



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:16 AM UTC

PDB ID : 4IJV / pdb_00004ijv
Title : Crystal structure of 11b-HSD1 double mutant (L262R, F278E) in complex with 3-[1-(4-chlorophenyl)cyclopropyl]-8-(2-fluorophenoxy)[1,2,4]triazolo[4,3-a]pyridine
Authors : Sheriff, S.
Deposited on : 2012-12-23
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 types of validation reports are described at

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

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

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

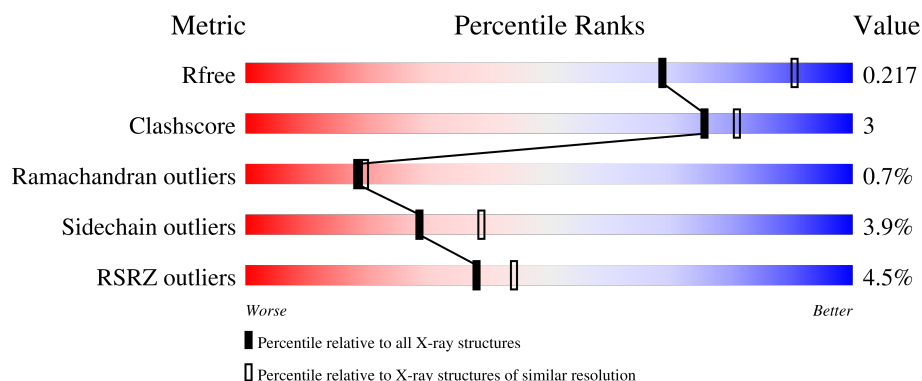
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	286	3% 83% 9% 7%
1	B	286	5% 87% 10% ..
1	D	286	4% 85% 11% .
1	E	286	5% 79% 12% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8918 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	1	0
			2055	1307	352	379	17			
1	B	281	Total	C	N	O	S	0	0	0
			2133	1351	365	397	20			
1	D	275	Total	C	N	O	S	0	1	0
			2089	1324	358	388	19			
1	E	264	Total	C	N	O	S	0	0	0
			2029	1290	346	376	17			

There are 72 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	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
B	9	HIS	-	expression tag	UNP P28845

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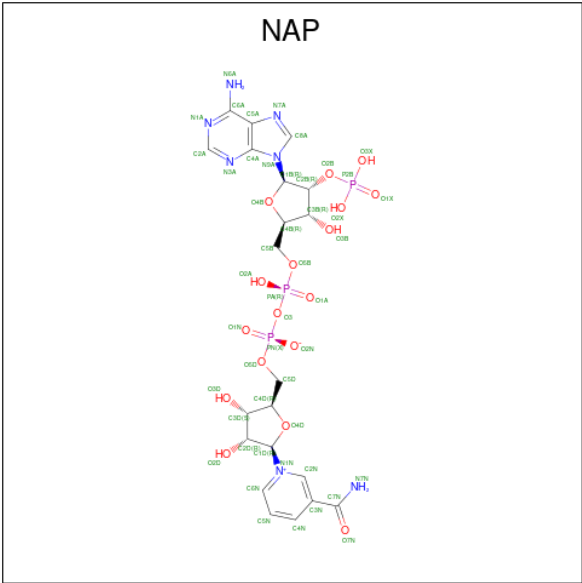
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	MET	-	expression tag	UNP P28845
B	12	SER	-	expression tag	UNP P28845
B	13	MET	-	expression tag	UNP P28845
B	14	THR	-	expression tag	UNP P28845
B	15	GLY	-	expression tag	UNP P28845
B	16	GLY	-	expression tag	UNP P28845
B	17	GLN	-	expression tag	UNP P28845
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	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	12	SER	-	expression tag	UNP P28845
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

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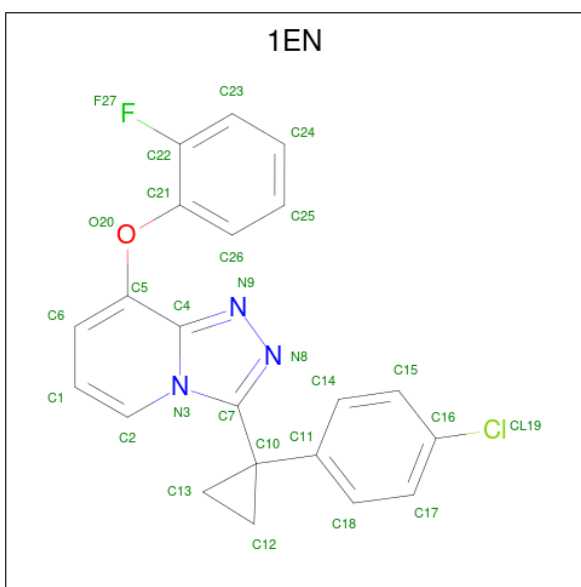
Chain	Residue	Modelled	Actual	Comment	Reference
E	17	GLN	-	expression tag	UNP P28845
E	18	GLN	-	expression tag	UNP P28845
E	19	MET	-	expression tag	UNP P28845
E	20	GLY	-	expression tag	UNP P28845
E	21	ARG	-	expression tag	UNP P28845
E	22	GLY	-	expression tag	UNP P28845
E	23	SER	-	expression tag	UNP P28845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

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 3-[1-(4-chlorophenyl)cyclopropyl]-8-(2-fluorophenoxy)[1,2,4]triazolo[4,3-a]pyridine (CCD ID: 1EN) (formula: C₂₁H₁₅ClFN₃O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 27	C 21	Cl 1	F 1	N 3	O 1	0	0
3	B	1	Total 27	C 21	Cl 1	F 1	N 3	O 1	0	0
3	D	1	Total 27	C 21	Cl 1	F 1	N 3	O 1	0	0
3	E	1	Total 27	C 21	Cl 1	F 1	N 3	O 1	0	0

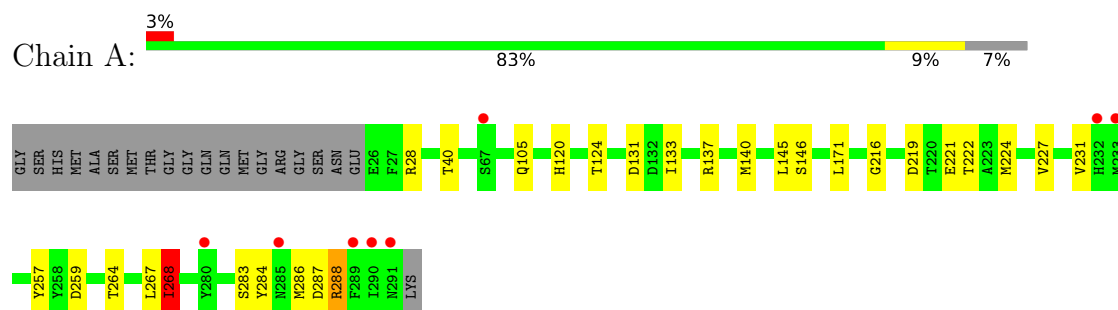
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	75	Total	O	0	0
			75	75		
4	D	97	Total	O	0	0
			97	97		
4	E	66	Total	O	0	0
			66	66		

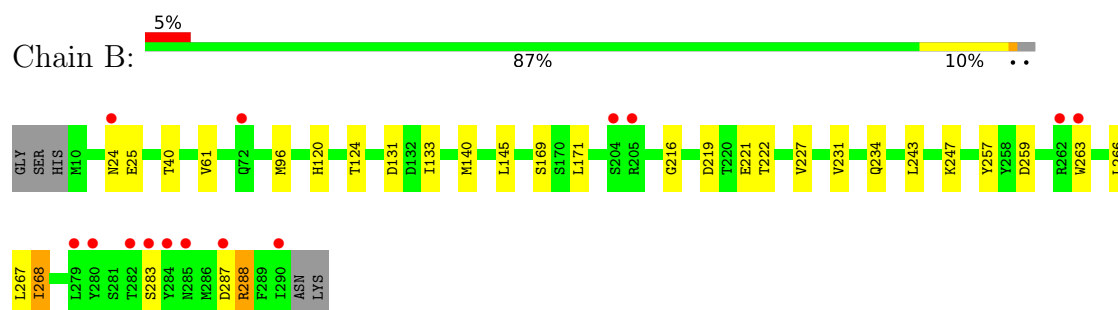
3 Residue-property plots [i](#)

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.

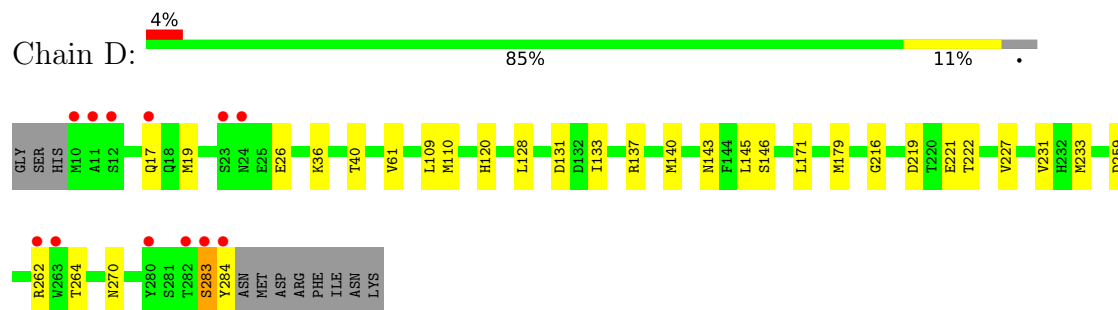
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



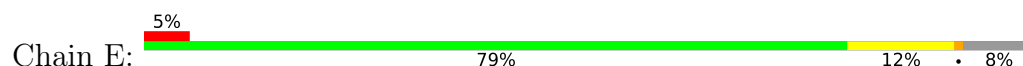
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

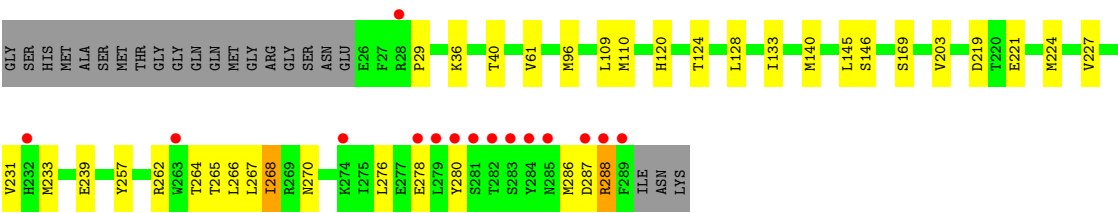


- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



- 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	74.40Å 94.00Å 167.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.98 – 2.35 35.98 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.4 (35.98-2.35) 98.3 (35.98-2.35)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.11 (at 2.34Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.2, BUSTER 2.11.2	Depositor
R, R_{free}	0.189 , 0.213 (Not available) , 0.217	Depositor DCC
R_{free} test set	1046 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8918	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: NAP, 1EN

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	0.77	1/2093 (0.0%)	1.34	6/2824 (0.2%)
1	B	0.79	0/2167	1.37	8/2921 (0.3%)
1	D	0.80	0/2126	1.35	6/2867 (0.2%)
1	E	0.80	1/2063 (0.0%)	1.36	8/2784 (0.3%)
All	All	0.79	2/8449 (0.0%)	1.36	28/11396 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	MET	SD-CE	-5.30	1.66	1.79
1	E	224	MET	SD-CE	-5.20	1.66	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ASN	CA-C-N	11.29	142.02	121.70
1	B	24	ASN	C-N-CA	11.29	142.02	121.70
1	A	267	LEU	N-CA-C	6.54	121.39	113.41
1	B	24	ASN	N-CA-C	6.18	120.99	112.90
1	E	29	PRO	CA-C-N	6.16	129.15	120.28
1	E	29	PRO	C-N-CA	6.16	129.15	120.28
1	A	268	ILE	N-CA-CB	5.95	120.83	110.65
1	B	267	LEU	N-CA-C	5.95	120.67	113.41
1	E	267	LEU	N-CA-C	5.88	121.49	113.97
1	A	131	ASP	CA-CB-CG	5.79	118.39	112.60
1	D	26	GLU	N-CA-C	5.79	117.95	108.52
1	D	171	LEU	N-CA-C	-5.61	105.16	111.28
1	E	265	THR	CA-C-N	5.53	127.69	120.28
1	E	265	THR	C-N-CA	5.53	127.69	120.28
1	E	270	ASN	CA-CB-CG	5.42	118.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	LEU	N-CA-C	-5.26	105.66	111.71
1	D	270	ASN	CA-CB-CG	5.23	117.83	112.60
1	D	131	ASP	N-CA-CB	-5.21	104.11	110.98
1	D	143	ASN	CA-CB-CG	5.18	117.78	112.60
1	A	171	LEU	N-CA-C	-5.13	105.81	111.71
1	E	287	ASP	CA-C-N	5.10	131.29	121.54
1	E	287	ASP	C-N-CA	5.10	131.29	121.54
1	B	287	ASP	CA-C-N	5.08	131.25	121.54
1	B	287	ASP	C-N-CA	5.08	131.25	121.54
1	A	287	ASP	CA-C-N	5.05	131.19	121.54
1	A	287	ASP	C-N-CA	5.05	131.19	121.54
1	D	131	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	131	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2055	0	2098	12	0
1	B	2133	0	2162	13	0
1	D	2089	0	2120	19	0
1	E	2029	0	2065	21	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	D	48	0	25	0	0
2	E	48	0	25	1	0
3	A	27	0	15	3	0
3	B	27	0	15	3	0
3	D	27	0	15	1	0
3	E	27	0	15	1	0
4	A	74	0	0	0	0
4	B	75	0	0	0	0
4	D	97	0	0	0	0
4	E	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8918	0	8605	51	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 (51) 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:E:227:VAL:HB	1:E:231:VAL:HB	1.61	0.82
1:B:227:VAL:HB	1:B:231:VAL:HB	1.77	0.67
1:D:283:SER:HB3	1:E:233:MET:HG2	1.79	0.65
1:D:128:LEU:HD21	1:E:286:MET:HE2	1.82	0.61
1:D:222:THR:HG22	3:D:302:1EN:H13	1.82	0.60
1:A:140:MET:HE2	1:B:140:MET:HE2	1.88	0.55
1:B:222:THR:HG22	3:B:302:1EN:H12	1.89	0.55
1:E:124:THR:O	3:E:302:1EN:H14	2.07	0.54
1:B:124:THR:O	3:B:302:1EN:H14	2.07	0.54
1:B:263:TRP:HH2	1:E:278:GLU:HG2	1.73	0.54
1:E:264:THR:O	1:E:268:ILE:HG13	2.09	0.52
1:E:203:VAL:HG21	1:E:286:MET:SD	2.50	0.52
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.93	0.52
1:D:284:TYR:HB3	1:E:231:VAL:HG22	1.92	0.51
1:D:231:VAL:HG12	1:D:233:MET:HG2	1.92	0.51
1:E:40:THR:OG1	1:E:120:HIS:HD2	1.94	0.51
1:D:227:VAL:HB	1:D:231:VAL:HB	1.93	0.51
1:D:283:SER:HB3	1:E:233:MET:CG	2.41	0.51
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.94	0.50
1:A:120:HIS:HE1	1:A:146:SER:OG	1.96	0.49
1:E:120:HIS:HE1	1:E:146:SER:OG	1.96	0.49
1:D:264:THR:HG23	1:E:280:TYR:OH	2.12	0.48
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.96	0.47
1:B:222:THR:HG22	3:B:302:1EN:C23	2.44	0.47
1:E:36:LYS:HG2	1:E:110:MET:HB3	1.96	0.47
1:A:284:TYR:CE1	1:A:286:MET:HE2	2.50	0.47
1:D:140:MET:HE2	1:E:140:MET:HE2	1.95	0.47
1:D:264:THR:HA	1:E:276:LEU:HD21	1.97	0.47
1:B:257:TYR:CD1	1:B:268:ILE:HD13	2.50	0.47
1:E:257:TYR:CD1	1:E:268:ILE:HD13	2.51	0.45
1:D:179:MET:HG3	1:E:286:MET:HE3	1.99	0.45
1:D:231:VAL:CG1	1:D:233:MET:HG2	2.46	0.45
1:D:128:LEU:HD21	1:E:286:MET:CE	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HB	1:A:231:VAL:HB	1.99	0.45
1:B:169:SER:O	2:B:301:NAP:H6N	2.17	0.45
1:D:36:LYS:HG2	1:D:110:MET:HB3	1.99	0.45
1:A:264:THR:O	1:A:268:ILE:HG13	2.18	0.44
1:A:137:ARG:HH22	1:B:96:MET:HG3	1.83	0.44
1:D:216:GLY:HA3	1:D:259:ASP:OD1	2.18	0.43
1:B:216:GLY:HA3	1:B:259:ASP:OD1	2.20	0.42
1:B:263:TRP:CH2	1:E:278:GLU:HG2	2.52	0.42
1:D:17:GLN:HE21	1:D:19:MET:HB2	1.85	0.42
1:A:216:GLY:HA3	1:A:259:ASP:OD1	2.19	0.42
1:A:222:THR:HG22	3:A:302:1EN:H12	2.02	0.41
1:E:169:SER:O	2:E:301:NAP:H6N	2.21	0.41
1:D:137:ARG:HH22	1:E:96:MET:HG3	1.84	0.41
1:A:124:THR:HG23	3:A:302:1EN:C25	2.49	0.41
1:B:243:LEU:HG	1:B:247:LYS:HE3	2.03	0.40
1:A:257:TYR:CD1	1:A:268:ILE:HD13	2.57	0.40
1:D:120:HIS:HE1	1:D:146:SER:OG	2.05	0.40
1:A:124:THR:O	3:A:302:1EN:H14	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/286 (93%)	256 (97%)	7 (3%)	2 (1%)	16	17
1	B	279/286 (98%)	265 (95%)	11 (4%)	3 (1%)	11	11
1	D	274/286 (96%)	265 (97%)	8 (3%)	1 (0%)	30	34
1	E	262/286 (92%)	252 (96%)	8 (3%)	2 (1%)	16	17
All	All	1080/1144 (94%)	1038 (96%)	34 (3%)	8 (1%)	18	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	GLU
1	B	288	ARG
1	E	288	ARG
1	A	288	ARG
1	A	219	ASP
1	B	219	ASP
1	D	219	ASP
1	E	219	ASP

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	224/237 (94%)	216 (96%)	8 (4%)	31	41
1	B	229/237 (97%)	220 (96%)	9 (4%)	28	39
1	D	224/237 (94%)	217 (97%)	7 (3%)	35	47
1	E	220/237 (93%)	209 (95%)	11 (5%)	22	27
All	All	897/948 (95%)	862 (96%)	35 (4%)	28	39

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	105	GLN
1	A	133	ILE
1	A	145	LEU
1	A	221	GLU
1	A	268	ILE
1	A	283	SER
1	A	288	ARG
1	B	61	VAL
1	B	133	ILE
1	B	145	LEU
1	B	221	GLU
1	B	234	GLN
1	B	266	LEU

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Mol	Chain	Res	Type
1	B	268	ILE
1	B	283	SER
1	B	288	ARG
1	D	61	VAL
1	D	109	LEU
1	D	133	ILE
1	D	145	LEU
1	D	221	GLU
1	D	262	ARG
1	D	283	SER
1	E	61	VAL
1	E	109	LEU
1	E	128	LEU
1	E	133	ILE
1	E	145	LEU
1	E	221	GLU
1	E	239	GLU
1	E	262	ARG
1	E	266	LEU
1	E	268	ILE
1	E	288	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	120	HIS
1	A	130	HIS
1	A	234	GLN
1	A	253	GLN
1	A	285	ASN
1	B	72	GLN
1	B	119	ASN
1	B	120	HIS
1	B	130	HIS
1	B	234	GLN
1	D	17	GLN
1	D	72	GLN
1	D	119	ASN
1	D	120	HIS
1	D	234	GLN
1	E	72	GLN

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Mol	Chain	Res	Type
1	E	105	GLN
1	E	120	HIS
1	E	234	GLN
1	E	285	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E	301	-	50,52,52	1.01	1 (2%)	71,80,80	0.66	2 (2%)
2	NAP	D	301	-	50,52,52	1.08	1 (2%)	71,80,80	0.71	1 (1%)
3	1EN	D	302	-	29,31,31	1.32	5 (17%)	38,46,46	1.17	4 (10%)
3	1EN	A	302	-	29,31,31	1.43	5 (17%)	38,46,46	1.35	5 (13%)
2	NAP	B	301	-	50,52,52	0.85	1 (2%)	71,80,80	0.68	3 (4%)
2	NAP	A	301	-	50,52,52	1.00	1 (2%)	71,80,80	0.70	2 (2%)
3	1EN	B	302	-	29,31,31	1.41	4 (13%)	38,46,46	1.35	5 (13%)
3	1EN	E	302	-	29,31,31	1.49	4 (13%)	38,46,46	1.22	5 (13%)

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	E	301	-	-	6/35/67/67	0/5/5/5
2	NAP	D	301	-	-	2/35/67/67	0/5/5/5
3	1EN	D	302	-	-	5/10/20/20	0/5/5/5
3	1EN	A	302	-	-	5/10/20/20	0/5/5/5
2	NAP	B	301	-	-	4/35/67/67	0/5/5/5
2	NAP	A	301	-	-	1/35/67/67	0/5/5/5
3	1EN	B	302	-	-	6/10/20/20	0/5/5/5
3	1EN	E	302	-	-	5/10/20/20	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAP	C2N-N1N	6.99	1.42	1.35
2	E	301	NAP	C2N-N1N	6.38	1.42	1.35
2	A	301	NAP	C2N-N1N	6.06	1.41	1.35
2	B	301	NAP	C2N-N1N	4.87	1.40	1.35
3	E	302	1EN	C12-C10	-3.23	1.48	1.52
3	B	302	1EN	C1-C6	3.05	1.48	1.41
3	E	302	1EN	C1-C6	2.99	1.48	1.41
3	A	302	1EN	C1-C6	2.92	1.48	1.41
3	A	302	1EN	C12-C10	-2.80	1.49	1.52
3	A	302	1EN	O20-C21	-2.66	1.35	1.41
3	D	302	1EN	C1-C6	2.65	1.47	1.41
3	A	302	1EN	C13-C10	-2.65	1.49	1.52
3	B	302	1EN	O20-C21	-2.54	1.36	1.41
3	E	302	1EN	C13-C10	-2.54	1.49	1.52
3	A	302	1EN	N9-N8	2.43	1.44	1.39
3	B	302	1EN	C13-C10	-2.22	1.50	1.52
3	D	302	1EN	O20-C21	-2.18	1.36	1.41
3	E	302	1EN	O20-C21	-2.17	1.36	1.41
3	D	302	1EN	N9-N8	2.09	1.44	1.39
3	B	302	1EN	C12-C10	-2.08	1.50	1.52
3	D	302	1EN	C12-C10	-2.03	1.50	1.52
3	D	302	1EN	C13-C10	-2.02	1.50	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	1EN	C10-C7-N3	-3.86	123.54	127.01
3	A	302	1EN	C13-C10-C12	3.79	60.15	58.45
3	B	302	1EN	C13-C10-C12	3.59	60.06	58.45
3	E	302	1EN	C13-C10-C12	3.24	59.90	58.45
2	B	301	NAP	P2B-O2B-C2B	3.07	131.64	123.43
2	A	301	NAP	P2B-O2B-C2B	2.96	131.34	123.43
2	D	301	NAP	P2B-O2B-C2B	2.64	130.47	123.43
3	D	302	1EN	C13-C10-C12	2.57	59.60	58.45
3	D	302	1EN	O20-C5-C4	2.48	119.24	114.21
3	E	302	1EN	C10-C7-N3	-2.41	124.85	127.01
2	E	301	NAP	C6N-N1N-C2N	-2.35	119.87	121.88
3	A	302	1EN	O20-C5-C4	2.34	118.97	114.21
3	B	302	1EN	C26-C21-C22	2.28	121.44	118.04
3	A	302	1EN	C13-C10-C11	2.26	121.22	118.58
3	D	302	1EN	N3-C7-N8	-2.22	108.77	110.79
3	E	302	1EN	O20-C5-C4	2.19	118.65	114.21
3	A	302	1EN	C26-C21-C22	2.18	121.30	118.04
2	E	301	NAP	P2B-O2B-C2B	2.16	129.20	123.43
2	A	301	NAP	O2B-P2B-O1X	2.13	116.92	109.33
3	E	302	1EN	C12-C13-C10	-2.12	59.81	60.78
3	A	302	1EN	C10-C7-N3	-2.12	125.11	127.01
3	E	302	1EN	C21-O20-C5	-2.11	115.01	118.49
3	B	302	1EN	C10-C7-N8	2.10	126.57	123.52
2	B	301	NAP	O2B-P2B-O1X	2.09	116.78	109.33
3	D	302	1EN	C26-C21-C22	2.04	121.09	118.04
2	B	301	NAP	C6N-N1N-C2N	-2.01	120.16	121.88
3	B	302	1EN	O20-C5-C4	2.01	118.29	114.21

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAP	C5D-O5D-PN-O1N
2	E	301	NAP	C5D-O5D-PN-O1N
3	A	302	1EN	C7-C10-C11-C14
3	A	302	1EN	C13-C10-C11-C14
3	A	302	1EN	C13-C10-C11-C18
3	D	302	1EN	C13-C10-C11-C18
3	E	302	1EN	C13-C10-C11-C14
3	E	302	1EN	C13-C10-C11-C18
2	B	301	NAP	C5D-O5D-PN-O3
2	E	301	NAP	C5D-O5D-PN-O3
3	A	302	1EN	C7-C10-C11-C18

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Mol	Chain	Res	Type	Atoms
3	B	302	1EN	C7-C10-C11-C14
3	B	302	1EN	C7-C10-C11-C18
3	D	302	1EN	C7-C10-C11-C14
3	D	302	1EN	C7-C10-C11-C18
3	E	302	1EN	C7-C10-C11-C14
3	E	302	1EN	C7-C10-C11-C18
3	B	302	1EN	C13-C10-C11-C14
3	B	302	1EN	C13-C10-C11-C18
3	D	302	1EN	C13-C10-C11-C14
2	E	301	NAP	C2B-O2B-P2B-O2X
2	E	301	NAP	C2B-O2B-P2B-O1X
3	B	302	1EN	C26-C21-O20-C5
3	A	302	1EN	C22-C21-O20-C5
3	B	302	1EN	C22-C21-O20-C5
3	D	302	1EN	C22-C21-O20-C5
3	E	302	1EN	C22-C21-O20-C5
2	E	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	PN-O3-PA-O2A
2	D	301	NAP	C2B-O2B-P2B-O3X
2	B	301	NAP	C3B-C2B-O2B-P2B
2	A	301	NAP	PN-O3-PA-O2A
2	D	301	NAP	PN-O3-PA-O2A
2	E	301	NAP	PN-O3-PA-O2A

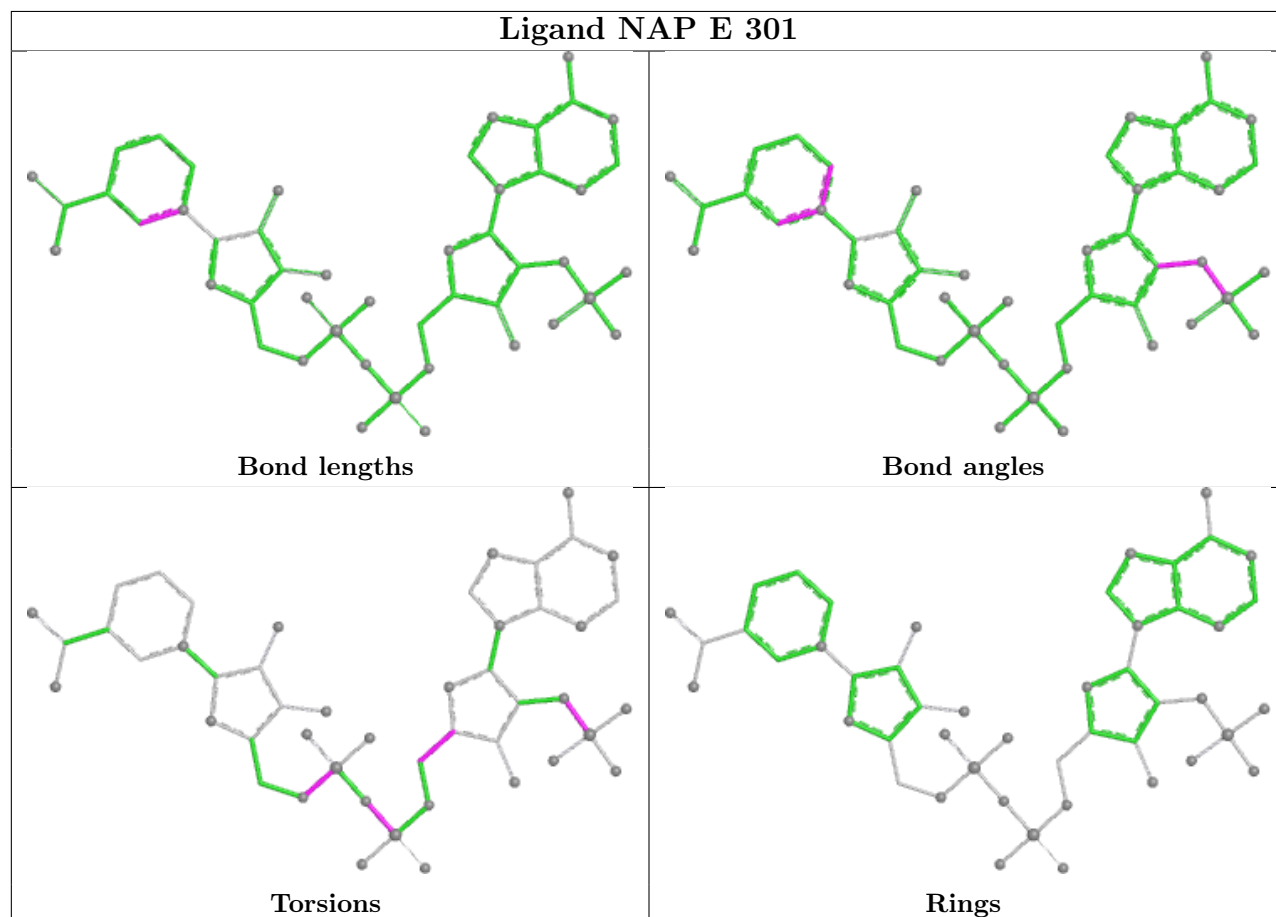
There are no ring outliers.

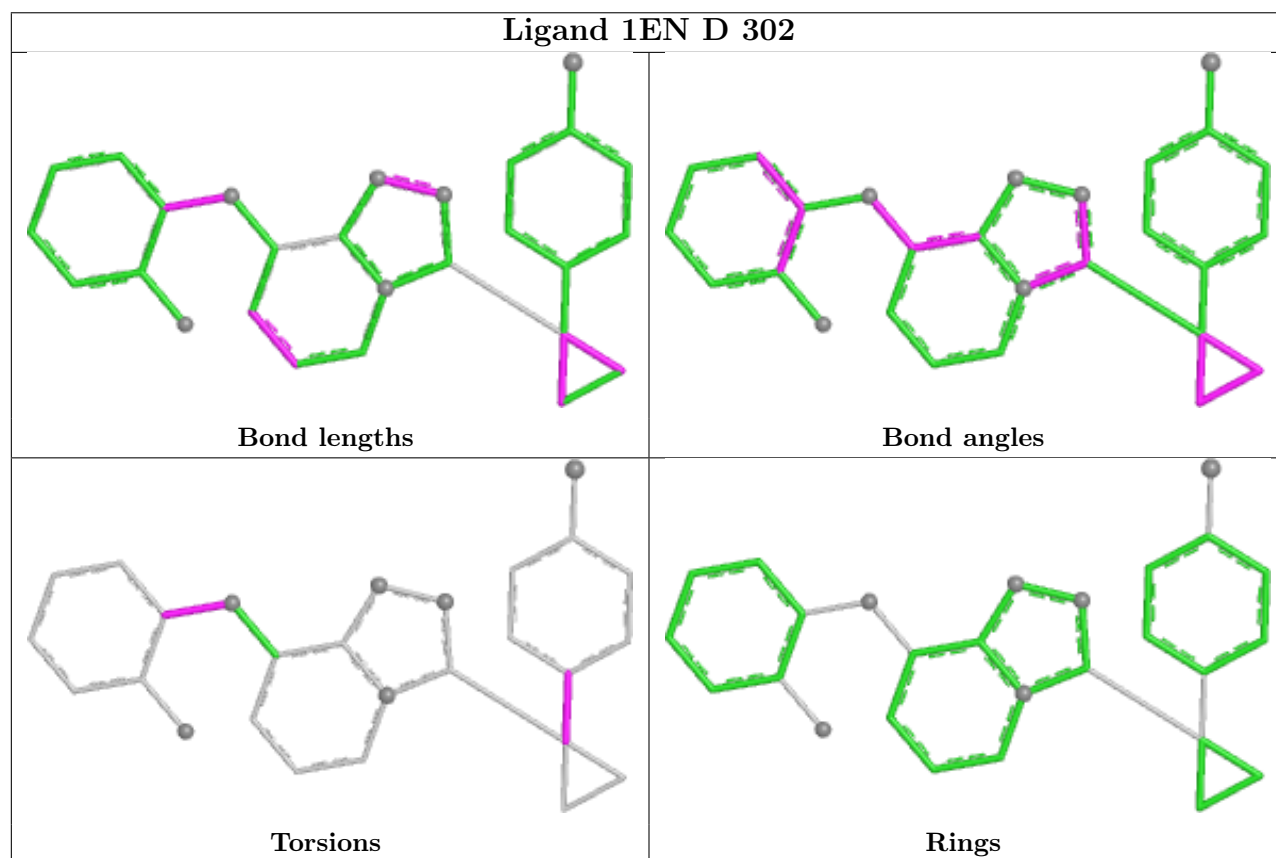
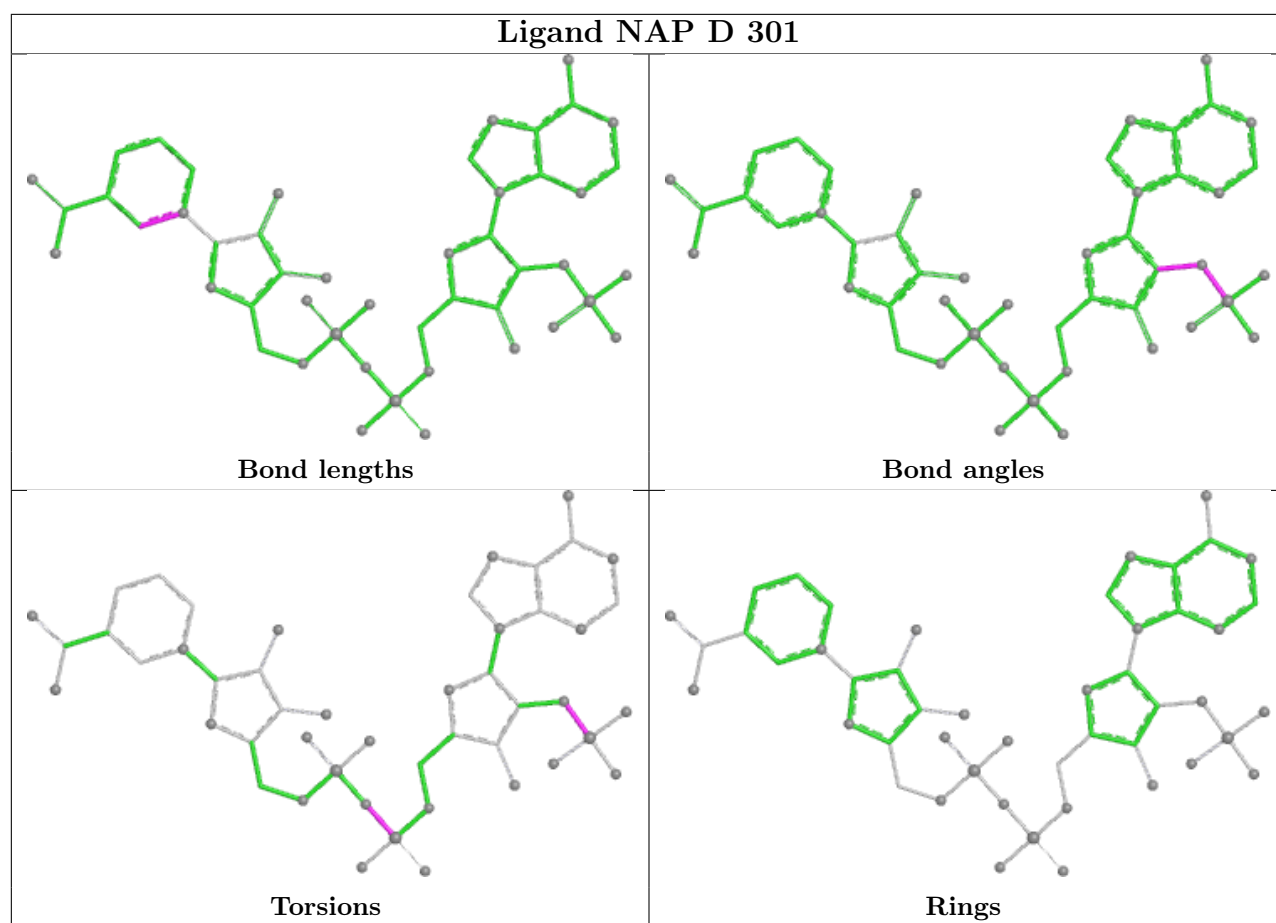
6 monomers are involved in 10 short contacts:

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

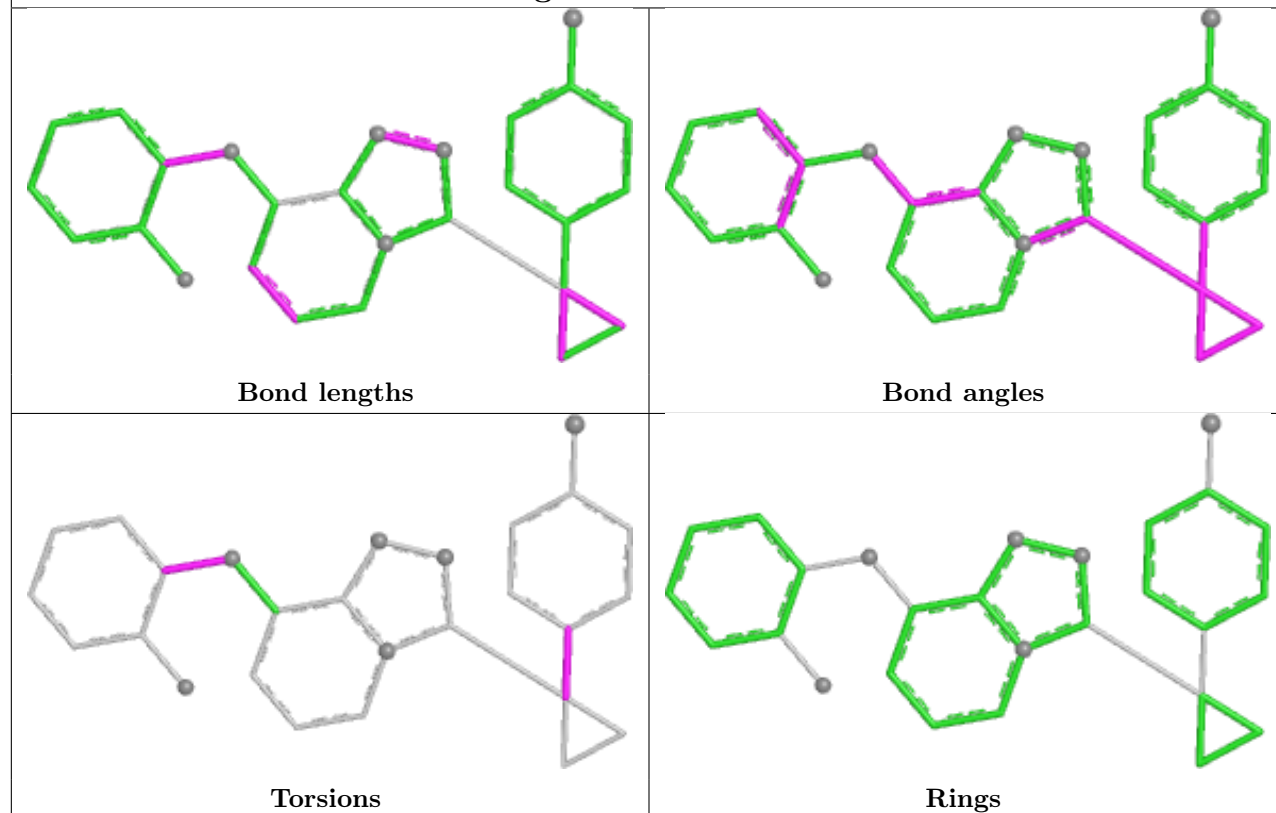
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

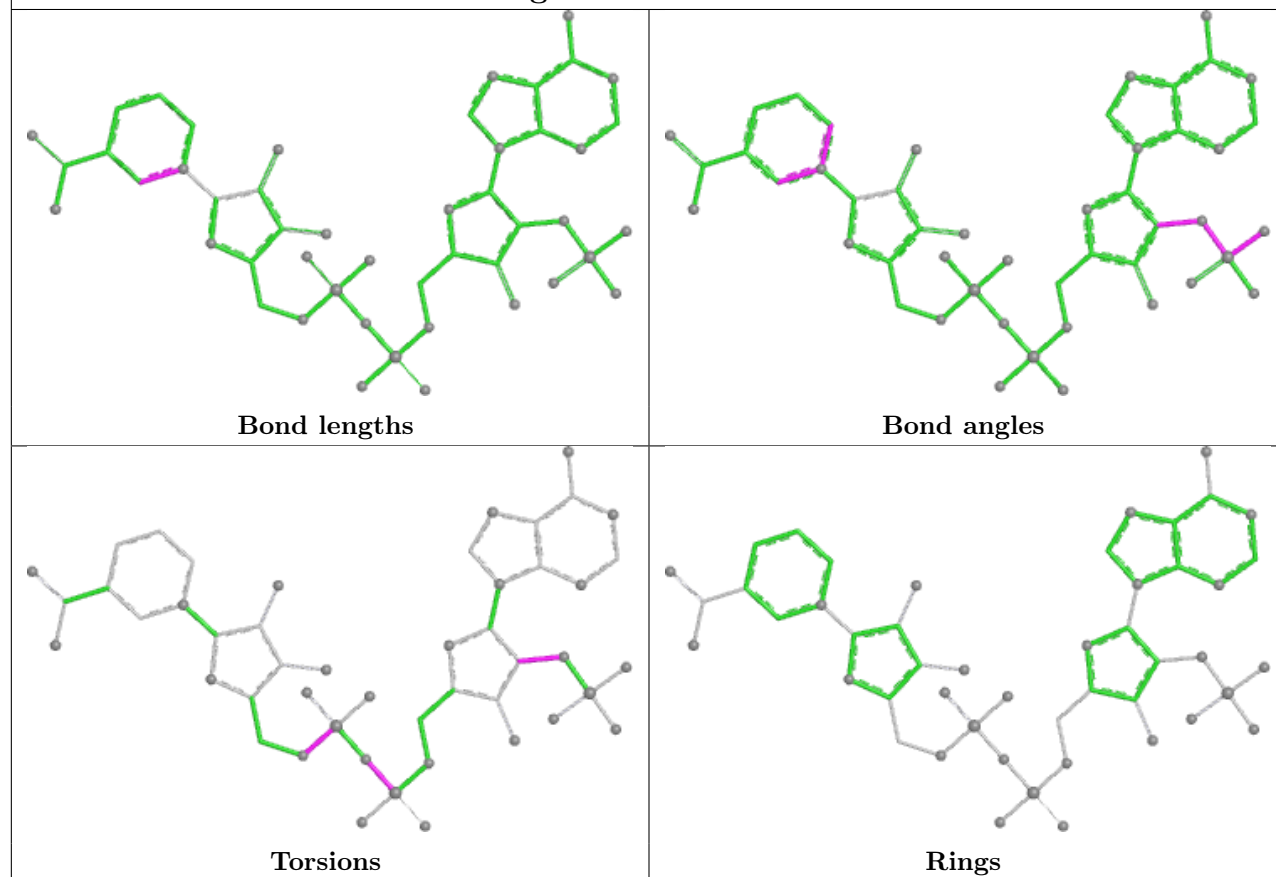


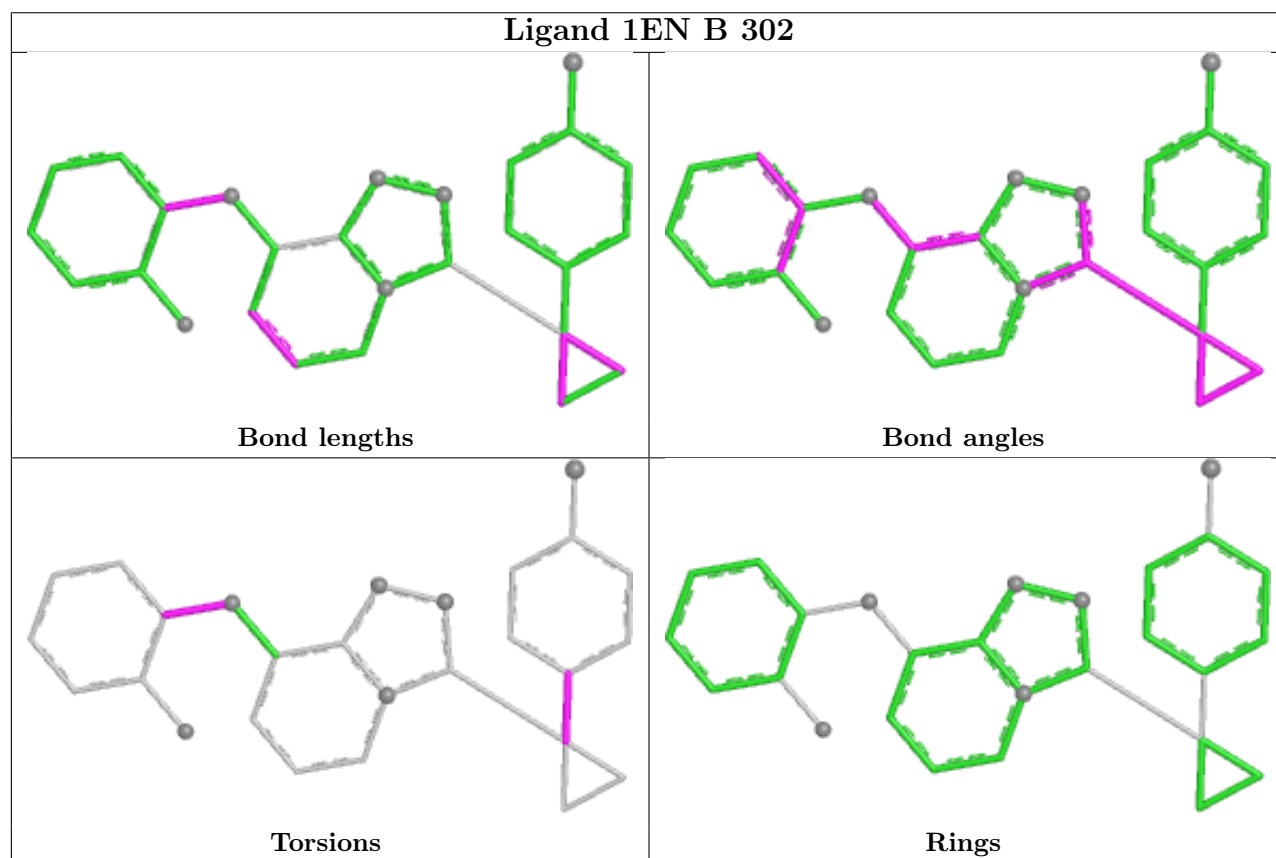
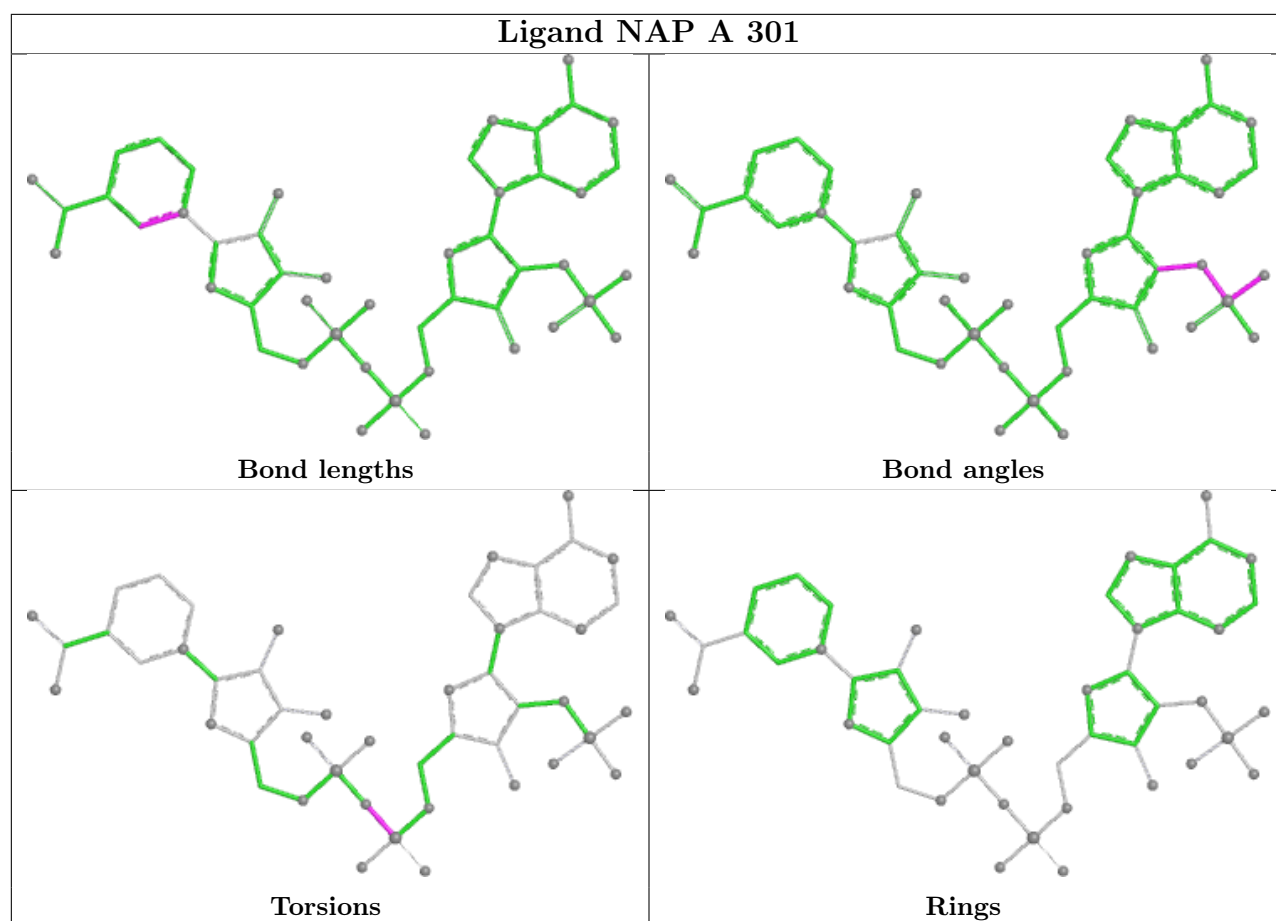


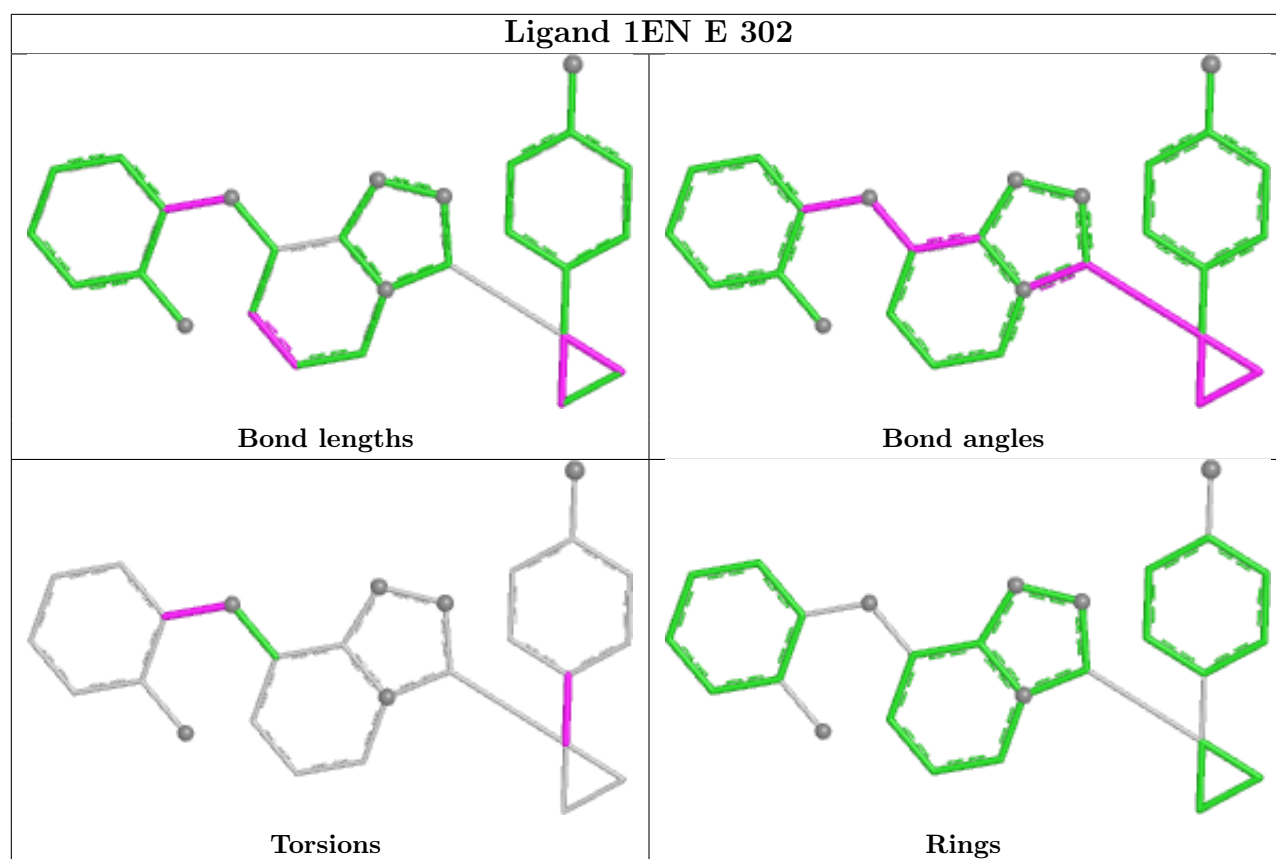
Ligand 1EN A 302



Ligand NAP B 301







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	266/286 (93%)	-0.08	8 (3%) 52 59	13, 24, 48, 105	1 (0%)
1	B	281/286 (98%)	0.08	14 (4%) 34 40	13, 27, 54, 85	0
1	D	275/286 (96%)	-0.17	12 (4%) 39 45	10, 21, 53, 71	1 (0%)
1	E	264/286 (92%)	0.07	15 (5%) 29 34	11, 26, 61, 81	0
All	All	1086/1144 (94%)	-0.02	49 (4%) 38 44	10, 25, 54, 105	2 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	ILE	8.1
1	E	282	THR	6.9
1	E	280	TYR	5.8
1	E	263	TRP	5.5
1	A	290	ILE	4.9
1	B	263	TRP	4.8
1	A	291	ASN	4.7
1	D	263	TRP	4.4
1	D	284	TYR	4.0
1	E	283	SER	3.9
1	E	281	SER	3.7
1	E	284	TYR	3.6
1	B	280	TYR	3.6
1	D	12	SER	3.6
1	D	282	THR	3.4
1	B	283	SER	3.4
1	D	10	MET	3.2
1	E	279	LEU	3.2
1	D	24	ASN	3.1
1	B	284	TYR	3.1
1	A	280	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	278	GLU	2.8
1	B	279	LEU	2.8
1	D	11	ALA	2.8
1	A	67	SER	2.7
1	D	17	GLN	2.7
1	E	274	LYS	2.6
1	E	288	ARG	2.6
1	A	233	MET	2.6
1	D	23	SER	2.5
1	B	262	ARG	2.5
1	B	205	ARG	2.4
1	B	287	ASP	2.4
1	B	24	ASN	2.4
1	E	285	ASN	2.4
1	A	232	HIS	2.4
1	B	285	ASN	2.3
1	D	280	TYR	2.3
1	B	282	THR	2.3
1	B	204	SER	2.3
1	E	289	PHE	2.3
1	E	232	HIS	2.2
1	B	72	GLN	2.2
1	E	28	ARG	2.1
1	A	289	PHE	2.1
1	A	285	ASN	2.0
1	D	262	ARG	2.0
1	D	283	SER	2.0
1	E	287	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

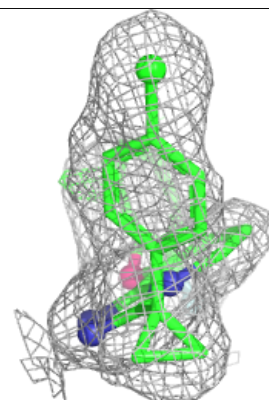
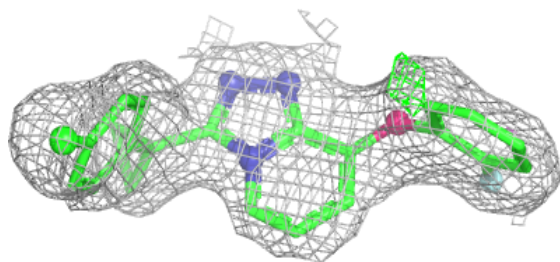
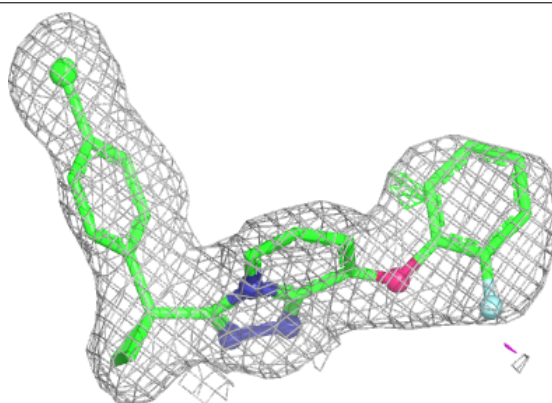
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	1EN	A	302	27/27	0.93	0.10	25,28,37,41	0
3	1EN	B	302	27/27	0.93	0.09	18,23,34,41	0
3	1EN	D	302	27/27	0.95	0.07	15,17,22,38	0
3	1EN	E	302	27/27	0.96	0.06	16,22,28,38	0
2	NAP	A	301	48/48	0.98	0.05	9,19,23,29	0
2	NAP	B	301	48/48	0.98	0.05	12,19,25,32	0
2	NAP	D	301	48/48	0.98	0.04	10,15,22,25	0
2	NAP	E	301	48/48	0.98	0.06	10,18,25,30	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.

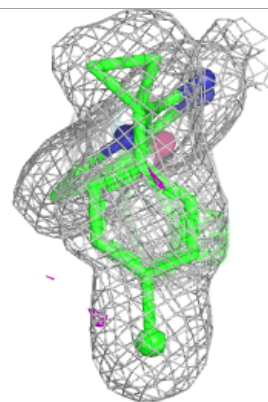
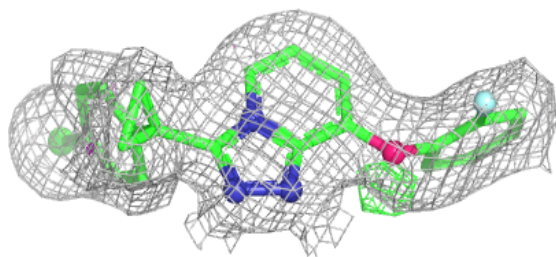
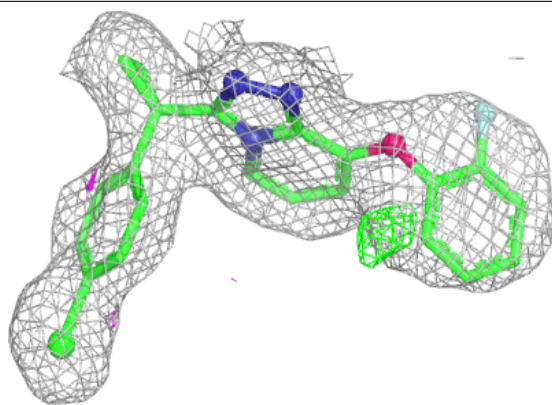
Electron density around 1EN A 302:

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

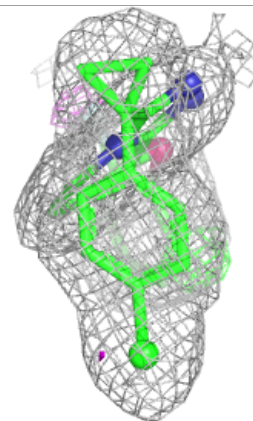
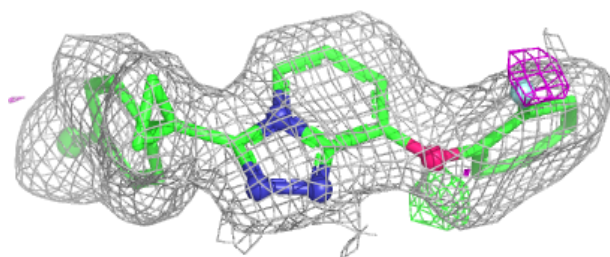
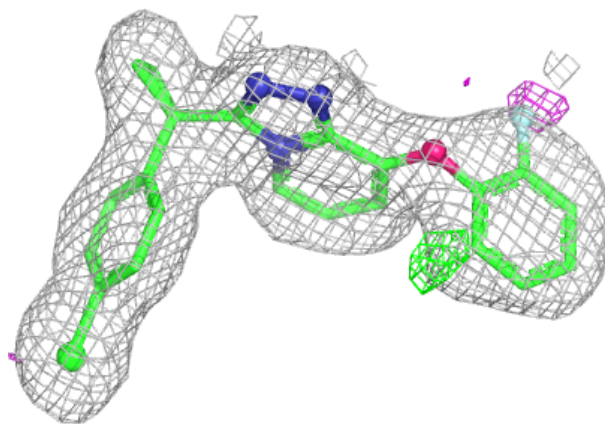


Electron density around 1EN B 302:

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

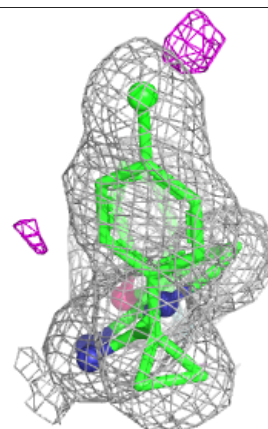
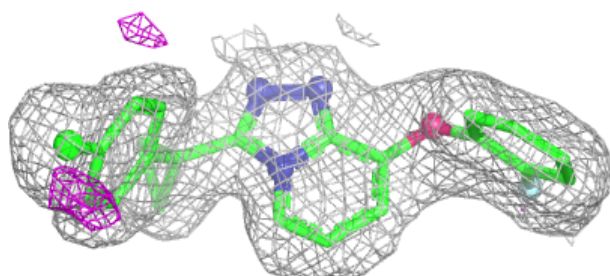
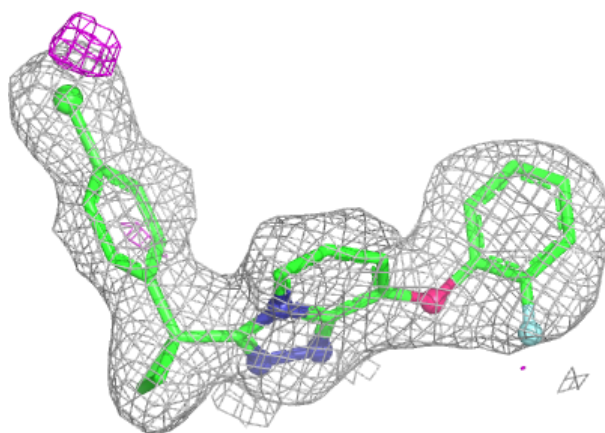
**Electron density around 1EN D 302:**

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

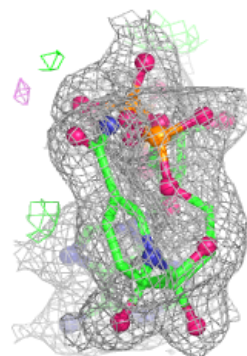
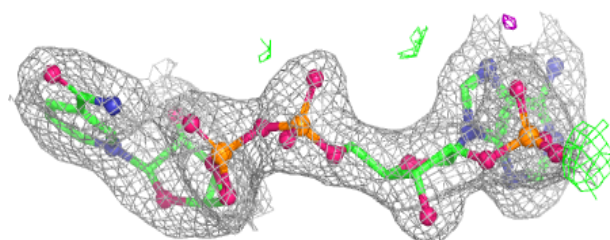
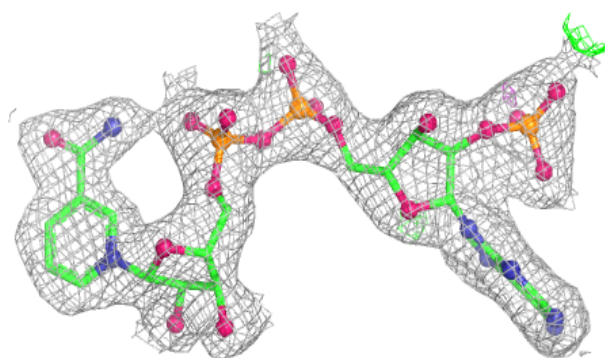


Electron density around 1EN E 302:

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

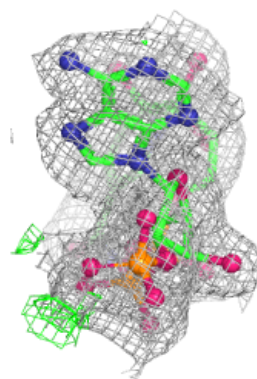
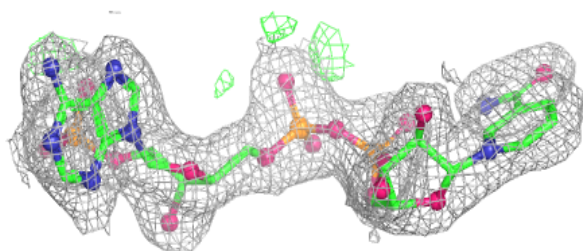
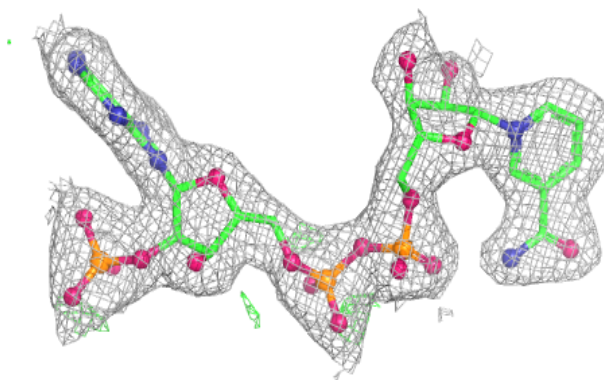
**Electron density around NAP A 301:**

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

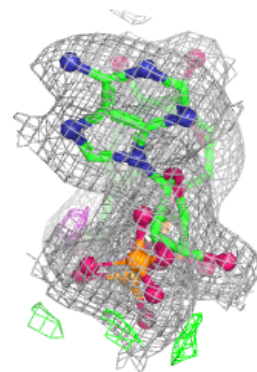
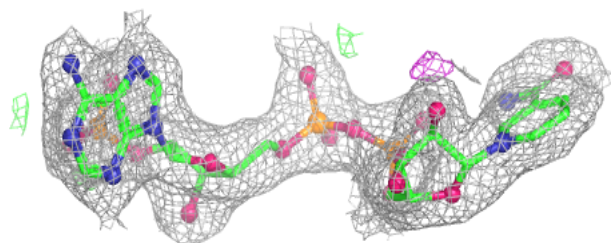
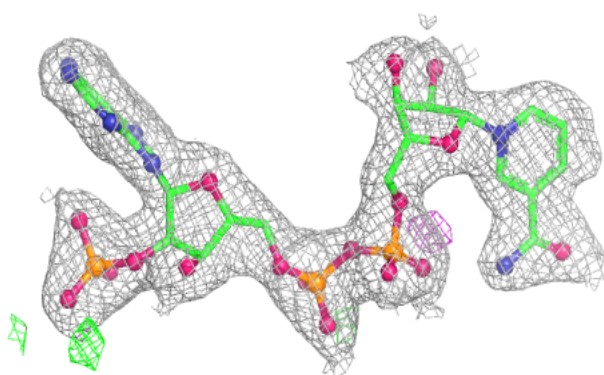


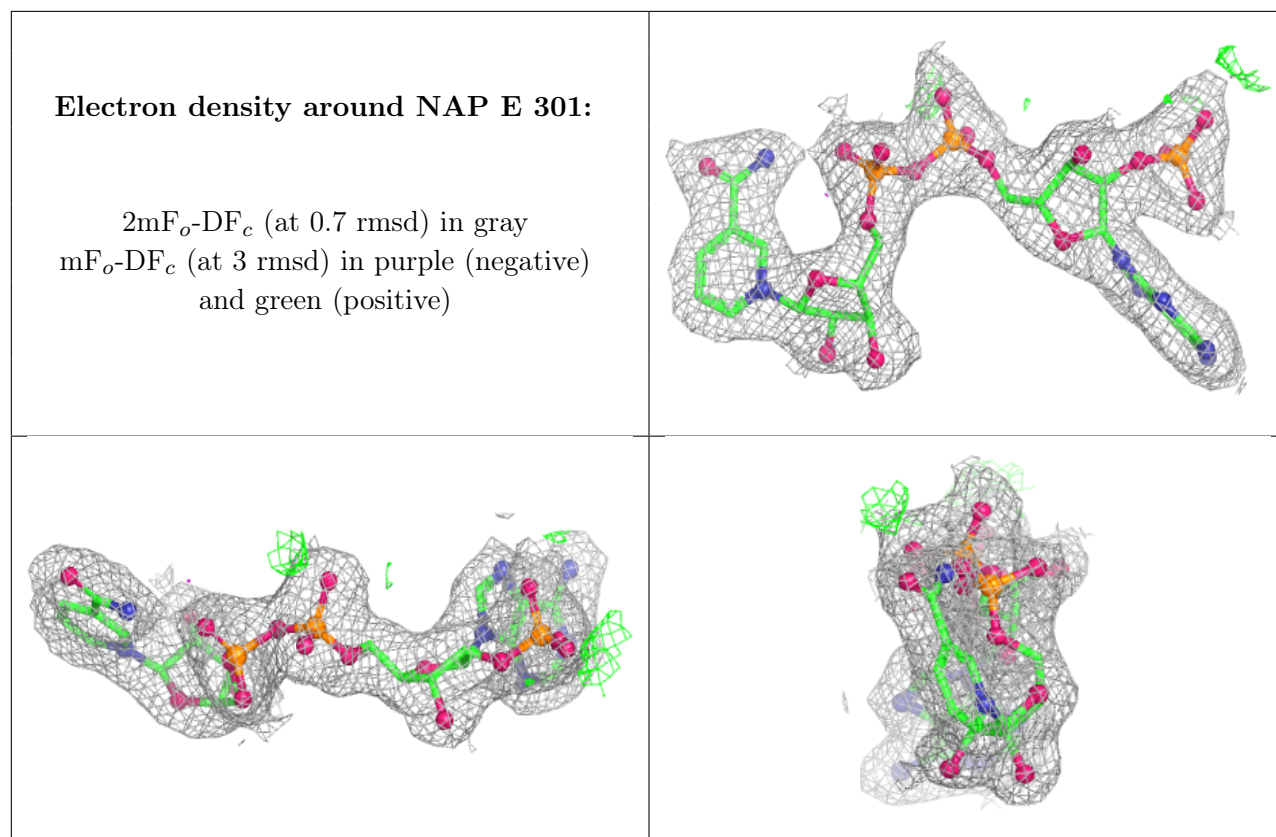
Electron density around NAP B 301:

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

**Electron density around 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.