



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 07:17 am BST

PDB ID : 1O02  
Title : Human mitochondrial aldehyde dehydrogenase complexed with NADH in the presence of Mg<sup>2+</sup>  
Authors : Perez-Miller, S.J.; Hurley, T.D.  
Deposited on : 2003-02-20  
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

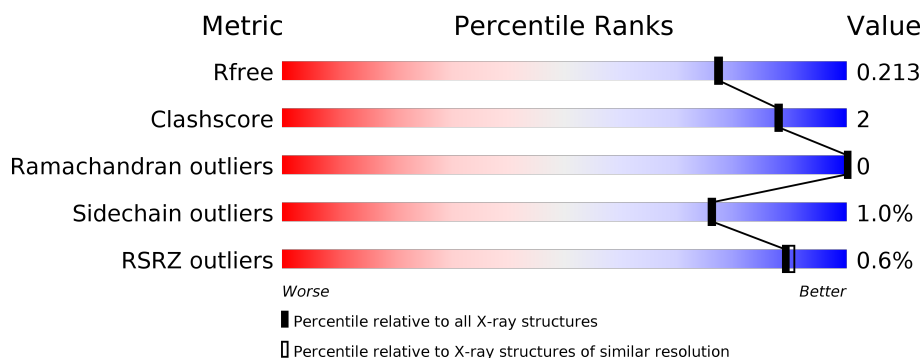
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	500	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>•</div> </div> </div>
1	B	500	<div> <div></div> <div>92%</div> <div>6%</div> <div>•</div> </div>
1	C	500	<div> <div></div> <div>96%</div> <div></div> <div>• •</div> </div>
1	D	500	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>•</div> </div> </div>
1	E	500	<div> <div></div> <div>94%</div> <div>5%</div> <div>•</div> </div>
1	F	500	<div> <div></div> <div>93%</div> <div>5%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	500	<div><div></div><div>94%</div><div>5%</div></div>
1	H	500	<div>%<div><div></div><div>93%</div><div>6%</div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34432 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	B	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	C	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	D	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	E	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	F	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	G	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	H	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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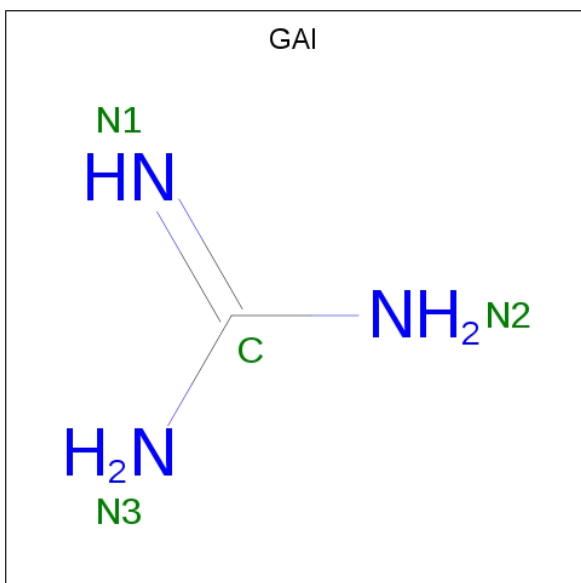
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is GUANIDINE (three-letter code: GAI) (formula:  $\text{CH}_5\text{N}_3$ ).



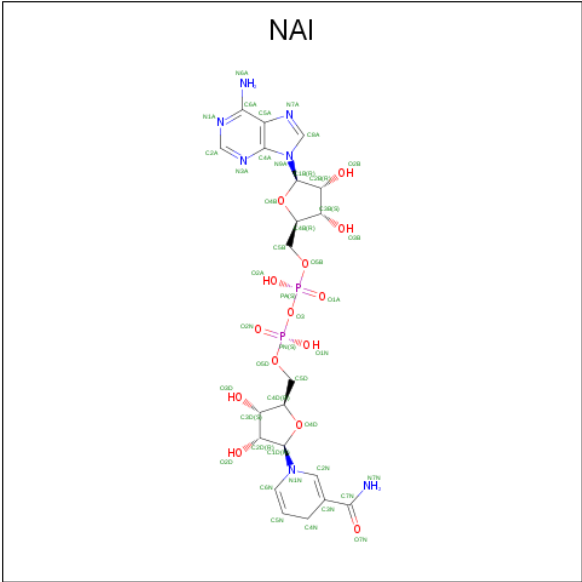
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 4 1 3	0	0
4	A	1	Total C N 4 1 3	0	0
4	B	1	Total C N 4 1 3	0	0
4	B	1	Total C N 4 1 3	0	0
4	C	1	Total C N 4 1 3	0	0
4	C	1	Total C N 4 1 3	0	0
4	D	1	Total C N 4 1 3	0	0
4	D	1	Total C N 4 1 3	0	0
4	E	1	Total C N 4 1 3	0	0
4	E	1	Total C N 4 1 3	0	0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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 6 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	418	Total	O	0	0
			418	418		
7	B	498	Total	O	0	0
			498	498		
7	C	470	Total	O	0	0
			470	470		
7	D	426	Total	O	0	0
			426	426		

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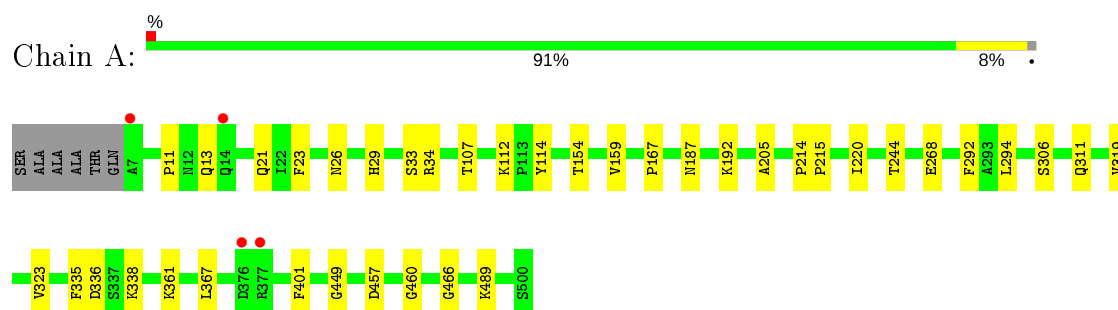
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	466	Total 466	O 466	0	0
7	F	498	Total 498	O 498	0	0
7	G	437	Total 437	O 437	0	0
7	H	371	Total 371	O 371	0	0

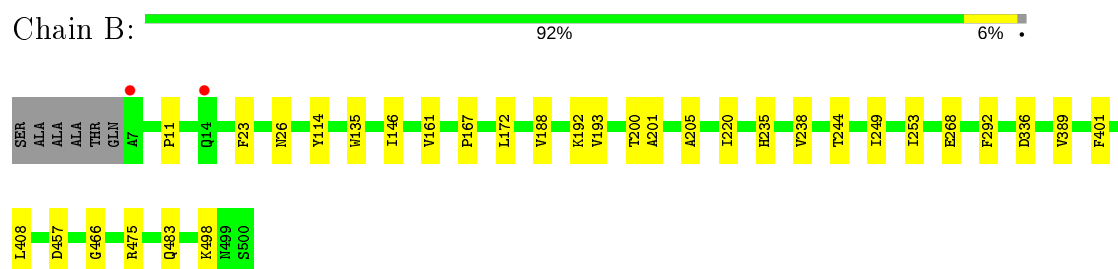
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

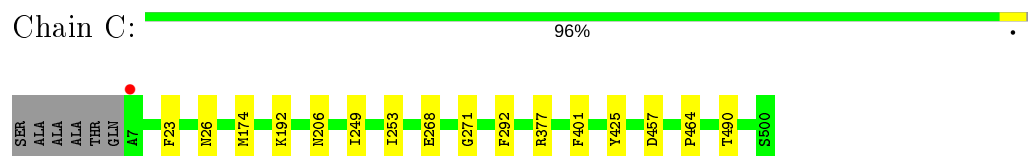
- Molecule 1: Aldehyde dehydrogenase



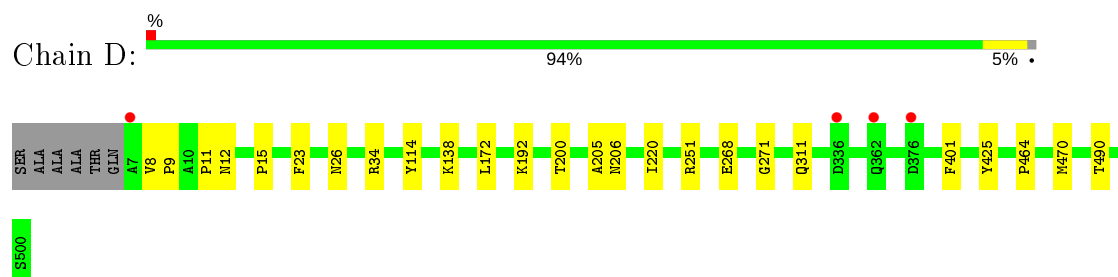
- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



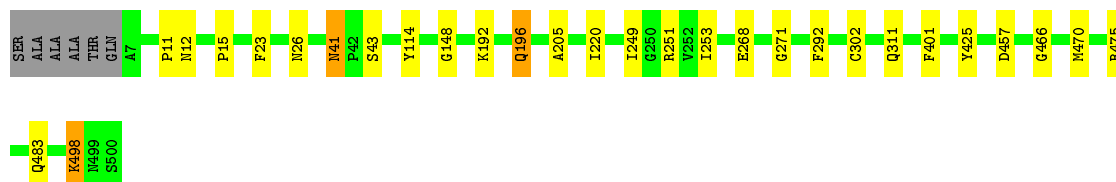
- Molecule 1: Aldehyde dehydrogenase

Chain E:  94% 5% •



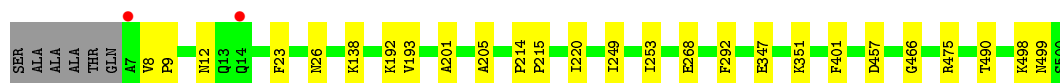
- Molecule 1: Aldehyde dehydrogenase

Chain F:  93% 5% ••

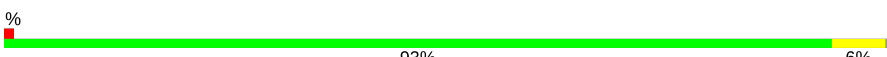


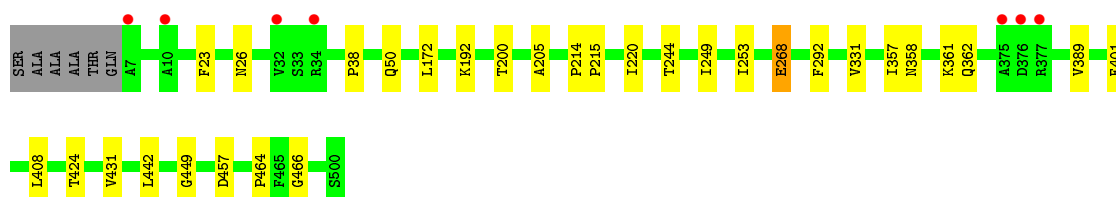
- Molecule 1: Aldehyde dehydrogenase

Chain G:  94% 5% •



- Molecule 1: Aldehyde dehydrogenase

Chain H:  93% 6% •



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.49Å 150.87Å 177.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.97 – 1.90 24.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (24.97-1.90) 98.5 (24.96-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.69 (at 1.90Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.181 , 0.213 0.180 , 0.213	Depositor DCC
$R_{free}$ test set	14729 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtrriage
Anisotropy	0.804	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	34432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4188e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, NAI, EDO, GAI

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	0.41	0/3882	0.62	0/5267
1	B	0.42	0/3882	0.63	0/5267
1	C	0.42	0/3882	0.64	0/5267
1	D	0.42	0/3882	0.63	0/5267
1	E	0.42	0/3882	0.63	0/5267
1	F	0.43	0/3882	0.65	0/5267
1	G	0.41	0/3882	0.63	1/5267 (0.0%)
1	H	0.39	0/3882	0.61	0/5267
All	All	0.41	0/31056	0.63	1/42136 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	12	ASN	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	0	3745	20	0
1	B	3798	0	3745	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3798	0	3745	7	0
1	D	3798	0	3745	13	0
1	E	3798	0	3745	21	0
1	F	3798	0	3745	21	0
1	G	3798	0	3745	13	0
1	H	3798	0	3745	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	8	0	9	0	0
4	B	8	0	10	0	0
4	C	8	0	9	0	0
4	D	8	0	10	0	0
4	E	8	0	10	0	0
4	F	8	0	9	0	0
4	G	12	0	14	0	0
4	H	4	0	5	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	4	0	6	0	0
5	D	4	0	6	0	0
5	E	4	0	6	0	0
5	F	8	0	12	0	0
5	H	4	0	6	0	0
6	A	44	0	27	0	0
6	B	44	0	27	0	0
6	C	44	0	27	0	0
6	D	44	0	27	0	0
6	E	44	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	44	0	27	0	0
6	G	44	0	27	0	0
6	H	44	0	27	0	0
7	A	418	0	0	2	0
7	B	498	0	0	2	0
7	C	470	0	0	0	0
7	D	426	0	0	1	0
7	E	466	0	0	1	0
7	F	498	0	0	3	0
7	G	437	0	0	0	0
7	H	371	0	0	1	0
All	All	34432	0	30300	121	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 2.

All (121) 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:F:196:GLN:HE21	1:F:196:GLN:H	1.24	0.85
1:H:357:ILE:HG22	1:H:361:LYS:HE3	1.64	0.80
1:A:336:ASP:HB3	7:A:5050:HOH:O	1.93	0.68
1:E:254:GLN:HE21	1:E:254:GLN:HA	1.59	0.67
1:E:124:MET:HE3	1:E:173:LEU:HD22	1.80	0.64
1:A:361:LYS:HE2	1:A:367:LEU:HD22	1.78	0.63
1:B:336:ASP:HB3	7:B:1167:HOH:O	1.97	0.63
1:F:41:ASN:HD22	1:F:41:ASN:C	2.03	0.61
1:F:302:CYS:SG	7:F:721:HOH:O	2.56	0.59
1:F:311:GLN:HG3	7:F:1167:HOH:O	2.03	0.58
1:E:120:VAL:HG12	1:E:124:MET:HE1	1.85	0.58
1:E:254:GLN:HA	1:E:254:GLN:NE2	2.19	0.58
1:E:358:ASN:HB2	7:E:912:HOH:O	2.03	0.58
1:F:41:ASN:ND2	1:F:43:SER:H	2.01	0.58
1:F:251:ARG:HH21	1:F:470:MET:HE1	1.72	0.55
1:F:41:ASN:HD22	1:F:43:SER:H	1.55	0.54
1:E:362:GLN:HE21	1:E:362:GLN:HA	1.72	0.54
1:F:292:PHE:HE1	1:F:457:ASP:HB2	1.73	0.54
1:F:148:GLY:O	1:F:498:LYS:HE2	2.08	0.53
1:F:196:GLN:NE2	1:F:196:GLN:H	2.00	0.53
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.44	0.52
1:F:249:ILE:O	1:F:253:ILE:HG12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.43	0.52
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.90	0.52
1:D:172:LEU:HD21	1:D:200:THR:HB	1.92	0.52
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.45	0.51
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.46	0.51
1:F:251:ARG:HH21	1:F:470:MET:CE	2.23	0.51
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.46	0.50
1:F:466:GLY:HA3	1:F:475:ARG:HD3	1.93	0.50
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.94	0.50
1:A:292:PHE:HE1	1:A:457:ASP:HB2	1.77	0.50
1:E:120:VAL:HG12	1:E:124:MET:CE	2.42	0.50
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.46	0.50
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.46	0.49
1:H:292:PHE:HE1	1:H:457:ASP:HB2	1.76	0.49
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.95	0.49
1:H:358:ASN:O	1:H:362:GLN:HG2	2.12	0.49
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.12	0.49
1:A:311:GLN:HG3	7:A:4711:HOH:O	2.12	0.49
1:C:292:PHE:HE1	1:C:457:ASP:HB2	1.77	0.49
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.95	0.49
1:C:249:ILE:O	1:C:253:ILE:HG12	2.12	0.48
1:D:251:ARG:NH2	1:D:470:MET:CE	2.77	0.48
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.96	0.48
1:D:251:ARG:NH2	1:D:470:MET:HE3	2.28	0.48
1:F:483:GLN:HB3	7:F:1145:HOH:O	2.13	0.48
1:H:389:VAL:HB	1:H:408:LEU:HG	1.96	0.47
1:C:174:MET:HA	1:C:174:MET:CE	2.45	0.47
1:D:311:GLN:HG3	7:D:955:HOH:O	2.13	0.47
1:B:292:PHE:HE1	1:B:457:ASP:HB2	1.79	0.47
1:H:38:PRO:HB3	1:H:50:GLN:HE22	1.80	0.47
1:E:271:GLY:HA2	1:E:425:TYR:CG	2.50	0.47
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.50	0.47
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.51	0.46
1:F:12:ASN:O	1:F:15:PRO:HD3	2.16	0.46
1:B:498:LYS:C	1:B:498:LYS:HD2	2.35	0.46
1:H:249:ILE:O	1:H:253:ILE:HG12	2.14	0.46
1:E:8:VAL:HA	1:E:9:PRO:HD3	1.82	0.45
1:F:196:GLN:N	1:F:196:GLN:HE21	2.03	0.45
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.52	0.45
1:B:466:GLY:HA3	1:B:475:ARG:HD3	1.99	0.45
1:A:159:VAL:HG12	1:A:187:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:498:LYS:HG2	1:G:499:ASN:N	2.32	0.45
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.17	0.45
1:F:271:GLY:HA2	1:F:425:TYR:CG	2.53	0.44
1:F:11:PRO:HB3	1:F:114:TYR:CE2	2.52	0.44
1:A:449:GLY:HA3	1:A:466:GLY:O	2.18	0.44
1:B:135:TRP:CE2	1:D:138:LYS:HD3	2.53	0.44
1:B:167:PRO:HD3	1:B:244:THR:HB	1.98	0.44
1:E:254:GLN:NE2	1:E:265:VAL:HG11	2.33	0.44
1:B:483:GLN:HB3	7:B:1028:HOH:O	2.17	0.43
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.53	0.43
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.19	0.43
1:B:249:ILE:O	1:B:253:ILE:HG12	2.18	0.43
1:G:292:PHE:HE1	1:G:457:ASP:HB2	1.84	0.43
1:H:449:GLY:HA3	1:H:466:GLY:O	2.19	0.43
1:E:254:GLN:HE21	1:E:254:GLN:CA	2.25	0.43
1:H:172:LEU:HD21	1:H:200:THR:HB	1.99	0.43
1:E:466:GLY:HA3	1:E:475:ARG:HD3	2.01	0.42
1:A:319:VAL:O	1:A:323:VAL:HG23	2.19	0.42
1:D:271:GLY:HA2	1:D:425:TYR:CG	2.55	0.42
1:A:460:GLY:HA3	1:B:146:ILE:HG13	2.02	0.42
1:D:205:ALA:HB2	1:D:220:ILE:HD12	2.00	0.42
1:H:424:THR:HG22	7:H:721:HOH:O	2.19	0.42
1:G:466:GLY:HA3	1:G:475:ARG:HD3	2.02	0.42
1:G:498:LYS:HE2	1:G:498:LYS:HB3	1.84	0.42
1:A:13:GLN:HG2	1:A:335:PHE:CG	2.54	0.42
1:A:33:SER:O	1:A:34:ARG:HB2	2.19	0.42
1:B:193:VAL:HG11	1:B:201:ALA:CB	2.49	0.42
1:H:214:PRO:HA	1:H:215:PRO:HD3	1.92	0.42
1:A:338:LYS:NZ	1:H:331:VAL:O	2.53	0.42
1:B:172:LEU:HD21	1:B:200:THR:HB	2.00	0.41
1:H:244:THR:HA	1:H:268:GLU:O	2.20	0.41
1:A:154:THR:HA	1:A:489:LYS:O	2.20	0.41
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.92	0.41
1:A:21:GLN:HB3	1:A:29:HIS:O	2.20	0.41
1:G:8:VAL:HA	1:G:9:PRO:HD3	1.89	0.41
1:A:107:THR:HG23	1:A:112:LYS:O	2.20	0.41
1:E:362:GLN:HA	1:E:362:GLN:NE2	2.34	0.41
1:B:235:HIS:HB3	1:B:238:VAL:HG23	2.02	0.41
1:B:389:VAL:HB	1:B:408:LEU:HG	2.02	0.41
1:A:167:PRO:HD3	1:A:244:THR:HB	2.03	0.41
1:G:214:PRO:HA	1:G:215:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:ASN:O	1:D:15:PRO:HD3	2.21	0.41
1:E:11:PRO:HB3	1:E:114:TYR:CE1	2.56	0.41
1:E:135:TRP:CE2	1:G:138:LYS:HD3	2.55	0.41
1:G:347:GLU:HG2	1:G:351:LYS:HE2	2.02	0.41
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.55	0.41
1:E:294:LEU:HD23	1:E:306:SER:HA	2.03	0.41
1:A:294:LEU:HD23	1:A:306:SER:HA	2.02	0.40
1:G:193:VAL:HG11	1:G:201:ALA:CB	2.51	0.40
1:D:8:VAL:HA	1:D:9:PRO:HD3	1.89	0.40
1:E:254:GLN:HE22	1:E:265:VAL:HB	1.85	0.40
1:G:249:ILE:O	1:G:253:ILE:HG12	2.22	0.40
1:C:271:GLY:HA2	1:C:425:TYR:CG	2.56	0.40
1:E:33:SER:O	1:E:34:ARG:HB2	2.21	0.40
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.56	0.40
1:H:431:VAL:HG21	1:H:442:LEU:HB3	2.03	0.40
1:B:161:VAL:HA	1:B:188:VAL:HG23	2.03	0.40
1:E:254:GLN:HE22	1:E:265:VAL:CB	2.35	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	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	B	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	C	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	D	492/500 (98%)	476 (97%)	16 (3%)	0	100	100
1	E	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	F	492/500 (98%)	476 (97%)	16 (3%)	0	100	100
1	G	492/500 (98%)	479 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	492/500 (98%)	475 (96%)	17 (4%)	0	100	100
All	All	3936/4000 (98%)	3818 (97%)	118 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	399/402 (99%)	396 (99%)	3 (1%)	81	82
1	B	399/402 (99%)	396 (99%)	3 (1%)	81	82
1	C	399/402 (99%)	394 (99%)	5 (1%)	69	68
1	D	399/402 (99%)	394 (99%)	5 (1%)	69	68
1	E	399/402 (99%)	396 (99%)	3 (1%)	81	82
1	F	399/402 (99%)	393 (98%)	6 (2%)	65	62
1	G	399/402 (99%)	396 (99%)	3 (1%)	81	82
1	H	399/402 (99%)	396 (99%)	3 (1%)	81	82
All	All	3192/3216 (99%)	3161 (99%)	31 (1%)	76	76

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LYS
1	A	268	GLU
1	A	401	PHE
1	B	192	LYS
1	B	268	GLU
1	B	401	PHE
1	C	192	LYS
1	C	206	ASN
1	C	268	GLU
1	C	377	ARG

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Mol	Chain	Res	Type
1	C	401	PHE
1	D	34	ARG
1	D	192	LYS
1	D	206	ASN
1	D	268	GLU
1	D	401	PHE
1	E	192	LYS
1	E	268	GLU
1	E	401	PHE
1	F	41	ASN
1	F	192	LYS
1	F	196	GLN
1	F	268	GLU
1	F	401	PHE
1	F	498	LYS
1	G	192	LYS
1	G	268	GLU
1	G	401	PHE
1	H	192	LYS
1	H	268	GLU
1	H	401	PHE

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

Mol	Chain	Res	Type
1	B	483	GLN
1	C	13	GLN
1	C	26	ASN
1	D	14	GLN
1	D	175	GLN
1	D	362	GLN
1	D	440	ASN
1	E	50	GLN
1	E	254	GLN
1	E	275	ASN
1	E	362	GLN
1	F	29	HIS
1	F	41	ASN
1	F	175	GLN
1	F	196	GLN
1	F	358	ASN
1	F	362	GLN

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Mol	Chain	Res	Type
1	G	13	GLN
1	G	29	HIS
1	G	50	GLN
1	H	50	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	GAI	H	603	-	3,3,3	1.79	1 (33%)	3,3,3	1.05	0
4	GAI	A	4604	-	3,3,3	1.05	0	3,3,3	1.06	0
6	NAI	D	606	2	42,48,48	2.16	9 (21%)	47,73,73	1.32	8 (17%)
6	NAI	B	606	2	42,48,48	2.17	8 (19%)	47,73,73	1.35	7 (14%)
6	NAI	G	606	2	42,48,48	2.09	7 (16%)	47,73,73	1.33	8 (17%)
4	GAI	G	604	-	3,3,3	1.13	0	3,3,3	0.99	0
6	NAI	H	605	2	42,48,48	2.14	8 (19%)	47,73,73	1.26	4 (8%)
5	EDO	F	605	-	3,3,3	0.64	0	2,2,2	0.22	0
5	EDO	D	605	-	3,3,3	0.43	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	E	605	-	3,3,3	0.48	0	2,2,2	0.29	0
6	NAI	E	606	2	42,48,48	2.20	7 (16%)	47,73,73	1.39	10 (21%)
5	EDO	A	4605	-	3,3,3	0.50	0	2,2,2	0.31	0
5	EDO	F	606	-	3,3,3	0.50	0	2,2,2	0.28	0
4	GAI	B	604	-	3,3,3	1.57	1 (33%)	3,3,3	0.98	0
6	NAI	A	4606	2	42,48,48	2.13	8 (19%)	47,73,73	1.30	6 (12%)
5	EDO	B	605	-	3,3,3	0.48	0	2,2,2	0.29	0
6	NAI	C	606	2	42,48,48	2.01	8 (19%)	47,73,73	1.50	8 (17%)
4	GAI	G	605	-	3,3,3	1.33	1 (33%)	3,3,3	0.97	0
5	EDO	C	605	-	3,3,3	0.51	0	2,2,2	0.32	0
4	GAI	C	604	-	3,3,3	1.32	1 (33%)	3,3,3	1.05	0
4	GAI	G	603	-	3,3,3	1.30	1 (33%)	3,3,3	1.04	0
4	GAI	E	603	-	3,3,3	1.37	1 (33%)	3,3,3	0.97	0
6	NAI	F	607	2	42,48,48	2.11	6 (14%)	47,73,73	1.47	7 (14%)
4	GAI	C	603	-	3,3,3	1.28	0	3,3,3	1.07	0
4	GAI	B	603	-	3,3,3	1.43	1 (33%)	3,3,3	0.96	0
4	GAI	F	603	-	3,3,3	1.49	1 (33%)	3,3,3	0.93	0
4	GAI	D	603	-	3,3,3	1.62	1 (33%)	3,3,3	1.06	0
4	GAI	F	604	-	3,3,3	1.23	1 (33%)	3,3,3	0.94	0
4	GAI	E	604	-	3,3,3	1.31	1 (33%)	3,3,3	0.99	0
5	EDO	H	604	-	3,3,3	0.48	0	2,2,2	0.29	0
4	GAI	A	4603	-	3,3,3	1.48	1 (33%)	3,3,3	1.04	0
4	GAI	D	604	-	3,3,3	1.53	1 (33%)	3,3,3	0.95	0

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
6	NAI	G	606	2	-	1/25/72/72	0/5/5/5
6	NAI	D	606	2	-	2/25/72/72	0/5/5/5
6	NAI	E	606	2	-	2/25/72/72	0/5/5/5
6	NAI	B	606	2	-	1/25/72/72	0/5/5/5
5	EDO	H	604	-	-	0/1/1/1	-
5	EDO	A	4605	-	-	0/1/1/1	-
5	EDO	F	606	-	-	0/1/1/1	-
5	EDO	C	605	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAI	H	605	2	-	1/25/72/72	0/5/5/5
5	EDO	E	605	-	-	0/1/1/1	-
6	NAI	A	4606	2	-	2/25/72/72	0/5/5/5
5	EDO	F	605	-	-	0/1/1/1	-
5	EDO	D	605	-	-	0/1/1/1	-
5	EDO	B	605	-	-	0/1/1/1	-
6	NAI	F	607	2	-	2/25/72/72	0/5/5/5
6	NAI	C	606	2	-	2/25/72/72	0/5/5/5

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	606	NAI	C4N-C3N	-7.83	1.34	1.49
6	E	606	NAI	C4N-C3N	-7.73	1.34	1.49
6	H	605	NAI	C4N-C3N	-7.47	1.35	1.49
6	C	606	NAI	C4N-C3N	-7.20	1.35	1.49
6	G	606	NAI	C4N-C3N	-7.17	1.35	1.49
6	D	606	NAI	C4N-C3N	-7.16	1.35	1.49
6	F	607	NAI	C4N-C3N	-7.06	1.36	1.49
6	A	4606	NAI	C4N-C3N	-6.97	1.36	1.49
6	E	606	NAI	C7N-C3N	-6.11	1.35	1.48
6	A	4606	NAI	C7N-C3N	-5.91	1.36	1.48
6	F	607	NAI	C7N-C3N	-5.90	1.36	1.48
6	D	606	NAI	C7N-C3N	-5.67	1.36	1.48
6	G	606	NAI	C7N-C3N	-5.56	1.36	1.48
6	A	4606	NAI	C4N-C5N	-5.50	1.34	1.48
6	H	605	NAI	C4N-C5N	-5.50	1.34	1.48
6	E	606	NAI	C4N-C5N	-5.47	1.34	1.48
6	B	606	NAI	C4N-C5N	-5.43	1.34	1.48
6	G	606	NAI	C4N-C5N	-5.39	1.34	1.48
6	B	606	NAI	C7N-C3N	-5.31	1.37	1.48
6	D	606	NAI	C4N-C5N	-5.23	1.35	1.48
6	H	605	NAI	C7N-C3N	-5.19	1.37	1.48
6	F	607	NAI	C2A-N3A	5.09	1.40	1.32
6	C	606	NAI	C7N-C3N	-5.08	1.37	1.48
6	H	605	NAI	C2A-N3A	4.93	1.40	1.32
6	B	606	NAI	C2A-N3A	4.83	1.39	1.32
6	E	606	NAI	C2A-N3A	4.81	1.39	1.32
6	G	606	NAI	C2A-N3A	4.66	1.39	1.32
6	C	606	NAI	C4N-C5N	-4.63	1.36	1.48
6	D	606	NAI	C2A-N3A	4.53	1.39	1.32
6	F	607	NAI	C4N-C5N	-4.43	1.37	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4606	NAI	C2A-N3A	4.35	1.39	1.32
6	C	606	NAI	C2A-N3A	4.22	1.38	1.32
6	H	605	NAI	C2A-N1A	3.83	1.41	1.33
6	F	607	NAI	C6N-C5N	3.59	1.39	1.33
6	D	606	NAI	C2A-N1A	3.49	1.40	1.33
6	B	606	NAI	C6N-C5N	3.42	1.39	1.33
6	D	606	NAI	C6N-C5N	3.37	1.39	1.33
6	C	606	NAI	C6N-C5N	3.23	1.39	1.33
6	G	606	NAI	C2A-N1A	3.19	1.39	1.33
6	A	4606	NAI	C8A-N7A	3.17	1.40	1.34
6	D	606	NAI	C8A-N7A	3.17	1.40	1.34
6	F	607	NAI	C2A-N1A	3.15	1.39	1.33
6	A	4606	NAI	C2A-N1A	3.09	1.39	1.33
4	H	603	GAI	C-N1	3.08	1.37	1.30
6	B	606	NAI	C2A-N1A	3.07	1.39	1.33
6	G	606	NAI	C8A-N7A	2.95	1.40	1.34
6	E	606	NAI	C6N-C5N	2.93	1.38	1.33
6	C	606	NAI	C2A-N1A	2.92	1.39	1.33
6	A	4606	NAI	C6N-C5N	2.85	1.38	1.33
6	B	606	NAI	C8A-N7A	2.83	1.39	1.34
6	G	606	NAI	C6N-C5N	2.83	1.38	1.33
6	E	606	NAI	C2A-N1A	2.82	1.39	1.33
4	D	603	GAI	C-N1	2.79	1.36	1.30
6	C	606	NAI	C8A-N7A	2.74	1.39	1.34
4	B	604	GAI	C-N1	2.68	1.36	1.30
6	H	605	NAI	C6N-C5N	2.63	1.38	1.33
4	F	603	GAI	C-N1	2.58	1.36	1.30
6	E	606	NAI	C8A-N7A	2.57	1.39	1.34
4	D	604	GAI	C-N1	2.56	1.36	1.30
4	A	4603	GAI	C-N1	2.53	1.36	1.30
6	H	605	NAI	C8A-N7A	2.48	1.39	1.34
4	B	603	GAI	C-N1	2.47	1.35	1.30
6	H	605	NAI	C4A-N3A	2.37	1.38	1.35
4	E	603	GAI	C-N1	2.35	1.35	1.30
4	G	605	GAI	C-N1	2.30	1.35	1.30
6	D	606	NAI	C4A-N3A	2.26	1.38	1.35
6	C	606	NAI	C4A-N3A	2.26	1.38	1.35
4	E	604	GAI	C-N1	2.25	1.35	1.30
4	G	603	GAI	C-N1	2.23	1.35	1.30
6	A	4606	NAI	C4A-N3A	2.21	1.38	1.35
4	C	604	GAI	C-N1	2.20	1.35	1.30
6	D	606	NAI	O4B-C1B	2.19	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	606	NAI	C4A-N3A	2.17	1.38	1.35
4	F	604	GAI	C-N1	2.12	1.35	1.30

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	607	NAI	N3A-C2A-N1A	-4.52	121.62	128.68
6	G	606	NAI	O4B-C1B-C2B	-4.42	100.47	106.93
6	A	4606	NAI	N3A-C2A-N1A	-4.32	121.93	128.68
6	H	605	NAI	N3A-C2A-N1A	-4.18	122.14	128.68
6	D	606	NAI	N3A-C2A-N1A	-4.03	122.38	128.68
6	C	606	NAI	N3A-C2A-N1A	-3.99	122.44	128.68
6	C	606	NAI	O4B-C1B-C2B	-3.84	101.32	106.93
6	E	606	NAI	N3A-C2A-N1A	-3.82	122.70	128.68
6	F	607	NAI	O4B-C1B-C2B	-3.78	101.40	106.93
6	B	606	NAI	C2B-C3B-C4B	-3.75	95.36	102.64
6	F	607	NAI	C3N-C7N-N7N	3.49	123.87	117.67
6	C	606	NAI	O7N-C7N-N7N	-3.26	115.27	122.88
6	B	606	NAI	N3A-C2A-N1A	-3.16	123.73	128.68
6	G	606	NAI	N3A-C2A-N1A	-3.10	123.83	128.68
6	F	607	NAI	C1D-N1N-C2N	-3.00	116.11	121.11
6	C	606	NAI	C2B-C3B-C4B	-2.97	96.87	102.64
6	D	606	NAI	PN-O3-PA	-2.96	122.66	132.83
6	A	4606	NAI	C3N-C7N-N7N	2.95	122.91	117.67
6	B	606	NAI	O4B-C1B-C2B	-2.81	102.82	106.93
6	C	606	NAI	C1D-N1N-C2N	-2.79	116.46	121.11
6	B	606	NAI	O7N-C7N-N7N	-2.78	116.37	122.88
6	E	606	NAI	C2B-C3B-C4B	-2.68	97.43	102.64
6	F	607	NAI	O7N-C7N-N7N	-2.67	116.64	122.88
6	E	606	NAI	C3N-C7N-N7N	2.66	122.39	117.67
6	G	606	NAI	O7N-C7N-N7N	-2.63	116.72	122.88
6	E	606	NAI	C1D-N1N-C2N	-2.62	116.75	121.11
6	D	606	NAI	O7N-C7N-N7N	-2.59	116.83	122.88
6	F	607	NAI	C2B-C3B-C4B	-2.54	97.71	102.64
6	B	606	NAI	O4D-C4D-C3D	-2.52	100.12	105.11
6	E	606	NAI	C5A-C6A-N6A	2.52	124.17	120.35
6	G	606	NAI	PN-O3-PA	-2.48	124.31	132.83
6	C	606	NAI	C3D-C2D-C1D	-2.44	96.79	101.43
6	G	606	NAI	C5A-C6A-N6A	2.44	124.06	120.35
6	A	4606	NAI	C1D-N1N-C2N	-2.40	117.12	121.11
6	E	606	NAI	O4D-C1D-N1N	2.39	112.73	108.06
6	B	606	NAI	O4B-C4B-C3B	2.36	109.79	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4606	NAI	O7N-C7N-N7N	-2.31	117.49	122.88
6	H	605	NAI	C3N-C2N-N1N	-2.30	119.81	123.10
6	G	606	NAI	C3N-C7N-N7N	2.29	121.74	117.67
6	G	606	NAI	C2D-C3D-C4D	-2.29	98.19	102.64
6	A	4606	NAI	C3N-C2N-N1N	-2.24	119.90	123.10
6	D	606	NAI	O4D-C4D-C3D	-2.24	100.68	105.11
6	E	606	NAI	O5B-C5B-C4B	2.21	116.59	108.99
6	C	606	NAI	C5A-C6A-N6A	2.20	123.70	120.35
6	H	605	NAI	O7N-C7N-N7N	-2.20	117.74	122.88
6	D	606	NAI	C3N-C2N-N1N	-2.19	119.97	123.10
6	D	606	NAI	O4B-C1B-C2B	-2.18	103.74	106.93
6	C	606	NAI	O7N-C7N-C3N	2.16	124.97	120.90
6	D	606	NAI	C5A-C6A-N6A	2.15	123.62	120.35
6	D	606	NAI	C1D-N1N-C2N	-2.15	117.53	121.11
6	H	605	NAI	C4A-C5A-N7A	2.14	111.63	109.40
6	E	606	NAI	C2D-C3D-C4D	-2.07	98.62	102.64
6	B	606	NAI	C5A-C6A-N6A	2.06	123.49	120.35
6	G	606	NAI	C1D-N1N-C2N	-2.04	117.71	121.11
6	E	606	NAI	C3N-C2N-N1N	-2.04	120.18	123.10
6	A	4606	NAI	C2B-C3B-C4B	-2.02	98.71	102.64
6	F	607	NAI	O4D-C1D-N1N	2.02	112.00	108.06
6	E	606	NAI	PN-O3-PA	-2.00	125.95	132.83

There are no chirality outliers.

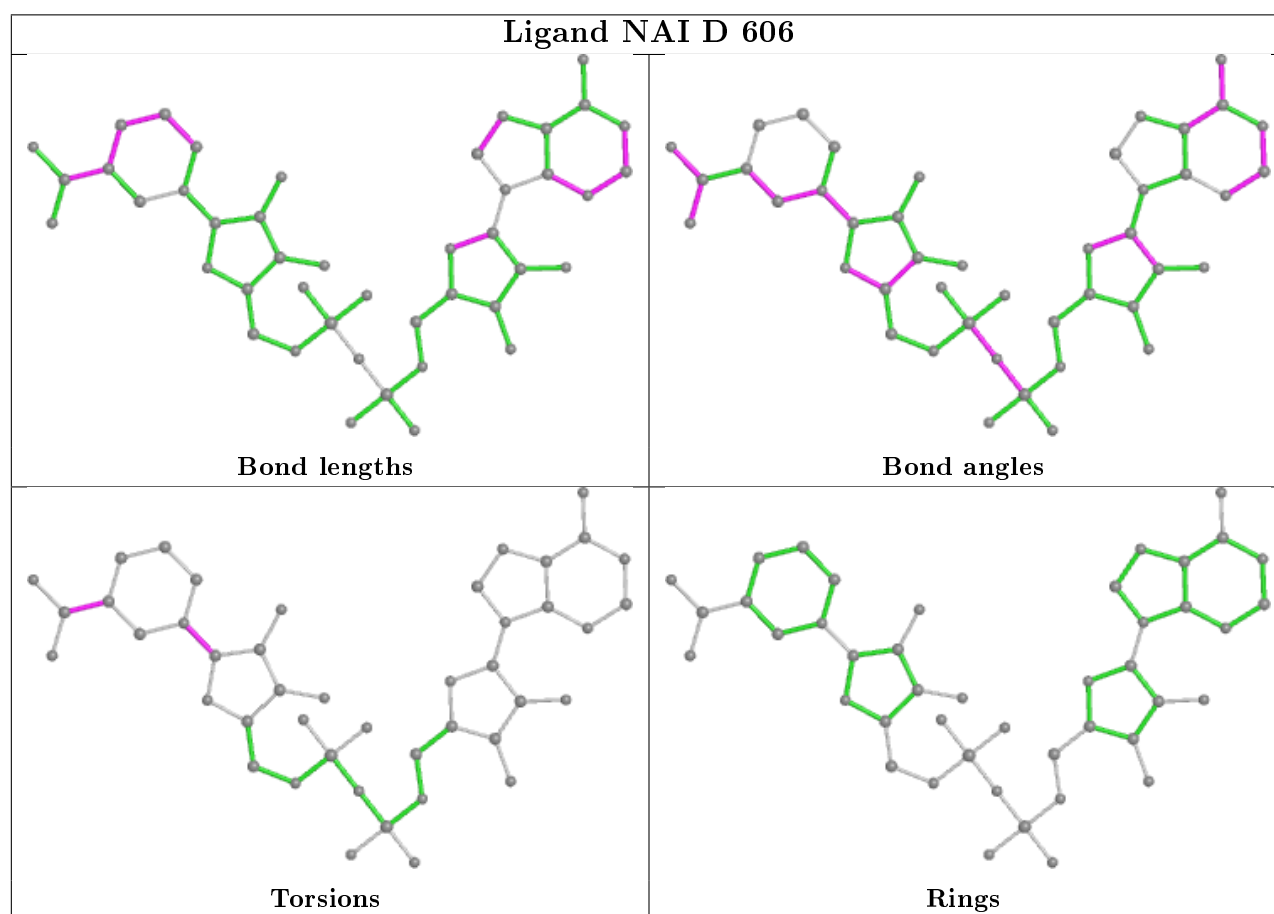
All (13) torsion outliers are listed below:

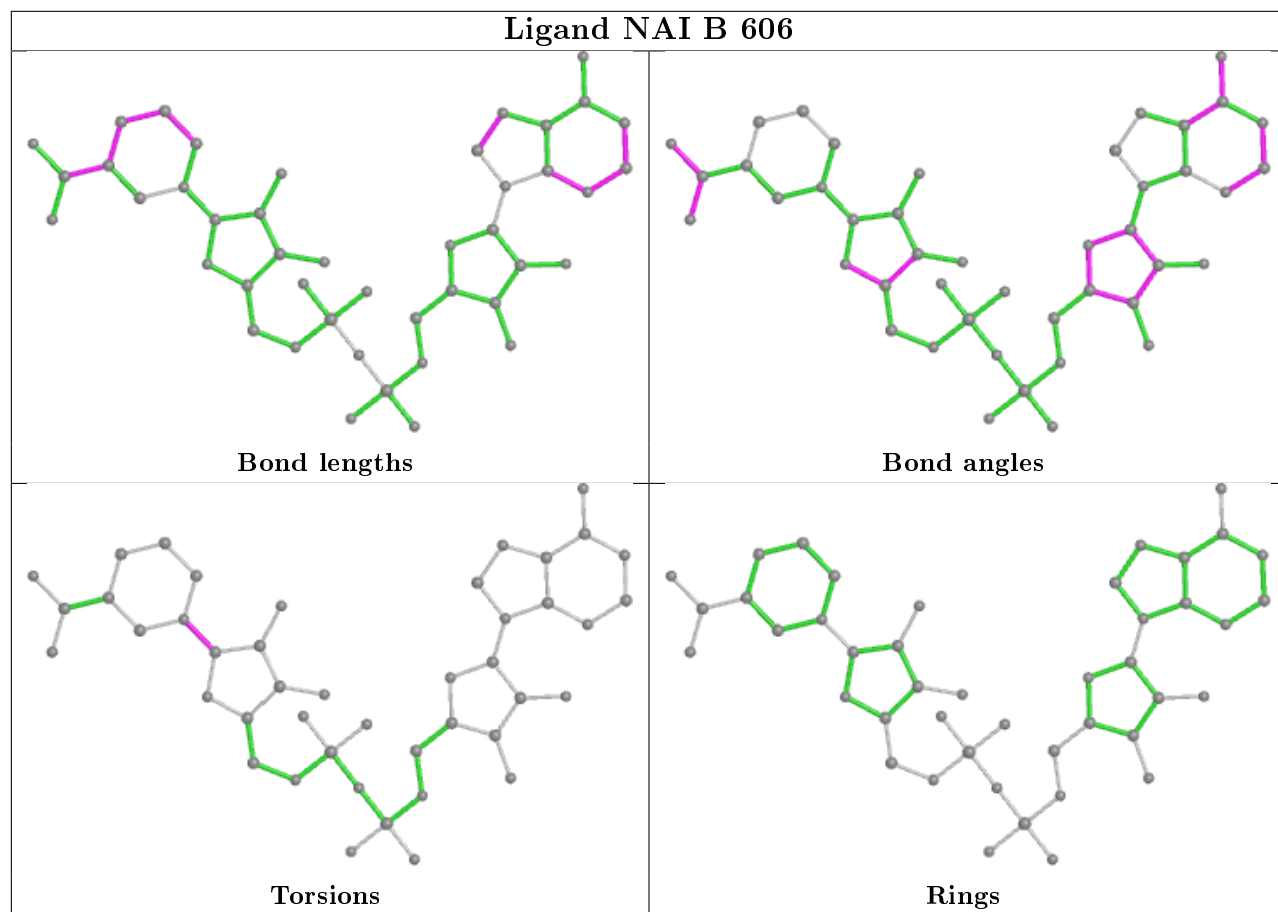
Mol	Chain	Res	Type	Atoms
6	H	605	NAI	O4D-C1D-N1N-C2N
6	G	606	NAI	O4D-C1D-N1N-C2N
6	B	606	NAI	O4D-C1D-N1N-C2N
6	E	606	NAI	O4D-C1D-N1N-C2N
6	A	4606	NAI	O4D-C1D-N1N-C2N
6	D	606	NAI	O4D-C1D-N1N-C2N
6	C	606	NAI	O4D-C1D-N1N-C2N
6	F	607	NAI	O4D-C1D-N1N-C2N
6	F	607	NAI	C2N-C3N-C7N-N7N
6	D	606	NAI	C2N-C3N-C7N-N7N
6	E	606	NAI	C5B-O5B-PA-O2A
6	A	4606	NAI	C2N-C3N-C7N-N7N
6	C	606	NAI	C2N-C3N-C7N-N7N

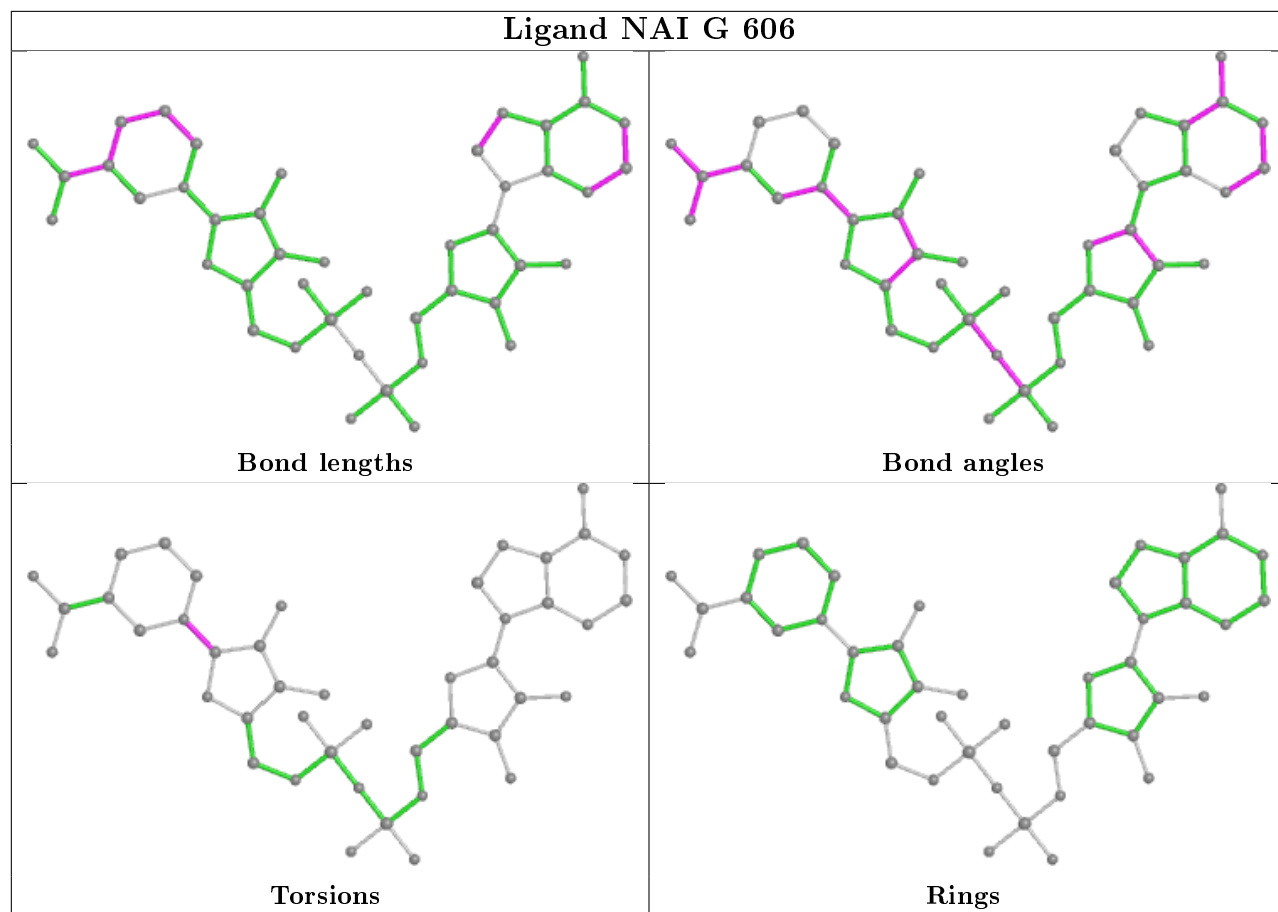
There are no ring outliers.

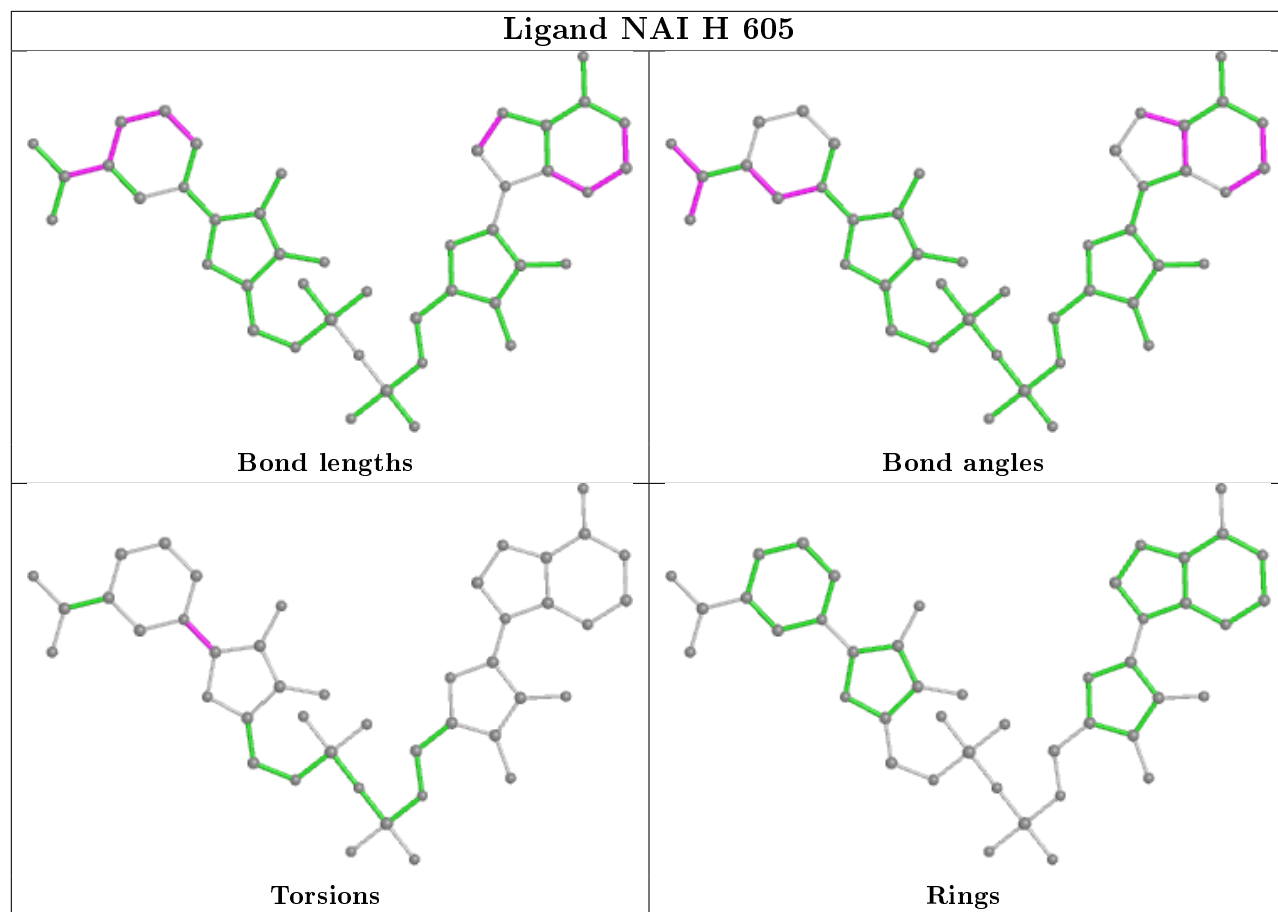
No monomer is involved in short contacts.

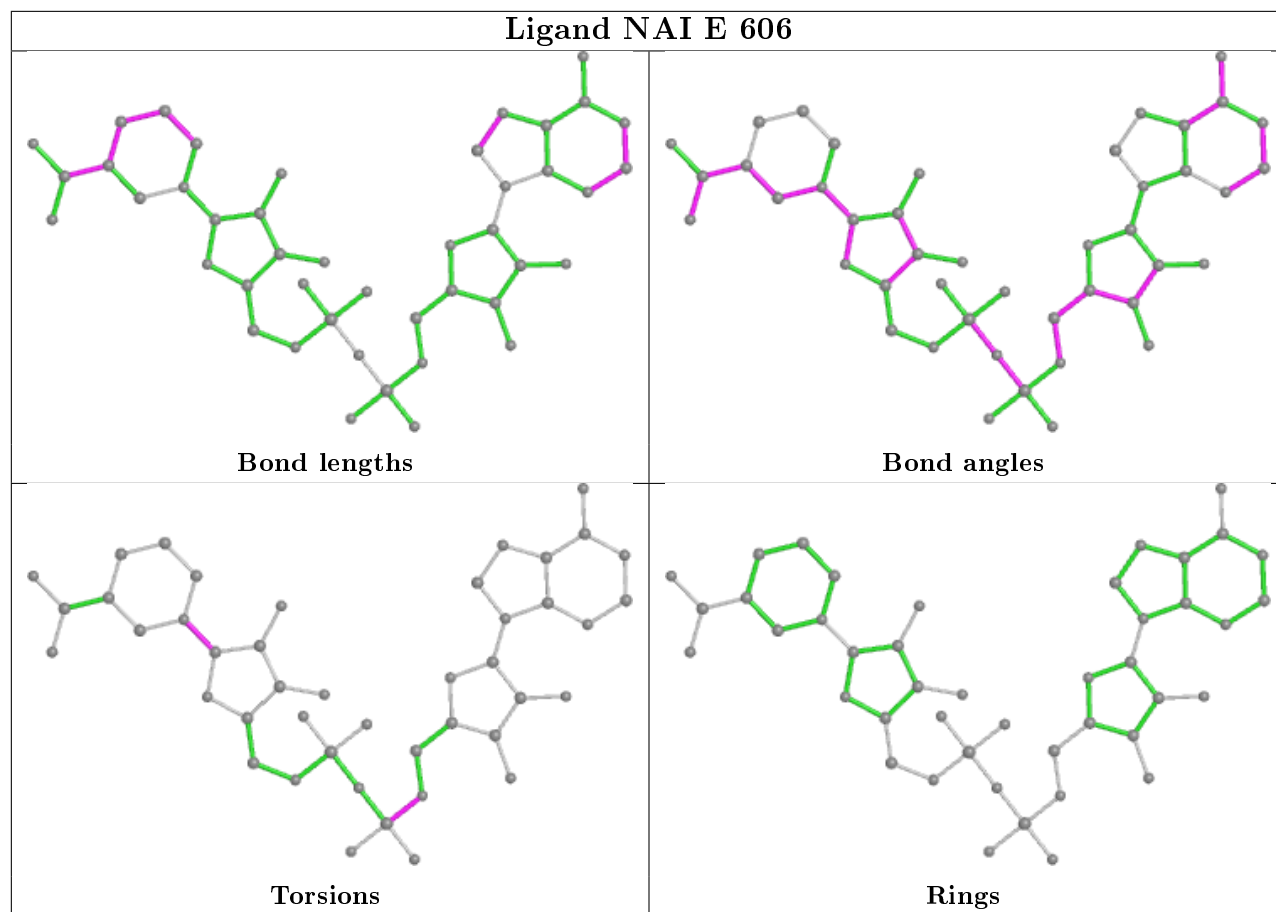
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

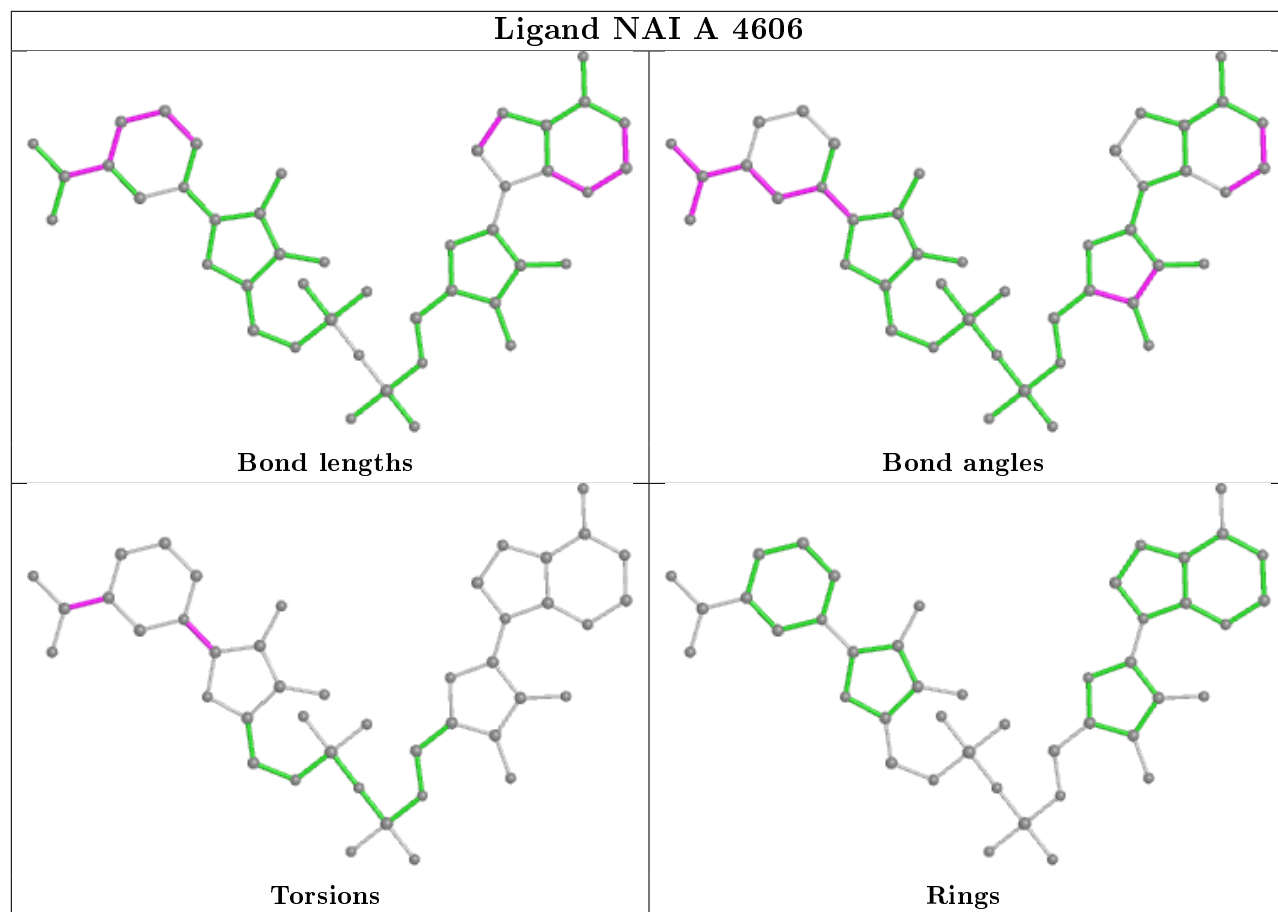




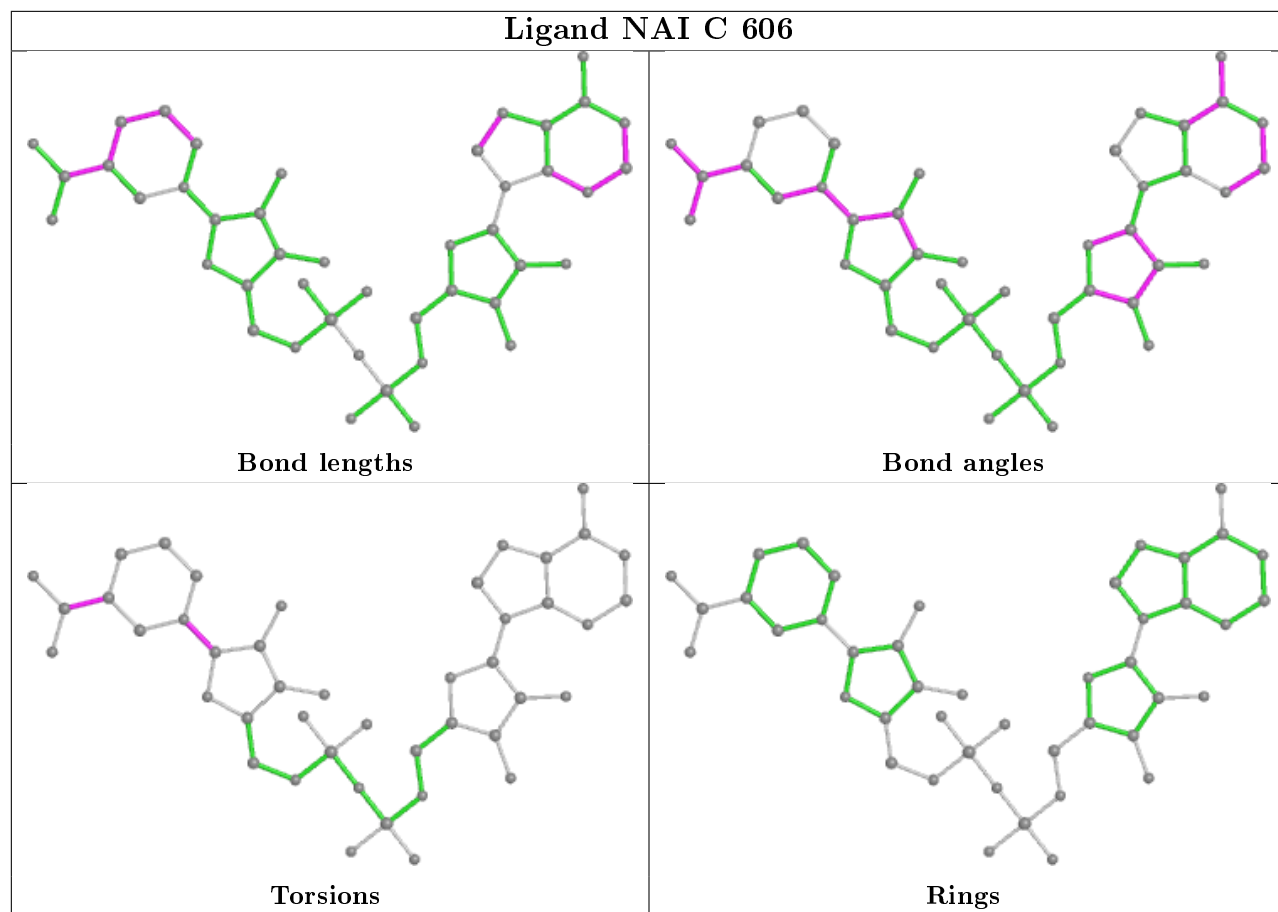


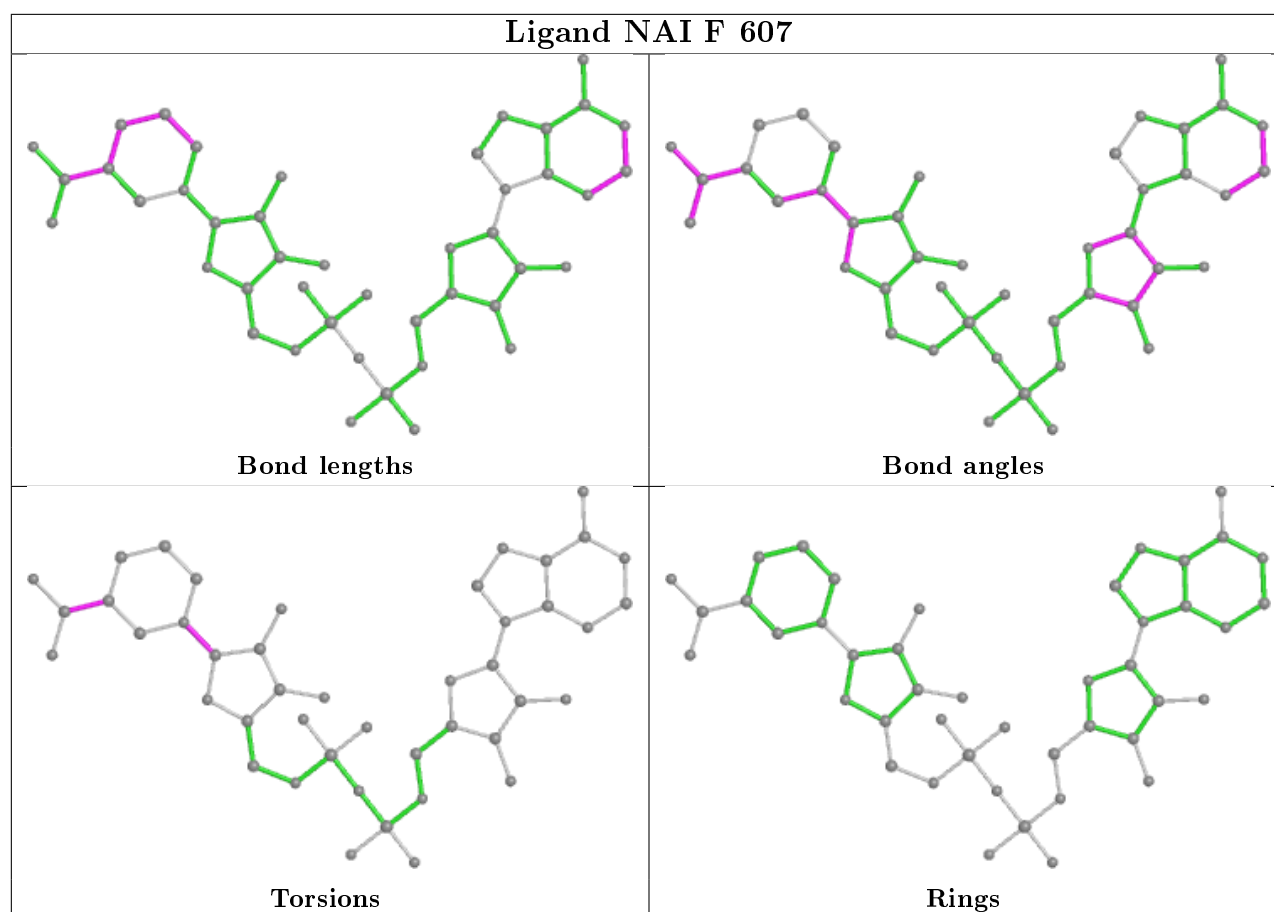












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	494/500 (98%)	-0.20	4 (0%) 86 87	12, 21, 35, 47	0
1	B	494/500 (98%)	-0.37	2 (0%) 92 93	13, 19, 27, 41	0
1	C	494/500 (98%)	-0.44	1 (0%) 95 95	12, 17, 27, 37	0
1	D	494/500 (98%)	-0.24	4 (0%) 86 87	12, 21, 33, 49	0
1	E	494/500 (98%)	-0.37	2 (0%) 92 93	12, 19, 31, 49	0
1	F	494/500 (98%)	-0.49	0 100 100	10, 16, 27, 34	0
1	G	494/500 (98%)	-0.28	2 (0%) 92 93	13, 21, 32, 49	0
1	H	494/500 (98%)	-0.02	7 (1%) 75 77	13, 24, 42, 58	0
All	All	3952/4000 (98%)	-0.30	22 (0%) 89 90	10, 20, 33, 58	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ALA	6.6
1	H	376	ASP	5.8
1	G	7	ALA	5.7
1	A	7	ALA	4.8
1	H	7	ALA	4.3
1	D	7	ALA	3.9
1	D	376	ASP	3.8
1	E	376	ASP	3.8
1	H	10	ALA	3.3
1	A	376	ASP	3.2
1	H	377	ARG	3.1
1	G	14	GLN	2.9
1	H	34	ARG	2.7
1	C	7	ALA	2.4
1	E	34	ARG	2.4
1	B	14	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	377	ARG	2.3
1	A	14	GLN	2.3
1	H	375	ALA	2.2
1	D	336	ASP	2.2
1	H	32	VAL	2.1
1	D	362	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GAI	C	604	4/4	0.84	0.22	34,35,37,37	0
4	GAI	G	605	4/4	0.86	0.29	37,39,40,40	0
4	GAI	B	604	4/4	0.88	0.27	34,35,35,36	0
4	GAI	G	604	4/4	0.91	0.27	34,35,35,37	0
2	MG	H	601	1/1	0.92	0.08	31,31,31,31	0
4	GAI	D	604	4/4	0.92	0.15	35,35,35,35	0
2	MG	G	601	1/1	0.93	0.09	28,28,28,28	0
4	GAI	A	4604	4/4	0.93	0.21	35,37,37,38	0
6	NAI	H	605	44/44	0.94	0.10	23,26,29,30	0
2	MG	E	601	1/1	0.94	0.07	30,30,30,30	0
4	GAI	E	604	4/4	0.94	0.12	32,33,33,34	0
4	GAI	F	604	4/4	0.94	0.15	39,40,40,41	0
5	EDO	C	605	4/4	0.95	0.11	23,28,30,30	0
5	EDO	F	606	4/4	0.95	0.12	24,27,28,29	0
4	GAI	H	603	4/4	0.95	0.11	23,24,25,26	0
5	EDO	B	605	4/4	0.95	0.17	25,25,27,27	0
4	GAI	B	603	4/4	0.95	0.11	24,27,28,29	0

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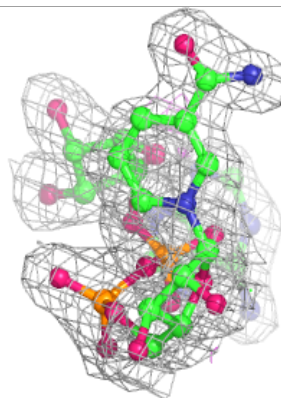
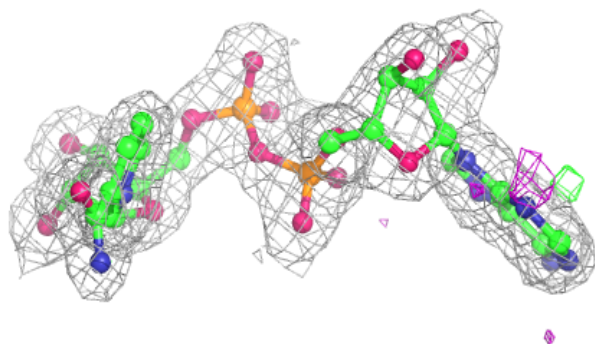
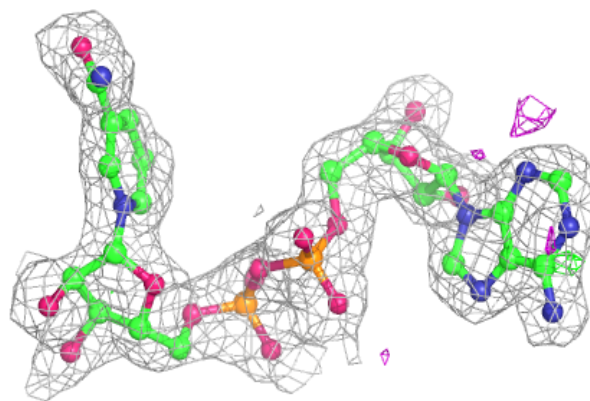
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GAI	D	603	4/4	0.95	0.11	23,29,30,30	0
3	NA	H	602	1/1	0.95	0.08	30,30,30,30	0
5	EDO	H	604	4/4	0.95	0.11	25,26,28,29	0
6	NAI	G	606	44/44	0.95	0.09	19,22,25,27	0
4	GAI	F	603	4/4	0.96	0.08	20,21,23,23	0
5	EDO	A	4605	4/4	0.96	0.10	23,26,28,29	0
6	NAI	D	606	44/44	0.96	0.09	17,22,26,27	0
5	EDO	E	605	4/4	0.96	0.13	20,26,27,28	0
5	EDO	D	605	4/4	0.96	0.17	22,27,28,28	0
4	GAI	A	4603	4/4	0.96	0.10	22,24,24,25	0
2	MG	C	601	1/1	0.96	0.04	27,27,27,27	0
2	MG	A	4601	1/1	0.96	0.12	32,32,32,32	0
2	MG	F	601	1/1	0.97	0.05	25,25,25,25	0
6	NAI	A	4606	44/44	0.97	0.08	19,23,25,26	0
5	EDO	F	605	4/4	0.97	0.08	22,25,27,27	0
6	NAI	B	606	44/44	0.97	0.08	18,21,23,24	0
3	NA	A	4602	1/1	0.97	0.07	25,25,25,25	0
6	NAI	C	606	44/44	0.97	0.07	15,19,21,23	0
2	MG	D	601	1/1	0.97	0.05	27,27,27,27	0
4	GAI	C	603	4/4	0.97	0.09	19,20,20,22	0
4	GAI	E	603	4/4	0.98	0.08	20,23,23,23	0
3	NA	D	602	1/1	0.98	0.06	27,27,27,27	0
6	NAI	E	606	44/44	0.98	0.06	16,20,23,24	0
3	NA	F	602	1/1	0.98	0.05	19,19,19,19	0
6	NAI	F	607	44/44	0.98	0.06	13,16,19,22	0
3	NA	G	602	1/1	0.98	0.05	21,21,21,21	0
4	GAI	G	603	4/4	0.98	0.09	24,25,26,28	0
3	NA	B	602	1/1	0.99	0.04	21,21,21,21	0
2	MG	B	601	1/1	0.99	0.05	29,29,29,29	0
3	NA	E	602	1/1	0.99	0.10	25,25,25,25	0
3	NA	C	602	1/1	1.00	0.03	21,21,21,21	0

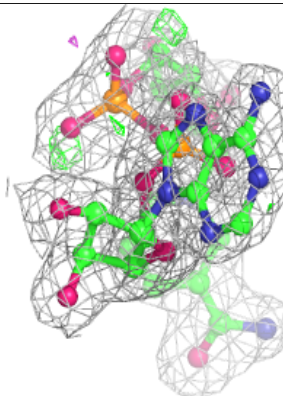
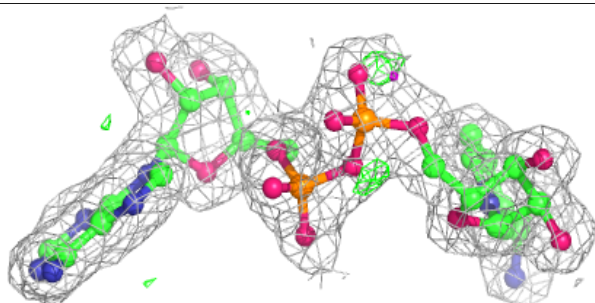
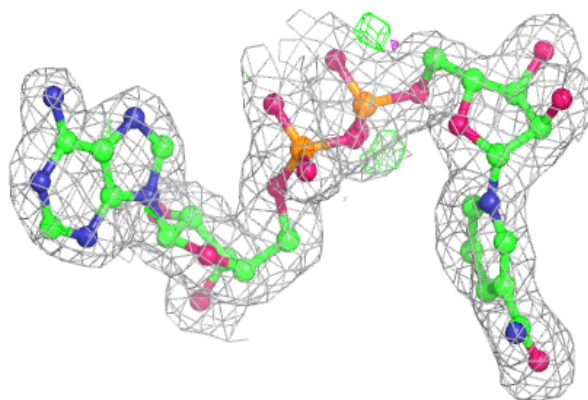
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAI H 605:**

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

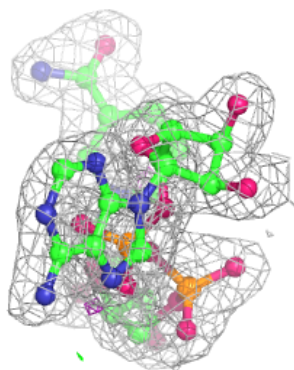
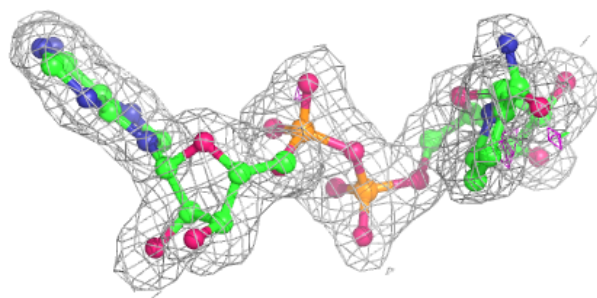
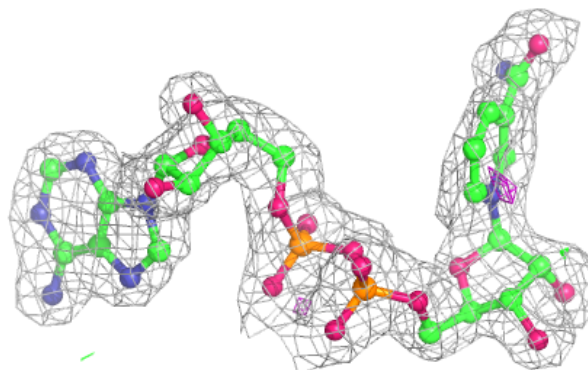
**Electron density around NAI G 606:**

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

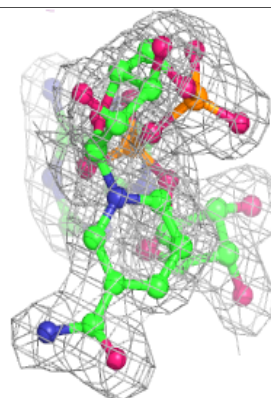
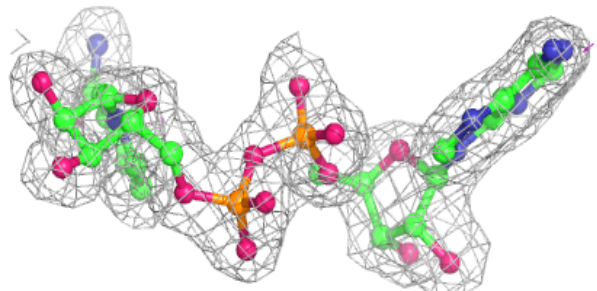
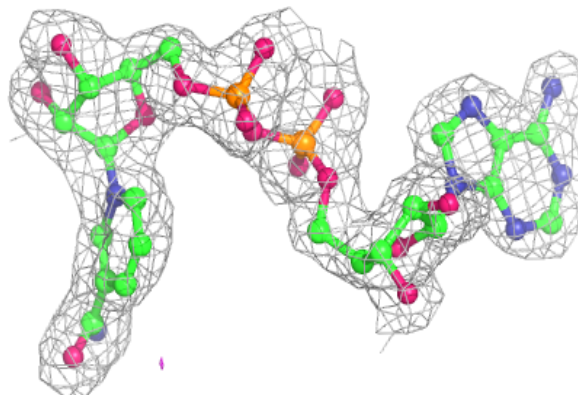


**Electron density around NAI D 606:**

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

**Electron density around NAI A 4606:**

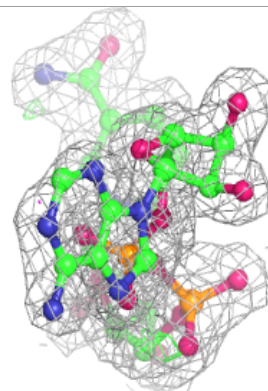
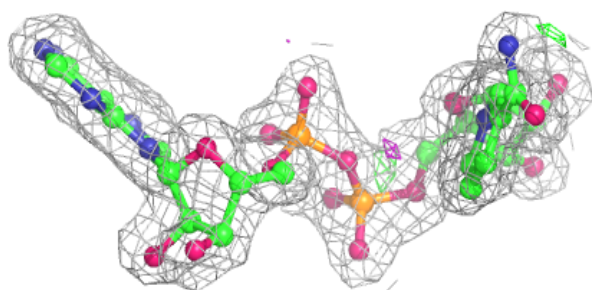
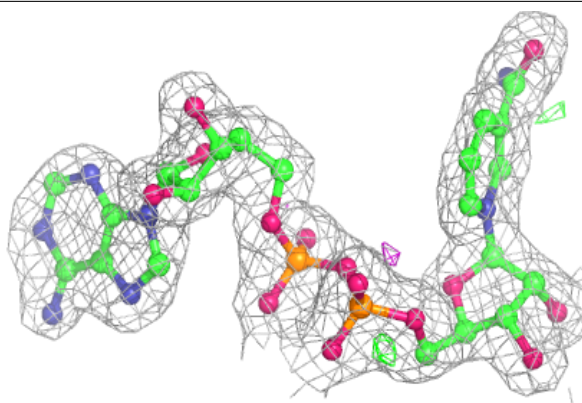
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



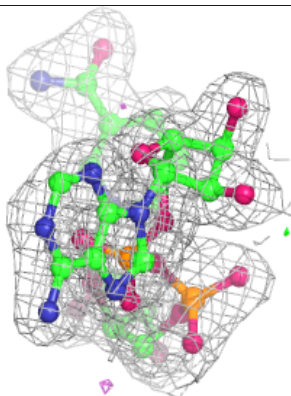
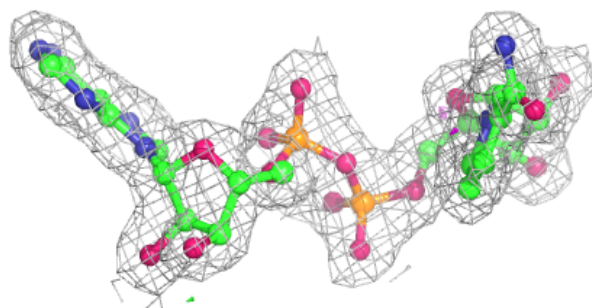
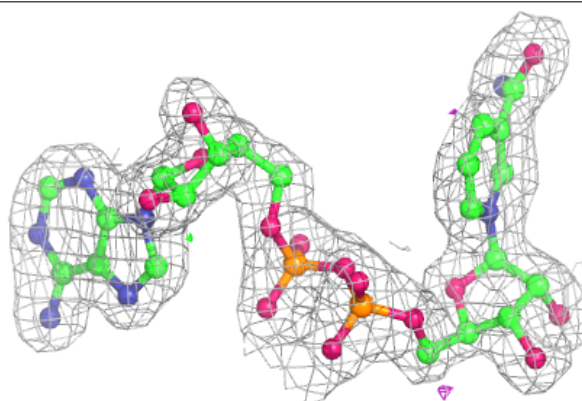


**Electron density around NAI B 606:**

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

**Electron density around NAI C 606:**

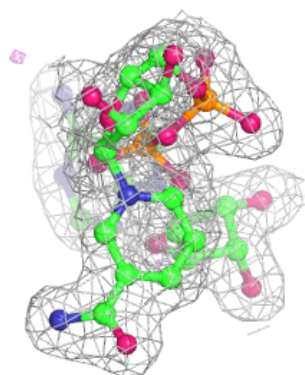
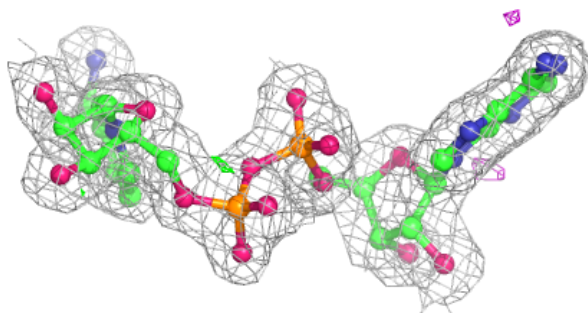
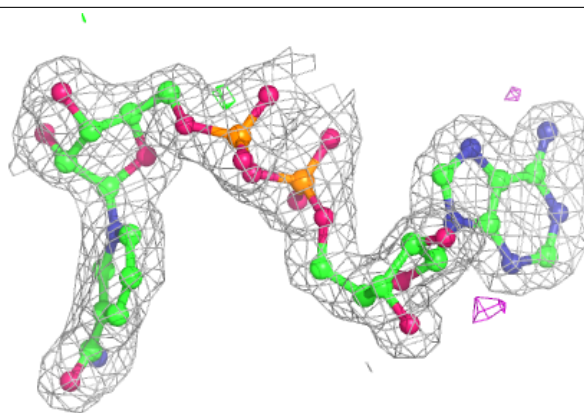
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



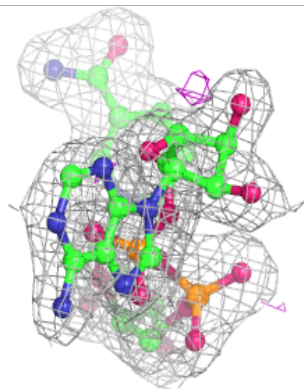
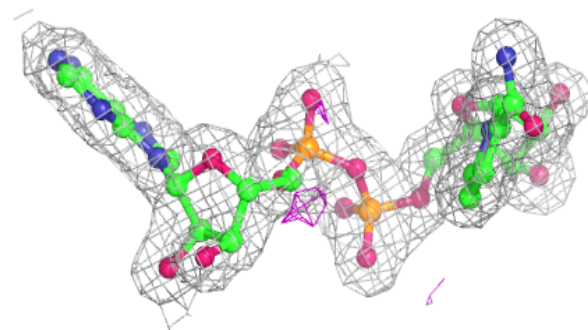
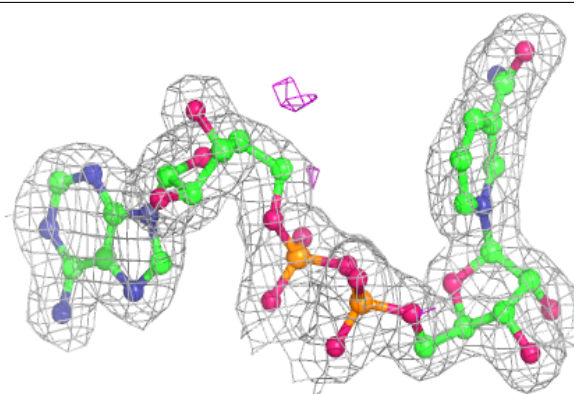


**Electron density around NAI E 606:**

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

**Electron density around NAI F 607:**

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



## 6.5 Other polymers

There are no such residues in this entry.