



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 10:11 PM JST

PDB ID : 8HFJ  
Title : Crystal Structure of CbAR mutant (H162F) in complex with NADP<sup>+</sup> and a bulky 1,3-cyclodiketone  
Authors : Hou, X.D.; Yin, D.J.; Rao, Y.J.  
Deposited on : 2022-11-10  
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

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

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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 : 2.36  
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) : 2.36

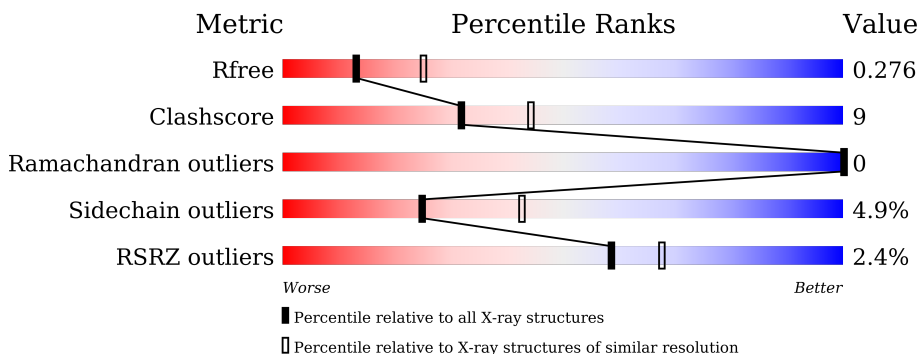
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 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	279	
1	B	279	
1	C	279	
1	D	279	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	L7Z	D	302	-	X	-	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7992 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 Versicolorin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	Total 1929	C 1216	N 343	O 366	S 4	0	0	0
1	B	252	Total 1881	C 1183	N 336	O 359	S 3	0	0	0
1	C	260	Total 1957	C 1232	N 351	O 370	S 4	0	1	0
1	D	253	Total 1898	C 1195	N 340	O 359	S 4	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
A	0	ALA	-	expression tag	UNP A0A2G5I2X5
A	162	PHE	HIS	engineered mutation	UNP A0A2G5I2X5
A	269	ALA	-	expression tag	UNP A0A2G5I2X5
A	270	LEU	-	expression tag	UNP A0A2G5I2X5
A	271	GLU	-	expression tag	UNP A0A2G5I2X5
A	272	HIS	-	expression tag	UNP A0A2G5I2X5
A	273	HIS	-	expression tag	UNP A0A2G5I2X5
A	274	HIS	-	expression tag	UNP A0A2G5I2X5
A	275	HIS	-	expression tag	UNP A0A2G5I2X5
A	276	HIS	-	expression tag	UNP A0A2G5I2X5
A	277	HIS	-	expression tag	UNP A0A2G5I2X5
B	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
B	0	ALA	-	expression tag	UNP A0A2G5I2X5
B	162	PHE	HIS	engineered mutation	UNP A0A2G5I2X5
B	269	ALA	-	expression tag	UNP A0A2G5I2X5
B	270	LEU	-	expression tag	UNP A0A2G5I2X5
B	271	GLU	-	expression tag	UNP A0A2G5I2X5
B	272	HIS	-	expression tag	UNP A0A2G5I2X5
B	273	HIS	-	expression tag	UNP A0A2G5I2X5
B	274	HIS	-	expression tag	UNP A0A2G5I2X5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	275	HIS	-	expression tag	UNP A0A2G5I2X5
B	276	HIS	-	expression tag	UNP A0A2G5I2X5
B	277	HIS	-	expression tag	UNP A0A2G5I2X5
C	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
C	0	ALA	-	expression tag	UNP A0A2G5I2X5
C	162	PHE	HIS	engineered mutation	UNP A0A2G5I2X5
C	269	ALA	-	expression tag	UNP A0A2G5I2X5
C	270	LEU	-	expression tag	UNP A0A2G5I2X5
C	271	GLU	-	expression tag	UNP A0A2G5I2X5
C	272	HIS	-	expression tag	UNP A0A2G5I2X5
C	273	HIS	-	expression tag	UNP A0A2G5I2X5
C	274	HIS	-	expression tag	UNP A0A2G5I2X5
C	275	HIS	-	expression tag	UNP A0A2G5I2X5
C	276	HIS	-	expression tag	UNP A0A2G5I2X5
C	277	HIS	-	expression tag	UNP A0A2G5I2X5
D	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
D	0	ALA	-	expression tag	UNP A0A2G5I2X5
D	162	PHE	HIS	engineered mutation	UNP A0A2G5I2X5
D	269	ALA	-	expression tag	UNP A0A2G5I2X5
D	270	LEU	-	expression tag	UNP A0A2G5I2X5
D	271	GLU	-	expression tag	UNP A0A2G5I2X5
D	272	HIS	-	expression tag	UNP A0A2G5I2X5
D	273	HIS	-	expression tag	UNP A0A2G5I2X5
D	274	HIS	-	expression tag	UNP A0A2G5I2X5
D	275	HIS	-	expression tag	UNP A0A2G5I2X5
D	276	HIS	-	expression tag	UNP A0A2G5I2X5
D	277	HIS	-	expression tag	UNP A0A2G5I2X5

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			16	14	2		
3	D	1	Total	C	O	0	0
			16	14	2		

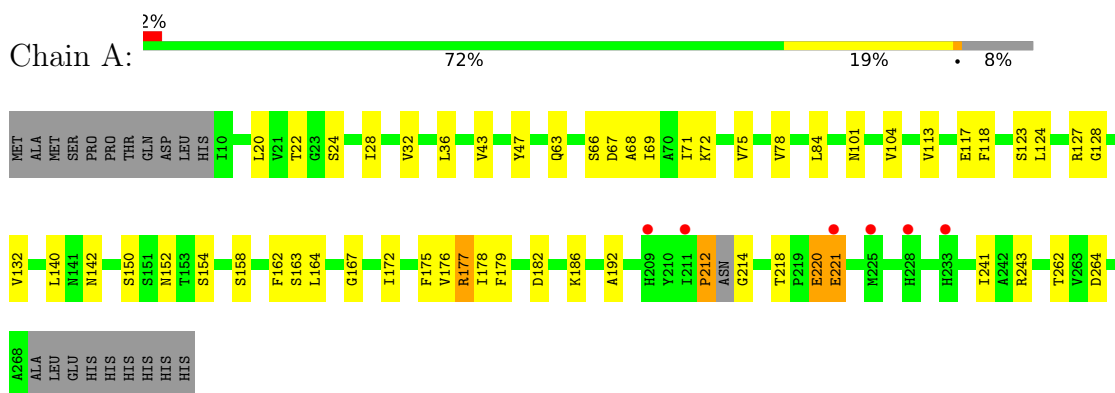
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	25	Total	O	0	0
			25	25		
4	C	26	Total	O	0	0
			26	26		
4	D	27	Total	O	0	0
			27	27		

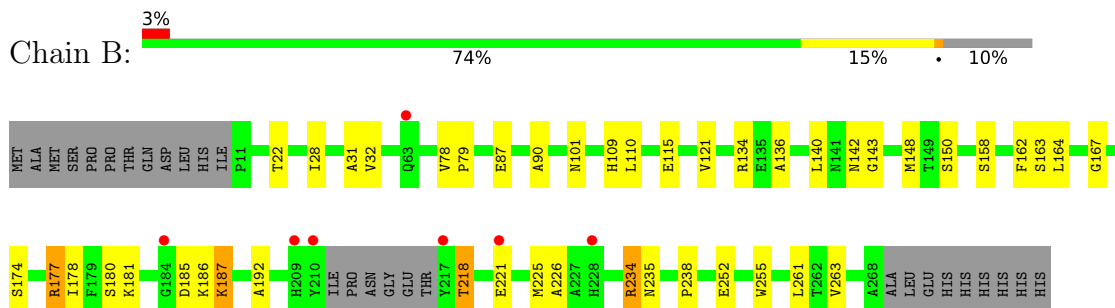
### 3 Residue-property plots i

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.

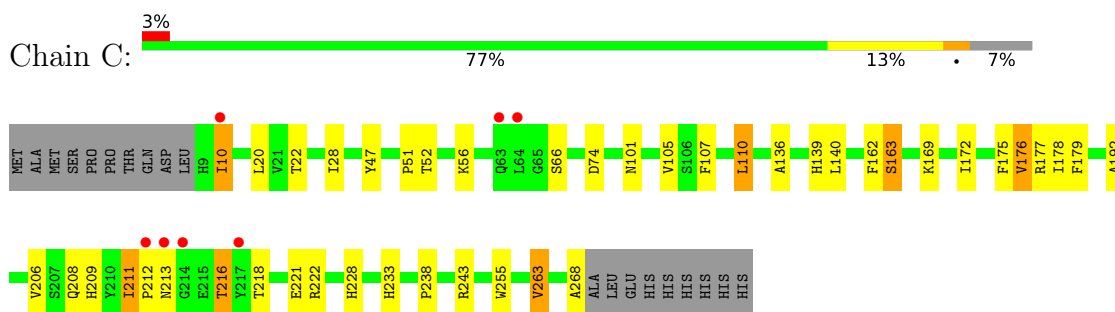
- Molecule 1: Versicolorin reductase



- Molecule 1: Versicolorin reductase



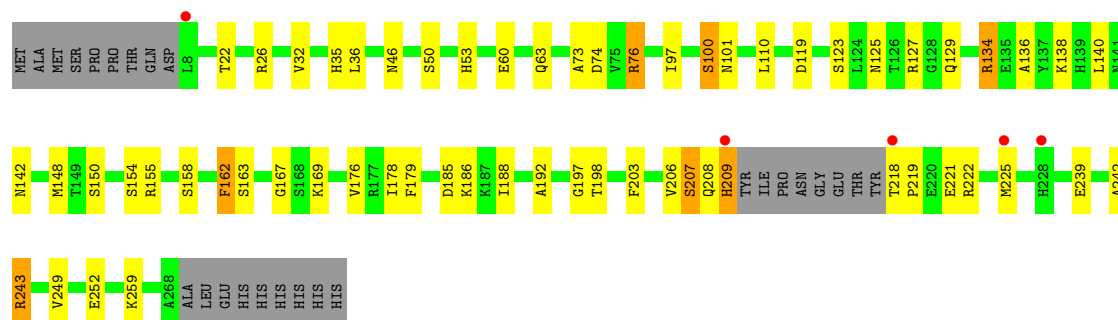
- Molecule 1: Versicolorin reductase



- Molecule 1: Versicolorin reductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.92Å 124.92Å 133.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.11 – 2.75 24.06 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.11-2.75) 99.9 (24.06-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.76Å)	Xtrriage
Refinement program	REFMAC 5.5	Depositor
R, $R_{free}$	0.205 , 0.270 0.218 , 0.276	Depositor DCC
$R_{free}$ test set	1383 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtrriage
Anisotropy	0.018	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 27.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7992	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L7Z, 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	0.75	0/1965	0.90	0/2659
1	B	0.72	0/1916	0.87	0/2593
1	C	0.74	0/1996	0.88	0/2703
1	D	0.67	0/1933	0.84	0/2615
All	All	0.72	0/7810	0.87	0/10570

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	4
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	234	ARG	Sidechain
1	D	127	ARG	Sidechain
1	D	134	ARG	Sidechain
1	D	243	ARG	Sidechain
1	D	26	ARG	Sidechain

## 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	1929	0	1898	44	0
1	B	1881	0	1836	38	0
1	C	1957	0	1918	33	0
1	D	1898	0	1875	48	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
2	C	48	0	25	1	0
2	D	48	0	25	5	0
3	C	16	0	0	3	0
3	D	16	0	0	3	0
4	A	25	0	0	0	0
4	B	25	0	0	1	0
4	C	26	0	0	1	0
4	D	27	0	0	3	0
All	All	7992	0	7627	138	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 9.

All (138) 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:C:206:VAL:HG11	3:C:302:L7Z:C11	2.13	0.77
1:D:136:ALA:O	1:D:140:LEU:HB2	1.85	0.75
2:D:301:NAP:H71N	3:D:302:L7Z:C16	2.00	0.74
1:B:143:GLY:HA2	1:B:187:LYS:O	1.89	0.71
1:D:60:GLU:O	1:D:63:GLN:HB3	1.91	0.71
2:D:301:NAP:H4N	3:D:302:L7Z:C16	2.21	0.69
1:A:158:SER:O	1:B:181:LYS:NZ	2.28	0.67
1:C:211:ILE:HD12	1:C:222:ARG:HG2	1.77	0.66
1:A:262:THR:HB	1:D:259:LYS:HE2	1.79	0.64
1:C:136:ALA:O	1:C:140:LEU:HB2	1.98	0.64
1:D:32:VAL:HG22	1:D:242:ALA:HA	1.80	0.62
1:A:182:ASP:HB3	1:B:109:HIS:CE1	2.34	0.62
1:C:176:VAL:HG11	1:C:192:ALA:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:THR:HB	1:D:221:GLU:HB3	1.82	0.62
1:A:167:GLY:HA2	1:B:174:SER:HB2	1.83	0.61
1:D:35:HIS:CE1	1:D:243:ARG:HG2	2.35	0.61
1:B:255:TRP:HB3	1:C:263:VAL:HG12	1.81	0.61
1:A:177:ARG:HB2	1:A:177:ARG:CZ	2.32	0.60
2:B:301:NAP:O1N	2:B:301:NAP:N7N	2.34	0.59
1:C:175:PHE:CE1	1:D:167:GLY:HA3	2.38	0.59
1:A:128:GLY:O	1:A:132:VAL:HG23	2.04	0.57
1:A:104:VAL:HG13	1:A:124:LEU:HD23	1.85	0.57
1:C:268:ALA:O	3:C:302:L7Z:C07	2.53	0.57
1:C:28:ILE:HA	1:C:238:PRO:HB3	1.86	0.57
1:D:239:GLU:CG	4:D:408:HOH:O	2.53	0.57
1:B:225:MET:CB	4:B:409:HOH:O	2.54	0.56
1:B:263:VAL:HG12	1:C:255:TRP:HB3	1.87	0.56
1:A:176:VAL:HG11	1:A:192:ALA:HB2	1.86	0.56
1:A:177:ARG:HG2	1:B:158:SER:OG	2.05	0.55
1:D:22:THR:HA	1:D:46:ASN:HB3	1.89	0.55
1:C:110:LEU:HD22	1:D:134:ARG:HB2	1.88	0.54
1:A:179:PHE:CE1	1:B:110:LEU:HD13	2.43	0.54
1:C:163:SER:N	1:D:178:ILE:HG21	2.22	0.54
1:A:212:PRO:C	1:A:214:GLY:HA3	2.28	0.54
1:A:264:ASP:OD1	1:D:259:LYS:NZ	2.39	0.53
1:D:197:GLY:HA2	3:D:302:L7Z:C16	2.39	0.53
1:C:110:LEU:HG	1:D:179:PHE:CE1	2.44	0.53
1:D:208:GLN:C	1:D:209:HIS:CG	2.81	0.52
1:D:239:GLU:HG3	4:D:408:HOH:O	2.09	0.52
1:B:252:GLU:HA	1:C:243:ARG:HD3	1.91	0.52
1:A:22:THR:O	1:A:101:ASN:HB3	2.09	0.52
1:C:179:PHE:CE1	1:D:110:LEU:HD13	2.46	0.51
1:A:75:VAL:HG23	1:A:124:LEU:HD12	1.91	0.51
1:C:47:TYR:CE2	1:C:51:PRO:HB3	2.46	0.51
1:B:143:GLY:CA	1:B:187:LYS:O	2.58	0.51
3:C:302:L7Z:C05	3:C:302:L7Z:O15	2.59	0.50
1:D:148:MET:O	1:D:192:ALA:HA	2.12	0.50
1:D:97:ILE:HG12	1:D:249:VAL:HB	1.94	0.49
1:B:136:ALA:O	1:B:140:LEU:HB2	2.11	0.49
1:D:176:VAL:HG11	1:D:192:ALA:HB2	1.94	0.49
1:D:206:VAL:HG23	1:D:206:VAL:O	2.12	0.49
1:A:78:VAL:HG21	1:B:115:GLU:HG2	1.93	0.49
1:A:43:VAL:O	1:A:68:ALA:HA	2.11	0.49
1:A:175:PHE:CE1	1:B:167:GLY:HA3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:VAL:N	1:B:79:PRO:CD	2.76	0.49
1:D:207:SER:OG	1:D:222:ARG:NH1	2.46	0.48
1:B:31:ALA:HB2	1:B:238:PRO:HB3	1.94	0.48
1:C:213:ASN:HB3	1:C:216:THR:OG1	2.12	0.48
1:A:150:SER:O	2:A:301:NAP:H6N	2.14	0.48
1:A:127:ARG:NH2	1:B:115:GLU:HB3	2.28	0.47
1:B:31:ALA:HB2	1:B:238:PRO:CB	2.45	0.47
1:B:28:ILE:O	1:B:32:VAL:HG23	2.15	0.47
1:C:10:ILE:HG22	1:C:10:ILE:O	2.14	0.47
1:D:46:ASN:ND2	1:D:73:ALA:HB3	2.29	0.47
1:B:148:MET:O	1:B:192:ALA:HA	2.15	0.47
1:C:177:ARG:NH2	1:D:155:ARG:HA	2.29	0.47
1:C:218:THR:OG1	1:C:221:GLU:HG3	2.15	0.47
1:C:233[A]:HIS:O	1:C:233[A]:HIS:CD2	2.68	0.47
1:C:110:LEU:HD13	1:D:134:ARG:HA	1.97	0.46
1:D:32:VAL:O	1:D:36:LEU:HG	2.15	0.46
1:C:74:ASP:OD1	2:C:301:NAP:N6A	2.43	0.46
1:D:162:PHE:HA	4:D:403:HOH:O	2.16	0.46
1:B:150:SER:O	2:B:301:NAP:H6N	2.16	0.46
1:B:226:ALA:HB3	1:B:235:ASN:ND2	2.31	0.46
1:D:239:GLU:O	1:D:243:ARG:HG3	2.16	0.46
1:A:117:GLU:HA	1:A:117:GLU:OE1	2.16	0.46
1:B:218:THR:H	1:B:221:GLU:HB2	1.81	0.46
1:D:222:ARG:HA	1:D:225:MET:HG2	1.98	0.46
1:A:178:ILE:HG21	1:B:163:SER:N	2.30	0.45
1:C:20:LEU:C	1:C:20:LEU:HD23	2.36	0.45
1:C:139:HIS:CD2	4:C:409:HOH:O	2.69	0.45
1:D:218:THR:N	1:D:219:PRO:CD	2.80	0.45
1:C:178:ILE:CD1	1:D:158:SER:HA	2.46	0.45
1:D:74:ASP:OD1	2:D:301:NAP:N6A	2.45	0.45
1:D:150:SER:O	2:D:301:NAP:H6N	2.16	0.45
1:A:172:ILE:O	1:A:176:VAL:HG13	2.17	0.45
1:A:177:ARG:CZ	1:A:177:ARG:CB	2.94	0.45
1:A:158:SER:HB2	1:B:181:LYS:HZ1	1.81	0.45
1:A:142:ASN:HA	1:A:186:LYS:O	2.17	0.45
1:B:252:GLU:OE1	1:B:252:GLU:N	2.47	0.45
1:A:63:GLN:HA	1:A:63:GLN:OE1	2.17	0.44
1:A:66:SER:OG	1:A:67:ASP:N	2.51	0.44
1:D:125:ASN:HB3	1:D:169:LYS:HE2	1.99	0.44
1:D:150:SER:OG	1:D:169:LYS:HB3	2.18	0.44
1:C:105:VAL:HG21	1:C:206:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:O	1:B:134:ARG:NH1	2.49	0.43
1:C:22:THR:O	1:C:101:ASN:HB3	2.19	0.43
1:B:142:ASN:HA	1:B:186:LYS:O	2.18	0.43
1:D:186:LYS:HB2	1:D:188:ILE:HD12	2.01	0.43
2:D:301:NAP:O1N	2:D:301:NAP:H2N	2.18	0.43
1:A:20:LEU:HD11	1:A:84:LEU:HG	2.01	0.43
1:D:119:ASP:O	1:D:123:SER:HB3	2.18	0.43
1:C:209:HIS:CD2	1:C:209:HIS:N	2.87	0.43
1:D:46:ASN:HD21	1:D:73:ALA:HB3	1.84	0.43
1:B:121:VAL:HG21	1:B:164:LEU:HD23	2.00	0.43
1:D:50:SER:HB3	1:D:53:HIS:HB2	2.01	0.43
1:D:208:GLN:O	1:D:209:HIS:ND1	2.52	0.43
1:A:243:ARG:HD3	1:D:252:GLU:HA	2.01	0.42
1:A:158:SER:HB2	1:B:181:LYS:NZ	2.34	0.42
1:A:154:SER:O	1:B:177:ARG:NH1	2.45	0.42
1:B:87:GLU:O	1:B:90:ALA:HB3	2.20	0.42
1:A:104:VAL:HG13	1:A:124:LEU:CD2	2.49	0.42
1:D:100:SER:OG	1:D:129:GLN:HG2	2.20	0.42
1:B:218:THR:HG23	1:B:221:GLU:CD	2.39	0.41
1:A:47:TYR:CZ	1:A:72:LYS:HB2	2.55	0.41
1:A:158:SER:HA	1:B:178:ILE:CD1	2.51	0.41
1:A:69:ILE:HD12	1:A:71:ILE:HD11	2.03	0.41
1:A:178:ILE:CD1	1:B:158:SER:HA	2.50	0.41
1:B:22:THR:O	1:B:101:ASN:HB3	2.20	0.41
1:B:177:ARG:HH21	1:B:178:ILE:HD11	1.86	0.41
1:B:218:THR:HG23	1:B:221:GLU:CG	2.51	0.41
1:C:178:ILE:HD13	1:D:158:SER:HA	2.03	0.41
1:A:28:ILE:HG21	1:A:241:ILE:HG21	2.02	0.41
1:C:228:HIS:CE1	1:C:233[A]:HIS:CE1	3.09	0.41
1:C:233[A]:HIS:O	1:C:233[A]:HIS:HD2	2.02	0.41
1:C:255:TRP:CE3	1:C:255:TRP:HA	2.56	0.41
1:A:152:ASN:HB3	1:A:262:THR:HG23	2.03	0.41
1:A:220:GLU:HG3	1:A:221:GLU:N	2.35	0.41
1:D:74:ASP:C	1:D:76:ARG:H	2.23	0.41
1:D:134:ARG:O	1:D:138:LYS:HD3	2.21	0.41
1:D:142:ASN:HA	1:D:186:LYS:O	2.21	0.40
1:C:169:LYS:O	1:C:172:ILE:HB	2.21	0.40
1:D:22:THR:O	1:D:101:ASN:HB3	2.21	0.40
1:A:123:SER:O	1:A:128:GLY:N	2.50	0.40
1:A:32:VAL:O	1:A:36:LEU:HG	2.22	0.40
1:A:118:PHE:HA	1:A:164:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:THR:O	1:D:203:PHE:HB2	2.21	0.40
1:A:75:VAL:HG23	1:A:124:LEU:CD1	2.51	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	254/279 (91%)	243 (96%)	11 (4%)	0	100	100
1	B	248/279 (89%)	234 (94%)	14 (6%)	0	100	100
1	C	259/279 (93%)	241 (93%)	18 (7%)	0	100	100
1	D	249/279 (89%)	236 (95%)	13 (5%)	0	100	100
All	All	1010/1116 (90%)	954 (94%)	56 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/225 (90%)	193 (96%)	9 (4%)	27	46
1	B	196/225 (87%)	188 (96%)	8 (4%)	30	50
1	C	205/225 (91%)	191 (93%)	14 (7%)	16	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	200/225 (89%)	192 (96%)	8 (4%)	31	51
All	All	803/900 (89%)	764 (95%)	39 (5%)	25	43

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	140	LEU
1	A	162	PHE
1	A	163	SER
1	A	177	ARG
1	A	212	PRO
1	A	218	THR
1	A	220	GLU
1	A	221	GLU
1	B	162	PHE
1	B	177	ARG
1	B	180	SER
1	B	185	ASP
1	B	187	LYS
1	B	218	THR
1	B	234	ARG
1	B	261	LEU
1	C	10	ILE
1	C	52	THR
1	C	56	LYS
1	C	66	SER
1	C	107	PHE
1	C	110	LEU
1	C	162	PHE
1	C	163	SER
1	C	176	VAL
1	C	208	GLN
1	C	211	ILE
1	C	212	PRO
1	C	216	THR
1	C	263	VAL
1	D	76	ARG
1	D	100	SER
1	D	154	SER
1	D	162	PHE
1	D	163	SER

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Mol	Chain	Res	Type
1	D	185	ASP
1	D	207	SER
1	D	209	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	B	235	ASN
1	C	209	HIS
1	D	208	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	A	301	-	45,52,52	2.13	19 (42%)	56,80,80	1.25	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAP	B	301	-	45,52,52	2.33	19 (42%)	56,80,80	1.53	9 (16%)
2	NAP	C	301	-	45,52,52	2.32	25 (55%)	56,80,80	1.60	10 (17%)
3	L7Z	C	302	-	17,17,17	7.79	11 (64%)	23,25,25	3.67	6 (26%)
3	L7Z	D	302	-	17,17,17	8.51	13 (76%)	23,25,25	3.11	9 (39%)
2	NAP	D	301	-	45,52,52	2.20	18 (40%)	56,80,80	1.44	10 (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
2	NAP	A	301	-	-	6/31/67/67	0/5/5/5
2	NAP	B	301	-	-	6/31/67/67	0/5/5/5
2	NAP	C	301	-	-	7/31/67/67	0/5/5/5
3	L7Z	C	302	-	-	3/5/22/22	0/2/2/2
3	L7Z	D	302	-	-	5/5/22/22	0/2/2/2
2	NAP	D	301	-	-	5/31/67/67	0/5/5/5

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	L7Z	C09-C10	-23.42	1.30	1.52
3	C	302	L7Z	C09-C13	17.32	1.69	1.52
3	C	302	L7Z	C09-C10	-17.18	1.36	1.52
3	D	302	L7Z	C09-C13	15.70	1.67	1.52
3	D	302	L7Z	C12-C13	-11.32	1.33	1.51
3	C	302	L7Z	C12-C13	-10.31	1.34	1.51
3	C	302	L7Z	C06-C01	8.61	1.54	1.38
3	D	302	L7Z	C06-C01	7.99	1.53	1.38
3	D	302	L7Z	C11-C10	7.34	1.63	1.51
3	C	302	L7Z	C04-C05	7.32	1.54	1.38
3	D	302	L7Z	C04-C03	7.21	1.51	1.38
3	C	302	L7Z	C04-C03	7.11	1.51	1.38
3	C	302	L7Z	C11-C10	6.50	1.61	1.51
3	C	302	L7Z	C06-C05	6.47	1.52	1.38
3	D	302	L7Z	C04-C05	6.44	1.52	1.38
3	D	302	L7Z	C06-C05	5.69	1.51	1.38
2	B	301	NAP	O7N-C7N	-5.13	1.14	1.24
3	D	302	L7Z	C03-C02	5.07	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	L7Z	C03-C02	5.02	1.52	1.38
3	C	302	L7Z	C01-C02	4.78	1.52	1.38
2	A	301	NAP	C2N-N1N	-4.72	1.29	1.35
2	A	301	NAP	PN-O1N	-4.58	1.34	1.50
3	D	302	L7Z	C01-C02	4.38	1.51	1.38
2	D	301	NAP	O7N-C7N	-4.24	1.16	1.24
2	C	301	NAP	P2B-O2B	-4.07	1.51	1.59
2	B	301	NAP	P2B-O2X	-3.92	1.39	1.54
2	D	301	NAP	P2B-O3X	-3.91	1.39	1.54
2	D	301	NAP	C2N-N1N	-3.87	1.30	1.35
2	C	301	NAP	C2N-N1N	-3.81	1.30	1.35
2	B	301	NAP	P2B-O1X	-3.79	1.38	1.50
2	B	301	NAP	P2B-O2B	-3.77	1.52	1.59
2	C	301	NAP	P2B-O1X	-3.74	1.38	1.50
2	B	301	NAP	P2B-O3X	-3.74	1.40	1.54
2	C	301	NAP	O7N-C7N	-3.71	1.17	1.24
2	B	301	NAP	C2N-N1N	-3.64	1.30	1.35
2	D	301	NAP	P2B-O2B	-3.64	1.52	1.59
2	D	301	NAP	PN-O1N	-3.58	1.38	1.50
2	A	301	NAP	P2B-O2B	-3.55	1.52	1.59
2	B	301	NAP	PA-O2A	-3.55	1.38	1.55
2	C	301	NAP	P2B-O3X	-3.51	1.41	1.54
2	D	301	NAP	PN-O2N	-3.48	1.39	1.55
2	C	301	NAP	PA-O1A	-3.42	1.38	1.50
2	C	301	NAP	C2D-C1D	-3.40	1.48	1.53
2	C	301	NAP	P2B-O2X	-3.40	1.41	1.54
2	D	301	NAP	C3N-C7N	-3.38	1.45	1.50
2	D	301	NAP	P2B-O2X	-3.30	1.42	1.54
2	B	301	NAP	PA-O1A	-3.27	1.39	1.50
2	B	301	NAP	C7N-N7N	-3.23	1.26	1.33
2	C	301	NAP	C3N-C7N	-3.23	1.45	1.50
2	C	301	NAP	PN-O1N	-3.15	1.39	1.50
2	A	301	NAP	O7N-C7N	-3.14	1.18	1.24
2	B	301	NAP	PN-O1N	-3.14	1.39	1.50
3	C	302	L7Z	C08-C05	3.13	1.56	1.51
2	A	301	NAP	P2B-O3X	-3.12	1.42	1.54
2	A	301	NAP	C4A-N3A	-3.11	1.31	1.35
2	D	301	NAP	PA-O2A	-3.10	1.40	1.55
2	A	301	NAP	P2B-O2X	-3.07	1.43	1.54
2	A	301	NAP	PN-O2N	-3.05	1.41	1.55
2	C	301	NAP	O4D-C4D	-3.03	1.38	1.45
2	A	301	NAP	O4B-C4B	-2.98	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	O4D-C4D	-2.95	1.38	1.45
2	A	301	NAP	PA-O2A	-2.93	1.41	1.55
2	D	301	NAP	P2B-O1X	-2.91	1.41	1.50
2	B	301	NAP	PN-O2N	-2.91	1.41	1.55
2	D	301	NAP	O4B-C4B	-2.86	1.38	1.45
2	C	301	NAP	PN-O2N	-2.82	1.42	1.55
2	D	301	NAP	C4A-N3A	-2.77	1.31	1.35
2	B	301	NAP	C2D-C1D	-2.77	1.49	1.53
2	B	301	NAP	C2A-N1A	-2.71	1.28	1.33
2	C	301	NAP	O4B-C1B	-2.67	1.37	1.41
3	D	302	L7Z	O15-C13	-2.63	1.17	1.21
2	D	301	NAP	PN-O5D	-2.63	1.48	1.59
2	B	301	NAP	O4B-C4B	-2.61	1.39	1.45
2	C	301	NAP	C7N-N7N	-2.61	1.28	1.33
2	B	301	NAP	PN-O5D	-2.60	1.48	1.59
2	A	301	NAP	P2B-O1X	-2.60	1.42	1.50
2	C	301	NAP	PA-O2A	-2.59	1.43	1.55
2	C	301	NAP	PN-O5D	-2.54	1.49	1.59
2	B	301	NAP	C3N-C7N	-2.50	1.46	1.50
2	A	301	NAP	C5A-N7A	-2.48	1.30	1.39
2	D	301	NAP	C5A-N7A	-2.46	1.30	1.39
2	A	301	NAP	O4D-C4D	-2.42	1.39	1.45
2	A	301	NAP	C2D-C1D	-2.41	1.50	1.53
2	A	301	NAP	C3B-C2B	-2.40	1.47	1.52
2	D	301	NAP	C2D-C1D	-2.39	1.50	1.53
2	C	301	NAP	C4A-N3A	-2.36	1.32	1.35
2	C	301	NAP	C2A-N1A	-2.34	1.29	1.33
2	C	301	NAP	C3B-C2B	-2.33	1.47	1.52
2	C	301	NAP	O4D-C1D	-2.29	1.37	1.41
2	C	301	NAP	O5B-C5B	-2.27	1.36	1.44
3	D	302	L7Z	C08-C09	-2.20	1.52	1.56
2	D	301	NAP	C7N-N7N	-2.20	1.28	1.33
2	B	301	NAP	C5A-N7A	-2.16	1.31	1.39
2	B	301	NAP	C4A-N3A	-2.16	1.32	1.35
2	A	301	NAP	PN-O5D	-2.14	1.50	1.59
2	A	301	NAP	PA-O1A	-2.12	1.43	1.50
2	C	301	NAP	O4B-C4B	-2.09	1.40	1.45
2	C	301	NAP	C2A-N3A	-2.07	1.28	1.32
2	C	301	NAP	PA-O5B	-2.07	1.50	1.59
2	D	301	NAP	O4D-C4D	-2.06	1.40	1.45
2	A	301	NAP	C8A-N7A	-2.06	1.31	1.34
2	A	301	NAP	C7N-N7N	-2.05	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAP	C2D-C3D	-2.05	1.47	1.53
3	D	302	L7Z	O14-C10	-2.02	1.18	1.21
2	D	301	NAP	C2D-C3D	-2.00	1.47	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	L7Z	O14-C10-C09	12.30	132.49	124.80
3	D	302	L7Z	C13-C09-C10	10.99	108.95	101.78
3	C	302	L7Z	C13-C09-C10	10.21	108.45	101.78
3	D	302	L7Z	C11-C12-C13	-5.19	103.52	106.55
2	C	301	NAP	C4A-C5A-N7A	-4.79	104.40	109.40
2	D	301	NAP	C4A-C5A-N7A	-4.60	104.61	109.40
3	C	302	L7Z	C08-C09-C13	-4.35	97.74	109.80
2	B	301	NAP	N3A-C2A-N1A	-4.24	122.05	128.68
2	C	301	NAP	N3A-C2A-N1A	-4.10	122.27	128.68
2	C	301	NAP	O4B-C1B-C2B	-4.06	99.54	106.59
2	B	301	NAP	O4B-C1B-C2B	-4.01	99.63	106.59
3	D	302	L7Z	C16-C09-C08	-3.78	104.63	109.96
2	A	301	NAP	N3A-C2A-N1A	-3.76	122.80	128.68
3	D	302	L7Z	O15-C13-C09	3.65	127.08	124.80
2	B	301	NAP	O7N-C7N-N7N	-3.62	117.44	122.58
2	C	301	NAP	O2B-P2B-O1X	-3.35	96.44	109.39
3	D	302	L7Z	C08-C09-C10	3.31	118.98	109.80
2	D	301	NAP	N3A-C2A-N1A	-3.30	123.53	128.68
2	B	301	NAP	O4D-C1D-C2D	-3.24	102.19	106.93
2	D	301	NAP	O4B-C1B-C2B	-3.12	101.18	106.59
2	A	301	NAP	C4A-C5A-N7A	-2.94	106.33	109.40
3	C	302	L7Z	O15-C13-C09	2.90	126.61	124.80
2	C	301	NAP	C2A-N1A-C6A	2.87	123.66	118.75
2	C	301	NAP	O4D-C1D-C2D	-2.86	102.74	106.93
2	B	301	NAP	C3N-C7N-N7N	2.84	121.16	117.75
2	B	301	NAP	O3X-P2B-O2X	2.83	118.44	107.64
2	B	301	NAP	C4A-C5A-N7A	-2.82	106.45	109.40
2	B	301	NAP	C2A-N1A-C6A	2.81	123.56	118.75
3	C	302	L7Z	C12-C11-C10	-2.74	104.95	106.55
2	A	301	NAP	O4B-C1B-C2B	-2.72	101.87	106.59
2	C	301	NAP	C5A-C6A-N6A	2.68	124.42	120.35
2	B	301	NAP	O2B-P2B-O1X	-2.66	99.11	109.39
2	D	301	NAP	O4D-C4D-C3D	2.59	110.25	105.11
2	C	301	NAP	O2B-C2B-C1B	2.50	119.09	110.10
3	D	302	L7Z	C16-C09-C10	-2.49	100.60	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAP	C2A-N1A-C6A	2.49	123.01	118.75
3	D	302	L7Z	O14-C10-C11	2.48	128.84	125.76
3	D	302	L7Z	C08-C05-C06	-2.40	117.86	121.07
2	D	301	NAP	O5D-PN-O1N	-2.37	99.79	109.07
2	D	301	NAP	C5N-C4N-C3N	-2.36	117.55	120.34
2	D	301	NAP	PN-O3-PA	2.25	140.54	132.83
2	D	301	NAP	O3X-P2B-O2X	2.16	115.88	107.64
2	C	301	NAP	C3N-C7N-N7N	2.14	120.31	117.75
2	D	301	NAP	C5A-C6A-N6A	2.11	123.56	120.35
2	C	301	NAP	O5D-PN-O1N	-2.08	100.95	109.07
2	D	301	NAP	O2N-PN-O1N	2.05	122.36	112.24
3	D	302	L7Z	O14-C10-C09	2.05	126.08	124.80
3	C	302	L7Z	C04-C03-C02	-2.04	118.64	121.38

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C2B-O2B-P2B-O3X
2	A	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	C5D-O5D-PN-O2N
2	B	301	NAP	C5D-O5D-PN-O1N
2	B	301	NAP	C5D-O5D-PN-O2N
2	C	301	NAP	C5D-O5D-PN-O2N
2	D	301	NAP	C5D-O5D-PN-O1N
2	D	301	NAP	C5D-O5D-PN-O2N
3	D	302	L7Z	C05-C08-C09-C10
3	D	302	L7Z	C05-C08-C09-C13
3	D	302	L7Z	C05-C08-C09-C16
2	B	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	C3B-C4B-C5B-O5B
3	C	302	L7Z	C04-C05-C08-C09
3	C	302	L7Z	C06-C05-C08-C09
3	D	302	L7Z	C06-C05-C08-C09
3	D	302	L7Z	C04-C05-C08-C09
2	C	301	NAP	C5D-O5D-PN-O3
2	D	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5B-O5B-PA-O1A
2	C	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	PN-O3-PA-O1A
2	C	301	NAP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	301	NAP	PA-O3-PN-O2N
2	B	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	C2B-O2B-P2B-O3X
2	A	301	NAP	O4B-C4B-C5B-O5B
2	A	301	NAP	PA-O3-PN-O2N
2	C	301	NAP	PN-O3-PA-O2A
3	C	302	L7Z	C05-C08-C09-C10
2	D	301	NAP	O4B-C4B-C5B-O5B

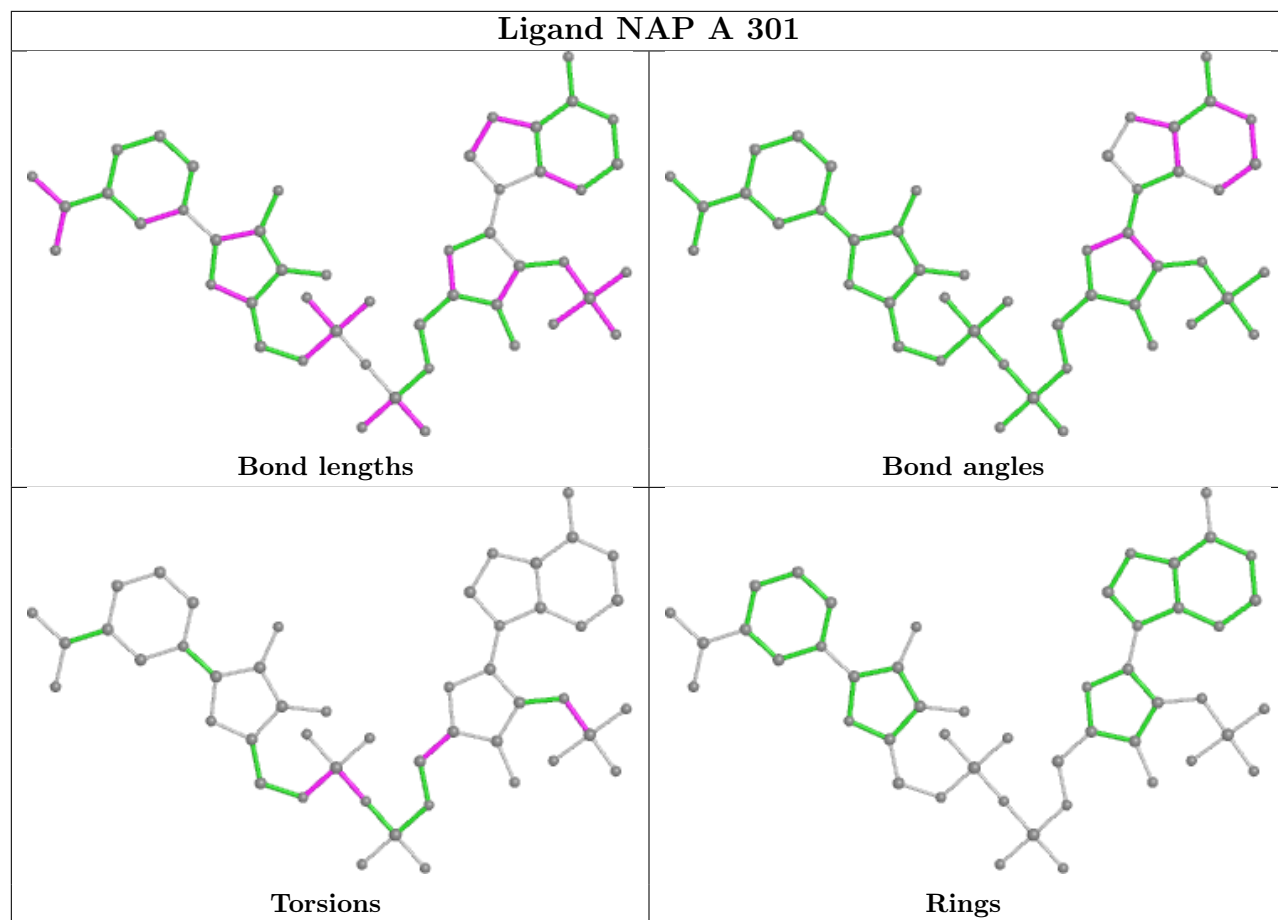
There are no ring outliers.

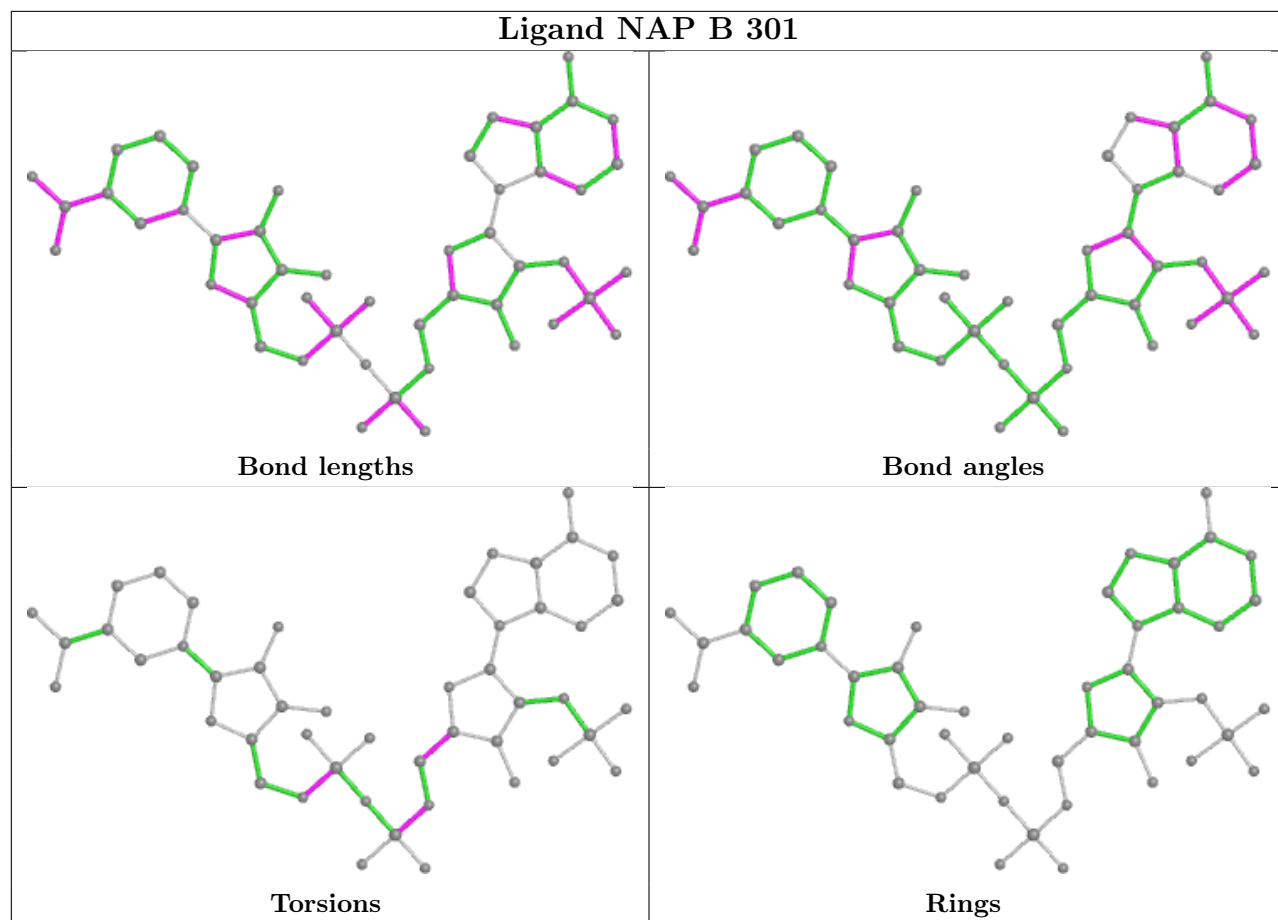
6 monomers are involved in 13 short contacts:

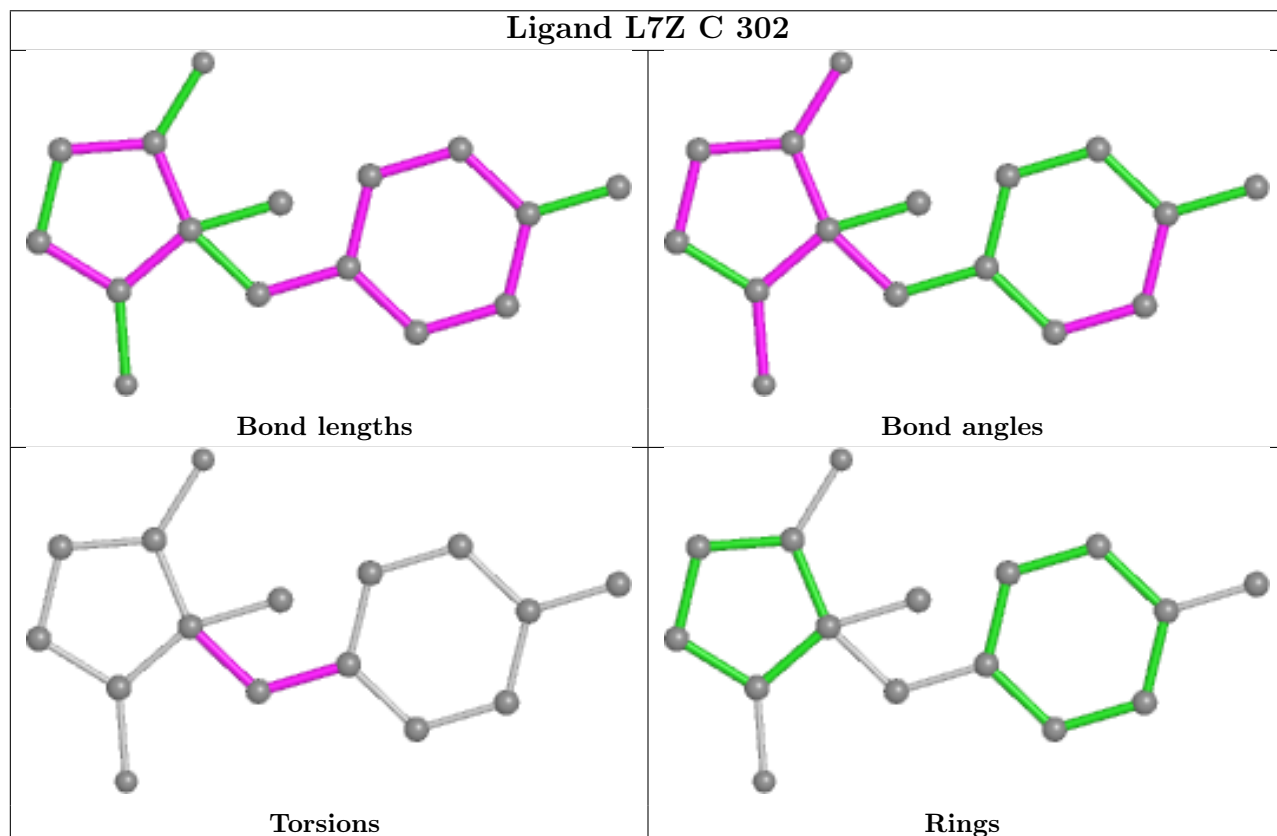
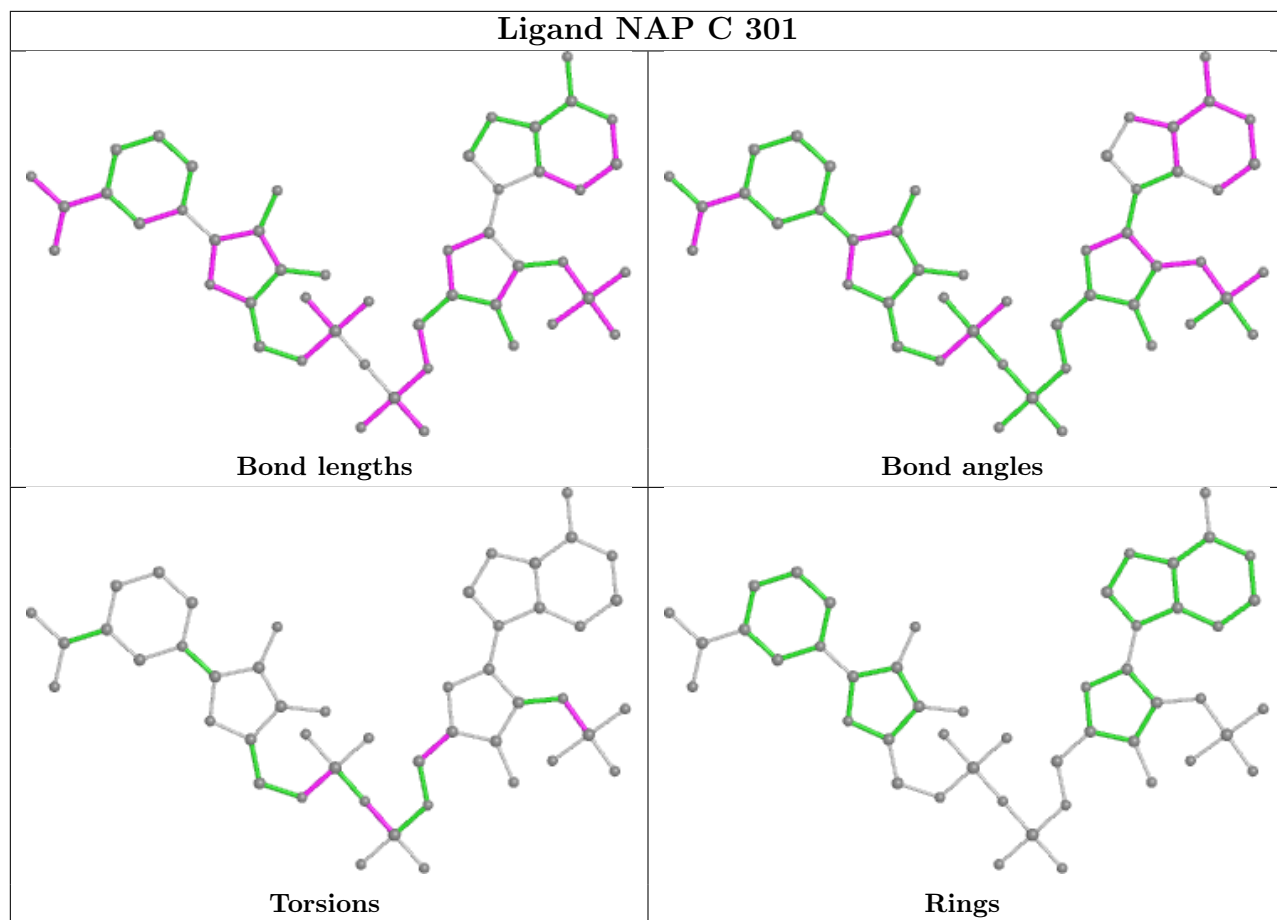
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAP	1	0
2	B	301	NAP	2	0
2	C	301	NAP	1	0
3	C	302	L7Z	3	0
3	D	302	L7Z	3	0
2	D	301	NAP	5	0

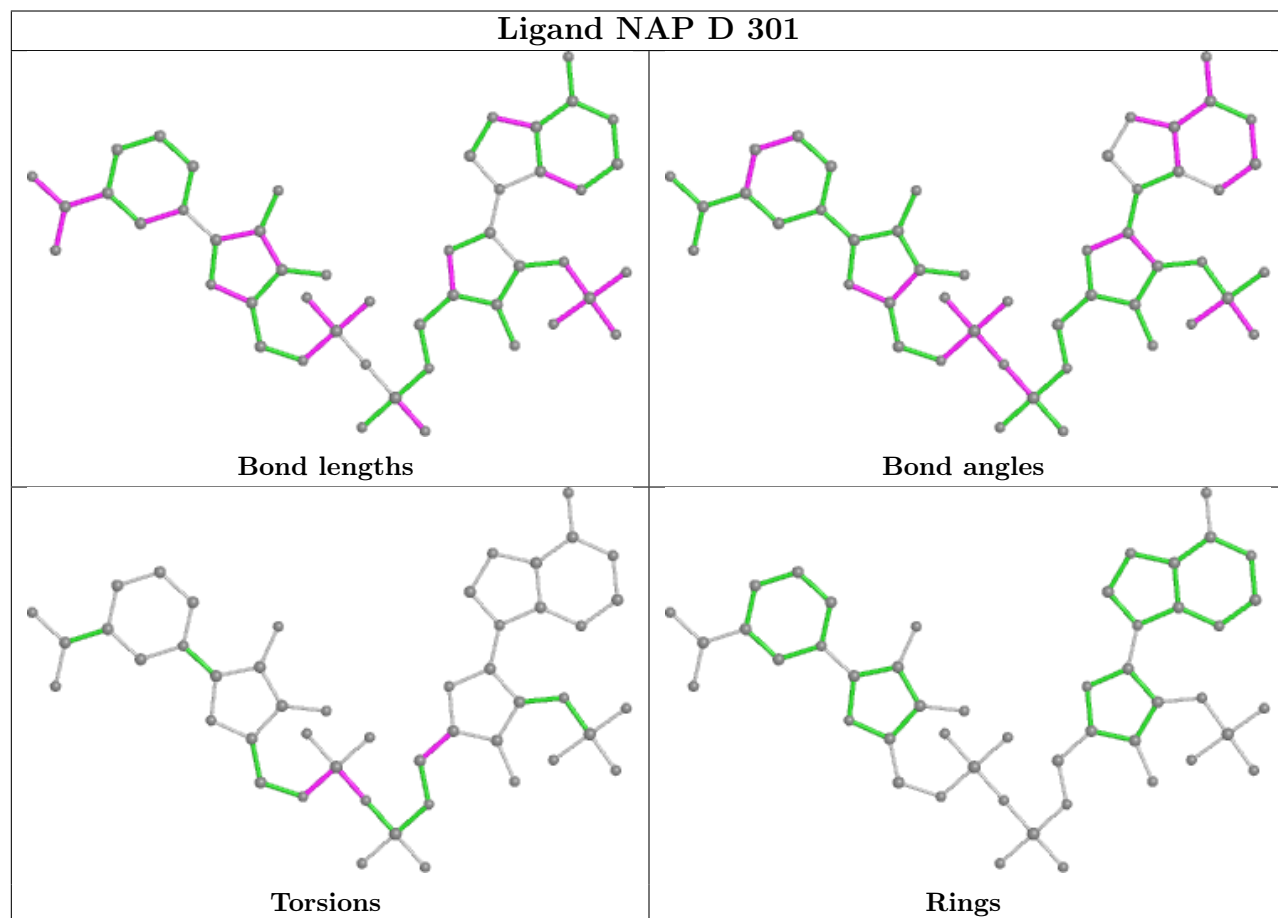
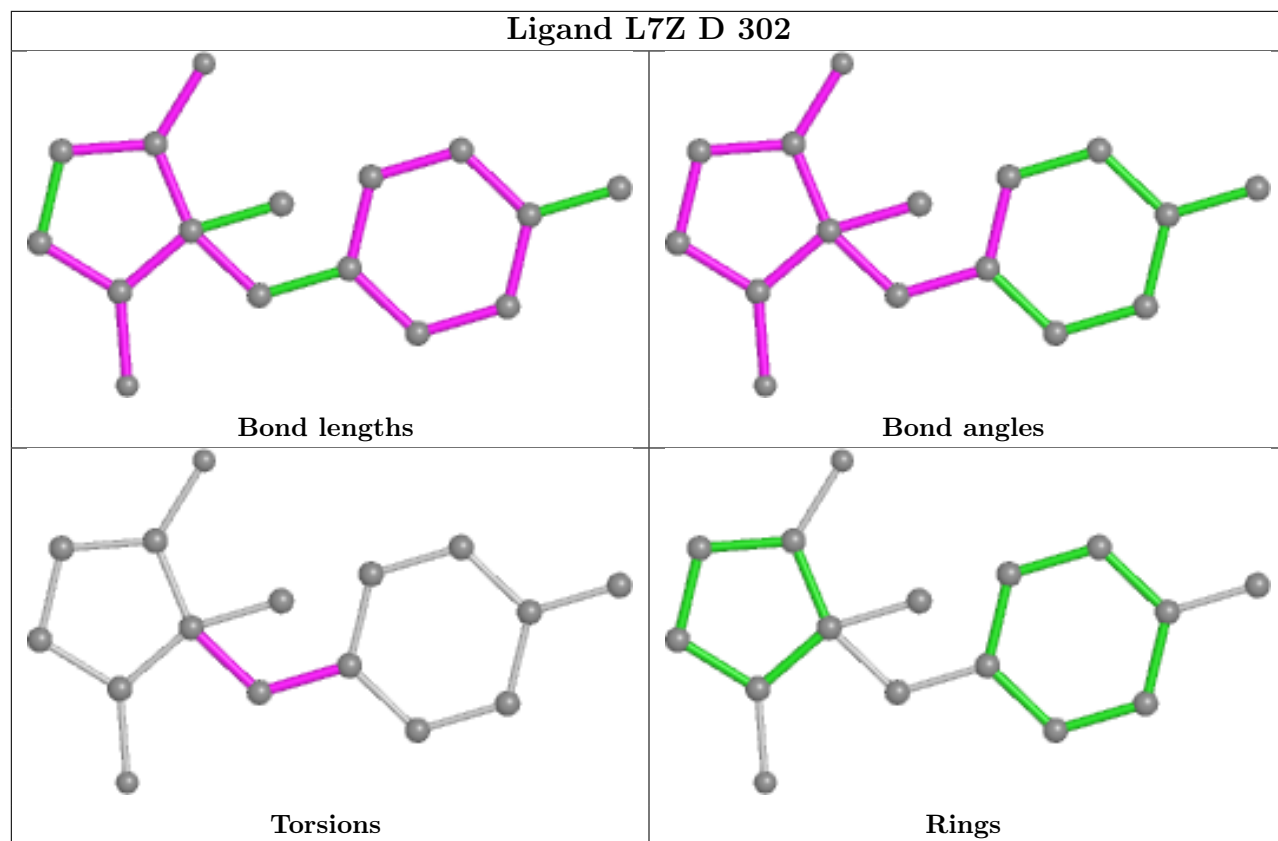
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	258/279 (92%)	-0.05	6 (2%) 60 69	13, 20, 44, 62	0
1	B	252/279 (90%)	-0.05	7 (2%) 53 62	11, 18, 44, 62	0
1	C	260/279 (93%)	-0.15	7 (2%) 54 63	10, 17, 40, 70	0
1	D	253/279 (90%)	-0.01	5 (1%) 65 73	10, 20, 43, 68	0
All	All	1023/1116 (91%)	-0.07	25 (2%) 59 68	10, 19, 43, 70	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	TYR	4.2
1	B	209	HIS	3.7
1	B	228	HIS	3.6
1	C	212	PRO	3.5
1	A	228	HIS	3.5
1	C	214	GLY	3.4
1	A	233	HIS	3.0
1	D	209	HIS	3.0
1	C	10	ILE	2.9
1	C	213	ASN	2.9
1	C	217	TYR	2.8
1	B	63	GLN	2.8
1	D	225	MET	2.7
1	C	64	LEU	2.7
1	B	210	TYR	2.6
1	D	8	LEU	2.5
1	B	184	GLY	2.4
1	B	221	GLU	2.3
1	D	228	HIS	2.2
1	D	218	THR	2.1
1	C	63	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	211	ILE	2.1
1	A	209	HIS	2.1
1	A	221	GLU	2.0
1	A	225	MET	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

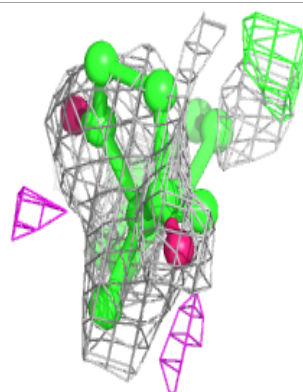
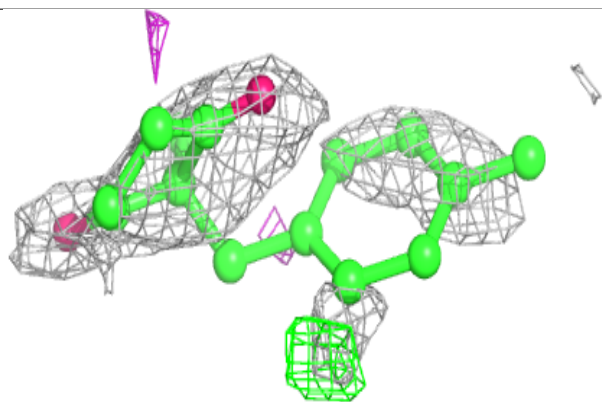
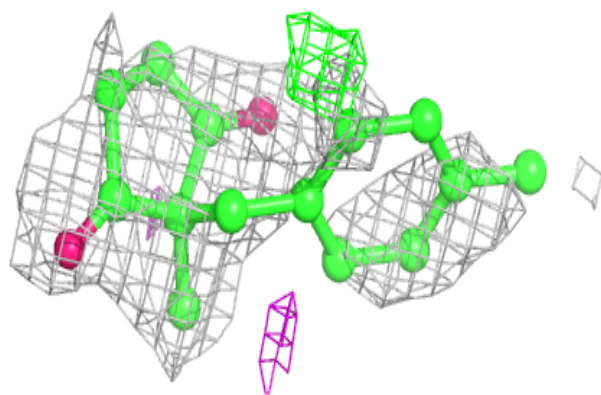
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	L7Z	C	302	16/16	0.79	0.31	55,63,72,73	0
3	L7Z	D	302	16/16	0.81	0.32	58,61,64,69	0
2	NAP	D	301	48/48	0.95	0.13	13,16,20,23	0
2	NAP	C	301	48/48	0.96	0.11	11,13,17,18	0
2	NAP	A	301	48/48	0.96	0.12	12,15,20,22	0
2	NAP	B	301	48/48	0.97	0.10	10,12,14,15	0

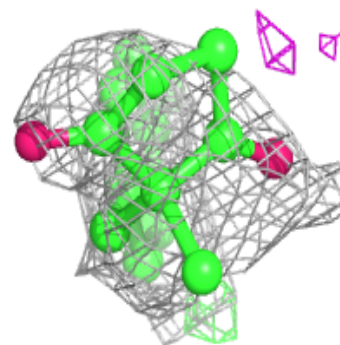
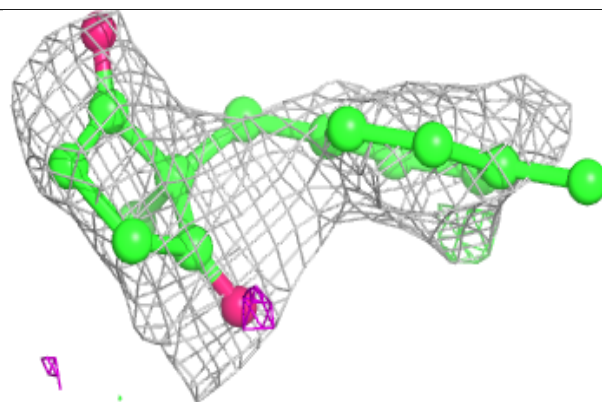
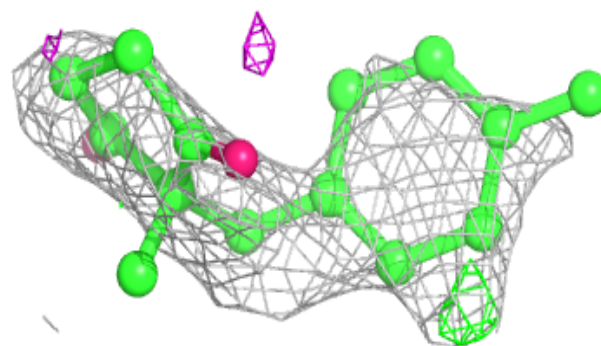
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around L7Z C 302:**

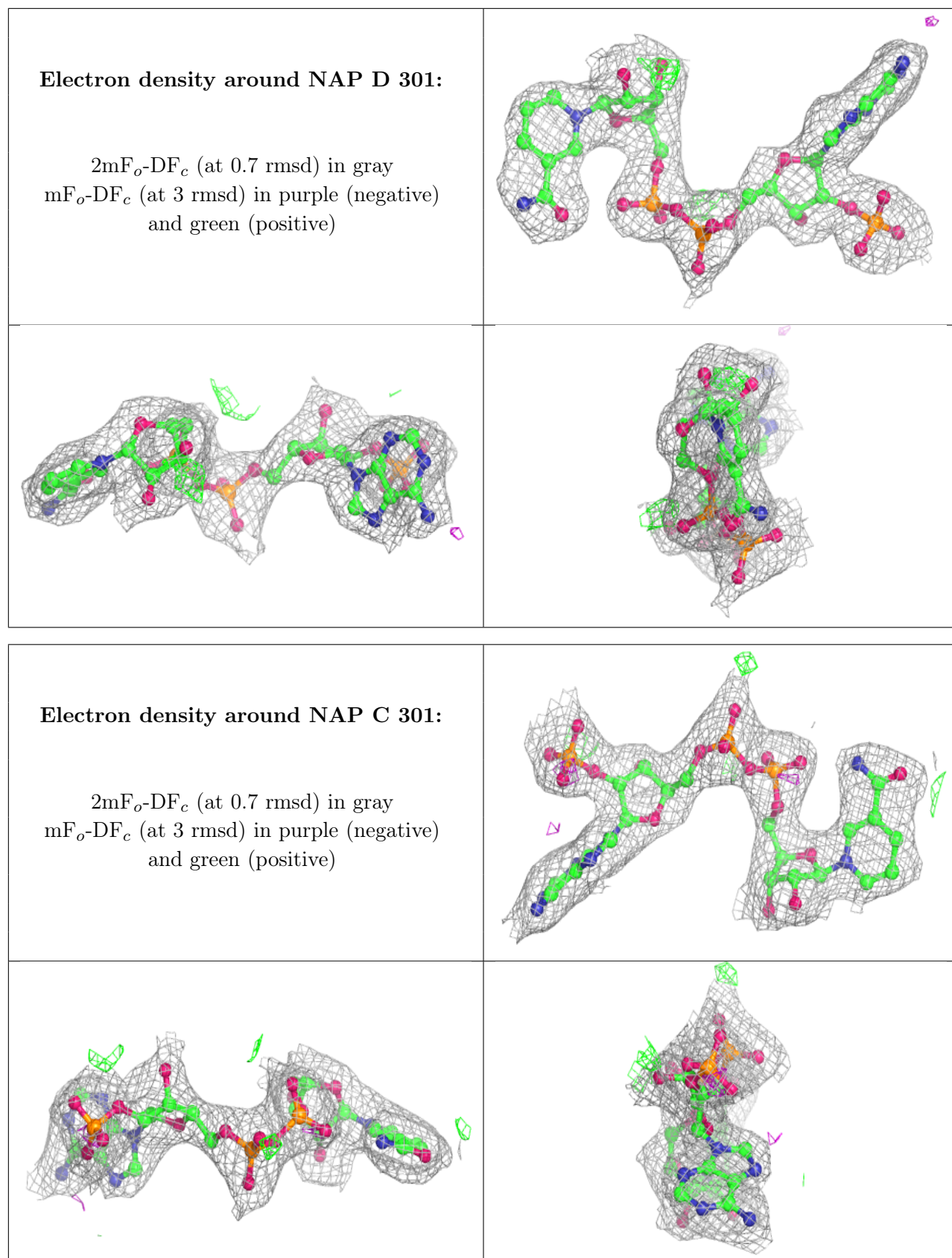
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around L7Z 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)

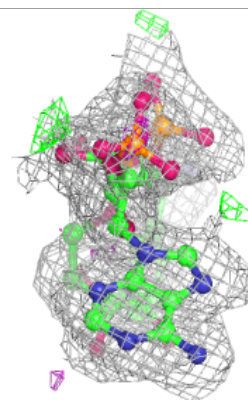
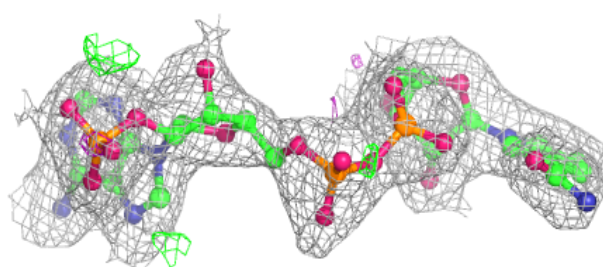
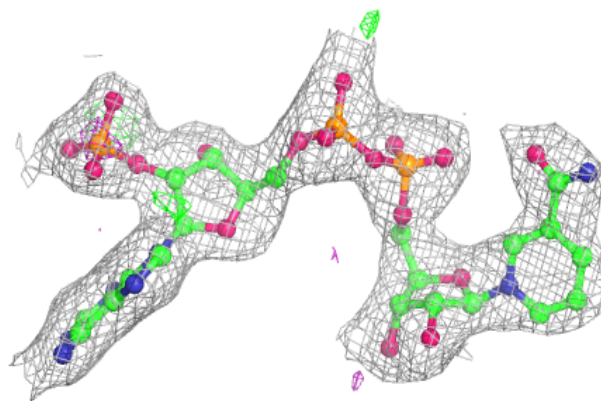




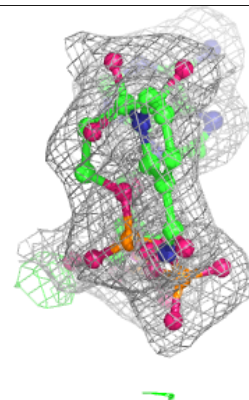
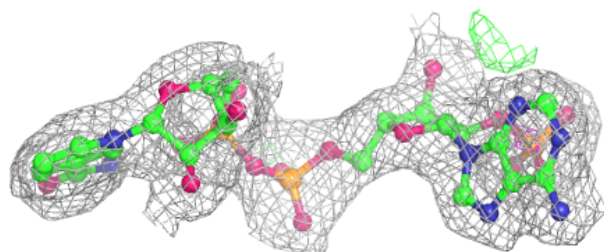
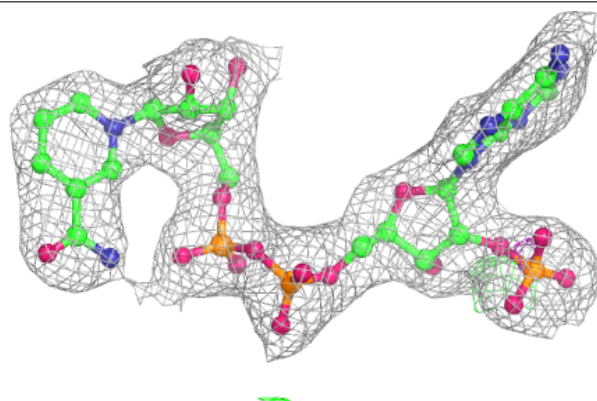


**Electron density around NAP A 301:**

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

**Electron density around NAP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.