



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:43 pm BST

PDB ID : 5ZJD  
Title : Lactate dehydrogenase with NADH and MLA  
Authors : Han, C.W.; Jang, S.B.  
Deposited on : 2018-03-20  
Resolution : 2.39 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

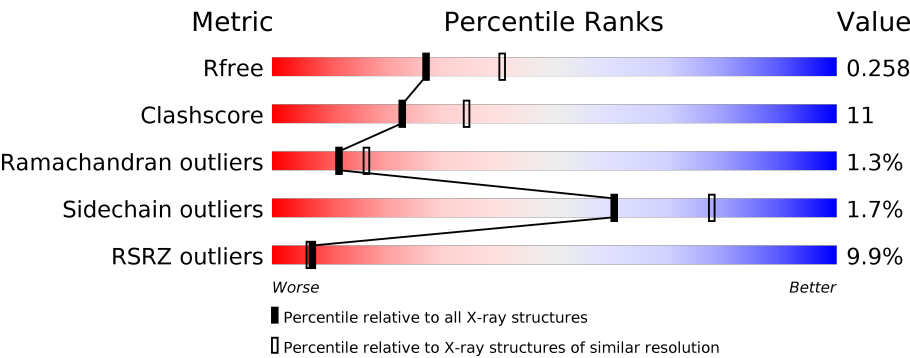
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	337	<div><div>6%</div><div><div></div><div>73%</div><div>25%</div><div>..</div></div></div>
1	B	337	<div><div>7%</div><div><div></div><div>73%</div><div>25%</div><div>..</div></div></div>
1	C	337	<div><div>12%</div><div><div></div><div>73%</div><div>23%</div><div>..</div></div></div>
1	D	337	<div><div>9%</div><div><div></div><div>74%</div><div>23%</div><div>.</div></div></div>
1	E	337	<div><div>9%</div><div><div></div><div>74%</div><div>23%</div><div>..</div></div></div>
1	F	337	<div><div>13%</div><div><div></div><div>72%</div><div>24%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	337	
1	H	337	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MLI	A	402	-	-	X	-
3	MLI	B	402	-	-	X	-
3	MLI	C	402	-	-	X	-
3	MLI	D	402	-	-	X	-
3	MLI	E	402	-	-	X	-
3	MLI	F	402	-	-	X	-
3	MLI	G	402	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21367 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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	B	331	Total	C	N	O	S	1	0	0
			2568	1639	439	477	13			
1	C	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	D	331	Total	C	N	O	S	5	0	0
			2568	1639	439	477	13			
1	E	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	F	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	G	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	H	331	Total	C	N	O	S	5	0	0
			2568	1639	439	477	13			

There are 48 discrepancies between the modelled and reference sequences:

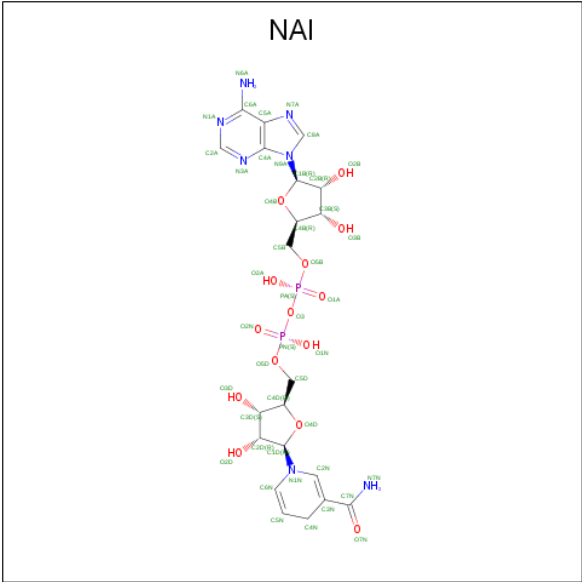
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P00338
A	-4	HIS	-	expression tag	UNP P00338
A	-3	HIS	-	expression tag	UNP P00338
A	-2	HIS	-	expression tag	UNP P00338
A	-1	HIS	-	expression tag	UNP P00338
A	0	HIS	-	expression tag	UNP P00338
B	-5	HIS	-	expression tag	UNP P00338
B	-4	HIS	-	expression tag	UNP P00338
B	-3	HIS	-	expression tag	UNP P00338
B	-2	HIS	-	expression tag	UNP P00338
B	-1	HIS	-	expression tag	UNP P00338
B	0	HIS	-	expression tag	UNP P00338
C	-5	HIS	-	expression tag	UNP P00338

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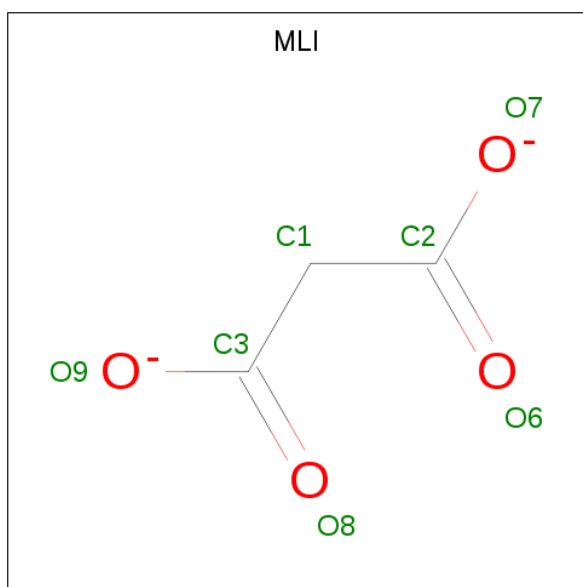
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P00338
C	-3	HIS	-	expression tag	UNP P00338
C	-2	HIS	-	expression tag	UNP P00338
C	-1	HIS	-	expression tag	UNP P00338
C	0	HIS	-	expression tag	UNP P00338
D	-5	HIS	-	expression tag	UNP P00338
D	-4	HIS	-	expression tag	UNP P00338
D	-3	HIS	-	expression tag	UNP P00338
D	-2	HIS	-	expression tag	UNP P00338
D	-1	HIS	-	expression tag	UNP P00338
D	0	HIS	-	expression tag	UNP P00338
E	-5	HIS	-	expression tag	UNP P00338
E	-4	HIS	-	expression tag	UNP P00338
E	-3	HIS	-	expression tag	UNP P00338
E	-2	HIS	-	expression tag	UNP P00338
E	-1	HIS	-	expression tag	UNP P00338
E	0	HIS	-	expression tag	UNP P00338
F	-5	HIS	-	expression tag	UNP P00338
F	-4	HIS	-	expression tag	UNP P00338
F	-3	HIS	-	expression tag	UNP P00338
F	-2	HIS	-	expression tag	UNP P00338
F	-1	HIS	-	expression tag	UNP P00338
F	0	HIS	-	expression tag	UNP P00338
G	-5	HIS	-	expression tag	UNP P00338
G	-4	HIS	-	expression tag	UNP P00338
G	-3	HIS	-	expression tag	UNP P00338
G	-2	HIS	-	expression tag	UNP P00338
G	-1	HIS	-	expression tag	UNP P00338
G	0	HIS	-	expression tag	UNP P00338
H	-5	HIS	-	expression tag	UNP P00338
H	-4	HIS	-	expression tag	UNP P00338
H	-3	HIS	-	expression tag	UNP P00338
H	-2	HIS	-	expression tag	UNP P00338
H	-1	HIS	-	expression tag	UNP P00338
H	0	HIS	-	expression tag	UNP P00338

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 3 4	0	0
3	B	1	Total C O 7 3 4	0	0
3	C	1	Total C O 7 3 4	0	0
3	D	1	Total C O 7 3 4	0	0
3	E	1	Total C O 7 3 4	0	0
3	F	1	Total C O 7 3 4	0	0
3	G	1	Total C O 7 3 4	0	0
3	H	1	Total C O 7 3 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	62	Total O 62 62	0	0
4	B	61	Total O 61 61	0	0
4	C	61	Total O 61 61	0	0
4	D	57	Total O 57 57	0	0

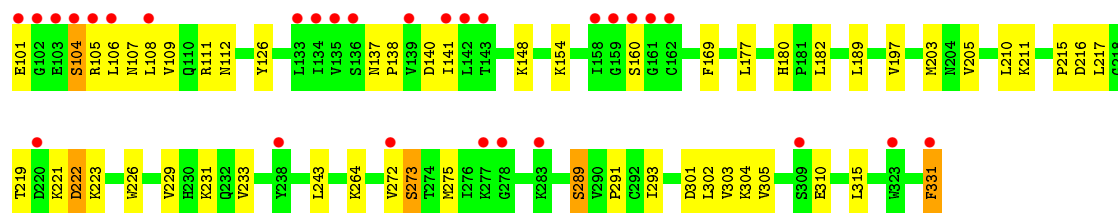
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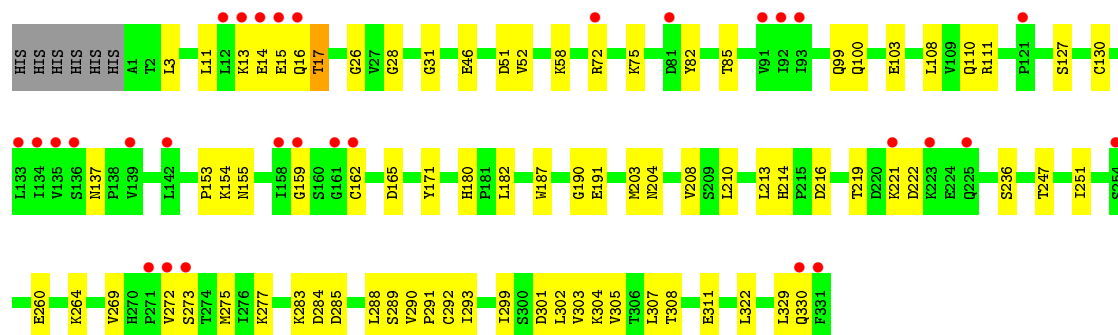
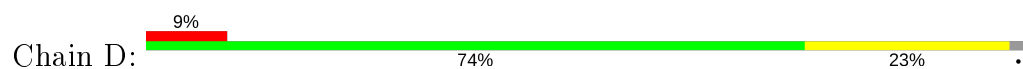
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	48	Total 48	O 48	0	0
4	F	42	Total 42	O 42	0	0
4	G	41	Total 41	O 41	0	0
4	H	43	Total 43	O 43	0	0



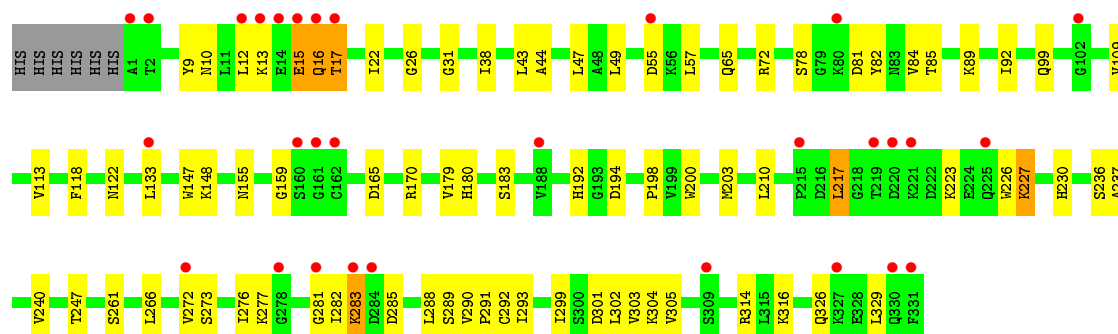




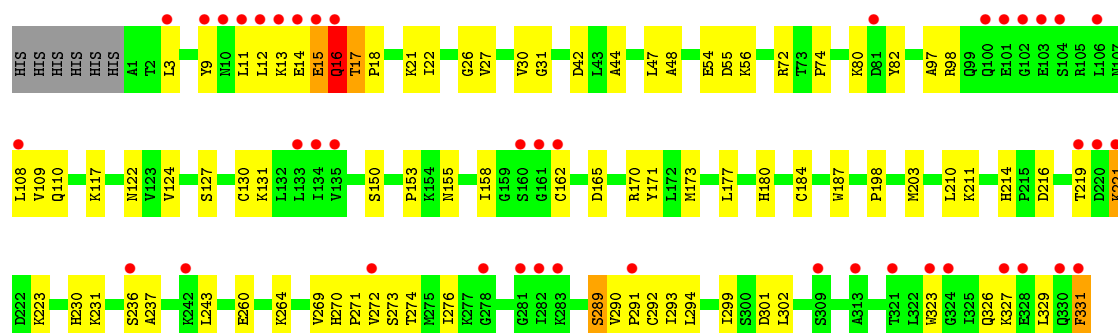
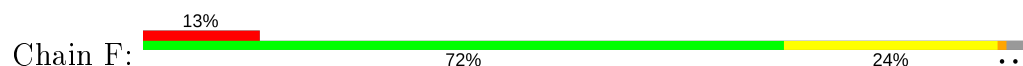
• Molecule 1: L-lactate dehydrogenase A chain



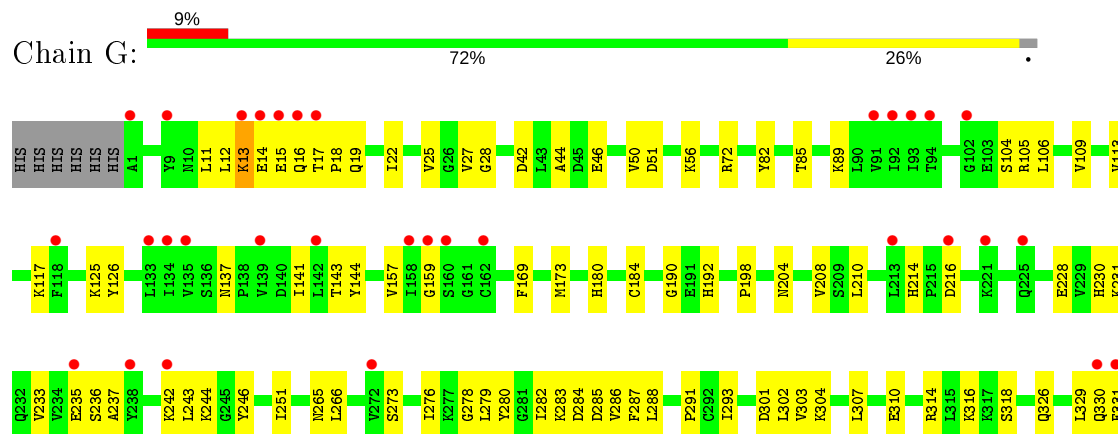
• Molecule 1: L-lactate dehydrogenase A chain



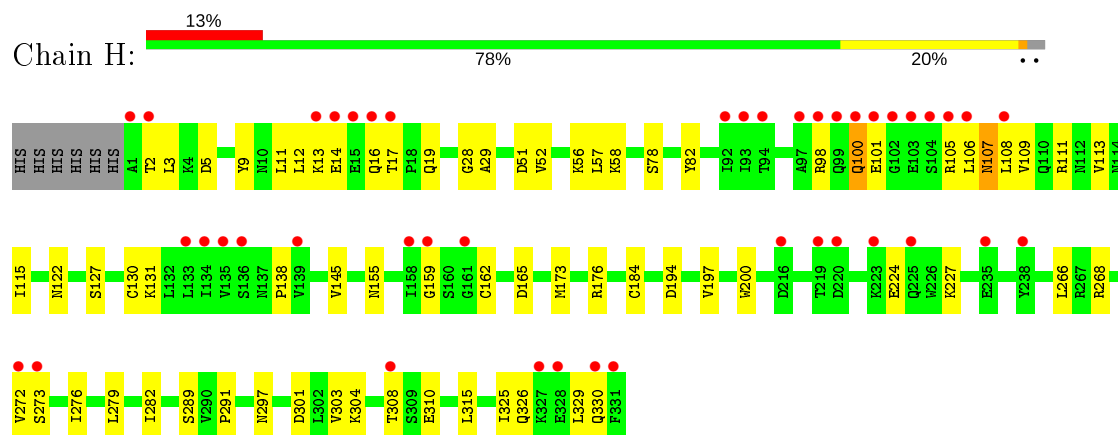
• Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.01Å 265.69Å 88.01Å 90.00° 103.17° 90.00°	Depositor
Resolution (Å)	29.80 – 2.39 29.80 – 2.39	Depositor EDS
% Data completeness (in resolution range)	91.3 (29.80-2.39) 91.3 (29.80-2.39)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.28 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.187 , 0.258 0.187 , 0.258	Depositor DCC
$R_{free}$ test set	5073 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.950	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: NAI, MLI

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	0.42	0/2612	0.59	0/3532
1	B	0.43	0/2612	0.57	0/3532
1	C	0.42	0/2612	0.60	2/3532 (0.1%)
1	D	0.42	0/2612	0.59	0/3532
1	E	0.41	0/2612	0.59	1/3532 (0.0%)
1	F	0.40	0/2612	0.58	1/3532 (0.0%)
1	G	0.42	0/2612	0.58	0/3532
1	H	0.41	0/2612	0.60	0/3532
All	All	0.42	0/20896	0.59	4/28256 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	GLN	C-N-CA	5.54	135.54	121.70
1	C	302	LEU	CA-CB-CG	5.48	127.90	115.30
1	E	170	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	F	16	GLN	C-N-CA	5.12	134.49	121.70

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	2568	0	2656	69	0
1	B	2568	0	2656	65	0
1	C	2568	0	2656	70	0
1	D	2568	0	2656	68	0
1	E	2568	0	2656	71	0
1	F	2568	0	2656	64	0
1	G	2568	0	2656	61	0
1	H	2568	0	2656	49	0
2	A	44	0	27	6	0
2	B	44	0	27	9	0
2	C	44	0	27	6	0
2	D	44	0	27	10	0
2	E	44	0	27	4	0
2	F	44	0	27	6	0
2	G	44	0	27	7	0
2	H	44	0	27	5	0
3	A	7	0	2	7	0
3	B	7	0	2	5	0
3	C	7	0	2	2	0
3	D	7	0	2	4	0
3	E	7	0	2	5	0
3	F	7	0	2	5	0
3	G	7	0	2	6	0
3	H	7	0	2	1	0
4	A	62	0	0	5	0
4	B	61	0	0	4	0
4	C	61	0	0	7	0
4	D	57	0	0	3	0
4	E	48	0	0	0	0
4	F	42	0	0	2	0
4	G	41	0	0	1	0
4	H	43	0	0	2	0
All	All	21367	0	21480	485	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 11.

All (485) 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:302:LEU:HD13	1:D:11:LEU:HD11	1.29	1.10
2:D:401:NAI:H42N	3:D:402:MLI:H12	1.35	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:HD3	1:C:182:LEU:HD23	1.34	1.07
1:F:16:GLN:HG3	1:F:17:THR:H	1.15	1.04
1:A:302:LEU:HD13	1:D:11:LEU:CD1	1.87	1.02
1:B:13:LYS:O	1:B:15:GLU:OE2	1.81	0.99
1:D:330:GLN:NE2	4:D:501:HOH:O	1.97	0.98
2:D:401:NAI:C4N	3:D:402:MLI:H12	1.99	0.92
1:C:107:ASN:O	4:C:501:HOH:O	1.87	0.90
1:A:137:ASN:ND2	3:A:402:MLI:O8	2.04	0.90
1:D:204:ASN:HA	1:D:210:LEU:HD13	1.51	0.90
1:C:154:LYS:HD3	1:C:275:MET:CE	2.03	0.89
1:G:56:LYS:NZ	2:G:401:NAI:O3B	2.05	0.88
1:B:263:MET:SD	4:B:538:HOH:O	2.32	0.87
1:F:54:GLU:OE1	1:F:80:LYS:HE3	1.77	0.84
1:A:170:ARG:HD3	1:A:184:CYS:O	1.76	0.83
1:A:302:LEU:CD1	1:D:11:LEU:HD11	2.09	0.83
1:C:154:LYS:HD3	1:C:275:MET:HE3	1.61	0.82
1:A:218:GLY:HA2	1:A:227:LYS:HG3	1.60	0.82
1:B:16:GLN:O	1:B:17:THR:HG22	1.79	0.81
2:E:401:NAI:H42N	3:E:402:MLI:C3	2.12	0.80
1:E:15:GLU:HB2	1:H:297:ASN:ND2	1.97	0.79
1:F:110:GLN:NE2	4:F:501:HOH:O	2.15	0.79
1:G:22:ILE:HD12	1:G:44:ALA:HB2	1.63	0.78
1:E:291:PRO:HB2	1:E:303:VAL:HB	1.65	0.78
1:D:204:ASN:HA	1:D:210:LEU:CD1	2.14	0.76
1:C:108:LEU:HD12	1:C:111:ARG:HE	1.50	0.76
1:C:211:LYS:NZ	1:C:215:PRO:O	2.18	0.75
1:D:216:ASP:O	1:D:222:ASP:HB2	1.85	0.75
1:H:308:THR:HG22	1:H:310:GLU:H	1.50	0.75
1:G:282:ILE:HD11	1:G:316:LYS:HG2	1.69	0.75
1:F:54:GLU:CD	1:F:80:LYS:HE3	2.08	0.73
1:F:293:ILE:HD12	1:F:301:ASP:HB2	1.71	0.73
1:G:192:HIS:NE2	3:G:402:MLI:O8	2.21	0.73
1:D:291:PRO:HB2	1:D:303:VAL:HB	1.70	0.73
1:E:227:LYS:NZ	1:E:314:ARG:HH12	1.86	0.72
1:D:251:ILE:HG12	2:D:401:NAI:H4N	1.72	0.72
1:H:291:PRO:HB2	1:H:303:VAL:HB	1.71	0.72
1:D:137:ASN:ND2	3:D:402:MLI:O8	2.20	0.72
1:F:302:LEU:HD13	1:G:11:LEU:HD11	1.70	0.72
1:D:216:ASP:O	1:D:219:THR:HG22	1.90	0.71
1:B:25:VAL:HG12	1:B:50:VAL:HB	1.73	0.71
1:F:54:GLU:CD	1:F:80:LYS:CE	2.60	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:VAL:HG12	1:B:80:LYS:HE2	1.74	0.70
1:F:13:LYS:O	1:F:15:GLU:N	2.25	0.70
1:A:192:HIS:NE2	3:A:402:MLI:O9	2.25	0.69
1:F:203:MET:HG2	1:F:210:LEU:HD12	1.73	0.69
1:F:16:GLN:HG3	1:F:17:THR:N	1.99	0.69
1:F:16:GLN:CG	1:F:17:THR:H	1.95	0.68
1:A:175:GLU:OE1	4:A:501:HOH:O	2.10	0.68
1:C:107:ASN:ND2	4:C:504:HOH:O	2.25	0.68
1:D:159:GLY:HA3	1:D:273:SER:HB2	1.75	0.68
1:C:148:LYS:CB	1:C:331:PHE:HE2	2.07	0.68
1:E:276:ILE:HD12	1:E:282:ILE:HD13	1.76	0.68
1:A:11:LEU:HD11	1:D:302:LEU:HD13	1.74	0.67
1:D:154:LYS:HD3	1:D:275:MET:HE3	1.76	0.67
1:D:13:LYS:O	1:D:15:GLU:N	2.28	0.66
1:C:293:ILE:HD12	1:C:301:ASP:HB2	1.78	0.66
1:C:154:LYS:HD3	1:C:275:MET:HE2	1.76	0.66
1:A:264:LYS:HD3	1:D:72:ARG:HG2	1.78	0.66
1:E:290:VAL:HG22	1:E:291:PRO:HD2	1.78	0.66
1:G:82:TYR:O	1:G:85:THR:HB	1.95	0.65
1:A:302:LEU:CD1	1:D:11:LEU:CD1	2.70	0.65
1:E:9:TYR:HB2	1:H:304:LYS:HD3	1.77	0.65
2:F:401:NAI:H42N	3:F:402:MLI:C2	2.26	0.65
1:E:276:ILE:HD13	1:E:288:LEU:HD11	1.79	0.64
1:B:268:ARG:HD3	1:D:182:LEU:HD23	1.78	0.64
1:E:198:PRO:HD3	1:E:230:HIS:CE1	2.33	0.64
1:G:125:LYS:HD3	1:G:126:TYR:CE2	2.33	0.64
1:B:251:ILE:HG21	2:B:401:NAI:H4N	1.79	0.64
1:D:191:GLU:HG3	1:D:322:LEU:HD21	1.78	0.64
1:E:15:GLU:O	1:E:15:GLU:HG2	1.98	0.64
1:A:219:THR:HG22	1:A:221:LYS:H	1.62	0.64
1:H:105:ARG:O	1:H:138:PRO:HB3	1.97	0.63
1:H:2:THR:HG23	1:H:5:ASP:H	1.62	0.63
1:H:127:SER:HB3	1:H:130:CYS:HB3	1.79	0.63
1:G:293:ILE:HD12	1:G:301:ASP:HB2	1.79	0.62
1:C:148:LYS:HB3	1:C:331:PHE:HE2	1.63	0.62
1:A:22:ILE:HD12	1:A:44:ALA:HB2	1.81	0.62
1:E:293:ILE:HD12	1:E:301:ASP:HB2	1.80	0.62
1:E:82:TYR:O	1:E:85:THR:HB	2.00	0.62
1:D:203:MET:HG2	1:D:210:LEU:HD22	1.82	0.62
1:G:251:ILE:HG12	2:G:401:NAI:H4N	1.82	0.62
1:A:293:ILE:HD12	1:A:301:ASP:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:GLN:HA	1:F:329:LEU:HD12	1.82	0.62
1:A:82:TYR:O	1:A:85:THR:HB	2.00	0.61
1:B:51:ASP:O	1:B:80:LYS:HD3	2.00	0.61
1:C:98:ARG:HD3	2:C:401:NAI:O3	1.99	0.61
1:E:276:ILE:CD1	1:E:282:ILE:HD13	2.29	0.61
1:E:227:LYS:NZ	1:E:314:ARG:HH22	1.99	0.61
1:B:203:MET:HG2	1:B:210:LEU:HD13	1.83	0.61
1:D:290:VAL:HG22	1:D:291:PRO:HD2	1.82	0.61
1:D:190:GLY:HA2	1:D:288:LEU:HD13	1.83	0.61
1:D:108:LEU:HD23	1:D:111:ARG:NH2	2.16	0.61
2:G:401:NAI:O7N	3:G:402:MLI:H11	2.01	0.60
1:C:106:LEU:HA	1:C:109:VAL:HG23	1.83	0.60
1:C:243:LEU:HD11	1:D:58:LYS:HD3	1.84	0.60
1:D:16:GLN:O	1:D:17:THR:OG1	2.17	0.60
1:A:277:LYS:HB2	1:A:284:ASP:O	2.01	0.59
1:F:216:ASP:O	1:F:219:THR:HB	2.02	0.59
1:D:162:CYS:HA	1:D:165:ASP:OD1	2.03	0.59
1:F:117:LYS:HD3	1:F:331:PHE:HB2	1.84	0.59
2:F:401:NAI:H42N	3:F:402:MLI:C3	2.32	0.59
1:G:113:VAL:O	1:G:117:LYS:HG3	2.03	0.59
1:C:99:GLN:HE22	1:C:112:ASN:HD21	1.49	0.59
1:G:13:LYS:O	1:G:15:GLU:N	2.36	0.59
1:G:19:GLN:O	1:G:89:LYS:HE3	2.02	0.59
1:D:330:GLN:N	1:D:330:GLN:OE1	2.31	0.59
1:H:115:ILE:HG23	2:H:401:NAI:N6A	2.18	0.59
1:C:100:GLN:N	1:C:100:GLN:OE1	2.34	0.58
1:H:82:TYR:CG	1:H:122:ASN:HB3	2.38	0.58
1:G:243:LEU:HD13	1:H:58:LYS:HG2	1.84	0.58
1:A:127:SER:HB3	1:A:130:CYS:HB3	1.85	0.58
1:B:168:ARG:NH1	3:B:402:MLI:O7	2.21	0.58
1:A:216:ASP:O	1:A:219:THR:HB	2.04	0.58
1:B:204:ASN:HA	1:B:210:LEU:HD12	1.86	0.58
1:A:323:TRP:HA	1:A:326:GLN:HG3	1.85	0.58
1:D:110:GLN:HG3	4:D:530:HOH:O	2.04	0.58
1:H:115:ILE:HG23	2:H:401:NAI:H61A	1.68	0.58
1:G:233:VAL:O	1:G:236:SER:OG	2.18	0.58
1:C:291:PRO:HB2	1:C:303:VAL:HB	1.86	0.57
1:E:15:GLU:HB2	1:H:297:ASN:HD21	1.70	0.57
1:F:16:GLN:HE22	1:G:265:ASN:ND2	2.03	0.57
2:G:401:NAI:C5N	3:G:402:MLI:H12	2.35	0.57
1:F:270:HIS:CD2	1:F:294:LEU:HD12	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:THR:HG23	1:G:157:VAL:HG12	1.86	0.57
1:E:22:ILE:HD12	1:E:44:ALA:HB2	1.86	0.56
2:H:401:NAI:H42N	3:H:402:MLI:C2	2.36	0.56
1:G:56:LYS:CE	2:G:401:NAI:O3B	2.53	0.56
1:E:302:LEU:HD13	1:H:11:LEU:CD1	2.35	0.56
2:A:401:NAI:H42N	3:A:402:MLI:C1	2.36	0.56
1:A:13:LYS:HG3	1:A:14:GLU:H	1.70	0.56
1:A:3:LEU:HD23	1:B:214:HIS:HB2	1.87	0.56
1:C:219:THR:OG1	1:C:221:LYS:HG2	2.06	0.56
1:C:140:ASP:OD1	1:C:273:SER:OG	2.23	0.55
1:A:99:GLN:HG3	1:A:241:ILE:HD13	1.88	0.55
1:C:97:ALA:O	4:C:502:HOH:O	2.18	0.55
1:C:38:ILE:HG23	1:C:43:LEU:HB2	1.88	0.55
2:A:401:NAI:H42N	3:A:402:MLI:C2	2.36	0.55
1:C:109:VAL:HG22	1:C:138:PRO:HG3	1.89	0.55
1:H:176:ARG:NH1	1:H:224:GLU:O	2.39	0.55
1:B:139:VAL:HG21	1:B:160:SER:HB2	1.88	0.55
1:H:105:ARG:NH1	1:H:194:ASP:OD2	2.40	0.55
1:A:276:ILE:HD13	1:A:288:LEU:HD11	1.88	0.55
1:D:204:ASN:CA	1:D:210:LEU:HD13	2.32	0.55
1:C:264:LYS:HE2	4:C:543:HOH:O	2.07	0.54
1:E:165:ASP:OD1	1:E:192:HIS:HD2	1.90	0.54
1:F:290:VAL:HG22	1:F:291:PRO:HD2	1.89	0.54
2:E:401:NAI:H42N	3:E:402:MLI:C2	2.38	0.54
1:A:216:ASP:O	1:A:222:ASP:HB2	2.08	0.54
1:F:16:GLN:HE22	1:G:265:ASN:HD21	1.54	0.54
1:A:260:GLU:OE2	1:D:72:ARG:HD3	2.07	0.54
1:F:9:TYR:HB2	1:G:304:LYS:HD2	1.90	0.54
1:G:291:PRO:HB2	1:G:303:VAL:HB	1.90	0.54
1:H:106:LEU:HD22	1:H:325:ILE:HD12	1.90	0.54
1:C:105:ARG:HD3	4:C:547:HOH:O	2.07	0.54
1:E:326:GLN:O	1:E:329:LEU:HB2	2.08	0.54
1:A:213:LEU:O	1:B:6:GLN:NE2	2.36	0.53
1:C:66:HIS:CE1	1:D:236:SER:HB2	2.43	0.53
1:F:272:VAL:O	1:F:289:SER:HA	2.08	0.53
2:F:401:NAI:H42N	3:F:402:MLI:O6	2.08	0.53
1:A:117:LYS:HD3	1:A:331:PHE:HB2	1.90	0.53
1:A:18:PRO:HB2	1:A:21:LYS:HB2	1.89	0.53
1:A:219:THR:HG22	1:A:221:LYS:N	2.23	0.53
1:F:214:HIS:CE1	1:F:216:ASP:HB2	2.44	0.53
1:D:308:THR:HG22	1:D:311:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:VAL:HG11	1:F:150:SER:HB2	1.90	0.53
1:F:292:CYS:HB3	1:F:299:ILE:HG23	1.91	0.53
1:E:302:LEU:HD13	1:H:11:LEU:HD11	1.90	0.53
1:G:329:LEU:HD12	1:G:330:GLN:H	1.74	0.53
1:A:18:PRO:HB3	1:A:46:GLU:OE1	2.08	0.52
1:G:106:LEU:O	1:G:109:VAL:HG12	2.09	0.52
1:G:18:PRO:HB3	1:G:46:GLU:OE1	2.09	0.52
1:G:28:GLY:HA3	2:G:401:NAI:O5B	2.09	0.52
1:H:279:LEU:O	1:H:282:ILE:HG12	2.09	0.52
1:A:13:LYS:HG3	1:A:15:GLU:HG3	1.91	0.52
1:B:326:GLN:HA	1:B:329:LEU:HD12	1.90	0.52
1:E:165:ASP:OD1	1:E:192:HIS:CD2	2.63	0.52
1:G:137:ASN:HD21	3:G:402:MLI:C3	2.22	0.52
1:C:180:HIS:ND1	1:C:182:LEU:HB2	2.25	0.52
1:F:260:GLU:HG3	1:F:264:LYS:HD2	1.91	0.52
1:E:12:LEU:HD11	1:H:155:ASN:CB	2.40	0.52
1:E:227:LYS:HZ1	1:E:314:ARG:HH12	1.54	0.52
1:G:244:LYS:HE2	1:G:246:TYR:O	2.08	0.52
1:A:55:ASP:OD1	4:A:502:HOH:O	2.19	0.52
1:C:65:GLN:HB3	1:D:171:TYR:CZ	2.44	0.52
1:F:74:PRO:O	4:F:502:HOH:O	2.19	0.52
1:A:105:ARG:HE	3:A:402:MLI:C3	2.22	0.52
1:E:203:MET:HE3	1:E:210:LEU:HD12	1.91	0.52
1:E:305:VAL:HA	1:G:208:VAL:HG21	1.91	0.52
1:F:18:PRO:HB2	1:F:21:LYS:HB2	1.91	0.51
1:A:275:MET:SD	1:A:277:LYS:HB3	2.49	0.51
1:A:3:LEU:HD11	1:B:210:LEU:HD23	1.92	0.51
1:A:266:LEU:O	1:C:180:HIS:HB2	2.11	0.51
1:B:99:GLN:HE22	1:B:105:ARG:HG2	1.75	0.51
1:A:218:GLY:O	1:A:227:LYS:HE3	2.10	0.51
1:C:25:VAL:HG22	1:C:50:VAL:CG1	2.40	0.51
1:G:105:ARG:NE	3:G:402:MLI:O8	2.31	0.51
1:C:46:GLU:HG3	1:C:75:LYS:HB3	1.92	0.51
1:D:247:THR:OG1	2:D:401:NAI:H5N	2.10	0.51
1:B:82:TYR:O	1:B:85:THR:HB	2.11	0.51
1:F:27:VAL:O	1:F:56:LYS:HE3	2.10	0.50
1:G:214:HIS:CE1	1:G:216:ASP:HB2	2.46	0.50
1:A:279:LEU:HB3	1:A:280:TYR:CD1	2.46	0.50
1:B:216:ASP:HB3	1:B:222:ASP:HA	1.93	0.50
1:C:216:ASP:O	1:C:222:ASP:HB2	2.12	0.50
1:F:170:ARG:HA	1:F:173:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:LEU:HD13	1:G:11:LEU:CD1	2.41	0.50
1:B:198:PRO:HD3	1:B:230:HIS:CE1	2.47	0.50
1:E:272:VAL:O	1:E:289:SER:HA	2.12	0.50
1:B:262:ILE:HG22	4:B:538:HOH:O	2.11	0.50
1:C:82:TYR:O	1:C:85:THR:HB	2.12	0.50
1:E:236:SER:O	1:E:240:VAL:HG23	2.12	0.50
1:F:198:PRO:HD3	1:F:230:HIS:CE1	2.47	0.50
1:H:2:THR:OG1	1:H:3:LEU:N	2.45	0.49
1:A:125:LYS:HE2	1:A:126:TYR:CZ	2.46	0.49
1:A:267:ARG:HD3	4:A:553:HOH:O	2.12	0.49
1:E:192:HIS:HE1	3:E:402:MLI:O8	1.95	0.49
1:B:27:VAL:HG22	1:B:51:ASP:HB2	1.95	0.49
1:C:16:GLN:O	1:C:17:THR:OG1	2.27	0.49
1:E:89:LYS:NZ	1:H:19:GLN:HG2	2.27	0.49
1:D:187:TRP:N	4:D:503:HOH:O	2.36	0.49
1:B:327:LYS:NZ	4:B:503:HOH:O	2.45	0.49
1:C:105:ARG:HB3	1:C:138:PRO:HB3	1.95	0.49
1:D:28:GLY:HA3	2:D:401:NAI:O5B	2.13	0.49
1:H:272:VAL:O	1:H:289:SER:HA	2.12	0.49
1:B:19:GLN:O	1:B:89:LYS:HE3	2.12	0.49
1:B:52:VAL:HA	1:B:80:LYS:HD3	1.94	0.49
1:B:159:GLY:HA3	1:B:273:SER:HB2	1.94	0.49
2:B:401:NAI:H42N	3:B:402:MLI:C1	2.43	0.49
1:D:159:GLY:CA	1:D:273:SER:HB2	2.42	0.49
1:G:169:PHE:CE1	1:G:173:MET:HE2	2.48	0.49
1:B:10:ASN:ND2	1:B:12:LEU:O	2.35	0.49
1:C:216:ASP:HB3	1:C:222:ASP:HA	1.94	0.49
1:E:109:VAL:O	1:E:113:VAL:HG23	2.12	0.48
1:B:227:LYS:NZ	4:B:504:HOH:O	2.47	0.48
1:C:197:VAL:HG21	1:C:315:LEU:CD1	2.44	0.48
1:F:158:ILE:HG12	1:F:299:ILE:HG13	1.95	0.48
1:B:13:LYS:O	1:B:15:GLU:CD	2.50	0.48
1:E:227:LYS:NZ	1:E:314:ARG:NH1	2.57	0.48
1:G:237:ALA:HB2	3:G:402:MLI:O6	2.14	0.48
1:D:272:VAL:O	1:D:289:SER:HA	2.13	0.48
1:A:326:GLN:O	1:A:329:LEU:HB2	2.14	0.48
1:C:3:LEU:HD13	1:D:214:HIS:HB2	1.96	0.48
1:B:251:ILE:HG12	2:B:401:NAI:H4N	1.95	0.48
1:F:219:THR:HG22	1:F:221:LYS:N	2.28	0.48
1:B:113:VAL:HG21	1:B:329:LEU:HD22	1.96	0.48
1:D:251:ILE:CG1	2:D:401:NAI:H4N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:LYS:HZ1	1:E:314:ARG:HH22	1.60	0.48
1:E:281:GLY:O	1:E:316:LYS:NZ	2.47	0.48
1:E:92:ILE:HG12	1:E:133:LEU:HD23	1.96	0.47
1:H:57:LEU:HD11	1:H:78:SER:HB2	1.95	0.47
1:E:281:GLY:HA3	1:E:316:LYS:HZ1	1.79	0.47
1:B:208:VAL:HG11	1:D:305:VAL:HA	1.95	0.47
1:A:74:PRO:O	1:A:75:LYS:HD2	2.14	0.47
1:F:323:TRP:O	1:F:327:LYS:HB2	2.15	0.47
1:H:98:ARG:HB3	2:H:401:NAI:H3D	1.97	0.47
1:C:108:LEU:HA	4:C:544:HOH:O	2.13	0.47
1:E:12:LEU:HD11	1:H:155:ASN:HB3	1.97	0.47
1:A:147:TRP:HB2	1:A:157:VAL:HG11	1.96	0.47
1:C:177:LEU:HD11	1:C:226:TRP:HH2	1.80	0.47
1:F:98:ARG:HD3	2:F:401:NAI:O3	2.15	0.47
1:G:141:ILE:HG12	1:G:326:GLN:HG3	1.97	0.47
1:A:292:CYS:HB3	1:A:299:ILE:HG23	1.96	0.47
1:B:221:LYS:O	1:B:221:LYS:HG2	2.16	0.46
1:E:266:LEU:O	1:G:180:HIS:HB2	2.16	0.46
1:E:292:CYS:HB3	1:E:299:ILE:HG23	1.97	0.46
2:A:401:NAI:H42N	3:A:402:MLI:H11	1.97	0.46
1:B:11:LEU:O	1:B:12:LEU:HD23	2.15	0.46
1:B:282:ILE:HG13	1:B:316:LYS:NZ	2.31	0.46
1:D:13:LYS:O	1:D:15:GLU:HG2	2.15	0.46
1:F:42:ASP:OD1	1:F:72:ARG:HB2	2.14	0.46
1:B:189:LEU:HD22	1:B:199:VAL:HG21	1.98	0.46
1:B:28:GLY:HA3	2:B:401:NAI:O5B	2.15	0.46
1:C:18:PRO:HB2	1:C:21:LYS:HB2	1.97	0.46
1:G:198:PRO:HD3	1:G:230:HIS:CE1	2.50	0.46
1:C:272:VAL:O	1:C:289:SER:HA	2.16	0.46
1:A:42:ASP:HB3	1:D:264:LYS:HZ1	1.80	0.46
1:G:15:GLU:OE1	1:G:15:GLU:N	2.47	0.46
1:E:26:GLY:O	1:E:31:GLY:HA3	2.16	0.46
1:E:38:ILE:HG23	1:E:43:LEU:HB2	1.97	0.46
1:B:26:GLY:O	1:B:31:GLY:HA3	2.16	0.46
1:C:6:GLN:HB3	1:D:213:LEU:HD12	1.98	0.46
1:D:46:GLU:HG3	1:D:75:LYS:HB3	1.98	0.46
1:F:47:LEU:HD12	1:F:48:ALA:N	2.31	0.46
1:F:97:ALA:O	1:F:108:LEU:HD13	2.16	0.46
1:E:72:ARG:HH22	1:H:268:ARG:NH2	2.14	0.46
1:A:275:MET:HG2	1:A:287:PHE:CE1	2.51	0.46
2:B:401:NAI:O7N	3:B:402:MLI:H11	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:LEU:HD11	1:E:78:SER:HB2	1.98	0.46
1:E:99:GLN:H	1:E:99:GLN:HG2	1.33	0.46
1:E:283:LYS:HE2	1:E:283:LYS:HB3	1.71	0.46
1:F:11:LEU:HD11	1:G:302:LEU:HD13	1.98	0.46
1:F:30:VAL:HG21	2:F:401:NAI:C6N	2.46	0.46
1:A:165:ASP:OD1	1:A:192:HIS:ND1	2.36	0.46
1:B:307:LEU:HB3	1:B:311:GLU:HB2	1.98	0.46
1:D:292:CYS:HB3	1:D:299:ILE:HG23	1.98	0.46
1:A:320:ASP:OD1	4:A:503:HOH:O	2.21	0.45
1:A:105:ARG:NE	3:A:402:MLI:O9	2.44	0.45
1:G:278:GLY:C	1:G:279:LEU:HD22	2.36	0.45
1:C:148:LYS:HA	1:C:148:LYS:HD2	1.73	0.45
1:E:226:TRP:CZ2	1:F:3:LEU:HD23	2.51	0.45
1:G:284:ASP:O	1:G:286:VAL:N	2.45	0.45
1:G:310:GLU:OE1	1:G:314:ARG:HD2	2.16	0.45
1:B:280:TYR:O	1:B:316:LYS:HD2	2.16	0.45
1:F:127:SER:HB3	1:F:130:CYS:HB3	1.97	0.45
1:H:107:ASN:ND2	4:H:501:HOH:O	2.17	0.45
1:H:131:LYS:HE2	1:H:131:LYS:HB2	1.65	0.45
1:B:9:TYR:HB2	1:C:304:LYS:HD3	1.98	0.45
1:D:293:ILE:HD12	1:D:301:ASP:HB2	1.98	0.45
1:E:16:GLN:HB2	1:E:17:THR:H	1.47	0.45
1:H:326:GLN:O	1:H:329:LEU:HB2	2.17	0.45
1:C:105:ARG:HG2	1:C:137:ASN:HB3	1.98	0.45
1:F:54:GLU:OE2	1:F:80:LYS:NZ	2.45	0.45
1:H:308:THR:HG22	1:H:310:GLU:N	2.24	0.45
1:B:114:ASN:HA	1:B:117:LYS:HD2	1.99	0.45
1:C:148:LYS:HB3	1:C:331:PHE:CE2	2.49	0.45
1:A:302:LEU:HD13	1:D:11:LEU:HD13	1.88	0.45
1:B:16:GLN:O	1:B:17:THR:CG2	2.58	0.45
2:B:401:NAI:H42N	3:B:402:MLI:H11	1.97	0.45
2:D:401:NAI:C3N	3:D:402:MLI:H12	2.46	0.45
1:D:51:ASP:OD1	1:D:52:VAL:N	2.50	0.45
1:F:22:ILE:HD12	1:F:44:ALA:HB2	1.99	0.45
1:A:55:ASP:HA	4:A:502:HOH:O	2.16	0.45
1:B:213:LEU:O	1:B:215:PRO:HD3	2.17	0.45
1:E:237:ALA:HB1	3:E:402:MLI:H12	1.97	0.45
1:E:277:LYS:HD3	1:E:285:ASP:OD1	2.17	0.45
1:E:81:ASP:O	1:E:84:VAL:HG22	2.17	0.45
1:C:99:GLN:HG2	2:C:401:NAI:O2D	2.17	0.44
2:E:401:NAI:H42N	3:E:402:MLI:C1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ASP:O	1:F:243:LEU:HB3	2.17	0.44
1:F:187:TRP:CZ3	1:F:271:PRO:HD3	2.52	0.44
1:G:173:MET:SD	1:G:184:CYS:HB3	2.58	0.44
1:A:36:ILE:O	1:A:40:MET:HG3	2.18	0.44
1:H:111:ARG:O	1:H:115:ILE:HG13	2.17	0.44
1:A:117:LYS:HD3	1:A:331:PHE:CB	2.48	0.44
1:B:165:ASP:OD1	1:B:192:HIS:ND1	2.44	0.44
1:B:292:CYS:HB3	1:B:299:ILE:HG23	1.98	0.44
1:D:329:LEU:HA	1:D:329:LEU:HD12	1.76	0.44
1:F:180:HIS:HB2	1:H:266:LEU:O	2.18	0.44
1:H:109:VAL:HG22	1:H:138:PRO:HG3	2.00	0.44
1:A:272:VAL:O	1:A:289:SER:HA	2.18	0.44
1:E:227:LYS:CE	1:E:314:ARG:HH22	2.30	0.44
1:F:173:MET:SD	1:F:184:CYS:HB3	2.57	0.44
1:G:159:GLY:HA3	1:G:273:SER:HB2	1.98	0.44
1:A:189:LEU:HD22	1:A:199:VAL:HG21	2.00	0.44
1:E:329:LEU:HD23	1:E:329:LEU:HA	1.70	0.44
1:F:11:LEU:CD1	1:G:302:LEU:HD13	2.48	0.44
1:H:276:ILE:HG12	1:H:276:ILE:O	2.18	0.44
1:F:237:ALA:HB1	3:F:402:MLI:H12	1.99	0.44
1:G:242:LYS:HE2	1:G:242:LYS:HB3	1.77	0.44
1:A:131:LYS:HE2	1:A:131:LYS:HB2	1.68	0.43
1:B:124:VAL:HG22	1:B:152:PHE:CZ	2.52	0.43
2:C:401:NAI:H42N	3:C:402:MLI:C2	2.48	0.43
1:B:293:ILE:HD12	1:B:301:ASP:HB2	1.99	0.43
1:B:7:LEU:HG	1:B:8:ILE:HG13	2.00	0.43
1:D:251:ILE:HG21	2:D:401:NAI:H4N	2.00	0.43
2:D:401:NAI:H6N	2:D:401:NAI:H2D	1.88	0.43
1:F:12:LEU:HA	1:F:12:LEU:HD23	1.78	0.43
1:E:15:GLU:CB	1:H:297:ASN:ND2	2.75	0.43
1:B:216:ASP:O	1:B:222:ASP:HB2	2.19	0.43
1:D:127:SER:HB3	1:D:130:CYS:HB3	1.99	0.43
1:D:277:LYS:HE2	1:D:285:ASP:OD1	2.19	0.43
1:C:138:PRO:HG2	1:C:141:ILE:HB	2.00	0.43
2:B:401:NAI:C4N	3:B:402:MLI:C1	2.97	0.43
1:B:80:LYS:HD2	1:B:80:LYS:HA	1.64	0.43
1:E:65:GLN:HB3	1:F:171:TYR:CZ	2.54	0.43
1:B:131:LYS:HB2	1:B:131:LYS:HE2	1.87	0.43
1:F:82:TYR:CG	1:F:122:ASN:HB3	2.54	0.43
1:D:82:TYR:O	1:D:85:THR:HB	2.18	0.43
1:E:227:LYS:NZ	1:E:314:ARG:NH2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LEU:CD1	1:C:226:TRP:HH2	2.31	0.43
1:D:260:GLU:HG3	1:D:264:LYS:HD2	2.00	0.43
1:D:277:LYS:HB2	1:D:284:ASP:O	2.18	0.43
1:D:99:GLN:HB2	1:D:103:GLU:HB3	2.01	0.43
1:G:273:SER:HA	1:G:288:LEU:O	2.18	0.43
1:B:22:ILE:HD12	1:B:44:ALA:HB2	2.01	0.42
1:C:104:SER:O	1:C:105:ARG:HG3	2.19	0.42
1:B:302:LEU:HD11	1:C:11:LEU:HD11	2.00	0.42
2:C:401:NAI:H42N	3:C:402:MLI:C3	2.48	0.42
1:E:147:TRP:CE3	1:E:148:LYS:HD3	2.54	0.42
1:F:231:LYS:HD2	1:F:231:LYS:HA	1.77	0.42
1:B:94:THR:O	2:B:401:NAI:H51N	2.19	0.42
1:C:105:ARG:O	1:C:106:LEU:HD23	2.19	0.42
1:C:203:MET:O	4:C:503:HOH:O	2.20	0.42
1:C:229:VAL:O	1:C:233:VAL:HG23	2.18	0.42
1:D:26:GLY:O	1:D:31:GLY:HA3	2.19	0.42
1:G:12:LEU:O	1:G:13:LYS:HG2	2.18	0.42
1:C:12:LEU:HD23	1:C:12:LEU:HA	1.72	0.42
1:C:98:ARG:HB2	2:C:401:NAI:O3	2.20	0.42
1:A:9:TYR:HB2	1:D:304:LYS:HD2	2.01	0.42
1:F:26:GLY:O	1:F:31:GLY:HA3	2.19	0.42
1:G:251:ILE:HG12	2:G:401:NAI:C4N	2.47	0.42
1:B:153:PRO:HB2	1:B:155:ASN:OD1	2.20	0.42
1:F:269:VAL:HA	1:F:292:CYS:O	2.20	0.42
1:H:100:GLN:HB3	1:H:101:GLU:H	1.60	0.42
1:B:282:ILE:HG13	1:B:316:LYS:HZ3	1.85	0.42
1:C:105:ARG:O	1:C:138:PRO:HB3	2.19	0.42
1:C:148:LYS:HB2	1:C:331:PHE:HE2	1.85	0.42
1:C:39:LEU:HD11	1:C:64:LEU:HD13	2.02	0.42
1:D:180:HIS:ND1	1:D:182:LEU:HB2	2.35	0.42
1:D:3:LEU:O	1:D:3:LEU:HD12	2.20	0.42
1:E:281:GLY:CA	1:E:316:LYS:HZ1	2.32	0.42
1:B:322:LEU:HD23	1:B:322:LEU:HA	1.90	0.42
1:B:326:GLN:HA	1:B:329:LEU:CD1	2.49	0.42
1:C:203:MET:HE1	1:C:217:LEU:HD11	2.02	0.42
1:D:269:VAL:HG22	1:D:293:ILE:HG12	2.01	0.42
1:D:307:LEU:HD23	1:D:307:LEU:HA	1.90	0.42
1:E:180:HIS:HB2	1:G:266:LEU:O	2.19	0.42
1:G:13:LYS:C	1:G:15:GLU:H	2.22	0.42
1:G:244:LYS:O	4:G:501:HOH:O	2.21	0.42
1:A:208:VAL:HG11	1:C:305:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:PHE:O	1:E:122:ASN:ND2	2.50	0.42
1:G:109:VAL:O	1:G:113:VAL:HG23	2.18	0.42
1:H:51:ASP:OD1	1:H:52:VAL:N	2.48	0.42
1:B:286:VAL:HG22	1:B:323:TRP:HB2	2.01	0.42
1:C:189:LEU:HB3	1:C:289:SER:O	2.20	0.42
2:F:401:NAI:C4N	3:F:402:MLI:C3	2.98	0.42
1:A:66:HIS:CE1	1:B:236:SER:HB2	2.55	0.42
1:C:26:GLY:O	1:C:31:GLY:HA3	2.20	0.42
1:E:302:LEU:HD13	1:H:11:LEU:HD13	2.01	0.42
1:G:280:TYR:CE1	1:G:307:LEU:HD12	2.55	0.42
1:H:197:VAL:HG21	1:H:315:LEU:HD12	2.00	0.42
1:A:52:VAL:HG13	2:A:401:NAI:C2A	2.50	0.41
1:C:169:PHE:HD1	1:C:233:VAL:HG21	1.85	0.41
1:E:49:LEU:O	1:E:78:SER:HA	2.20	0.41
1:G:231:LYS:O	1:G:235:GLU:HG2	2.20	0.41
1:H:56:LYS:NZ	4:H:504:HOH:O	2.43	0.41
1:D:208:VAL:O	1:D:210:LEU:HD12	2.19	0.41
2:E:401:NAI:H6N	2:E:401:NAI:H2D	1.86	0.41
1:F:264:LYS:NZ	1:G:42:ASP:HB3	2.35	0.41
1:B:276:ILE:HG12	1:B:288:LEU:CD1	2.51	0.41
1:E:240:VAL:HB	1:E:247:THR:HG22	2.01	0.41
1:E:47:LEU:HD21	1:E:49:LEU:HD21	2.02	0.41
1:A:290:VAL:HG22	1:A:291:PRO:HD2	2.02	0.41
1:D:153:PRO:HB2	1:D:155:ASN:OD1	2.20	0.41
1:F:274:THR:O	1:F:276:ILE:HG23	2.21	0.41
1:G:25:VAL:HG22	1:G:50:VAL:CG1	2.50	0.41
1:C:203:MET:HG2	1:C:210:LEU:HD22	2.01	0.41
1:C:98:ARG:HD3	2:C:401:NAI:PN	2.61	0.41
1:C:51:ASP:OD1	1:C:52:VAL:N	2.49	0.41
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.69	0.41
1:G:190:GLY:HA2	1:G:288:LEU:HD22	2.01	0.41
1:G:276:ILE:HD12	1:G:276:ILE:O	2.21	0.41
2:B:401:NAI:H2D	2:B:401:NAI:H6N	1.82	0.41
1:C:148:LYS:CB	1:C:331:PHE:CE2	2.96	0.41
1:D:100:GLN:HG2	1:D:103:GLU:OE1	2.21	0.41
1:B:208:VAL:HG12	1:D:305:VAL:HG13	2.02	0.41
1:G:204:ASN:HA	1:G:210:LEU:HD13	2.03	0.41
1:A:158:ILE:HG23	1:A:299:ILE:HD11	2.02	0.41
1:B:112:ASN:ND2	1:B:137:ASN:O	2.43	0.41
1:F:219:THR:HG22	1:F:221:LYS:H	1.86	0.41
1:F:223:LYS:HE3	1:F:223:LYS:HB3	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:VAL:HG22	1:H:145:VAL:HG21	2.03	0.41
1:A:38:ILE:HG23	1:A:43:LEU:HB2	2.03	0.41
1:E:261:SER:HA	1:E:266:LEU:HD12	2.03	0.41
1:F:162:CYS:HA	1:F:165:ASP:OD1	2.21	0.41
1:H:173:MET:SD	1:H:184:CYS:HB3	2.61	0.41
1:E:304:LYS:HD3	1:H:9:TYR:HB2	2.03	0.41
1:A:28:GLY:HA3	2:A:401:NAI:O5B	2.20	0.41
1:B:276:ILE:HD13	1:B:282:ILE:HD13	2.03	0.41
1:E:159:GLY:HA3	1:E:273:SER:HB2	2.01	0.41
1:F:211:LYS:HA	1:F:211:LYS:HD2	1.94	0.41
1:G:27:VAL:HG22	1:G:51:ASP:HB2	2.03	0.41
1:E:155:ASN:ND2	1:H:12:LEU:HD11	2.35	0.41
1:E:200:TRP:CE3	1:E:217:LEU:HD21	2.55	0.40
1:F:274:THR:HB	1:F:299:ILE:HD13	2.03	0.40
1:G:144:TYR:HB2	1:G:287:PHE:CD1	2.57	0.40
1:D:251:ILE:CB	2:D:401:NAI:H4N	2.50	0.40
1:E:10:ASN:HA	1:H:301:ASP:OD2	2.22	0.40
1:E:179:VAL:CG1	1:E:183:SER:HB2	2.51	0.40
1:F:153:PRO:HB2	1:F:155:ASN:OD1	2.22	0.40
1:H:28:GLY:HA3	2:H:401:NAI:O5B	2.22	0.40
1:A:30:VAL:HG21	2:A:401:NAI:C6N	2.52	0.40
1:G:25:VAL:HA	1:G:50:VAL:HG13	2.04	0.40
1:H:200:TRP:CH2	1:H:227:LYS:HA	2.56	0.40
1:A:218:GLY:CA	1:A:227:LYS:HG3	2.42	0.40
1:C:177:LEU:HD23	1:C:205:VAL:HG21	2.04	0.40
1:C:86:ALA:HA	1:C:126:TYR:HB3	2.04	0.40
1:E:13:LYS:C	1:E:15:GLU:H	2.25	0.40
1:H:159:GLY:HA3	1:H:273:SER:HB2	2.02	0.40
1:A:273:SER:HA	1:A:288:LEU:O	2.22	0.40
1:E:148:LYS:HA	1:E:148:LYS:HD2	1.89	0.40
1:F:198:PRO:HG3	1:F:230:HIS:CG	2.56	0.40
1:H:162:CYS:HB2	1:H:289:SER:CB	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/337 (98%)	313 (95%)	13 (4%)	3 (1%)	17	25
1	B	329/337 (98%)	310 (94%)	16 (5%)	3 (1%)	17	25
1	C	329/337 (98%)	306 (93%)	15 (5%)	8 (2%)	6	6
1	D	329/337 (98%)	315 (96%)	12 (4%)	2 (1%)	25	36
1	E	329/337 (98%)	311 (94%)	16 (5%)	2 (1%)	25	36
1	F	329/337 (98%)	309 (94%)	15 (5%)	5 (2%)	10	14
1	G	329/337 (98%)	308 (94%)	16 (5%)	5 (2%)	10	14
1	H	329/337 (98%)	306 (93%)	17 (5%)	6 (2%)	8	10
All	All	2632/2696 (98%)	2478 (94%)	120 (5%)	34 (1%)	12	17

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	B	14	GLU
1	B	17	THR
1	C	13	LYS
1	C	16	GLN
1	C	17	THR
1	C	98	ARG
1	C	104	SER
1	D	14	GLU
1	D	17	THR
1	F	14	GLU
1	F	16	GLN
1	F	17	THR
1	F	109	VAL
1	G	14	GLU
1	H	14	GLU
1	H	16	GLN
1	H	100	GLN
1	A	15	GLU
1	B	285	ASP
1	C	15	GLU
1	C	101	GLU
1	G	13	LYS

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Mol	Chain	Res	Type
1	G	16	GLN
1	G	285	ASP
1	H	29	ALA
1	E	16	GLN
1	G	17	THR
1	A	17	THR
1	C	222	ASP
1	E	17	THR
1	F	221	LYS
1	H	17	THR
1	H	107	ASN

### 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	287/293 (98%)	282 (98%)	5 (2%)	60	78
1	B	287/293 (98%)	286 (100%)	1 (0%)	92	97
1	C	287/293 (98%)	279 (97%)	8 (3%)	43	63
1	D	287/293 (98%)	285 (99%)	2 (1%)	84	92
1	E	287/293 (98%)	281 (98%)	6 (2%)	53	72
1	F	287/293 (98%)	279 (97%)	8 (3%)	43	63
1	G	287/293 (98%)	281 (98%)	6 (2%)	53	72
1	H	287/293 (98%)	283 (99%)	4 (1%)	67	82
All	All	2296/2344 (98%)	2256 (98%)	40 (2%)	60	78

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	131	LYS
1	A	173	MET
1	A	283	LYS

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Mol	Chain	Res	Type
1	A	317	LYS
1	B	160	SER
1	C	13	LYS
1	C	160	SER
1	C	223	LYS
1	C	231	LYS
1	C	273	SER
1	C	289	SER
1	C	310	GLU
1	C	331	PHE
1	D	221	LYS
1	D	283	LYS
1	E	15	GLU
1	E	194	ASP
1	E	217	LEU
1	E	223	LYS
1	E	227	LYS
1	E	283	LYS
1	F	15	GLU
1	F	55	ASP
1	F	131	LYS
1	F	177	LEU
1	F	236	SER
1	F	273	SER
1	F	289	SER
1	F	331	PHE
1	G	72	ARG
1	G	104	SER
1	G	228	GLU
1	G	283	LYS
1	G	318	SER
1	G	331	PHE
1	H	13	LYS
1	H	108	LEU
1	H	165	ASP
1	H	330	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	326	GLN

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Mol	Chain	Res	Type
1	B	99	GLN
1	C	99	GLN
1	E	19	GLN
1	E	192	HIS
1	F	16	GLN
1	H	297	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	MLI	A	402	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	H	402	-	0,6,6	0.00	-	0,7,7	0.00	-
2	NAI	F	401	-	42,48,48	4.94	25 (59%)	47,73,73	3.31	10 (21%)
3	MLI	D	402	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	G	402	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	F	402	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	C	402	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	B	402	-	0,6,6	0.00	-	0,7,7	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MLI	E	402	-	0,6,6	0.00	-	0,7,7	0.00	-
2	NAI	G	401	-	42,48,48	4.93	24 (57%)	47,73,73	3.62	10 (21%)
2	NAI	E	401	-	42,48,48	4.99	24 (57%)	47,73,73	3.54	6 (12%)
2	NAI	C	401	-	42,48,48	4.95	22 (52%)	47,73,73	3.25	7 (14%)
2	NAI	A	401	-	42,48,48	4.89	21 (50%)	47,73,73	3.31	7 (14%)
2	NAI	B	401	-	42,48,48	4.85	22 (52%)	47,73,73	3.24	9 (19%)
2	NAI	H	401	-	42,48,48	4.92	21 (50%)	47,73,73	3.30	7 (14%)
2	NAI	D	401	-	42,48,48	4.96	22 (52%)	47,73,73	3.32	9 (19%)

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	MLI	A	402	-	-	0/0/4/4	-
3	MLI	H	402	-	-	0/0/4/4	-
2	NAI	F	401	-	-	5/25/72/72	0/5/5/5
3	MLI	D	402	-	-	0/0/4/4	-
3	MLI	G	402	-	-	0/0/4/4	-
3	MLI	F	402	-	-	0/0/4/4	-
3	MLI	C	402	-	-	0/0/4/4	-
3	MLI	B	402	-	-	0/0/4/4	-
3	MLI	E	402	-	-	0/0/4/4	-
2	NAI	G	401	-	-	5/25/72/72	0/5/5/5
2	NAI	E	401	-	-	9/25/72/72	0/5/5/5
2	NAI	C	401	-	-	9/25/72/72	0/5/5/5
2	NAI	A	401	-	-	6/25/72/72	0/5/5/5
2	NAI	B	401	-	-	5/25/72/72	0/5/5/5
2	NAI	H	401	-	-	5/25/72/72	0/5/5/5
2	NAI	D	401	-	-	5/25/72/72	0/5/5/5

All (181) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	NAI	C2B-C1B	-17.78	1.26	1.53
2	E	401	NAI	C2B-C1B	-17.65	1.27	1.53
2	A	401	NAI	C2B-C1B	-17.47	1.27	1.53
2	D	401	NAI	C2B-C1B	-17.38	1.27	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	NAI	C2B-C1B	-17.36	1.27	1.53
2	C	401	NAI	C2B-C1B	-17.15	1.27	1.53
2	F	401	NAI	C2B-C1B	-16.75	1.28	1.53
2	B	401	NAI	C2B-C1B	-16.63	1.28	1.53
2	C	401	NAI	C6N-C5N	11.74	1.54	1.33
2	E	401	NAI	C6N-C5N	11.63	1.54	1.33
2	H	401	NAI	C6N-C5N	11.43	1.53	1.33
2	D	401	NAI	C6N-C5N	11.08	1.53	1.33
2	G	401	NAI	C6N-C5N	11.08	1.53	1.33
2	F	401	NAI	C6N-C5N	10.98	1.52	1.33
2	B	401	NAI	C6N-C5N	10.88	1.52	1.33
2	A	401	NAI	C6N-C5N	10.84	1.52	1.33
2	B	401	NAI	C3B-C4B	-10.37	1.26	1.53
2	F	401	NAI	O4B-C1B	10.29	1.55	1.41
2	D	401	NAI	O4B-C1B	10.29	1.55	1.41
2	G	401	NAI	O4B-C1B	10.20	1.55	1.41
2	F	401	NAI	C3B-C4B	-10.20	1.26	1.53
2	C	401	NAI	C3B-C4B	-10.15	1.27	1.53
2	D	401	NAI	C3B-C4B	-10.09	1.27	1.53
2	A	401	NAI	C3B-C4B	-10.01	1.27	1.53
2	E	401	NAI	C3B-C4B	-9.93	1.27	1.53
2	G	401	NAI	C3B-C4B	-9.92	1.27	1.53
2	H	401	NAI	C3B-C4B	-9.88	1.27	1.53
2	B	401	NAI	O4B-C1B	9.49	1.54	1.41
2	C	401	NAI	O4B-C1B	9.49	1.54	1.41
2	E	401	NAI	O4B-C1B	9.43	1.54	1.41
2	H	401	NAI	O4B-C1B	9.32	1.54	1.41
2	A	401	NAI	O4B-C1B	9.21	1.53	1.41
2	F	401	NAI	C2D-C1D	-7.61	1.29	1.53
2	A	401	NAI	C2D-C1D	-7.48	1.29	1.53
2	H	401	NAI	C2D-C1D	-7.42	1.29	1.53
2	B	401	NAI	C2D-C1D	-7.40	1.29	1.53
2	D	401	NAI	C2D-C1D	-7.33	1.30	1.53
2	C	401	NAI	O4D-C1D	7.28	1.59	1.42
2	G	401	NAI	C2D-C1D	-7.27	1.30	1.53
2	E	401	NAI	C2D-C1D	-7.24	1.30	1.53
2	C	401	NAI	C2D-C1D	-7.22	1.30	1.53
2	B	401	NAI	O4D-C1D	7.14	1.58	1.42
2	F	401	NAI	O4D-C1D	7.12	1.58	1.42
2	C	401	NAI	C2N-C3N	7.10	1.54	1.34
2	E	401	NAI	O4D-C1D	7.09	1.58	1.42
2	E	401	NAI	C2N-C3N	7.08	1.54	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	NAI	O4D-C1D	7.08	1.58	1.42
2	D	401	NAI	O4D-C1D	7.04	1.58	1.42
2	G	401	NAI	O4D-C1D	7.01	1.58	1.42
2	A	401	NAI	O4D-C1D	6.95	1.58	1.42
2	F	401	NAI	C2N-C3N	6.94	1.54	1.34
2	G	401	NAI	C2N-C3N	6.86	1.54	1.34
2	B	401	NAI	C2N-C3N	6.83	1.54	1.34
2	D	401	NAI	C2N-C3N	6.76	1.53	1.34
2	H	401	NAI	C2N-C3N	6.67	1.53	1.34
2	A	401	NAI	C2N-C3N	6.64	1.53	1.34
2	E	401	NAI	O4D-C4D	-6.22	1.31	1.45
2	A	401	NAI	O4D-C4D	-6.09	1.31	1.45
2	D	401	NAI	C7N-N7N	6.07	1.49	1.33
2	C	401	NAI	C7N-N7N	6.05	1.49	1.33
2	F	401	NAI	O4D-C4D	-6.01	1.31	1.45
2	G	401	NAI	C7N-N7N	5.78	1.48	1.33
2	H	401	NAI	C7N-N7N	5.75	1.48	1.33
2	F	401	NAI	O4B-C4B	5.72	1.57	1.45
2	C	401	NAI	O4D-C4D	-5.70	1.32	1.45
2	F	401	NAI	C7N-N7N	5.58	1.48	1.33
2	E	401	NAI	C7N-N7N	5.56	1.48	1.33
2	A	401	NAI	C7N-N7N	5.55	1.48	1.33
2	H	401	NAI	O4D-C4D	-5.55	1.32	1.45
2	D	401	NAI	O4B-C4B	5.54	1.57	1.45
2	B	401	NAI	C7N-N7N	5.53	1.48	1.33
2	E	401	NAI	C2B-C3B	5.52	1.68	1.53
2	G	401	NAI	C2B-C3B	5.51	1.68	1.53
2	F	401	NAI	C2B-C3B	5.44	1.68	1.53
2	G	401	NAI	O4D-C4D	-5.41	1.32	1.45
2	A	401	NAI	O4B-C4B	5.40	1.57	1.45
2	B	401	NAI	O4B-C4B	5.37	1.57	1.45
2	D	401	NAI	O4D-C4D	-5.33	1.33	1.45
2	E	401	NAI	O4B-C4B	5.33	1.56	1.45
2	B	401	NAI	C2B-C3B	5.23	1.67	1.53
2	A	401	NAI	C2B-C3B	5.22	1.67	1.53
2	C	401	NAI	C2B-C3B	5.21	1.67	1.53
2	D	401	NAI	C2B-C3B	5.19	1.67	1.53
2	G	401	NAI	O4B-C4B	5.19	1.56	1.45
2	H	401	NAI	C2B-C3B	5.14	1.67	1.53
2	H	401	NAI	O4B-C4B	5.09	1.56	1.45
2	B	401	NAI	O4D-C4D	-5.03	1.33	1.45
2	C	401	NAI	O4B-C4B	4.92	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	NAI	C6A-N6A	4.85	1.51	1.34
2	E	401	NAI	C6A-N6A	4.70	1.51	1.34
2	G	401	NAI	C6A-N6A	4.63	1.51	1.34
2	H	401	NAI	C6A-N6A	4.61	1.50	1.34
2	C	401	NAI	C6A-N6A	4.57	1.50	1.34
2	D	401	NAI	C6A-N6A	4.53	1.50	1.34
2	A	401	NAI	C6A-N6A	4.52	1.50	1.34
2	B	401	NAI	C6A-N6A	4.40	1.50	1.34
2	D	401	NAI	C2A-N3A	4.30	1.39	1.32
2	F	401	NAI	C2A-N3A	3.96	1.38	1.32
2	C	401	NAI	C2A-N3A	3.92	1.38	1.32
2	A	401	NAI	C2A-N3A	3.84	1.38	1.32
2	H	401	NAI	C2A-N3A	3.83	1.38	1.32
2	E	401	NAI	C2A-N3A	3.79	1.38	1.32
2	B	401	NAI	C2A-N3A	3.76	1.38	1.32
2	B	401	NAI	C6N-N1N	3.72	1.46	1.37
2	C	401	NAI	C6N-N1N	3.72	1.46	1.37
2	G	401	NAI	C2A-N3A	3.57	1.37	1.32
2	F	401	NAI	C6N-N1N	3.56	1.46	1.37
2	D	401	NAI	C6N-N1N	3.55	1.46	1.37
2	H	401	NAI	C6N-N1N	3.55	1.46	1.37
2	G	401	NAI	C6N-N1N	3.47	1.46	1.37
2	E	401	NAI	C6N-N1N	3.46	1.45	1.37
2	A	401	NAI	C6N-N1N	3.41	1.45	1.37
2	B	401	NAI	C7N-C3N	3.33	1.55	1.48
2	D	401	NAI	C7N-C3N	3.31	1.55	1.48
2	C	401	NAI	C7N-C3N	3.19	1.55	1.48
2	C	401	NAI	O2D-C2D	3.17	1.50	1.43
2	E	401	NAI	O2D-C2D	3.16	1.50	1.43
2	G	401	NAI	C7N-C3N	3.15	1.55	1.48
2	C	401	NAI	C4N-C5N	3.09	1.57	1.48
2	H	401	NAI	C4N-C5N	3.06	1.56	1.48
2	E	401	NAI	C7N-C3N	2.96	1.55	1.48
2	F	401	NAI	C4N-C5N	2.94	1.56	1.48
2	E	401	NAI	C4N-C5N	2.92	1.56	1.48
2	B	401	NAI	O2D-C2D	2.89	1.49	1.43
2	D	401	NAI	O2D-C2D	2.88	1.49	1.43
2	F	401	NAI	O2D-C2D	2.84	1.49	1.43
2	D	401	NAI	C4N-C5N	2.83	1.56	1.48
2	H	401	NAI	O2D-C2D	2.82	1.49	1.43
2	G	401	NAI	C4N-C5N	2.82	1.56	1.48
2	A	401	NAI	O7N-C7N	-2.74	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAI	C4N-C5N	2.73	1.56	1.48
2	E	401	NAI	O7N-C7N	-2.72	1.18	1.24
2	C	401	NAI	C5A-C4A	-2.71	1.33	1.40
2	A	401	NAI	O2D-C2D	2.67	1.49	1.43
2	A	401	NAI	C4N-C5N	2.67	1.55	1.48
2	G	401	NAI	O2D-C2D	2.67	1.49	1.43
2	A	401	NAI	C7N-C3N	2.63	1.54	1.48
2	D	401	NAI	C5A-C4A	-2.61	1.34	1.40
2	B	401	NAI	O7N-C7N	-2.59	1.18	1.24
2	A	401	NAI	C5A-C4A	-2.56	1.34	1.40
2	A	401	NAI	PN-O5D	2.56	1.69	1.59
2	H	401	NAI	O7N-C7N	-2.56	1.18	1.24
2	G	401	NAI	O7N-C7N	-2.53	1.18	1.24
2	F	401	NAI	O7N-C7N	-2.52	1.18	1.24
2	F	401	NAI	C5B-C4B	2.51	1.59	1.51
2	B	401	NAI	C5A-C4A	-2.51	1.34	1.40
2	B	401	NAI	PN-O5D	2.50	1.69	1.59
2	F	401	NAI	C7N-C3N	2.46	1.54	1.48
2	G	401	NAI	C4N-C3N	2.42	1.54	1.49
2	H	401	NAI	C5A-C4A	-2.40	1.34	1.40
2	E	401	NAI	C5A-C4A	-2.37	1.34	1.40
2	H	401	NAI	C7N-C3N	2.37	1.53	1.48
2	G	401	NAI	C5B-C4B	2.37	1.59	1.51
2	F	401	NAI	C5A-C4A	-2.37	1.34	1.40
2	E	401	NAI	PN-O5D	2.36	1.68	1.59
2	D	401	NAI	PN-O5D	2.35	1.68	1.59
2	F	401	NAI	O3D-C3D	-2.33	1.37	1.43
2	G	401	NAI	C5A-C4A	-2.33	1.34	1.40
2	G	401	NAI	PN-O5D	2.30	1.68	1.59
2	E	401	NAI	O3D-C3D	-2.27	1.37	1.43
2	D	401	NAI	O3D-C3D	-2.25	1.37	1.43
2	C	401	NAI	O7N-C7N	-2.25	1.19	1.24
2	E	401	NAI	O3B-C3B	2.22	1.48	1.43
2	C	401	NAI	O3D-C3D	-2.19	1.37	1.43
2	F	401	NAI	PN-O5D	2.18	1.68	1.59
2	C	401	NAI	PN-O5D	2.18	1.68	1.59
2	E	401	NAI	C5B-C4B	2.16	1.58	1.51
2	A	401	NAI	O3B-C3B	2.16	1.48	1.43
2	G	401	NAI	O3D-C3D	-2.15	1.37	1.43
2	D	401	NAI	C5B-C4B	2.14	1.58	1.51
2	B	401	NAI	C5B-C4B	2.13	1.58	1.51
2	H	401	NAI	O3D-C3D	-2.10	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAI	C4N-C3N	2.10	1.54	1.49
2	D	401	NAI	O3B-C3B	2.09	1.47	1.43
2	G	401	NAI	O3B-C3B	2.05	1.47	1.43
2	E	401	NAI	C2A-N1A	2.05	1.37	1.33
2	F	401	NAI	O3B-C3B	2.03	1.47	1.43
2	H	401	NAI	C5B-C4B	2.02	1.57	1.51
2	F	401	NAI	C4N-C3N	2.02	1.53	1.49
2	F	401	NAI	PA-O5B	2.01	1.67	1.59
2	C	401	NAI	C5B-C4B	2.01	1.57	1.51

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	NAI	C5A-C6A-N6A	16.67	145.69	120.35
2	E	401	NAI	C5A-C6A-N6A	16.04	144.73	120.35
2	H	401	NAI	C5A-C6A-N6A	15.38	143.73	120.35
2	F	401	NAI	C5A-C6A-N6A	15.19	143.43	120.35
2	D	401	NAI	C5A-C6A-N6A	15.04	143.21	120.35
2	A	401	NAI	C5A-C6A-N6A	14.96	143.09	120.35
2	C	401	NAI	C5A-C6A-N6A	14.78	142.81	120.35
2	B	401	NAI	C5A-C6A-N6A	14.72	142.71	120.35
2	G	401	NAI	N6A-C6A-N1A	-11.75	94.18	118.57
2	D	401	NAI	N6A-C6A-N1A	-11.30	95.12	118.57
2	E	401	NAI	N6A-C6A-N1A	-11.14	95.45	118.57
2	E	401	NAI	C1B-N9A-C4A	-10.76	107.73	126.64
2	F	401	NAI	N6A-C6A-N1A	-10.71	96.34	118.57
2	H	401	NAI	N6A-C6A-N1A	-10.62	96.53	118.57
2	C	401	NAI	N6A-C6A-N1A	-10.53	96.71	118.57
2	A	401	NAI	N6A-C6A-N1A	-10.39	97.00	118.57
2	B	401	NAI	N6A-C6A-N1A	-10.26	97.28	118.57
2	G	401	NAI	C1B-N9A-C4A	-10.13	108.84	126.64
2	C	401	NAI	C1B-N9A-C4A	-9.39	110.15	126.64
2	A	401	NAI	C1B-N9A-C4A	-8.99	110.84	126.64
2	F	401	NAI	C1B-N9A-C4A	-8.95	110.91	126.64
2	B	401	NAI	C1B-N9A-C4A	-8.77	111.23	126.64
2	H	401	NAI	C1B-N9A-C4A	-8.70	111.36	126.64
2	D	401	NAI	C1B-N9A-C4A	-8.03	112.53	126.64
2	A	401	NAI	N3A-C2A-N1A	-6.17	119.03	128.68
2	D	401	NAI	N3A-C2A-N1A	-5.97	119.35	128.68
2	E	401	NAI	N3A-C2A-N1A	-5.96	119.36	128.68
2	H	401	NAI	N3A-C2A-N1A	-5.94	119.40	128.68
2	F	401	NAI	N3A-C2A-N1A	-5.73	119.72	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAI	N3A-C2A-N1A	-5.59	119.94	128.68
2	B	401	NAI	N3A-C2A-N1A	-5.49	120.09	128.68
2	G	401	NAI	N3A-C2A-N1A	-5.46	120.14	128.68
2	G	401	NAI	C3N-C2N-N1N	-3.75	117.74	123.10
2	D	401	NAI	O4B-C1B-C2B	-3.42	101.93	106.93
2	E	401	NAI	PN-O3-PA	-3.41	121.12	132.83
2	A	401	NAI	PN-O3-PA	-3.19	121.86	132.83
2	H	401	NAI	C1D-N1N-C2N	-3.09	115.97	121.11
2	D	401	NAI	PN-O3-PA	-2.99	122.57	132.83
2	B	401	NAI	C3N-C2N-N1N	-2.98	118.84	123.10
2	G	401	NAI	PN-O3-PA	-2.90	122.87	132.83
2	A	401	NAI	C3B-C2B-C1B	2.87	105.31	100.98
2	B	401	NAI	C4D-O4D-C1D	-2.74	103.42	109.47
2	F	401	NAI	O4B-C1B-C2B	-2.74	102.92	106.93
2	G	401	NAI	C2B-C3B-C4B	2.71	107.91	102.64
2	H	401	NAI	PN-O3-PA	-2.65	123.74	132.83
2	B	401	NAI	C3B-C2B-C1B	2.59	104.88	100.98
2	F	401	NAI	PN-O3-PA	-2.58	123.97	132.83
2	F	401	NAI	C2B-C3B-C4B	2.51	107.52	102.64
2	D	401	NAI	C1D-N1N-C2N	-2.47	116.99	121.11
2	B	401	NAI	O4B-C1B-C2B	-2.45	103.35	106.93
2	D	401	NAI	C4D-O4D-C1D	-2.43	104.12	109.47
2	C	401	NAI	O5B-C5B-C4B	-2.38	100.78	108.99
2	G	401	NAI	C3B-C2B-C1B	2.34	104.50	100.98
2	C	401	NAI	C3B-C2B-C1B	2.30	104.44	100.98
2	F	401	NAI	O4D-C1D-C2D	-2.27	101.70	106.64
2	D	401	NAI	O4D-C1D-C2D	-2.25	101.73	106.64
2	F	401	NAI	C3B-C2B-C1B	2.18	104.26	100.98
2	H	401	NAI	O4B-C1B-C2B	-2.13	103.82	106.93
2	B	401	NAI	PN-O3-PA	-2.12	125.54	132.83
2	E	401	NAI	C4D-O4D-C1D	-2.12	104.79	109.47
2	C	401	NAI	C1D-N1N-C2N	-2.10	117.61	121.11
2	G	401	NAI	C1D-N1N-C2N	-2.10	117.62	121.11
2	F	401	NAI	C3N-C2N-N1N	-2.06	120.16	123.10
2	G	401	NAI	C4D-O4D-C1D	-2.03	105.00	109.47
2	A	401	NAI	O4B-C1B-C2B	-2.01	103.99	106.93

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	401	NAI	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	C	401	NAI	PN-O3-PA-O5B
2	A	401	NAI	C2D-C1D-N1N-C2N
2	G	401	NAI	C2D-C1D-N1N-C2N
2	C	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	C2D-C1D-N1N-C2N
2	E	401	NAI	C2D-C1D-N1N-C2N
2	E	401	NAI	C5B-O5B-PA-O3
2	A	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	C2D-C1D-N1N-C2N
2	C	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	O4D-C1D-N1N-C2N
2	H	401	NAI	C2D-C1D-N1N-C2N
2	E	401	NAI	O4D-C1D-N1N-C2N
2	B	401	NAI	O4D-C1D-N1N-C2N
2	D	401	NAI	O4D-C1D-N1N-C2N
2	D	401	NAI	C2D-C1D-N1N-C6N
2	G	401	NAI	O4D-C1D-N1N-C2N
2	H	401	NAI	O4D-C1D-N1N-C2N
2	F	401	NAI	C2D-C1D-N1N-C2N
2	G	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	C2D-C1D-N1N-C6N
2	F	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	O4D-C1D-N1N-C6N
2	E	401	NAI	C2D-C1D-N1N-C6N
2	C	401	NAI	C2D-C1D-N1N-C6N
2	H	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	O4B-C4B-C5B-O5B
2	G	401	NAI	O4D-C1D-N1N-C6N
2	E	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	O4D-C1D-N1N-C6N
2	H	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C6N
2	D	401	NAI	O4D-C1D-N1N-C6N
2	E	401	NAI	C5D-O5D-PN-O3
2	F	401	NAI	O4B-C4B-C5B-O5B
2	C	401	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	O4B-C4B-C5B-O5B
2	H	401	NAI	O4B-C4B-C5B-O5B
2	D	401	NAI	O4B-C4B-C5B-O5B
2	C	401	NAI	PA-O3-PN-O1N
2	C	401	NAI	PA-O3-PN-O2N
2	F	401	NAI	C5B-O5B-PA-O1A

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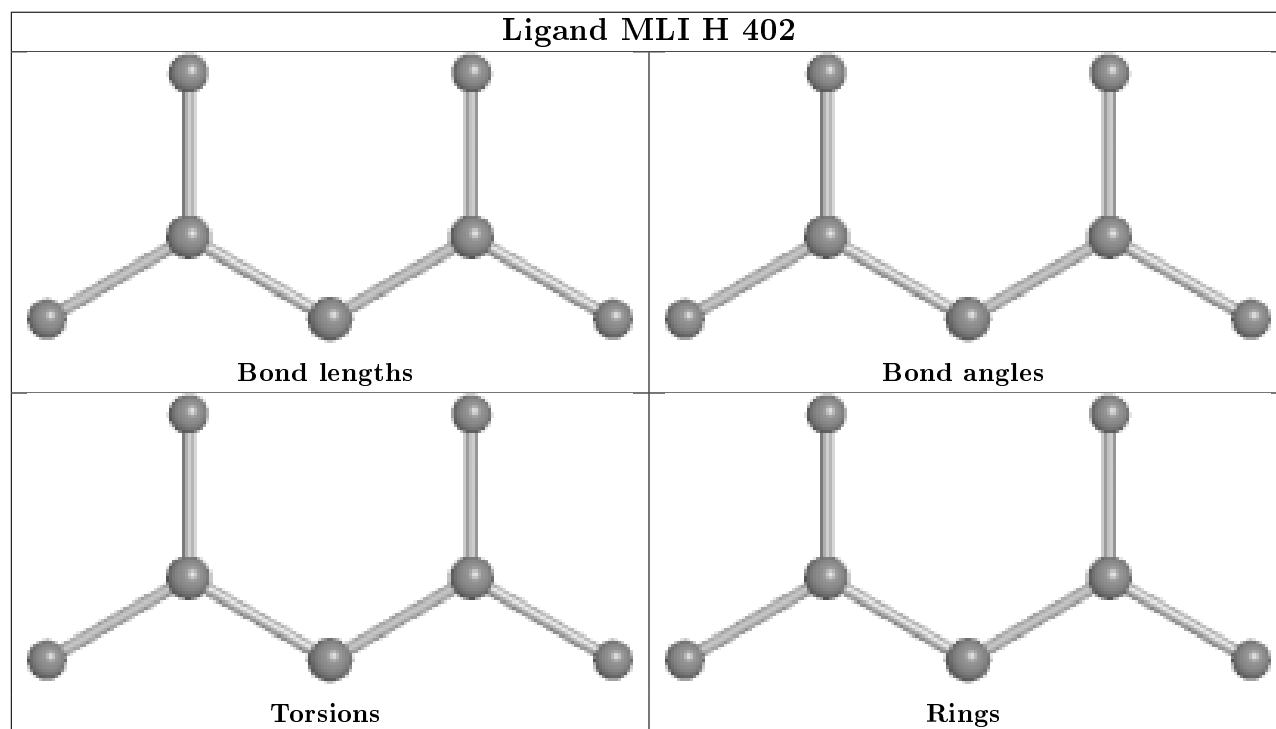
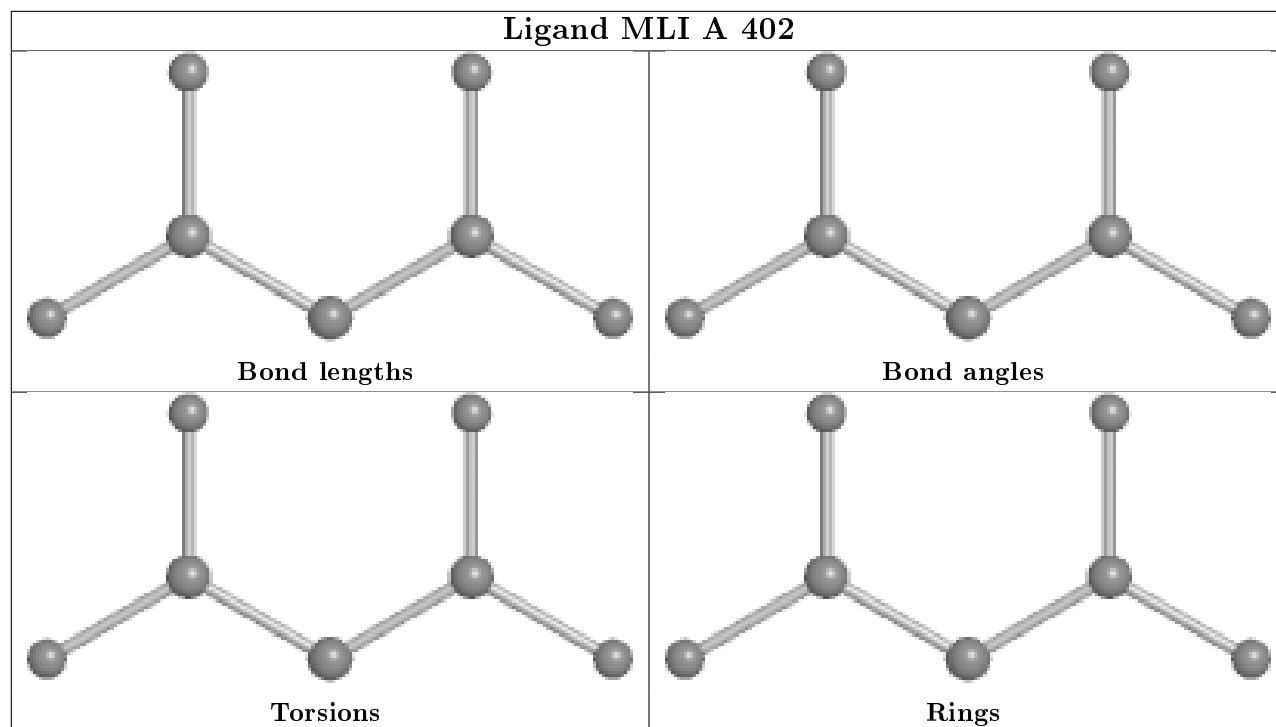
Mol	Chain	Res	Type	Atoms
2	C	401	NAI	C2N-C3N-C7N-N7N
2	A	401	NAI	C5B-O5B-PA-O1A
2	G	401	NAI	O4B-C4B-C5B-O5B
2	E	401	NAI	O4B-C4B-C5B-O5B
2	E	401	NAI	O4D-C4D-C5D-O5D
2	F	401	NAI	C2D-C1D-N1N-C6N

There are no ring outliers.

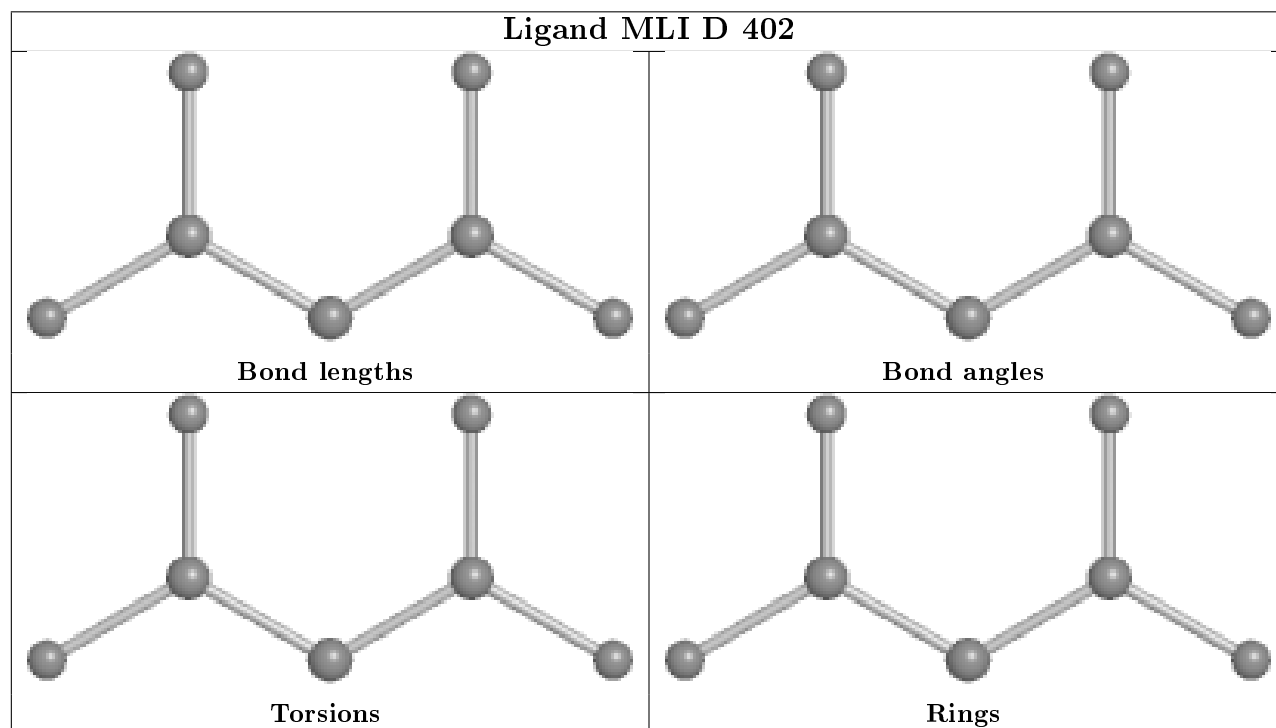
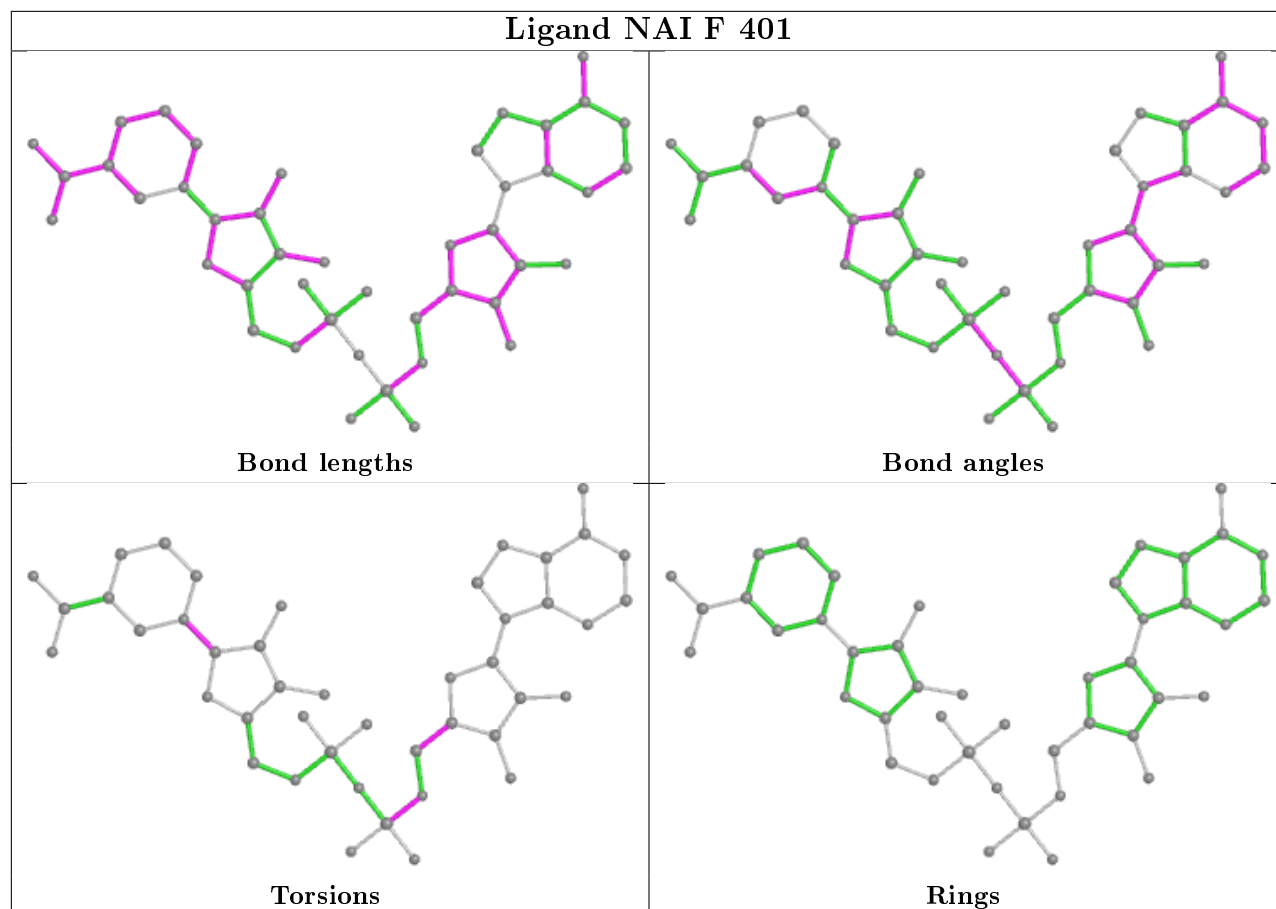
16 monomers are involved in 66 short contacts:

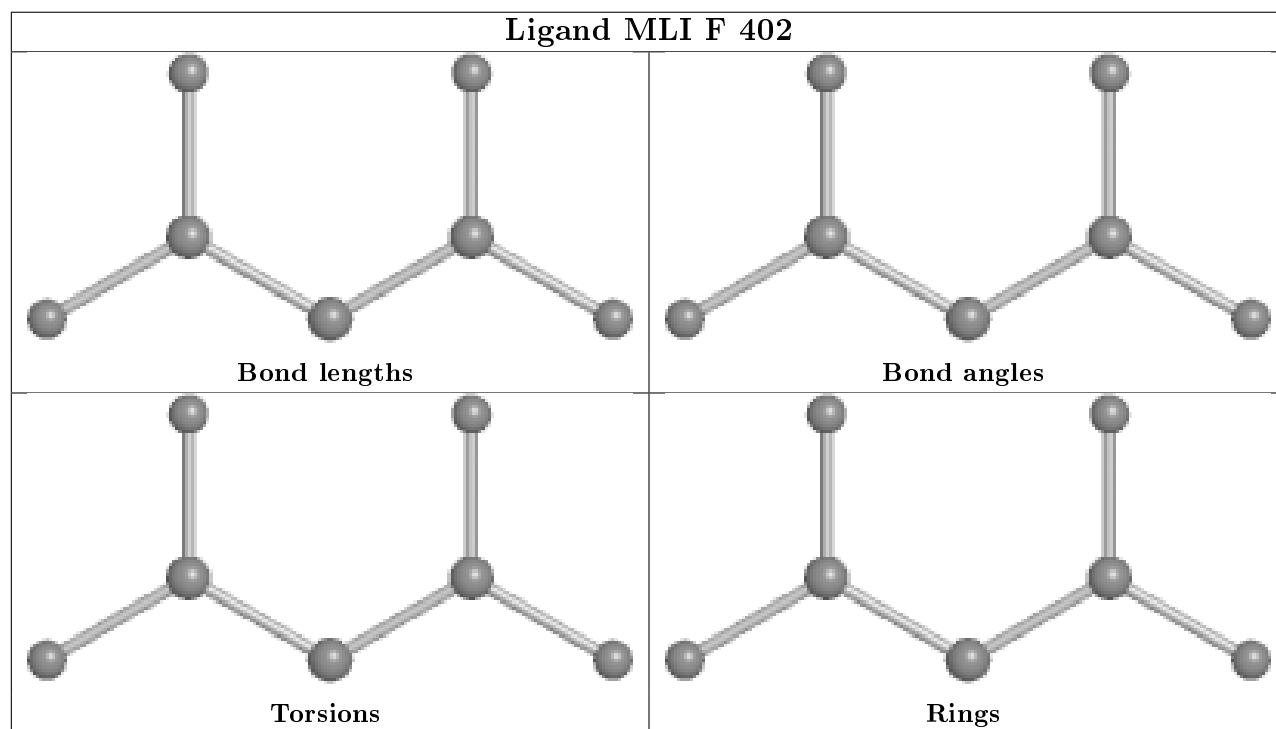
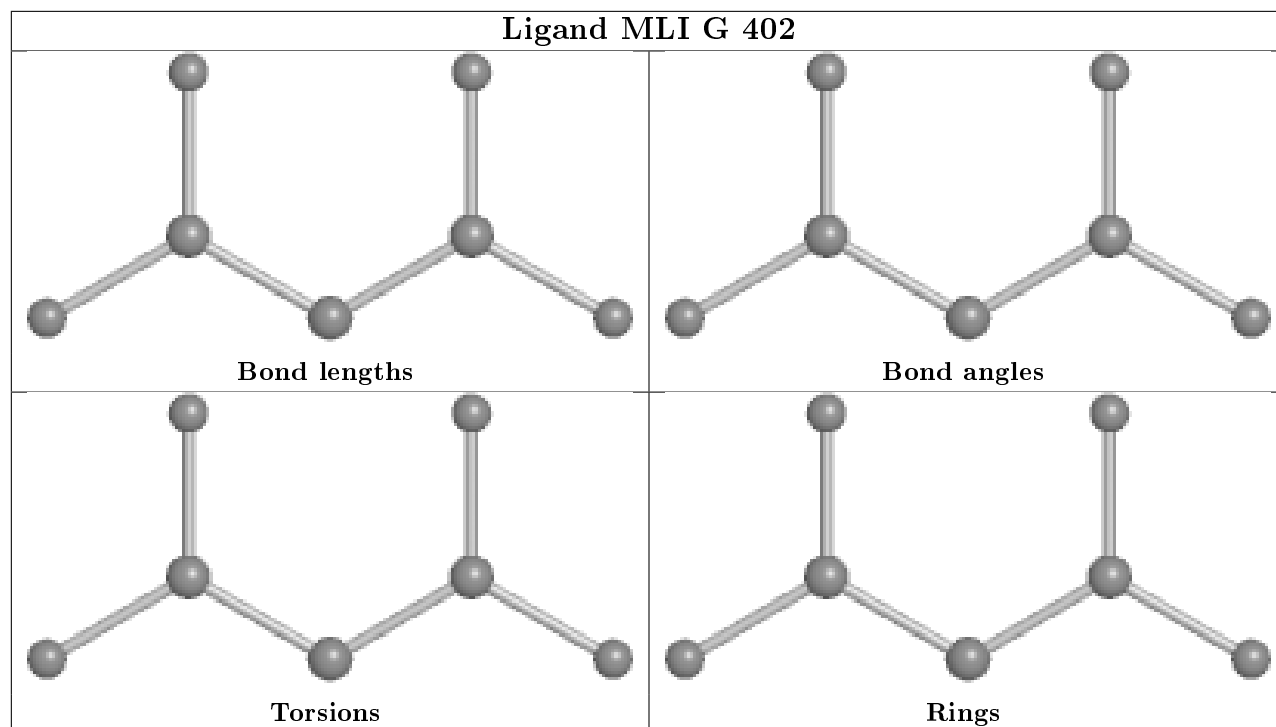
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	MLI	7	0
3	H	402	MLI	1	0
2	F	401	NAI	6	0
3	D	402	MLI	4	0
3	G	402	MLI	6	0
3	F	402	MLI	5	0
3	C	402	MLI	2	0
3	B	402	MLI	5	0
3	E	402	MLI	5	0
2	G	401	NAI	7	0
2	E	401	NAI	4	0
2	C	401	NAI	6	0
2	A	401	NAI	6	0
2	B	401	NAI	9	0
2	H	401	NAI	5	0
2	D	401	NAI	10	0

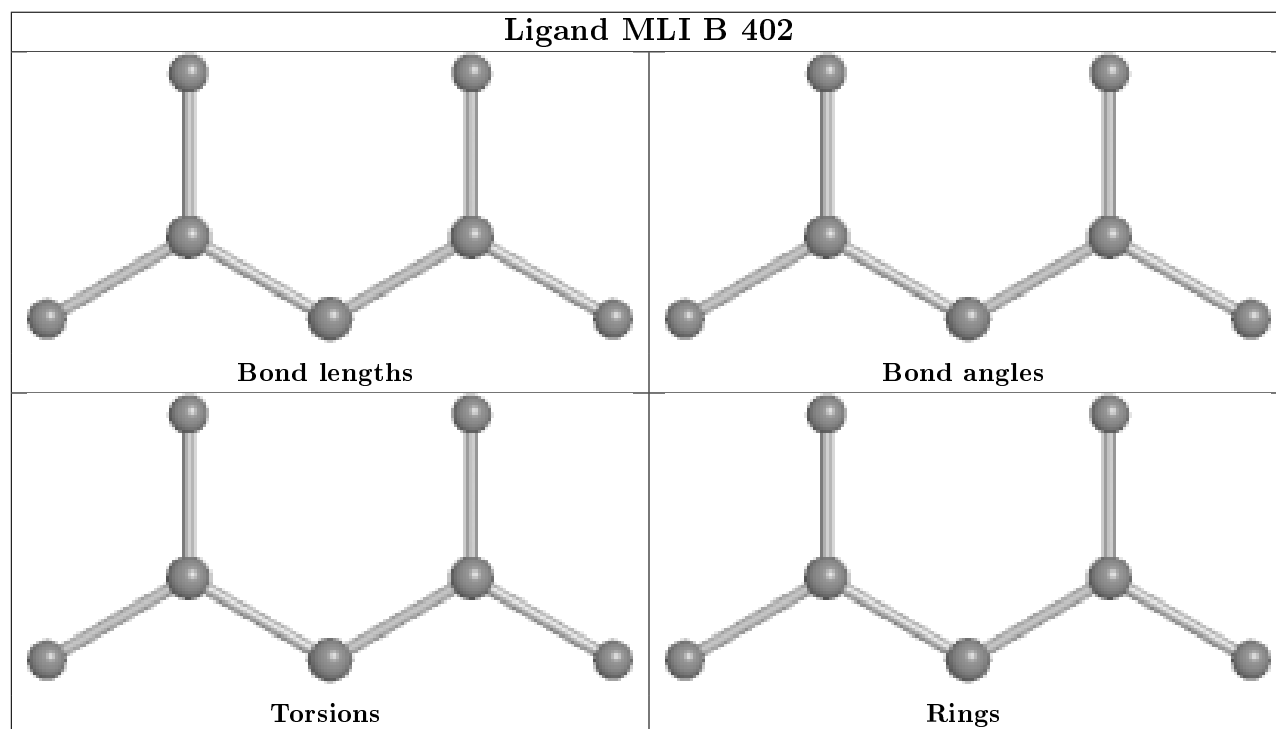
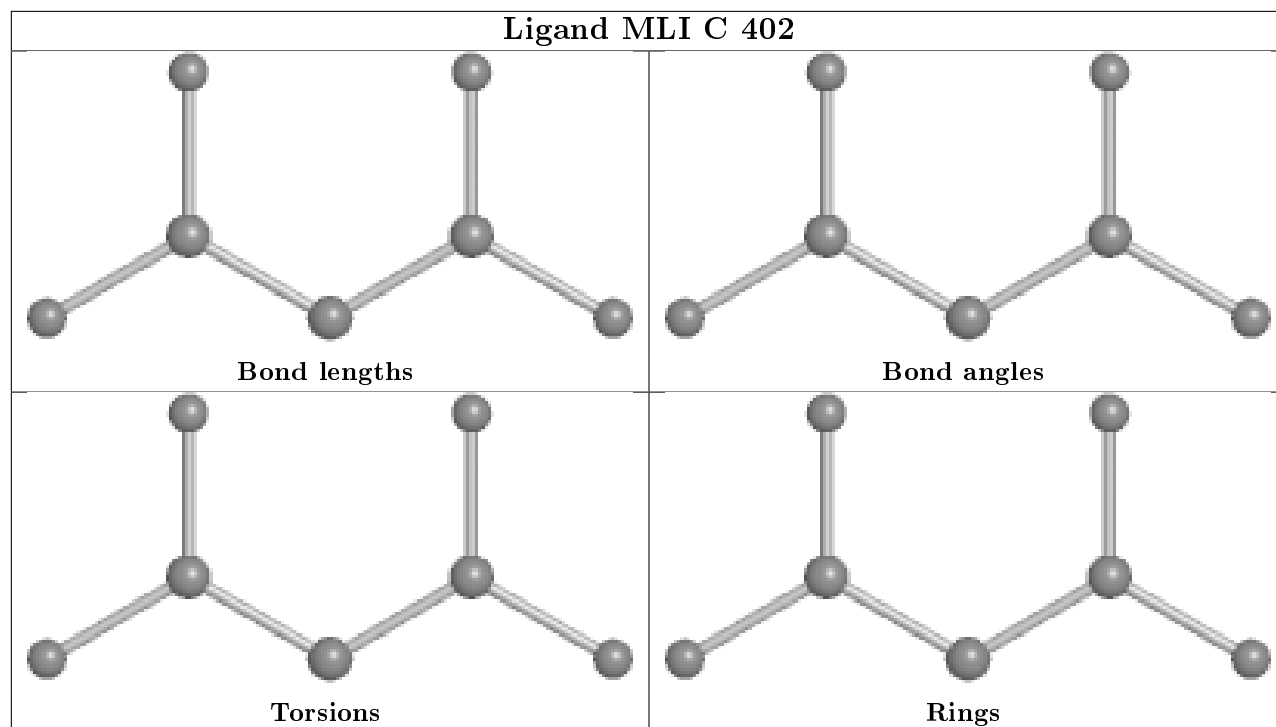
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

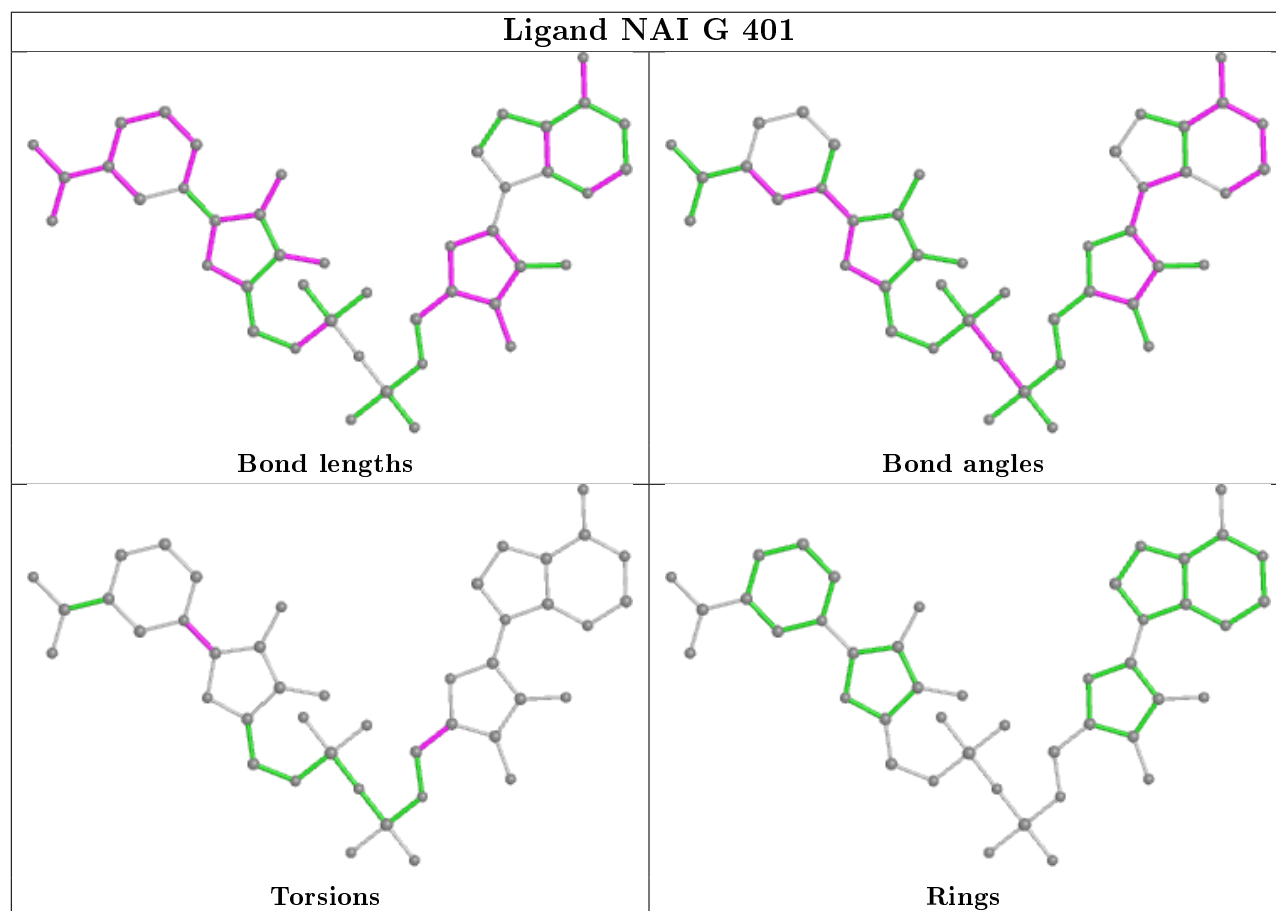
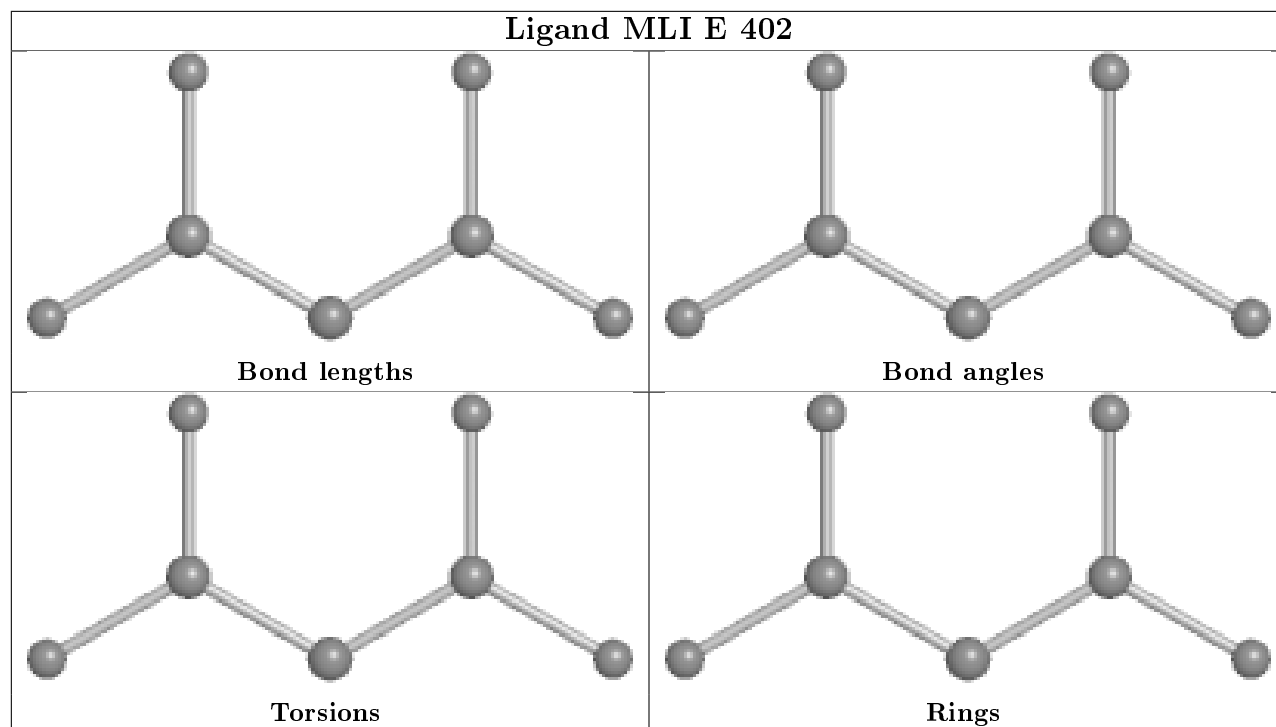




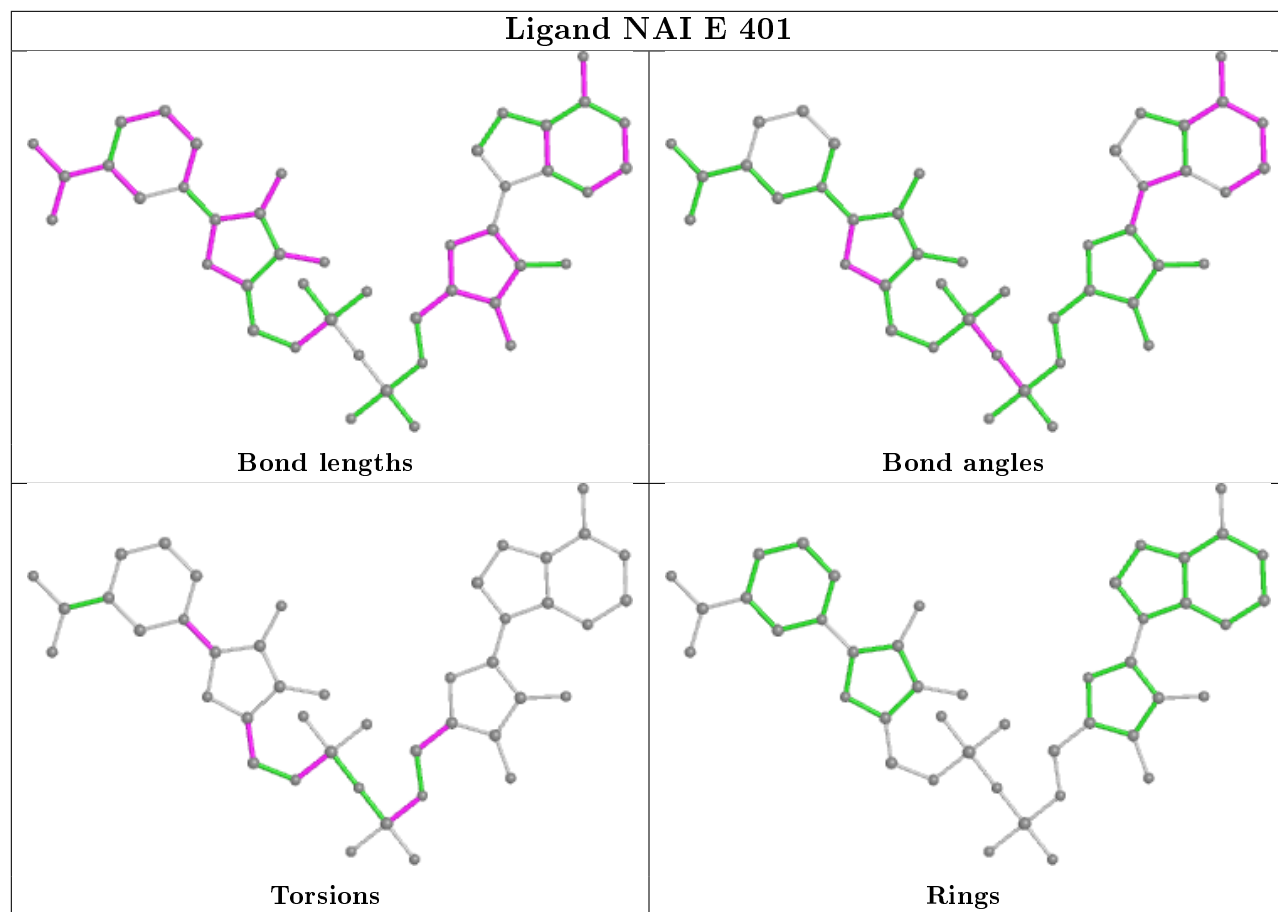


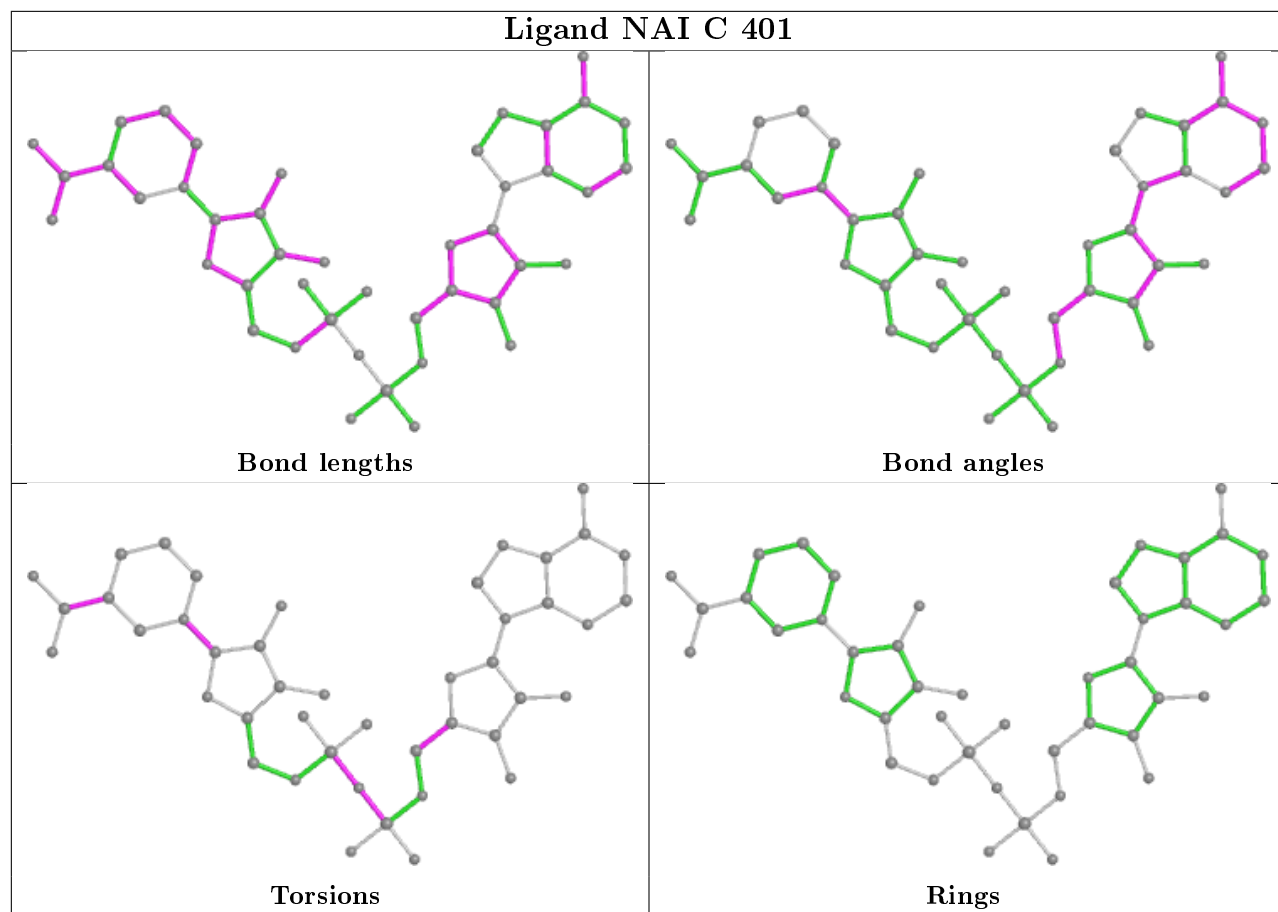


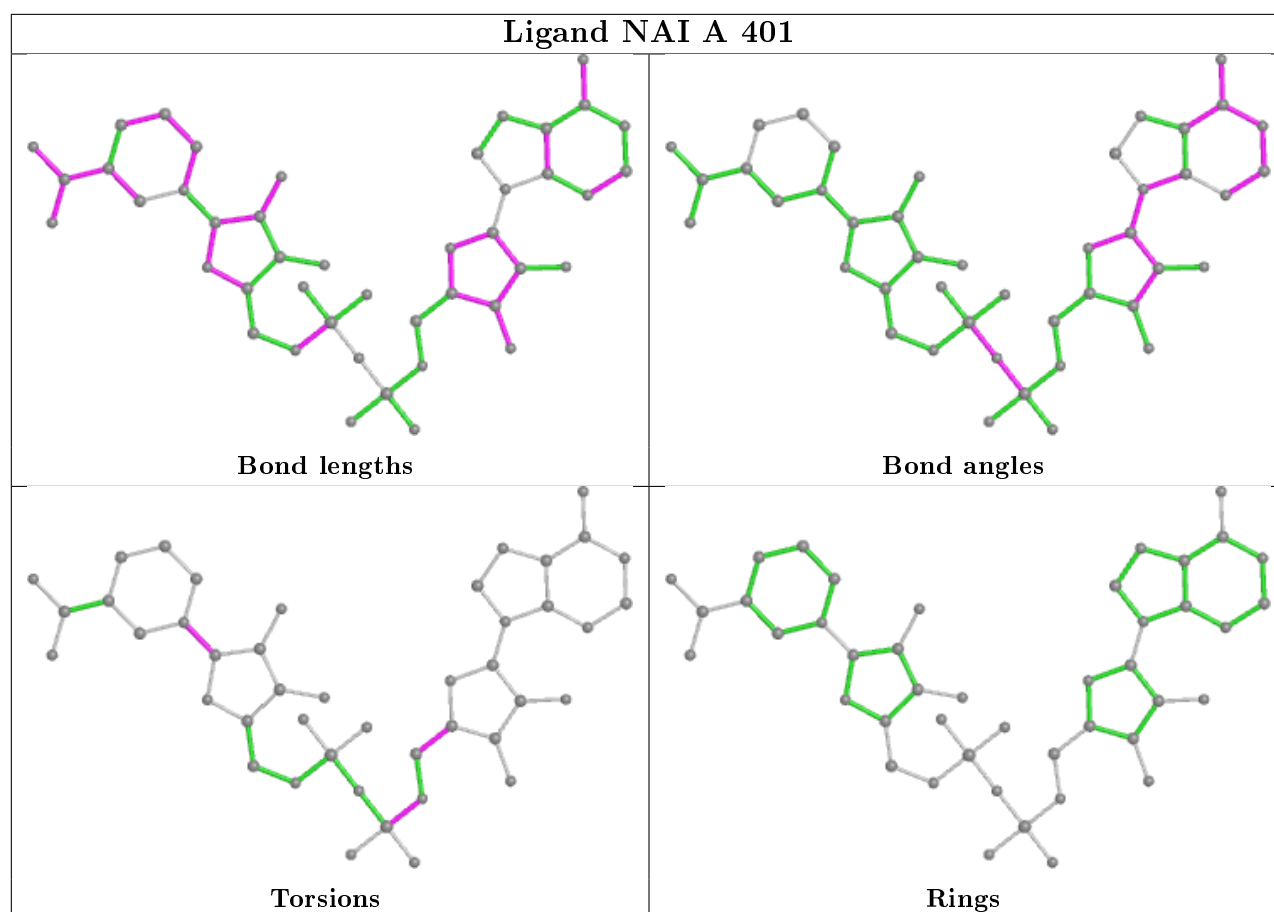


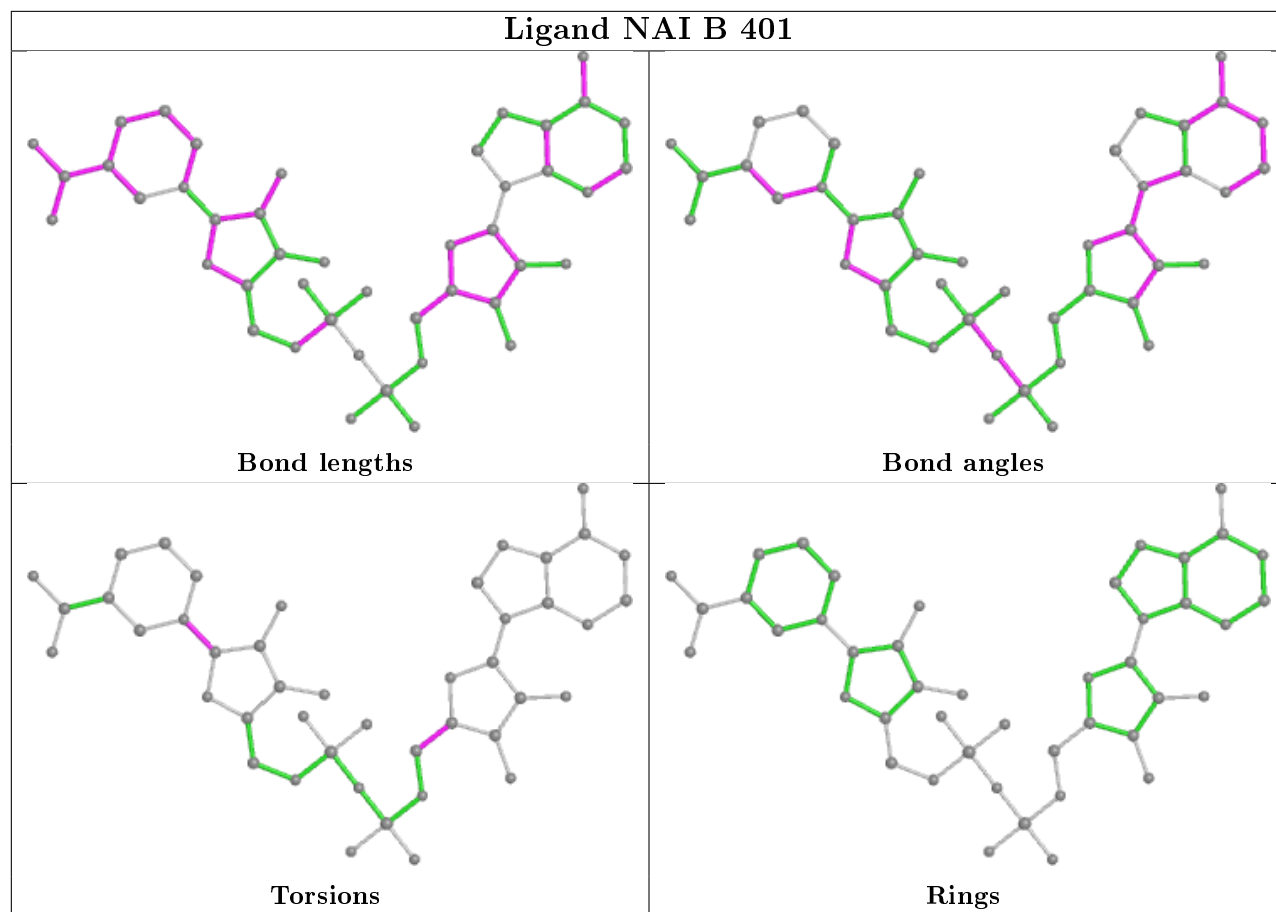


## Ligand NAI E 401

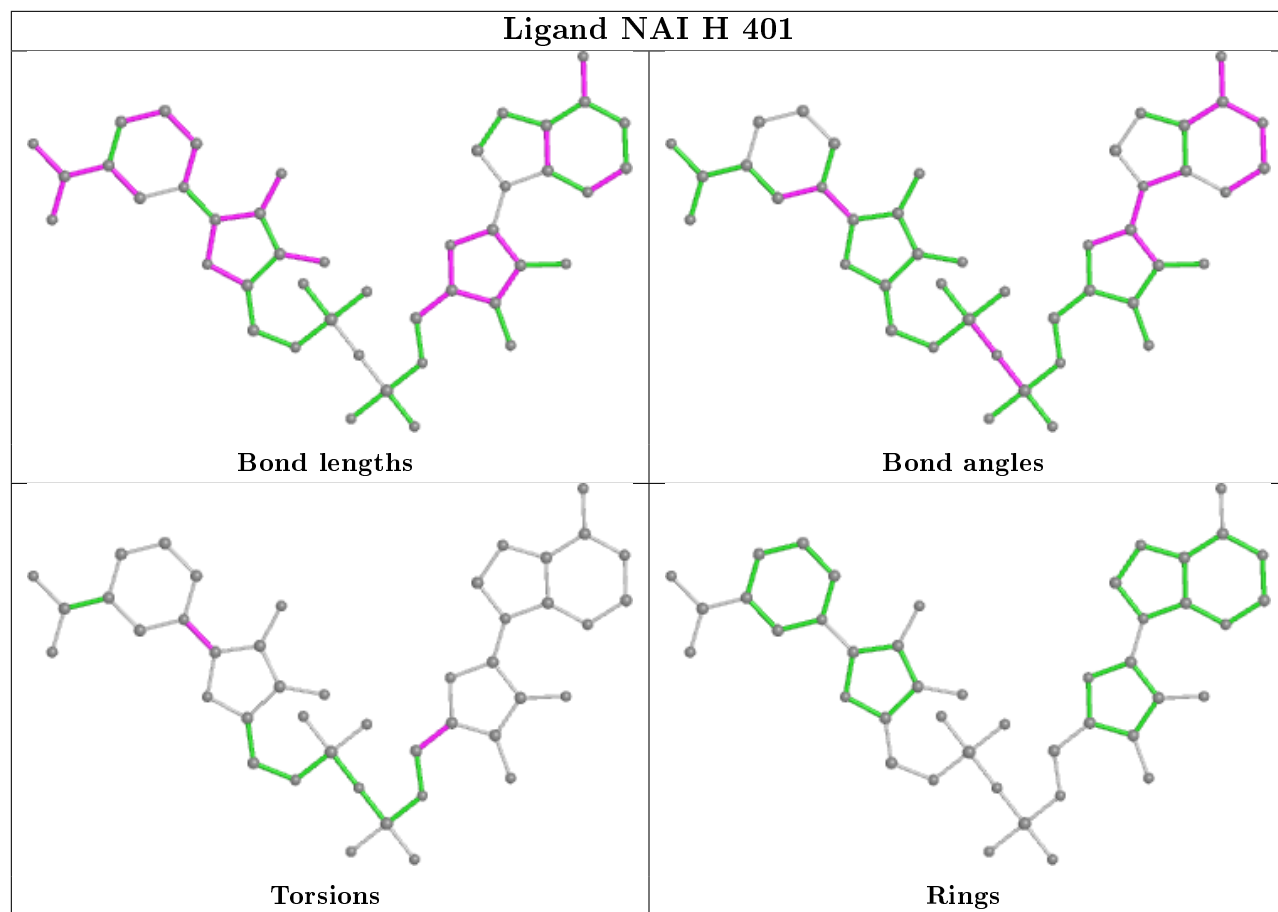


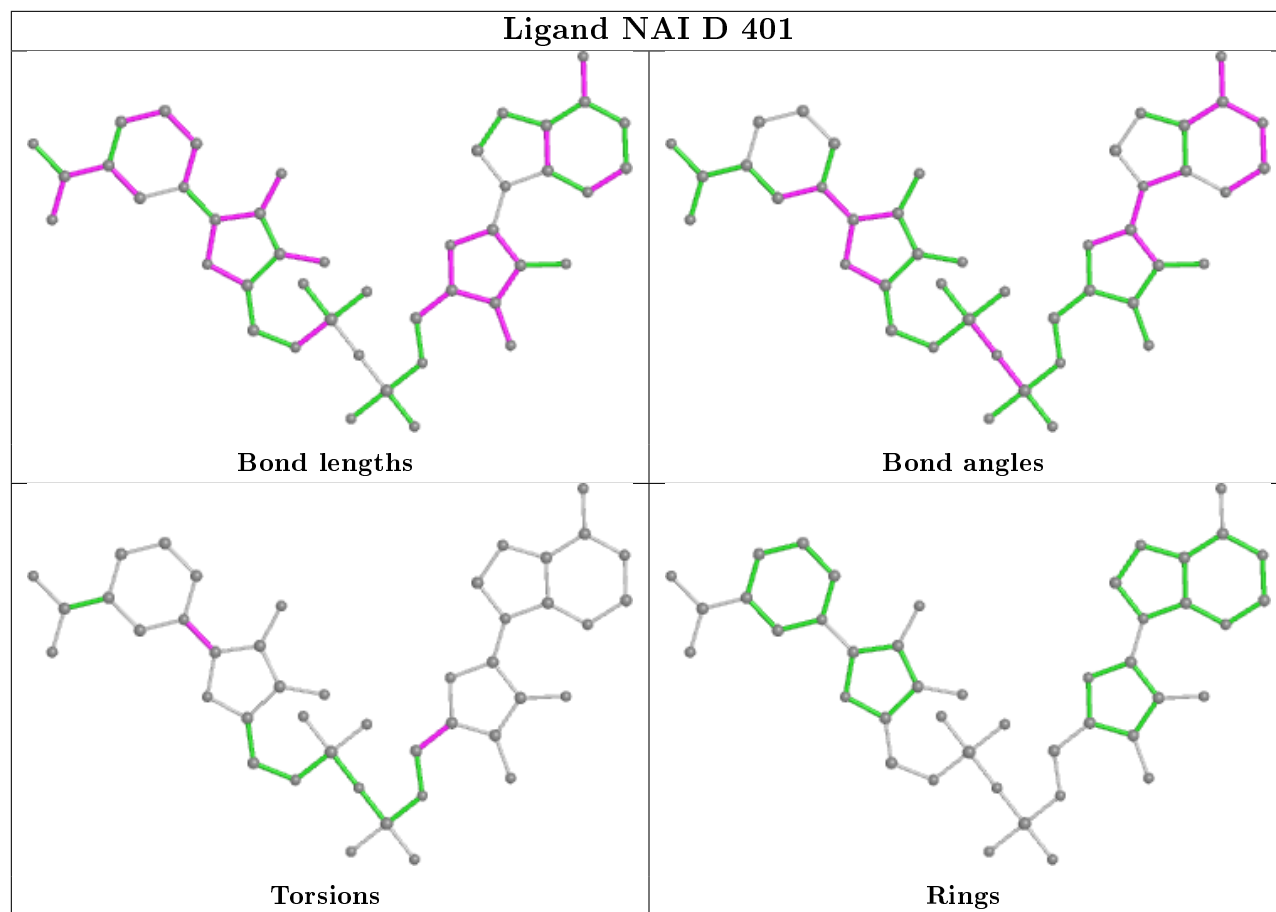












## 5.7 Other polymers [i](#)

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	331/337 (98%)	0.39	20 (6%) 21 20	19, 32, 57, 89	0
1	B	331/337 (98%)	0.37	24 (7%) 15 13	19, 31, 56, 98	1 (0%)
1	C	331/337 (98%)	0.81	41 (12%) 4 3	23, 35, 60, 109	0
1	D	331/337 (98%)	0.55	30 (9%) 9 8	23, 34, 56, 87	1 (0%)
1	E	331/337 (98%)	0.48	30 (9%) 9 8	21, 33, 58, 96	0
1	F	331/337 (98%)	0.67	43 (12%) 3 3	20, 37, 67, 95	1 (0%)
1	G	331/337 (98%)	0.63	32 (9%) 7 7	24, 37, 58, 93	0
1	H	331/337 (98%)	0.73	43 (12%) 3 3	24, 37, 65, 96	1 (0%)
All	All	2648/2696 (98%)	0.58	263 (9%) 7 6	19, 35, 61, 109	4 (0%)

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	102	GLY	13.4
1	B	14	GLU	12.2
1	C	106	LEU	11.1
1	H	102	GLY	10.1
1	G	330	GLN	10.1
1	G	331	PHE	9.1
1	C	104	SER	9.0
1	H	101	GLU	8.9
1	C	99	GLN	8.6
1	G	14	GLU	8.6
1	C	103	GLU	8.1
1	C	101	GLU	7.9
1	H	100	GLN	7.6
1	H	14	GLU	7.5
1	H	99	GLN	7.0
1	H	106	LEU	6.9

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Mol	Chain	Res	Type	RSRZ
1	C	100	GLN	6.8
1	E	14	GLU	6.7
1	F	14	GLU	6.4
1	H	15	GLU	6.4
1	C	105	ARG	6.2
1	E	15	GLU	6.0
1	C	14	GLU	5.9
1	C	98	ARG	5.6
1	D	14	GLU	5.1
1	F	331	PHE	5.1
1	H	103	GLU	5.1
1	B	13	LYS	5.0
1	A	1	ALA	4.9
1	H	219	THR	4.7
1	C	133	LEU	4.7
1	D	134	ILE	4.6
1	B	15	GLU	4.6
1	C	134	ILE	4.5
1	F	281	GLY	4.5
1	H	98	ARG	4.4
1	G	1	ALA	4.4
1	H	330	GLN	4.3
1	H	1	ALA	4.3
1	F	102	GLY	4.2
1	G	17	THR	4.1
1	H	104	SER	4.1
1	G	102	GLY	4.1
1	H	135	VAL	4.1
1	A	15	GLU	4.1
1	C	283	LYS	4.0
1	G	139	VAL	4.0
1	F	221	LYS	4.0
1	F	15	GLU	4.0
1	H	159	GLY	3.9
1	D	331	PHE	3.9
1	D	15	GLU	3.9
1	F	101	GLU	3.9
1	G	13	LYS	3.9
1	C	13	LYS	3.9
1	A	14	GLU	3.9
1	D	13	LYS	3.9
1	A	13	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	13	LYS	3.8
1	E	331	PHE	3.8
1	C	16	GLN	3.8
1	D	93	ILE	3.7
1	C	331	PHE	3.7
1	F	219	THR	3.7
1	D	16	GLN	3.7
1	F	323	TRP	3.6
1	F	16	GLN	3.6
1	C	272	VAL	3.5
1	G	16	GLN	3.5
1	E	102	GLY	3.5
1	H	97	ALA	3.5
1	H	133	LEU	3.5
1	C	278	GLY	3.5
1	C	9	TYR	3.5
1	H	134	ILE	3.4
1	F	106	LEU	3.4
1	G	118	PHE	3.4
1	G	134	ILE	3.4
1	B	12	LEU	3.4
1	C	92	ILE	3.4
1	E	12	LEU	3.3
1	E	281	GLY	3.3
1	D	221	LYS	3.3
1	H	16	GLN	3.3
1	H	223	LYS	3.3
1	E	1	ALA	3.3
1	F	330	GLN	3.2
1	F	327	LYS	3.2
1	C	159	GLY	3.2
1	F	13	LYS	3.2
1	F	160	SER	3.2
1	C	93	ILE	3.2
1	G	135	VAL	3.2
1	C	139	VAL	3.1
1	E	330	GLN	3.1
1	G	133	LEU	3.1
1	B	220	ASP	3.1
1	H	331	PHE	3.1
1	F	283	LYS	3.1
1	F	11	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	139	VAL	3.1
1	G	216	ASP	3.1
1	E	219	THR	3.1
1	A	221	LYS	3.1
1	H	13	LYS	3.1
1	D	135	VAL	3.1
1	F	328	GLU	3.1
1	G	15	GLU	3.1
1	C	160	SER	3.1
1	E	161	GLY	3.1
1	F	104	SER	3.0
1	F	12	LEU	3.0
1	B	221	LYS	3.0
1	F	100	GLN	3.0
1	D	92	ILE	3.0
1	H	161	GLY	3.0
1	F	108	LEU	3.0
1	F	309	SER	3.0
1	F	134	ILE	2.9
1	D	158	ILE	2.9
1	C	135	VAL	2.9
1	F	220	ASP	2.9
1	E	220	ASP	2.9
1	B	160	SER	2.9
1	A	220	ASP	2.9
1	H	238	TYR	2.9
1	G	93	ILE	2.8
1	D	159	GLY	2.8
1	H	17	THR	2.8
1	E	17	THR	2.8
1	G	9	TYR	2.8
1	B	331	PHE	2.8
1	C	277	LYS	2.8
1	H	328	GLU	2.8
1	H	273	SER	2.7
1	A	330	GLN	2.7
1	E	162	CYS	2.7
1	B	118	PHE	2.7
1	C	15	GLU	2.7
1	B	314	ARG	2.7
1	F	236	SER	2.7
1	B	161	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	92	ILE	2.7
1	G	272	VAL	2.7
1	F	161	GLY	2.7
1	G	221	LYS	2.7
1	D	136	SER	2.6
1	H	225	GLN	2.6
1	D	133	LEU	2.6
1	D	223	LYS	2.6
1	A	327	LYS	2.6
1	E	16	GLN	2.6
1	C	142	LEU	2.6
1	D	91	VAL	2.6
1	E	284	ASP	2.6
1	F	9	TYR	2.5
1	F	272	VAL	2.5
1	H	105	ARG	2.5
1	E	278	GLY	2.5
1	G	162	CYS	2.5
1	H	220	ASP	2.5
1	H	92	ILE	2.5
1	B	16	GLN	2.5
1	C	158	ILE	2.5
1	H	158	ILE	2.5
1	F	278	GLY	2.5
1	G	158	ILE	2.5
1	E	55	ASP	2.5
1	A	331	PHE	2.4
1	B	9	TYR	2.4
1	D	72	ARG	2.4
1	H	235	GLU	2.4
1	G	94	THR	2.4
1	G	159	GLY	2.4
1	G	238	TYR	2.4
1	F	282	ILE	2.4
1	C	12	LEU	2.4
1	C	220	ASP	2.4
1	E	272	VAL	2.4
1	F	321	THR	2.4
1	H	2	THR	2.4
1	C	108	LEU	2.4
1	B	273	SER	2.4
1	D	225	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	323	TRP	2.4
1	A	162	CYS	2.4
1	C	162	CYS	2.4
1	D	273	SER	2.4
1	H	94	THR	2.3
1	F	135	VAL	2.3
1	A	225	GLN	2.3
1	B	327	LYS	2.3
1	E	133	LEU	2.3
1	G	142	LEU	2.3
1	D	81	ASP	2.3
1	G	213	LEU	2.3
1	H	93	ILE	2.3
1	D	162	CYS	2.3
1	H	308	THR	2.3
1	A	161	GLY	2.3
1	E	80	LYS	2.3
1	B	313	ALA	2.3
1	D	161	GLY	2.3
1	D	330	GLN	2.3
1	H	327	LYS	2.2
1	C	91	VAL	2.2
1	G	235	GLU	2.2
1	A	2	THR	2.2
1	E	283	LYS	2.2
1	C	323	TRP	2.2
1	E	160	SER	2.2
1	B	134	ILE	2.2
1	D	12	LEU	2.2
1	E	327	LYS	2.2
1	F	324	GLY	2.2
1	B	133	LEU	2.2
1	F	81	ASP	2.2
1	G	242	LYS	2.2
1	A	9	TYR	2.2
1	H	136	SER	2.2
1	F	10	ASN	2.2
1	G	91	VAL	2.2
1	B	3	LEU	2.2
1	F	3	LEU	2.2
1	B	272	VAL	2.1
1	H	139	VAL	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	135	VAL	2.1
1	B	310	GLU	2.1
1	A	3	LEU	2.1
1	F	242	LYS	2.1
1	F	313	ALA	2.1
1	C	136	SER	2.1
1	E	215	PRO	2.1
1	F	103	GLU	2.1
1	F	162	CYS	2.1
1	E	2	THR	2.1
1	C	309	SER	2.1
1	D	271	PRO	2.1
1	C	161	GLY	2.1
1	G	160	SER	2.1
1	F	291	PRO	2.1
1	A	12	LEU	2.1
1	G	225	GLN	2.1
1	B	54	GLU	2.1
1	A	283	LYS	2.1
1	C	143	THR	2.1
1	D	272	VAL	2.1
1	A	118	PHE	2.1
1	A	16	GLN	2.0
1	C	141	ILE	2.0
1	F	133	LEU	2.0
1	A	317	LYS	2.0
1	D	254	SER	2.0
1	E	309	SER	2.0
1	D	121	PRO	2.0
1	E	225	GLN	2.0
1	H	272	VAL	2.0
1	C	238	TYR	2.0
1	E	221	LYS	2.0
1	D	142	LEU	2.0
1	H	108	LEU	2.0
1	H	216	ASP	2.0
1	E	188	VAL	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 ⓘ

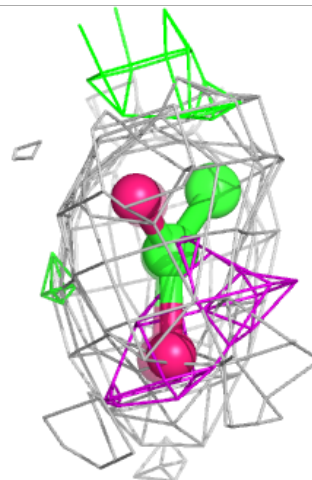
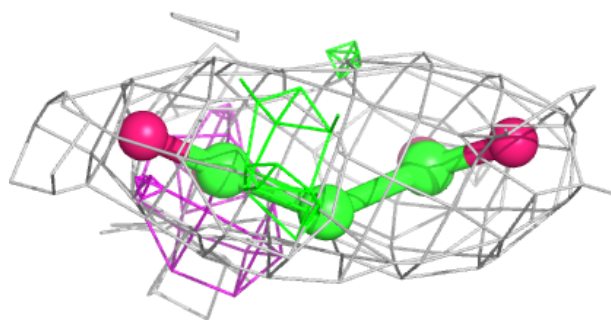
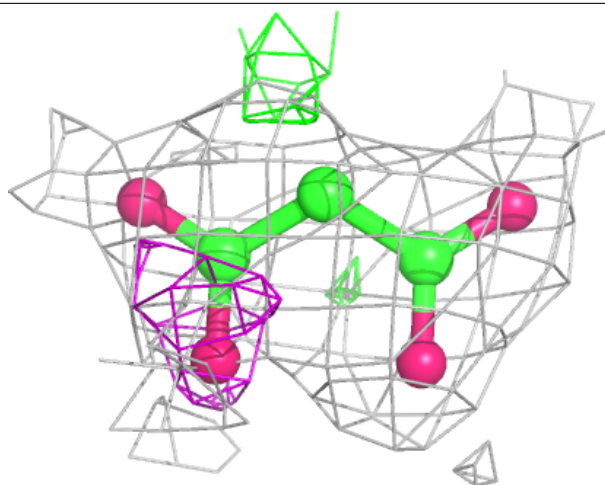
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MLI	A	402	7/7	0.86	0.23	25,28,39,40	0
3	MLI	H	402	7/7	0.88	0.19	35,38,49,61	0
3	MLI	F	402	7/7	0.90	0.20	31,35,45,50	0
3	MLI	E	402	7/7	0.90	0.20	39,40,40,40	0
3	MLI	G	402	7/7	0.91	0.19	39,40,41,42	0
3	MLI	C	402	7/7	0.92	0.15	39,40,44,51	0
3	MLI	D	402	7/7	0.92	0.21	32,33,38,42	0
2	NAI	F	401	44/44	0.94	0.16	26,34,40,41	0
2	NAI	H	401	44/44	0.94	0.15	27,32,41,42	0
2	NAI	C	401	44/44	0.95	0.14	26,33,40,45	0
2	NAI	A	401	44/44	0.95	0.15	22,28,34,36	0
2	NAI	B	401	44/44	0.95	0.14	21,28,35,36	0
2	NAI	E	401	44/44	0.95	0.13	25,30,36,39	0
2	NAI	D	401	44/44	0.95	0.17	26,33,39,47	0
3	MLI	B	402	7/7	0.96	0.13	25,27,34,35	0
2	NAI	G	401	44/44	0.96	0.15	26,34,40,42	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.

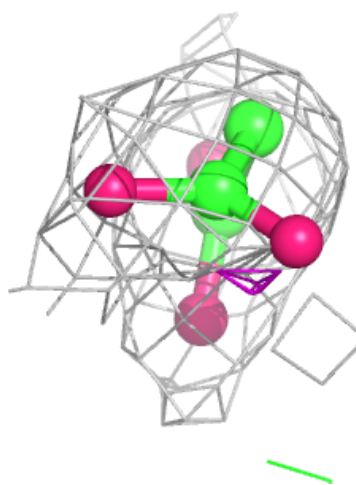
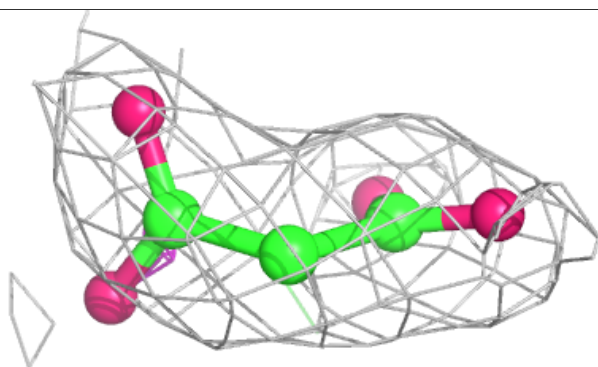
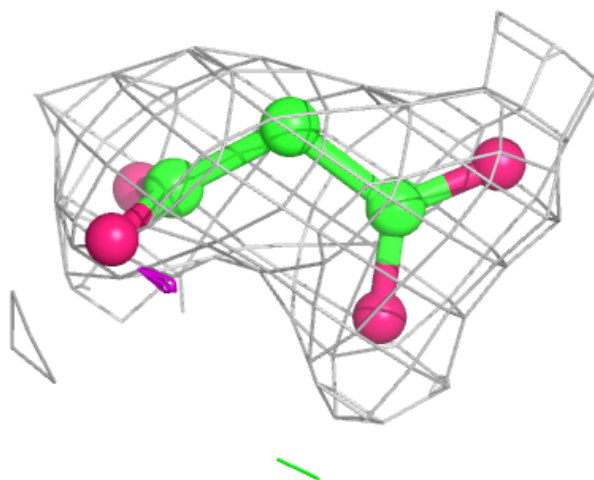
**Electron density around MLI A 402:**

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



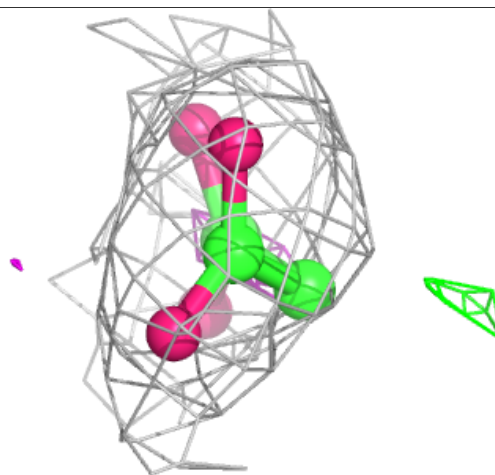
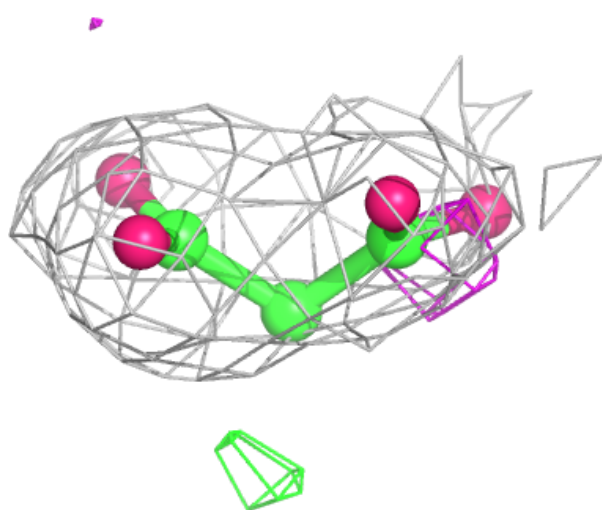
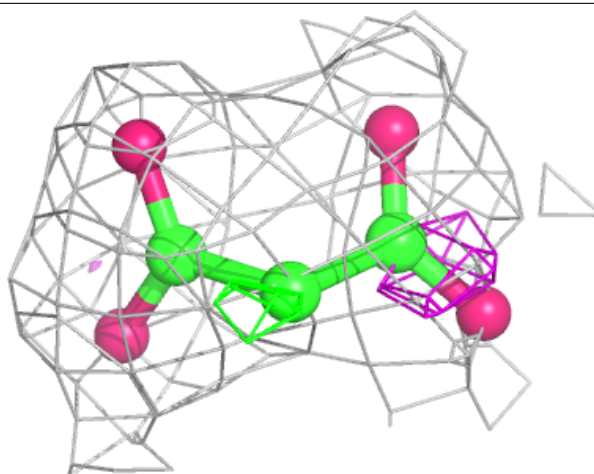
**Electron density around MLI H 402:**

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



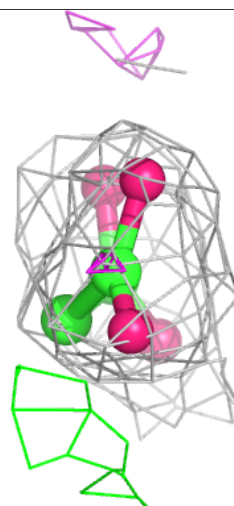
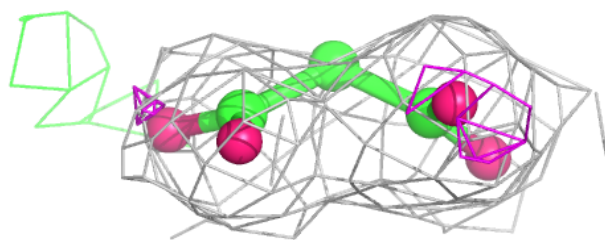
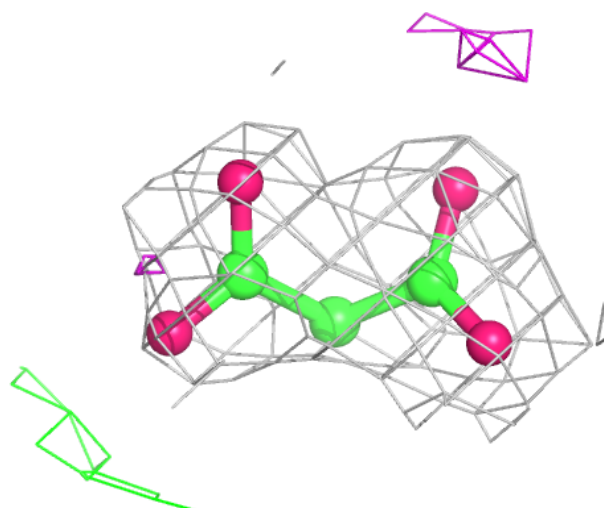
**Electron density around MLI F 402:**

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



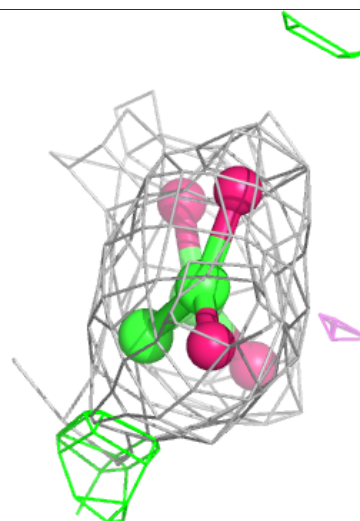
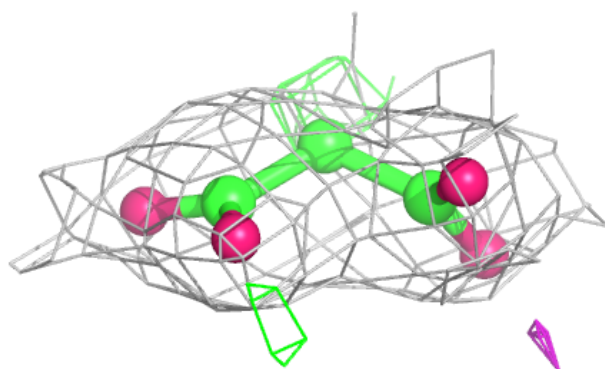
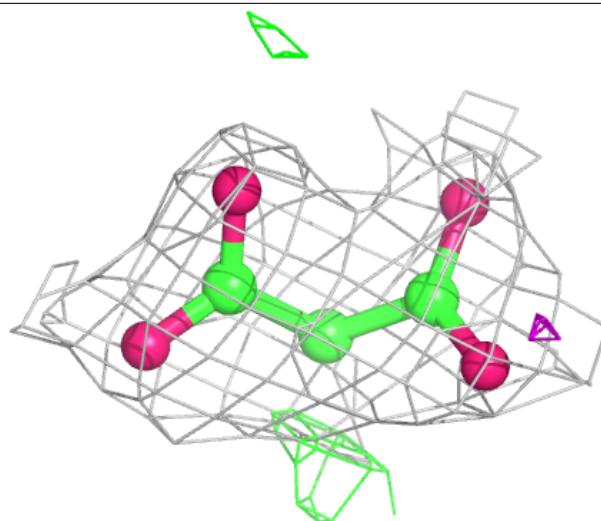
**Electron density around MLI E 402:**

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



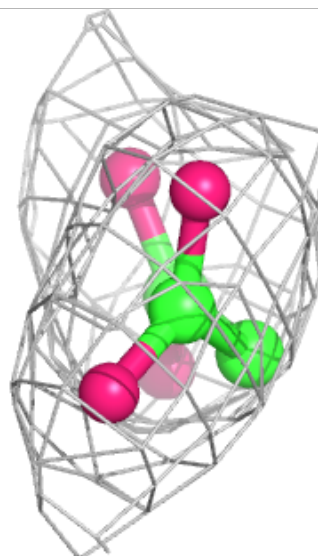
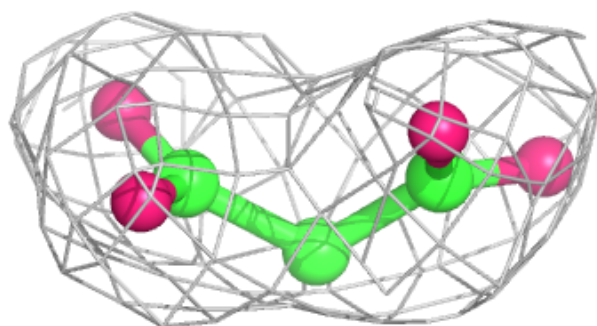
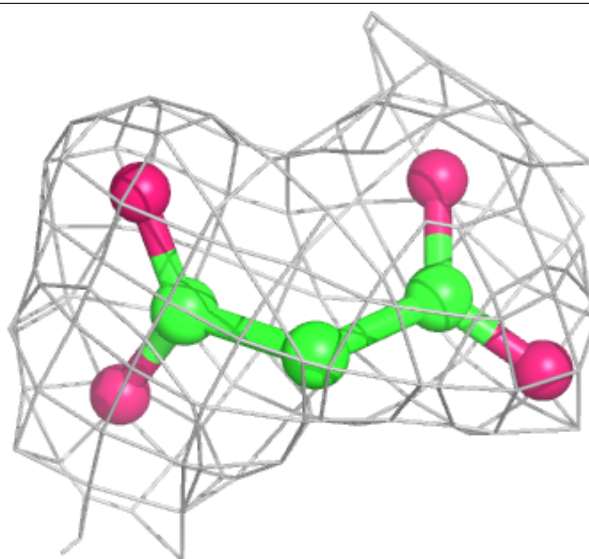
**Electron density around MLI G 402:**

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



**Electron density around MLI C 402:**

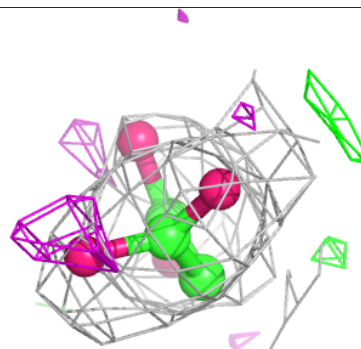
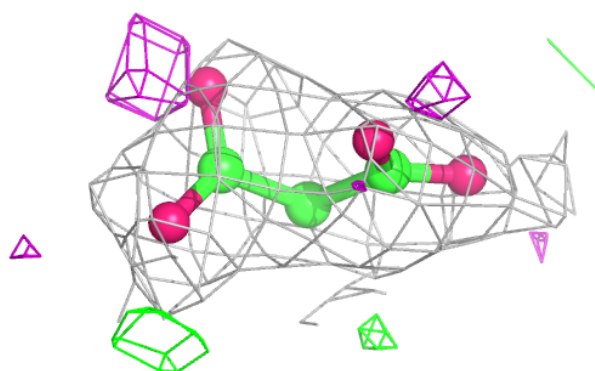
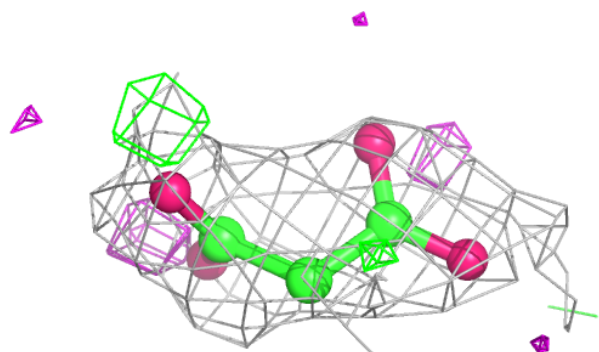
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



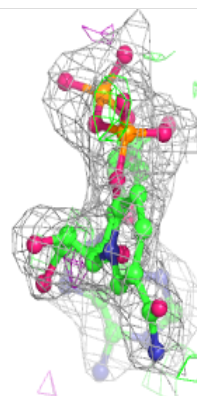
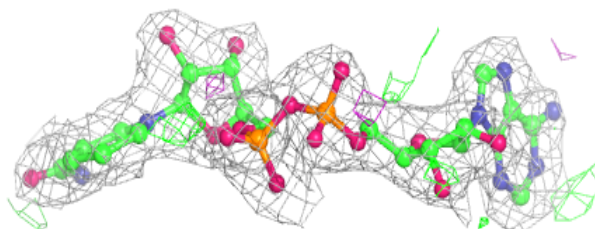
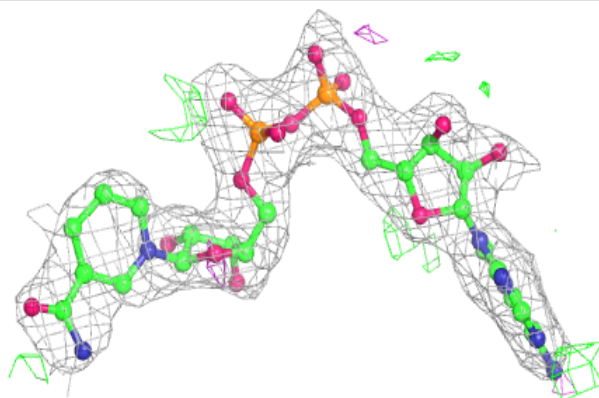


**Electron density around MLI D 402:**

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

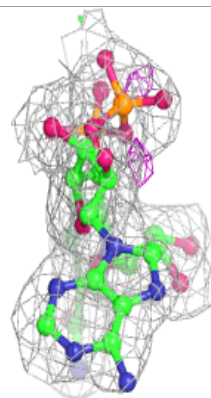
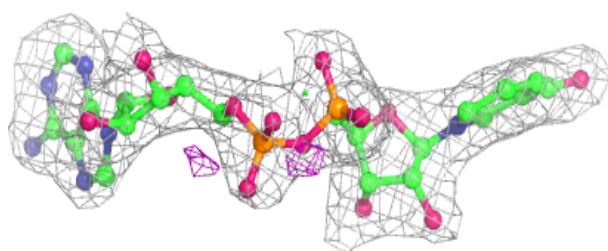
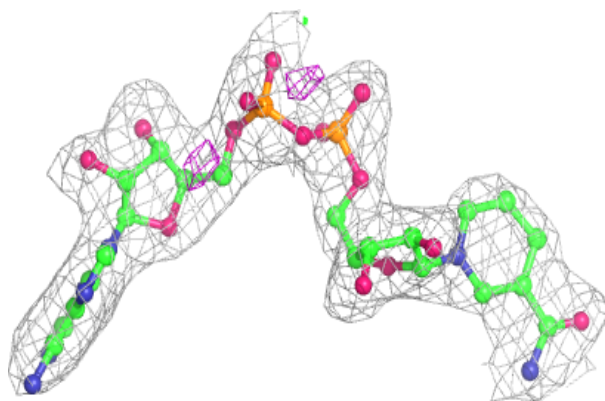
**Electron density around NAI F 401:**

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

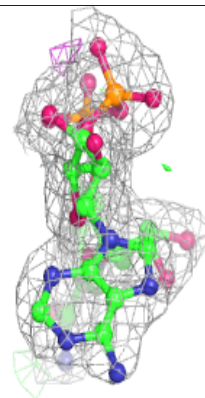
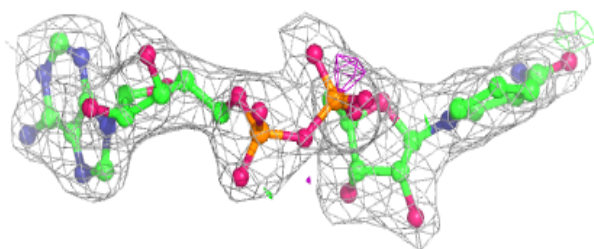
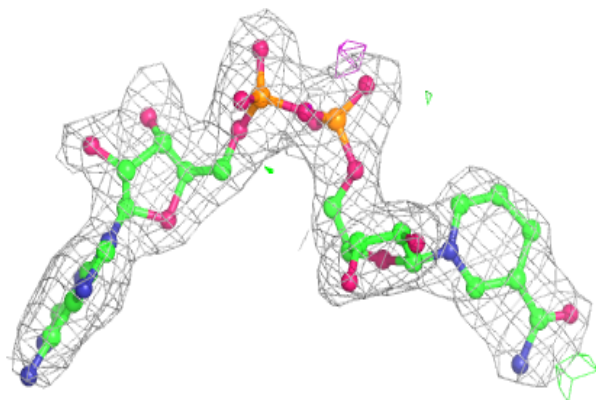


**Electron density around NAI H 401:**

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

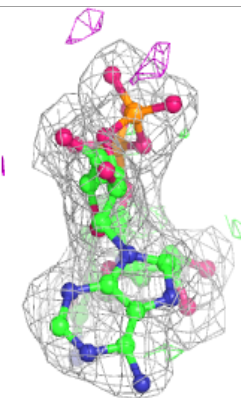
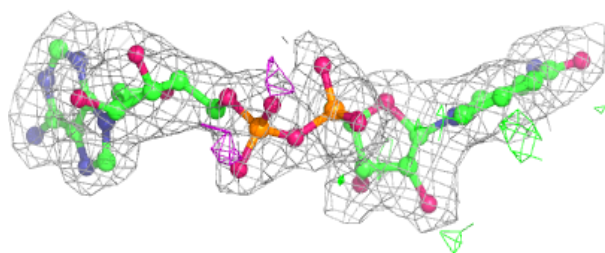
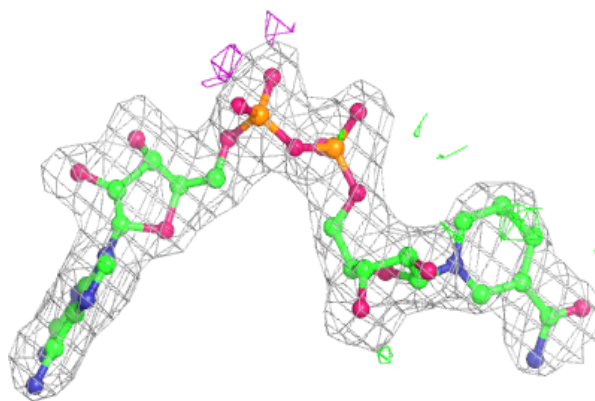
**Electron density around NAI C 401:**

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

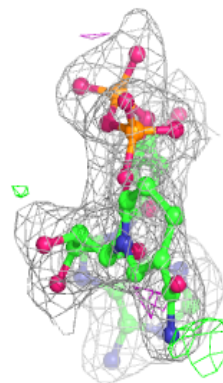
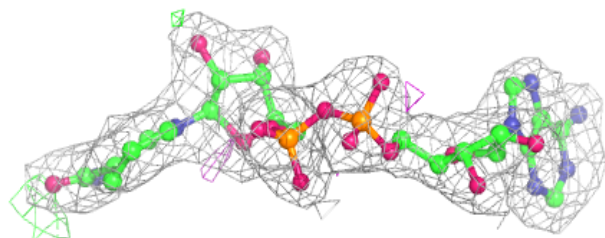
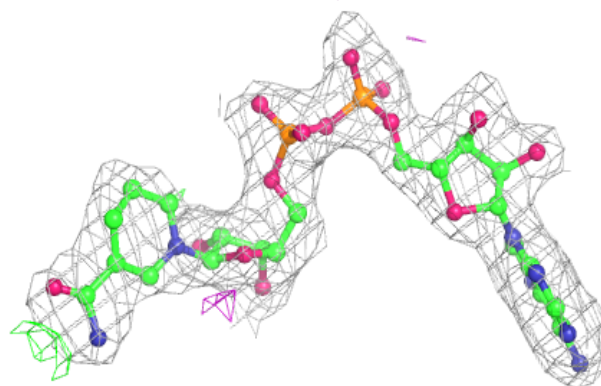


**Electron density around NAI A 401:**

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

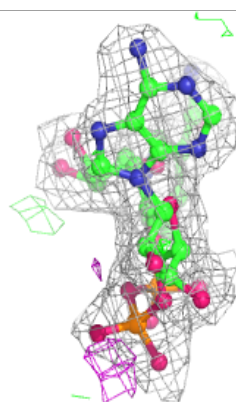
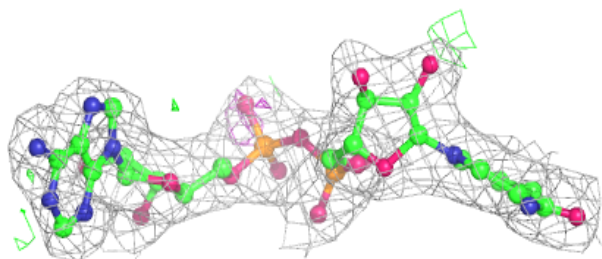
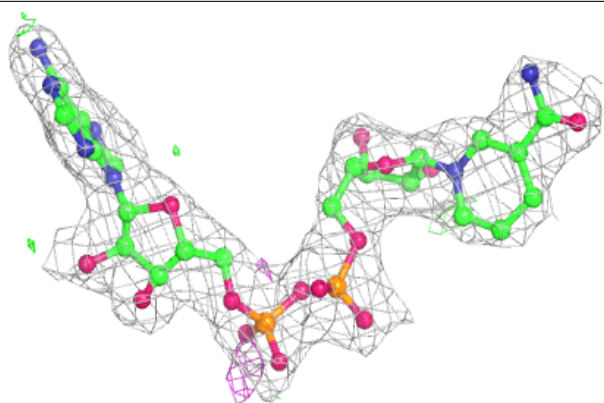
**Electron density around NAI B 401:**

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and green (positive)

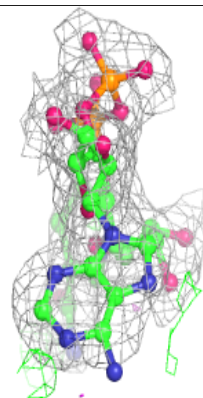
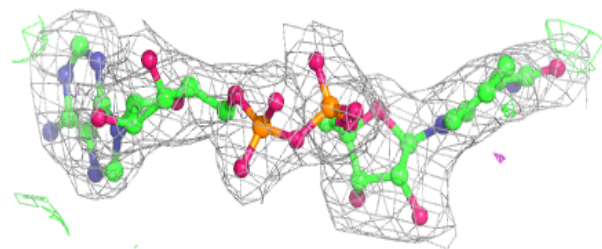
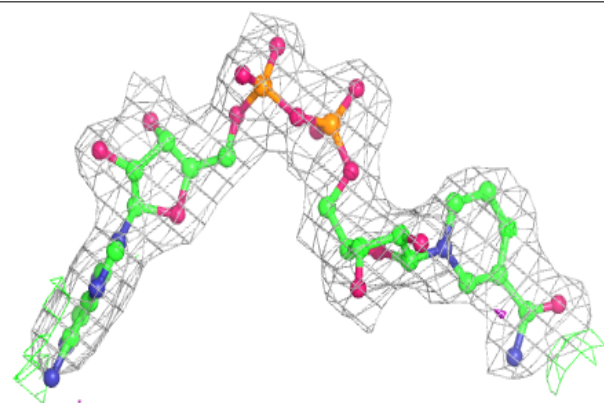


**Electron density around NAI E 401:**

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

**Electron density around NAI D 401:**

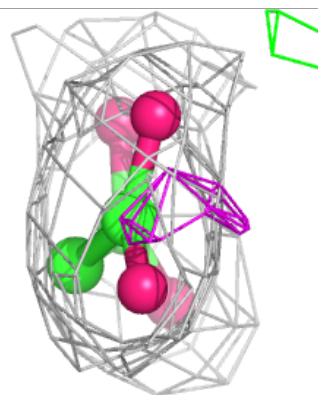
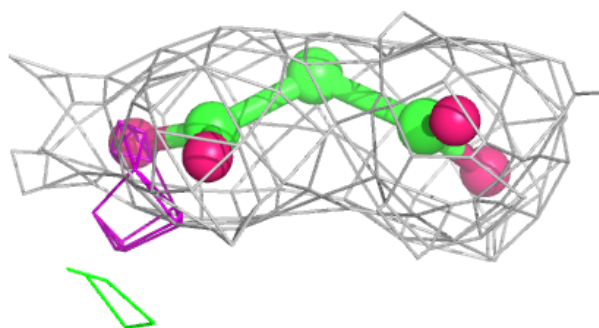
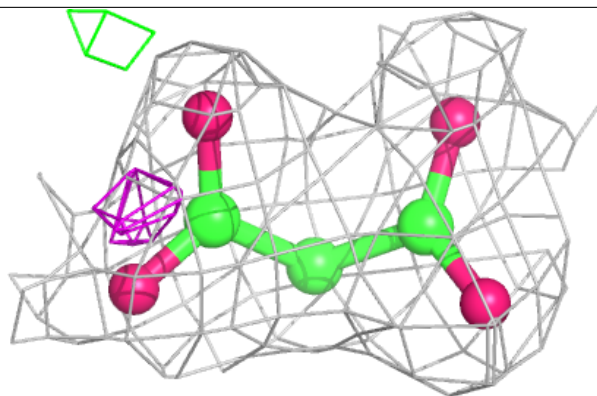
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



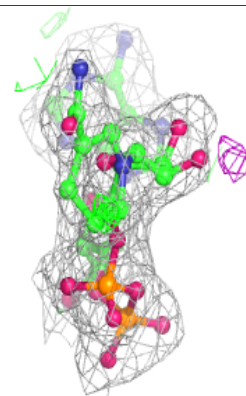
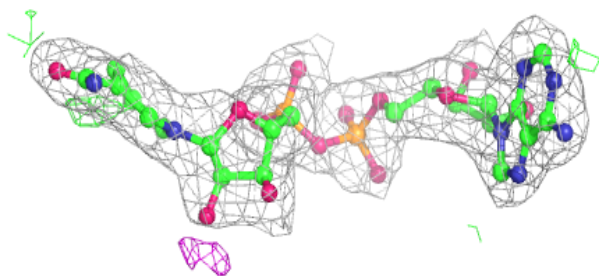
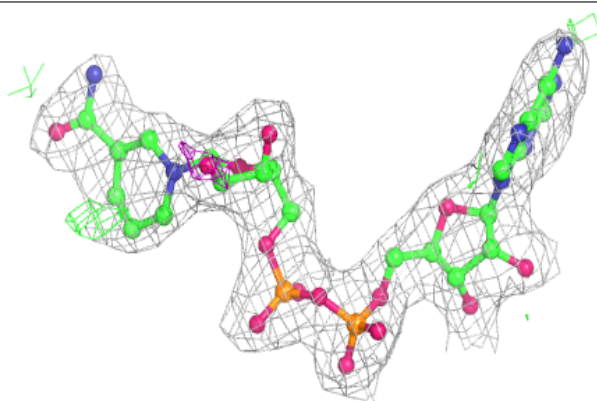


**Electron density around MLI B 402:**

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

**Electron density around NAI G 401:**

$2mF_o-DF_c$  (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.