



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:18 am BST

PDB ID : 3VDR  
Title : Crystal structure of D-3-hydroxybutyrate dehydrogenase, prepared in the presence of the substrate D-3-hydroxybutyrate and NAD(+)  
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Deposited on : 2012-01-06  
Resolution : 3.00 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

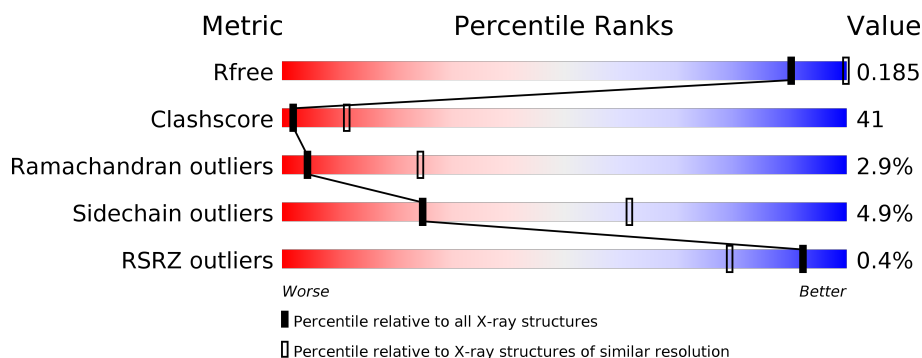
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	260	<div> <div></div> <div>53% 40% 7%</div> </div>
1	B	260	<div> <div></div> <div>52% 44% .</div> </div>
1	C	260	<div> <div></div> <div>55% 40% 5%</div> </div>
1	D	260	<div> <div></div> <div>54% 42% .</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	3HR	A	305[A]	-	-	X	-
6	3HR	B	305[A]	-	-	X	-
7	AAE	B	306[B]	-	-	X	-
7	AAE	C	304[B]	-	-	X	-
7	AAE	D	305[B]	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8281 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 D-3-hydroxybutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1906	1203	331	366	6			
1	B	260	Total	C	N	O	S	0	0	0
			1906	1203	331	366	6			
1	C	260	Total	C	N	O	S	0	0	0
			1906	1203	331	366	6			
1	D	260	Total	C	N	O	S	0	0	0
			1906	1203	331	366	6			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

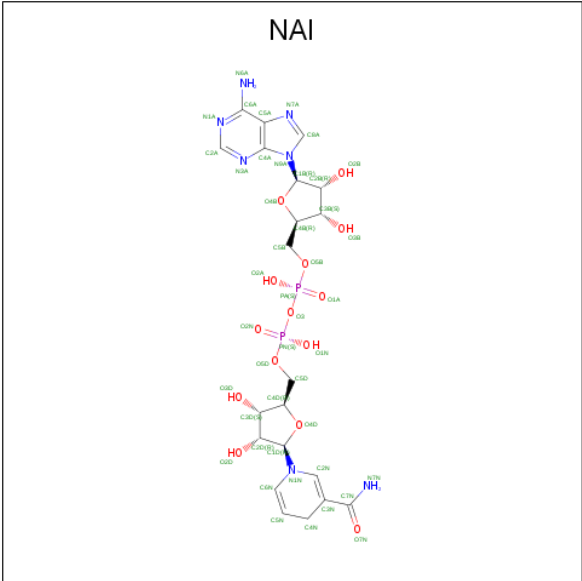
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



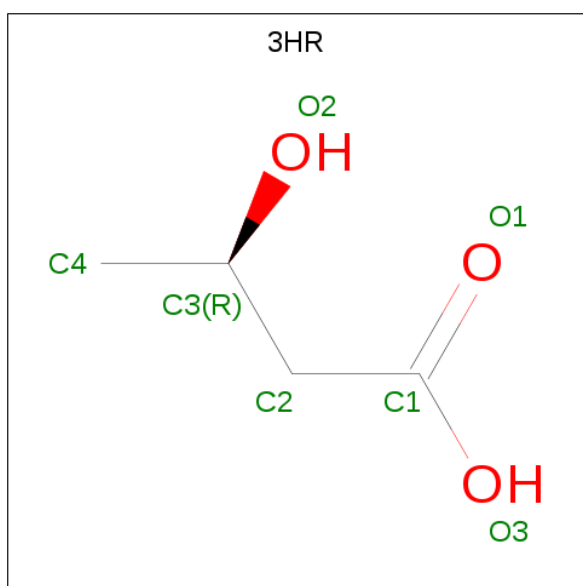
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	1
			44	21	7	14	2		

- Molecule 5 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>).



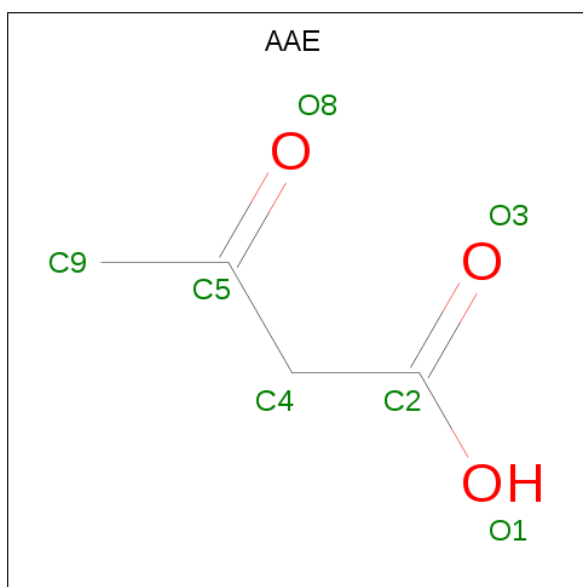
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
5	C	1	Total	C	N	O	P	0	1
			44	21	7	14	2		
5	D	1	Total	C	N	O	P	0	1
			44	21	7	14	2		

- Molecule 6 is (3R)-3-hydroxybutanoic acid (three-letter code: 3HR) (formula:  $C_4H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			7	4	3		
6	B	1	Total	C	O	0	1
			7	4	3		
6	C	1	Total	C	O	0	1
			7	4	3		
6	D	1	Total	C	O	0	1
			7	4	3		

- Molecule 7 is ACETOACETIC ACID (three-letter code: AAE) (formula:  $C_4H_6O_3$ ).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	67	Total O 67 67	0	0
8	B	51	Total O 51 51	0	0
8	C	73	Total O 73 73	0	0
8	D	53	Total O 53 53	0	0

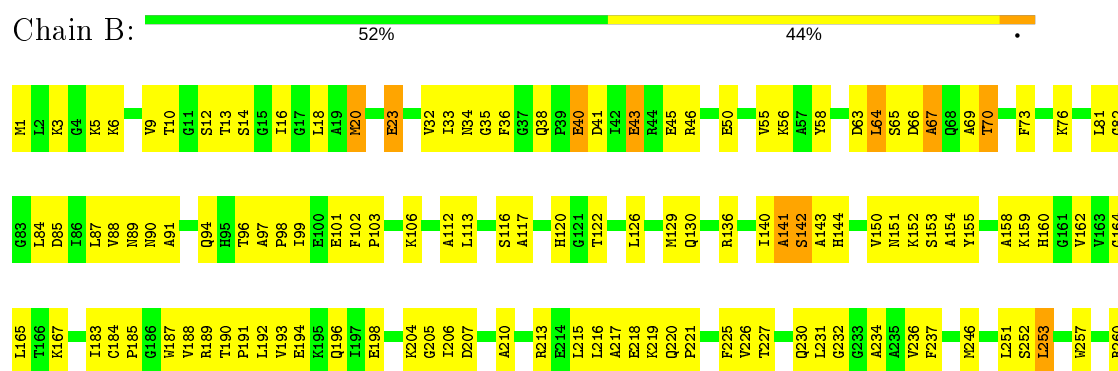
### 3 Residue-property plots

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.

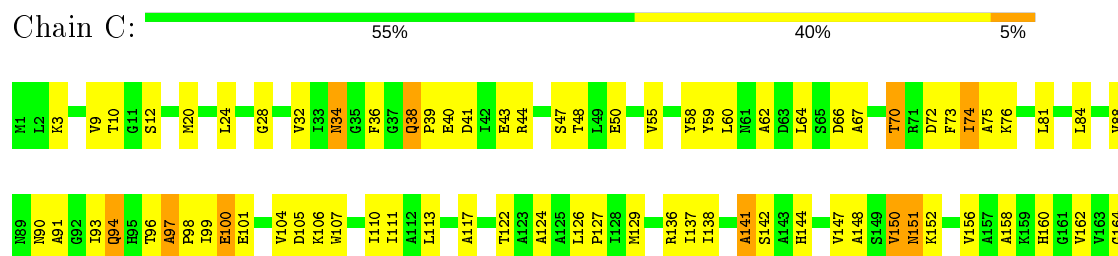
- Molecule 1: D-3-hydroxybutyrate dehydrogenase



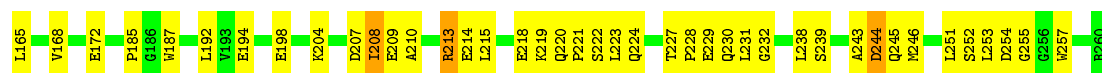
- Molecule 1: D-3-hydroxybutyrate dehydrogenase



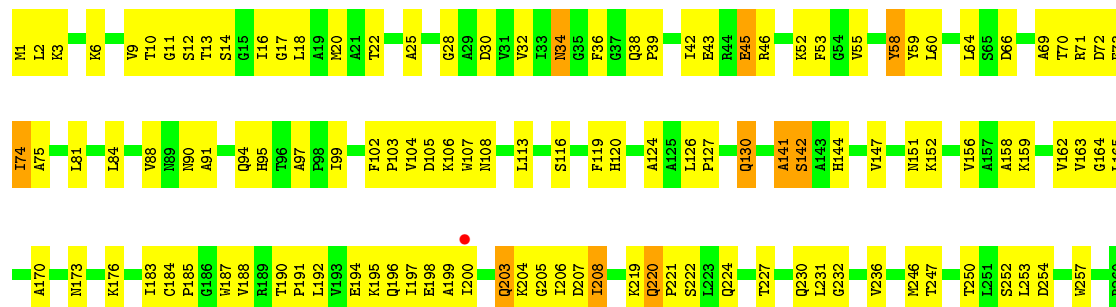
- Molecule 1: D-3-hydroxybutyrate dehydrogenase







• Molecule 1: D-3-hydroxybutyrate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.10 Å 91.10 Å 262.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.00 – 3.00 43.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.0 (43.00-3.00) 91.2 (43.02-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.59 (at 3.01 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.176 , 0.241 0.185 , 0.185	Depositor DCC
$R_{free}$ test set	2062 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.3	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: AAE, 3HR, NAD, CL, CA, 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	0.32	0/1935	0.61	0/2623
1	B	0.30	0/1935	0.60	0/2623
1	C	0.32	0/1935	0.61	0/2623
1	D	0.30	0/1935	0.59	0/2623
All	All	0.31	0/7740	0.60	0/10492

There are no bond length outliers.

There are no bond angle outliers.

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	1906	0	1941	185	0
1	B	1906	0	1941	184	0
1	C	1906	0	1941	152	0
1	D	1906	0	1941	162	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	44	0	26	11	0
4	B	44	0	26	11	0
4	C	44	0	26	10	0
4	D	44	0	26	10	0
5	A	44	0	27	9	0
5	B	44	0	27	8	0
5	C	44	0	27	13	0
5	D	44	0	27	14	0
6	A	7	0	7	4	0
6	B	7	0	7	6	0
6	C	7	0	7	3	0
6	D	7	0	7	2	0
7	A	7	0	5	3	0
7	B	7	0	5	5	0
7	C	7	0	5	5	0
7	D	7	0	5	4	0
8	A	67	0	0	9	0
8	B	51	0	0	6	0
8	C	73	0	0	4	0
8	D	53	0	0	4	0
All	All	8281	0	8024	664	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 41.

All (664) 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:D:74:ILE:HD12	1:D:75:ALA:N	1.41	1.33
1:B:56:LYS:HG3	8:B:402:HOH:O	1.14	1.26
1:C:74:ILE:HD12	1:C:75:ALA:N	1.56	1.19
1:D:64:LEU:HA	1:D:70:THR:HG22	1.31	1.11
1:C:246:MET:HB2	1:D:253:LEU:HD22	1.26	1.11
1:A:213:ARG:NH1	1:A:213:ARG:HB2	1.67	1.09
1:D:74:ILE:HG12	1:D:124:ALA:HB3	1.35	1.08
1:D:203:GLN:OE1	1:D:203:GLN:O	1.72	1.07
1:D:208:ILE:O	1:D:208:ILE:HD13	1.55	1.06
1:A:90:ASN:HB2	1:A:140:ILE:HD12	1.34	1.05
1:C:210:ALA:HA	1:C:213:ARG:HH12	1.15	1.05
1:A:208:ILE:O	1:A:208:ILE:HD13	1.55	1.05
1:A:213:ARG:HH11	1:A:213:ARG:CB	1.69	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ILE:HD12	1:C:74:ILE:C	1.79	1.03
1:A:74:ILE:HD13	1:A:74:ILE:N	1.74	1.00
1:D:227:THR:OG1	1:D:230:GLN:HG3	1.63	0.99
1:A:40:GLU:HG2	8:A:444:HOH:O	1.63	0.98
1:A:71:ARG:HA	1:A:74:ILE:HD11	1.44	0.98
1:C:253:LEU:HD22	1:D:246:MET:HB2	1.45	0.98
1:B:99:ILE:HG13	1:C:172:GLU:OE1	1.62	0.98
1:D:90:ASN:OD1	4:D:302[A]:NAD:H4D	1.62	0.98
1:C:253:LEU:CD2	1:D:246:MET:HG3	1.95	0.97
1:D:90:ASN:OD1	5:D:303[B]:NAI:H4D	1.61	0.97
1:A:187:TRP:HZ3	7:A:306[B]:AAE:H41	1.29	0.96
1:B:227:THR:OG1	1:B:230:GLN:HG3	1.63	0.96
1:B:251:LEU:HD13	1:B:253:LEU:HD21	1.48	0.94
5:C:302[B]:NAI:H4N	7:C:304[B]:AAE:C5	1.98	0.93
1:D:74:ILE:C	1:D:74:ILE:HD12	1.88	0.93
1:A:70:THR:O	1:A:74:ILE:CD1	2.17	0.92
1:C:253:LEU:HD23	1:D:246:MET:HG3	1.52	0.92
1:A:187:TRP:CZ3	7:A:306[B]:AAE:H41	2.03	0.92
1:B:188:VAL:O	1:B:193:VAL:HG21	1.69	0.92
1:B:20:MET:CE	1:B:232:GLY:HA2	2.01	0.91
1:C:210:ALA:HA	1:C:213:ARG:NH1	1.86	0.91
1:B:66:ASP:O	1:B:70:THR:HG22	1.69	0.91
1:D:64:LEU:HA	1:D:70:THR:CG2	2.01	0.90
1:A:74:ILE:H	1:A:74:ILE:HD13	1.35	0.90
1:B:142:SER:O	1:B:184:CYS:HB3	1.71	0.90
1:D:74:ILE:HG12	1:D:124:ALA:CB	2.02	0.90
1:A:1:MET:HG3	8:A:454:HOH:O	1.72	0.89
1:B:187:TRP:CZ3	7:B:306[B]:AAE:H41	2.08	0.88
1:A:61:ASN:HD22	1:A:62:ALA:N	1.72	0.88
1:B:207:ASP:HB3	1:B:210:ALA:CB	2.02	0.88
4:C:301[A]:NAD:C4N	6:C:303[A]:3HR:H3	2.04	0.88
1:B:1:MET:CE	1:B:236:VAL:HG12	2.01	0.88
1:A:187:TRP:HZ3	6:A:305[A]:3HR:H2	1.38	0.87
1:A:71:ARG:CA	1:A:74:ILE:HD11	2.04	0.87
1:A:16:ILE:O	1:A:20:MET:HG3	1.74	0.86
1:C:208:ILE:HD13	1:C:208:ILE:O	1.75	0.86
1:A:213:ARG:NH1	1:A:213:ARG:CB	2.34	0.86
1:A:252:SER:O	1:A:253:LEU:HD23	1.77	0.85
1:B:87:LEU:HG	1:B:89:ASN:ND2	1.92	0.84
1:B:237:PHE:HE2	1:B:246:MET:HE1	1.40	0.83
1:C:246:MET:HB2	1:D:253:LEU:CD2	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:302[B]:NAI:H4N	7:C:304[B]:AAE:C9	2.09	0.82
1:B:90:ASN:OD1	5:B:304[B]:NAI:H4D	1.77	0.82
1:A:99:ILE:O	1:A:101:GLU:N	2.12	0.82
1:B:251:LEU:CD1	1:B:253:LEU:HD21	2.10	0.81
1:B:87:LEU:HG	1:B:89:ASN:HD21	1.43	0.81
1:D:72:ASP:OD1	8:D:404:HOH:O	1.98	0.81
1:C:44:ARG:HD3	8:C:449:HOH:O	1.81	0.81
1:C:100:GLU:N	1:C:100:GLU:OE1	2.12	0.81
1:A:192:LEU:HD23	1:A:192:LEU:O	1.80	0.80
1:B:90:ASN:OD1	4:B:303[A]:NAD:H4D	1.79	0.80
1:B:9:VAL:HG22	1:B:88:VAL:HB	1.63	0.80
1:B:207:ASP:HB3	1:B:210:ALA:HB3	1.63	0.80
1:A:74:ILE:H	1:A:74:ILE:CD1	1.95	0.79
1:B:1:MET:HE2	1:B:236:VAL:HG12	1.64	0.79
1:A:213:ARG:HH11	1:A:213:ARG:HB3	1.47	0.78
1:A:64:LEU:HD22	1:A:70:THR:HG23	1.64	0.78
1:C:74:ILE:CD1	1:C:75:ALA:N	2.43	0.78
1:B:87:LEU:CG	1:B:89:ASN:HD21	1.96	0.78
1:A:61:ASN:HD22	1:A:62:ALA:H	1.29	0.77
1:A:74:ILE:HG13	1:A:124:ALA:HB3	1.64	0.77
1:B:204:LYS:O	1:B:206:ILE:HG23	1.85	0.77
1:C:64:LEU:HD12	4:C:301[A]:NAD:H2A	1.65	0.77
1:A:198:GLU:O	1:A:202:GLN:HG3	1.84	0.77
1:C:227:THR:O	1:C:230:GLN:HB2	1.85	0.77
1:A:91:ALA:HB1	5:A:304[B]:NAI:C2A	2.15	0.77
1:D:205:GLY:O	1:D:206:ILE:HG23	1.84	0.77
1:D:74:ILE:CD1	1:D:75:ALA:N	2.36	0.77
1:A:104:VAL:HG23	1:D:120:HIS:HE1	1.49	0.76
1:D:74:ILE:HD11	1:D:124:ALA:HB1	1.66	0.76
1:C:74:ILE:HD12	1:C:75:ALA:CA	2.14	0.76
1:D:9:VAL:HG22	1:D:88:VAL:HB	1.67	0.76
1:C:253:LEU:HD22	1:D:246:MET:CB	2.15	0.76
1:A:122:THR:HG23	1:A:137:ILE:HD13	1.66	0.76
1:D:36:PHE:CD1	4:D:302[A]:NAD:N7A	2.54	0.76
1:B:183:ILE:O	1:B:185:PRO:HD3	1.85	0.76
1:C:64:LEU:HD12	5:C:302[B]:NAI:H2A	1.66	0.76
1:B:232:GLY:O	1:B:236:VAL:HG23	1.86	0.76
1:B:190:THR:HB	1:B:191:PRO:CD	2.15	0.75
1:C:34:ASN:HB2	1:C:60:LEU:O	1.84	0.75
1:A:213:ARG:O	8:A:462:HOH:O	2.03	0.75
1:A:44:ARG:O	1:A:48:THR:HG22	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:THR:O	1:C:97:ALA:HB2	1.87	0.75
1:C:224:GLN:HG2	8:C:447:HOH:O	1.87	0.75
1:A:91:ALA:HB1	4:A:303[A]:NAD:C2A	2.16	0.74
1:A:187:TRP:CZ3	6:A:305[A]:3HR:H2	2.22	0.74
5:B:304[B]:NAI:H4N	7:B:306[B]:AAE:C5	2.16	0.74
1:C:38:GLN:HA	1:C:38:GLN:OE1	1.86	0.74
1:D:20:MET:HG2	1:D:88:VAL:HG11	1.69	0.74
1:D:222:SER:O	1:D:224:GLN:HG3	1.87	0.74
1:D:74:ILE:CD1	1:D:74:ILE:C	2.55	0.74
1:B:64:LEU:HD12	5:B:304[B]:NAI:H2A	1.69	0.74
1:C:74:ILE:C	1:C:74:ILE:CD1	2.54	0.73
1:B:122:THR:HG22	1:B:126:LEU:CD1	2.18	0.73
1:B:120:HIS:HE1	1:C:104:VAL:HG12	1.53	0.73
1:A:70:THR:O	1:A:73:PHE:HB3	1.89	0.73
1:D:196:GLN:NE2	7:D:305[B]:AAE:O3	2.22	0.73
1:A:91:ALA:CB	4:A:303[A]:NAD:C2A	2.66	0.73
1:A:91:ALA:CB	5:A:304[B]:NAI:C2A	2.66	0.72
1:D:74:ILE:HD12	1:D:75:ALA:CA	2.17	0.72
1:B:251:LEU:HD13	1:B:253:LEU:CD2	2.18	0.72
1:B:64:LEU:HD12	4:B:303[A]:NAD:H2A	1.69	0.72
1:B:40:GLU:N	1:B:40:GLU:OE1	2.22	0.72
1:A:218:GLU:OE2	1:A:219:LYS:HE2	1.90	0.72
1:A:90:ASN:CB	1:A:140:ILE:HD12	2.18	0.71
1:B:219:LYS:O	1:B:221:PRO:HD3	1.88	0.71
1:D:36:PHE:CD1	5:D:303[B]:NAI:N7A	2.58	0.71
1:C:187:TRP:CZ2	1:C:215:LEU:HD11	2.25	0.71
1:D:91:ALA:HB1	5:D:303[B]:NAI:C2A	2.20	0.71
1:D:43:GLU:OE2	1:D:46:ARG:NE	2.18	0.71
1:A:64:LEU:HD12	4:A:303[A]:NAD:H2A	1.73	0.71
1:A:252:SER:C	1:A:253:LEU:HD23	2.12	0.70
1:A:20:MET:HE1	1:A:235:ALA:HB2	1.72	0.70
1:D:74:ILE:CG1	1:D:124:ALA:HB3	2.19	0.70
1:D:32:VAL:HG23	1:D:81:LEU:HD21	1.72	0.70
1:A:253:LEU:CD2	1:B:246:MET:HG3	2.21	0.70
1:A:150:VAL:HG23	3:A:302:CL:CL	2.28	0.70
1:B:237:PHE:HE2	1:B:246:MET:CE	2.05	0.70
1:B:257:TRP:O	1:B:257:TRP:HD1	1.75	0.70
1:B:20:MET:HE3	1:B:232:GLY:HA2	1.72	0.70
1:D:197:ILE:CG2	1:D:208:ILE:HD13	2.21	0.69
1:D:142:SER:HA	1:D:185:PRO:HD2	1.73	0.69
1:D:91:ALA:HB1	4:D:302[A]:NAD:C2A	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HD22	1:B:246:MET:HB2	1.73	0.69
1:A:189:ARG:NH2	1:A:194:GLU:OE2	2.25	0.69
1:A:64:LEU:HD12	5:A:304[B]:NAI:H2A	1.74	0.69
1:B:103:PRO:HB2	1:B:106:LYS:HG2	1.75	0.69
1:C:59:TYR:O	1:C:60:LEU:HD23	1.91	0.69
1:C:9:VAL:HG22	1:C:88:VAL:HB	1.75	0.69
1:D:10:THR:HB	1:D:64:LEU:HD11	1.74	0.69
1:B:20:MET:HE1	1:B:231:LEU:O	1.93	0.68
1:B:237:PHE:CE2	1:B:246:MET:CE	2.76	0.68
1:C:126:LEU:HB2	1:C:127:PRO:HD3	1.75	0.68
1:C:204:LYS:HE2	1:C:214:GLU:OE1	1.92	0.68
1:D:74:ILE:CG1	1:D:124:ALA:CB	2.71	0.68
1:D:60:LEU:HB2	1:D:73:PHE:HE1	1.58	0.68
1:D:74:ILE:CD1	1:D:124:ALA:HB1	2.24	0.68
1:B:66:ASP:OD1	1:B:69:ALA:HB2	1.93	0.68
1:D:208:ILE:CD1	1:D:208:ILE:O	2.39	0.68
1:A:206:ILE:O	1:A:207:ASP:O	2.13	0.67
1:B:164:GLY:HA2	1:B:167:LYS:HD2	1.76	0.67
1:D:197:ILE:CG2	1:D:208:ILE:CD1	2.72	0.67
1:C:243:ALA:O	1:C:246:MET:N	2.24	0.67
1:A:20:MET:CE	1:A:235:ALA:HB2	2.24	0.67
1:B:160:HIS:O	1:C:160:HIS:HB3	1.95	0.67
1:A:87:LEU:HD12	1:A:88:VAL:N	2.10	0.67
1:B:225:PHE:HB3	8:B:416:HOH:O	1.95	0.66
1:C:221:PRO:HG2	1:C:255:GLY:O	1.94	0.66
1:C:20:MET:HE1	1:C:232:GLY:HA2	1.76	0.66
1:C:32:VAL:HG23	1:C:81:LEU:HD21	1.78	0.66
1:B:193:VAL:CG2	4:B:303[A]:NAD:H72N	2.07	0.66
1:C:253:LEU:CD2	1:D:246:MET:CG	2.72	0.66
1:D:197:ILE:HG21	1:D:208:ILE:CD1	2.25	0.66
1:B:193:VAL:HG23	4:B:303[A]:NAD:H72N	1.61	0.66
1:C:165:LEU:HD23	1:C:165:LEU:O	1.96	0.65
1:C:213:ARG:HH11	1:C:213:ARG:HB2	1.60	0.65
1:D:72:ASP:O	1:D:75:ALA:HB3	1.97	0.65
1:C:251:LEU:HD21	1:D:246:MET:HE1	1.79	0.65
1:D:197:ILE:HG21	1:D:208:ILE:HD13	1.78	0.65
1:B:165:LEU:O	1:B:165:LEU:HD23	1.96	0.64
1:B:213:ARG:NH1	1:B:213:ARG:HB2	2.13	0.64
1:B:23:GLU:HG3	8:B:406:HOH:O	1.96	0.64
1:D:194:GLU:O	1:D:198:GLU:HG3	1.97	0.64
1:D:10:THR:HB	1:D:64:LEU:CD1	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LEU:HD23	1:C:192:LEU:C	2.17	0.64
1:A:246:MET:HE3	1:B:251:LEU:HD22	1.79	0.64
1:A:71:ARG:C	1:A:74:ILE:HD11	2.18	0.64
1:A:212:ALA:C	1:A:214:GLU:H	1.99	0.64
1:C:136:ARG:HE	1:C:239:SER:HA	1.62	0.64
1:A:45:GLU:HA	1:A:48:THR:CG2	2.27	0.64
1:C:66:ASP:O	1:C:70:THR:HG22	1.98	0.63
1:C:91:ALA:HB1	5:C:302[B]:NAI:N3A	2.13	0.63
1:B:207:ASP:HB3	1:B:210:ALA:HB2	1.80	0.63
1:D:32:VAL:HG23	1:D:81:LEU:CD2	2.28	0.63
1:A:122:THR:HG23	1:A:137:ILE:CD1	2.29	0.63
1:B:3:LYS:H	1:B:3:LYS:HD3	1.64	0.62
1:B:56:LYS:HD2	1:B:56:LYS:N	2.14	0.62
1:D:1:MET:O	1:D:2:LEU:HD23	1.99	0.62
1:B:192:LEU:O	1:B:192:LEU:HD23	1.99	0.62
1:A:91:ALA:HB1	5:A:304[B]:NAI:N3A	2.14	0.62
1:D:32:VAL:HG23	1:D:81:LEU:CG	2.29	0.62
1:A:208:ILE:C	1:A:208:ILE:HD13	2.20	0.62
1:A:32:VAL:HG23	1:A:81:LEU:HD11	1.81	0.62
1:A:70:THR:O	1:A:74:ILE:HD12	2.00	0.62
1:B:85:ASP:O	1:B:129:MET:HE2	2.00	0.61
1:C:3:LYS:HA	1:C:28:GLY:O	2.00	0.61
1:A:216:LEU:O	1:A:218:GLU:N	2.33	0.61
1:A:201:SER:HB2	1:A:211:ALA:CB	2.30	0.61
1:A:45:GLU:O	1:A:48:THR:HG23	2.00	0.61
1:A:91:ALA:CB	5:A:304[B]:NAI:H2A	2.30	0.61
1:B:40:GLU:H	1:B:40:GLU:CD	2.03	0.61
1:C:136:ARG:NE	1:C:239:SER:HA	2.15	0.61
1:B:122:THR:HG22	1:B:126:LEU:HD11	1.83	0.61
1:C:208:ILE:HD13	1:C:208:ILE:C	2.20	0.61
1:A:91:ALA:HB1	4:A:303[A]:NAD:N3A	2.15	0.61
1:C:144:HIS:HA	1:C:147:VAL:O	2.01	0.61
1:A:45:GLU:O	1:A:48:THR:CG2	2.49	0.61
1:B:190:THR:HB	1:B:191:PRO:HD2	1.83	0.60
1:B:194:GLU:O	1:B:198:GLU:HG3	2.01	0.60
1:B:90:ASN:O	1:B:90:ASN:CG	2.39	0.60
1:A:91:ALA:CB	4:A:303[A]:NAD:H2A	2.30	0.60
1:B:189:ARG:HD2	1:B:225:PHE:CE1	2.36	0.60
1:C:208:ILE:HG23	1:C:209:GLU:N	2.15	0.60
1:D:116:SER:O	1:D:119:PHE:HB3	2.02	0.60
1:B:237:PHE:CE2	1:B:246:MET:HE1	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:VAL:HG12	1:C:12:SER:HB3	1.83	0.59
1:C:91:ALA:HB1	4:C:301[A]:NAD:N3A	2.16	0.59
1:C:251:LEU:HD21	1:D:246:MET:CE	2.31	0.59
1:B:196:GLN:NE2	7:B:306[B]:AAE:O3	2.29	0.59
1:B:36:PHE:CE1	4:B:303[A]:NAD:N7A	2.70	0.59
1:A:100:GLU:HG2	1:A:101:GLU:HG3	1.84	0.59
1:D:64:LEU:CA	1:D:70:THR:HG22	2.21	0.59
1:A:26:LYS:HA	1:A:53:PHE:CD1	2.38	0.59
1:B:63:ASP:O	1:B:65:SER:N	2.36	0.59
1:D:91:ALA:CB	5:D:303[B]:NAI:H2A	2.33	0.59
6:A:305[A]:3HR:O1	6:A:305[A]:3HR:H4A	2.02	0.59
1:D:91:ALA:HB1	5:D:303[B]:NAI:H2A	1.83	0.59
1:B:43:GLU:OE2	1:B:46:ARG:NE	2.26	0.59
1:A:61:ASN:ND2	1:A:62:ALA:N	2.47	0.59
1:C:36:PHE:CD1	4:C:301[A]:NAD:N7A	2.71	0.59
1:A:71:ARG:O	1:A:74:ILE:HD11	2.03	0.58
1:D:158:ALA:O	1:D:162:VAL:HG23	2.03	0.58
1:B:150:VAL:HG13	3:B:302:CL:CL	2.41	0.58
1:B:158:ALA:O	1:B:162:VAL:HG23	2.02	0.58
1:C:10:THR:HB	1:C:64:LEU:CD1	2.33	0.58
5:B:304[B]:NAI:H4N	7:B:306[B]:AAE:O8	2.03	0.58
1:B:183:ILE:C	1:B:185:PRO:HD3	2.22	0.58
1:D:142:SER:O	1:D:184:CYS:HB3	2.03	0.58
1:D:69:ALA:HA	8:D:430:HOH:O	2.02	0.58
1:C:187:TRP:CH2	1:C:215:LEU:HD11	2.39	0.58
1:A:139:ASN:O	1:A:182:ALA:HA	2.04	0.58
1:A:165:LEU:O	1:A:165:LEU:HD23	2.02	0.58
1:A:167:LYS:HE2	8:A:404:HOH:O	2.04	0.58
1:B:257:TRP:CD1	1:B:257:TRP:O	2.55	0.58
6:B:305[A]:3HR:O1	6:B:305[A]:3HR:H4A	2.01	0.58
1:D:22:THR:HG23	1:D:53:PHE:CE2	2.39	0.58
1:D:91:ALA:HB1	4:D:302[A]:NAD:H2A	1.84	0.58
1:A:190:THR:HB	1:A:191:PRO:CD	2.33	0.58
1:B:192:LEU:HD23	1:B:192:LEU:C	2.24	0.58
1:A:207:ASP:HB3	1:A:210:ALA:CB	2.34	0.58
1:B:67:ALA:O	1:B:70:THR:HG23	2.04	0.58
1:B:159:LYS:NZ	5:B:304[B]:NAI:O2D	2.28	0.58
1:C:36:PHE:CE1	4:C:301[A]:NAD:N7A	2.72	0.58
1:D:64:LEU:O	1:D:70:THR:HG21	2.03	0.58
1:B:101:GLU:OE2	8:B:437:HOH:O	2.17	0.57
1:D:64:LEU:HD23	1:D:70:THR:HG22	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CE	1:B:236:VAL:CG1	2.80	0.57
1:B:167:LYS:HB3	1:C:148:ALA:HB3	1.85	0.57
1:C:91:ALA:HB1	5:C:302[B]:NAI:C2A	2.35	0.57
1:C:168:VAL:O	1:C:172:GLU:HG3	2.04	0.57
1:A:74:ILE:HG13	1:A:124:ALA:CB	2.33	0.57
1:A:20:MET:SD	1:A:140:ILE:HD11	2.45	0.57
1:A:206:ILE:O	1:A:207:ASP:C	2.42	0.57
1:A:71:ARG:O	1:A:74:ILE:CD1	2.52	0.57
1:B:70:THR:O	1:B:73:PHE:HB3	2.05	0.57
1:D:190:THR:HB	1:D:191:PRO:HD2	1.87	0.57
1:D:17:GLY:HA3	1:D:90:ASN:ND2	2.19	0.57
1:A:166:THR:HG23	1:A:180:CYS:SG	2.44	0.57
1:A:32:VAL:HG23	1:A:81:LEU:CD1	2.35	0.57
1:D:17:GLY:CA	1:D:90:ASN:ND2	2.68	0.57
1:D:205:GLY:O	1:D:206:ILE:CG2	2.52	0.57
1:A:10:THR:O	1:A:11:GLY:C	2.43	0.56
1:A:207:ASP:HB3	1:A:210:ALA:HB2	1.87	0.56
1:B:36:PHE:CE1	5:B:304[B]:NAI:N7A	2.73	0.56
1:C:10:THR:HB	1:C:64:LEU:HD11	1.87	0.56
1:D:64:LEU:HD12	5:D:303[B]:NAI:H2A	1.87	0.56
1:A:212:ALA:C	1:A:214:GLU:N	2.58	0.56
1:B:89:ASN:HD22	1:B:89:ASN:N	2.03	0.56
1:B:159:LYS:NZ	4:B:303[A]:NAD:O2D	2.30	0.56
1:D:197:ILE:HG22	1:D:208:ILE:CD1	2.35	0.56
1:D:91:ALA:CB	4:D:302[A]:NAD:H2A	2.34	0.56
1:A:232:GLY:O	1:A:236:VAL:HG23	2.05	0.56
1:A:88:VAL:HG22	1:A:138:ILE:HB	1.86	0.56
1:D:9:VAL:HG12	1:D:12:SER:HB3	1.87	0.56
1:A:153:SER:HB3	8:A:445:HOH:O	2.04	0.56
1:D:52:LYS:HE3	1:D:53:PHE:CZ	2.41	0.56
1:B:155:TYR:CZ	1:B:159:LYS:HE3	2.41	0.56
1:C:36:PHE:CE1	5:C:302[B]:NAI:N7A	2.74	0.56
1:C:94:GLN:OE1	1:C:94:GLN:HA	2.06	0.56
1:B:144:HIS:O	1:B:159:LYS:HB2	2.06	0.56
1:C:208:ILE:C	1:C:208:ILE:CD1	2.75	0.56
1:D:32:VAL:HG23	1:D:81:LEU:HG	1.88	0.56
1:B:122:THR:CG2	1:B:126:LEU:HD11	2.35	0.55
1:C:74:ILE:HG12	1:C:124:ALA:CB	2.36	0.55
1:C:90:ASN:OD1	4:C:301[A]:NAD:H4D	2.06	0.55
1:C:39:PRO:HG2	1:C:40:GLU:OE2	2.06	0.55
1:C:36:PHE:CD1	5:C:302[B]:NAI:N7A	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ALA:H	1:C:151:ASN:HB3	1.71	0.55
1:B:260:ARG:OXT	1:D:147:VAL:HG11	2.06	0.55
1:B:18:LEU:HD11	1:B:45:GLU:HG3	1.88	0.55
1:D:64:LEU:HD12	4:D:302[A]:NAD:H2A	1.89	0.55
1:B:16:ILE:HD11	1:B:188:VAL:HG21	1.87	0.55
1:C:185:PRO:HG3	1:C:231:LEU:HD22	1.89	0.55
1:D:36:PHE:CE1	4:D:302[A]:NAD:N7A	2.74	0.55
1:D:59:TYR:O	1:D:60:LEU:HD23	2.06	0.55
1:A:96:THR:O	1:A:97:ALA:HB2	2.07	0.55
4:B:303[A]:NAD:C4N	6:B:305[A]:3HR:H3	2.37	0.55
1:D:200:ILE:O	1:D:204:LYS:HB2	2.07	0.55
1:D:190:THR:HB	1:D:191:PRO:CD	2.37	0.55
1:A:104:VAL:HG23	1:D:120:HIS:CE1	2.35	0.55
1:A:189:ARG:CZ	1:A:194:GLU:OE1	2.55	0.55
1:B:167:LYS:HB2	1:C:148:ALA:HB2	1.89	0.55
5:C:302[B]:NAI:C4N	7:C:304[B]:AAE:C9	2.83	0.55
1:D:60:LEU:HB2	1:D:73:PHE:CE1	2.40	0.54
1:D:64:LEU:CA	1:D:70:THR:CG2	2.82	0.54
1:D:199:ALA:O	1:D:203:GLN:CB	2.55	0.54
1:B:10:THR:HB	1:B:64:LEU:CD1	2.38	0.54
1:D:103:PRO:HB2	1:D:106:LYS:HB2	1.90	0.54
1:A:45:GLU:CA	1:A:48:THR:HG22	2.37	0.54
1:A:104:VAL:CG1	8:A:464:HOH:O	2.55	0.54
1:A:93:ILE:HG23	1:A:113:LEU:CD2	2.36	0.54
1:B:94:GLN:HE22	1:B:152:LYS:HD3	1.73	0.54
1:B:120:HIS:CE1	1:C:104:VAL:HG12	2.39	0.54
1:D:64:LEU:CD2	1:D:70:THR:HG22	2.37	0.54
1:A:254:ASP:HB2	1:A:257:TRP:CB	2.37	0.54
1:A:45:GLU:HA	1:A:48:THR:HG22	1.90	0.54
1:B:167:LYS:HB3	1:C:148:ALA:CB	2.37	0.54
1:D:141:ALA:O	1:D:142:SER:HB2	2.07	0.54
1:A:91:ALA:CB	5:A:304[B]:NAI:N3A	2.71	0.54
1:B:190:THR:CB	1:B:191:PRO:CD	2.86	0.54
1:C:90:ASN:OD1	5:C:302[B]:NAI:H4D	2.07	0.54
1:C:129:MET:HE1	1:C:136:ARG:H	1.71	0.54
6:D:304[A]:3HR:H4A	6:D:304[A]:3HR:O1	2.08	0.54
1:A:32:VAL:HG23	1:A:81:LEU:CG	2.38	0.53
1:B:87:LEU:CD2	1:B:89:ASN:HD21	2.21	0.53
1:B:87:LEU:CG	1:B:89:ASN:ND2	2.64	0.53
5:C:302[B]:NAI:H4N	7:C:304[B]:AAE:H93	1.87	0.53
1:B:253:LEU:HD23	1:B:253:LEU:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:THR:O	1:B:97:ALA:HB2	2.08	0.53
1:A:136:ARG:NE	1:A:238:LEU:O	2.39	0.53
1:A:70:THR:O	1:A:74:ILE:HD13	2.03	0.53
1:C:91:ALA:HB1	4:C:301[A]:NAD:C2A	2.38	0.53
1:B:1:MET:HE2	1:B:236:VAL:CG1	2.38	0.53
1:C:20:MET:CE	1:C:232:GLY:HA2	2.37	0.53
1:D:141:ALA:O	1:D:142:SER:CB	2.57	0.53
1:D:152:LYS:O	1:D:156:VAL:HG23	2.07	0.53
1:A:194:GLU:HB2	8:A:402:HOH:O	2.09	0.53
1:C:165:LEU:HD23	1:C:165:LEU:C	2.28	0.53
1:C:74:ILE:CG1	1:C:124:ALA:HB1	2.39	0.53
1:C:208:ILE:CG2	1:C:209:GLU:N	2.72	0.53
1:B:122:THR:HG22	1:B:126:LEU:HD12	1.90	0.53
1:C:257:TRP:CD1	1:C:257:TRP:C	2.83	0.53
1:A:32:VAL:CG2	1:A:81:LEU:HG	2.39	0.53
1:D:203:GLN:CD	1:D:203:GLN:O	2.44	0.53
1:A:93:ILE:HG12	1:A:113:LEU:HD23	1.91	0.52
1:B:66:ASP:CG	1:B:69:ALA:HB2	2.30	0.52
1:D:18:LEU:HD21	1:D:45:GLU:HG2	1.91	0.52
1:A:253:LEU:HD22	1:B:246:MET:CB	2.39	0.52
1:D:32:VAL:CG2	1:D:81:LEU:HG	2.39	0.52
1:D:113:LEU:HD11	4:D:302[A]:NAD:C2A	2.38	0.52
1:A:251:LEU:C	1:A:251:LEU:CD2	2.77	0.52
1:A:45:GLU:C	1:A:48:THR:HG22	2.30	0.52
1:A:246:MET:HE3	1:B:251:LEU:CD2	2.38	0.52
1:D:36:PHE:CE1	5:D:303[B]:NAI:N7A	2.77	0.52
1:A:193:VAL:HG23	4:A:303[A]:NAD:H72N	1.75	0.52
1:B:43:GLU:OE1	1:B:43:GLU:O	2.27	0.52
1:C:150:VAL:CG1	1:C:151:ASN:N	2.71	0.52
1:B:94:GLN:HG2	1:B:155:TYR:CD2	2.45	0.52
1:B:6:LYS:HE3	1:B:82:GLY:O	2.09	0.52
1:C:43:GLU:O	1:C:47:SER:HB2	2.10	0.52
1:B:213:ARG:HH11	1:B:213:ARG:CB	2.23	0.52
1:A:91:ALA:CB	4:A:303[A]:NAD:N3A	2.72	0.52
1:A:246:MET:CE	1:B:251:LEU:HD22	2.39	0.52
1:D:113:LEU:HD11	5:D:303[B]:NAI:C2A	2.39	0.52
1:B:227:THR:HG1	1:B:230:GLN:HG3	1.74	0.51
1:C:94:GLN:NE2	1:C:152:LYS:HD3	2.25	0.51
1:A:210:ALA:O	1:A:214:GLU:HB2	2.10	0.51
1:C:194:GLU:O	1:C:198:GLU:HG3	2.10	0.51
1:D:38:GLN:OE1	1:D:38:GLN:HA	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:O	1:A:256:GLY:N	2.43	0.51
1:C:96:THR:O	1:C:97:ALA:CB	2.53	0.51
1:D:74:ILE:HD12	1:D:75:ALA:H	1.59	0.51
1:A:90:ASN:OD1	4:A:303[A]:NAD:H4D	2.10	0.51
1:D:104:VAL:HG23	1:D:105:ASP:N	2.24	0.51
1:B:5:LYS:CE	8:B:411:HOH:O	2.58	0.51
1:C:99:ILE:C	1:C:101:GLU:H	2.14	0.51
1:A:32:VAL:HG23	1:A:81:LEU:HG	1.92	0.51
1:A:94:GLN:OE1	1:A:95:HIS:N	2.44	0.51
1:B:142:SER:O	1:B:184:CYS:CB	2.53	0.51
1:C:20:MET:CE	1:C:231:LEU:C	2.80	0.51
6:C:303[A]:3HR:O1	6:C:303[A]:3HR:H4A	2.09	0.51
1:C:70:THR:O	1:C:73:PHE:HB3	2.11	0.51
1:A:99:ILE:C	1:A:101:GLU:N	2.64	0.50
1:B:90:ASN:HB2	1:B:140:ILE:HG13	1.91	0.50
1:C:74:ILE:HG12	1:C:124:ALA:HB1	1.93	0.50
1:D:58:TYR:CD1	1:D:58:TYR:N	2.79	0.50
1:B:16:ILE:O	1:B:20:MET:HG2	2.11	0.50
1:C:38:GLN:OE1	1:C:38:GLN:CA	2.58	0.50
1:D:95:HIS:O	1:D:102:PHE:HE1	1.94	0.50
1:B:167:LYS:CB	1:C:148:ALA:HB2	2.42	0.50
1:B:204:LYS:O	1:B:205:GLY:C	2.50	0.50
1:A:254:ASP:HB2	1:A:257:TRP:HB2	1.92	0.50
1:C:122:THR:HG23	1:C:137:ILE:HD13	1.93	0.50
1:A:104:VAL:HG12	8:A:464:HOH:O	2.12	0.50
1:C:76:LYS:HD2	8:C:415:HOH:O	2.10	0.50
1:D:97:ALA:HB3	1:D:102:PHE:CD1	2.47	0.50
1:D:197:ILE:CG2	1:D:208:ILE:HD11	2.40	0.50
1:B:187:TRP:CZ3	6:B:305[A]:3HR:H2	2.47	0.50
1:B:20:MET:HE3	1:B:232:GLY:CA	2.42	0.50
1:A:97:ALA:C	1:A:151:ASN:HB3	2.33	0.49
1:A:254:ASP:O	1:A:255:GLY:C	2.50	0.49
1:B:32:VAL:HG23	1:B:81:LEU:HD11	1.93	0.49
1:C:50:GLU:HG3	1:C:55:VAL:O	2.12	0.49
1:A:141:ALA:O	1:A:142:SER:CB	2.59	0.49
1:C:66:ASP:O	1:C:70:THR:CG2	2.61	0.49
1:A:192:LEU:HD23	1:A:192:LEU:C	2.31	0.49
1:A:200:ILE:O	1:A:200:ILE:HG22	2.11	0.49
1:A:153:SER:CB	8:A:445:HOH:O	2.58	0.49
1:B:112:ALA:O	1:B:116:SER:HB2	2.11	0.49
1:C:106:LYS:O	1:C:110:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ALA:O	1:A:214:GLU:N	2.46	0.49
5:C:302[B]:NAI:C4N	7:C:304[B]:AAE:H93	2.41	0.49
1:A:253:LEU:HD23	1:B:246:MET:HG3	1.92	0.49
1:C:76:LYS:CD	8:C:415:HOH:O	2.61	0.49
1:A:127:PRO:HA	1:A:130:GLN:NE2	2.27	0.49
1:A:187:TRP:CE3	1:A:187:TRP:HA	2.48	0.49
1:A:252:SER:O	1:B:246:MET:HG3	2.13	0.49
1:D:185:PRO:HB3	1:D:231:LEU:HD21	1.95	0.49
1:A:193:VAL:HG21	5:A:304[B]:NAI:O7N	2.12	0.49
1:C:213:ARG:HB2	1:C:213:ARG:NH1	2.28	0.49
1:B:237:PHE:CE2	1:B:246:MET:HE3	2.48	0.48
1:A:246:MET:CE	1:B:251:LEU:CD2	2.91	0.48
1:D:104:VAL:CG2	1:D:105:ASP:N	2.75	0.48
1:A:90:ASN:OD1	5:A:304[B]:NAI:H4D	2.13	0.48
1:B:67:ALA:O	1:B:70:THR:CG2	2.61	0.48
1:D:199:ALA:O	1:D:203:GLN:HB2	2.13	0.48
1:B:129:MET:CE	1:B:136:ARG:H	2.26	0.48
1:A:186:GLY:O	4:A:303[A]:NAD:H4N	2.13	0.48
1:B:187:TRP:HZ3	7:B:306[B]:AAE:H41	1.73	0.48
1:D:199:ALA:O	1:D:203:GLN:HB3	2.14	0.48
1:B:207:ASP:CB	1:B:210:ALA:HB3	2.40	0.48
1:C:113:LEU:O	1:C:117:ALA:HB3	2.14	0.48
1:A:251:LEU:C	1:A:251:LEU:HD23	2.34	0.48
1:B:257:TRP:C	1:B:257:TRP:CD1	2.86	0.48
1:C:67:ALA:O	1:C:70:THR:HG23	2.14	0.48
1:D:11:GLY:O	1:D:90:ASN:ND2	2.46	0.48
1:D:173:ASN:HA	1:D:176:LYS:HD2	1.96	0.48
1:A:172:GLU:OE2	1:D:151:ASN:N	2.47	0.48
1:A:187:TRP:CZ3	6:A:305[A]:3HR:H4B	2.48	0.48
1:A:44:ARG:O	1:A:48:THR:CG2	2.61	0.48
1:B:213:ARG:NH1	1:B:213:ARG:CB	2.77	0.48
1:D:232:GLY:O	1:D:236:VAL:HG23	2.14	0.48
1:B:142:SER:OG	1:B:143:ALA:N	2.47	0.48
1:D:9:VAL:CG1	1:D:12:SER:HB3	2.43	0.48
1:A:99:ILE:C	1:A:101:GLU:H	2.17	0.48
1:B:142:SER:HA	1:B:185:PRO:HD2	1.96	0.48
1:D:103:PRO:HB2	1:D:106:LYS:CG	2.43	0.48
1:D:22:THR:HG23	1:D:53:PHE:CZ	2.49	0.48
1:A:26:LYS:HB2	1:A:53:PHE:CE1	2.49	0.47
1:A:187:TRP:HB2	1:A:220:GLN:OE1	2.14	0.47
1:B:20:MET:HE2	1:B:232:GLY:HA2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLN:HE22	1:B:152:LYS:CD	2.27	0.47
1:D:39:PRO:O	1:D:43:GLU:HB2	2.14	0.47
1:A:150:VAL:HG12	1:A:151:ASN:CG	2.35	0.47
1:A:99:ILE:O	1:A:102:PHE:N	2.47	0.47
1:B:252:SER:C	1:B:253:LEU:HD23	2.34	0.47
1:B:66:ASP:CG	1:B:69:ALA:CB	2.82	0.47
1:B:36:PHE:CD1	4:B:303[A]:NAD:N7A	2.82	0.47
1:B:58:TYR:CE1	1:B:81:LEU:HD23	2.50	0.47
1:C:204:LYS:CE	1:C:214:GLU:OE1	2.60	0.47
1:D:107:TRP:CD1	1:D:107:TRP:C	2.88	0.47
1:A:19:ALA:O	1:A:22:THR:HB	2.15	0.47
1:B:191:PRO:HA	1:B:194:GLU:HB2	1.97	0.47
1:B:187:TRP:CD2	1:B:215:LEU:HD21	2.50	0.47
1:A:219:LYS:O	1:A:221:PRO:HD3	2.14	0.47
1:B:130:GLN:OE1	1:C:100:GLU:OE2	2.33	0.47
1:A:187:TRP:CD1	1:A:216:LEU:HD23	2.50	0.47
1:B:113:LEU:O	1:B:117:ALA:HB3	2.13	0.47
1:B:89:ASN:N	1:B:89:ASN:ND2	2.63	0.47
1:A:99:ILE:O	1:A:100:GLU:C	2.52	0.47
1:D:42:ILE:HG21	1:D:59:TYR:CZ	2.50	0.47
1:B:129:MET:HE1	1:B:136:ARG:O	2.15	0.47
1:B:91:ALA:HB1	5:B:304[B]:NAI:C2A	2.45	0.47
1:D:18:LEU:HD21	1:D:45:GLU:CG	2.45	0.47
1:A:193:VAL:O	1:A:197:ILE:HG13	2.15	0.46
1:D:91:ALA:CB	5:D:303[B]:NAI:C2A	2.91	0.46
1:B:12:SER:OG	1:B:33:ILE:HA	2.15	0.46
1:D:126:LEU:HB2	1:D:127:PRO:HD3	1.96	0.46
1:A:95:HIS:CD2	1:A:106:LYS:HG3	2.50	0.46
1:A:244:ASP:HB2	1:B:230:GLN:NE2	2.31	0.46
1:D:219:LYS:O	1:D:221:PRO:HD3	2.16	0.46
1:D:220:GLN:HG3	1:D:254:ASP:O	2.15	0.46
1:C:136:ARG:NE	1:C:238:LEU:O	2.48	0.46
1:A:183:ILE:O	1:A:185:PRO:HD3	2.16	0.46
4:B:303[A]:NAD:H4N	6:B:305[A]:3HR:H3	1.96	0.46
1:C:9:VAL:HG22	1:C:88:VAL:CB	2.45	0.46
1:A:201:SER:HB2	1:A:211:ALA:HB3	1.96	0.46
1:B:3:LYS:N	1:B:3:LYS:HD3	2.31	0.46
1:B:56:LYS:CD	1:B:56:LYS:N	2.78	0.46
1:C:91:ALA:CB	5:C:302[B]:NAI:C2A	2.94	0.46
1:A:190:THR:HB	1:A:191:PRO:HD2	1.96	0.46
1:B:84:LEU:HD23	1:B:84:LEU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LEU:HD22	1:D:246:MET:CG	2.43	0.46
1:C:44:ARG:O	1:C:48:THR:HG23	2.15	0.46
1:B:196:GLN:NE2	6:B:305[A]:3HR:O3	2.42	0.46
1:B:6:LYS:HB3	1:B:81:LEU:HD13	1.97	0.45
1:C:20:MET:HE3	1:C:231:LEU:C	2.36	0.45
1:C:91:ALA:CB	5:C:302[B]:NAI:N3A	2.78	0.45
1:D:127:PRO:HA	1:D:130:GLN:HE21	1.81	0.45
1:D:187:TRP:CZ3	7:D:305[B]:AAE:H41	2.50	0.45
1:C:243:ALA:O	1:C:245:GLN:N	2.50	0.45
1:D:1:MET:N	8:D:407:HOH:O	2.49	0.45
1:A:190:THR:O	1:A:194:GLU:HB2	2.17	0.45
1:C:207:ASP:O	1:C:210:ALA:HB3	2.16	0.45
5:D:303[B]:NAI:H4N	7:D:305[B]:AAE:C5	2.46	0.45
1:C:74:ILE:HD12	1:C:75:ALA:HA	1.94	0.45
1:A:113:LEU:O	1:A:117:ALA:HB3	2.16	0.45
1:A:213:ARG:CZ	1:A:213:ARG:HB2	2.41	0.45
1:C:20:MET:O	1:C:24:LEU:HG	2.16	0.45
1:B:38:GLN:O	1:B:40:GLU:N	2.50	0.45
1:D:227:THR:HG1	1:D:230:GLN:HG3	1.78	0.45
1:B:183:ILE:HG22	1:B:185:PRO:HG3	1.98	0.45
1:B:32:VAL:HG23	1:B:81:LEU:HD21	1.98	0.45
1:D:195:LYS:HA	8:D:405:HOH:O	2.16	0.45
1:D:91:ALA:CB	4:D:302[A]:NAD:C2A	2.93	0.45
1:D:3:LYS:HA	1:D:28:GLY:O	2.17	0.45
5:D:303[B]:NAI:H4N	7:D:305[B]:AAE:O8	2.17	0.45
1:B:91:ALA:HB1	4:B:303[A]:NAD:C2A	2.46	0.45
1:A:106:LYS:HA	1:A:106:LYS:HD3	1.78	0.44
1:B:167:LYS:CB	1:C:148:ALA:CB	2.95	0.44
1:D:74:ILE:CG1	1:D:124:ALA:HB1	2.42	0.44
1:D:6:LYS:NZ	1:D:30:ASP:OD2	2.48	0.44
1:B:221:PRO:HG3	1:B:260:ARG:CZ	2.47	0.44
1:A:208:ILE:CD1	1:A:208:ILE:C	2.86	0.44
1:B:98:PRO:HG3	1:B:151:ASN:OD1	2.18	0.44
4:C:301[A]:NAD:H4N	6:C:303[A]:3HR:H3	1.95	0.44
1:B:14:SER:HB2	8:B:410:HOH:O	2.17	0.44
1:C:99:ILE:C	1:C:101:GLU:N	2.70	0.44
1:D:257:TRP:CD1	1:D:257:TRP:C	2.91	0.44
1:D:91:ALA:HB1	5:D:303[B]:NAI:N3A	2.32	0.44
1:D:66:ASP:O	1:D:70:THR:HG23	2.18	0.44
1:C:32:VAL:HG23	1:C:81:LEU:CD2	2.47	0.44
1:A:188:VAL:HG12	1:A:190:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:THR:HG23	1:B:35:GLY:HA3	1.99	0.44
1:C:220:GLN:HA	1:C:221:PRO:HD2	1.81	0.44
1:D:144:HIS:O	1:D:159:LYS:HB2	2.18	0.44
1:D:9:VAL:HG22	1:D:88:VAL:CB	2.43	0.43
1:A:45:GLU:HA	1:A:48:THR:HG21	2.00	0.43
1:B:141:ALA:O	1:B:142:SER:HB2	2.17	0.43
1:C:219:LYS:HB3	1:C:257:TRP:CE2	2.53	0.43
1:C:257:TRP:HD1	1:C:257:TRP:O	2.01	0.43
1:D:162:VAL:O	1:D:163:VAL:C	2.54	0.43
1:A:187:TRP:HE3	1:A:187:TRP:HA	1.82	0.43
1:A:193:VAL:HG23	4:A:303[A]:NAD:N7N	2.33	0.43
1:A:73:PHE:O	1:A:74:ILE:C	2.56	0.43
1:B:234:ALA:HB2	1:B:253:LEU:HD11	2.01	0.43
1:B:36:PHE:CD1	5:B:304[B]:NAI:N7A	2.86	0.43
1:A:254:ASP:HB2	1:A:257:TRP:HB3	1.99	0.43
1:C:94:GLN:HE22	1:C:152:LYS:HD3	1.83	0.43
1:C:243:ALA:O	1:C:244:ASP:C	2.57	0.43
1:D:95:HIS:O	1:D:102:PHE:CE1	2.71	0.43
1:D:107:TRP:CD1	1:D:108:ASN:N	2.87	0.43
1:D:191:PRO:O	1:D:192:LEU:C	2.57	0.43
1:C:218:GLU:HG2	1:C:219:LYS:HG2	2.00	0.43
1:C:254:ASP:HB2	1:C:257:TRP:HB3	2.01	0.43
1:C:91:ALA:CB	4:C:301[A]:NAD:C2A	2.97	0.43
1:C:91:ALA:CB	4:C:301[A]:NAD:N3A	2.80	0.43
1:C:141:ALA:O	1:C:142:SER:HB2	2.18	0.43
1:C:97:ALA:N	1:C:151:ASN:HB3	2.34	0.43
1:D:91:ALA:HB1	4:D:302[A]:NAD:N3A	2.33	0.43
1:D:196:GLN:NE2	6:D:304[A]:3HR:O3	2.50	0.43
1:A:104:VAL:CG1	1:A:105:ASP:N	2.81	0.43
1:C:228:PRO:O	1:C:229:GLU:C	2.56	0.43
1:B:9:VAL:CG1	1:B:12:SER:HB3	2.49	0.43
1:C:94:GLN:OE1	1:C:94:GLN:CA	2.66	0.43
1:D:103:PRO:HB2	1:D:106:LYS:CB	2.49	0.43
1:B:102:PHE:CE2	1:B:154:ALA:HB2	2.54	0.43
1:C:66:ASP:C	1:C:66:ASP:OD2	2.58	0.43
1:C:76:LYS:HB2	1:C:76:LYS:HE3	1.83	0.43
1:D:197:ILE:HG21	1:D:208:ILE:HD11	1.99	0.43
1:D:205:GLY:C	1:D:206:ILE:HG23	2.38	0.43
1:A:165:LEU:O	1:A:165:LEU:CD2	2.67	0.42
1:A:32:VAL:CG2	1:A:81:LEU:CD1	2.97	0.42
1:C:245:GLN:HA	1:C:245:GLN:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:THR:O	1:D:14:SER:HB3	2.19	0.42
1:D:197:ILE:HG22	1:D:208:ILE:HD13	1.97	0.42
1:B:155:TYR:O	1:B:159:LYS:HG2	2.18	0.42
1:C:222:SER:O	1:C:223:LEU:HB2	2.19	0.42
1:D:254:ASP:OD1	1:D:257:TRP:N	2.52	0.42
1:D:188:VAL:HB	5:D:303[B]:NAI:C7N	2.49	0.42
1:B:188:VAL:O	1:B:193:VAL:CG2	2.55	0.42
1:B:33:ILE:HD11	1:B:46:ARG:HB2	2.00	0.42
1:B:50:GLU:HG2	1:B:55:VAL:O	2.19	0.42
1:A:85:ASP:HB3	1:A:134:TRP:HZ3	1.84	0.42
1:A:78:ALA:O	1:A:82:GLY:N	2.50	0.42
1:B:46:ARG:HH11	1:B:46:ARG:HG2	1.83	0.42
1:B:63:ASP:C	1:B:65:SER:H	2.23	0.42
1:C:99:ILE:O	1:C:101:GLU:N	2.53	0.42
1:D:116:SER:O	1:D:119:PHE:N	2.53	0.42
1:A:152:LYS:O	1:A:156:VAL:HG23	2.19	0.42
1:A:193:VAL:HG21	4:A:303[A]:NAD:O7N	2.19	0.42
1:B:216:LEU:C	1:B:218:GLU:H	2.23	0.42
1:B:219:LYS:HB3	1:B:257:TRP:CD2	2.54	0.42
1:C:227:THR:OG1	1:C:230:GLN:HG3	2.20	0.42
1:C:36:PHE:N	1:C:36:PHE:CD2	2.88	0.42
1:A:187:TRP:CE3	7:A:306[B]:AAE:H93	2.55	0.42
1:A:216:LEU:O	1:A:219:LYS:N	2.45	0.42
1:A:60:LEU:CD1	1:A:77:ALA:HA	2.50	0.42
1:C:165:LEU:CD2	1:C:165:LEU:C	2.87	0.42
1:D:184:CYS:SG	1:D:250:THR:HB	2.59	0.42
1:A:112:ALA:HA	1:A:116:SER:HB2	2.02	0.42
1:A:138:ILE:HG22	1:A:138:ILE:O	2.19	0.42
1:B:38:GLN:HB2	1:B:41:ASP:OD2	2.19	0.42
1:B:153:SER:O	1:B:154:ALA:C	2.58	0.41
1:B:193:VAL:CG2	4:B:303[A]:NAD:N7N	2.79	0.41
1:C:38:GLN:HB2	1:C:41:ASP:OD2	2.19	0.41
1:C:144:HIS:HB3	1:C:156:VAL:HG22	2.02	0.41
1:D:71:ARG:HG3	1:D:120:HIS:HB3	2.02	0.41
1:B:66:ASP:OD2	1:B:66:ASP:C	2.59	0.41
1:C:9:VAL:CG1	1:C:12:SER:HB3	2.48	0.41
1:A:165:LEU:CD2	1:A:165:LEU:C	2.89	0.41
1:C:72:ASP:O	1:C:76:LYS:HB2	2.20	0.41
1:D:25:ALA:HB1	1:D:55:VAL:HG21	2.02	0.41
1:D:18:LEU:CD2	1:D:45:GLU:HG2	2.51	0.41
1:A:227:THR:O	1:A:230:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:THR:O	1:A:74:ILE:HD11	2.16	0.41
1:B:9:VAL:HG22	1:B:88:VAL:CB	2.42	0.41
1:C:9:VAL:HG22	1:C:88:VAL:CG2	2.50	0.41
1:D:34:ASN:HB2	1:D:73:PHE:CZ	2.55	0.41
1:A:185:PRO:HB2	5:A:304[B]:NAI:C5N	2.51	0.41
1:B:188:VAL:HG13	1:B:226:VAL:O	2.20	0.41
1:C:20:MET:HE1	1:C:231:LEU:O	2.21	0.41
1:A:143:ALA:C	1:A:145:GLY:H	2.24	0.41
1:B:187:TRP:HZ3	6:B:305[A]:3HR:H2	1.86	0.41
1:D:14:SER:HA	1:D:18:LEU:HD22	2.03	0.41
1:A:197:ILE:HG23	1:A:212:ALA:HB2	2.03	0.41
1:A:6:LYS:N	1:A:6:LYS:HD2	2.36	0.41
1:A:32:VAL:CG2	1:A:81:LEU:HD11	2.50	0.41
1:C:88:VAL:HA	1:C:138:ILE:O	2.21	0.41
1:A:104:VAL:HG13	1:A:105:ASP:N	2.35	0.41
1:A:197:ILE:O	1:A:197:ILE:HG22	2.21	0.41
1:C:93:ILE:HG13	1:C:110:ILE:HG12	2.03	0.41
1:C:58:TYR:N	1:C:58:TYR:CD1	2.89	0.41
1:D:183:ILE:O	1:D:185:PRO:HD3	2.21	0.41
1:A:242:ALA:O	1:B:230:GLN:HB3	2.21	0.41
1:B:160:HIS:CG	1:C:164:GLY:HA3	2.56	0.41
1:B:50:GLU:HA	1:B:55:VAL:O	2.21	0.40
1:D:11:GLY:O	1:D:17:GLY:HA3	2.22	0.40
1:D:170:ALA:HB1	1:D:247:THR:OG1	2.21	0.40
1:D:16:ILE:HD12	5:D:303[B]:NAI:C2N	2.50	0.40
1:B:210:ALA:HA	1:B:213:ARG:NH2	2.36	0.40
1:B:76:LYS:HB2	1:B:76:LYS:HE3	1.78	0.40
1:D:162:VAL:C	1:D:164:GLY:N	2.73	0.40
1:A:87:LEU:HD12	1:A:88:VAL:H	1.80	0.40
1:C:252:SER:O	1:C:253:LEU:HD23	2.21	0.40
1:C:38:GLN:O	1:C:40:GLU:N	2.54	0.40
1:C:107:TRP:O	1:C:111:ILE:HG12	2.22	0.40
1:C:158:ALA:O	1:C:162:VAL:HG23	2.22	0.40
1:C:192:LEU:HD23	1:C:192:LEU:O	2.21	0.40
1:B:66:ASP:HB3	1:B:69:ALA:HB3	2.03	0.40
1:C:106:LYS:HA	1:C:106:LYS:HD3	1.88	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	258/260 (99%)	221 (86%)	24 (9%)	13 (5%)	2	12
1	B	258/260 (99%)	230 (89%)	23 (9%)	5 (2%)	8	36
1	C	258/260 (99%)	225 (87%)	25 (10%)	8 (3%)	4	23
1	D	258/260 (99%)	222 (86%)	32 (12%)	4 (2%)	9	40
All	All	1032/1040 (99%)	898 (87%)	104 (10%)	30 (3%)	4	24

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	GLU
1	A	207	ASP
1	A	217	ALA
1	B	141	ALA
1	C	150	VAL
1	D	99	ILE
1	A	73	PHE
1	A	99	ILE
1	A	142	SER
1	A	255	GLY
1	B	64	LEU
1	B	217	ALA
1	C	97	ALA
1	C	151	ASN
1	C	244	ASP
1	D	141	ALA
1	D	142	SER
1	B	67	ALA
1	B	142	SER
1	C	141	ALA
1	C	62	ALA
1	C	100	GLU

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Mol	Chain	Res	Type
1	A	141	ALA
1	A	213	ARG
1	A	144	HIS
1	D	207	ASP
1	A	74	ILE
1	A	97	ALA
1	C	98	PRO
1	A	11	GLY

### 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	192/192 (100%)	183 (95%)	9 (5%)	26	63
1	B	192/192 (100%)	184 (96%)	8 (4%)	30	66
1	C	192/192 (100%)	183 (95%)	9 (5%)	26	63
1	D	192/192 (100%)	180 (94%)	12 (6%)	18	51
All	All	768/768 (100%)	730 (95%)	38 (5%)	25	61

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	61	ASN
1	A	74	ILE
1	A	84	LEU
1	A	165	LEU
1	A	187	TRP
1	A	208	ILE
1	A	220	GLN
1	A	251	LEU
1	B	20	MET
1	B	23	GLU
1	B	34	ASN
1	B	40	GLU

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Mol	Chain	Res	Type
1	B	43	GLU
1	B	70	THR
1	B	220	GLN
1	B	253	LEU
1	C	34	ASN
1	C	38	GLN
1	C	70	THR
1	C	74	ILE
1	C	84	LEU
1	C	94	GLN
1	C	105	ASP
1	C	208	ILE
1	C	213	ARG
1	D	34	ASN
1	D	45	GLU
1	D	58	TYR
1	D	74	ILE
1	D	84	LEU
1	D	94	GLN
1	D	130	GLN
1	D	165	LEU
1	D	203	GLN
1	D	208	ILE
1	D	220	GLN
1	D	252	SER

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

Mol	Chain	Res	Type
1	A	61	ASN
1	A	89	ASN
1	A	130	GLN
1	A	132	GLN
1	A	139	ASN
1	A	173	ASN
1	A	202	GLN
1	B	89	ASN
1	B	108	ASN
1	B	130	GLN
1	B	139	ASN
1	B	173	ASN
1	C	89	ASN

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Mol	Chain	Res	Type
1	C	130	GLN
1	C	139	ASN
1	C	173	ASN
1	D	130	GLN
1	D	132	GLN
1	D	139	ASN
1	D	173	ASN
1	D	202	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 21 ligands modelled in this entry, 5 are monoatomic - leaving 16 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	NAD	A	303[A]	-	42,48,48	1.71	11 (26%)	50,73,73	2.18	12 (24%)
6	3HR	C	303[A]	-	2,6,6	1.36	0	2,7,7	1.28	0
5	NAI	D	303[B]	-	42,48,48	1.66	7 (16%)	47,73,73	2.22	10 (21%)
7	AAE	A	306[B]	-	3,6,6	0.18	0	4,7,7	0.84	0
7	AAE	B	306[B]	-	3,6,6	0.18	0	4,7,7	0.81	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAI	C	302[B]	-	42,48,48	1.66	7 (16%)	47,73,73	2.25	12 (25%)
6	3HR	D	304[A]	-	2,6,6	1.37	0	2,7,7	1.29	0
4	NAD	B	303[A]	-	42,48,48	1.72	12 (28%)	50,73,73	2.20	14 (28%)
4	NAD	D	302[A]	-	42,48,48	1.72	12 (28%)	50,73,73	2.19	12 (24%)
6	3HR	A	305[A]	-	2,6,6	1.36	0	2,7,7	1.69	1 (50%)
4	NAD	C	301[A]	-	42,48,48	1.76	12 (28%)	50,73,73	2.21	14 (28%)
5	NAI	A	304[B]	-	42,48,48	1.64	6 (14%)	47,73,73	2.22	11 (23%)
7	AAE	C	304[B]	-	3,6,6	0.26	0	4,7,7	0.93	0
7	AAE	D	305[B]	-	3,6,6	0.19	0	4,7,7	0.83	0
5	NAI	B	304[B]	-	42,48,48	1.66	6 (14%)	47,73,73	2.24	12 (25%)
6	3HR	B	305[A]	-	2,6,6	1.33	0	2,7,7	1.70	1 (50%)

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	NAD	A	303[A]	-	-	7/26/62/62	0/5/5/5
6	3HR	C	303[A]	-	-	0/2/4/4	-
5	NAI	D	303[B]	-	-	8/25/72/72	0/5/5/5
7	AAE	A	306[B]	-	-	2/2/4/4	-
7	AAE	B	306[B]	-	-	2/2/4/4	-
5	NAI	C	302[B]	-	-	8/25/72/72	0/5/5/5
6	3HR	D	304[A]	-	-	0/2/4/4	-
4	NAD	B	303[A]	-	-	5/26/62/62	0/5/5/5
4	NAD	D	302[A]	-	-	5/26/62/62	0/5/5/5
6	3HR	A	305[A]	-	-	0/2/4/4	-
4	NAD	C	301[A]	-	-	6/26/62/62	0/5/5/5
5	NAI	A	304[B]	-	-	8/25/72/72	0/5/5/5
7	AAE	C	304[B]	-	-	2/2/4/4	-
7	AAE	D	305[B]	-	-	2/2/4/4	-
5	NAI	B	304[B]	-	-	8/25/72/72	0/5/5/5
6	3HR	B	305[A]	-	-	0/2/4/4	-

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	304[B]	NAI	O4B-C1B	4.90	1.47	1.41
4	B	303[A]	NAD	O4B-C1B	4.88	1.47	1.41
4	C	301[A]	NAD	O4B-C1B	4.87	1.47	1.41
5	C	302[B]	NAI	O4B-C1B	4.80	1.47	1.41
5	A	304[B]	NAI	C6N-C5N	4.79	1.41	1.33
5	D	303[B]	NAI	O4B-C1B	4.68	1.47	1.41
5	D	303[B]	NAI	C6N-C5N	4.66	1.41	1.33
4	D	302[A]	NAD	O4B-C1B	4.66	1.47	1.41
5	C	302[B]	NAI	C6N-C5N	4.60	1.41	1.33
5	B	304[B]	NAI	C6N-C5N	4.49	1.41	1.33
5	A	304[B]	NAI	O4B-C1B	4.36	1.47	1.41
4	A	303[A]	NAD	O4B-C1B	4.35	1.47	1.41
4	D	302[A]	NAD	C2N-N1N	3.59	1.39	1.35
4	B	303[A]	NAD	C2N-N1N	3.50	1.39	1.35
5	C	302[B]	NAI	C4N-C3N	-3.43	1.43	1.49
4	C	301[A]	NAD	C2D-C1D	-3.42	1.48	1.53
5	B	304[B]	NAI	C4N-C3N	-3.41	1.43	1.49
5	D	303[B]	NAI	C4N-C3N	-3.40	1.43	1.49
4	C	301[A]	NAD	C2N-N1N	3.38	1.39	1.35
4	D	302[A]	NAD	C2D-C1D	-3.36	1.48	1.53
5	A	304[B]	NAI	C4N-C3N	-3.35	1.43	1.49
4	A	303[A]	NAD	C2N-N1N	3.30	1.39	1.35
4	B	303[A]	NAD	C2D-C1D	-3.17	1.48	1.53
4	A	303[A]	NAD	C2D-C1D	-3.09	1.49	1.53
4	D	302[A]	NAD	C2A-N3A	2.99	1.36	1.32
5	D	303[B]	NAI	C2A-N3A	2.97	1.36	1.32
4	C	301[A]	NAD	C5N-C4N	2.95	1.45	1.38
4	A	303[A]	NAD	C2A-N3A	2.94	1.36	1.32
4	B	303[A]	NAD	C5N-C4N	2.88	1.45	1.38
4	A	303[A]	NAD	C5N-C4N	2.88	1.45	1.38
5	A	304[B]	NAI	C2A-N3A	2.86	1.36	1.32
4	D	302[A]	NAD	C5N-C4N	2.84	1.44	1.38
5	B	304[B]	NAI	C2A-N3A	2.83	1.36	1.32
4	B	303[A]	NAD	C2A-N3A	2.79	1.36	1.32
4	C	301[A]	NAD	C2A-N3A	2.78	1.36	1.32
4	C	301[A]	NAD	C3N-C7N	-2.75	1.46	1.50
5	C	302[B]	NAI	C2A-N3A	2.74	1.36	1.32
4	A	303[A]	NAD	C3N-C7N	-2.59	1.46	1.50
4	A	303[A]	NAD	O7N-C7N	2.57	1.29	1.24
5	B	304[B]	NAI	O4D-C4D	2.56	1.50	1.45
4	A	303[A]	NAD	O4D-C4D	2.53	1.50	1.45
4	B	303[A]	NAD	O4D-C4D	2.52	1.50	1.45
5	A	304[B]	NAI	O4D-C4D	2.49	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301[A]	NAD	O7N-C7N	2.40	1.28	1.24
5	D	303[B]	NAI	O4D-C4D	2.39	1.50	1.45
4	D	302[A]	NAD	O7N-C7N	2.39	1.28	1.24
4	D	302[A]	NAD	O4D-C4D	2.39	1.50	1.45
4	D	302[A]	NAD	C6N-N1N	2.36	1.41	1.35
4	C	301[A]	NAD	O3D-C3D	2.35	1.48	1.43
4	C	301[A]	NAD	C6N-N1N	2.34	1.41	1.35
5	C	302[B]	NAI	O3D-C3D	2.32	1.48	1.43
4	A	303[A]	NAD	C6N-N1N	2.29	1.41	1.35
4	B	303[A]	NAD	O7N-C7N	2.29	1.28	1.24
5	D	303[B]	NAI	O3D-C3D	2.29	1.48	1.43
4	D	302[A]	NAD	O3D-C3D	2.29	1.48	1.43
4	B	303[A]	NAD	C6N-N1N	2.28	1.41	1.35
4	A	303[A]	NAD	O3D-C3D	2.27	1.48	1.43
5	A	304[B]	NAI	O3D-C3D	2.25	1.48	1.43
4	B	303[A]	NAD	C3N-C7N	-2.22	1.47	1.50
4	C	301[A]	NAD	O4D-C4D	2.21	1.49	1.45
4	C	301[A]	NAD	C2B-C1B	-2.20	1.50	1.53
5	C	302[B]	NAI	O4D-C4D	2.16	1.49	1.45
4	B	303[A]	NAD	O3D-C3D	2.15	1.48	1.43
4	D	302[A]	NAD	C3N-C7N	-2.10	1.47	1.50
4	B	303[A]	NAD	PN-O2N	-2.09	1.45	1.55
5	B	304[B]	NAI	O3D-C3D	2.09	1.47	1.43
5	C	302[B]	NAI	C2B-C1B	-2.08	1.50	1.53
4	A	303[A]	NAD	PN-O2N	-2.07	1.45	1.55
4	D	302[A]	NAD	PN-O2N	-2.07	1.45	1.55
4	D	302[A]	NAD	O4B-C4B	2.06	1.49	1.45
4	B	303[A]	NAD	C2B-C1B	-2.04	1.50	1.53
4	C	301[A]	NAD	PN-O2N	-2.03	1.45	1.55
5	D	303[B]	NAI	O4B-C4B	2.01	1.49	1.45

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301[A]	NAD	O3D-C3D-C4D	7.82	133.66	111.05
5	C	302[B]	NAI	O3D-C3D-C4D	7.80	133.61	111.05
4	D	302[A]	NAD	O3D-C3D-C4D	7.76	133.49	111.05
4	B	303[A]	NAD	O3D-C3D-C4D	7.72	133.37	111.05
4	A	303[A]	NAD	O3D-C3D-C4D	7.72	133.36	111.05
5	D	303[B]	NAI	O3D-C3D-C4D	7.70	133.30	111.05
5	A	304[B]	NAI	O3D-C3D-C4D	7.69	133.28	111.05
5	B	304[B]	NAI	O3D-C3D-C4D	7.68	133.25	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	304[B]	NAI	O2D-C2D-C1D	-6.07	89.72	110.02
5	D	303[B]	NAI	O2D-C2D-C1D	-6.02	89.89	110.02
5	C	302[B]	NAI	O2D-C2D-C1D	-6.00	89.98	110.02
5	B	304[B]	NAI	O2D-C2D-C1D	-5.98	90.02	110.02
4	D	302[A]	NAD	PN-O3-PA	-5.82	112.86	132.83
5	D	303[B]	NAI	PN-O3-PA	-5.73	113.17	132.83
4	A	303[A]	NAD	O2D-C2D-C1D	-5.66	89.95	110.85
4	D	302[A]	NAD	O2D-C2D-C1D	-5.64	90.02	110.85
4	C	301[A]	NAD	O2D-C2D-C1D	-5.62	90.11	110.85
4	B	303[A]	NAD	O2D-C2D-C1D	-5.59	90.20	110.85
4	B	303[A]	NAD	PN-O3-PA	-5.35	114.45	132.83
5	B	304[B]	NAI	PN-O3-PA	-5.23	114.90	132.83
4	C	301[A]	NAD	PN-O3-PA	-5.13	115.23	132.83
4	A	303[A]	NAD	PN-O3-PA	-5.13	115.23	132.83
5	C	302[B]	NAI	PN-O3-PA	-5.10	115.34	132.83
5	A	304[B]	NAI	PN-O3-PA	-5.08	115.39	132.83
4	C	301[A]	NAD	O4B-C1B-C2B	-4.87	99.82	106.93
5	C	302[B]	NAI	O4B-C1B-C2B	-4.86	99.82	106.93
5	B	304[B]	NAI	O4B-C1B-C2B	-4.64	100.15	106.93
5	A	304[B]	NAI	O4B-C1B-C2B	-4.60	100.20	106.93
4	B	303[A]	NAD	O4B-C1B-C2B	-4.59	100.22	106.93
4	A	303[A]	NAD	O4B-C1B-C2B	-4.56	100.26	106.93
5	D	303[B]	NAI	O4B-C1B-C2B	-4.30	100.64	106.93
4	D	302[A]	NAD	O4B-C1B-C2B	-4.28	100.68	106.93
5	C	302[B]	NAI	N3A-C2A-N1A	-3.09	123.84	128.68
5	B	304[B]	NAI	N3A-C2A-N1A	-3.09	123.85	128.68
4	A	303[A]	NAD	N3A-C2A-N1A	-3.07	123.88	128.68
4	C	301[A]	NAD	N3A-C2A-N1A	-3.07	123.88	128.68
4	B	303[A]	NAD	N3A-C2A-N1A	-3.06	123.89	128.68
5	A	304[B]	NAI	N3A-C2A-N1A	-3.02	123.96	128.68
4	D	302[A]	NAD	N3A-C2A-N1A	-2.96	124.05	128.68
5	B	304[B]	NAI	C4D-O4D-C1D	-2.96	102.95	109.47
5	D	303[B]	NAI	N3A-C2A-N1A	-2.95	124.06	128.68
5	C	302[B]	NAI	C4D-O4D-C1D	-2.87	103.13	109.47
5	A	304[B]	NAI	C4D-O4D-C1D	-2.80	103.29	109.47
5	C	302[B]	NAI	C2A-N1A-C6A	2.78	123.50	118.75
4	C	301[A]	NAD	C2A-N1A-C6A	2.76	123.47	118.75
4	B	303[A]	NAD	C2A-N1A-C6A	2.74	123.44	118.75
5	B	304[B]	NAI	C2A-N1A-C6A	2.72	123.41	118.75
4	C	301[A]	NAD	C5N-C6N-N1N	-2.72	116.51	120.40
4	A	303[A]	NAD	C2A-N1A-C6A	2.71	123.39	118.75
5	D	303[B]	NAI	C2A-N1A-C6A	2.70	123.37	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	303[B]	NAI	C4D-O4D-C1D	-2.69	103.53	109.47
4	D	302[A]	NAD	C2A-N1A-C6A	2.69	123.36	118.75
5	A	304[B]	NAI	C2A-N1A-C6A	2.67	123.32	118.75
4	D	302[A]	NAD	O5B-C5B-C4B	-2.66	99.83	108.99
4	B	303[A]	NAD	C5N-C6N-N1N	-2.66	116.59	120.40
5	D	303[B]	NAI	O5B-C5B-C4B	-2.62	99.98	108.99
4	A	303[A]	NAD	C5N-C6N-N1N	-2.62	116.65	120.40
4	D	302[A]	NAD	C5N-C6N-N1N	-2.61	116.66	120.40
4	A	303[A]	NAD	O5B-C5B-C4B	-2.60	100.05	108.99
5	A	304[B]	NAI	O5B-C5B-C4B	-2.57	100.16	108.99
4	C	301[A]	NAD	C2N-C3N-C4N	2.56	121.16	118.26
4	B	303[A]	NAD	O5B-C5B-C4B	-2.55	100.22	108.99
5	B	304[B]	NAI	C1D-N1N-C6N	-2.54	115.35	120.83
5	B	304[B]	NAI	O5B-C5B-C4B	-2.54	100.26	108.99
4	A	303[A]	NAD	C2N-C3N-C4N	2.49	121.08	118.26
4	C	301[A]	NAD	O4D-C1D-C2D	2.48	110.56	106.93
5	C	302[B]	NAI	C1D-N1N-C6N	-2.42	115.61	120.83
4	B	303[A]	NAD	O4D-C1D-C2D	2.41	110.45	106.93
4	D	302[A]	NAD	C2N-C3N-C4N	2.41	120.99	118.26
4	B	303[A]	NAD	C2N-C3N-C4N	2.40	120.97	118.26
4	C	301[A]	NAD	O5B-C5B-C4B	-2.34	100.95	108.99
5	C	302[B]	NAI	O5B-C5B-C4B	-2.32	101.02	108.99
4	D	302[A]	NAD	O4D-C1D-C2D	2.31	110.30	106.93
4	A	303[A]	NAD	O4D-C1D-C2D	2.25	110.21	106.93
5	C	302[B]	NAI	O2D-C2D-C3D	-2.24	104.59	111.82
5	A	304[B]	NAI	C5B-C4B-C3B	-2.21	106.89	115.18
6	B	305[A]	3HR	C1-C2-C3	-2.20	109.91	113.92
5	A	304[B]	NAI	C1D-N1N-C6N	-2.19	116.10	120.83
4	C	301[A]	NAD	O2D-C2D-C3D	-2.19	104.75	111.82
4	A	303[A]	NAD	C5B-C4B-C3B	-2.18	107.02	115.18
6	A	305[A]	3HR	C1-C2-C3	-2.18	109.96	113.92
4	A	303[A]	NAD	O2D-C2D-C3D	-2.17	104.81	111.82
4	D	302[A]	NAD	O2D-C2D-C3D	-2.17	104.81	111.82
5	A	304[B]	NAI	O2D-C2D-C3D	-2.17	104.81	111.82
4	B	303[A]	NAD	C4N-C3N-C7N	-2.16	115.26	121.04
5	B	304[B]	NAI	O2D-C2D-C3D	-2.16	104.83	111.82
5	D	303[B]	NAI	C1D-N1N-C6N	-2.15	116.19	120.83
5	D	303[B]	NAI	O2D-C2D-C3D	-2.15	104.86	111.82
4	B	303[A]	NAD	O2D-C2D-C3D	-2.14	104.90	111.82
4	C	301[A]	NAD	C4N-C3N-C7N	-2.14	115.32	121.04
4	D	302[A]	NAD	C4N-C3N-C7N	-2.14	115.32	121.04
5	C	302[B]	NAI	C5B-C4B-C3B	-2.12	107.23	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301[A]	NAD	C5B-C4B-C3B	-2.12	107.25	115.18
5	B	304[B]	NAI	C5B-C4B-C3B	-2.04	107.53	115.18
4	B	303[A]	NAD	C6N-N1N-C2N	2.03	123.83	121.97
5	B	304[B]	NAI	C3N-C2N-N1N	-2.02	120.22	123.10
4	C	301[A]	NAD	C6N-N1N-C2N	2.01	123.81	121.97
4	B	303[A]	NAD	C5B-C4B-C3B	-2.01	107.65	115.18
5	C	302[B]	NAI	C2D-C1D-N1N	2.01	118.34	113.30

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303[A]	NAD	C5D-O5D-PN-O1N
4	A	303[A]	NAD	C5D-O5D-PN-O2N
4	A	303[A]	NAD	O4D-C1D-N1N-C2N
7	D	305[B]	AAE	C2-C4-C5-C9
5	D	303[B]	NAI	C5D-O5D-PN-O2N
7	A	306[B]	AAE	C2-C4-C5-C9
7	B	306[B]	AAE	C2-C4-C5-C9
5	C	302[B]	NAI	C5D-O5D-PN-O2N
4	B	303[A]	NAD	C5D-O5D-PN-O1N
4	B	303[A]	NAD	C5D-O5D-PN-O2N
4	D	302[A]	NAD	C5D-O5D-PN-O1N
4	D	302[A]	NAD	C5D-O5D-PN-O2N
4	C	301[A]	NAD	C5D-O5D-PN-O1N
4	C	301[A]	NAD	C5D-O5D-PN-O2N
4	C	301[A]	NAD	O4D-C1D-N1N-C2N
5	A	304[B]	NAI	C5D-O5D-PN-O2N
7	C	304[B]	AAE	C2-C4-C5-C9
5	B	304[B]	NAI	C5D-O5D-PN-O2N
5	D	303[B]	NAI	O4D-C1D-N1N-C6N
7	D	305[B]	AAE	C2-C4-C5-O8
7	A	306[B]	AAE	C2-C4-C5-O8
7	B	306[B]	AAE	C2-C4-C5-O8
7	C	304[B]	AAE	C2-C4-C5-O8
5	B	304[B]	NAI	O4D-C1D-N1N-C6N
5	C	302[B]	NAI	O4D-C1D-N1N-C6N
5	A	304[B]	NAI	O4D-C1D-N1N-C6N
5	D	303[B]	NAI	C5D-O5D-PN-O1N
5	C	302[B]	NAI	C5D-O5D-PN-O1N
5	A	304[B]	NAI	C5D-O5D-PN-O1N
5	B	304[B]	NAI	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
4	A	303[A]	NAD	PA-O3-PN-O2N
4	B	303[A]	NAD	PA-O3-PN-O2N
4	D	302[A]	NAD	PA-O3-PN-O2N
4	C	301[A]	NAD	PA-O3-PN-O2N
5	B	304[B]	NAI	PA-O3-PN-O2N
5	D	303[B]	NAI	O4B-C4B-C5B-O5B
5	C	302[B]	NAI	O4B-C4B-C5B-O5B
4	B	303[A]	NAD	O4B-C4B-C5B-O5B
4	D	302[A]	NAD	O4B-C4B-C5B-O5B
4	C	301[A]	NAD	O4B-C4B-C5B-O5B
5	B	304[B]	NAI	O4B-C4B-C5B-O5B
4	A	303[A]	NAD	C5D-O5D-PN-O3
5	D	303[B]	NAI	C5D-O5D-PN-O3
5	C	302[B]	NAI	C5D-O5D-PN-O3
4	B	303[A]	NAD	C5D-O5D-PN-O3
4	D	302[A]	NAD	C5D-O5D-PN-O3
4	C	301[A]	NAD	C5D-O5D-PN-O3
5	A	304[B]	NAI	C5D-O5D-PN-O3
5	B	304[B]	NAI	C5D-O5D-PN-O3
4	A	303[A]	NAD	O4B-C4B-C5B-O5B
5	A	304[B]	NAI	O4B-C4B-C5B-O5B
4	A	303[A]	NAD	PA-O3-PN-O1N
5	D	303[B]	NAI	PA-O3-PN-O1N
5	D	303[B]	NAI	PA-O3-PN-O2N
5	C	302[B]	NAI	PA-O3-PN-O1N
5	C	302[B]	NAI	PA-O3-PN-O2N
5	A	304[B]	NAI	PA-O3-PN-O1N
5	A	304[B]	NAI	PA-O3-PN-O2N
5	B	304[B]	NAI	PA-O3-PN-O1N
5	D	303[B]	NAI	C2N-C3N-C7N-N7N
5	C	302[B]	NAI	C2N-C3N-C7N-N7N
5	A	304[B]	NAI	C2N-C3N-C7N-N7N
5	B	304[B]	NAI	C2N-C3N-C7N-N7N

There are no ring outliers.

16 monomers are involved in 105 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303[A]	NAD	11	0
6	C	303[A]	3HR	3	0
5	D	303[B]	NAI	14	0
7	A	306[B]	AAE	3	0

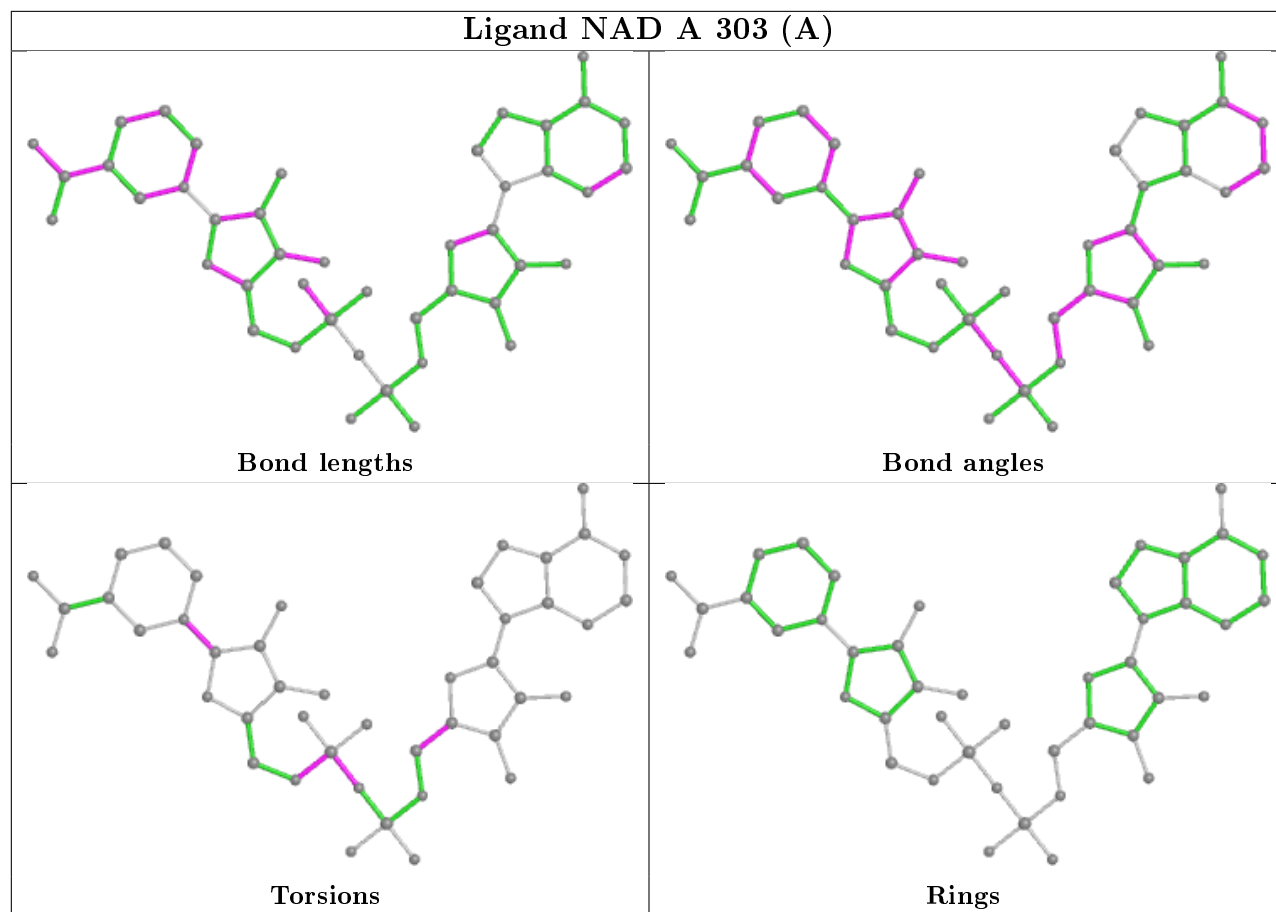
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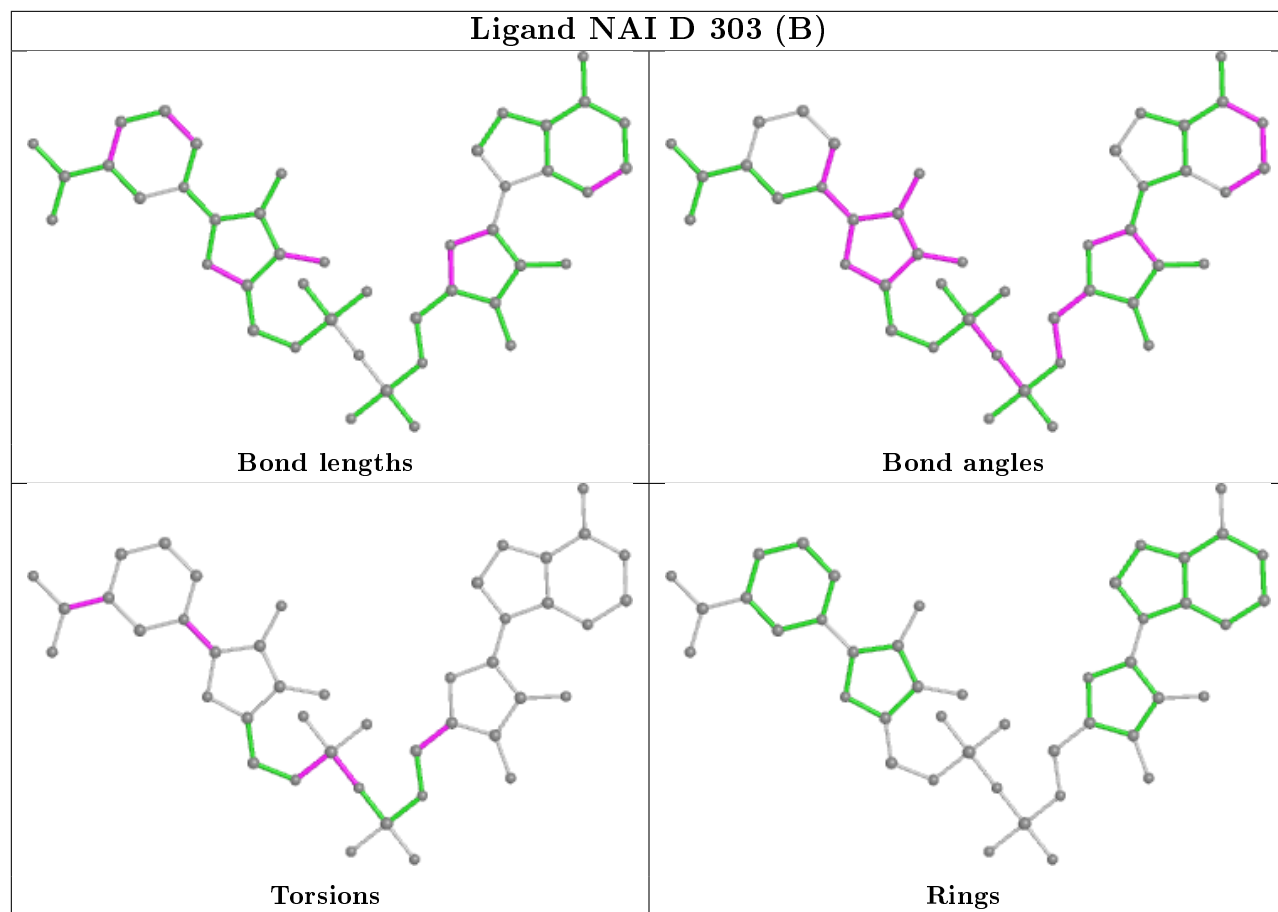
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	306[B]	AAE	5	0
5	C	302[B]	NAI	13	0
6	D	304[A]	3HR	2	0
4	B	303[A]	NAD	11	0
4	D	302[A]	NAD	10	0
6	A	305[A]	3HR	4	0
4	C	301[A]	NAD	10	0
5	A	304[B]	NAI	9	0
7	C	304[B]	AAE	5	0
7	D	305[B]	AAE	4	0
5	B	304[B]	NAI	8	0
6	B	305[A]	3HR	6	0

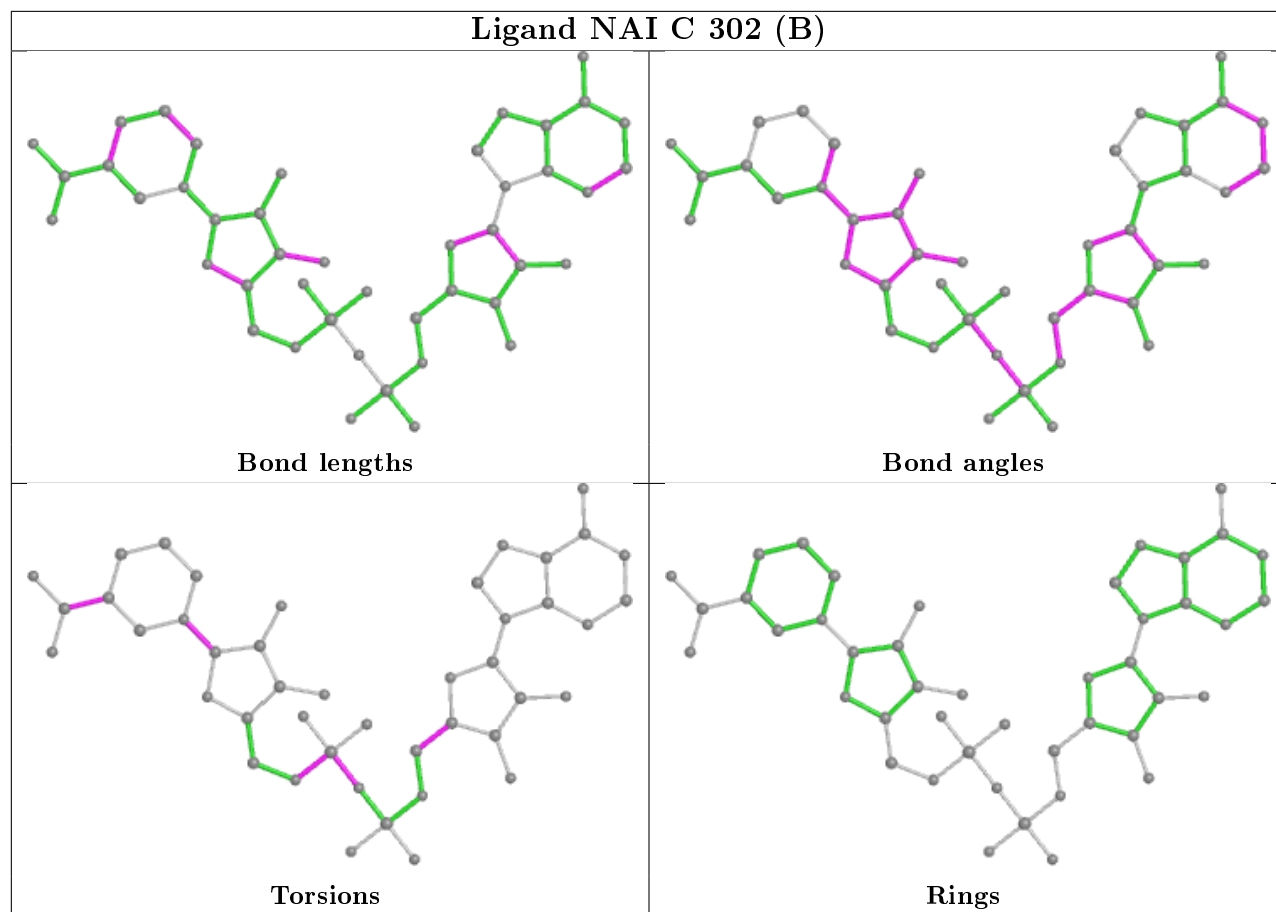
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

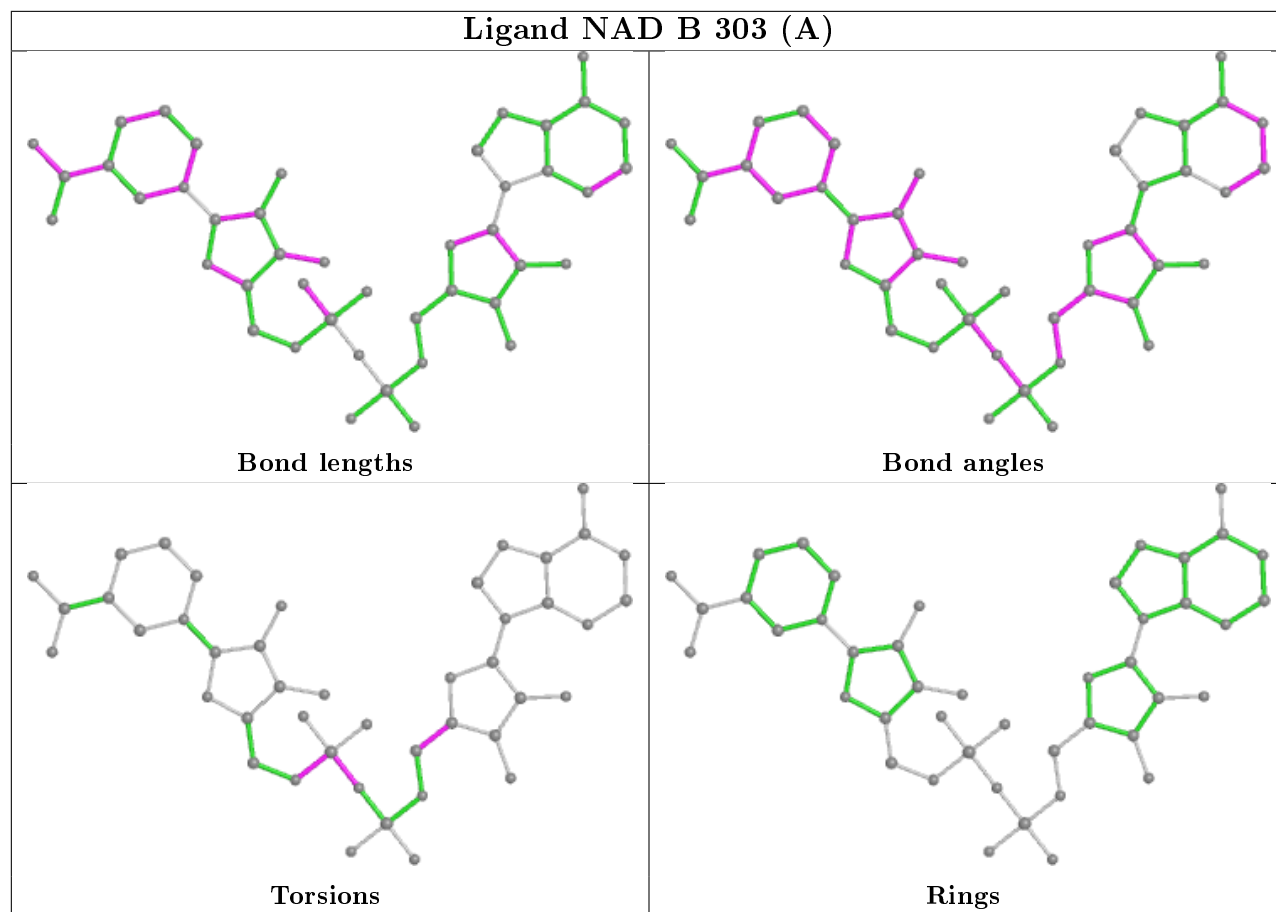


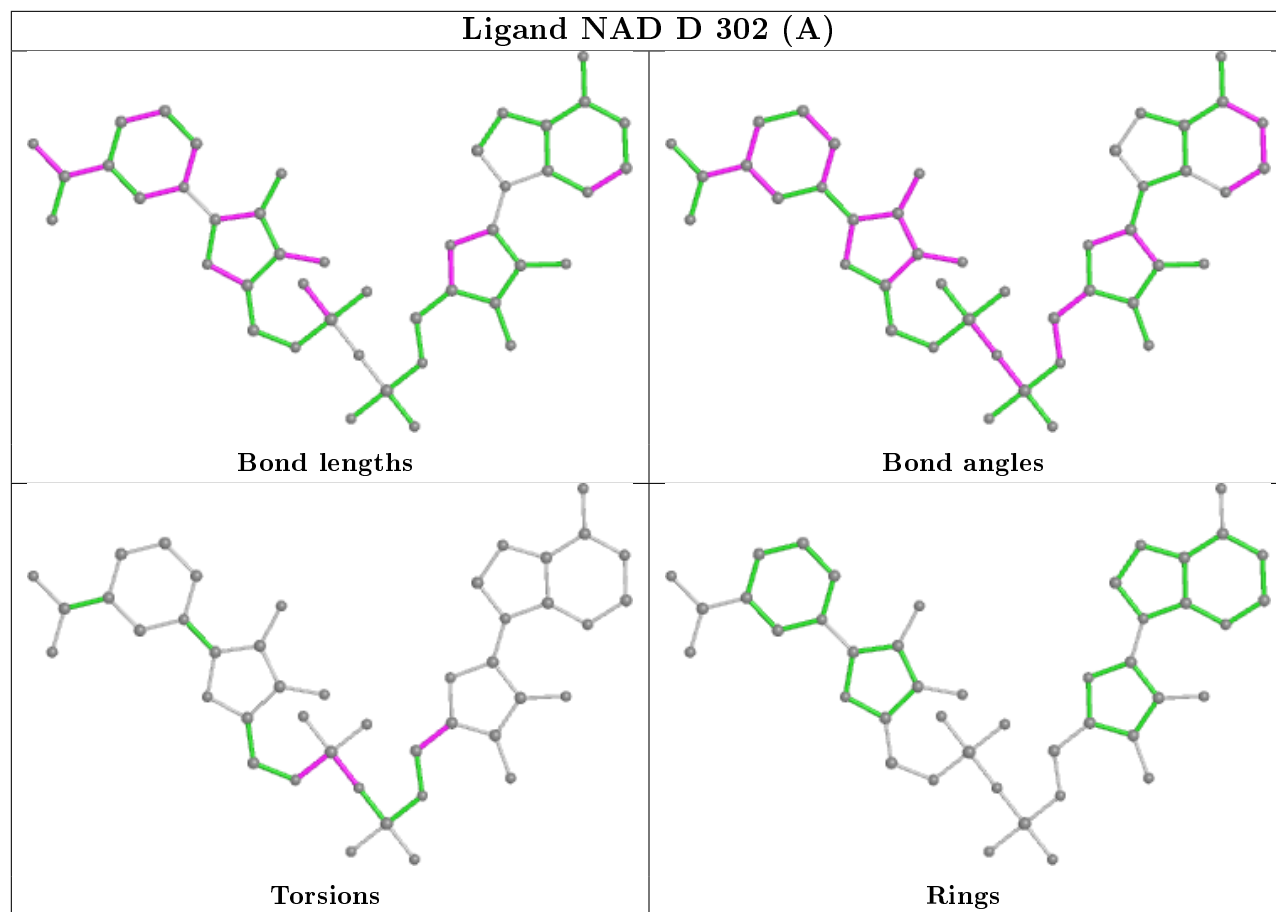


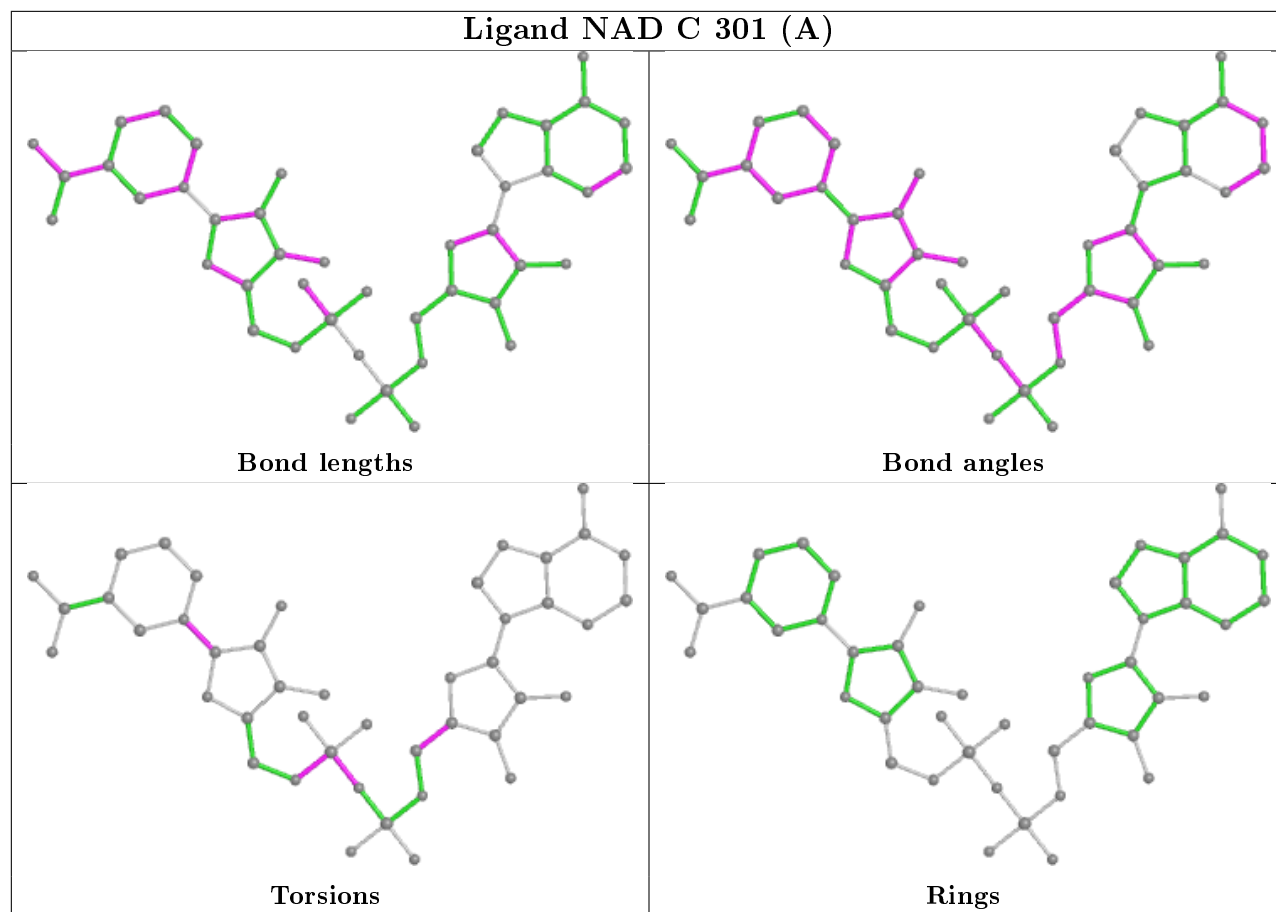
## Ligand NAI D 303 (B)



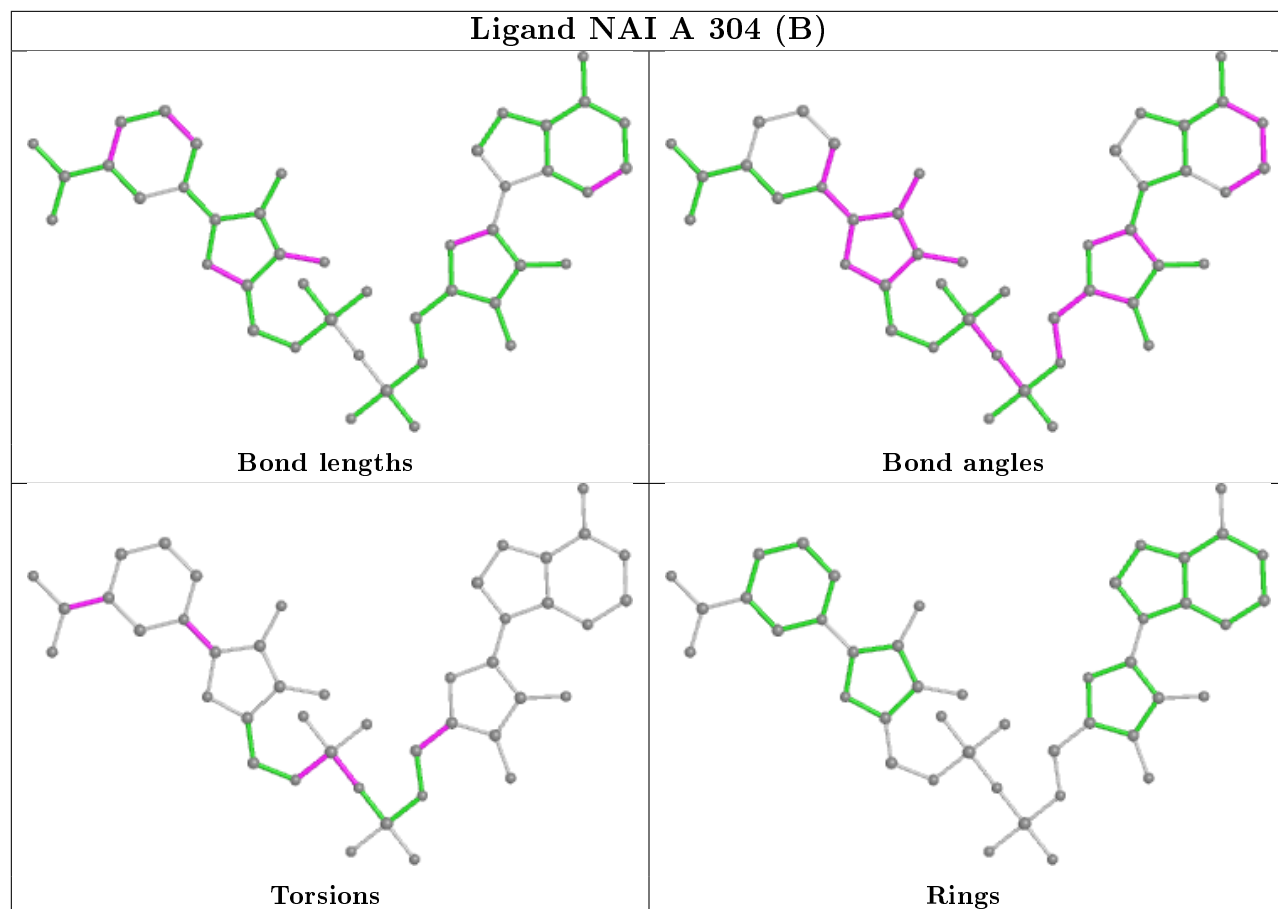


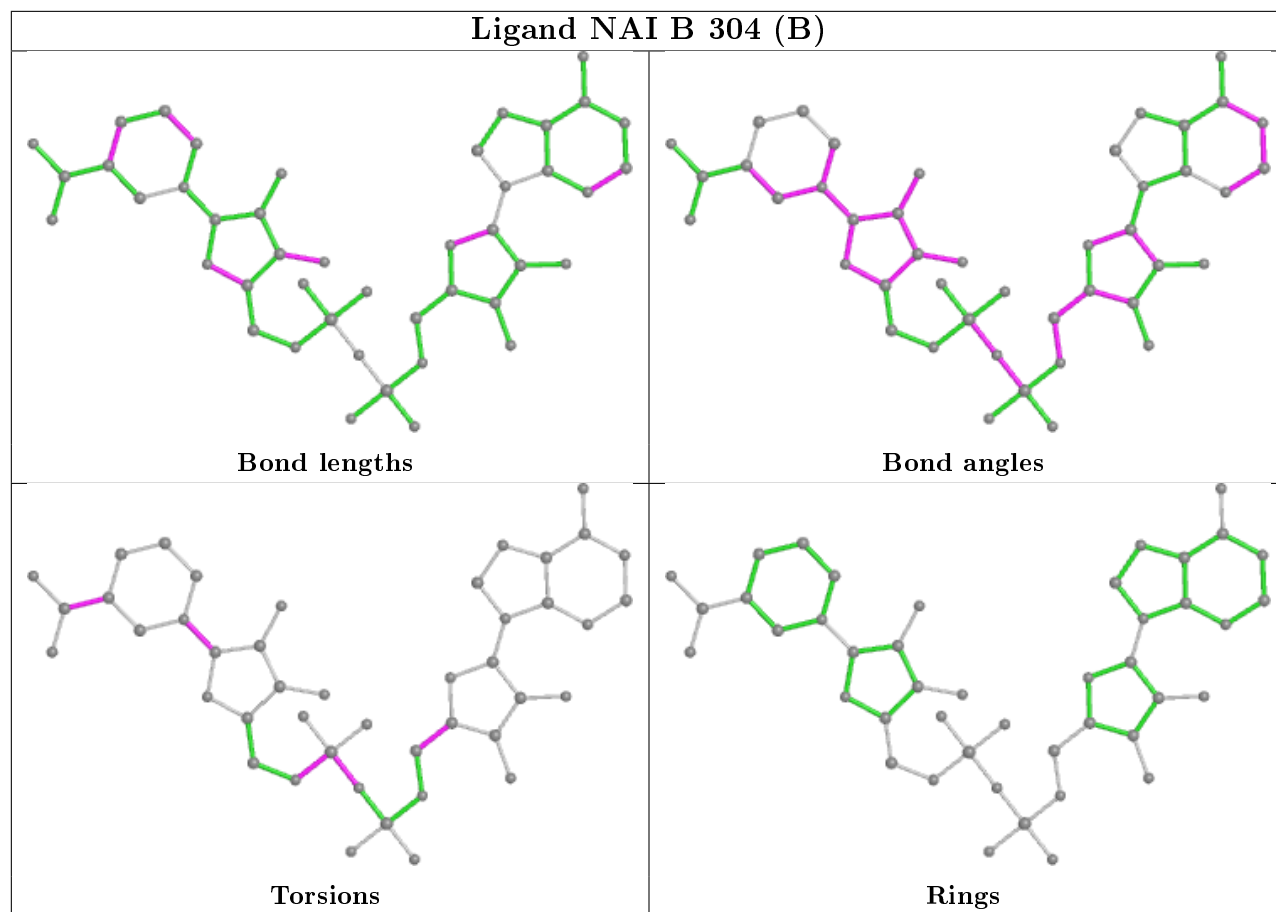






## Ligand NAI A 304 (B)





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	260/260 (100%)	-0.63	3 (1%) 79 54	21, 35, 92, 108	0
1	B	260/260 (100%)	-0.65	0 100 100	20, 38, 63, 80	0
1	C	260/260 (100%)	-0.66	0 100 100	19, 35, 64, 77	0
1	D	260/260 (100%)	-0.46	1 (0%) 92 79	26, 40, 82, 93	0
All	All	1040/1040 (100%)	-0.60	4 (0%) 92 79	19, 37, 72, 108	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	SER	2.4
1	A	203	GLN	2.3
1	D	200	ILE	2.3
1	A	202	GLN	2.3

### 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](#)

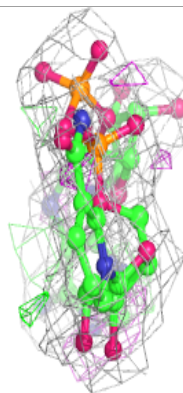
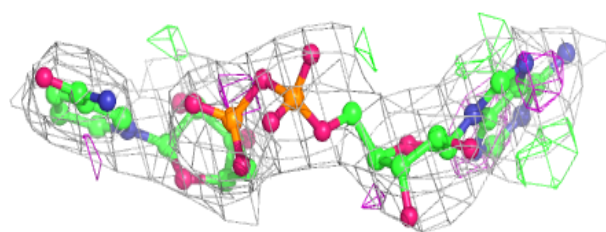
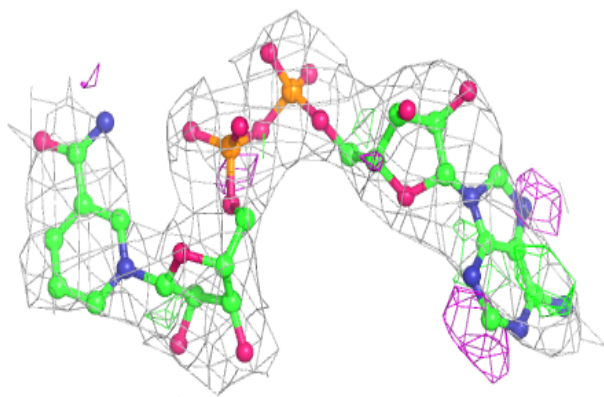
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	3HR	A	305[A]	7/7	0.89	0.27	60,61,64,65	7
5	NAI	D	303[B]	44/44	0.91	0.20	48,53,58,59	44
7	AAE	A	306[B]	7/7	0.91	0.28	69,70,71,72	7
4	NAD	D	302[A]	44/44	0.91	0.20	48,53,57,59	44
6	3HR	B	305[A]	7/7	0.91	0.21	44,44,47,47	7
5	NAI	A	304[B]	44/44	0.92	0.20	47,51,54,55	44
4	NAD	A	303[A]	44/44	0.92	0.20	46,51,54,55	44
3	CL	B	302	1/1	0.93	0.18	69,69,69,69	0
4	NAD	C	301[A]	44/44	0.94	0.18	35,40,52,53	44
5	NAI	C	302[B]	44/44	0.94	0.18	35,40,52,53	44
4	NAD	B	303[A]	44/44	0.94	0.18	42,45,51,52	44
5	NAI	B	304[B]	44/44	0.94	0.18	41,45,51,52	44
7	AAE	B	306[B]	7/7	0.94	0.21	47,48,50,51	7
6	3HR	D	304[A]	7/7	0.95	0.17	48,49,51,52	7
7	AAE	D	305[B]	7/7	0.95	0.16	50,51,53,54	7
2	CA	B	301	1/1	0.96	0.21	43,43,43,43	0
3	CL	A	302	1/1	0.97	0.16	81,81,81,81	0
7	AAE	C	304[B]	7/7	0.97	0.15	41,42,43,43	7
2	CA	A	301	1/1	0.97	0.28	51,51,51,51	0
3	CL	D	301	1/1	0.97	0.14	54,54,54,54	0
6	3HR	C	303[A]	7/7	0.97	0.15	36,37,37,38	7

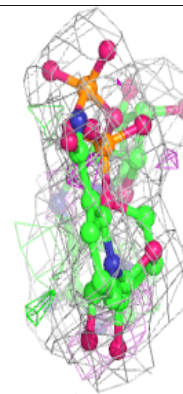
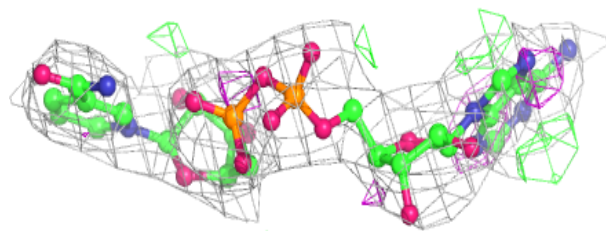
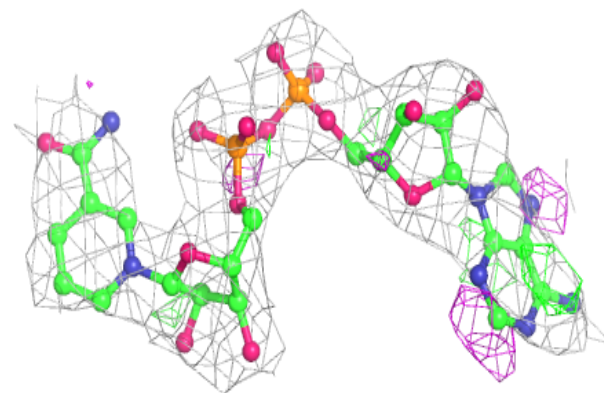
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAI D 303 (B):**

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

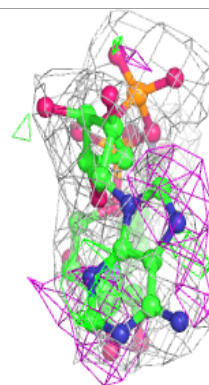
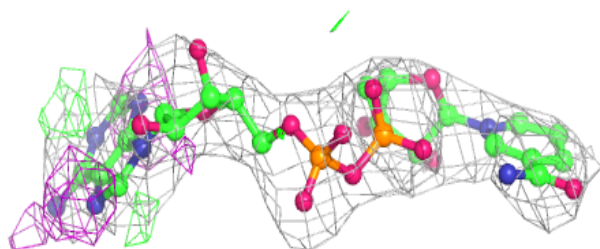
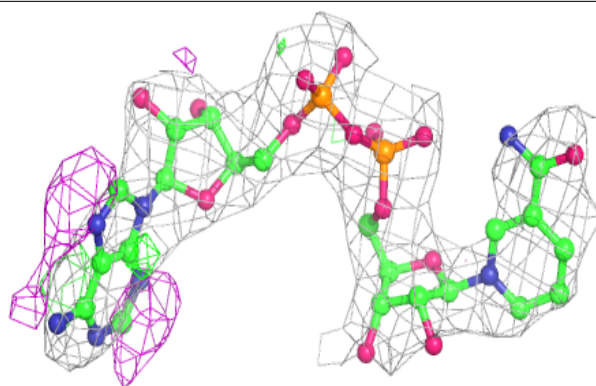
**Electron density around NAD D 302 (A):**

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

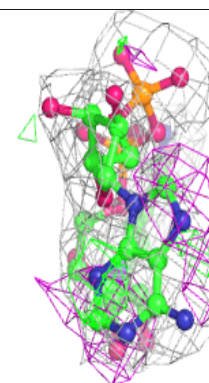
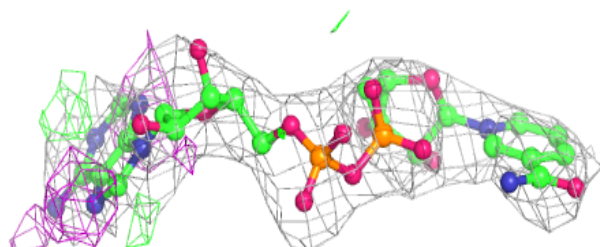
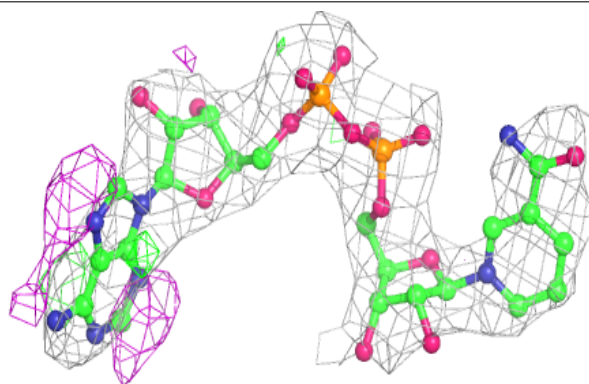


**Electron density around NAI A 304 (B):**

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

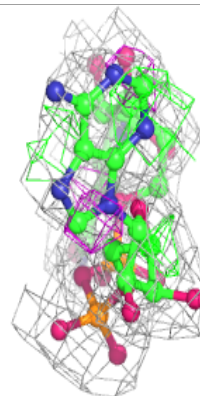
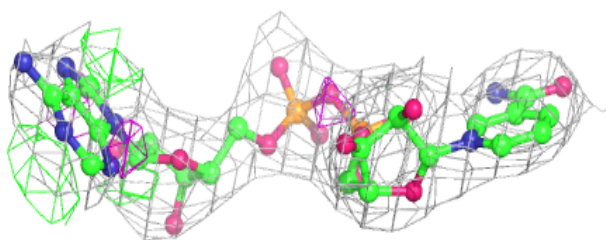
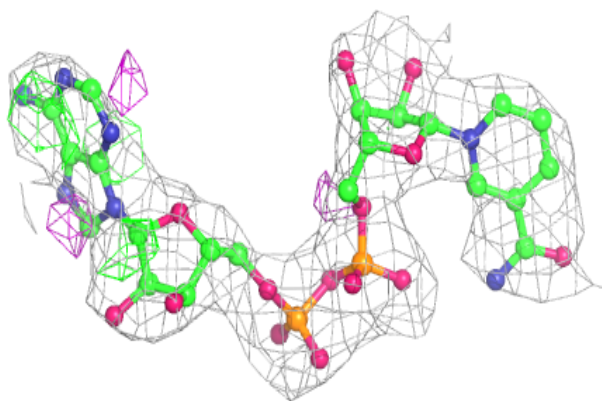
**Electron density around NAD A 303 (A):**

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

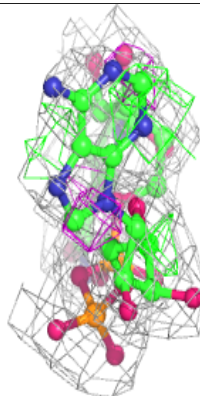
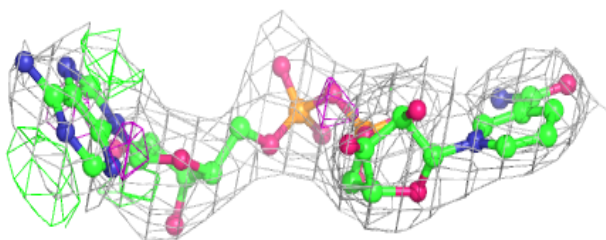
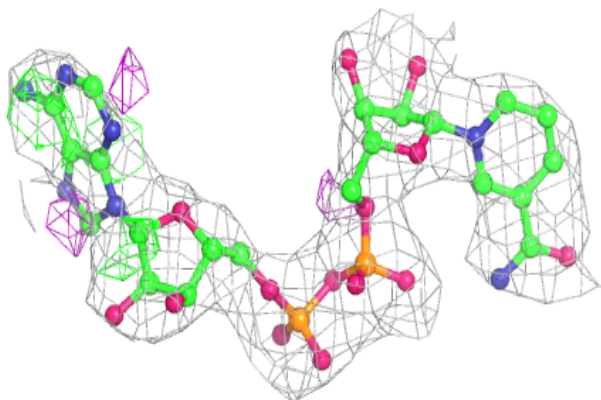


**Electron density around NAD C 301 (A):**

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

**Electron density around NAI C 302 (B):**

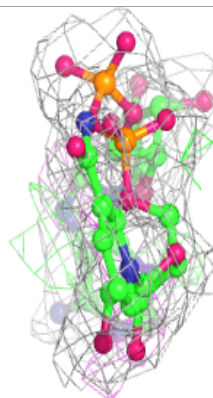
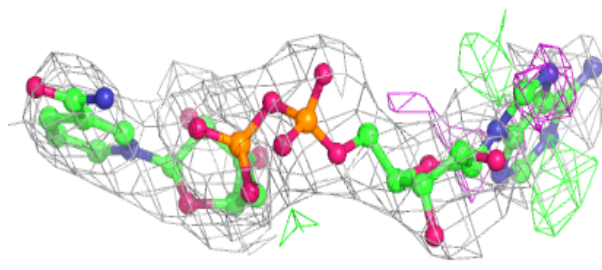
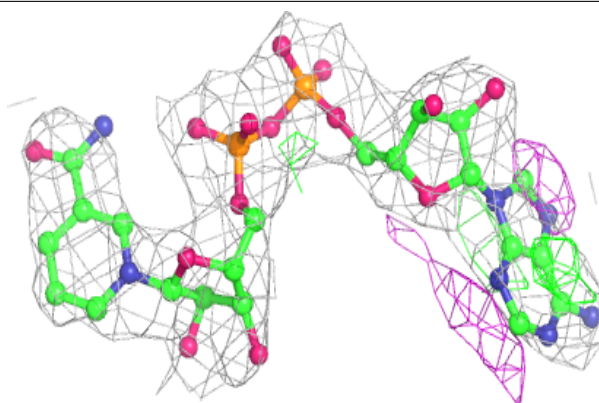
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



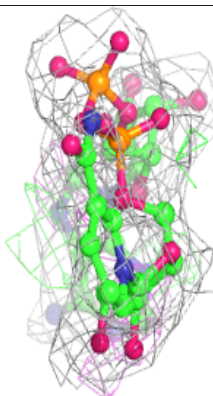
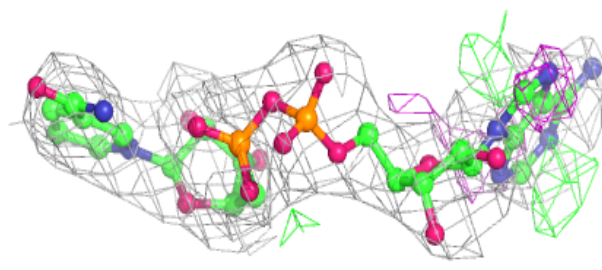
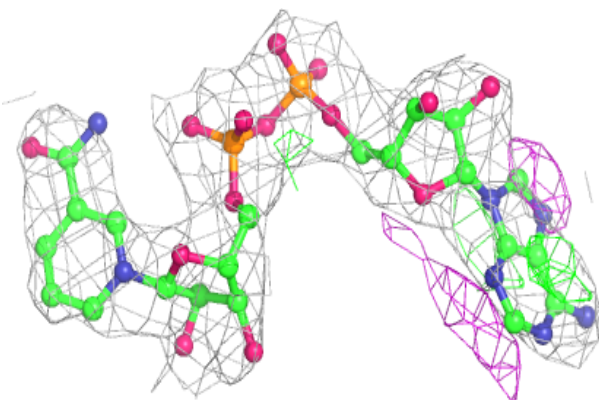


**Electron density around NAD B 303 (A):**

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

**Electron density around NAI B 304 (B):**

$2mF_o-DF_c$  (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.