



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:18 am BST

PDB ID : 4IJU  
Title : Crystal structure of 11b-HSD1 double mutant (L262R, F278E) in complex with (1S,4S)-4-[8-(2-fluorophenoxy)[1,2,4]triazolo[4,3-a]pyridin-3-yl]bicyclo[2.2.1]heptan-1-ol  
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](mailto: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.

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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

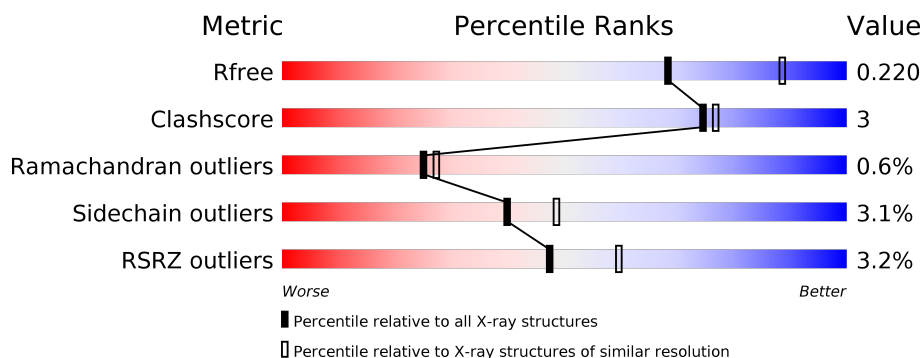
# 1 Overall quality at a glance

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  $\geq 3$ , 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 85%, yellow 85%, yellow 92%, grey 92%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>7% • 7%</span> </div> </div>
1	B	286	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 90%, yellow 90%, yellow 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>90%</span> <span>7% ••</span> </div> </div>
1	D	286	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 90%, yellow 90%, yellow 95%, grey 95%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>90%</span> <span>5% •••</span> </div> </div>
1	E	286	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 84%, yellow 84%, yellow 93%, grey 93%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>84%</span> <span>9% • 7%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9143 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	282	Total	C	N	O	S	0	0	0
			2144	1356	369	399	20			
1	D	275	Total	C	N	O	S	0	0	0
			2082	1319	356	388	19			
1	E	267	Total	C	N	O	S	0	0	0
			2057	1307	351	382	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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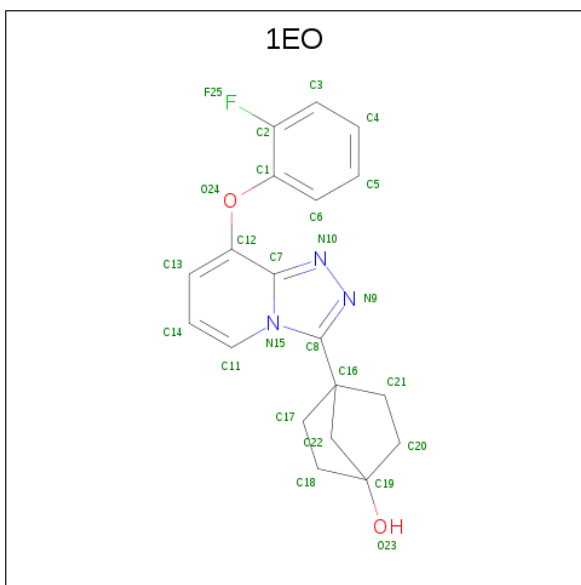
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	MET	-	EXPRESSION TAG	UNP P28845
B	12	SER	-	EXPRESSION TAG	UNP P28845
B	13	MET	-	EXPRESSION TAG	UNP P28845
B	14	THR	-	EXPRESSION TAG	UNP P28845
B	15	GLY	-	EXPRESSION TAG	UNP P28845
B	16	GLY	-	EXPRESSION TAG	UNP P28845
B	17	GLN	-	EXPRESSION TAG	UNP P28845
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

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- The chemical structure of Naproxen (NAP) is shown. It consists of a naphthalene ring system with a carboxylic acid group (-COOH) at position 1 and a 6-methoxy group (-OCH<sub>3</sub>) at position 2. The stereochemistry is indicated with (R) and (S) labels.

- Molecule 3 is (1s,4s)-4-[8-(2-fluorophenoxy)[1,2,4]triazolo[4,3-a]pyridin-3-yl]bicyclo[2.2.1]heptan-1-ol (three-letter code: 1EO) (formula: C<sub>19</sub>H<sub>18</sub>FN<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			25	19	1	3	2		
3	B	1	Total	C	F	N	O	0	0
			25	19	1	3	2		
3	D	1	Total	C	F	N	O	0	0
			25	19	1	3	2		
3	E	1	Total	C	F	N	O	0	0
			25	19	1	3	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total	O	0	0
			136	136		
5	B	152	Total	O	0	0
			152	152		
5	D	123	Total	O	0	0
			123	123		

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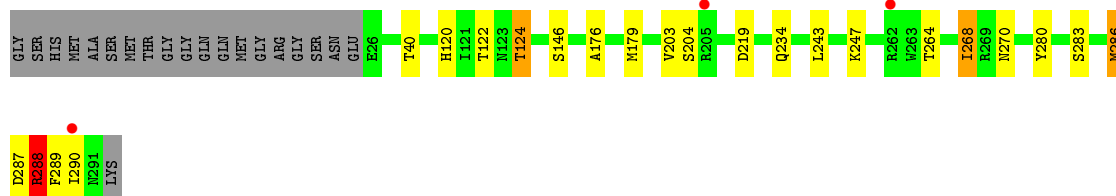
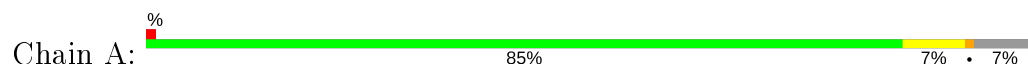
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	100	Total	O	0	0
			100	100		

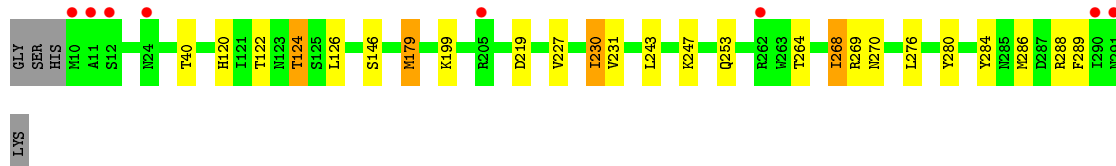
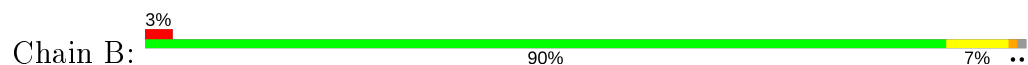
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

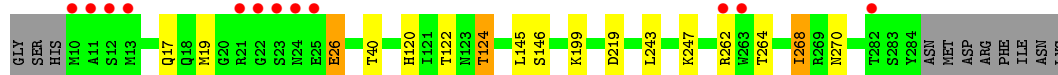
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



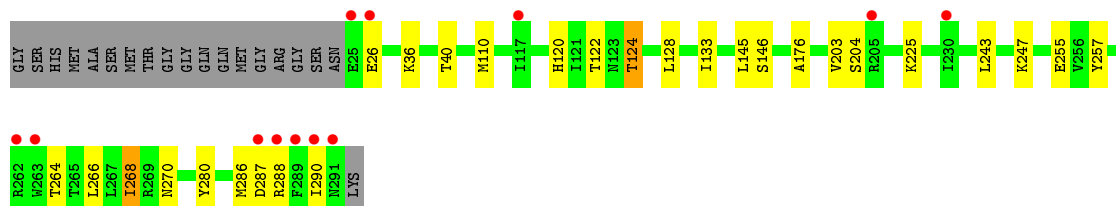
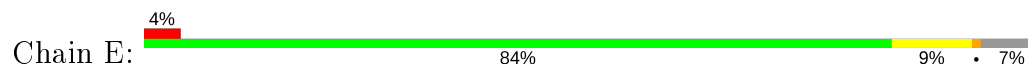
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



- 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, $\alpha$ , $\beta$ , $\gamma$	74.40 Å 94.20 Å 167.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.33 – 2.35 31.33 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.33-2.35) 99.7 (31.33-2.35)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.82 (at 2.34 Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.2, BUSTER 2.11.2	Depositor
R, $R_{free}$	0.182 , 0.218 0.177 , 0.220	Depositor DCC
$R_{free}$ test set	1184 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 1EO, CL

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	0.50	0/2093	0.68	0/2824
1	B	0.51	1/2178 (0.0%)	0.68	0/2936
1	D	0.48	0/2115	0.66	0/2852
1	E	0.47	0/2091	0.66	0/2821
All	All	0.49	1/8477 (0.0%)	0.67	0/11433

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	MET	SD-CE	-5.21	1.48	1.77

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	2055	0	2098	21	0
1	B	2144	0	2174	24	0
1	D	2082	0	2113	7	0
1	E	2057	0	2097	14	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	25	0	0
2	E	48	0	25	0	0
3	A	25	0	18	2	0
3	B	25	0	18	2	0
3	D	25	0	18	3	0
3	E	25	0	18	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	136	0	0	0	0
5	B	152	0	0	2	0
5	D	123	0	0	0	0
5	E	100	0	0	1	0
All	All	9143	0	8654	56	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 (56) 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:HG3	1:B:179:MET:HE3	1.53	0.89
1:A:288:ARG:HH21	1:A:288:ARG:HG2	1.45	0.81
1:A:286:MET:HG3	1:B:179:MET:CE	2.21	0.69
1:B:269:ARG:NH2	5:B:508:HOH:O	2.23	0.69
1:B:126:LEU:HD12	1:B:230:ILE:HD11	1.77	0.66
3:D:302:1EO:H2	1:E:280:TYR:CD2	2.29	0.66
1:A:288:ARG:CG	1:A:288:ARG:HH21	2.07	0.65
1:D:122:THR:O	1:D:124:THR:HG22	1.97	0.65
1:E:203:VAL:HG21	1:E:286:MET:SD	2.36	0.64
1:A:179:MET:HE2	1:B:286:MET:HG3	1.80	0.64
1:E:36:LYS:HG2	1:E:110:MET:HB3	1.80	0.64
1:B:122:THR:O	1:B:124:THR:HG22	2.00	0.62
1:A:179:MET:CE	1:B:286:MET:HG3	2.29	0.61
1:A:288:ARG:HG2	1:A:288:ARG:NH2	2.16	0.60
1:E:122:THR:O	1:E:124:THR:HG22	2.03	0.58
1:A:122:THR:O	1:A:124:THR:HG22	2.04	0.57
1:B:227:VAL:HB	1:B:231:VAL:HB	1.87	0.57
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.90	0.55
1:E:264:THR:O	1:E:268:ILE:HG13	2.08	0.54
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.91	0.53
1:E:40:THR:OG1	1:E:120:HIS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:TYR:CD1	1:B:286:MET:HE1	2.46	0.51
1:B:264:THR:O	1:B:268:ILE:HG13	2.10	0.51
1:A:264:THR:O	1:A:268:ILE:HG13	2.10	0.51
3:D:302:1EO:H2	1:E:280:TYR:CE2	2.45	0.51
1:A:289:PHE:HE2	1:B:179:MET:HE1	1.75	0.51
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.93	0.50
1:D:264:THR:O	1:D:268:ILE:HG13	2.12	0.50
1:B:284:TYR:CE1	1:B:286:MET:HE1	2.46	0.50
1:A:289:PHE:CE2	1:B:179:MET:HE1	2.47	0.50
3:A:302:1EO:H2	1:B:280:TYR:CD2	2.47	0.49
1:A:280:TYR:CD2	3:B:302:1EO:H2	2.49	0.48
1:E:255:GLU:OE2	1:E:257:TYR:OH	2.30	0.48
3:A:302:1EO:H2	1:B:280:TYR:CG	2.49	0.48
1:D:17:GLN:HG2	1:D:19:MET:H	1.79	0.47
1:A:176:ALA:HB3	1:B:199:LYS:HE2	1.97	0.47
1:A:204:SER:HA	1:A:290:ILE:HG12	1.97	0.47
1:E:204:SER:HA	1:E:290:ILE:HG12	1.98	0.46
1:A:203:VAL:HG21	1:A:286:MET:SD	2.56	0.46
1:A:179:MET:HE1	1:B:289:PHE:CE2	2.51	0.46
3:D:302:1EO:H2	1:E:280:TYR:CG	2.50	0.46
1:A:120:HIS:HE1	1:A:146:SER:OG	1.99	0.45
1:E:120:HIS:HE1	1:E:146:SER:OG	2.01	0.44
1:B:243:LEU:HG	1:B:247:LYS:HE3	2.01	0.43
1:B:120:HIS:HE1	1:B:146:SER:OG	2.01	0.43
1:D:199:LYS:HE2	1:E:176:ALA:HB3	2.01	0.42
1:B:253:GLN:NE2	5:B:520:HOH:O	2.53	0.42
1:A:280:TYR:CG	3:B:302:1EO:H2	2.54	0.42
1:D:120:HIS:HE1	1:D:146:SER:OG	2.02	0.42
1:D:243:LEU:HG	1:D:247:LYS:HE3	2.02	0.42
1:B:276:LEU:HD22	1:B:280:TYR:CZ	2.55	0.41
1:A:179:MET:HE1	1:B:289:PHE:HE2	1.84	0.41
1:E:243:LEU:HG	1:E:247:LYS:HE3	2.02	0.41
1:E:133:ILE:HG21	5:E:500:HOH:O	2.20	0.41
1:A:243:LEU:HG	1:A:247:LYS:HE3	2.01	0.41
1:B:230:ILE:HG21	1:B:230:ILE:HD12	1.87	0.41

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	265/286 (93%)	256 (97%)	7 (3%)	2 (1%)	19	20
1	B	280/286 (98%)	271 (97%)	8 (3%)	1 (0%)	34	38
1	D	273/286 (96%)	263 (96%)	8 (3%)	2 (1%)	22	23
1	E	265/286 (93%)	255 (96%)	9 (3%)	1 (0%)	34	38
All	All	1083/1144 (95%)	1045 (96%)	32 (3%)	6 (1%)	25	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	26	GLU
1	E	288	ARG
1	A	219	ASP
1	A	288	ARG
1	B	219	ASP
1	D	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%)	35	43
1	B	231/237 (98%)	226 (98%)	5 (2%)	52	63
1	D	223/237 (94%)	217 (97%)	6 (3%)	44	55
1	E	224/237 (94%)	215 (96%)	9 (4%)	31	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	902/948 (95%)	874 (97%)	28 (3%)	40	48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	THR
1	A	234	GLN
1	A	268	ILE
1	A	270	ASN
1	A	283	SER
1	A	286	MET
1	A	287	ASP
1	A	288	ARG
1	B	124	THR
1	B	230	ILE
1	B	268	ILE
1	B	270	ASN
1	B	288	ARG
1	D	26	GLU
1	D	124	THR
1	D	145	LEU
1	D	262	ARG
1	D	268	ILE
1	D	270	ASN
1	E	26	GLU
1	E	124	THR
1	E	128	LEU
1	E	145	LEU
1	E	225	LYS
1	E	266	LEU
1	E	268	ILE
1	E	270	ASN
1	E	287	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	253	GLN
1	B	17	GLN
1	B	33	GLN

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Mol	Chain	Res	Type
1	B	119	ASN
1	B	120	HIS
1	B	134	HIS
1	B	234	GLN
1	B	253	GLN
1	B	270	ASN
1	D	119	ASN
1	D	120	HIS
1	D	270	ASN
1	E	119	ASN
1	E	120	HIS
1	E	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](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	1EO	A	302	-	25,29,29	1.64	3 (12%)	28,45,45	1.94	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAP	E	301	-	45,52,52	0.99	1 (2%)	56,80,80	0.74	2 (3%)
3	1EO	E	302	-	25,29,29	1.73	3 (12%)	28,45,45	1.94	5 (17%)
2	NAP	A	301	-	45,52,52	1.14	1 (2%)	56,80,80	0.78	2 (3%)
3	1EO	B	302	-	25,29,29	1.61	3 (12%)	28,45,45	1.79	5 (17%)
2	NAP	B	301	-	45,52,52	1.06	1 (2%)	56,80,80	0.90	3 (5%)
2	NAP	D	301	-	45,52,52	1.16	1 (2%)	56,80,80	0.88	3 (5%)
3	1EO	D	302	-	25,29,29	1.69	3 (12%)	28,45,45	1.77	5 (17%)

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	1EO	A	302	-	-	0/4/30/30	0/6/5/5
2	NAP	E	301	-	-	3/31/67/67	0/5/5/5
3	1EO	E	302	-	-	0/4/30/30	0/6/5/5
2	NAP	A	301	-	-	6/31/67/67	0/5/5/5
3	1EO	B	302	-	-	0/4/30/30	0/6/5/5
2	NAP	B	301	-	-	7/31/67/67	0/5/5/5
2	NAP	D	301	-	-	7/31/67/67	0/5/5/5
3	1EO	D	302	-	-	0/4/30/30	0/6/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAP	C2N-N1N	6.76	1.43	1.35
2	A	301	NAP	C2N-N1N	6.01	1.42	1.35
2	B	301	NAP	C2N-N1N	5.47	1.41	1.35
2	E	301	NAP	C2N-N1N	5.15	1.41	1.35
3	D	302	1EO	C14-C13	5.01	1.49	1.38
3	A	302	1EO	C14-C13	5.00	1.49	1.38
3	E	302	1EO	C14-C13	4.84	1.49	1.38
3	B	302	1EO	C14-C13	4.84	1.49	1.38
3	E	302	1EO	C12-C7	4.27	1.47	1.42
3	B	302	1EO	C12-C7	3.89	1.47	1.42
3	E	302	1EO	N10-N9	3.85	1.45	1.37
3	D	302	1EO	C12-C7	3.75	1.47	1.42
3	A	302	1EO	C12-C7	3.71	1.47	1.42
3	A	302	1EO	N10-N9	3.45	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	1EO	N10-N9	3.38	1.44	1.37
3	D	302	1EO	N10-N9	3.25	1.44	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	1EO	C19-C22-C16	-7.41	95.33	100.04
3	A	302	1EO	C19-C22-C16	-6.48	95.92	100.04
3	B	302	1EO	C19-C22-C16	-5.54	96.52	100.04
3	D	302	1EO	C19-C22-C16	-5.17	96.75	100.04
3	A	302	1EO	O23-C19-C18	4.50	120.06	109.80
3	B	302	1EO	O23-C19-C18	4.04	118.99	109.80
3	B	302	1EO	O23-C19-C20	3.95	118.80	109.80
3	D	302	1EO	O23-C19-C18	3.76	118.38	109.80
3	D	302	1EO	O23-C19-C20	3.62	118.04	109.80
2	B	301	NAP	O4D-C1D-C2D	-3.61	101.64	106.93
3	E	302	1EO	O23-C19-C18	3.61	118.02	109.80
2	D	301	NAP	O4D-C1D-C2D	-3.42	101.92	106.93
3	E	302	1EO	O23-C19-C20	3.35	117.43	109.80
3	A	302	1EO	C18-C19-C22	-3.33	95.01	103.41
3	A	302	1EO	O23-C19-C20	3.33	117.38	109.80
3	D	302	1EO	C18-C19-C22	-3.02	95.82	103.41
3	E	302	1EO	C18-C19-C22	-2.96	95.96	103.41
3	B	302	1EO	C18-C19-C22	-2.68	96.67	103.41
3	D	302	1EO	C6-C1-C2	2.58	122.14	118.07
2	E	301	NAP	C5A-C6A-N6A	2.47	124.11	120.35
2	A	301	NAP	O4D-C1D-C2D	-2.47	103.32	106.93
2	B	301	NAP	C5A-C6A-N6A	2.43	124.05	120.35
2	A	301	NAP	C5A-C6A-N6A	2.40	124.00	120.35
3	A	302	1EO	C6-C1-C2	2.39	121.83	118.07
2	D	301	NAP	C5A-C6A-N6A	2.35	123.92	120.35
3	B	302	1EO	C6-C1-C2	2.24	121.60	118.07
2	E	301	NAP	O4D-C1D-C2D	-2.20	103.71	106.93
3	E	302	1EO	C6-C1-C2	2.13	121.43	118.07
2	D	301	NAP	C6N-N1N-C2N	-2.12	120.04	121.97
2	B	301	NAP	O2B-P2B-O1X	2.03	117.24	109.39

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	NAP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
2	E	301	NAP	C2B-O2B-P2B-O2X
2	A	301	NAP	C2B-O2B-P2B-O2X
2	A	301	NAP	C5D-O5D-PN-O1N
2	B	301	NAP	C5D-O5D-PN-O1N
2	D	301	NAP	C2B-O2B-P2B-O1X
2	D	301	NAP	C2B-O2B-P2B-O2X
2	D	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	C2B-O2B-P2B-O1X
2	A	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5D-O5D-PN-O3
2	D	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	PN-O3-PA-O1A
2	D	301	NAP	PN-O3-PA-O1A
2	B	301	NAP	C3B-C2B-O2B-P2B
2	A	301	NAP	O4B-C4B-C5B-O5B
2	A	301	NAP	PN-O3-PA-O2A
2	B	301	NAP	C5D-O5D-PN-O2N
2	D	301	NAP	C5D-O5D-PN-O2N
2	E	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	C1B-C2B-O2B-P2B

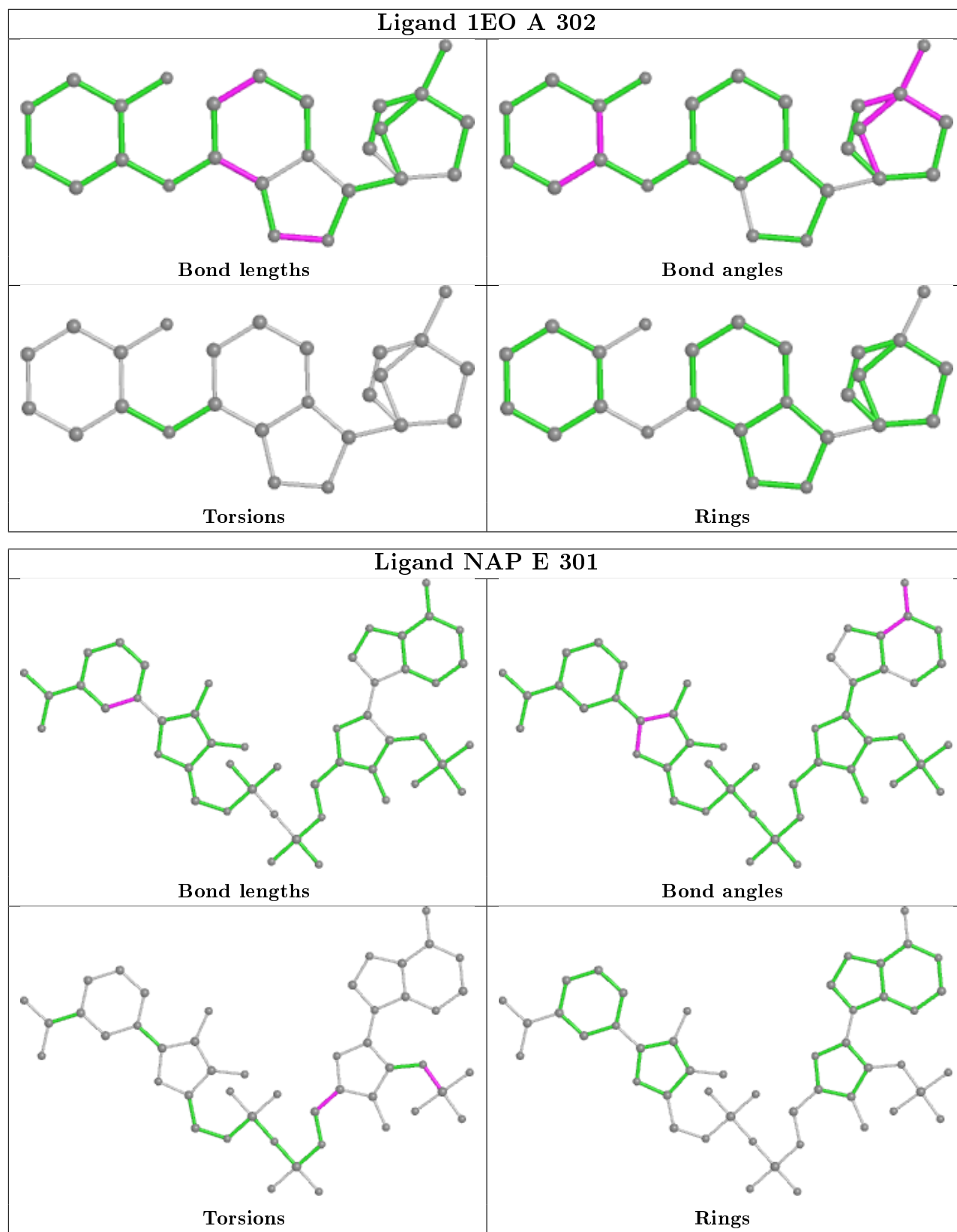
There are no ring outliers.

3 monomers are involved in 7 short contacts:

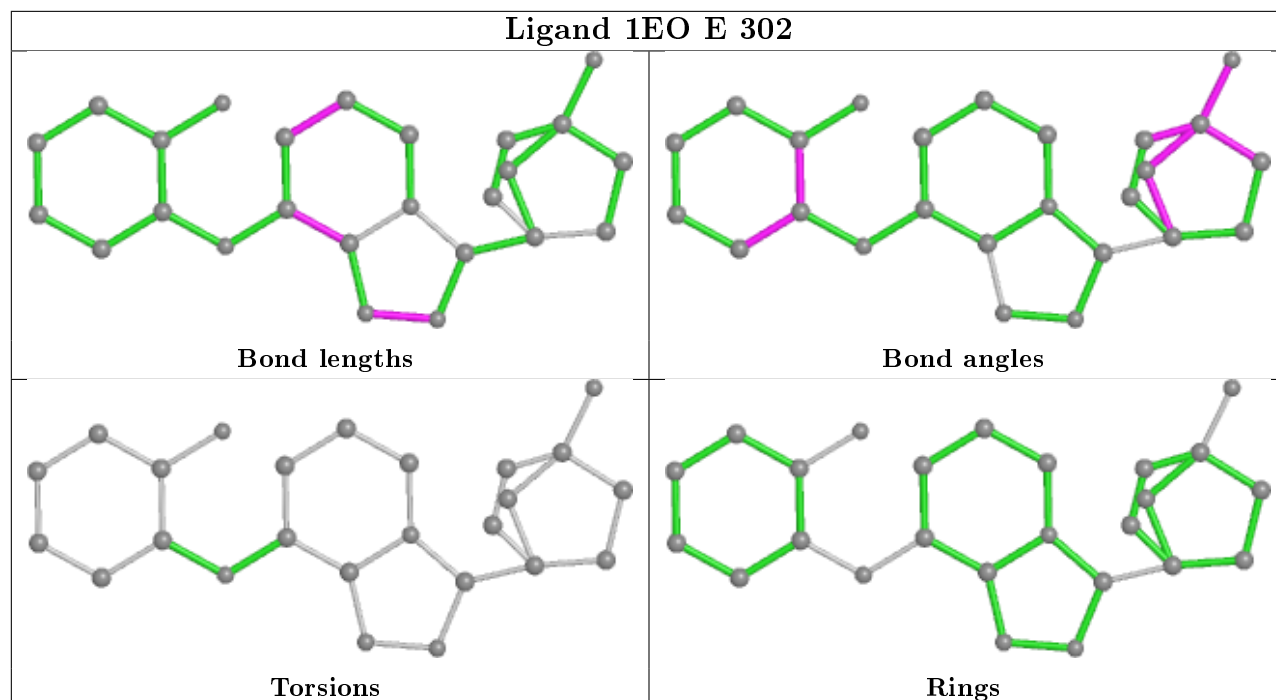
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	1EO	2	0
3	B	302	1EO	2	0
3	D	302	1EO	3	0

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

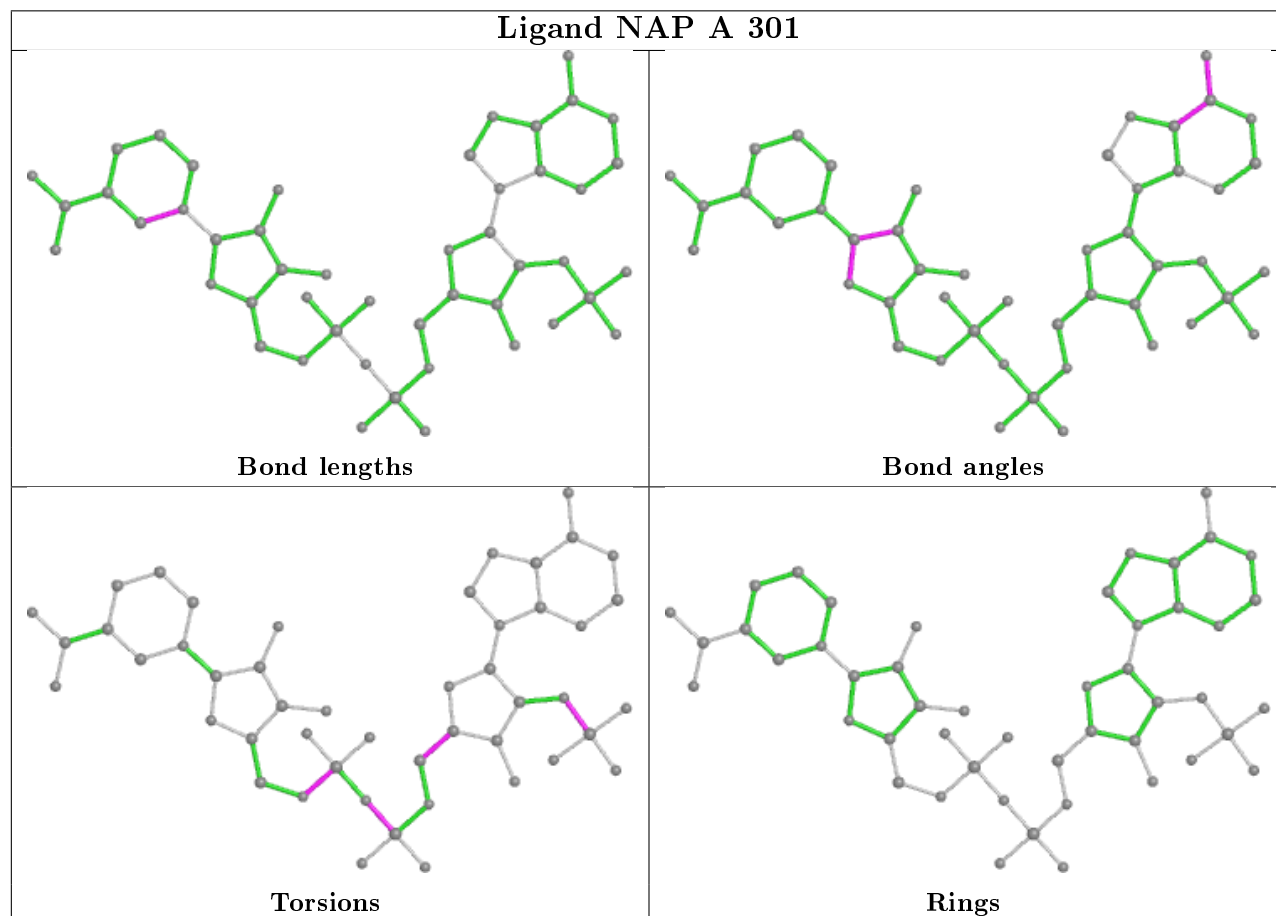
equivalents in the CSD to analyse the geometry.



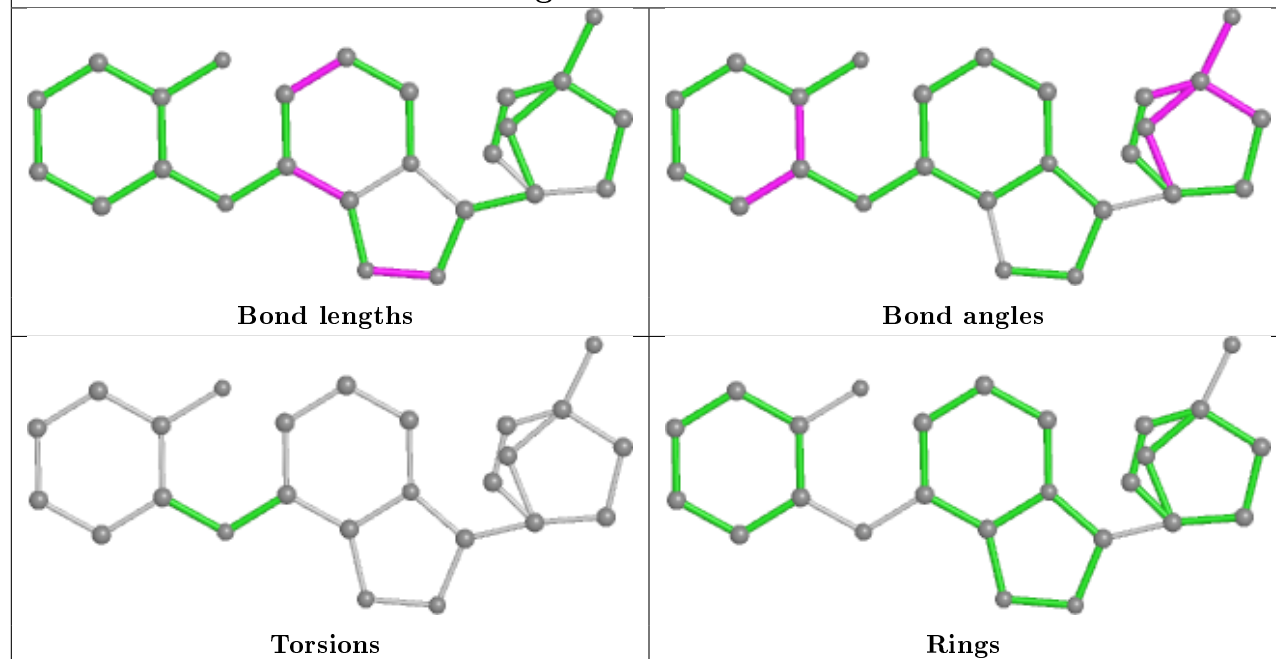
## Ligand 1EO E 302



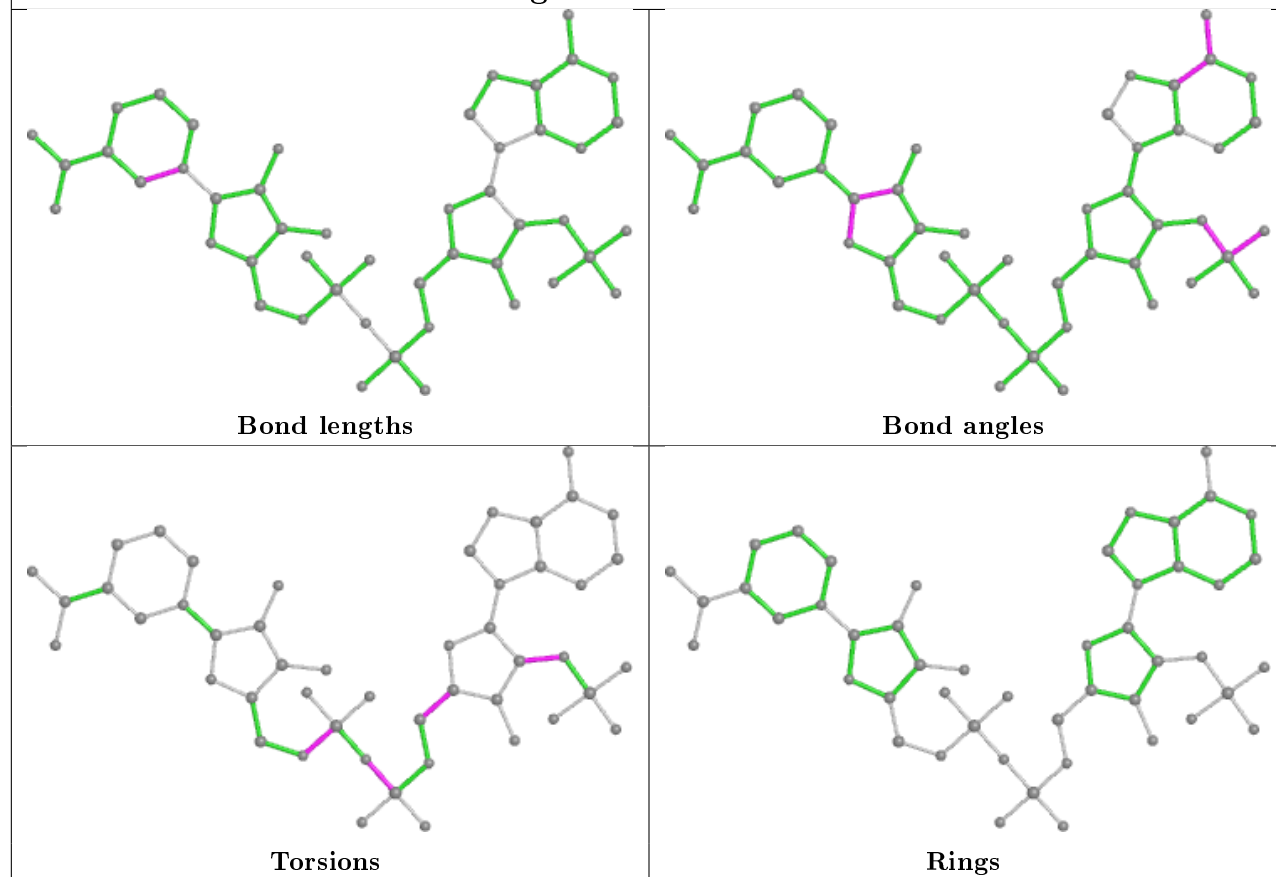
## Ligand NAP A 301

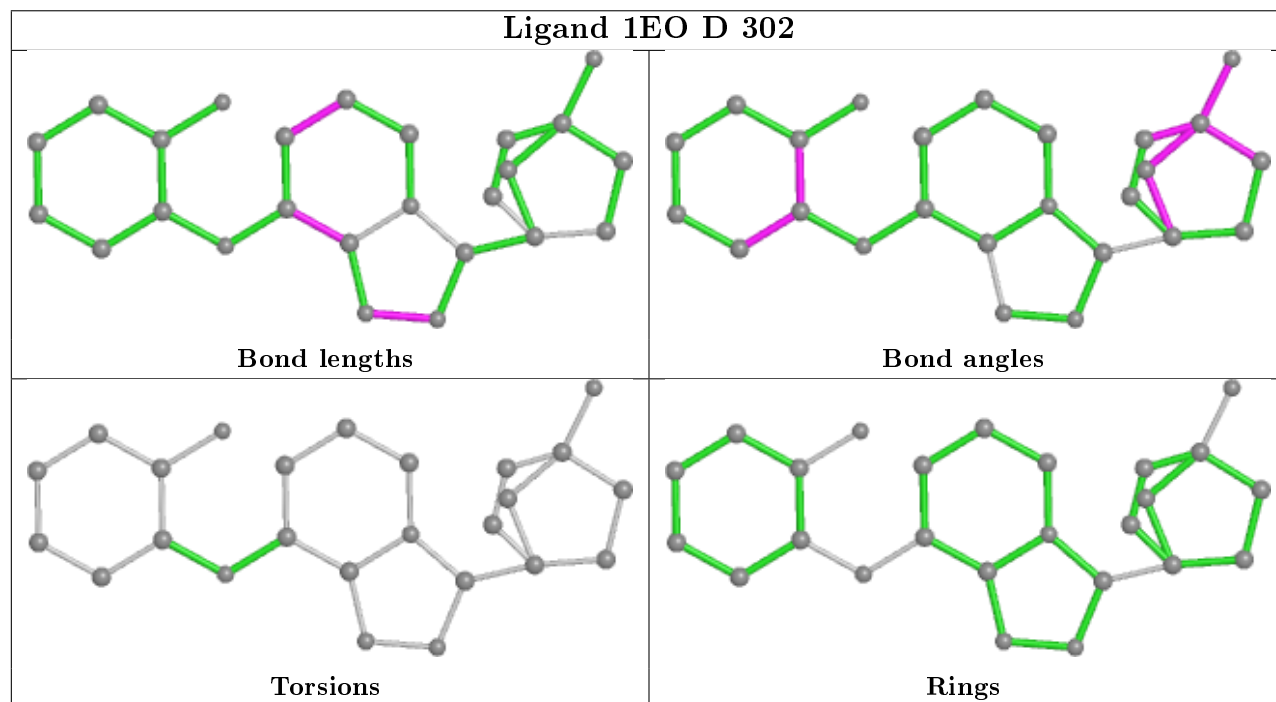
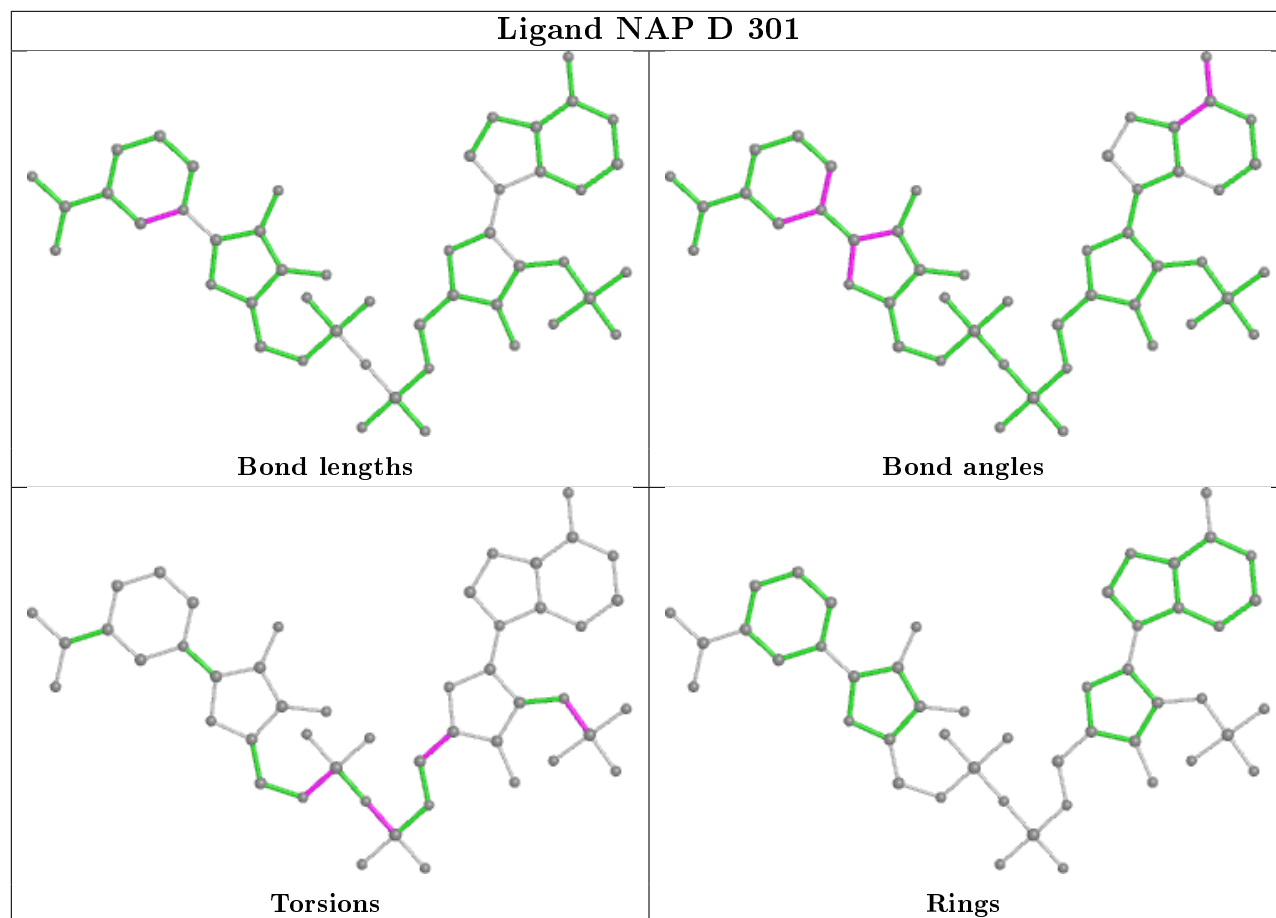


## Ligand 1EO B 302



## Ligand NAP B 301





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	266/286 (93%)	-0.29	3 (1%) 80 87	10, 19, 42, 93	0
1	B	282/286 (98%)	-0.19	8 (2%) 53 64	8, 21, 44, 100	0
1	D	275/286 (96%)	-0.24	12 (4%) 34 46	11, 21, 52, 71	0
1	E	267/286 (93%)	0.12	12 (4%) 33 46	14, 28, 54, 110	0
All	All	1090/1144 (95%)	-0.15	35 (3%) 47 59	8, 22, 50, 110	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	290	ILE	7.4
1	B	24	ASN	6.8
1	D	11	ALA	6.2
1	E	291	ASN	5.4
1	D	10	MET	5.0
1	A	290	ILE	4.6
1	E	262	ARG	4.2
1	B	290	ILE	4.0
1	B	262	ARG	3.9
1	E	25	GLU	3.7
1	D	23	SER	3.7
1	D	12	SER	3.6
1	D	22	GLY	3.6
1	B	291	ASN	3.2
1	A	262	ARG	3.1
1	E	205	ARG	3.1
1	E	288	ARG	3.0
1	E	263	TRP	3.0
1	D	21	ARG	3.0
1	A	205	ARG	3.0
1	D	24	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	25	GLU	2.9
1	D	262	ARG	2.9
1	D	263	TRP	2.8
1	E	289	PHE	2.7
1	B	11	ALA	2.7
1	B	205	ARG	2.5
1	E	230	ILE	2.5
1	B	12	SER	2.4
1	E	26	GLU	2.4
1	D	13	MET	2.3
1	E	117	ILE	2.2
1	D	282	THR	2.1
1	E	287	ASP	2.1
1	B	10	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	1EO	A	302	25/25	0.94	0.10	14,20,22,31	0
3	1EO	E	302	25/25	0.95	0.10	13,22,28,35	0
3	1EO	D	302	25/25	0.95	0.11	14,17,20,29	0
2	NAP	E	301	48/48	0.97	0.10	11,22,26,31	0
4	CL	E	303	1/1	0.97	0.07	47,47,47,47	0
3	1EO	B	302	25/25	0.97	0.13	15,18,20,28	0
4	CL	D	303	1/1	0.97	0.08	34,34,34,34	0
2	NAP	B	301	48/48	0.98	0.09	6,15,20,23	0
2	NAP	D	301	48/48	0.98	0.09	10,15,19,22	0

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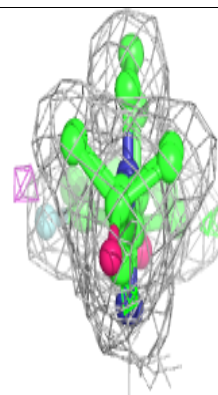
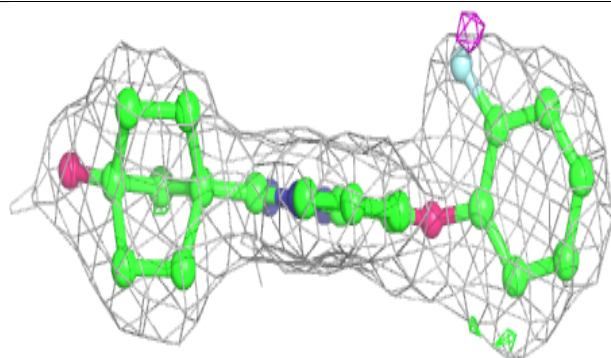
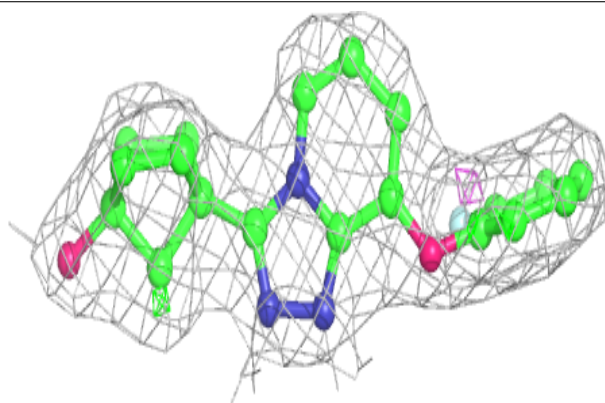
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	A	301	48/48	0.98	0.09	11,15,19,21	0

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.

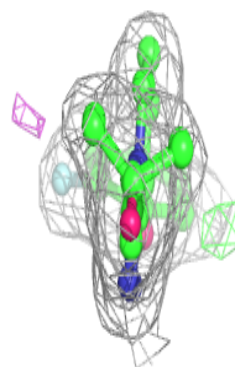
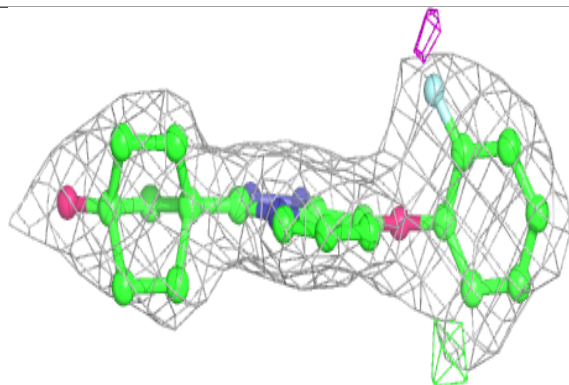
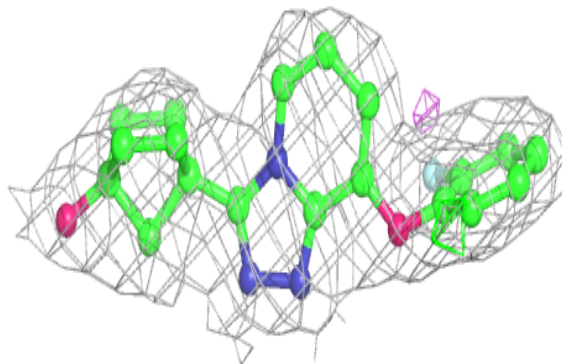
**Electron density around 1EO A 302:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

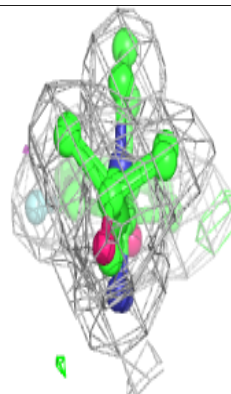
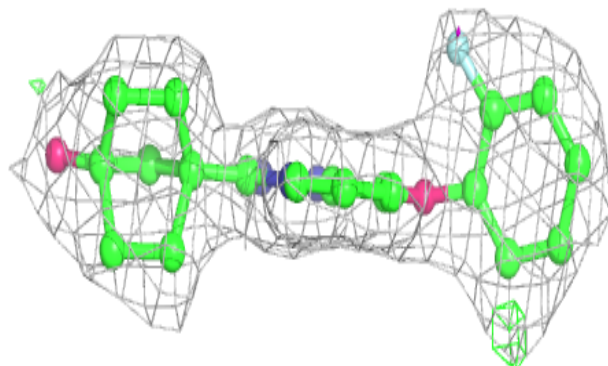
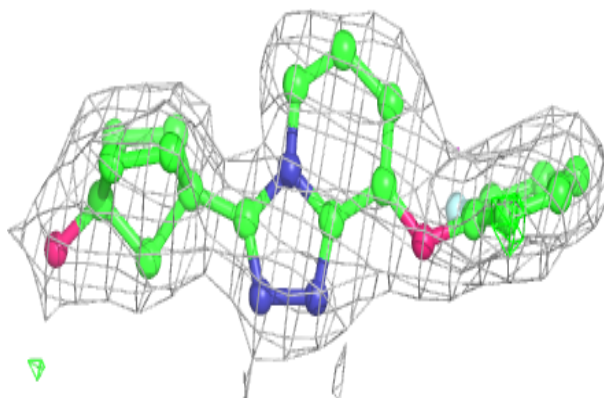


**Electron density around 1EO E 302:**

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

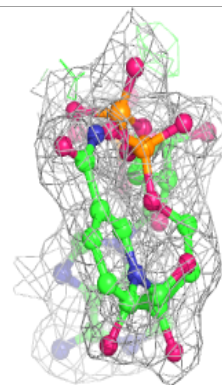
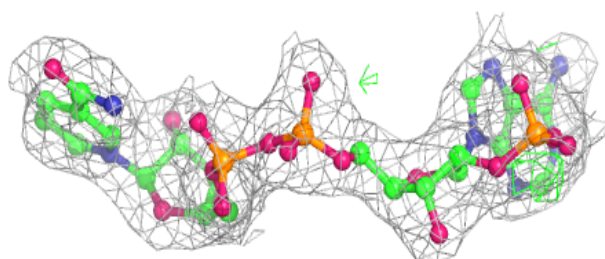
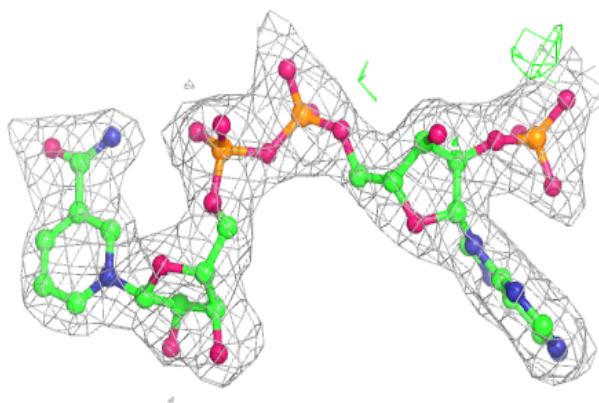
**Electron density around 1EO D 302:**

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

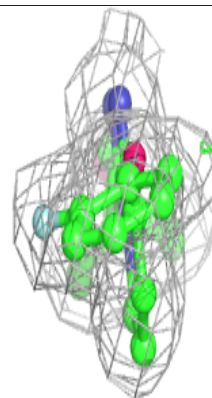
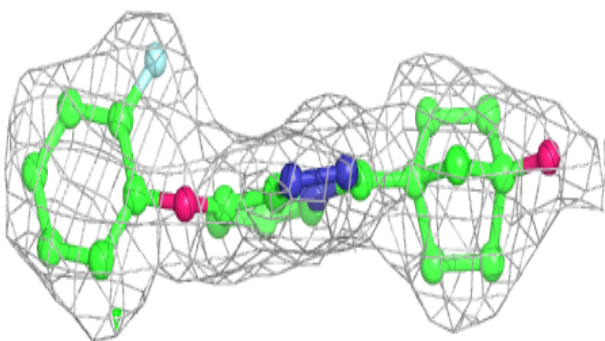
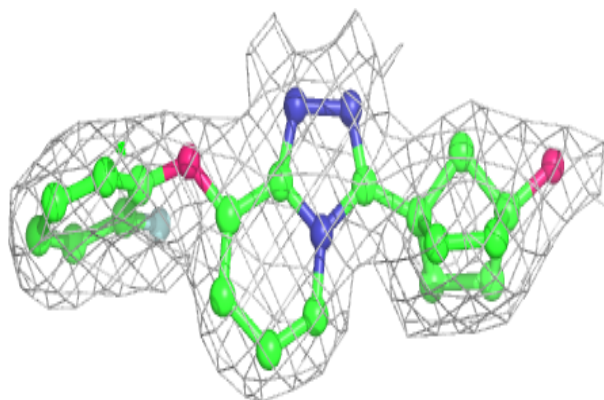


**Electron density around NAP E 301:**

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

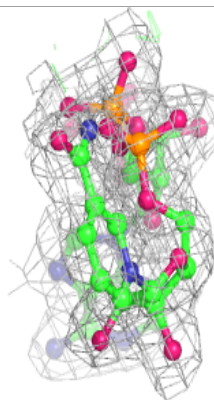
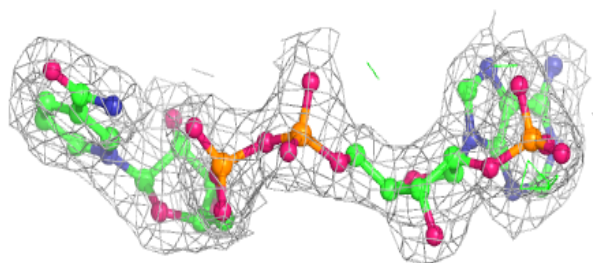
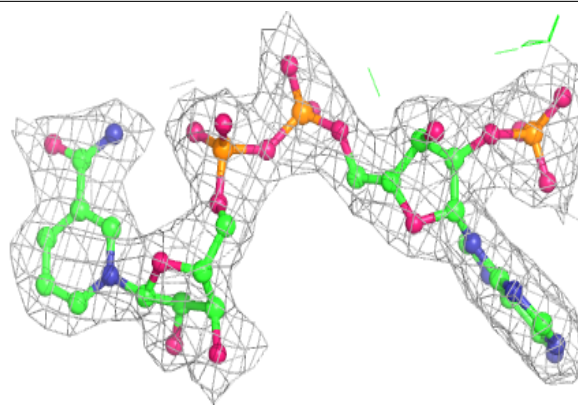
**Electron density around 1EO B 302:**

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

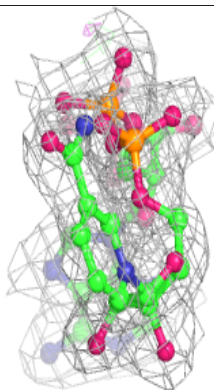
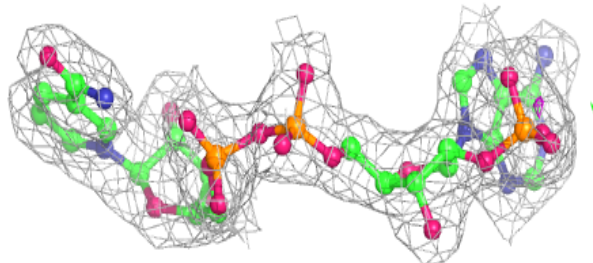
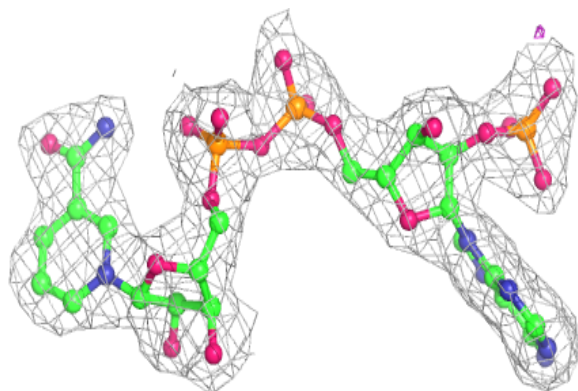


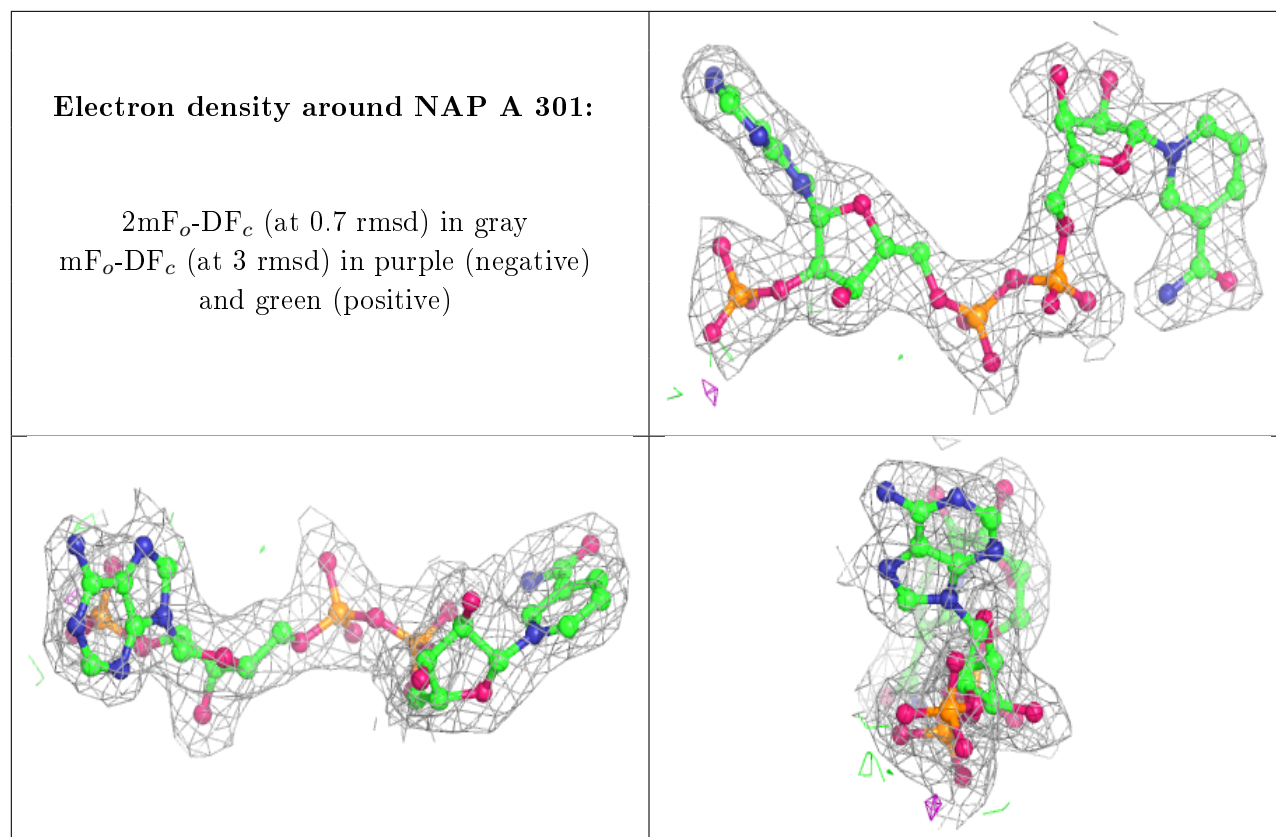
**Electron density around NAP B 301:**

$2mF_o-DF_c$  (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.