



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 12:53 am BST

PDB ID : 1I10  
Title : HUMAN MUSCLE L-LACTATE DEHYDROGENASE M CHAIN,  
TERNARY COMPLEX WITH NADH AND OXAMATE  
Authors : Read, J.A.; Winter, V.J.; Eszes, C.M.; Sessions, R.B.; Brady, R.L.  
Deposited on : 2001-01-30  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

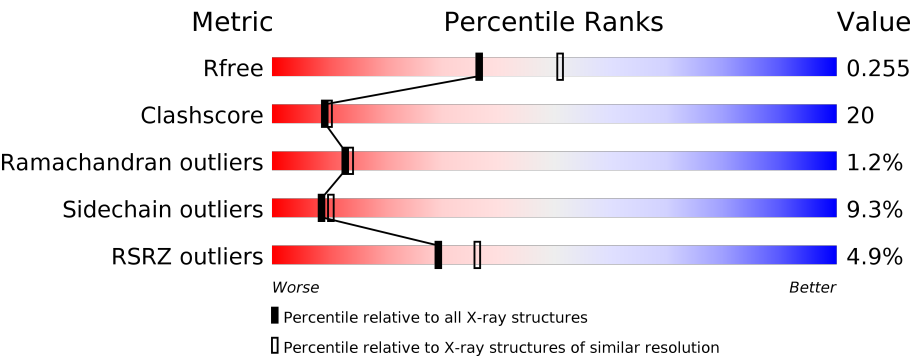
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	331	<div><div>2%</div><div><div></div><div>69%</div><div>27%</div><div></div></div><div></div></div>
1	B	331	<div><div>2%</div><div><div></div><div>73%</div><div>24%</div><div></div></div><div></div></div>
1	C	331	<div><div>4%</div><div><div></div><div>67%</div><div>27%</div><div>5%</div></div><div></div></div>
1	D	331	<div><div>3%</div><div><div></div><div>67%</div><div>27%</div><div>5%</div></div><div></div></div>
1	E	331	<div><div>10%</div><div><div></div><div>57%</div><div>33%</div><div>9%</div></div><div></div></div>
1	F	331	<div><div>4%</div><div><div></div><div>64%</div><div>29%</div><div>6%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	331	
1	H	331	

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
2	ACT	A	803	-	-	X	-
2	ACT	B	806	-	-	X	-
2	ACT	C	809	-	-	X	-
2	ACT	D	812	-	-	X	-
2	ACT	F	818	-	-	X	-
4	OXM	D	811	-	-	X	-
4	OXM	E	814	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21581 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 M CHAIN.

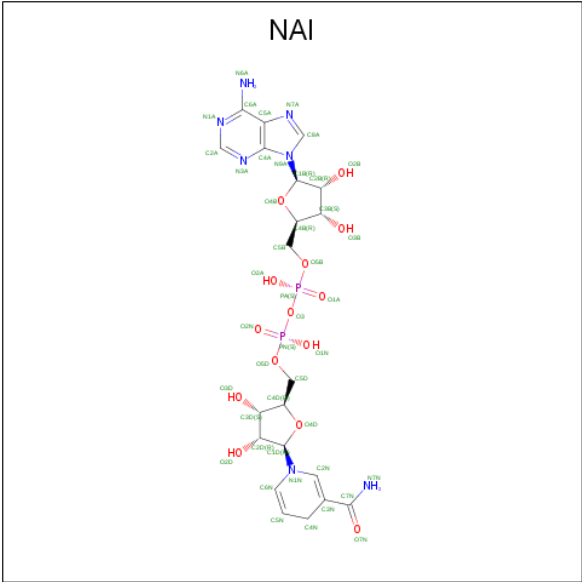
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	11	0	0
			2568	1639	439	477	13			
1	B	331	Total	C	N	O	S	21	0	0
			2568	1639	439	477	13			
1	C	331	Total	C	N	O	S	9	0	0
			2568	1639	439	477	13			
1	D	331	Total	C	N	O	S	60	0	0
			2568	1639	439	477	13			
1	E	331	Total	C	N	O	S	75	0	0
			2568	1639	439	477	13			
1	F	331	Total	C	N	O	S	36	0	0
			2568	1639	439	477	13			
1	G	325	Total	C	N	O	S	45	0	0
			2521	1612	430	466	13			
1	H	331	Total	C	N	O	S	36	0	0
			2568	1639	439	477	13			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



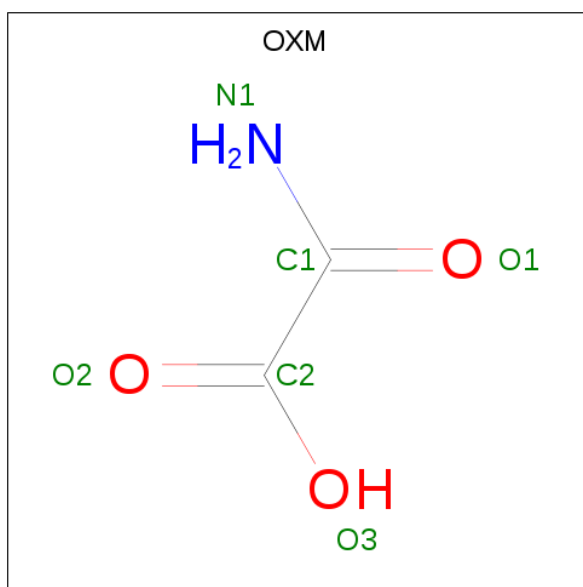
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 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>).



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

- Molecule 4 is OXAMIC ACID (three-letter code: OXM) (formula: C<sub>2</sub>H<sub>3</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			6	2	1	3		
4	B	1	Total	C	N	O	0	0
			6	2	1	3		
4	C	1	Total	C	N	O	0	0
			6	2	1	3		
4	D	1	Total	C	N	O	0	0
			6	2	1	3		
4	E	1	Total	C	N	O	0	0
			6	2	1	3		
4	F	1	Total	C	N	O	0	0
			6	2	1	3		
4	G	1	Total	C	N	O	0	0
			6	2	1	3		
4	H	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	135	Total	O	0	0
			135	135		
5	B	136	Total	O	0	0
			136	136		
5	C	78	Total	O	0	0
			78	78		
5	D	87	Total	O	0	0
			87	87		

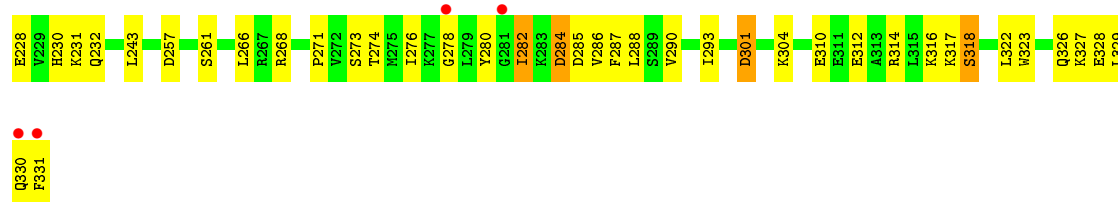
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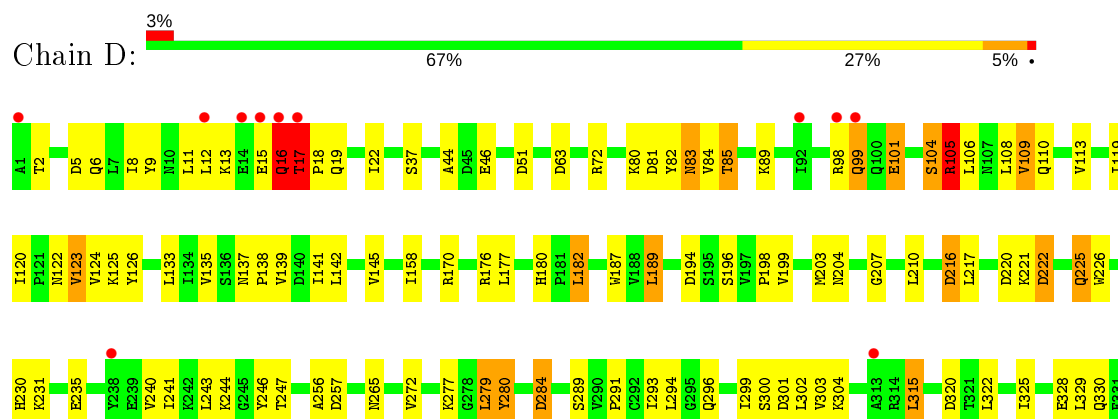
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	44	Total 44	O 44	0	0
5	F	51	Total 51	O 51	0	0
5	G	56	Total 56	O 56	0	0
5	H	65	Total 65	O 65	0	0



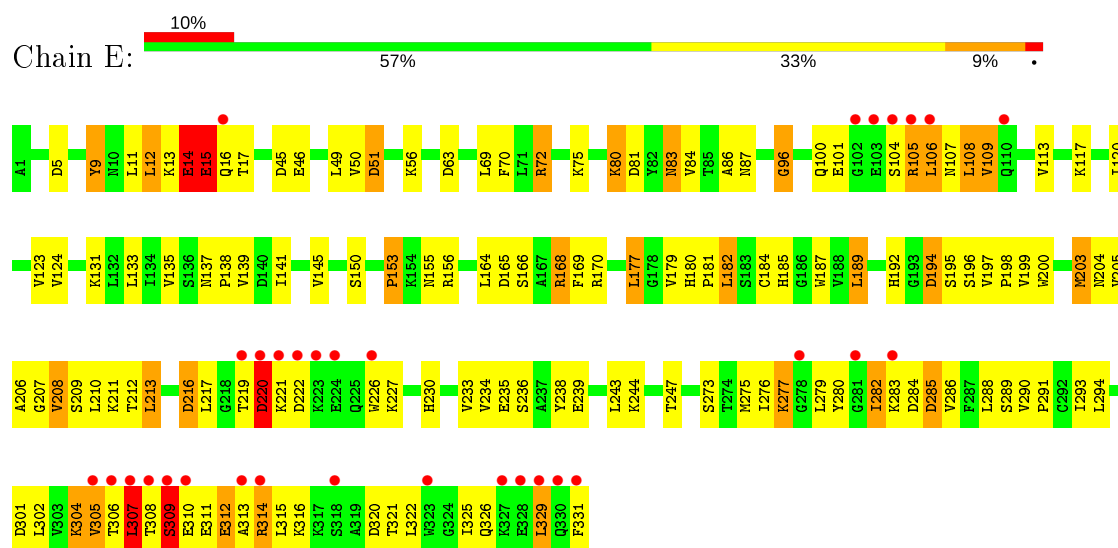




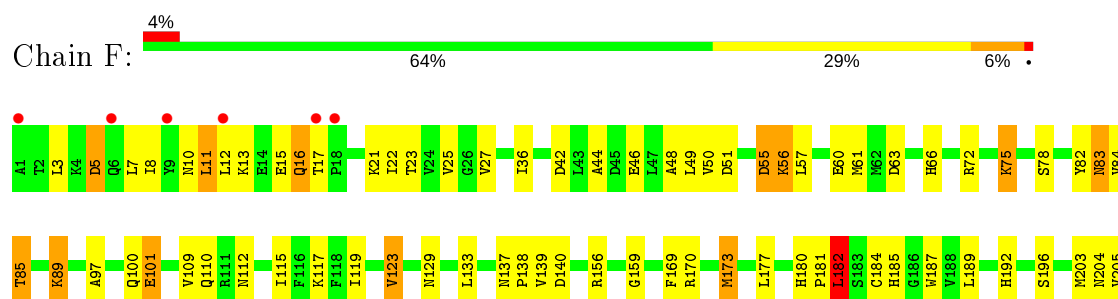
• Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN

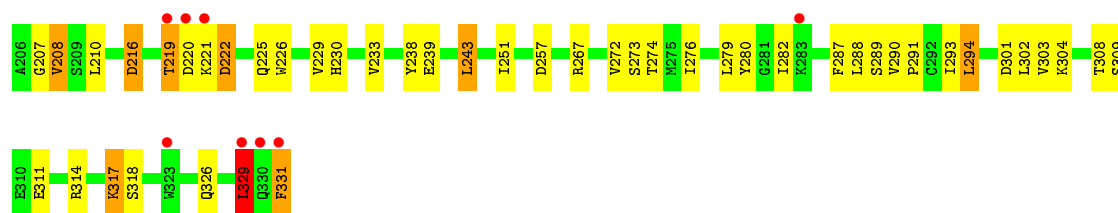


• Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN

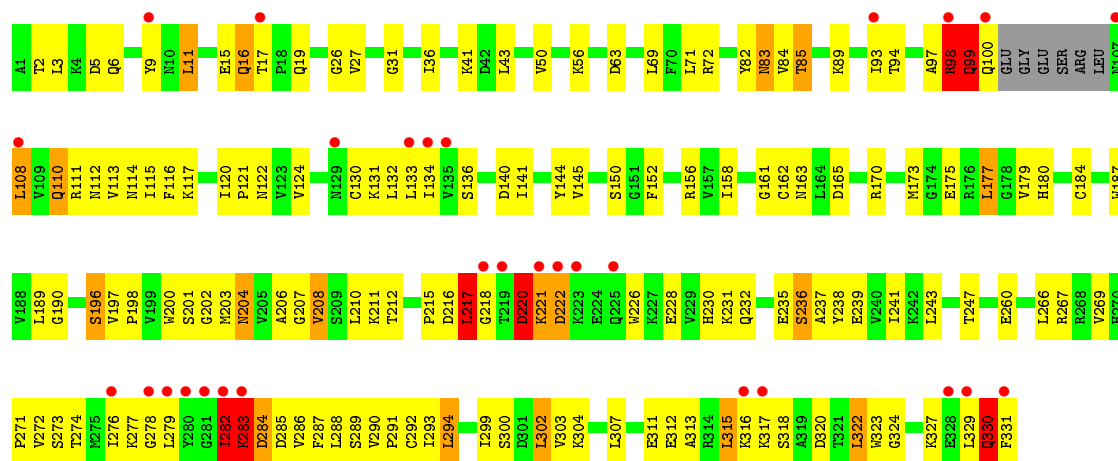


• Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN

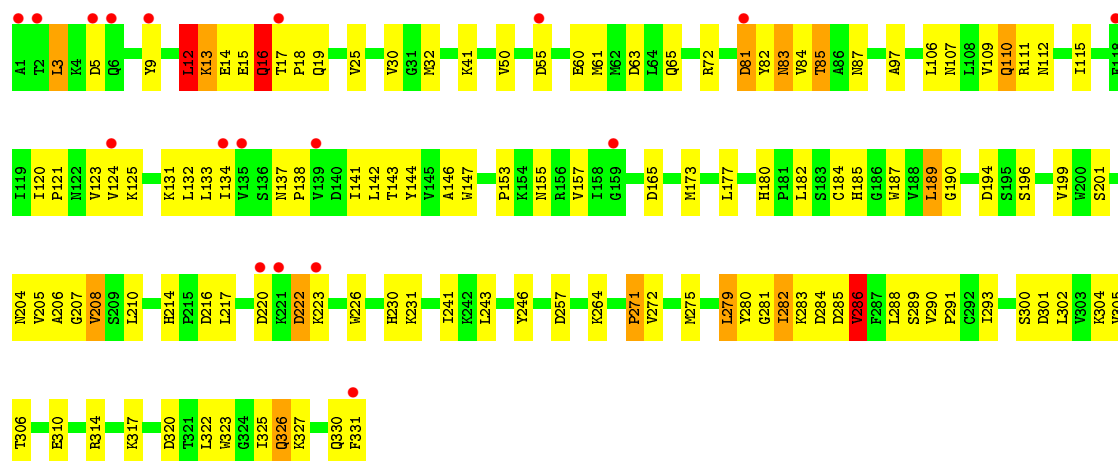




● Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN



● Molecule 1: L-LACTATE DEHYDROGENASE M CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.94Å 158.54Å 266.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 29.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (20.00-2.30) 91.1 (29.94-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.98 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.197 , 0.257 0.197 , 0.255	Depositor DCC
$R_{free}$ test set	6181 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21581	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: OXM, NAI, ACT

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	0.89	1/2612 (0.0%)	1.02	10/3532 (0.3%)
1	B	0.85	0/2612	0.98	8/3532 (0.2%)
1	C	0.82	3/2612 (0.1%)	1.01	15/3532 (0.4%)
1	D	0.89	4/2612 (0.2%)	0.99	16/3532 (0.5%)
1	E	0.78	2/2612 (0.1%)	1.00	14/3532 (0.4%)
1	F	0.78	1/2612 (0.0%)	0.97	12/3532 (0.3%)
1	G	0.78	3/2564 (0.1%)	0.97	11/3467 (0.3%)
1	H	0.82	1/2612 (0.0%)	1.02	15/3532 (0.4%)
All	All	0.83	15/20848 (0.1%)	1.00	101/28191 (0.4%)

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	D	0	2
1	E	0	1
1	F	0	1
1	H	0	3
All	All	0	7

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	12	LEU	C-N	-18.70	0.91	1.34
1	D	231	LYS	C-O	-16.70	0.91	1.23
1	G	226	TRP	CB-CG	-14.33	1.24	1.50
1	A	13	LYS	CB-CG	-14.12	1.14	1.52
1	F	16	GLN	C-N	13.99	1.66	1.34

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	217	LEU	CB-CG-CD1	14.68	135.96	111.00
1	H	16	GLN	O-C-N	-12.08	103.37	122.70
1	H	63	ASP	CB-CG-OD2	10.81	128.03	118.30
1	F	16	GLN	C-N-CA	-10.43	95.63	121.70
1	H	12	LEU	O-C-N	-10.34	106.16	122.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	104	SER	Mainchain,Peptide
1	E	96	GLY	Mainchain
1	F	12	LEU	Peptide
1	H	12	LEU	Mainchain
1	H	16	GLN	Mainchain

## 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	80	0
1	B	2568	0	2656	75	0
1	C	2568	0	2656	88	0
1	D	2568	0	2654	84	0
1	E	2568	0	2655	158	0
1	F	2568	0	2656	116	0
1	G	2521	0	2611	154	0
1	H	2568	0	2655	107	0
2	A	4	0	3	6	0
2	B	4	0	3	4	0
2	C	4	0	3	2	0
2	D	4	0	3	2	0
2	E	4	0	3	1	0
2	F	4	0	3	3	0
2	G	4	0	3	1	0
2	H	4	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	44	0	27	2	0
3	B	44	0	27	2	0
3	C	44	0	27	1	0
3	D	44	0	27	4	0
3	E	44	0	27	3	0
3	F	44	0	27	2	0
3	G	44	0	27	1	0
3	H	44	0	27	3	0
4	A	6	0	2	0	0
4	B	6	0	2	0	0
4	C	6	0	2	1	0
4	D	6	0	2	2	0
4	E	6	0	2	2	0
4	F	6	0	2	1	0
4	G	6	0	2	0	0
4	H	6	0	2	0	0
5	A	135	0	0	10	0
5	B	136	0	0	3	0
5	C	78	0	0	3	0
5	D	87	0	0	3	0
5	E	44	0	0	3	0
5	F	51	0	0	4	0
5	G	56	0	0	3	0
5	H	65	0	0	2	0
All	All	21581	0	21455	828	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 20.

The worst 5 of 828 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:ARG:O	1:E:106:LEU:HG	1.20	1.29
1:D:279:LEU:HB3	1:D:280:TYR:CE1	1.74	1.22
1:E:308:THR:CA	1:E:309:SER:HB3	1.70	1.22
1:G:282:ILE:HG13	1:G:283:LYS:N	1.39	1.20
1:D:280:TYR:N	1:D:280:TYR:HD1	1.32	1.19

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	329/331 (99%)	316 (96%)	11 (3%)	2 (1%)	25	31
1	B	329/331 (99%)	313 (95%)	12 (4%)	4 (1%)	13	14
1	C	329/331 (99%)	313 (95%)	15 (5%)	1 (0%)	41	50
1	D	329/331 (99%)	308 (94%)	16 (5%)	5 (2%)	10	10
1	E	329/331 (99%)	290 (88%)	30 (9%)	9 (3%)	5	3
1	F	329/331 (99%)	310 (94%)	17 (5%)	2 (1%)	25	31
1	G	321/331 (97%)	291 (91%)	23 (7%)	7 (2%)	6	5
1	H	329/331 (99%)	314 (95%)	13 (4%)	2 (1%)	25	31
All	All	2624/2648 (99%)	2455 (94%)	137 (5%)	32 (1%)	13	14

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	GLU
1	B	16	GLN
1	D	13	LYS
1	D	101	GLU
1	E	15	GLU

### 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	287/287 (100%)	264 (92%)	23 (8%)	12	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	287/287 (100%)	274 (96%)	13 (4%)	27	39
1	C	287/287 (100%)	265 (92%)	22 (8%)	13	16
1	D	287/287 (100%)	262 (91%)	25 (9%)	10	12
1	E	287/287 (100%)	247 (86%)	40 (14%)	3	3
1	F	287/287 (100%)	260 (91%)	27 (9%)	8	10
1	G	282/287 (98%)	245 (87%)	37 (13%)	4	4
1	H	287/287 (100%)	260 (91%)	27 (9%)	8	10
All	All	2291/2296 (100%)	2077 (91%)	214 (9%)	9	10

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	107	ASN
1	E	309	SER
1	H	85	THR
1	E	153	PRO
1	E	243	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	122	ASN
1	E	110	GLN
1	H	107	ASN
1	D	330	GLN
1	E	129	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

24 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
4	OXM	A	802	-	2,5,5	0.84	0	2,6,6	0.82	0
2	ACT	G	821	-	1,3,3	0.15	0	0,3,3	0.00	-
2	ACT	H	824	-	1,3,3	1.00	0	0,3,3	0.00	-
2	ACT	E	815	-	1,3,3	1.90	0	0,3,3	0.00	-
4	OXM	H	823	-	2,5,5	0.33	0	2,6,6	2.16	1 (50%)
4	OXM	D	811	-	2,5,5	1.59	0	2,6,6	0.71	0
4	OXM	G	820	-	2,5,5	0.30	0	2,6,6	2.01	1 (50%)
3	NAI	B	804	-	42,48,48	1.87	6 (14%)	47,73,73	1.35	4 (8%)
3	NAI	H	822	-	42,48,48	1.83	6 (14%)	47,73,73	1.57	8 (17%)
4	OXM	F	817	-	2,5,5	1.08	0	2,6,6	1.67	1 (50%)
3	NAI	F	816	-	42,48,48	1.78	5 (11%)	47,73,73	1.54	4 (8%)
4	OXM	B	805	-	2,5,5	1.37	0	2,6,6	1.32	0
4	OXM	E	814	-	2,5,5	1.41	0	2,6,6	0.07	0
3	NAI	E	813	-	42,48,48	1.99	6 (14%)	47,73,73	1.29	5 (10%)
3	NAI	C	807	-	42,48,48	1.95	9 (21%)	47,73,73	1.51	8 (17%)
3	NAI	D	810	-	42,48,48	1.96	6 (14%)	47,73,73	1.48	9 (19%)
2	ACT	A	803	-	1,3,3	1.07	0	0,3,3	0.00	-
2	ACT	F	818	-	1,3,3	0.50	0	0,3,3	0.00	-
2	ACT	B	806	-	1,3,3	0.69	0	0,3,3	0.00	-
4	OXM	C	808	-	2,5,5	0.75	0	2,6,6	2.03	1 (50%)
2	ACT	C	809	-	1,3,3	1.72	0	0,3,3	0.00	-
3	NAI	G	819	-	42,48,48	1.90	6 (14%)	47,73,73	1.34	6 (12%)
2	ACT	D	812	-	1,3,3	0.07	0	0,3,3	0.00	-
3	NAI	A	801	-	42,48,48	1.79	6 (14%)	47,73,73	1.63	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
4	OXM	B	805	-	-	0/0/4/4	-
4	OXM	E	814	-	-	0/0/4/4	-
4	OXM	H	823	-	-	0/0/4/4	-
3	NAI	E	813	-	-	5/25/72/72	0/5/5/5
4	OXM	D	811	-	-	0/0/4/4	-
3	NAI	D	810	-	-	7/25/72/72	0/5/5/5
4	OXM	A	802	-	-	0/0/4/4	-
4	OXM	G	820	-	-	0/0/4/4	-
3	NAI	B	804	-	-	4/25/72/72	0/5/5/5
3	NAI	H	822	-	-	5/25/72/72	0/5/5/5
3	NAI	G	819	-	-	5/25/72/72	0/5/5/5
4	OXM	F	817	-	-	0/0/4/4	-
3	NAI	F	816	-	-	6/25/72/72	0/5/5/5
3	NAI	A	801	-	-	6/25/72/72	0/5/5/5
3	NAI	C	807	-	-	4/25/72/72	0/5/5/5
4	OXM	C	808	-	-	0/0/4/4	-

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	810	NAI	O7N-C7N	7.90	1.43	1.24
3	E	813	NAI	O7N-C7N	7.80	1.43	1.24
3	G	819	NAI	O7N-C7N	7.36	1.41	1.24
3	B	804	NAI	O7N-C7N	6.88	1.40	1.24
3	H	822	NAI	O7N-C7N	6.15	1.39	1.24

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	816	NAI	N3A-C2A-N1A	-6.58	118.40	128.68
3	A	801	NAI	N3A-C2A-N1A	-5.93	119.41	128.68
3	D	810	NAI	N3A-C2A-N1A	-5.11	120.69	128.68
3	H	822	NAI	N3A-C2A-N1A	-4.82	121.15	128.68
3	E	813	NAI	N3A-C2A-N1A	-4.78	121.20	128.68

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	810	NAI	C5B-O5B-PA-O1A
3	G	819	NAI	C2D-C1D-N1N-C2N
3	G	819	NAI	C2D-C1D-N1N-C6N
3	F	816	NAI	C2D-C1D-N1N-C2N
3	E	813	NAI	C2D-C1D-N1N-C2N

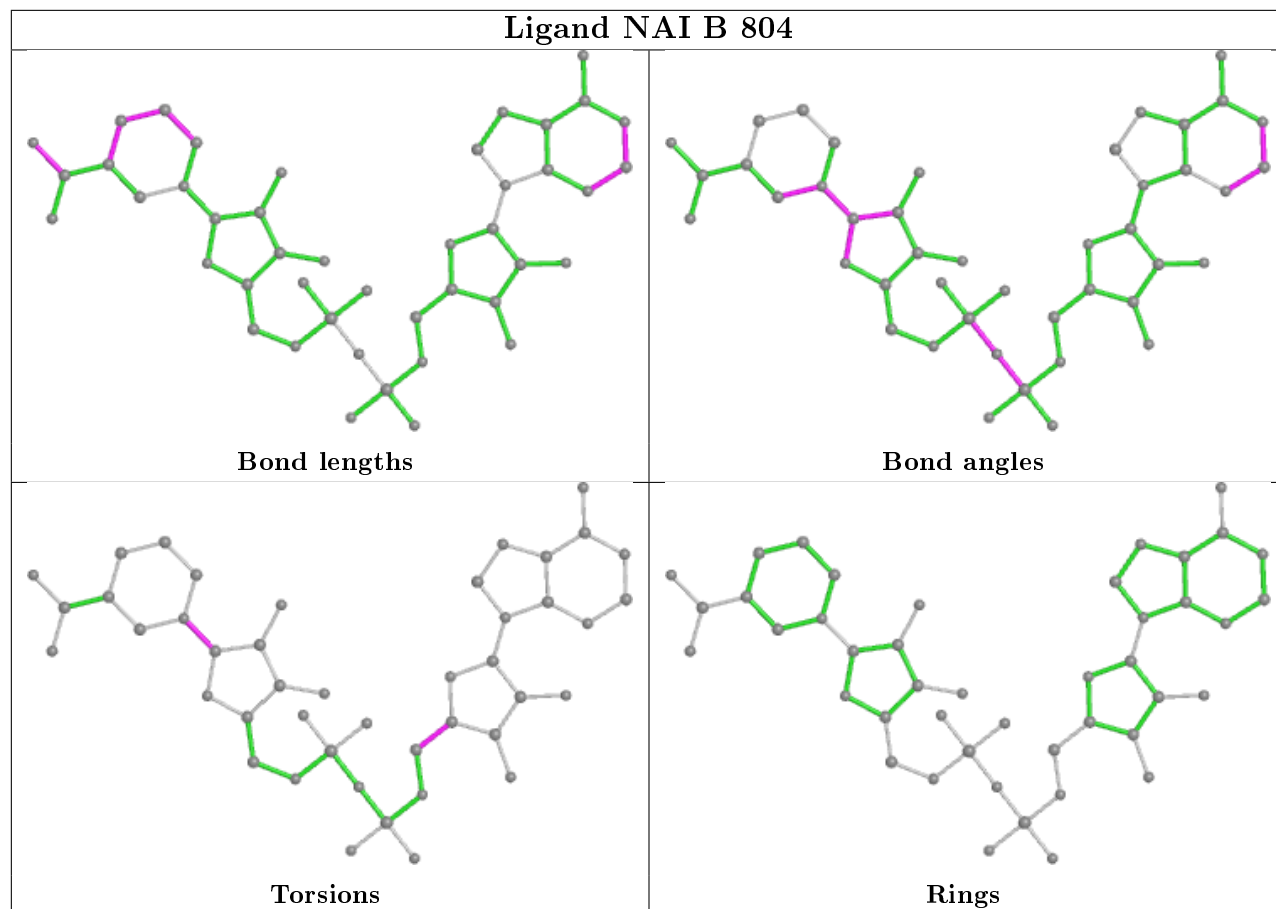
There are no ring outliers.

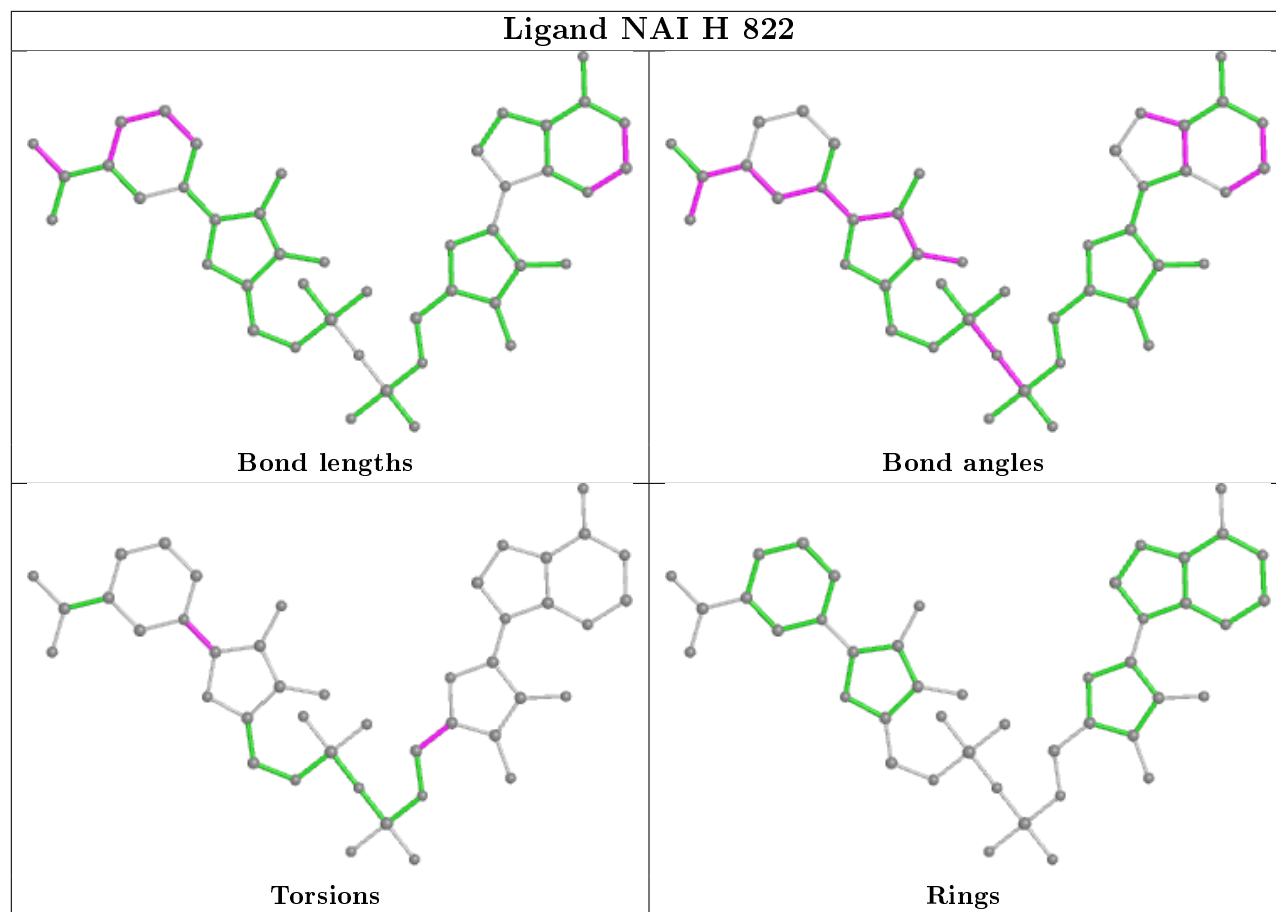
20 monomers are involved in 38 short contacts:

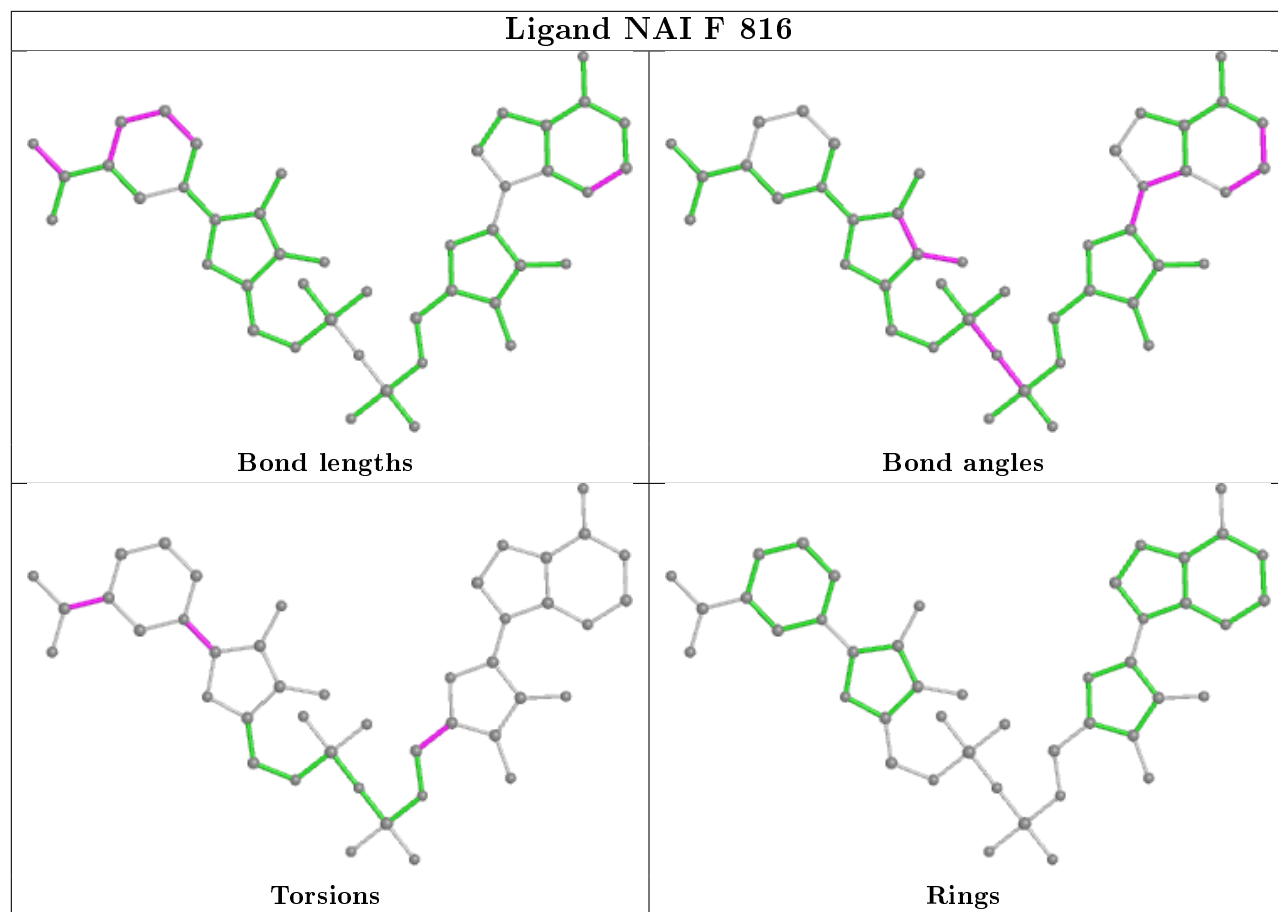
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	821	ACT	1	0
2	H	824	ACT	1	0
2	E	815	ACT	1	0
4	D	811	OXM	2	0
3	B	804	NAI	2	0
3	H	822	NAI	3	0
4	F	817	OXM	1	0
3	F	816	NAI	2	0
4	E	814	OXM	2	0
3	E	813	NAI	3	0
3	C	807	NAI	1	0
3	D	810	NAI	4	0
2	A	803	ACT	6	0
2	F	818	ACT	3	0
2	B	806	ACT	4	0
4	C	808	OXM	1	0
2	C	809	ACT	2	0
3	G	819	NAI	1	0
2	D	812	ACT	2	0
3	A	801	NAI	2	0

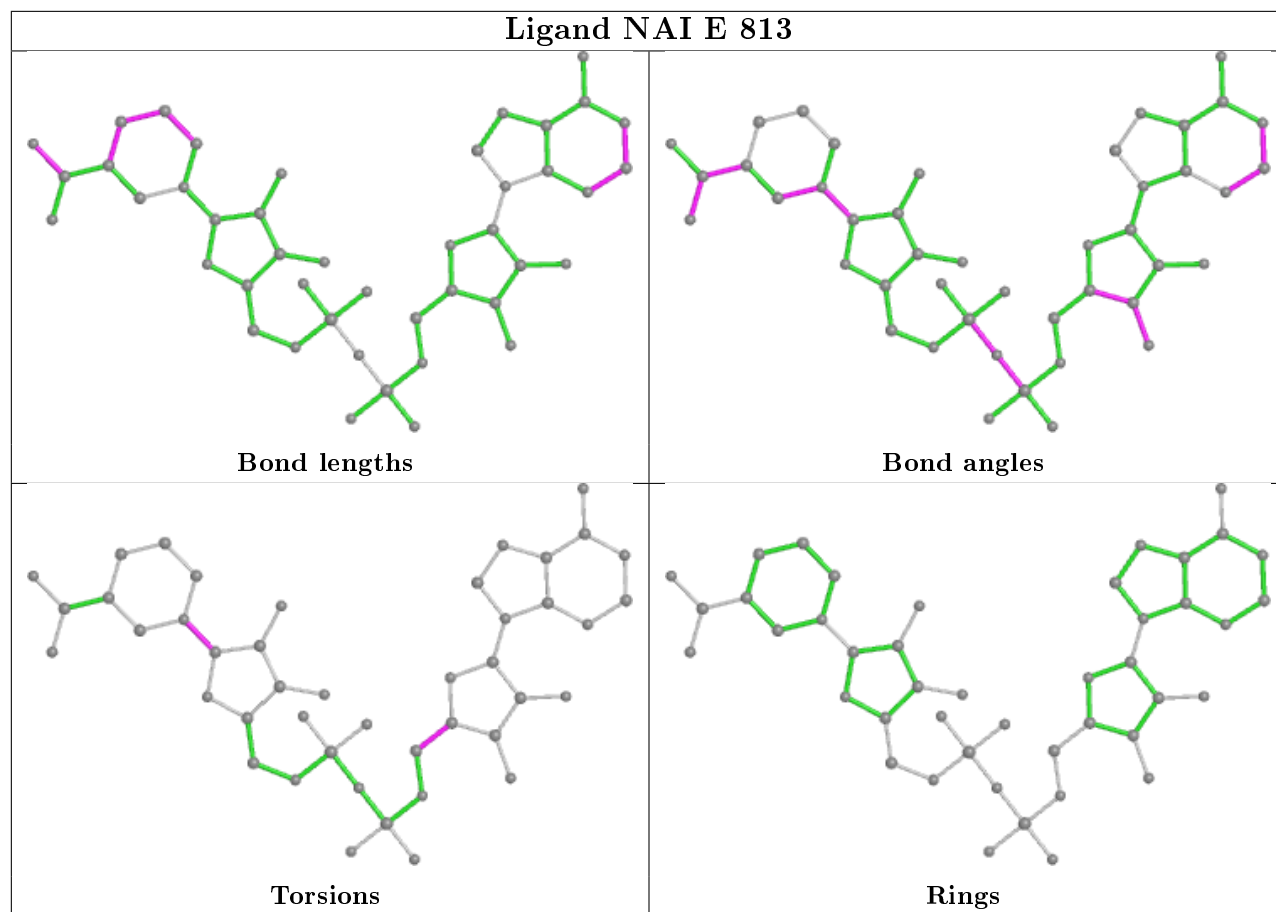
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

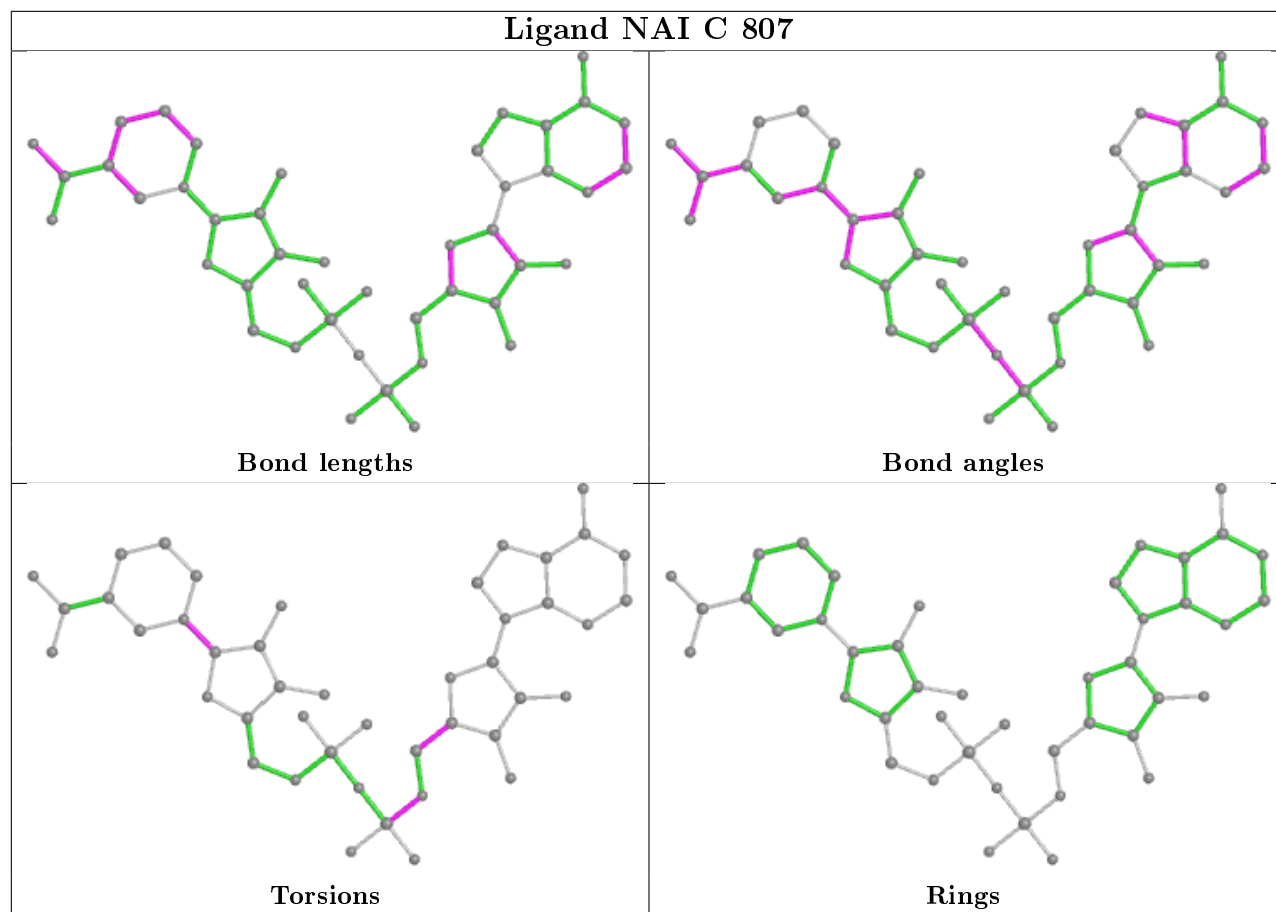


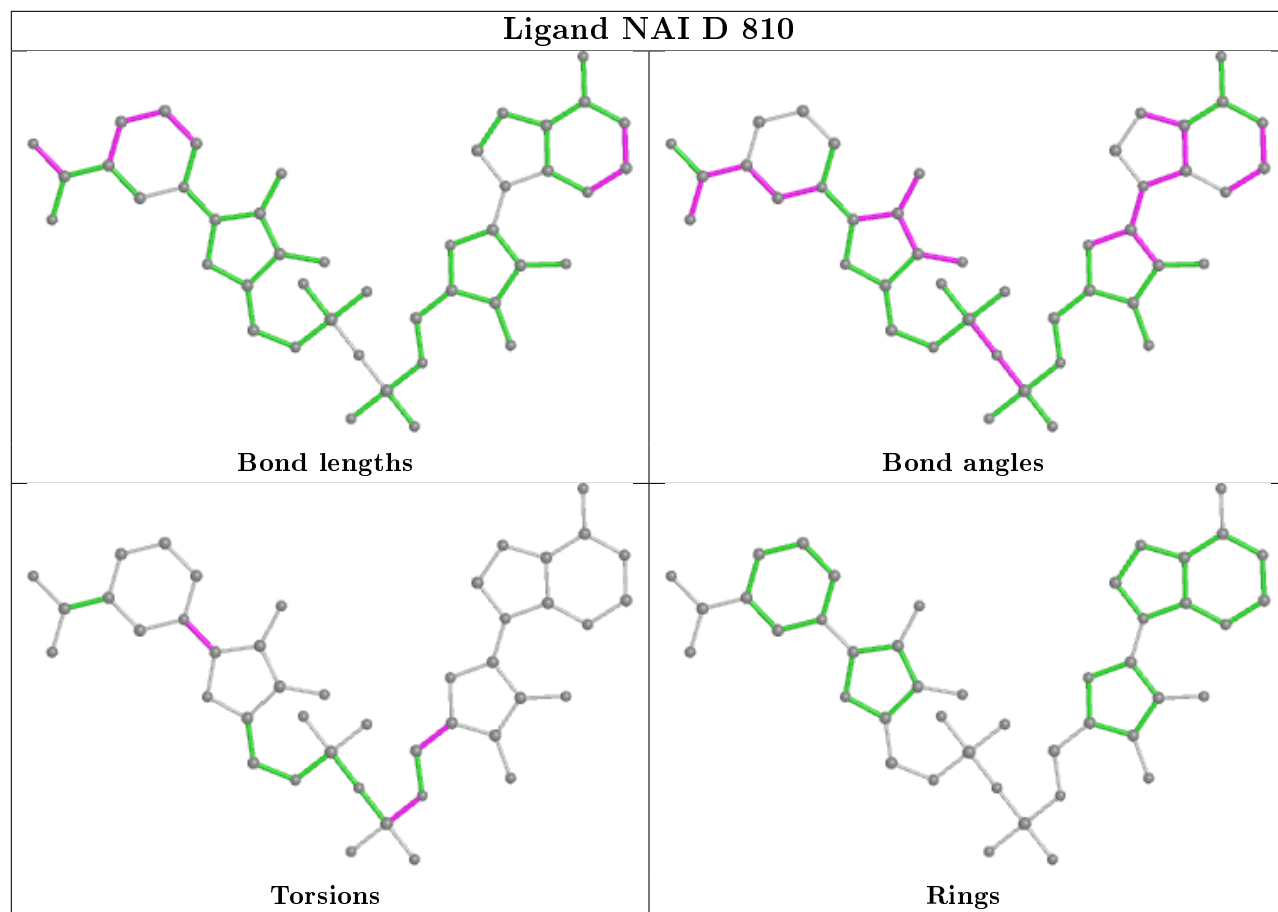




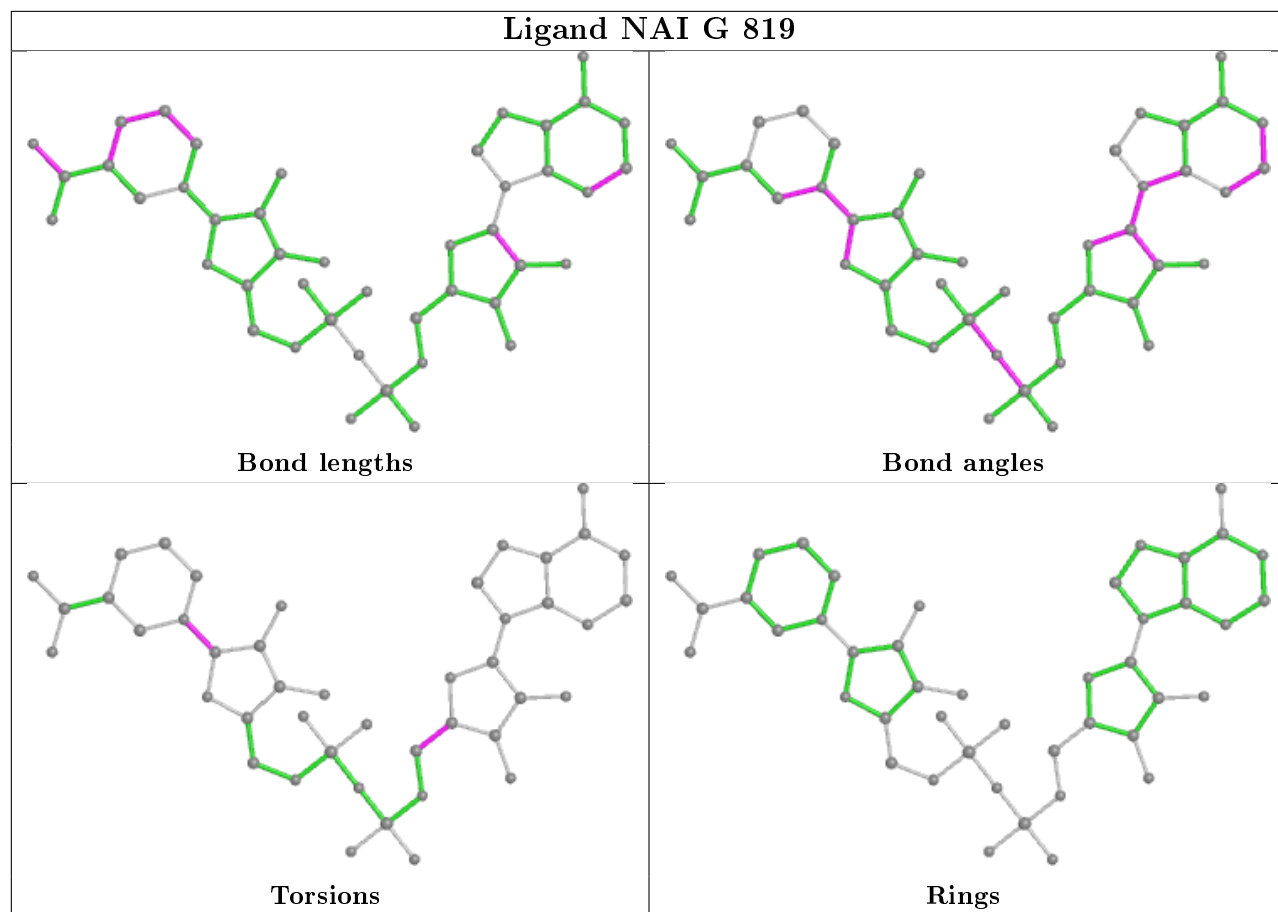


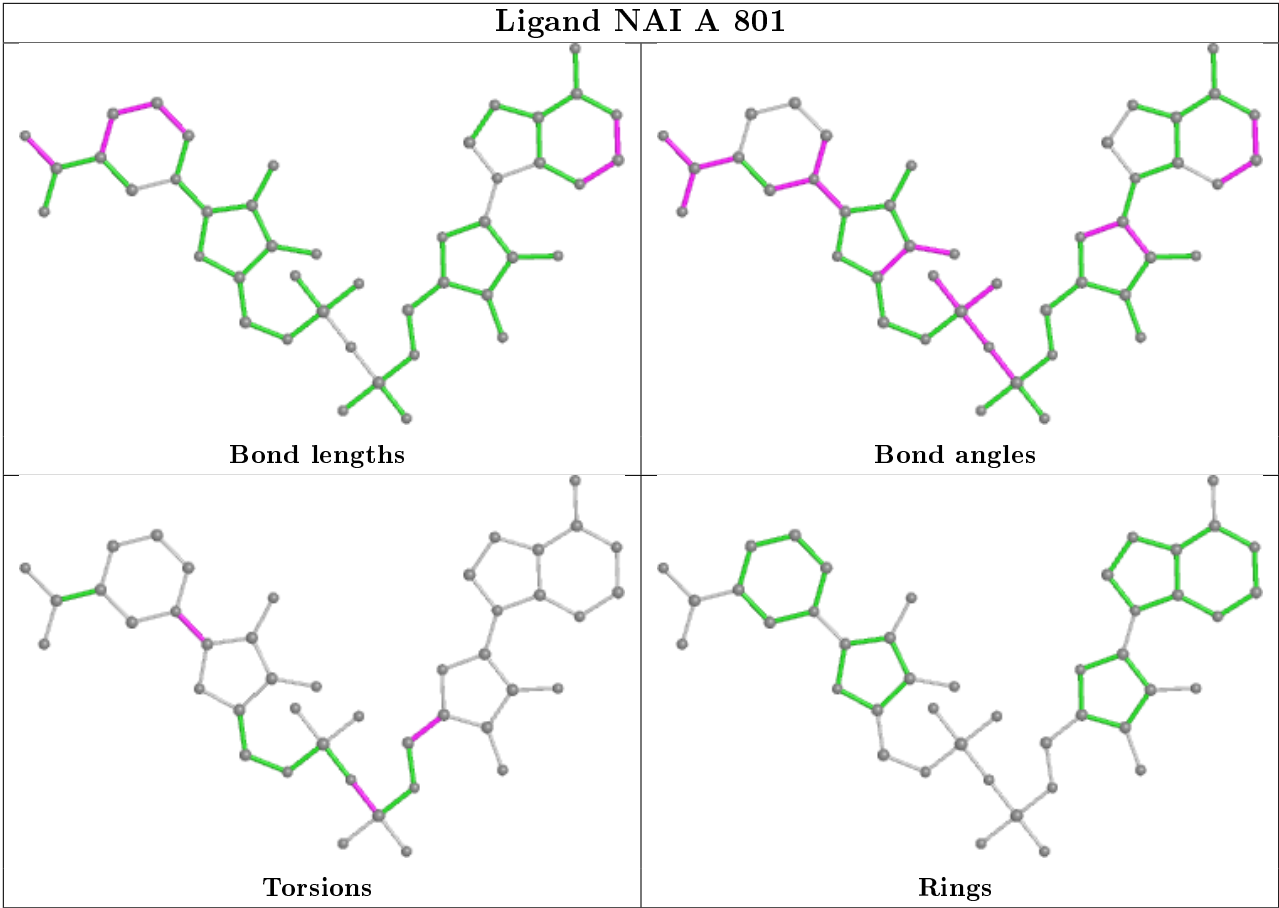






## Ligand NAI G 819





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	H	1
1	F	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	16:GLN	C	17:THR	N	1.66
1	D	99:GLN	C	100:GLN	N	1.13
1	D	104:SER	C	105:ARG	N	1.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	96:GLY	C	97:ALA	N	1.07
1	H	12:LEU	C	13:LYS	N	0.91

## 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	331/331 (100%)	-0.28	6 (1%) 68 74	5, 16, 37, 52	5 (1%)
1	B	330/331 (99%)	-0.26	7 (2%) 63 70	8, 16, 41, 66	5 (1%)
1	C	331/331 (100%)	-0.03	12 (3%) 42 49	11, 21, 49, 74	3 (0%)
1	D	326/331 (98%)	-0.08	11 (3%) 45 52	12, 22, 40, 56	6 (1%)
1	E	324/331 (97%)	0.30	32 (9%) 7 10	10, 29, 73, 150	4 (1%)
1	F	327/331 (98%)	0.02	14 (4%) 35 42	11, 24, 57, 79	0
1	G	325/331 (98%)	0.42	29 (8%) 9 13	12, 33, 67, 80	10 (3%)
1	H	327/331 (98%)	0.13	18 (5%) 25 31	11, 27, 52, 61	0
All	All	2621/2648 (98%)	0.03	129 (4%) 29 36	5, 23, 56, 150	33 (1%)

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	106	LEU	13.6
1	E	105	ARG	9.8
1	E	104	SER	6.5
1	D	14	GLU	6.2
1	H	331	PHE	6.1

### 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 ⓘ

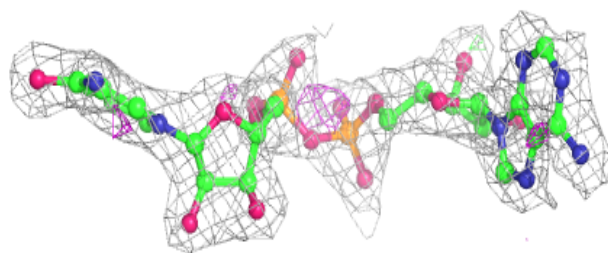
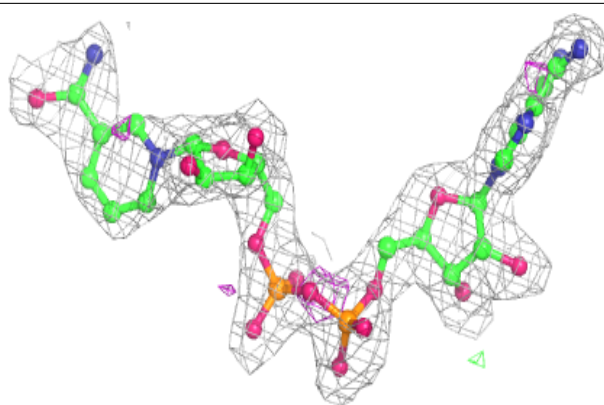
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	OXM	D	811	6/6	0.57	0.31	46,49,49,50	0
4	OXM	G	820	6/6	0.73	0.25	43,44,47,50	0
2	ACT	G	821	4/4	0.88	0.32	45,45,46,46	0
4	OXM	E	814	6/6	0.89	0.16	32,36,38,38	0
3	NAI	E	813	44/44	0.91	0.16	24,34,37,37	0
3	NAI	D	810	44/44	0.91	0.17	23,32,39,40	0
2	ACT	H	824	4/4	0.92	0.31	37,37,38,38	0
2	ACT	A	803	4/4	0.93	0.20	17,19,21,22	0
3	NAI	G	819	44/44	0.94	0.11	21,29,35,37	0
3	NAI	H	822	44/44	0.95	0.11	16,21,32,34	0
2	ACT	E	815	4/4	0.95	0.26	30,30,30,31	0
2	ACT	F	818	4/4	0.96	0.19	31,31,32,32	0
2	ACT	B	806	4/4	0.96	0.22	19,20,22,22	0
3	NAI	F	816	44/44	0.96	0.09	11,21,30,30	0
3	NAI	C	807	44/44	0.97	0.12	15,18,21,22	0
2	ACT	C	809	4/4	0.97	0.16	10,13,13,15	0
4	OXM	H	823	6/6	0.97	0.09	15,17,17,18	0
2	ACT	D	812	4/4	0.97	0.17	21,21,22,22	0
3	NAI	A	801	44/44	0.97	0.10	9,13,16,16	0
3	NAI	B	804	44/44	0.98	0.10	8,13,21,21	0
4	OXM	B	805	6/6	0.98	0.10	7,12,13,15	0
4	OXM	F	817	6/6	0.98	0.08	15,18,20,22	0
4	OXM	C	808	6/6	0.98	0.07	11,13,14,14	0
4	OXM	A	802	6/6	0.99	0.11	5,9,11,12	0

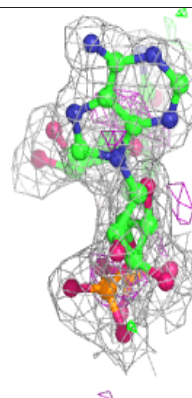
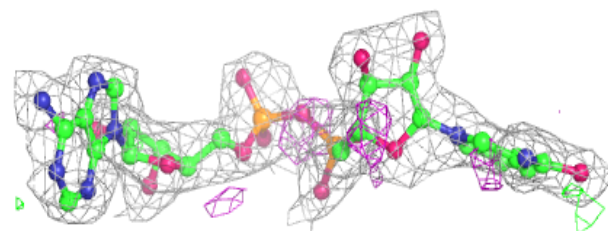
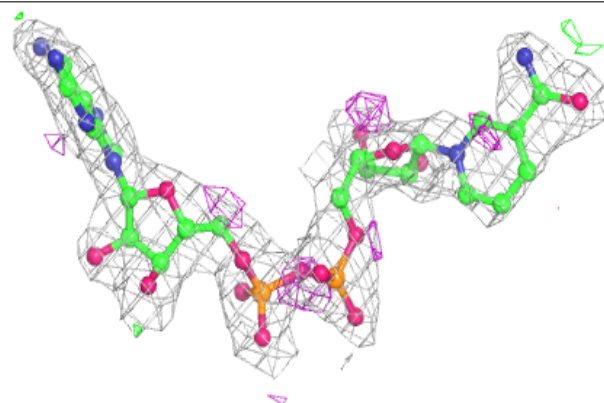
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAI E 813:**

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

**Electron density around NAI D 810:**

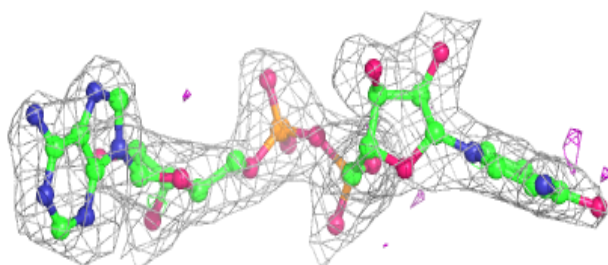
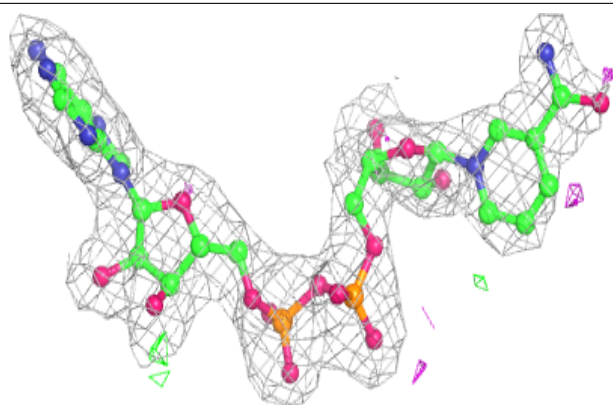
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



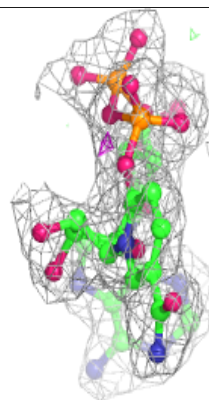
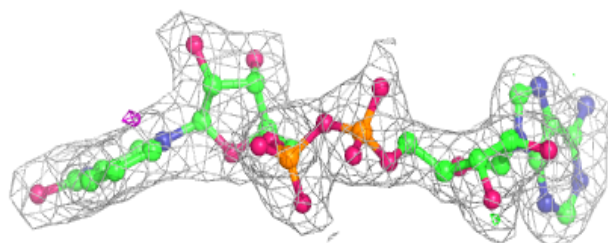
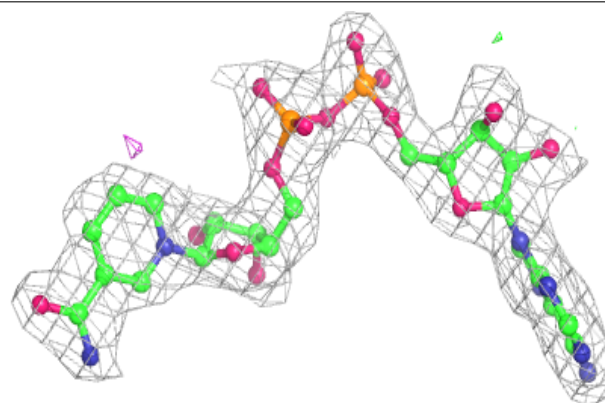


**Electron density around NAI G 819:**

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

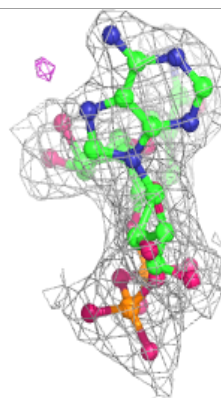
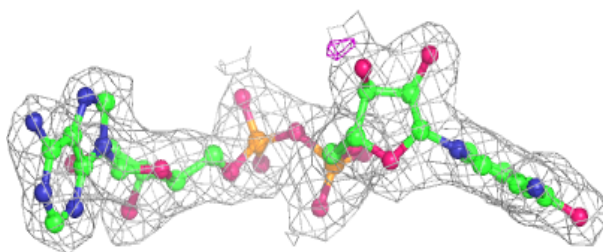
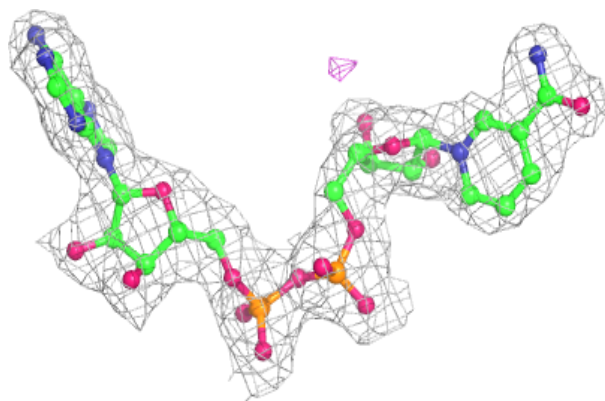
**Electron density around NAI H 822:**

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

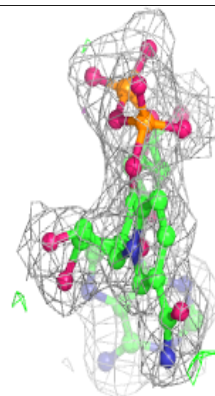
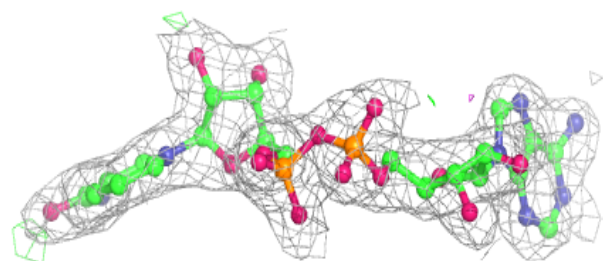
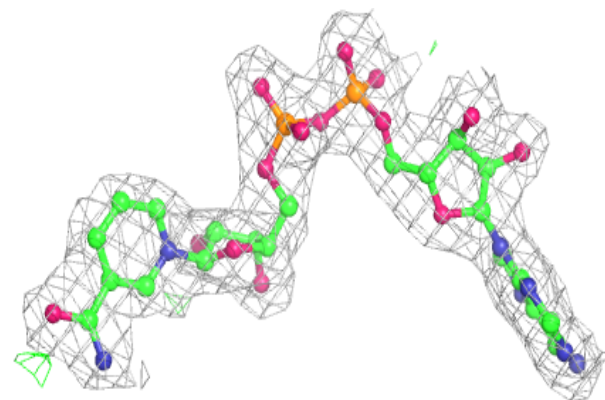


**Electron density around NAI F 816:**

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

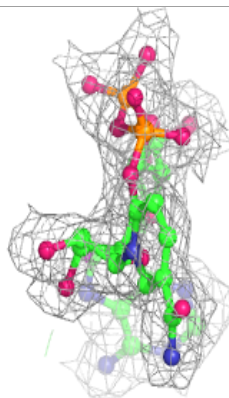
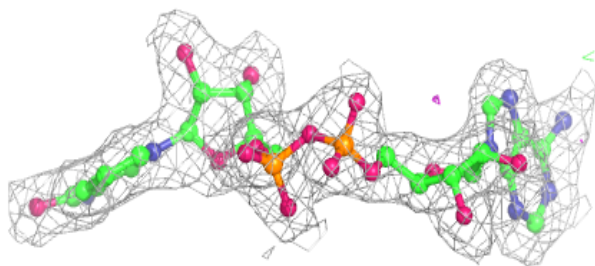
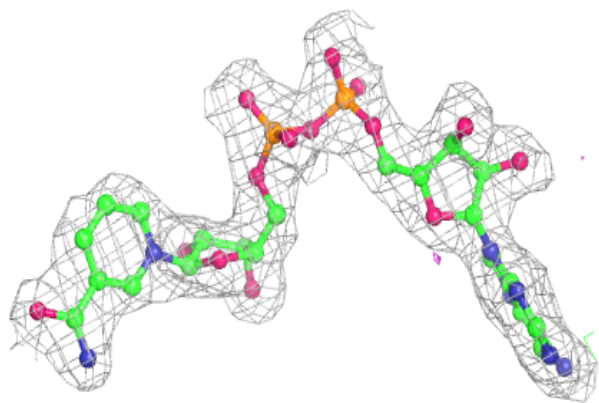
**Electron density around NAI C 807:**

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

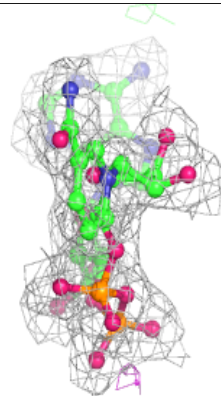
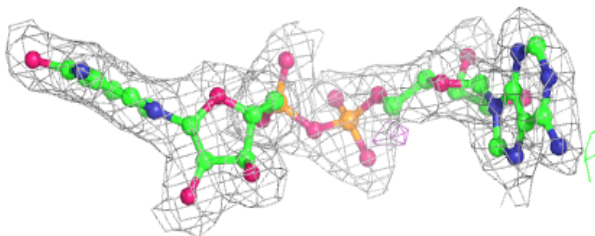
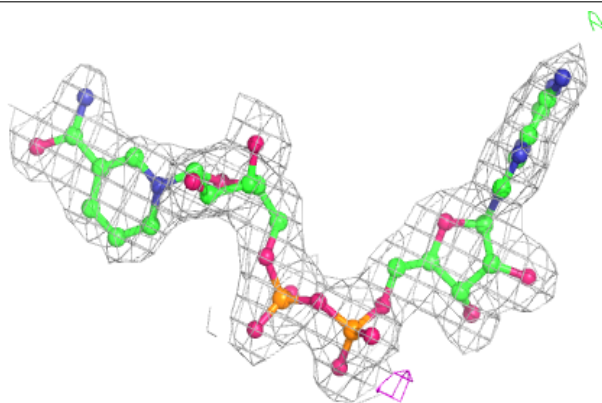


**Electron density around NAI A 801:**

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

**Electron density around NAI B 804:**

$2mF_o-DF_c$  (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.