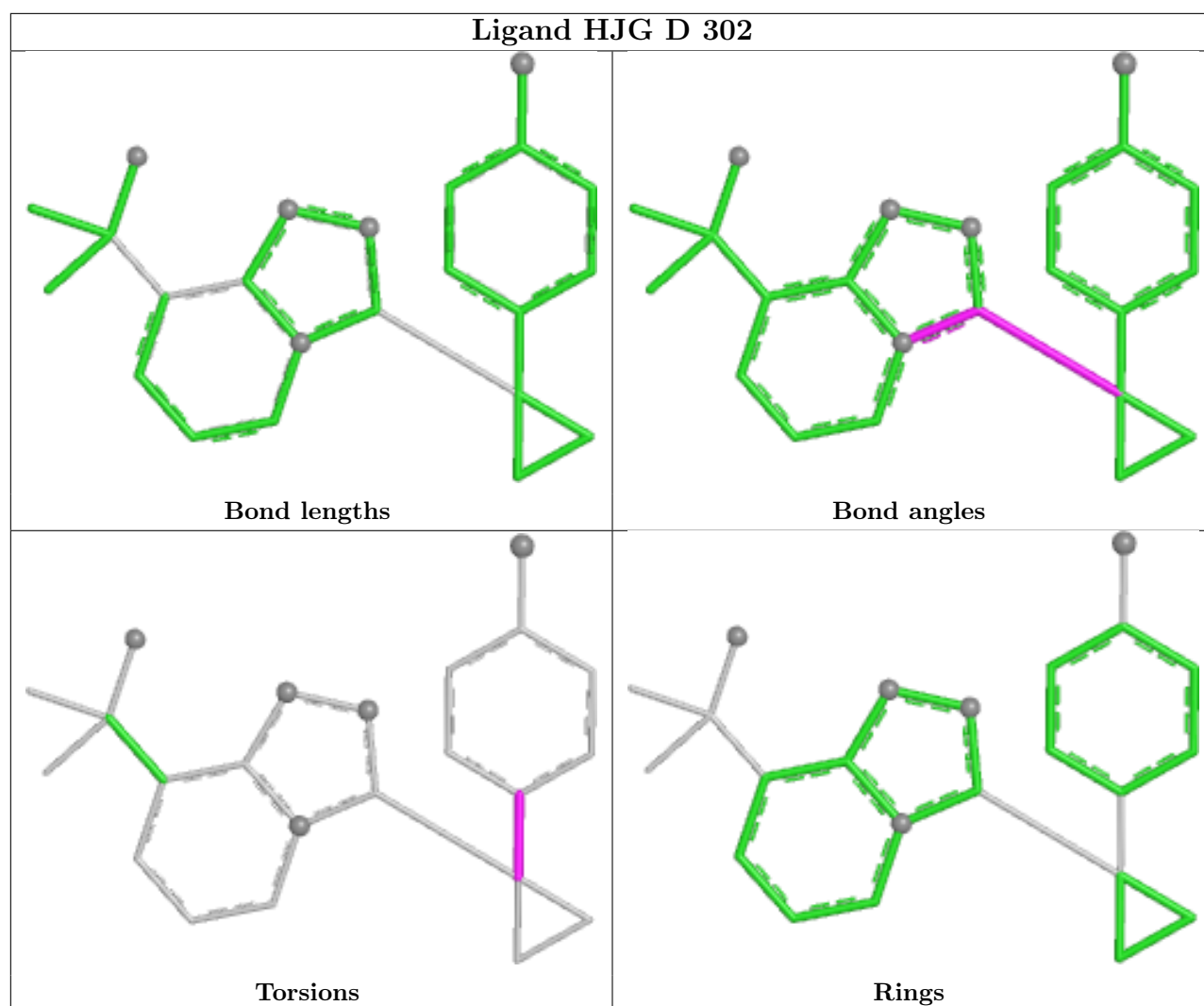
There are no ring outliers.

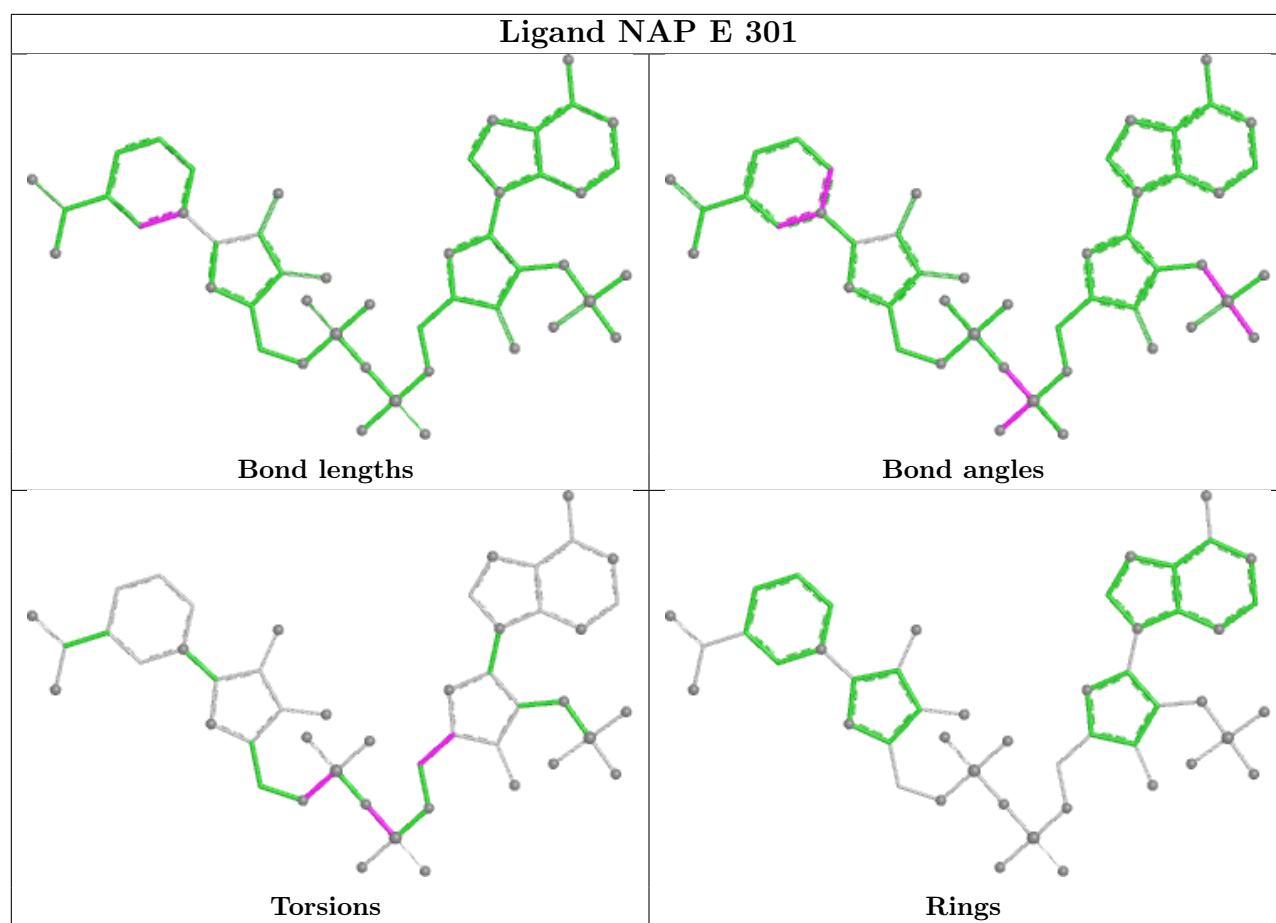
No monomer is involved in short contacts.

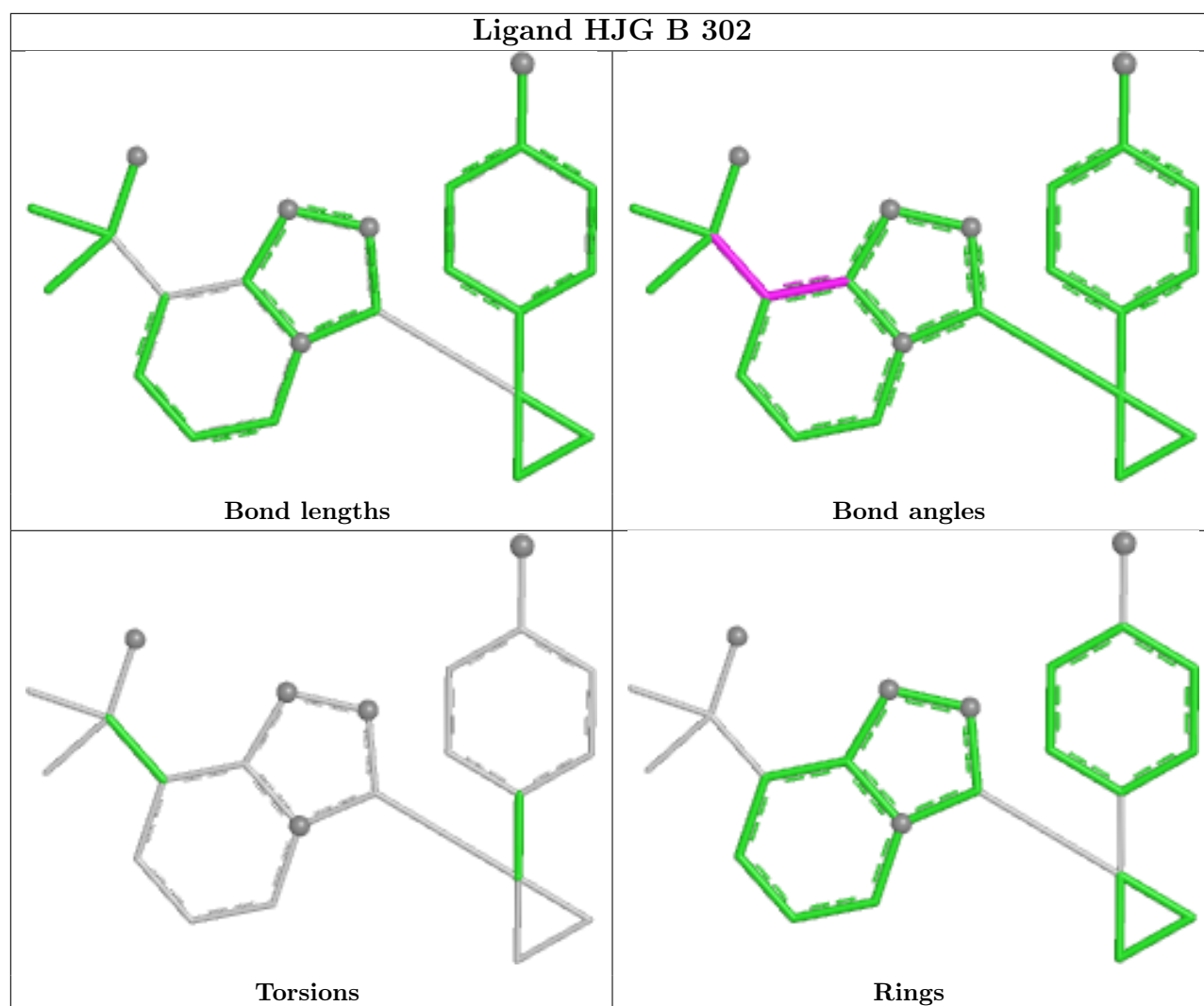
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

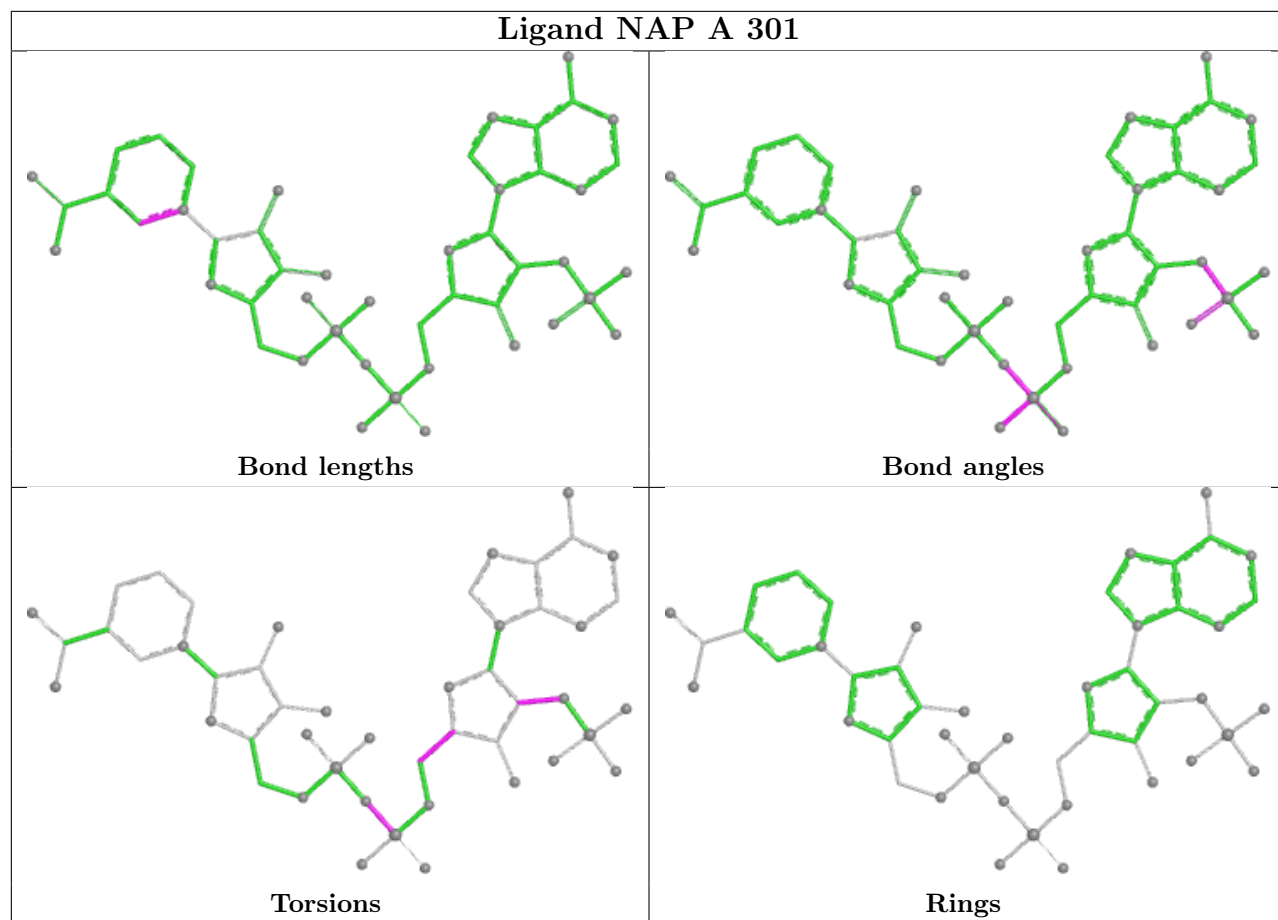
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

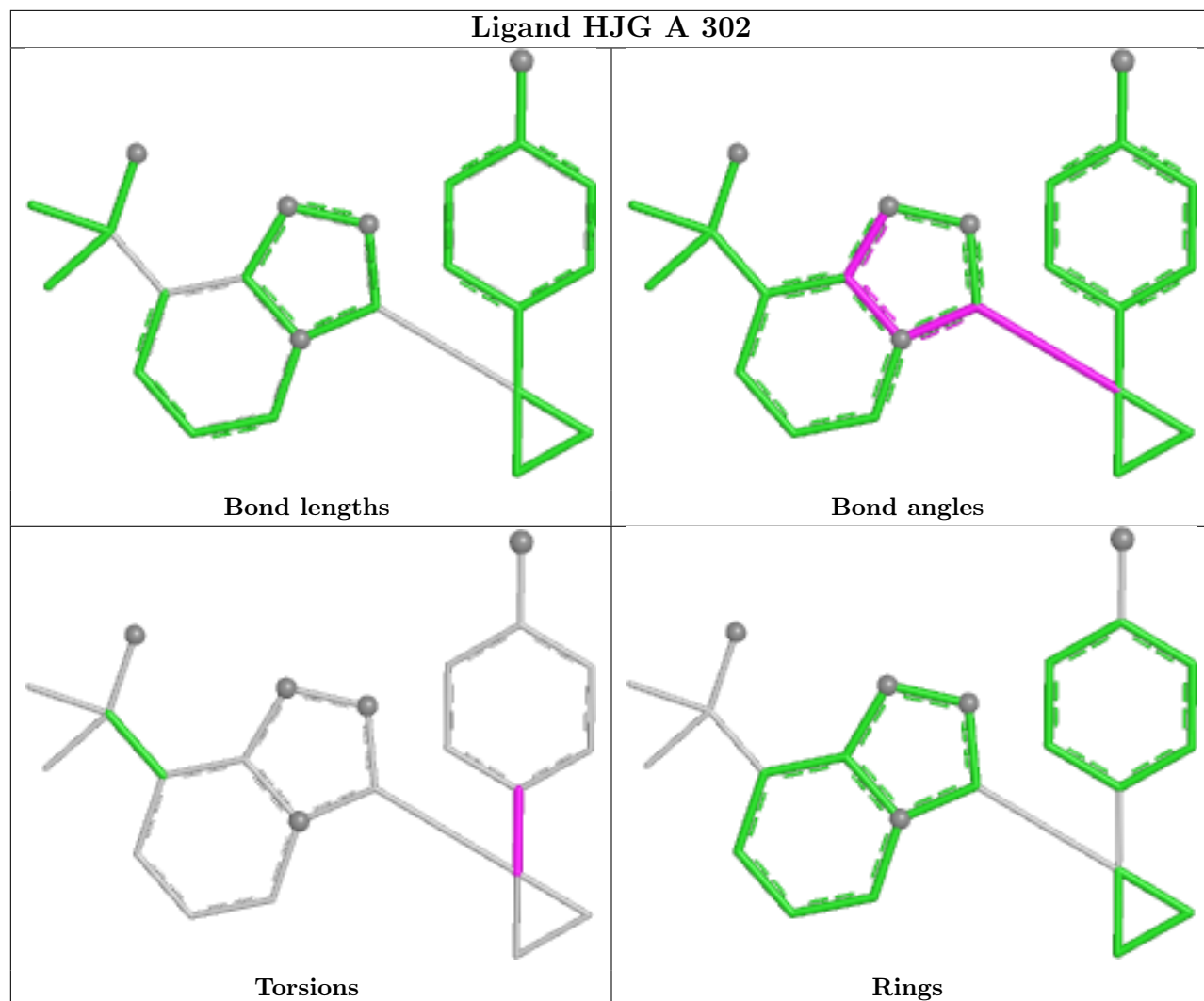


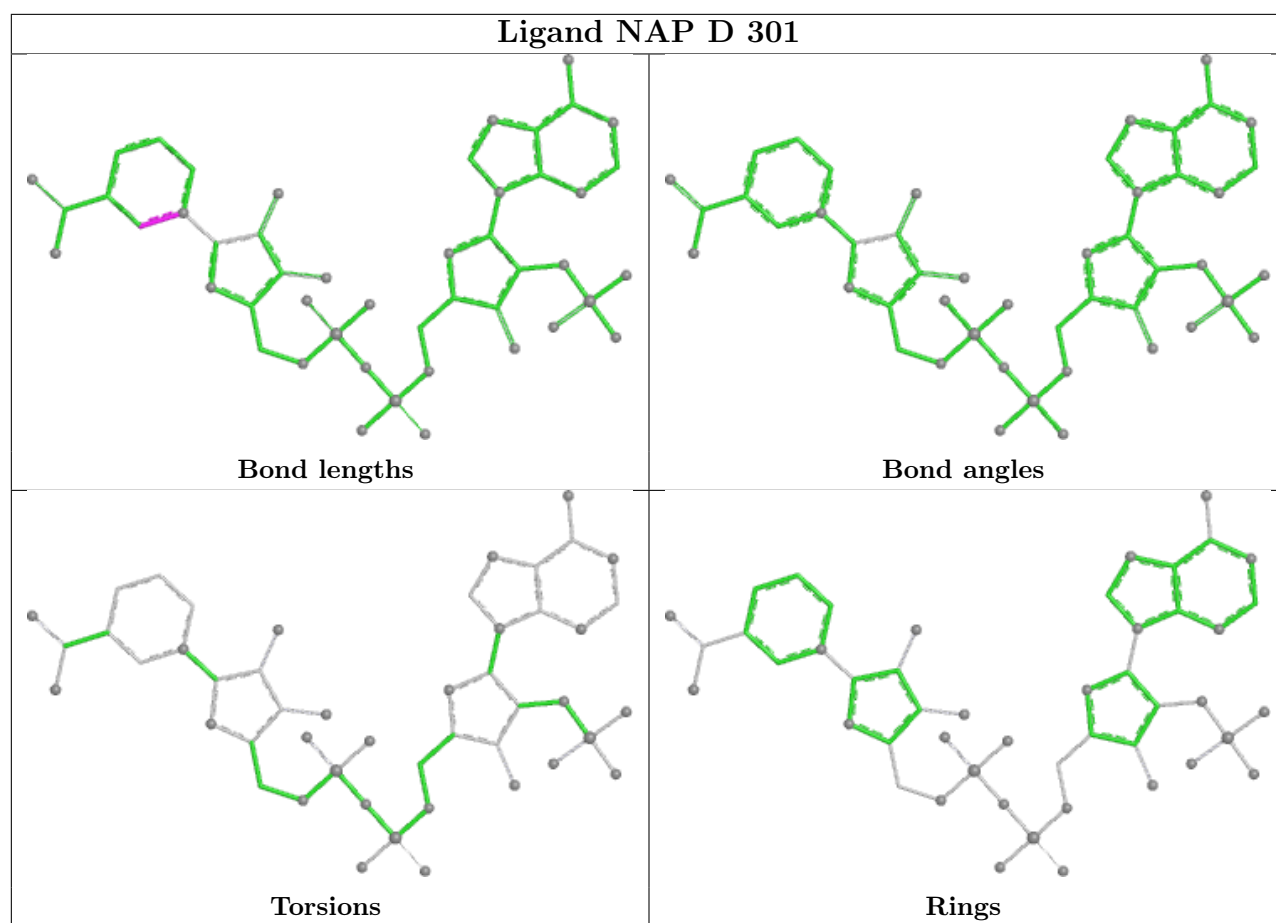


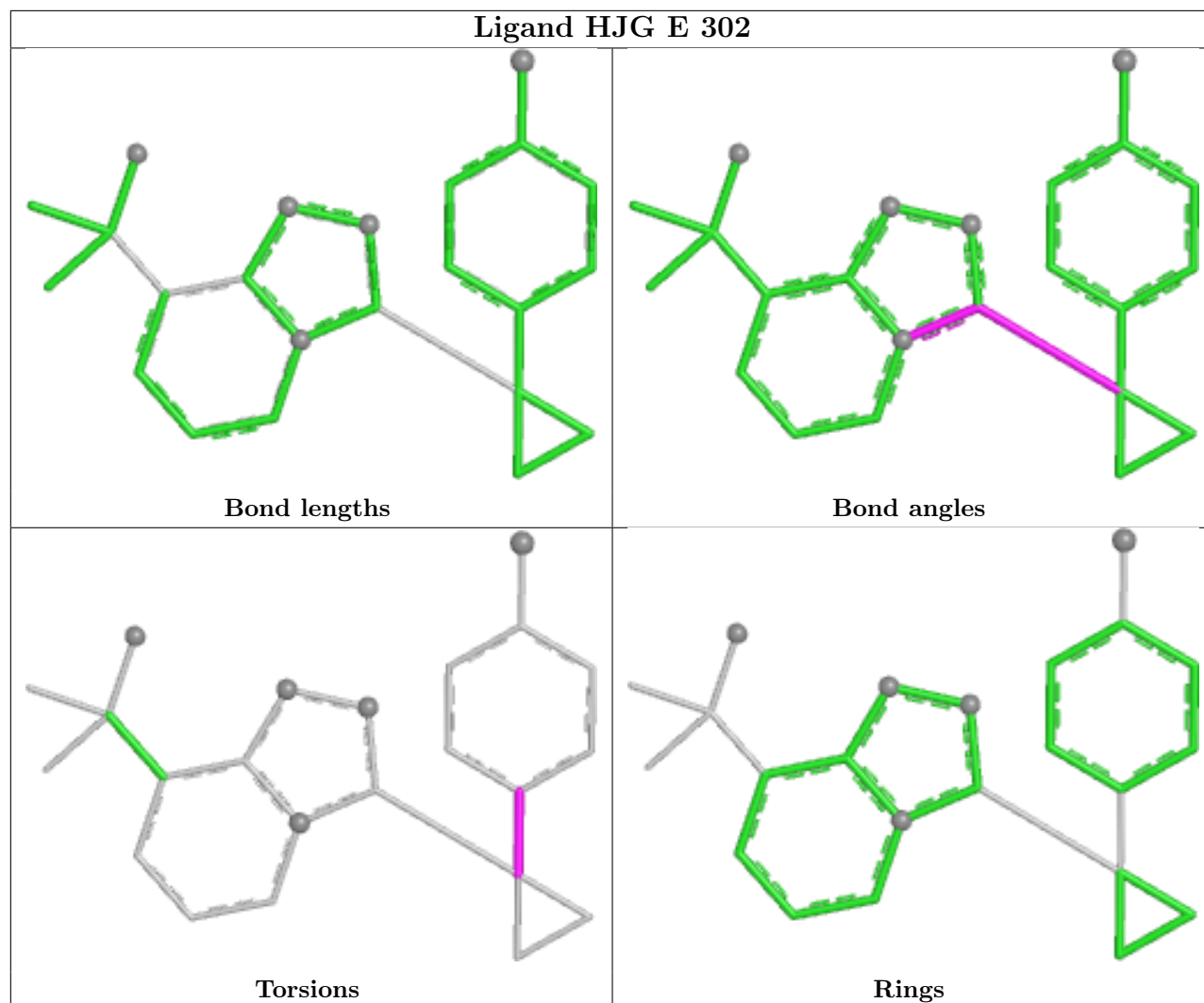












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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%)	0.92	52 (19%) 3 2	13, 38, 69, 89	1 (0%)
1	B	265/286 (92%)	1.47	89 (33%) 1 1	13, 47, 78, 91	0
1	D	273/286 (95%)	-0.15	1 (0%) 88 89	8, 22, 46, 69	0
1	E	265/286 (92%)	0.15	9 (3%) 48 48	8, 27, 56, 79	0
All	All	1065/1144 (93%)	0.59	151 (14%) 6 5	8, 31, 71, 91	1 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	89	ILE	5.1
1	B	25	GLU	4.8
1	A	86	ALA	4.5
1	B	284	TYR	4.4
1	B	87	HIS	4.4
1	B	280	TYR	4.2
1	A	232	HIS	4.1
1	A	84	ALA	3.9
1	E	279	LEU	3.9
1	E	225	LYS	3.9
1	B	84	ALA	3.8
1	A	108	LYS	3.8
1	A	235	ALA	3.8
1	B	76	SER	3.7
1	A	287	ASP	3.7
1	B	88	TYR	3.6
1	A	76	SER	3.6
1	B	62	VAL	3.6
1	B	83	ALA	3.6
1	B	105	GLN	3.6
1	A	83	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	59	ALA	3.5
1	B	79	LEU	3.5
1	B	54	LEU	3.5
1	A	67	SER	3.5
1	B	282	THR	3.4
1	B	27	PHE	3.3
1	A	233	MET	3.3
1	B	90	ALA	3.3
1	A	85	SER	3.3
1	B	85	SER	3.3
1	A	79	LEU	3.3
1	B	32	LEU	3.3
1	A	231	VAL	3.3
1	B	61	VAL	3.3
1	B	91	GLY	3.3
1	A	87	HIS	3.2
1	A	112	GLY	3.2
1	E	289	PHE	3.2
1	B	205	ARG	3.2
1	A	279	LEU	3.2
1	D	130	HIS	3.2
1	E	284	TYR	3.2
1	B	104	ALA	3.1
1	B	72	GLN	3.1
1	B	278	GLU	3.1
1	B	30	GLU	3.1
1	B	34	GLY	3.1
1	B	37	VAL	3.1
1	B	208	VAL	3.1
1	A	111	GLY	3.1
1	B	133	ILE	3.1
1	B	274	LYS	3.0
1	A	81	LEU	3.0
1	A	203	VAL	3.0
1	B	75	VAL	3.0
1	A	69	GLU	3.0
1	B	102	PHE	3.0
1	B	250	ALA	2.9
1	A	234	GLN	2.9
1	B	101	GLN	2.9
1	A	131	ASP	2.9
1	A	68	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	230	ILE	2.8
1	B	26	GLU	2.8
1	B	73	LYS	2.8
1	B	78	CYS	2.8
1	B	58	GLY	2.8
1	B	283	SER	2.8
1	B	29	PRO	2.8
1	B	40	THR	2.8
1	B	64	THR	2.8
1	B	33	GLN	2.8
1	B	108	LYS	2.8
1	A	82	GLY	2.8
1	B	281	SER	2.8
1	B	80	GLU	2.8
1	B	77	HIS	2.8
1	B	43	SER	2.7
1	A	61	VAL	2.7
1	B	71	LEU	2.7
1	B	263	TRP	2.7
1	B	74	VAL	2.7
1	A	88	TYR	2.7
1	A	229	GLY	2.7
1	B	98	PHE	2.7
1	B	251	LEU	2.7
1	B	279	LEU	2.7
1	B	106	ALA	2.7
1	A	286	MET	2.6
1	B	148	VAL	2.6
1	B	86	ALA	2.6
1	B	56	LYS	2.6
1	B	206	VAL	2.6
1	A	60	HIS	2.6
1	B	289	PHE	2.6
1	B	81	LEU	2.6
1	B	63	VAL	2.6
1	B	161	SER	2.6
1	B	225	LYS	2.6
1	B	127	ASN	2.5
1	B	237	PRO	2.5
1	B	47	GLY	2.4
1	B	60	HIS	2.4
1	B	31	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	282	THR	2.4
1	A	107	GLY	2.4
1	A	55	ALA	2.4
1	B	99	ALA	2.4
1	B	288	ARG	2.3
1	A	75	VAL	2.3
1	E	263	TRP	2.3
1	B	103	VAL	2.3
1	B	28	ARG	2.3
1	A	158	LEU	2.3
1	A	78	CYS	2.3
1	B	39	VAL	2.3
1	A	59	ALA	2.3
1	A	155	LEU	2.3
1	B	109	LEU	2.2
1	B	287	ASP	2.2
1	A	28	ARG	2.2
1	A	156	PRO	2.2
1	B	203	VAL	2.2
1	A	285	ASN	2.2
1	A	157	MET	2.2
1	A	225	LYS	2.2
1	B	93	MET	2.2
1	A	160	GLN	2.2
1	B	36	LYS	2.2
1	E	287	ASP	2.2
1	A	32	LEU	2.2
1	B	107	GLY	2.1
1	A	77[A]	HIS	2.1
1	A	130	HIS	2.1
1	B	82	GLY	2.1
1	A	80	GLU	2.1
1	B	69	GLU	2.1
1	E	280	TYR	2.1
1	B	114	ASP	2.1
1	B	159	LYS	2.1
1	A	236	ALA	2.1
1	A	109	LEU	2.1
1	B	38	ILE	2.1
1	E	286	MET	2.1
1	B	126	LEU	2.1
1	A	58	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	70	THR	2.1
1	B	67	SER	2.0
1	A	33	GLN	2.0
1	A	29	PRO	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](#)

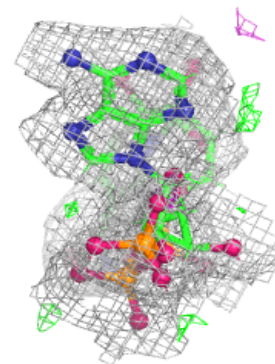
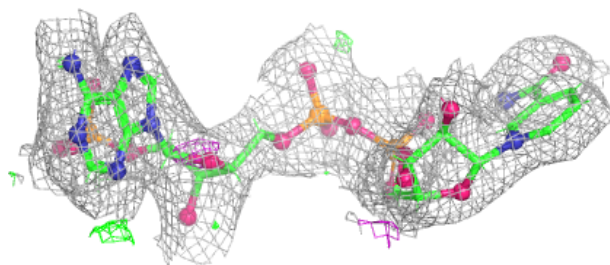
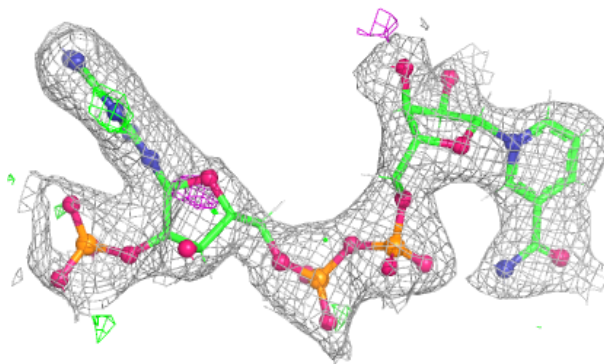
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	B	301	48/48	0.89	0.09	20,27,40,44	28
3	HJG	A	302	23/23	0.90	0.10	27,27,31,40	18
3	HJG	B	302	23/23	0.94	0.08	25,27,30,31	18
3	HJG	E	302	23/23	0.94	0.09	23,27,28,29	18
3	HJG	D	302	23/23	0.95	0.08	17,25,27,27	18
2	NAP	A	301	48/48	0.96	0.07	20,25,32,34	28
2	NAP	E	301	48/48	0.96	0.07	17,23,28,32	28
2	NAP	D	301	48/48	0.98	0.06	13,23,28,32	28

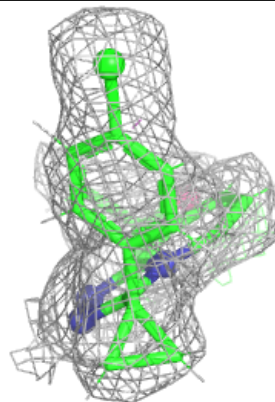
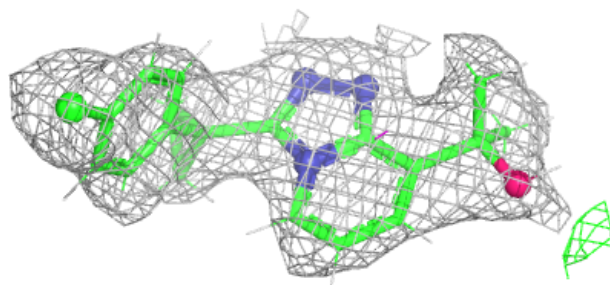
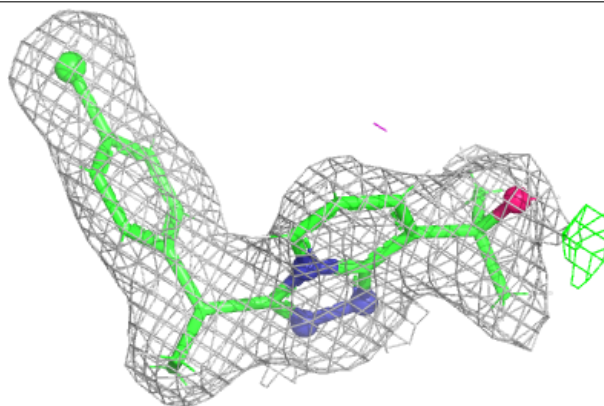
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP B 301:

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

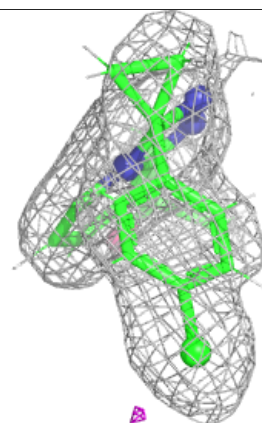
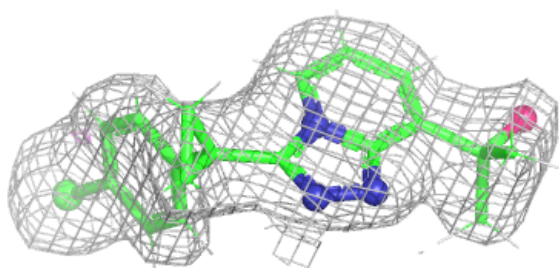
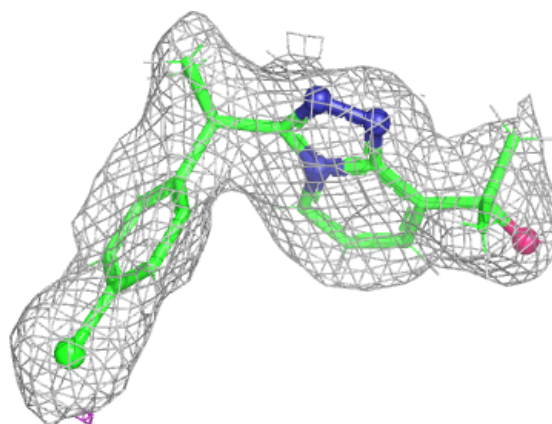
**Electron density around HJG A 302:**

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

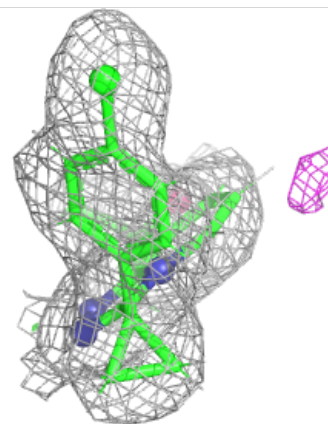
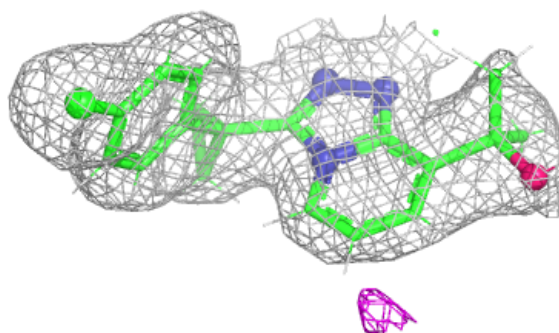
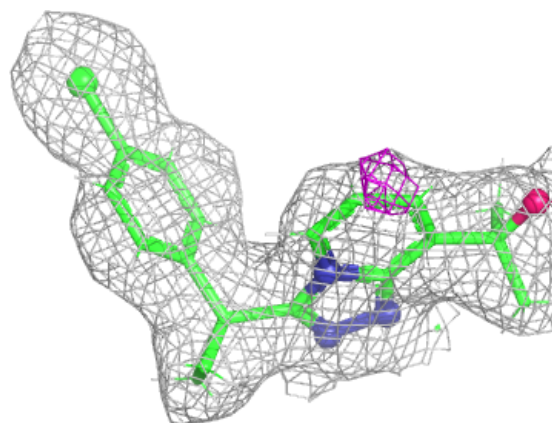


Electron density around HJG B 302:

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

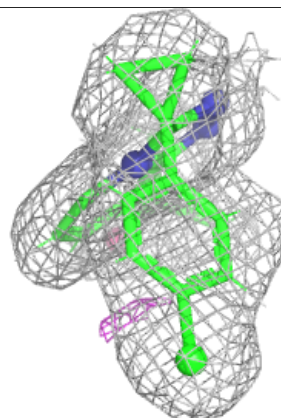
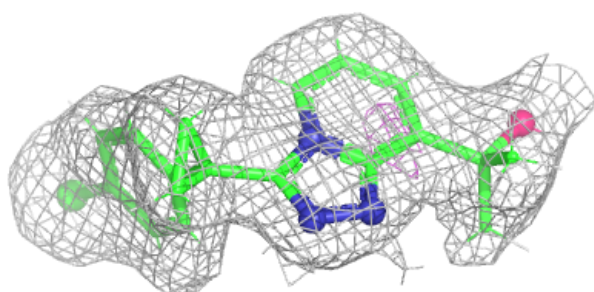
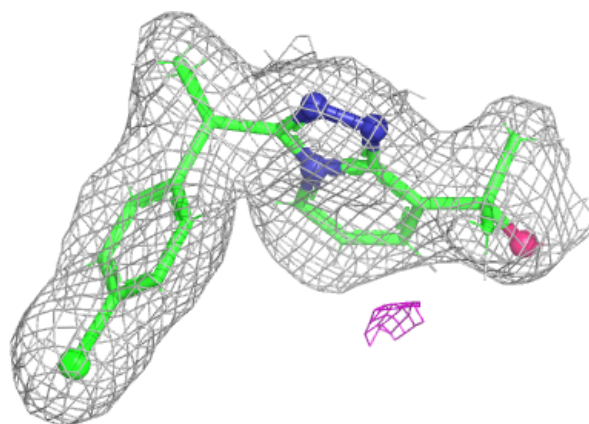
**Electron density around HJG E 302:**

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

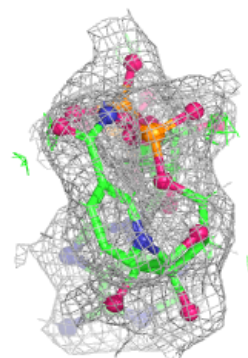
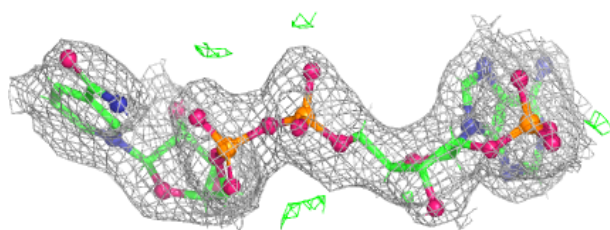
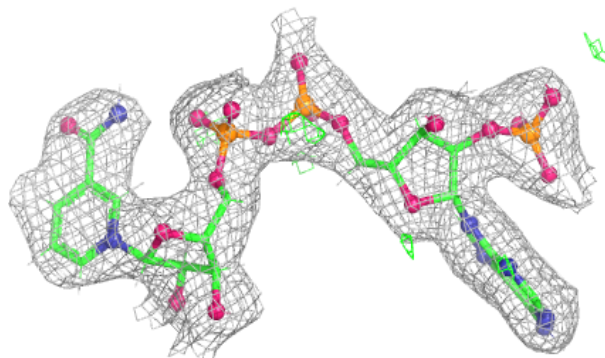


Electron density around HJG D 302:

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

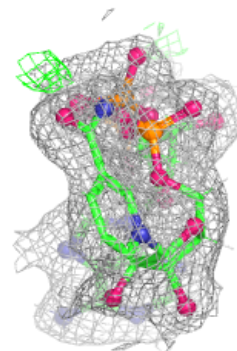
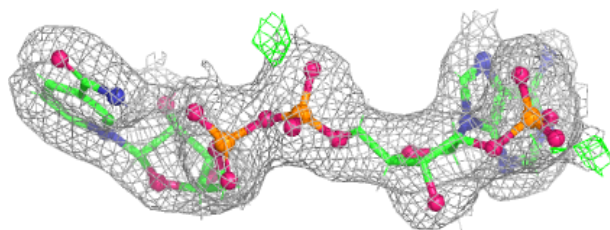
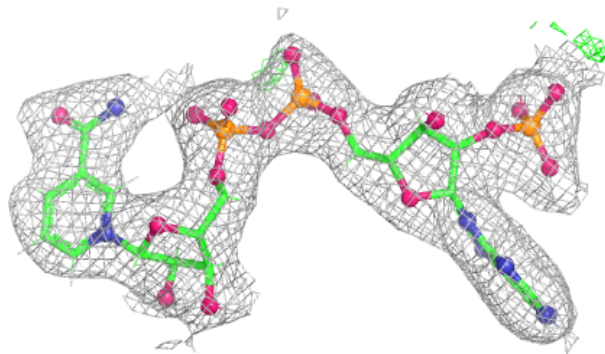
**Electron density around NAP A 301:**

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

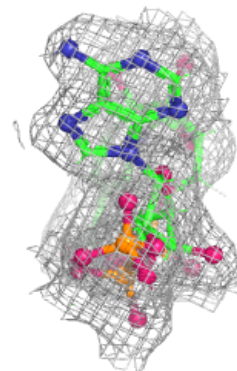
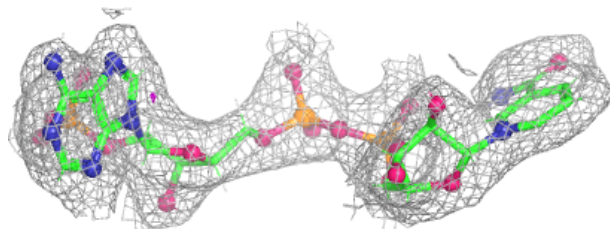
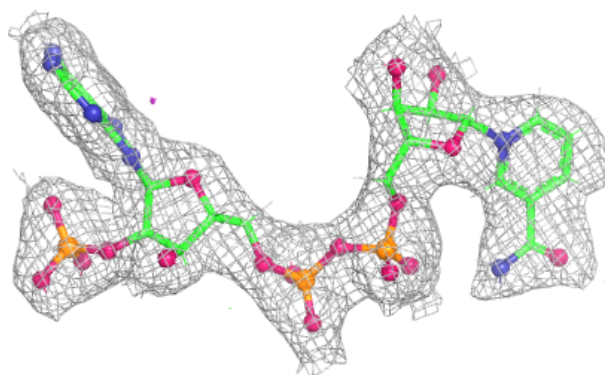


Electron density around NAP E 301:

$2mF_o - DF_c$ (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 [i](#)

There are no such residues in this entry.