



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2024 – 04:10 PM JST

PDB ID : 8K32  
Title : The complex structure of SLKARI with NADH at 2.12-angstrom resolution  
Authors : Chen, C.Y.; Huang, C.H.  
Deposited on : 2023-07-14  
Resolution : 2.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

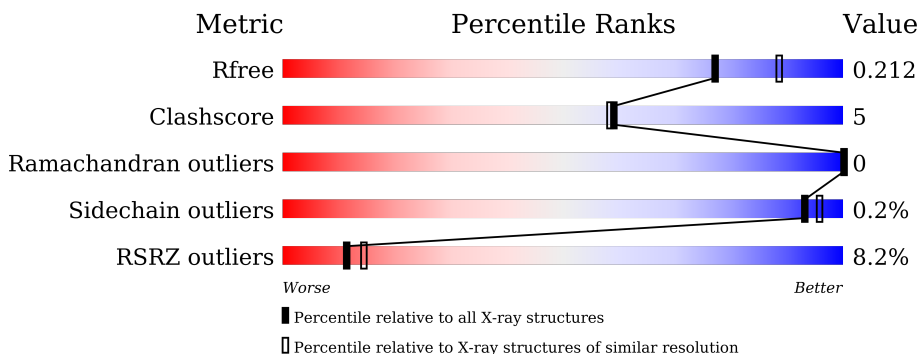
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	<p>2% 92% 7%</p>
1	B	334	<p>22% 85% 14%</p>
1	C	334	<p>7% 88% 12%</p>
1	D	334	<p>% 93% 6%</p>

## 2 Entry composition [i](#)

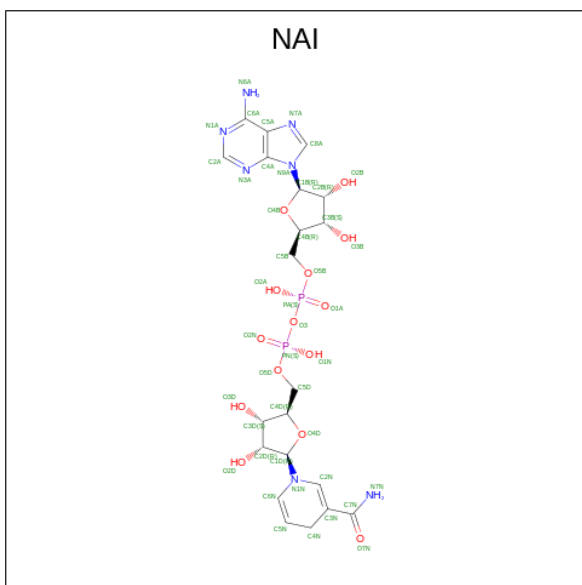
There are 7 unique types of molecules in this entry. The entry contains 11652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ketol-acid reductoisomerase (NADP(+)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	332	Total 2561	C 1631	N 438	O 481	S 11	0	0	0
1	B	332	Total 2561	C 1631	N 438	O 481	S 11	0	0	0
1	C	333	Total 2570	C 1637	N 440	O 482	S 11	0	0	0
1	D	332	Total 2561	C 1631	N 438	O 481	S 11	0	0	0

- 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 depositor).



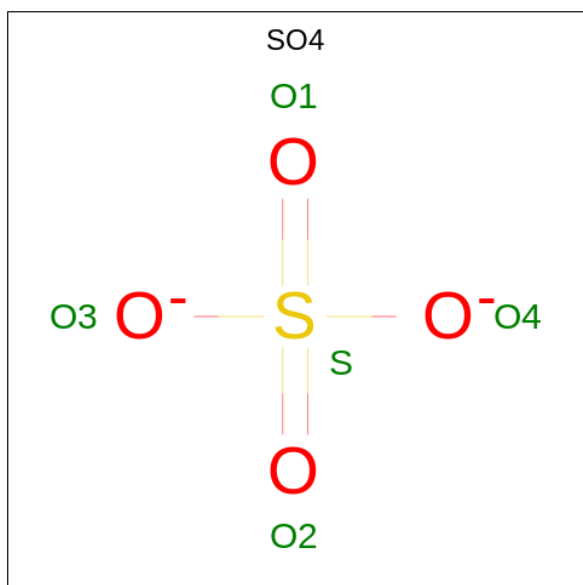
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

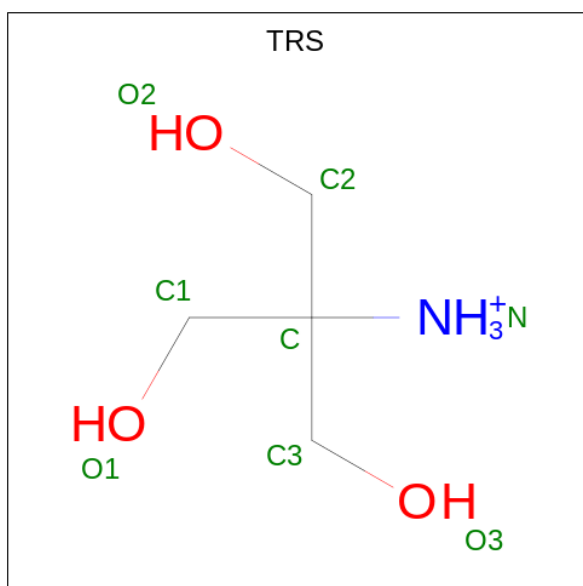
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

- 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	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is water.

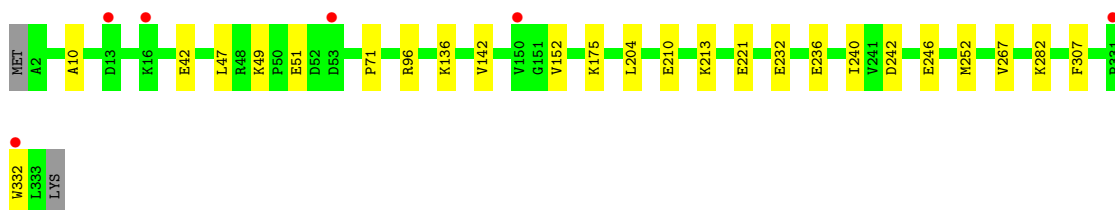
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	371	Total	O	0	0
			371	371		
7	B	179	Total	O	0	0
			179	179		
7	C	221	Total	O	0	0
			221	221		
7	D	311	Total	O	0	0
			311	311		

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


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

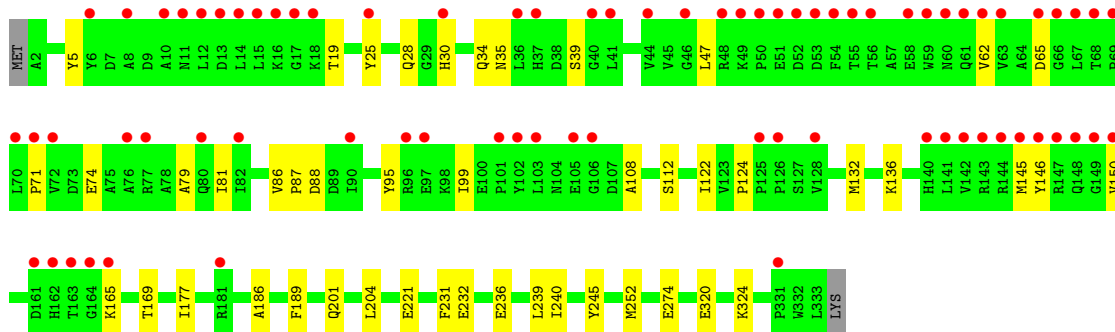
- Molecule 1: Ketol-acid reductoisomerase (NADP(+))

Chain A: 




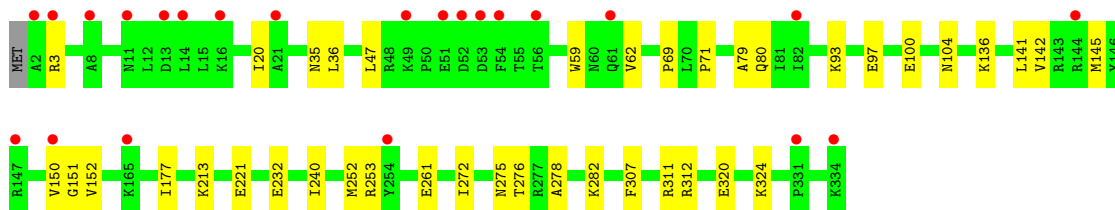
- Molecule 1: Ketol-acid reductoisomerase (NADP(+))

Chain B: 



- Molecule 1: Ketol-acid reductoisomerase (NADP(+))

Chain C: 



- Molecule 1: Ketol-acid reductoisomerase (NADP(+))



Chain D:  %



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.56Å 131.56Å 297.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.09 – 2.12 29.09 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.09-2.12) 97.4 (29.09-2.12)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.67 (at 2.12Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, $R_{free}$	0.179 , 0.212 0.179 , 0.212	Depositor DCC
$R_{free}$ test set	5081 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtrriage
Anisotropy	0.074	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11652	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

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

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, TRS, EDO, MG, NAI

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	0.48	0/2612	0.63	1/3540 (0.0%)
1	B	0.37	0/2612	0.53	0/3540
1	C	0.39	0/2621	0.55	2/3551 (0.1%)
1	D	0.43	0/2612	0.57	0/3540
All	All	0.42	0/10457	0.57	3/14171 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	42	GLU	CA-CB-CG	5.70	125.94	113.40
1	C	141	LEU	CB-CG-CD2	-5.43	101.77	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	2561	0	2556	19	0
1	B	2561	0	2556	33	0
1	C	2570	0	2569	31	0
1	D	2561	0	2556	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	26	1	0
2	B	44	0	26	7	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	30	0	0	2	0
3	B	20	0	0	1	0
3	C	25	0	0	0	0
3	D	30	0	0	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	4	0	6	0	0
5	C	8	0	12	3	0
6	A	8	0	12	0	0
6	B	8	0	12	0	0
7	A	371	0	0	7	1
7	B	179	0	0	4	0
7	C	221	0	0	6	0
7	D	311	0	0	5	0
All	All	11652	0	10383	98	1

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 5.

All (98) 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:282:LYS:NZ	7:A:501:HOH:O	2.02	0.91
1:D:253:ARG:NH2	7:D:503:HOH:O	2.16	0.77
1:C:312:ARG:NH1	7:C:503:HOH:O	2.19	0.76
1:B:221:GLU:OE1	7:B:501:HOH:O	2.06	0.74
1:C:100:GLU:OE1	7:C:501:HOH:O	2.04	0.74
1:C:145:MET:HE3	1:C:150:VAL:HB	1.69	0.72
1:D:149:GLY:O	1:D:181:ARG:NH1	2.24	0.71
1:D:221:GLU:OE1	7:D:501:HOH:O	2.09	0.70
1:C:307:PHE:HE2	1:C:311:ARG:NH1	1.90	0.70
1:C:213:LYS:NZ	7:D:503:HOH:O	2.22	0.69
1:B:274:GLU:OE2	7:B:502:HOH:O	2.13	0.66
3:D:406:SO4:O1	7:D:502:HOH:O	2.14	0.65
1:C:307:PHE:HE2	1:C:311:ARG:HH11	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:SER:OG	1:B:146:TYR:OH	2.08	0.65
3:A:404:SO4:O4	7:A:502:HOH:O	2.11	0.65
1:C:282:LYS:N	1:C:282:LYS:HD2	2.11	0.64
1:B:87:PRO:HD3	2:B:401:NAI:H51A	1.80	0.61
3:B:404:SO4:O2	7:B:503:HOH:O	2.16	0.61
1:A:136:LYS:NZ	1:B:232:GLU:OE2	2.33	0.61
1:C:282:LYS:NZ	7:C:507:HOH:O	2.33	0.60
1:A:142:VAL:HG22	1:A:152:VAL:HG21	1.82	0.60
1:D:11:ASN:HB3	1:D:14:LEU:HD13	1.85	0.59
1:C:232:GLU:OE2	1:D:136:LYS:NZ	2.35	0.58
1:B:231:PHE:O	1:B:236:GLU:HG3	2.03	0.58
3:A:406:SO4:O2	7:A:503:HOH:O	2.17	0.57
3:D:404:SO4:O4	7:D:504:HOH:O	2.16	0.57
1:A:221:GLU:OE2	7:A:504:HOH:O	2.18	0.56
1:A:232:GLU:OE2	1:B:136:LYS:NZ	2.36	0.56
1:C:320:GLU:O	1:C:324:LYS:HG3	2.06	0.56
1:A:96:ARG:NH1	7:A:505:HOH:O	2.18	0.56
1:B:239:LEU:HD12	7:B:599:HOH:O	2.05	0.56
1:C:278:ALA:O	1:C:282:LYS:HD3	2.09	0.53
1:B:35:ASN:HB3	1:B:177:ILE:HA	1.91	0.52
1:B:47:LEU:HD11	1:B:62:VAL:HG21	1.90	0.52
1:C:100:GLU:HG2	7:C:659:HOH:O	2.09	0.52
1:C:35:ASN:HB3	1:C:177:ILE:HA	1.92	0.52
1:A:240:ILE:HG21	1:B:204:LEU:O	2.10	0.51
1:B:28:GLN:HE21	2:B:401:NAI:C7N	2.23	0.51
1:C:80:GLN:HE21	5:C:410:EDO:H22	1.76	0.51
1:C:136:LYS:NZ	1:D:232:GLU:OE1	2.43	0.51
1:B:25:TYR:CE1	1:B:30:HIS:HA	2.48	0.48
1:C:253:ARG:HG2	1:C:261:GLU:HG3	1.95	0.48
1:B:71:PRO:HG2	1:B:74:GLU:HB2	1.95	0.48
1:B:320:GLU:O	1:B:324:LYS:HG3	2.13	0.48
1:B:88:ASP:OD1	2:B:401:NAI:O3D	2.32	0.48
1:A:236:GLU:HA	7:A:697:HOH:O	2.13	0.47
1:B:132:MET:HB2	1:B:189:PHE:CZ	2.49	0.47
1:C:240:ILE:HG23	1:C:252:MET:HG3	1.97	0.47
1:D:240:ILE:HG23	1:D:252:MET:HG3	1.96	0.47
1:D:136:LYS:HE2	1:D:136:LYS:HA	1.95	0.47
1:C:142:VAL:HG22	1:C:152:VAL:HG21	1.97	0.46
1:A:136:LYS:HA	1:A:136:LYS:HE2	1.97	0.46
1:B:165:LYS:O	1:B:169:THR:OG1	2.14	0.46
1:A:10:ALA:HB3	1:A:175:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ASN:OD1	5:C:410:EDO:H12	2.17	0.45
1:C:93:LYS:HE3	1:C:97:GLU:OE2	2.16	0.45
1:C:47:LEU:HD11	1:C:62:VAL:HG21	1.99	0.45
1:C:240:ILE:HG21	1:D:204:LEU:O	2.17	0.45
1:A:49:LYS:HG3	7:A:642:HOH:O	2.17	0.45
1:A:242:ASP:O	1:A:246:GLU:HG3	2.15	0.45
1:B:122:ILE:HG22	1:B:124:PRO:HD3	1.99	0.45
1:B:112:SER:HB3	2:B:401:NAI:H6N	1.99	0.45
1:B:47:LEU:O	1:B:71:PRO:HA	2.17	0.44
1:C:221:GLU:HG3	7:C:653:HOH:O	2.18	0.44
2:D:401:NAI:H8A	2:D:401:NAI:H2B	1.83	0.44
1:A:210:GLU:OE2	1:A:213:LYS:HE2	2.18	0.44
1:D:324:LYS:HG2	3:D:407:SO4:O4	2.18	0.44
1:B:5:TYR:HE2	1:B:186:ALA:HB2	1.83	0.44
2:B:401:NAI:H2N	2:B:401:NAI:H2D	1.78	0.44
1:B:81:ILE:HG12	1:B:108:ALA:HB3	2.00	0.43
1:B:240:ILE:HG23	1:B:252:MET:HG3	1.99	0.43
1:C:20:ILE:HG21	1:C:36:LEU:HD13	2.00	0.43
1:C:275:ASN:ND2	7:C:520:HOH:O	2.51	0.43
1:A:204:LEU:O	1:B:240:ILE:HG21	2.19	0.43
1:A:49:LYS:O	1:A:51:GLU:HG2	2.19	0.43
1:A:47:LEU:O	1:A:71:PRO:HA	2.18	0.43
1:A:267:VAL:HG11	1:B:201:GLN:HB3	2.00	0.43
1:B:86:VAL:HB	1:B:87:PRO:HD2	2.01	0.42
2:B:401:NAI:H8A	2:B:401:NAI:H2B	1.81	0.42
1:D:140:HIS:N	3:D:402:SO4:O1	2.53	0.42
1:C:272:ILE:HG23	1:C:276:THR:HG21	2.02	0.42
1:B:19:THR:HB	1:B:79:ALA:HA	2.01	0.42
1:A:332:TRP:HZ3	1:B:245:TYR:HH	1.63	0.41
1:B:95:TYR:HA	1:B:99:ILE:HB	2.02	0.41
2:C:401:NAI:H2N	2:C:401:NAI:H2D	1.79	0.41
1:D:30:HIS:CG	1:D:31:ALA:N	2.87	0.41
1:B:145:MET:HG3	1:B:150:VAL:O	2.21	0.41
1:B:34:GLN:NE2	1:B:65:ASP:OD2	2.53	0.41
1:D:84:ILE:HD11	1:D:109:LEU:HD11	2.02	0.41
1:C:59:TRP:CE2	1:C:69:PRO:HG2	2.56	0.41
1:C:79:ALA:O	5:C:410:EDO:H21	2.21	0.41
1:C:136:LYS:HA	1:C:136:LYS:HE2	2.01	0.41
1:C:47:LEU:O	1:C:71:PRO:HA	2.21	0.40
1:C:150:VAL:HG12	1:C:151:GLY:H	1.86	0.40
1:A:240:ILE:HG23	1:A:252:MET:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:NAI:H8A	2:A:401:NAI:H2B	1.77	0.40
1:B:28:GLN:NE2	2:B:401:NAI:O7N	2.53	0.40
1:D:150:VAL:HG12	1:D:151:GLY:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:727:HOH:O	7:A:806:HOH:O[3_555]	2.13	0.07

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/334 (99%)	319 (97%)	11 (3%)	0	100	100
1	B	330/334 (99%)	316 (96%)	14 (4%)	0	100	100
1	C	331/334 (99%)	318 (96%)	13 (4%)	0	100	100
1	D	330/334 (99%)	316 (96%)	14 (4%)	0	100	100
All	All	1321/1336 (99%)	1269 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/269 (99%)	266 (100%)	1 (0%)	91	94
1	B	267/269 (99%)	267 (100%)	0	100	100
1	C	268/269 (100%)	268 (100%)	0	100	100
1	D	267/269 (99%)	266 (100%)	1 (0%)	91	94
All	All	1069/1076 (99%)	1067 (100%)	2 (0%)	93	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	PHE
1	D	307	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

Of 38 ligands modelled in this entry, 8 are monoatomic - leaving 30 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
2	NAI	D	401	-	42,48,48	4.60	18 (42%)	47,73,73	1.92	5 (10%)
3	SO4	D	406	-	4,4,4	0.16	0	6,6,6	0.06	0
3	SO4	C	402	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	A	402	-	4,4,4	0.21	0	6,6,6	0.31	0
3	SO4	A	406	-	4,4,4	0.18	0	6,6,6	0.08	0
3	SO4	A	405	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	A	404	-	4,4,4	0.24	0	6,6,6	0.24	0
3	SO4	C	404	-	4,4,4	0.14	0	6,6,6	0.18	0
2	NAI	A	401	-	42,48,48	4.53	18 (42%)	47,73,73	1.93	7 (14%)
3	SO4	C	406	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	D	405	-	4,4,4	0.18	0	6,6,6	0.12	0
5	EDO	C	410	-	3,3,3	0.46	0	2,2,2	0.21	0
3	SO4	D	407	-	4,4,4	0.18	0	6,6,6	0.10	0
3	SO4	B	402	-	4,4,4	0.15	0	6,6,6	0.06	0
2	NAI	B	401	-	42,48,48	4.92	21 (50%)	47,73,73	1.91	4 (8%)
3	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.21	0
3	SO4	C	405	-	4,4,4	0.16	0	6,6,6	0.15	0
6	TRS	B	408	-	7,7,7	0.34	0	9,9,9	0.30	0
3	SO4	D	402	-	4,4,4	0.11	0	6,6,6	0.12	0
6	TRS	A	411	-	7,7,7	0.35	0	9,9,9	0.11	0
3	SO4	A	403	-	4,4,4	0.15	0	6,6,6	0.19	0
3	SO4	A	407	-	4,4,4	0.16	0	6,6,6	0.16	0
3	SO4	D	404	-	4,4,4	0.27	0	6,6,6	0.21	0
3	SO4	C	403	-	4,4,4	0.16	0	6,6,6	0.43	0
5	EDO	C	409	-	3,3,3	0.50	0	2,2,2	0.33	0
3	SO4	B	405	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	B	404	-	4,4,4	0.13	0	6,6,6	0.10	0
2	NAI	C	401	-	42,48,48	4.78	18 (42%)	47,73,73	2.15	3 (6%)
3	SO4	D	403	-	4,4,4	0.21	0	6,6,6	0.17	0
5	EDO	A	410	-	3,3,3	0.45	0	2,2,2	0.41	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	TRS	B	408	-	-	2/9/9/9	-
2	NAI	A	401	-	-	6/25/72/72	0/5/5/5
2	NAI	D	401	-	-	8/25/72/72	0/5/5/5
5	EDO	C	409	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TRS	A	411	-	-	6/9/9/9	-
5	EDO	C	410	-	-	1/1/1/1	-
2	NAI	B	401	-	-	11/25/72/72	0/5/5/5
2	NAI	C	401	-	-	7/25/72/72	0/5/5/5
5	EDO	A	410	-	-	1/1/1/1	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAI	C2B-C1B	-15.92	1.29	1.53
2	C	401	NAI	C2B-C1B	-15.57	1.30	1.53
2	B	401	NAI	O4B-C1B	15.43	1.62	1.41
2	D	401	NAI	C2B-C1B	-15.20	1.30	1.53
2	C	401	NAI	O4B-C1B	15.13	1.62	1.41
2	A	401	NAI	C2B-C1B	-14.81	1.31	1.53
2	D	401	NAI	O4B-C1B	13.73	1.60	1.41
2	A	401	NAI	O4B-C1B	13.30	1.59	1.41
2	B	401	NAI	C6N-C5N	11.75	1.54	1.33
2	C	401	NAI	C6N-C5N	11.67	1.54	1.33
2	D	401	NAI	C6N-C5N	11.36	1.53	1.33
2	A	401	NAI	C6N-C5N	11.02	1.53	1.33
2	B	401	NAI	O4D-C1D	8.96	1.63	1.42
2	A	401	NAI	O4D-C1D	8.04	1.61	1.42
2	C	401	NAI	O4D-C1D	7.90	1.60	1.42
2	D	401	NAI	O4D-C1D	7.60	1.60	1.42
2	D	401	NAI	C2N-C3N	7.29	1.55	1.34
2	A	401	NAI	C2N-C3N	7.26	1.55	1.34
2	B	401	NAI	C2N-C3N	7.12	1.54	1.34
2	C	401	NAI	C2N-C3N	6.98	1.54	1.34
2	C	401	NAI	C2D-C1D	-6.51	1.32	1.53
2	D	401	NAI	C2D-C1D	-6.45	1.32	1.53
2	B	401	NAI	C2D-C1D	-6.44	1.32	1.53
2	A	401	NAI	C2D-C1D	-6.39	1.33	1.53
2	B	401	NAI	O4D-C4D	-6.32	1.30	1.45
2	C	401	NAI	O4D-C4D	-6.20	1.31	1.45
2	A	401	NAI	O4D-C4D	-6.07	1.31	1.45
2	D	401	NAI	O4D-C4D	-6.05	1.31	1.45
2	D	401	NAI	O4B-C4B	-5.56	1.32	1.45
2	B	401	NAI	O4B-C4B	-5.53	1.32	1.45
2	C	401	NAI	O4B-C4B	-5.38	1.33	1.45
2	A	401	NAI	O4B-C4B	-5.29	1.33	1.45
2	C	401	NAI	C7N-N7N	4.34	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAI	C7N-N7N	4.31	1.44	1.33
2	A	401	NAI	C7N-N7N	4.16	1.44	1.33
2	D	401	NAI	C7N-N7N	4.08	1.44	1.33
2	B	401	NAI	C6N-N1N	3.76	1.46	1.37
2	C	401	NAI	C6N-N1N	3.70	1.46	1.37
2	C	401	NAI	O3D-C3D	-3.62	1.34	1.43
2	B	401	NAI	C7N-C3N	3.62	1.56	1.48
2	C	401	NAI	C7N-C3N	3.45	1.56	1.48
2	B	401	NAI	O3D-C3D	-3.38	1.35	1.43
2	D	401	NAI	C6N-N1N	3.32	1.45	1.37
2	D	401	NAI	C5A-C4A	-3.26	1.32	1.40
2	D	401	NAI	C7N-C3N	3.23	1.55	1.48
2	A	401	NAI	C6N-N1N	3.21	1.45	1.37
2	A	401	NAI	C7N-C3N	3.20	1.55	1.48
2	A	401	NAI	C5A-C4A	-3.16	1.32	1.40
2	C	401	NAI	C5A-C4A	-3.11	1.32	1.40
2	B	401	NAI	C5A-C4A	-3.01	1.33	1.40
2	A	401	NAI	O3D-C3D	-2.91	1.36	1.43
2	B	401	NAI	O2D-C2D	2.90	1.49	1.43
2	D	401	NAI	O3D-C3D	-2.66	1.36	1.43
2	A	401	NAI	C2A-N3A	2.47	1.36	1.32
2	A	401	NAI	C6A-N6A	2.40	1.42	1.34
2	B	401	NAI	C6A-N6A	2.35	1.42	1.34
2	B	401	NAI	C4N-C5N	2.26	1.54	1.48
2	A	401	NAI	O5D-C5D	-2.25	1.36	1.44
2	B	401	NAI	O3B-C3B	-2.24	1.37	1.43
2	C	401	NAI	C6A-N6A	2.22	1.42	1.34
2	D	401	NAI	O2D-C2D	2.20	1.48	1.43
2	C	401	NAI	O2D-C2D	2.19	1.48	1.43
2	D	401	NAI	C2A-N3A	2.19	1.35	1.32
2	D	401	NAI	C6A-N6A	2.16	1.41	1.34
2	A	401	NAI	O2D-C2D	2.14	1.48	1.43
2	C	401	NAI	O2B-C2B	2.12	1.48	1.43
2	C	401	NAI	PN-O5D	2.06	1.67	1.59
2	A	401	NAI	O3B-C3B	-2.05	1.38	1.43
2	C	401	NAI	C4N-C5N	2.04	1.54	1.48
2	B	401	NAI	O5D-C5D	-2.03	1.37	1.44
2	D	401	NAI	O5D-C5D	-2.03	1.37	1.44
2	D	401	NAI	C4N-C5N	2.02	1.54	1.48
2	B	401	NAI	O2B-C2B	2.02	1.47	1.43
2	B	401	NAI	C2A-N3A	2.01	1.35	1.32
2	B	401	NAI	PN-O5D	2.00	1.67	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAI	C5A-C6A-N6A	9.87	135.35	120.35
2	B	401	NAI	C5A-C6A-N6A	8.60	133.42	120.35
2	D	401	NAI	C5A-C6A-N6A	7.29	131.43	120.35
2	A	401	NAI	C5A-C6A-N6A	6.89	130.82	120.35
2	C	401	NAI	N6A-C6A-N1A	-6.73	104.61	118.57
2	A	401	NAI	N3A-C2A-N1A	-6.46	118.58	128.68
2	C	401	NAI	N3A-C2A-N1A	-6.11	119.13	128.68
2	D	401	NAI	N3A-C2A-N1A	-6.00	119.30	128.68
2	B	401	NAI	N6A-C6A-N1A	-5.65	106.86	118.57
2	B	401	NAI	N3A-C2A-N1A	-5.59	119.94	128.68
2	D	401	NAI	N6A-C6A-N1A	-4.84	108.52	118.57
2	A	401	NAI	N6A-C6A-N1A	-4.43	109.39	118.57
2	D	401	NAI	O4B-C1B-C2B	-3.44	101.90	106.93
2	D	401	NAI	PN-O3-PA	-3.21	121.83	132.83
2	A	401	NAI	O4B-C1B-C2B	-3.19	102.27	106.93
2	A	401	NAI	PN-O3-PA	-2.72	123.50	132.83
2	A	401	NAI	O3B-C3B-C2B	-2.52	103.68	111.82
2	A	401	NAI	O4D-C1D-C2D	-2.47	101.25	106.64
2	B	401	NAI	C3B-C2B-C1B	2.19	104.27	100.98

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAI	C5B-O5B-PA-O3
2	B	401	NAI	C5D-O5D-PN-O2N
2	D	401	NAI	C2N-C3N-C7N-N7N
2	B	401	NAI	O4B-C4B-C5B-O5B
2	B	401	NAI	C2D-C1D-N1N-C6N
2	C	401	NAI	C2D-C1D-N1N-C6N
2	D	401	NAI	C2D-C1D-N1N-C6N
5	C	410	EDO	O1-C1-C2-O2
2	C	401	NAI	PN-O3-PA-O1A
2	B	401	NAI	C2D-C1D-N1N-C2N
2	C	401	NAI	C2D-C1D-N1N-C2N
2	B	401	NAI	C3B-C4B-C5B-O5B
2	D	401	NAI	C2D-C1D-N1N-C2N
2	A	401	NAI	C2D-C1D-N1N-C6N
2	A	401	NAI	PN-O3-PA-O1A
6	A	411	TRS	C3-C-C1-O1
6	A	411	TRS	N-C-C1-O1

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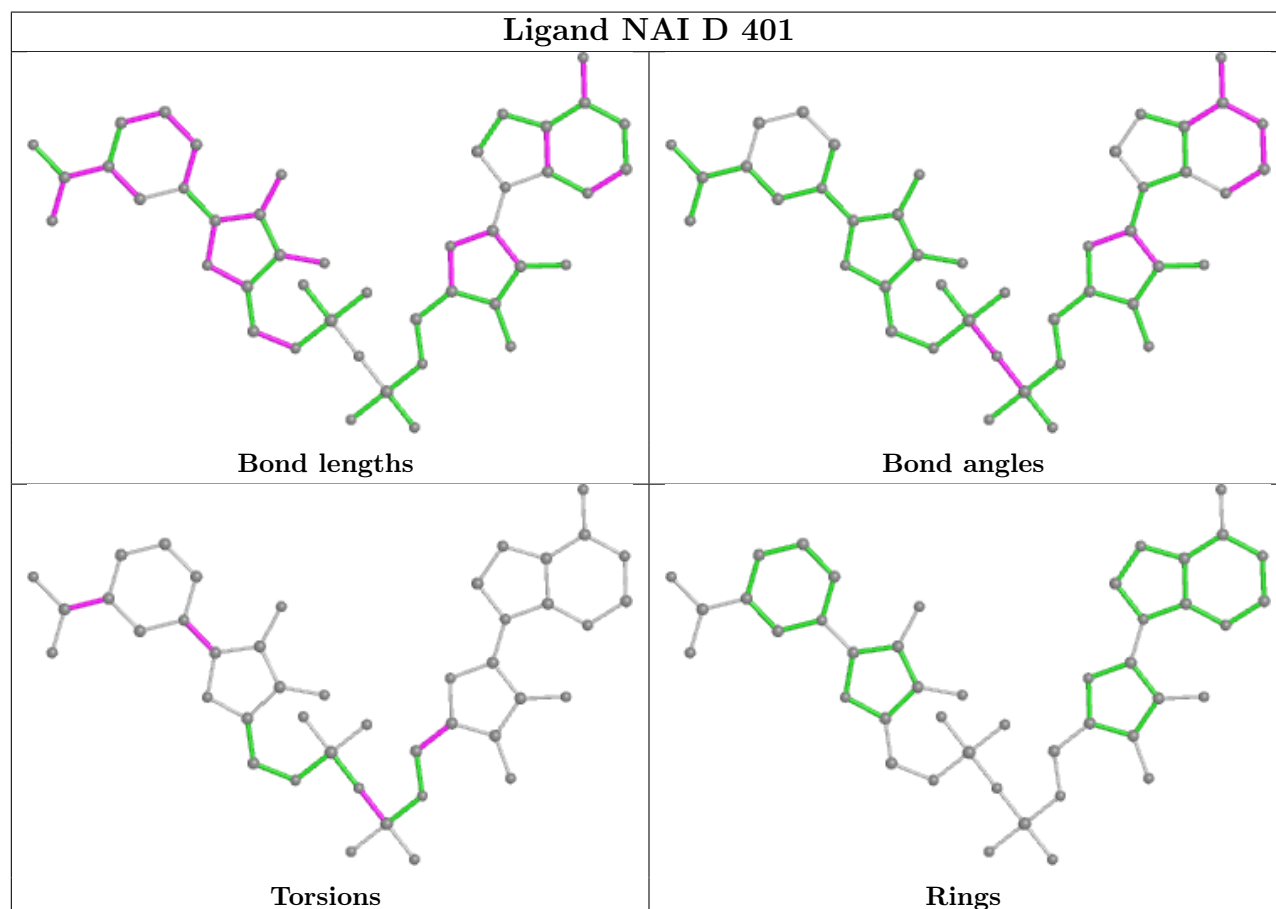
Mol	Chain	Res	Type	Atoms
6	B	408	TRS	C1-C-C3-O3
6	B	408	TRS	N-C-C3-O3
2	B	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	C5B-O5B-PA-O1A
2	B	401	NAI	O4D-C1D-N1N-C2N
2	D	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	PN-O3-PA-O2A
2	D	401	NAI	PN-O3-PA-O2A
6	A	411	TRS	C2-C-C1-O1
6	A	411	TRS	C1-C-C2-O2
6	A	411	TRS	C3-C-C2-O2
2	D	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	C2D-C1D-N1N-C2N
2	C	401	NAI	O4D-C1D-N1N-C2N
5	A	410	EDO	O1-C1-C2-O2
2	C	401	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	O4B-C4B-C5B-O5B
2	B	401	NAI	PN-O3-PA-O2A
2	C	401	NAI	PN-O3-PA-O2A
2	D	401	NAI	PN-O3-PA-O1A
6	A	411	TRS	N-C-C2-O2
2	B	401	NAI	C5B-O5B-PA-O2A
2	D	401	NAI	O4B-C4B-C5B-O5B

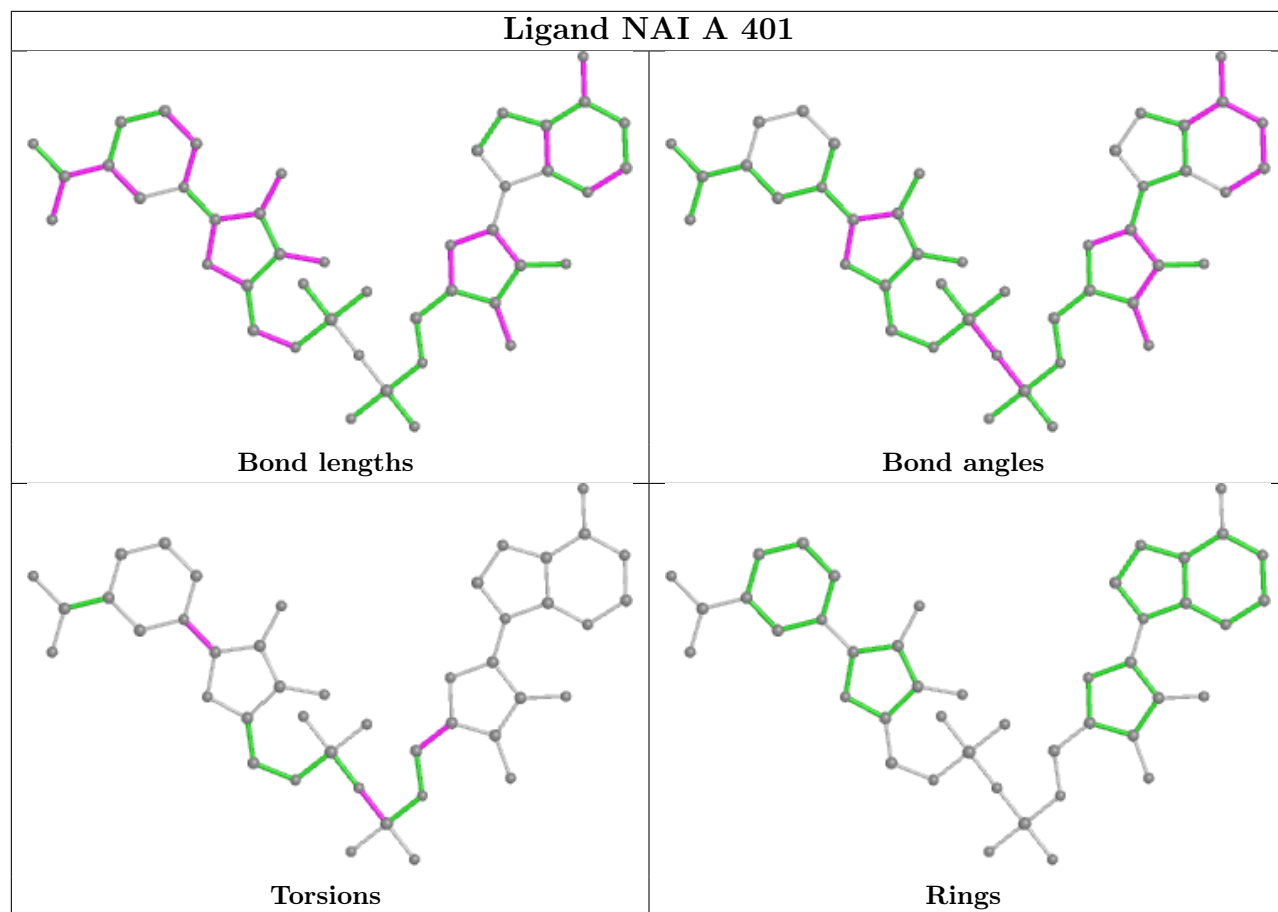
There are no ring outliers.

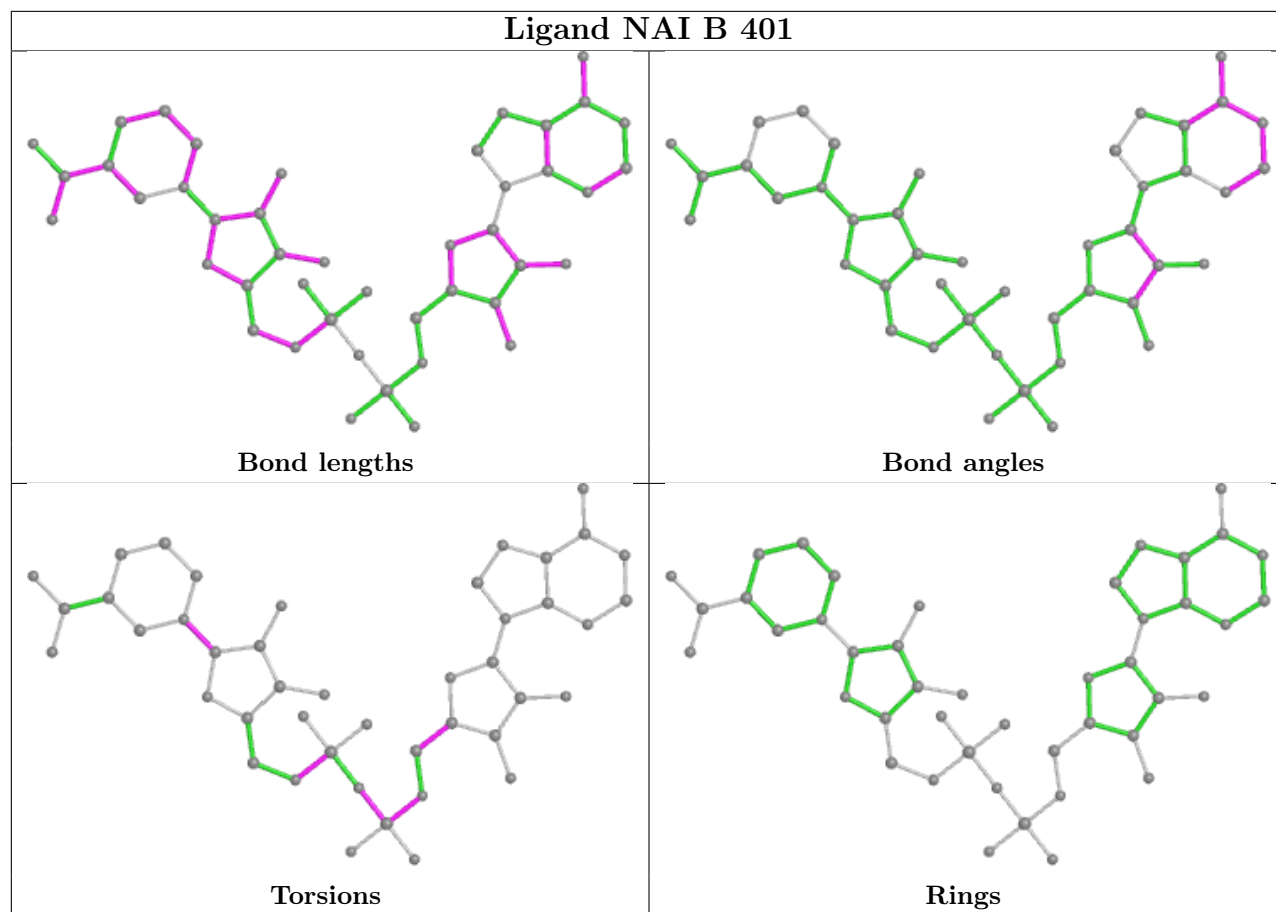
12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	NAI	1	0
3	D	406	SO4	1	0
3	A	406	SO4	1	0
3	A	404	SO4	1	0
2	A	401	NAI	1	0
5	C	410	EDO	3	0
3	D	407	SO4	1	0
2	B	401	NAI	7	0
3	D	402	SO4	1	0
3	D	404	SO4	1	0
3	B	404	SO4	1	0
2	C	401	NAI	1	0

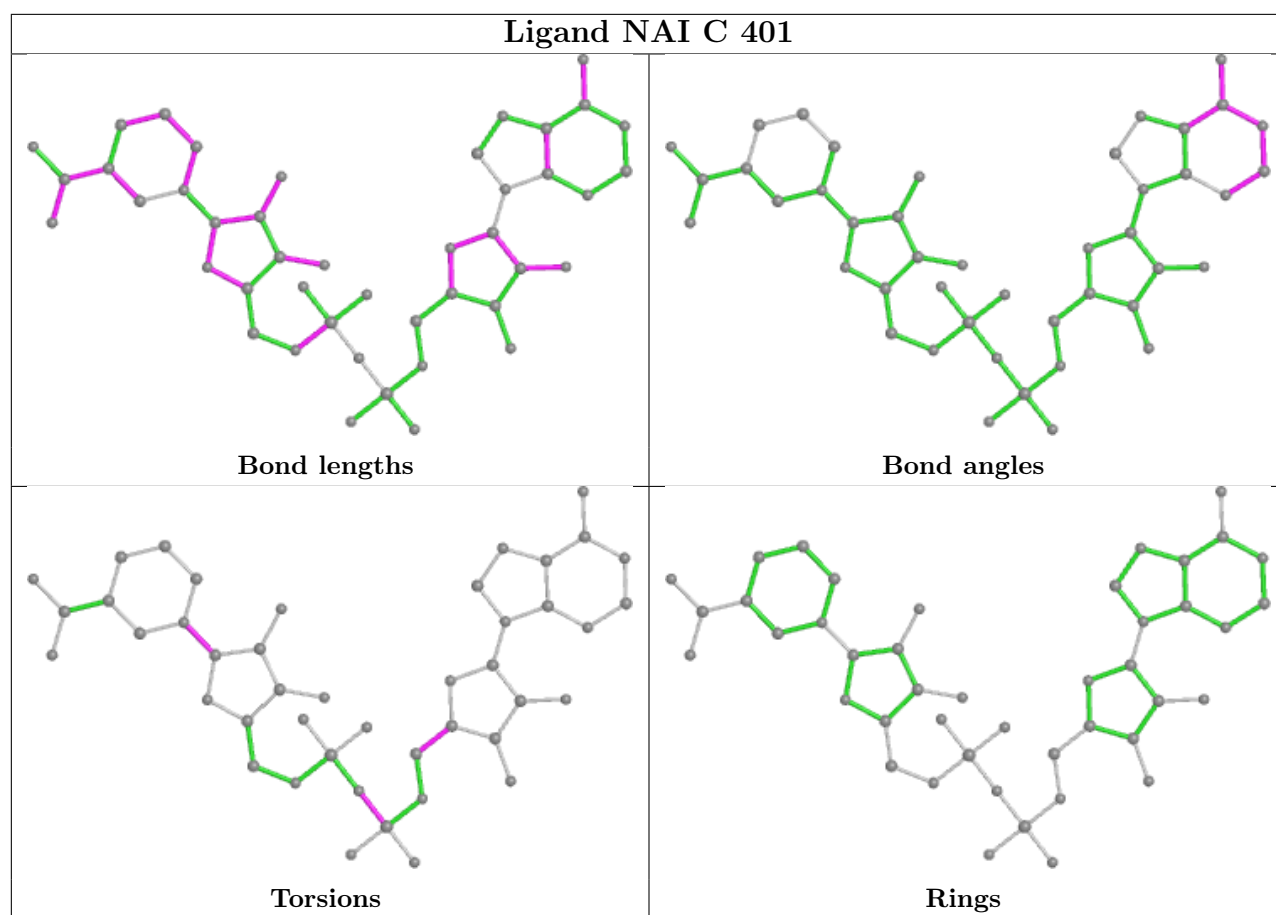
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	332/334 (99%)	-0.25	6 (1%) 68 72	12, 26, 44, 90	0
1	B	332/334 (99%)	0.88	75 (22%) 0 0	14, 57, 108, 125	0
1	C	333/334 (99%)	0.13	23 (6%) 16 20	18, 38, 69, 123	0
1	D	332/334 (99%)	-0.15	5 (1%) 73 77	17, 30, 49, 73	0
All	All	1329/1336 (99%)	0.15	109 (8%) 11 14	12, 31, 94, 125	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	PHE	8.1
1	B	150	VAL	7.6
1	B	55	THR	6.6
1	B	51	GLU	5.9
1	B	53	ASP	5.8
1	B	162	HIS	5.7
1	B	12	LEU	5.6
1	B	145	MET	5.5
1	C	51	GLU	5.5
1	C	54	PHE	5.4
1	B	56	THR	5.1
1	B	52	ASP	4.9
1	B	13	ASP	4.8
1	B	50	PRO	4.7
1	B	49	LYS	4.6
1	B	15	LEU	4.5
1	B	14	LEU	4.5
1	B	25	TYR	4.5
1	B	163	THR	4.4
1	B	164	GLY	4.4
1	B	146	TYR	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	17	GLY	4.2
1	B	8	ALA	4.2
1	A	331	PRO	4.1
1	B	16	LYS	4.1
1	B	11	ASN	4.0
1	B	101	PRO	4.0
1	C	2	ALA	3.9
1	B	77	ARG	3.9
1	B	40	GLY	3.8
1	C	150	VAL	3.8
1	B	59	TRP	3.7
1	B	147	ARG	3.7
1	B	144	ARG	3.7
1	B	72	VAL	3.7
1	B	63	VAL	3.6
1	B	142	VAL	3.6
1	C	53	ASP	3.5
1	B	148	GLN	3.5
1	B	141	LEU	3.5
1	C	16	LYS	3.4
1	B	62	VAL	3.4
1	B	103	LEU	3.3
1	B	66	GLY	3.3
1	C	14	LEU	3.2
1	B	96	ARG	3.2
1	B	60	ASN	3.2
1	C	56	THR	3.1
1	C	331	PRO	3.0
1	B	46	GLY	3.0
1	C	52	ASP	2.9
1	C	147	ARG	2.9
1	B	80	GLN	2.9
1	B	161	ASP	2.9
1	B	102	TYR	2.9
1	B	68	THR	2.8
1	B	67	LEU	2.8
1	B	36	LEU	2.7
1	B	143	ARG	2.7
1	B	165	LYS	2.7
1	C	13	ASP	2.6
1	B	70	LEU	2.6
1	B	69	PRO	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	71	PRO	2.6
1	B	30	HIS	2.5
1	B	149	GLY	2.5
1	C	334	LYS	2.5
1	B	44	VAL	2.5
1	C	8	ALA	2.5
1	B	48	ARG	2.5
1	C	144	ARG	2.5
1	D	332	TRP	2.5
1	B	65	ASP	2.5
1	B	126	PRO	2.5
1	B	140	HIS	2.5
1	B	106	GLY	2.5
1	B	58	GLU	2.4
1	B	6	TYR	2.4
1	A	150	VAL	2.4
1	D	133	VAL	2.4
1	A	332	TRP	2.4
1	B	331	PRO	2.4
1	B	128	VAL	2.3
1	B	61	GLN	2.3
1	C	82	ILE	2.3
1	A	13	ASP	2.3
1	C	11	ASN	2.3
1	D	333	LEU	2.3
1	A	53	ASP	2.2
1	B	82	ILE	2.2
1	B	76	ALA	2.2
1	C	61	GLN	2.2
1	B	10	ALA	2.2
1	C	254	TYR	2.2
1	C	3	ARG	2.2
1	D	331	PRO	2.2
1	B	41	LEU	2.1
1	D	53	ASP	2.1
1	B	181	ARG	2.1
1	C	21	ALA	2.1
1	B	90	ILE	2.1
1	B	125	PRO	2.1
1	B	97	GLU	2.1
1	B	18	LYS	2.1
1	B	105	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	49	LYS	2.1
1	B	37	HIS	2.0
1	A	16	LYS	2.0
1	C	165	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	C	402	5/5	0.78	0.24	127,127,128,128	0
3	SO4	B	402	5/5	0.81	0.27	99,99,102,106	0
3	SO4	D	402	5/5	0.82	0.34	90,90,90,95	0
4	MG	C	407	1/1	0.84	0.09	38,38,38,38	0
6	TRS	A	411	8/8	0.84	0.18	45,52,57,58	8
5	EDO	C	409	4/4	0.85	0.16	43,43,50,50	0
3	SO4	D	406	5/5	0.85	0.21	125,126,126,126	0
3	SO4	A	402	5/5	0.86	0.28	74,75,76,83	0
6	TRS	B	408	8/8	0.89	0.12	46,49,50,52	0
3	SO4	D	404	5/5	0.90	0.27	35,45,54,57	0
3	SO4	A	407	5/5	0.90	0.23	82,82,82,91	0
3	SO4	C	404	5/5	0.91	0.25	62,62,69,77	0
2	NAI	B	401	44/44	0.91	0.15	54,72,82,87	0
4	MG	B	407	1/1	0.92	0.09	51,51,51,51	0
3	SO4	A	406	5/5	0.93	0.23	61,61,68,78	0
3	SO4	B	404	5/5	0.93	0.19	77,77,80,92	0
3	SO4	A	404	5/5	0.93	0.22	58,58,59,64	0
3	SO4	C	403	5/5	0.94	0.19	53,54,62,66	0
3	SO4	C	405	5/5	0.94	0.19	78,78,81,93	0

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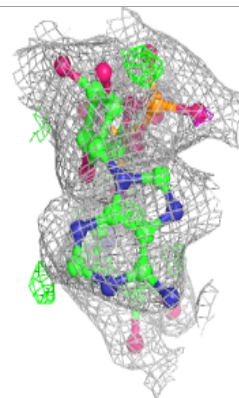
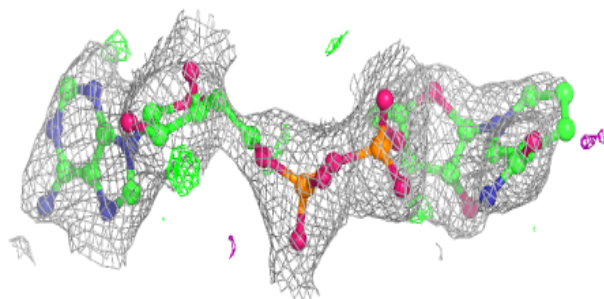
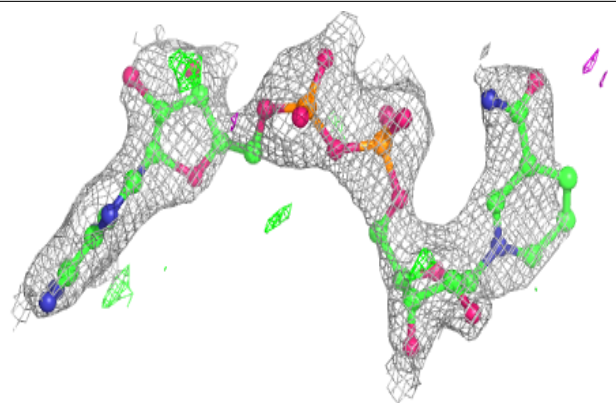
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	D	409	1/1	0.95	0.09	39,39,39,39	0
5	EDO	A	410	4/4	0.95	0.44	35,37,37,44	0
3	SO4	A	405	5/5	0.95	0.27	62,67,73,82	0
3	SO4	B	403	5/5	0.95	0.27	53,57,64,71	0
4	MG	C	408	1/1	0.95	0.23	51,51,51,51	0
4	MG	D	408	1/1	0.96	0.12	51,51,51,51	0
3	SO4	A	403	5/5	0.96	0.12	51,56,64,68	0
2	NAI	D	401	44/44	0.96	0.10	21,27,34,38	0
3	SO4	B	405	5/5	0.96	0.25	75,75,80,82	0
5	EDO	C	410	4/4	0.96	0.30	48,48,48,50	0
3	SO4	C	406	5/5	0.96	0.19	55,56,66,67	0
2	NAI	C	401	44/44	0.96	0.10	30,41,46,51	0
2	NAI	A	401	44/44	0.97	0.10	15,22,28,34	0
3	SO4	D	405	5/5	0.97	0.19	61,62,70,78	0
3	SO4	D	403	5/5	0.97	0.13	49,54,57,64	0
3	SO4	D	407	5/5	0.97	0.27	73,73,79,81	0
4	MG	A	408	1/1	0.97	0.08	41,41,41,41	0
4	MG	A	409	1/1	0.98	0.11	50,50,50,50	0
4	MG	B	406	1/1	0.99	0.07	43,43,43,43	0

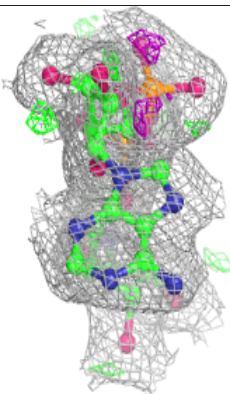
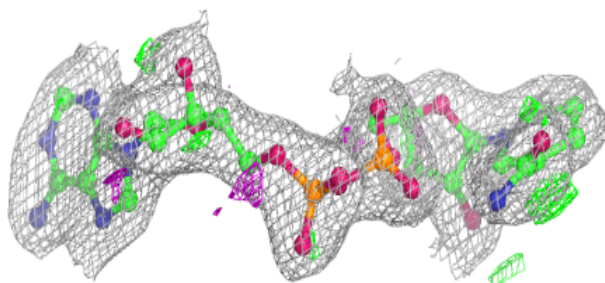
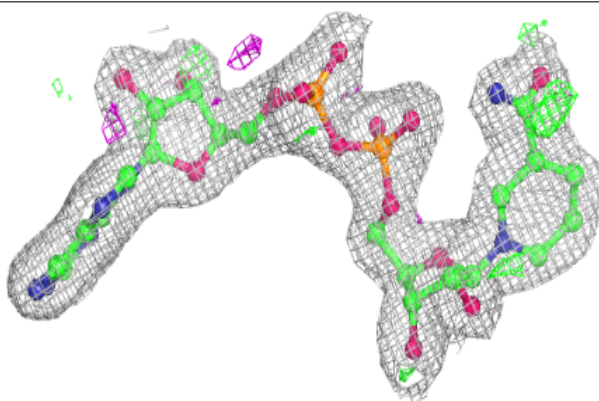
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAI B 401:**

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

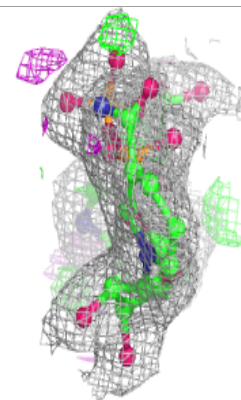
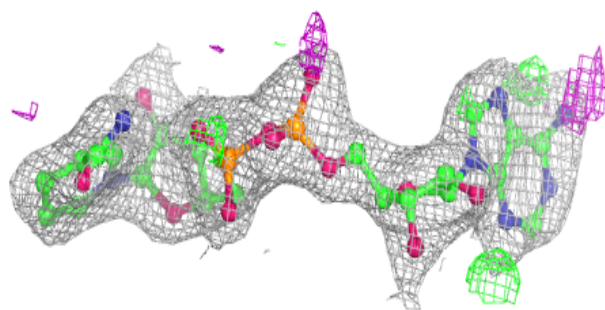
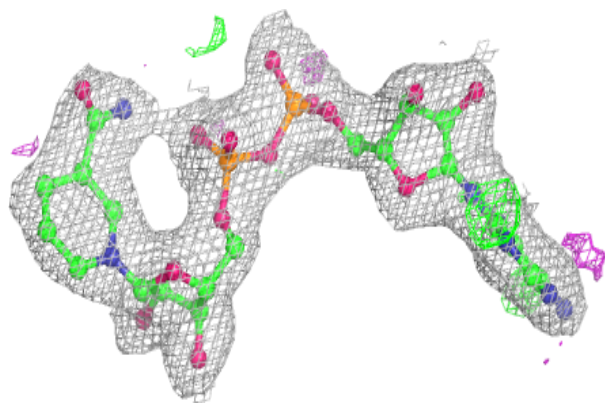
**Electron density around NAI D 401:**

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

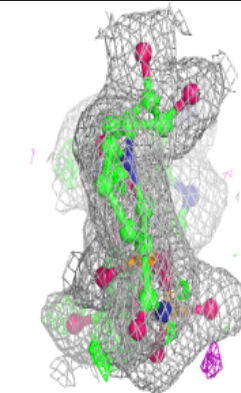
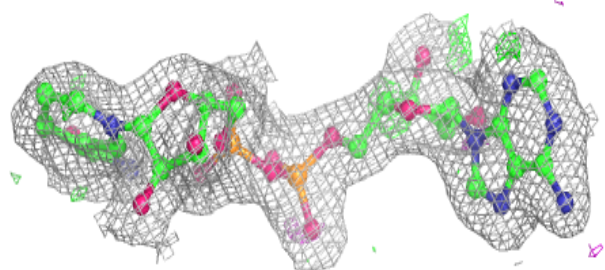
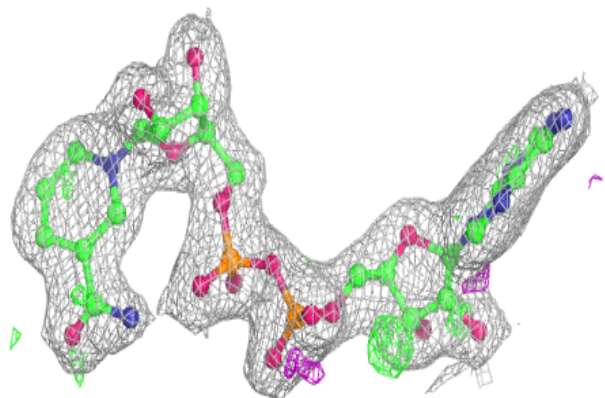


**Electron density around NAI C 401:**

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

**Electron density around NAI 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.