



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:54 am BST

PDB ID : 4ZGS  
Title : Identification of the pyruvate reductase of *Chlamydomonas reinhardtii*  
Authors : Burgess, S.J.; Hussein, T.; Yeoman, J.A.; Iamshanova, O.; Boehm, M.; Bundy, J.; Bialek, W.; Murray, J.W.; Nixon, P.J.  
Deposited on : 2015-04-23  
Resolution : 2.46 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

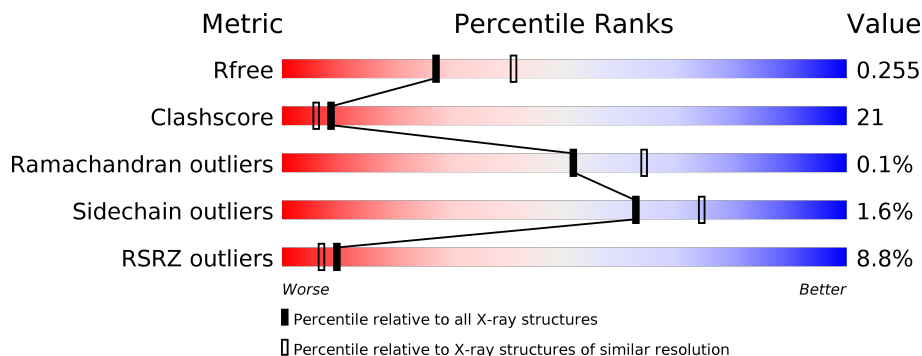
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	386	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">13% 59% 30% 10%</p>
1	B	386	<div style="display: flex; align-items: center;"> <div style="width: 13%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">12% 54% 33% 12%</p>
1	C	386	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">6% 59% 29% 10%</p>
1	D	386	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">10% 62% 25% 11%</p>
1	E	386	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	F	386	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	386	
1	H	386	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	B	1000	-	-	-	X
2	NAD	C	1000	-	-	-	X
2	NAD	F	1000	-	-	-	X
2	NAD	H	1000	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21903 atoms, of which 208 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 Putative D-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	346	Total 2661	C 1695	N 459	O 492	S 15	0	0	0
1	B	338	Total 2599	C 1657	N 449	O 478	S 15	0	0	0
1	C	342	Total 2633	C 1677	N 454	O 487	S 15	0	0	0
1	D	346	Total 2664	C 1697	N 458	O 494	S 15	0	0	0
1	E	344	Total 2648	C 1687	N 456	O 490	S 15	0	0	0
1	F	343	Total 2640	C 1682	N 455	O 488	S 15	0	0	0
1	G	343	Total 2640	C 1682	N 455	O 488	S 15	0	0	0
1	H	343	Total 2640	C 1681	N 455	O 489	S 15	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B0LUZ5
A	379	LEU	-	expression tag	UNP B0LUZ5
A	380	GLU	-	expression tag	UNP B0LUZ5
A	381	HIS	-	expression tag	UNP B0LUZ5
A	382	HIS	-	expression tag	UNP B0LUZ5
A	383	HIS	-	expression tag	UNP B0LUZ5
A	384	HIS	-	expression tag	UNP B0LUZ5
A	385	HIS	-	expression tag	UNP B0LUZ5
A	386	HIS	-	expression tag	UNP B0LUZ5
B	1	MET	-	initiating methionine	UNP B0LUZ5
B	379	LEU	-	expression tag	UNP B0LUZ5
B	380	GLU	-	expression tag	UNP B0LUZ5
B	381	HIS	-	expression tag	UNP B0LUZ5

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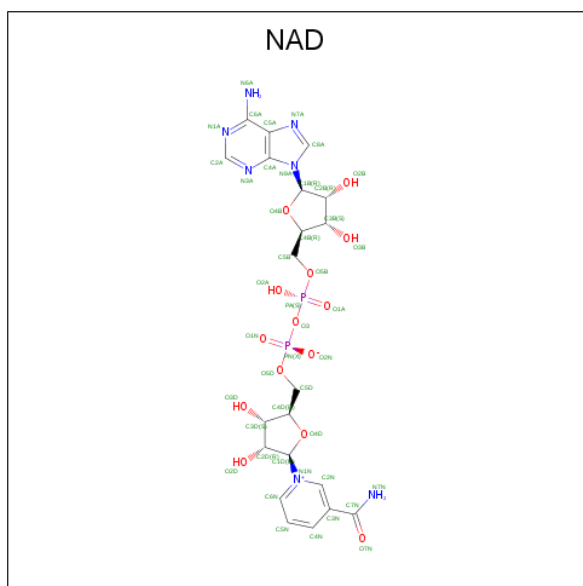
Chain	Residue	Modelled	Actual	Comment	Reference
B	382	HIS	-	expression tag	UNP B0LUZ5
B	383	HIS	-	expression tag	UNP B0LUZ5
B	384	HIS	-	expression tag	UNP B0LUZ5
B	385	HIS	-	expression tag	UNP B0LUZ5
B	386	HIS	-	expression tag	UNP B0LUZ5
C	1	MET	-	initiating methionine	UNP B0LUZ5
C	379	LEU	-	expression tag	UNP B0LUZ5
C	380	GLU	-	expression tag	UNP B0LUZ5
C	381	HIS	-	expression tag	UNP B0LUZ5
C	382	HIS	-	expression tag	UNP B0LUZ5
C	383	HIS	-	expression tag	UNP B0LUZ5
C	384	HIS	-	expression tag	UNP B0LUZ5
C	385	HIS	-	expression tag	UNP B0LUZ5
C	386	HIS	-	expression tag	UNP B0LUZ5
D	1	MET	-	initiating methionine	UNP B0LUZ5
D	379	LEU	-	expression tag	UNP B0LUZ5
D	380	GLU	-	expression tag	UNP B0LUZ5
D	381	HIS	-	expression tag	UNP B0LUZ5
D	382	HIS	-	expression tag	UNP B0LUZ5
D	383	HIS	-	expression tag	UNP B0LUZ5
D	384	HIS	-	expression tag	UNP B0LUZ5
D	385	HIS	-	expression tag	UNP B0LUZ5
D	386	HIS	-	expression tag	UNP B0LUZ5
E	1	MET	-	initiating methionine	UNP B0LUZ5
E	379	LEU	-	expression tag	UNP B0LUZ5
E	380	GLU	-	expression tag	UNP B0LUZ5
E	381	HIS	-	expression tag	UNP B0LUZ5
E	382	HIS	-	expression tag	UNP B0LUZ5
E	383	HIS	-	expression tag	UNP B0LUZ5
E	384	HIS	-	expression tag	UNP B0LUZ5
E	385	HIS	-	expression tag	UNP B0LUZ5
E	386	HIS	-	expression tag	UNP B0LUZ5
F	1	MET	-	initiating methionine	UNP B0LUZ5
F	379	LEU	-	expression tag	UNP B0LUZ5
F	380	GLU	-	expression tag	UNP B0LUZ5
F	381	HIS	-	expression tag	UNP B0LUZ5
F	382	HIS	-	expression tag	UNP B0LUZ5
F	383	HIS	-	expression tag	UNP B0LUZ5
F	384	HIS	-	expression tag	UNP B0LUZ5
F	385	HIS	-	expression tag	UNP B0LUZ5
F	386	HIS	-	expression tag	UNP B0LUZ5
G	1	MET	-	initiating methionine	UNP B0LUZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	379	LEU	-	expression tag	UNP B0LUZ5
G	380	GLU	-	expression tag	UNP B0LUZ5
G	381	HIS	-	expression tag	UNP B0LUZ5
G	382	HIS	-	expression tag	UNP B0LUZ5
G	383	HIS	-	expression tag	UNP B0LUZ5
G	384	HIS	-	expression tag	UNP B0LUZ5
G	385	HIS	-	expression tag	UNP B0LUZ5
G	386	HIS	-	expression tag	UNP B0LUZ5
H	1	MET	-	initiating methionine	UNP B0LUZ5
H	379	LEU	-	expression tag	UNP B0LUZ5
H	380	GLU	-	expression tag	UNP B0LUZ5
H	381	HIS	-	expression tag	UNP B0LUZ5
H	382	HIS	-	expression tag	UNP B0LUZ5
H	383	HIS	-	expression tag	UNP B0LUZ5
H	384	HIS	-	expression tag	UNP B0LUZ5
H	385	HIS	-	expression tag	UNP B0LUZ5
H	386	HIS	-	expression tag	UNP B0LUZ5

- Molecule 2 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	
			Total	C	H	N	O			P
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	C	1	70	21	26	7	14	2	0	0
2	D	1	70	21	26	7	14	2	0	0
2	E	1	70	21	26	7	14	2	0	0
2	F	1	70	21	26	7	14	2	0	0
2	G	1	70	21	26	7	14	2	0	0
2	H	1	70	21	26	7	14	2	0	0

- Molecule 3 is water.

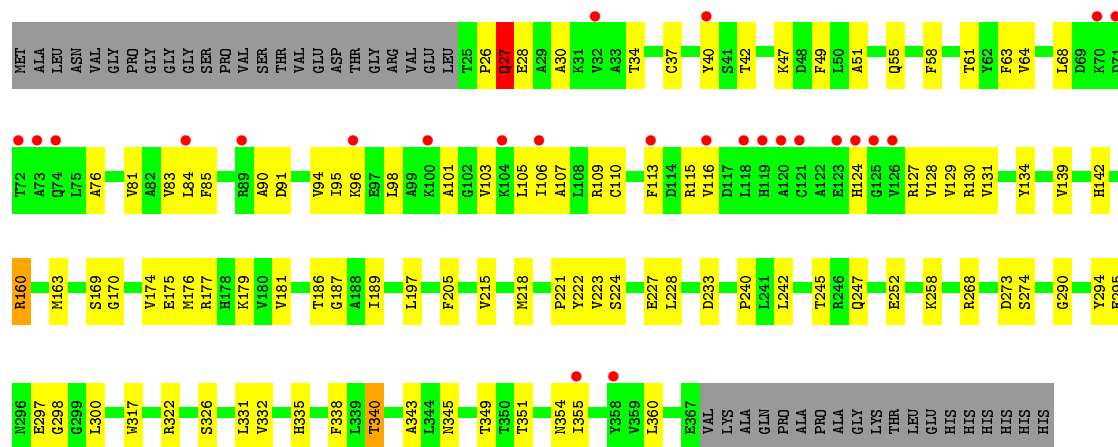
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	33	Total	O	0	0
			33	33		
3	C	25	Total	O	0	0
			25	25		
3	D	27	Total	O	0	0
			27	27		
3	E	33	Total	O	0	0
			33	33		
3	F	21	Total	O	0	0
			21	21		
3	G	20	Total	O	0	0
			20	20		
3	H	29	Total	O	0	0
			29	29		











## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.76Å 110.92Å 193.16Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	66.84 – 2.46 66.84 – 2.46	Depositor EDS
% Data completeness (in resolution range)	98.5 (66.84-2.46) 89.9 (66.84-2.46)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.202 , 0.254 0.205 , 0.255	Depositor DCC
$R_{free}$ test set	6341 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtrriage
Anisotropy	0.918	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.076 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21903	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0818e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
NAD

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	0.55	0/2710	0.75	1/3679 (0.0%)
1	B	0.52	0/2647	0.73	2/3593 (0.1%)
1	C	0.51	0/2682	0.73	2/3640 (0.1%)
1	D	0.51	0/2713	0.71	1/3684 (0.0%)
1	E	0.51	0/2697	0.72	2/3662 (0.1%)
1	F	0.53	0/2689	0.73	1/3650 (0.0%)
1	G	0.56	0/2689	0.76	1/3650 (0.0%)
1	H	0.51	0/2689	0.71	2/3651 (0.1%)
All	All	0.52	0/21516	0.73	12/29209 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	SER	C-N-CA	7.24	137.50	122.30
1	F	169	SER	C-N-CA	7.08	137.16	122.30
1	G	169	SER	C-N-CA	6.87	136.72	122.30
1	B	169	SER	C-N-CA	6.84	136.66	122.30
1	H	169	SER	C-N-CA	6.18	135.27	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	169	SER	C-N-CA	6.03	134.97	122.30
1	E	70	LYS	C-N-CA	5.78	136.16	121.70
1	B	160	ARG	CB-CG-CD	-5.52	97.25	111.60
1	C	152	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	D	169	SER	C-N-CA	5.40	133.64	122.30
1	H	160	ARG	CB-CG-CD	-5.38	97.61	111.60
1	A	169	SER	C-N-CA	5.05	132.90	122.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	ARG	Peptide
1	C	89	ARG	Peptide
1	E	71	ASP	Peptide

## 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	2661	0	2707	107	0
1	B	2599	0	2646	137	0
1	C	2633	0	2674	134	0
1	D	2664	0	2706	109	0
1	E	2648	0	2691	112	0
1	F	2640	0	2683	106	0
1	G	2640	0	2683	142	0
1	H	2640	0	2680	89	0
2	A	44	26	26	6	0
2	B	44	26	26	8	0
2	C	44	26	26	6	0
2	D	44	26	26	5	0
2	E	44	26	26	3	0
2	F	44	26	26	4	0
2	G	44	26	26	9	0
2	H	44	26	26	5	0
3	A	30	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	0	6	0
3	C	25	0	0	1	0
3	D	27	0	0	3	0
3	E	33	0	0	3	0
3	F	21	0	0	2	0
3	G	20	0	0	1	0
3	H	29	0	0	2	0
All	All	21695	208	21678	889	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 21.

All (889) 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:C:89:ARG:HB3	1:C:90:ALA:HA	1.21	1.16
1:F:38:ILE:HG22	1:F:62:TYR:HB3	1.18	1.15
1:E:70:LYS:HB3	1:E:71:ASP:HB2	1.31	1.12
1:C:106:ILE:HD11	1:C:128:VAL:HG13	1.31	1.09
1:G:89:ARG:HG3	1:G:115:ARG:HE	1.17	1.04
1:F:90:ALA:HB3	1:F:116:VAL:HA	1.38	1.00
1:C:89:ARG:CB	1:C:90:ALA:HA	1.90	1.00
1:E:90:ALA:HA	1:E:94:VAL:HG11	1.43	1.00
1:A:89:ARG:HG3	1:A:115:ARG:HH21	1.21	0.99
1:G:81:VAL:HG22	1:G:105:LEU:HB3	1.44	0.99
1:C:36:ARG:HH12	1:C:78:GLY:HA3	1.27	0.99
1:D:25:THR:HG21	1:D:29:ALA:N	1.77	0.99
1:E:25:THR:HG23	1:E:29:ALA:HB2	1.45	0.99
1:E:70:LYS:HB3	1:E:71:ASP:CB	1.94	0.96
1:D:215:VAL:HA	1:D:218:MET:HE3	1.47	0.95
1:A:246:ARG:NH1	1:F:315:GLN:O	2.00	0.95
1:C:89:ARG:HB3	1:C:90:ALA:CA	1.98	0.94
1:G:90:ALA:HA	1:G:94:VAL:HG21	1.50	0.92
1:D:215:VAL:HA	1:D:218:MET:CE	1.99	0.91
1:G:118:LEU:HD11	1:G:368:VAL:HG22	1.53	0.89
1:H:96:LYS:HB3	1:H:124:HIS:CE1	2.07	0.89
1:A:90:ALA:HA	1:A:94:VAL:CG2	2.03	0.89
1:B:129:VAL:HG11	1:B:354:ASN:HB3	1.54	0.89
1:C:160:ARG:NH2	1:C:169:SER:O	2.05	0.89
1:E:81:VAL:HG21	1:E:355:ILE:HD12	1.54	0.88
1:G:74:GLN:NE2	1:G:97:GLU:OE1	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:ILE:HG23	1:F:79:TYR:CD2	2.10	0.86
1:H:105:LEU:HD11	1:H:129:VAL:HG23	1.57	0.86
1:B:85:PHE:HB2	1:B:109:ARG:NH1	1.90	0.85
1:G:90:ALA:O	1:G:116:VAL:HA	1.75	0.85
1:C:36:ARG:NH1	1:C:78:GLY:HA3	1.92	0.85
1:D:304:ASP:OD1	1:D:306:THR:HB	1.76	0.85
1:B:62:TYR:CE1	1:B:64:VAL:HG12	2.13	0.84
1:H:233:ASP:OD1	1:H:258:LYS:NZ	2.11	0.84
1:D:113:PHE:O	1:D:116:VAL:HG12	1.77	0.83
1:D:90:ALA:HA	1:D:94:VAL:HG21	1.59	0.83
1:B:90:ALA:HA	1:B:94:VAL:HG21	1.59	0.83
1:F:38:ILE:HD11	1:F:76:ALA:HB2	1.61	0.83
1:A:90:ALA:HB1	1:A:95:ILE:HD11	1.61	0.82
1:B:69:ASP:OD1	1:B:72:THR:HG22	1.77	0.82
1:D:90:ALA:HA	1:D:94:VAL:CG2	2.10	0.82
1:B:68:LEU:N	1:B:88:ASP:OD1	2.11	0.82
1:F:38:ILE:HG22	1:F:62:TYR:CB	2.06	0.82
1:D:25:THR:HG22	1:D:28:GLU:HB2	1.60	0.82
1:G:68:LEU:HD22	1:G:84:LEU:HD21	1.60	0.81
1:A:89:ARG:CG	1:A:115:ARG:HH21	1.94	0.81
1:G:118:LEU:HD21	1:G:368:VAL:HG13	1.63	0.81
1:C:95:ILE:HG12	1:C:121:CYS:SG	2.21	0.81
1:D:233:ASP:OD1	1:D:258:LYS:NZ	2.14	0.81
1:E:340:THR:HG22	1:E:343:ALA:H	1.45	0.81
1:G:38:ILE:HD12	1:G:62:TYR:HD2	1.46	0.80
1:A:89:ARG:HG3	1:A:115:ARG:NH2	1.97	0.79
1:G:93:SER:O	1:G:96:LYS:HG2	1.82	0.79
1:H:90:ALA:HA	1:H:94:VAL:CG2	2.12	0.79
1:H:331:LEU:HD12	1:H:332:VAL:N	1.98	0.79
1:C:90:ALA:HB3	1:C:116:VAL:HG23	1.63	0.78
1:H:90:ALA:HA	1:H:94:VAL:HG21	1.65	0.78
1:G:93:SER:O	1:G:96:LYS:HE2	1.84	0.78
1:C:95:ILE:HG21	1:C:121:CYS:HA	1.65	0.78
1:G:36:ARG:HG2	1:G:79:TYR:CD2	2.19	0.78
1:E:70:LYS:CB	1:E:71:ASP:HB2	2.13	0.78
1:E:95:ILE:CD1	1:E:121:CYS:HA	2.14	0.78
1:A:92:ALA:HB3	1:H:247:GLN:HE22	1.48	0.77
1:H:91:ASP:O	1:H:95:ILE:HD12	1.83	0.77
1:E:28:GLU:HB3	1:E:360:LEU:HD21	1.66	0.77
1:E:241:LEU:HD11	1:E:246:ARG:HG2	1.65	0.77
1:H:223:VAL:CG1	1:H:227:GLU:HB2	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ALA:HA	1:G:94:VAL:CG2	2.14	0.77
1:D:187:GLY:HA3	2:D:1000:NAD:O5B	1.86	0.76
1:E:134:TYR:HA	3:E:1113:HOH:O	1.84	0.76
1:C:95:ILE:HD13	1:C:120:ALA:HB3	1.66	0.76
1:C:128:VAL:O	1:C:367:GLU:HA	1.86	0.76
1:F:55:GLN:NE2	3:F:1101:HOH:O	2.13	0.75
1:C:72:THR:HA	1:C:75:LEU:HD13	1.68	0.75
1:E:69:ASP:H	1:E:72:THR:HG22	1.51	0.74
1:C:62:TYR:HE2	1:C:64:VAL:HG22	1.52	0.74
1:E:90:ALA:HA	1:E:94:VAL:CG1	2.15	0.74
1:E:68:LEU:HD22	1:E:84:LEU:HD21	1.69	0.74
1:G:240:PRO:HD3	2:G:1000:NAD:H52A	1.70	0.74
1:G:181:VAL:HG11	1:G:197:LEU:HD13	1.69	0.74
1:A:39:CYS:SG	1:A:83:VAL:HB	2.28	0.74
1:G:106:ILE:HD11	1:G:128:VAL:HG23	1.68	0.74
1:G:128:VAL:HG11	1:G:368:VAL:HG13	1.70	0.74
1:A:51:ALA:O	1:A:55:GLN:HG3	1.88	0.73
1:E:331:LEU:HD12	1:E:332:VAL:N	2.04	0.73
1:H:187:GLY:HA3	2:H:1000:NAD:O5B	1.89	0.73
1:B:90:ALA:HA	1:B:94:VAL:CG2	2.19	0.73
1:F:74:GLN:NE2	1:F:97:GLU:OE1	2.21	0.73
1:E:67:PRO:O	1:E:72:THR:HG21	1.89	0.73
1:H:181:VAL:HG11	1:H:197:LEU:HD13	1.69	0.73
1:A:317:TRP:CZ2	1:A:322:ARG:HG3	2.24	0.72
1:C:106:ILE:HD11	1:C:128:VAL:CG1	2.14	0.72
1:C:111:ALA:O	1:C:130:ARG:NH1	2.22	0.72
1:C:267:SER:HA	2:C:1000:NAD:H1D	1.71	0.72
1:F:77:ARG:HA	1:F:101:ALA:HB1	1.70	0.72
1:B:186:THR:HG1	1:B:222:TYR:HH	1.29	0.72
1:D:223:VAL:CG1	1:D:227:GLU:HB2	2.19	0.72
1:E:326:SER:OG	1:G:322:ARG:HB3	1.89	0.72
1:D:105:LEU:HD12	1:D:127:ARG:O	1.88	0.72
1:E:51:ALA:O	1:E:55:GLN:HG3	1.89	0.72
1:E:323:THR:HG22	1:G:323:THR:HG23	1.71	0.72
1:H:223:VAL:HG13	1:H:227:GLU:HB2	1.71	0.72
1:C:90:ALA:HB1	1:C:94:VAL:CG2	2.19	0.72
1:H:215:VAL:HA	1:H:218:MET:CE	2.19	0.72
1:B:81:VAL:HG21	1:B:355:ILE:HD12	1.72	0.72
1:B:40:TYR:HA	1:B:64:VAL:HG22	1.72	0.71
1:E:297:GLU:OE1	3:E:1101:HOH:O	2.08	0.71
1:A:331:LEU:HD12	1:A:332:VAL:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:TYR:HA	3:G:1104:HOH:O	1.90	0.71
1:G:89:ARG:HG3	1:G:115:ARG:NE	2.00	0.71
1:F:223:VAL:HG22	1:F:227:GLU:OE1	1.90	0.71
1:G:113:PHE:CE1	1:G:368:VAL:HG21	2.26	0.71
1:C:240:PRO:HD3	2:C:1000:NAD:H52A	1.72	0.70
1:C:118:LEU:CD2	1:C:128:VAL:HG21	2.21	0.70
1:F:39:CYS:CB	1:F:83:VAL:HG13	2.21	0.70
1:E:95:ILE:HD11	1:E:121:CYS:HA	1.72	0.70
1:B:51:ALA:O	1:B:55:GLN:HG3	1.91	0.70
1:G:51:ALA:O	1:G:55:GLN:HG3	1.91	0.70
1:D:59:THR:HG22	3:D:1102:HOH:O	1.91	0.70
1:H:115:ARG:HH22	1:H:298:GLY:HA3	1.57	0.70
1:F:113:PHE:O	1:F:116:VAL:HG12	1.91	0.70
1:G:89:ARG:HA	1:G:115:ARG:NE	2.06	0.70
1:G:91:ASP:OD1	1:G:94:VAL:N	2.22	0.70
1:F:181:VAL:HG11	1:F:197:LEU:HD13	1.73	0.70
1:E:187:GLY:HA3	2:E:1000:NAD:O5B	1.92	0.69
1:H:37:CYS:HB2	1:H:61:THR:HG22	1.74	0.69
1:B:326:SER:OG	1:D:322:ARG:HB3	1.92	0.69
1:C:36:ARG:HG2	1:C:79:TYR:CD2	2.27	0.69
1:B:317:TRP:CZ2	1:B:322:ARG:HG3	2.26	0.69
1:G:38:ILE:HD12	1:G:62:TYR:CD2	2.27	0.69
1:E:70:LYS:HD3	1:E:71:ASP:OD2	1.93	0.69
1:G:53:PRO:O	1:G:56:LYS:HB3	1.93	0.69
1:B:340:THR:HG22	1:B:343:ALA:H	1.58	0.69
1:E:25:THR:HG23	1:E:29:ALA:CB	2.23	0.69
1:H:223:VAL:HG13	1:H:227:GLU:OE1	1.93	0.69
1:G:67:PRO:O	1:G:72:THR:HG21	1.93	0.69
1:H:90:ALA:HB3	1:H:116:VAL:HG23	1.73	0.69
1:D:223:VAL:HG13	1:D:227:GLU:HB2	1.74	0.68
1:D:241:LEU:HD11	1:D:246:ARG:HG2	1.76	0.68
1:D:317:TRP:CZ2	1:D:322:ARG:HG3	2.28	0.68
1:F:322:ARG:HB3	1:H:326:SER:OG	1.93	0.68
1:A:240:PRO:HD3	2:A:1000:NAD:H52A	1.75	0.68
1:F:148:PHE:CZ	1:F:176:MET:HE3	2.28	0.68
1:C:96:LYS:HG2	1:C:100:LYS:HE2	1.73	0.68
1:E:70:LYS:HB3	1:E:71:ASP:CG	2.13	0.68
1:B:148:PHE:CZ	1:B:176:MET:HE3	2.29	0.68
1:D:25:THR:HB	1:D:26:PRO:C	2.14	0.68
1:B:67:PRO:O	1:B:72:THR:HG21	1.93	0.68
1:A:89:ARG:HA	1:A:115:ARG:HE	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:LEU:CD2	1:G:128:VAL:HG11	2.24	0.67
1:B:322:ARG:HB3	1:D:326:SER:OG	1.94	0.67
1:E:26:PRO:HD2	1:E:28:GLU:OE1	1.94	0.67
1:A:129:VAL:HG11	1:A:354:ASN:HB3	1.75	0.67
1:C:68:LEU:N	1:C:88:ASP:OD1	2.24	0.67
1:A:90:ALA:HB1	1:A:95:ILE:CD1	2.24	0.67
1:G:241:LEU:HD11	1:G:246:ARG:HG2	1.75	0.67
1:C:317:TRP:CZ2	1:C:322:ARG:HG3	2.30	0.66
1:H:51:ALA:O	1:H:55:GLN:HG3	1.94	0.66
1:C:84:LEU:HB2	1:C:108:LEU:HD23	1.77	0.66
1:H:115:ARG:HH22	1:H:298:GLY:CA	2.07	0.66
1:A:96:LYS:O	1:A:100:LYS:HG2	1.95	0.66
1:D:26:PRO:HB2	1:D:27:GLN:OE1	1.94	0.66
1:G:317:TRP:CZ2	1:G:322:ARG:HG3	2.30	0.66
1:F:51:ALA:O	1:F:55:GLN:HG3	1.95	0.66
1:H:215:VAL:HA	1:H:218:MET:HE2	1.77	0.66
1:F:70:LYS:CA	1:F:94:VAL:HG12	2.25	0.66
1:B:181:VAL:HG11	1:B:197:LEU:HD13	1.79	0.65
1:H:27:GLN:OE1	1:H:27:GLN:HA	1.93	0.65
1:G:160:ARG:NH2	1:G:169:SER:O	2.25	0.65
1:H:113:PHE:O	1:H:116:VAL:HG12	1.97	0.65
1:G:118:LEU:HD22	1:G:128:VAL:HG11	1.79	0.65
1:F:70:LYS:HA	1:F:94:VAL:HG12	1.77	0.65
1:C:268:ARG:HG2	2:C:1000:NAD:O2D	1.96	0.65
1:D:25:THR:CG2	1:D:28:GLU:HB2	2.26	0.64
1:H:105:LEU:HD12	1:H:127:ARG:O	1.96	0.64
1:H:294:TYR:O	1:H:297:GLU:HG3	1.97	0.64
1:B:187:GLY:HA3	2:B:1000:NAD:O5B	1.97	0.64
1:H:105:LEU:HD11	1:H:129:VAL:CG2	2.27	0.64
1:G:223:VAL:HG21	1:G:231:MET:CE	2.27	0.64
1:C:91:ASP:O	1:C:95:ILE:HD12	1.97	0.64
1:D:90:ALA:HB3	1:D:116:VAL:HG23	1.78	0.64
1:B:351:THR:O	1:B:355:ILE:HG12	1.97	0.64
1:F:39:CYS:HB2	1:F:83:VAL:HG13	1.79	0.64
1:B:39:CYS:CB	1:B:83:VAL:HG13	2.28	0.64
1:B:62:TYR:HE1	1:B:64:VAL:HG12	1.62	0.64
1:G:111:ALA:HB2	1:G:131:VAL:O	1.98	0.64
1:G:240:PRO:HD3	2:G:1000:NAD:C5B	2.29	0.63
1:D:252:GLU:N	1:D:252:GLU:OE1	2.30	0.63
1:G:89:ARG:CG	1:G:115:ARG:HE	2.02	0.63
1:H:83:VAL:HA	1:H:107:ALA:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PHE:O	1:B:116:VAL:HG12	1.97	0.63
1:C:90:ALA:HB1	1:C:94:VAL:HG23	1.81	0.63
1:D:181:VAL:HG11	1:D:197:LEU:HD13	1.80	0.63
1:A:226:ASP:OD1	1:A:256:LYS:NZ	2.17	0.63
1:B:35:THR:HB	1:B:58:PHE:CD1	2.33	0.63
1:C:106:ILE:CD1	1:C:128:VAL:HG13	2.20	0.63
1:D:351:THR:O	1:D:355:ILE:HG12	1.99	0.63
1:E:68:LEU:HA	1:E:72:THR:CG2	2.29	0.63
1:G:38:ILE:HD11	1:G:64:VAL:HG21	1.80	0.63
1:A:127:ARG:NH2	1:A:364:LEU:HD12	2.13	0.63
1:A:87:ASN:ND2	3:A:1104:HOH:O	2.32	0.63
1:D:72:THR:HB	1:D:75:LEU:HD12	1.80	0.63
1:E:319:ARG:O	1:E:323:THR:HG23	1.99	0.62
1:F:187:GLY:HA3	2:F:1000:NAD:O5B	1.99	0.62
1:C:96:LYS:O	1:C:100:LYS:HG3	1.98	0.62
1:E:175:GLU:OE2	1:F:135:SER:OG	2.16	0.62
1:G:85:PHE:HB2	1:G:109:ARG:NH1	2.14	0.62
1:F:326:SER:OG	1:H:322:ARG:HB3	1.99	0.62
1:F:95:ILE:HD11	1:F:121:CYS:HA	1.81	0.62
1:A:113:PHE:CD2	1:A:368:VAL:HG21	2.33	0.62
1:B:117:ASP:OD2	1:B:120:ALA:HB2	1.99	0.62
1:G:267:SER:HB3	2:G:1000:NAD:O2D	1.99	0.62
1:D:345:ASN:O	1:D:349:THR:HG23	2.00	0.62
1:E:115:ARG:HH22	1:E:298:GLY:HA2	1.64	0.62
1:F:38:ILE:HD11	1:F:76:ALA:CB	2.27	0.62
1:H:186:THR:HG21	1:H:222:TYR:CE2	2.35	0.61
1:G:105:LEU:HD12	1:G:127:ARG:O	1.99	0.61
1:A:238:HIS:HA	1:A:267:SER:OG	2.00	0.61
1:B:106:ILE:HG13	1:B:128:VAL:HA	1.82	0.61
1:F:90:ALA:HB3	1:F:116:VAL:CA	2.21	0.61
1:C:226:ASP:OD1	1:C:256:LYS:HD3	1.99	0.61
1:G:69:ASP:C	1:G:94:VAL:HG12	2.21	0.61
1:G:69:ASP:OD1	1:G:72:THR:HG22	2.00	0.61
1:B:118:LEU:CD2	1:B:128:VAL:HG11	2.30	0.61
1:B:90:ALA:O	1:B:116:VAL:HA	2.01	0.61
1:C:36:ARG:NH1	1:C:78:GLY:CA	2.63	0.61
1:F:340:THR:HG22	1:F:343:ALA:H	1.66	0.61
1:A:81:VAL:HG21	1:A:355:ILE:HD12	1.83	0.61
1:B:106:ILE:HD11	1:B:128:VAL:HB	1.83	0.61
1:B:306:THR:O	1:D:160:ARG:NH2	2.34	0.61
1:G:39:CYS:HA	1:G:83:VAL:HG13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG11	1:A:197:LEU:HD13	1.83	0.60
1:A:351:THR:O	1:A:355:ILE:HG12	2.01	0.60
1:A:340:THR:HG22	1:A:343:ALA:H	1.66	0.60
1:A:345:ASN:O	1:A:349:THR:HG23	2.01	0.60
1:G:189:ILE:HD12	2:G:1000:NAD:O5D	2.01	0.60
1:D:69:ASP:N	1:D:69:ASP:OD1	2.34	0.60
1:A:322:ARG:HB3	1:C:326:SER:OG	2.02	0.60
1:H:340:THR:HG22	1:H:343:ALA:H	1.67	0.60
1:B:205:PHE:CD2	1:B:231:MET:HE1	2.36	0.60
1:C:267:SER:HB3	2:C:1000:NAD:O2D	2.01	0.60
1:G:68:LEU:N	1:G:88:ASP:OD1	2.34	0.60
1:H:174:VAL:HG13	1:H:179:LYS:HZ2	1.67	0.60
1:A:326:SER:OG	1:C:322:ARG:HB3	2.02	0.59
1:A:90:ALA:HA	1:A:94:VAL:HG21	1.80	0.59
1:D:25:THR:HB	1:D:26:PRO:O	2.02	0.59
1:E:30:ALA:O	1:E:34:THR:HG23	2.02	0.59
1:B:108:LEU:HD13	1:B:112:GLY:O	2.02	0.59
1:F:38:ILE:CD1	1:F:76:ALA:HB2	2.31	0.59
1:F:38:ILE:HG23	1:F:79:TYR:CG	2.37	0.59
1:B:338:PHE:HB3	2:B:1000:NAD:H71N	1.68	0.59
1:G:345:ASN:O	1:G:349:THR:HG23	2.02	0.59
1:H:317:TRP:CZ2	1:H:322:ARG:HG3	2.36	0.59
1:B:76:ALA:HB3	1:B:98:LEU:CD2	2.32	0.59
1:F:111:ALA:O	1:F:130:ARG:HD2	2.03	0.59
1:H:252:GLU:N	1:H:252:GLU:OE1	2.36	0.59
1:D:79:TYR:O	1:D:103:VAL:HG12	2.03	0.59
1:C:154:LEU:HD11	1:D:145:ALA:HB1	1.84	0.59
1:C:106:ILE:HG13	1:C:128:VAL:HA	1.84	0.59
1:E:68:LEU:HD22	1:E:84:LEU:CD2	2.32	0.59
1:F:317:TRP:CZ2	1:F:322:ARG:HG3	2.38	0.59
1:H:174:VAL:HG13	1:H:179:LYS:NZ	2.18	0.59
1:F:111:ALA:HB2	1:F:131:VAL:O	2.03	0.58
1:A:90:ALA:HB3	1:A:116:VAL:HG23	1.85	0.58
1:D:223:VAL:HG13	1:D:227:GLU:OE1	2.03	0.58
1:E:175:GLU:O	1:E:179:LYS:NZ	2.29	0.58
1:E:81:VAL:HG21	1:E:355:ILE:CD1	2.29	0.58
1:A:134:TYR:N	3:A:1103:HOH:O	2.32	0.58
1:B:189:ILE:HD12	2:B:1000:NAD:O5D	2.04	0.58
1:H:331:LEU:HD12	1:H:332:VAL:H	1.69	0.58
1:F:90:ALA:CB	1:F:116:VAL:HA	2.25	0.58
1:A:89:ARG:O	1:A:94:VAL:HG21	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:LEU:CD2	1:D:84:LEU:HD21	2.34	0.58
1:D:25:THR:OG1	1:D:29:ALA:HB2	2.03	0.58
1:E:27:GLN:N	1:E:27:GLN:OE1	2.37	0.58
1:F:39:CYS:HB2	1:F:83:VAL:CG1	2.34	0.58
1:G:128:VAL:CG2	1:G:368:VAL:HG12	2.34	0.58
1:D:111:ALA:O	1:D:130:ARG:HD2	2.04	0.58
1:H:139:VAL:HG11	1:H:189:ILE:HD13	1.85	0.58
1:B:241:LEU:HD21	1:B:246:ARG:NH1	2.19	0.57
1:G:121:CYS:HB3	1:G:126:VAL:O	2.04	0.57
1:H:106:ILE:HB	1:H:128:VAL:HG12	1.86	0.57
1:D:236:THR:HG23	1:D:264:ILE:HB	1.85	0.57
1:F:252:GLU:N	1:F:252:GLU:OE1	2.37	0.57
1:G:39:CYS:CB	1:G:83:VAL:HG13	2.34	0.57
1:C:215:VAL:HA	1:C:218:MET:HE3	1.86	0.57
1:D:338:PHE:HB3	2:D:1000:NAD:H71N	1.69	0.57
1:E:74:GLN:NE2	1:E:97:GLU:OE1	2.37	0.57
1:D:236:THR:HG22	3:D:1112:HOH:O	2.03	0.57
1:B:68:LEU:HD22	1:B:84:LEU:HD21	1.86	0.57
1:B:95:ILE:HD12	1:B:117:ASP:OD1	2.04	0.57
1:B:40:TYR:CD2	1:B:64:VAL:HG21	2.40	0.57
1:B:134:TYR:CD1	1:B:347:ILE:HD11	2.40	0.57
1:B:40:TYR:HA	1:B:64:VAL:CG2	2.35	0.56
1:C:85:PHE:HB2	1:C:109:ARG:NH1	2.20	0.56
1:D:51:ALA:HA	1:D:63:PHE:CZ	2.40	0.56
1:G:39:CYS:HB3	1:G:63:PHE:CD1	2.41	0.56
1:H:215:VAL:HA	1:H:218:MET:HE3	1.88	0.56
1:F:267:SER:HB3	2:F:1000:NAD:O2D	2.05	0.56
1:G:174:VAL:HG13	1:G:179:LYS:NZ	2.20	0.56
1:C:95:ILE:HD13	1:C:120:ALA:CB	2.35	0.56
1:E:238:HIS:HA	1:E:267:SER:OG	2.06	0.56
1:F:32:VAL:HG22	1:F:359:VAL:HG11	1.87	0.56
1:G:340:THR:HG22	1:G:343:ALA:H	1.70	0.56
1:A:50:LEU:O	1:A:53:PRO:HD2	2.06	0.56
1:A:37:CYS:HB2	1:A:61:THR:HG22	1.88	0.56
1:C:42:THR:HG22	1:C:47:LYS:HG3	1.88	0.56
1:H:130:ARG:HG2	1:H:131:VAL:N	2.20	0.56
1:E:111:ALA:O	1:E:130:ARG:HD2	2.06	0.56
1:B:329:GLN:OE1	1:B:329:GLN:N	2.31	0.56
1:D:215:VAL:HA	1:D:218:MET:HE2	1.87	0.56
1:D:58:PHE:CZ	1:D:355:ILE:HG21	2.41	0.56
1:D:37:CYS:HB2	1:D:61:THR:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:ARG:O	1:F:94:VAL:HG21	2.06	0.56
1:A:85:PHE:HB2	1:A:109:ARG:NH1	2.20	0.56
1:D:106:ILE:HB	1:D:128:VAL:HG22	1.87	0.56
1:F:77:ARG:CA	1:F:101:ALA:HB1	2.35	0.56
1:F:351:THR:O	1:F:355:ILE:HG12	2.06	0.56
1:G:208:ASP:OD1	1:G:209:ILE:N	2.39	0.56
1:E:84:LEU:HD12	1:E:106:ILE:CG2	2.36	0.56
1:E:317:TRP:CZ2	1:E:322:ARG:HG3	2.40	0.56
1:E:148:PHE:HD1	1:F:145:ALA:HB2	1.71	0.56
1:B:130:ARG:HH21	1:B:132:PRO:HB3	1.71	0.55
1:C:62:TYR:CE2	1:C:64:VAL:HG22	2.37	0.55
1:G:91:ASP:OD1	1:G:94:VAL:HG13	2.05	0.55
1:D:331:LEU:HD12	1:D:332:VAL:N	2.22	0.55
1:F:338:PHE:HB3	2:F:1000:NAD:H71N	1.72	0.55
1:H:134:TYR:HE2	2:H:1000:NAD:C4N	2.19	0.55
1:C:331:LEU:HD12	1:C:332:VAL:N	2.20	0.55
1:E:338:PHE:HB3	2:E:1000:NAD:H71N	1.70	0.55
1:C:91:ASP:H	1:C:94:VAL:HG22	1.70	0.55
1:G:267:SER:HA	2:G:1000:NAD:H1D	1.88	0.55
1:G:30:ALA:O	1:G:34:THR:HG23	2.07	0.55
1:B:121:CYS:HB3	1:B:126:VAL:O	2.07	0.55
1:C:62:TYR:HB2	1:C:79:TYR:CZ	2.42	0.55
1:A:30:ALA:O	1:A:34:THR:HG23	2.06	0.55
1:C:148:PHE:CZ	1:C:176:MET:HE3	2.42	0.55
1:B:36:ARG:NH1	3:B:1104:HOH:O	2.40	0.55
1:E:345:ASN:O	1:E:349:THR:HG23	2.07	0.55
1:E:53:PRO:HA	1:E:56:LYS:HD2	1.89	0.55
1:F:90:ALA:HB1	1:F:116:VAL:HG23	1.89	0.55
1:G:118:LEU:CD2	1:G:368:VAL:HG13	2.35	0.55
1:C:135:SER:OG	1:D:175:GLU:OE2	2.23	0.55
1:H:30:ALA:O	1:H:34:THR:HG23	2.07	0.55
1:A:28:GLU:O	1:A:32:VAL:HG23	2.07	0.54
1:G:252:GLU:OE1	1:G:252:GLU:N	2.40	0.54
1:C:96:LYS:HE2	1:C:100:LYS:CE	2.37	0.54
1:C:46:VAL:O	1:C:50:LEU:HB3	2.08	0.54
1:G:113:PHE:CD1	1:G:368:VAL:HG21	2.42	0.54
1:G:128:VAL:HG22	1:G:368:VAL:HG12	1.89	0.54
1:G:268:ARG:HG2	2:G:1000:NAD:O2D	2.06	0.54
1:G:135:SER:OG	1:H:175:GLU:OE2	2.23	0.54
1:C:223:VAL:HG21	1:C:231:MET:CE	2.37	0.54
1:D:111:ALA:HB2	1:D:131:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ALA:HB3	1:H:247:GLN:NE2	2.20	0.54
1:E:322:ARG:HB3	1:G:326:SER:OG	2.07	0.54
1:F:107:ALA:HA	1:F:129:VAL:HG12	1.90	0.54
1:E:329:GLN:N	1:E:329:GLN:OE1	2.35	0.54
1:F:228:LEU:HA	1:F:231:MET:HE2	1.89	0.54
1:G:70:LYS:N	1:G:94:VAL:HG12	2.23	0.54
1:G:117:ASP:OD2	1:G:120:ALA:HB2	2.08	0.54
1:F:117:ASP:OD2	1:F:120:ALA:HB2	2.08	0.54
1:H:338:PHE:HB3	2:H:1000:NAD:H71N	1.72	0.54
1:H:58:PHE:CZ	1:H:355:ILE:HG21	2.43	0.54
1:A:253:SER:HA	1:A:256:LYS:HE2	1.90	0.53
1:A:208:ASP:OD1	1:A:209:ILE:N	2.42	0.53
1:G:148:PHE:CZ	1:G:176:MET:HE3	2.43	0.53
1:H:205:PHE:CD2	1:H:221:PRO:HG2	2.43	0.53
1:E:76:ALA:O	1:E:101:ALA:HB1	2.08	0.53
1:E:105:LEU:HD12	1:E:127:ARG:O	2.07	0.53
1:E:175:GLU:HG3	1:F:340:THR:HG21	1.89	0.53
1:D:51:ALA:O	1:D:55:GLN:HG3	2.07	0.53
1:F:95:ILE:HD12	1:F:121:CYS:SG	2.48	0.53
1:F:65:GLU:N	1:F:66:PRO:HD2	2.24	0.53
1:G:72:THR:O	1:G:72:THR:HG23	2.08	0.53
1:D:27:GLN:N	1:D:27:GLN:OE1	2.41	0.53
1:E:50:LEU:O	1:E:53:PRO:HD2	2.09	0.53
1:G:38:ILE:HD11	1:G:64:VAL:CG2	2.39	0.53
1:E:160:ARG:NH1	1:E:169:SER:O	2.39	0.53
1:G:72:THR:OG1	1:G:75:LEU:HD12	2.09	0.53
1:B:106:ILE:HD11	1:B:128:VAL:CB	2.38	0.53
1:C:94:VAL:O	1:C:98:LEU:HG	2.09	0.53
1:G:91:ASP:H	1:G:94:VAL:HG22	1.74	0.53
1:A:252:GLU:OE1	1:A:252:GLU:N	2.42	0.53
1:E:115:ARG:NH2	1:E:298:GLY:HA2	2.24	0.53
1:F:148:PHE:CE1	1:F:176:MET:HE3	2.44	0.53
1:G:89:ARG:NE	1:G:115:ARG:HH21	2.07	0.53
1:E:351:THR:O	1:E:355:ILE:HG12	2.09	0.53
1:E:297:GLU:HG3	3:E:1114:HOH:O	2.09	0.52
1:F:130:ARG:HG2	1:F:131:VAL:N	2.24	0.52
1:B:65:GLU:N	1:B:66:PRO:HD2	2.24	0.52
1:E:130:ARG:HG2	1:E:131:VAL:N	2.25	0.52
1:A:70:LYS:HG3	3:A:1109:HOH:O	2.08	0.52
1:B:186:THR:OG1	1:B:222:TYR:OH	2.10	0.52
1:B:223:VAL:HG21	1:B:231:MET:CE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ASN:O	1:B:349:THR:HG23	2.10	0.52
1:D:89:ARG:HG2	1:D:115:ARG:HE	1.75	0.52
1:B:267:SER:HA	2:B:1000:NAD:H1D	1.89	0.52
1:D:130:ARG:HG2	1:D:131:VAL:N	2.23	0.52
1:F:38:ILE:HD12	1:F:40:TYR:CE2	2.44	0.52
1:B:72:THR:OG1	1:B:75:LEU:HD13	2.09	0.52
1:D:96:LYS:O	1:D:100:LYS:HG2	2.09	0.52
1:D:25:THR:HG21	1:D:28:GLU:C	2.28	0.52
1:H:81:VAL:HG21	1:H:355:ILE:HD12	1.91	0.52
1:A:83:VAL:CG1	1:A:109:ARG:HG3	2.40	0.52
1:B:113:PHE:CE1	1:B:130:ARG:NH1	2.77	0.52
1:G:42:THR:HG22	1:G:47:LYS:HG3	1.92	0.52
1:C:338:PHE:HB3	2:C:1000:NAD:H71N	1.75	0.52
1:D:293:VAL:HA	1:D:297:GLU:OE2	2.10	0.52
1:E:252:GLU:N	1:E:252:GLU:OE1	2.39	0.52
1:G:93:SER:HA	1:G:96:LYS:HD3	1.92	0.52
1:C:51:ALA:O	1:C:55:GLN:HG3	2.08	0.52
1:E:205:PHE:CD2	1:E:231:MET:HE1	2.44	0.52
1:A:338:PHE:HB3	2:A:1000:NAD:H71N	1.75	0.52
1:B:98:LEU:HA	1:B:101:ALA:HB3	1.91	0.52
1:C:92:ALA:O	1:C:120:ALA:HB1	2.10	0.52
1:F:39:CYS:HA	1:F:83:VAL:HG13	1.92	0.52
1:H:351:THR:O	1:H:355:ILE:HG12	2.10	0.52
1:E:28:GLU:HB3	1:E:360:LEU:CD2	2.35	0.51
1:G:128:VAL:CG1	1:G:368:VAL:HG13	2.39	0.51
1:C:300:LEU:O	1:D:166:TYR:HD2	1.92	0.51
1:C:72:THR:CA	1:C:75:LEU:HD13	2.38	0.51
1:G:68:LEU:CD2	1:G:84:LEU:HD21	2.36	0.51
1:C:36:ARG:NH1	1:C:78:GLY:C	2.64	0.51
1:G:134:TYR:HE2	2:G:1000:NAD:C4N	2.23	0.51
1:G:88:ASP:O	1:G:115:ARG:HD3	2.11	0.51
1:C:105:LEU:HD22	1:C:358:TYR:CD2	2.45	0.51
1:D:356:ALA:HA	1:D:359:VAL:HG12	1.91	0.51
1:H:129:VAL:HG12	1:H:130:ARG:N	2.25	0.51
1:C:79:TYR:O	1:C:103:VAL:HG12	2.11	0.51
1:H:290:GLY:HA2	1:H:331:LEU:O	2.10	0.51
1:A:224:SER:OG	1:A:227:GLU:HG3	2.10	0.51
1:E:92:ALA:HA	1:E:120:ALA:CB	2.41	0.51
1:F:85:PHE:HB2	1:F:109:ARG:NH1	2.25	0.51
1:G:105:LEU:HD22	1:G:358:TYR:CD2	2.45	0.51
1:A:84:LEU:HD22	1:A:106:ILE:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLN:HG2	1:B:273:ASP:HB2	1.92	0.51
1:H:240:PRO:HD3	2:H:1000:NAD:H52A	1.93	0.51
1:A:289:LEU:HB3	1:A:330:VAL:HG22	1.93	0.51
1:B:79:TYR:O	1:B:103:VAL:HG12	2.10	0.51
1:C:160:ARG:HH22	1:C:169:SER:C	2.10	0.51
1:C:317:TRP:CE2	1:C:322:ARG:HG3	2.46	0.51
1:G:50:LEU:O	1:G:53:PRO:HD2	2.10	0.51
1:A:25:THR:N	1:A:26:PRO:CD	2.73	0.51
1:B:160:ARG:NH2	1:B:169:SER:O	2.41	0.51
1:C:252:GLU:OE1	1:C:252:GLU:N	2.43	0.51
1:E:92:ALA:O	1:E:95:ILE:HG22	2.11	0.51
1:F:208:ASP:OD1	1:F:209:ILE:N	2.44	0.51
1:H:228:LEU:HD23	1:H:228:LEU:C	2.31	0.51
1:A:113:PHE:O	1:A:116:VAL:HG12	2.11	0.51
1:A:177:ARG:HD2	1:B:137:GLU:HG2	1.93	0.51
1:E:51:ALA:HA	1:E:63:PHE:CZ	2.45	0.51
1:A:51:ALA:HA	1:A:63:PHE:CZ	2.45	0.50
1:B:323:THR:O	1:B:326:SER:HB3	2.11	0.50
1:B:129:VAL:CG1	1:B:354:ASN:HB3	2.36	0.50
1:H:83:VAL:CG1	1:H:109:ARG:HG3	2.41	0.50
1:F:70:LYS:N	1:F:94:VAL:HG12	2.27	0.50
1:F:39:CYS:CA	1:F:83:VAL:HG13	2.40	0.50
1:G:57:VAL:HG12	1:G:58:PHE:CD1	2.47	0.50
1:C:113:PHE:O	1:C:116:VAL:HG12	2.11	0.50
1:E:76:ALA:C	1:E:101:ALA:HB1	2.31	0.50
1:G:96:LYS:HA	1:G:124:HIS:CE1	2.47	0.50
1:E:137:GLU:O	1:E:141:GLU:HG3	2.11	0.50
1:F:79:TYR:O	1:F:103:VAL:HG12	2.12	0.50
1:G:340:THR:HG21	1:H:175:GLU:HG3	1.94	0.50
1:G:95:ILE:HD12	1:G:117:ASP:OD1	2.11	0.50
1:B:268:ARG:HG2	2:B:1000:NAD:O2D	2.11	0.50
1:B:98:LEU:HB3	1:B:103:VAL:HG22	1.94	0.50
1:C:57:VAL:HG12	1:C:58:PHE:CD1	2.47	0.50
1:F:68:LEU:N	1:F:88:ASP:OD1	2.24	0.50
1:C:27:GLN:HG3	1:C:27:GLN:O	2.12	0.50
1:F:233:ASP:OD1	1:F:258:LYS:NZ	2.31	0.50
1:A:40:TYR:CD2	1:A:64:VAL:HG21	2.47	0.50
1:E:241:LEU:HD21	1:E:246:ARG:NH1	2.26	0.50
1:C:181:VAL:HG11	1:C:197:LEU:HD13	1.94	0.50
1:E:90:ALA:O	1:E:116:VAL:HA	2.11	0.50
1:C:340:THR:HG22	1:C:342:GLU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LYS:HE2	1:C:100:LYS:HE2	1.94	0.50
1:D:240:PRO:HD3	2:D:1000:NAD:H52A	1.94	0.50
1:E:214:ALA:O	1:E:218:MET:HG3	2.12	0.50
1:E:331:LEU:HD12	1:E:332:VAL:H	1.76	0.50
1:F:38:ILE:HG23	1:F:79:TYR:CE2	2.47	0.50
1:G:95:ILE:HD12	1:G:120:ALA:HB3	1.94	0.50
1:C:351:THR:O	1:C:355:ILE:HG12	2.12	0.49
1:B:90:ALA:HB3	1:B:116:VAL:HG23	1.93	0.49
1:E:148:PHE:CD1	1:F:145:ALA:HB2	2.47	0.49
1:B:46:VAL:O	1:B:50:LEU:HB3	2.12	0.49
1:C:57:VAL:HG12	1:C:58:PHE:CE1	2.47	0.49
1:G:81:VAL:HG21	1:G:105:LEU:HD23	1.93	0.49
1:A:294:TYR:O	1:A:297:GLU:HG3	2.13	0.49
1:B:76:ALA:HB3	1:B:98:LEU:HD22	1.94	0.49
1:C:205:PHE:CD2	1:C:231:MET:HE1	2.47	0.49
1:F:331:LEU:HD12	1:F:332:VAL:N	2.28	0.49
1:G:79:TYR:O	1:G:103:VAL:HG12	2.13	0.49
1:B:177:ARG:O	1:B:201:GLY:O	2.31	0.49
1:F:92:ALA:HA	1:F:95:ILE:HG22	1.94	0.49
1:G:95:ILE:HD13	1:G:121:CYS:SG	2.53	0.49
1:B:215:VAL:HA	1:B:218:MET:HE3	1.95	0.49
1:C:81:VAL:CG2	1:C:105:LEU:HD23	2.42	0.49
1:D:229:LEU:O	1:D:257:MET:HA	2.12	0.49
1:E:253:SER:HA	1:E:256:LYS:HE2	1.95	0.49
1:B:76:ALA:CB	1:B:98:LEU:HD22	2.43	0.49
1:C:175:GLU:HG3	1:D:340:THR:HG21	1.95	0.49
1:E:58:PHE:HB2	1:E:61:THR:HG23	1.95	0.49
1:F:98:LEU:O	1:F:101:ALA:HB3	2.13	0.49
1:H:317:TRP:CE2	1:H:322:ARG:HG3	2.47	0.49
1:B:230:ALA:HB2	3:B:1117:HOH:O	2.13	0.48
1:B:134:TYR:HD1	1:B:347:ILE:HD11	1.78	0.48
1:C:81:VAL:HB	1:C:105:LEU:HD23	1.96	0.48
1:A:58:PHE:CZ	1:A:355:ILE:HG21	2.49	0.48
1:B:50:LEU:O	1:B:53:PRO:HD2	2.13	0.48
1:D:253:SER:HA	1:D:256:LYS:HE2	1.95	0.48
1:A:339:LEU:HG	1:B:172:VAL:HG22	1.95	0.48
1:B:39:CYS:HB2	1:B:83:VAL:HG13	1.95	0.48
1:E:242:LEU:O	1:E:246:ARG:HG3	2.13	0.48
1:H:51:ALA:HA	1:H:63:PHE:CZ	2.48	0.48
1:A:129:VAL:HG13	1:A:130:ARG:N	2.28	0.48
1:H:129:VAL:HG12	1:H:130:ARG:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ASN:O	1:B:254:ILE:HG13	2.13	0.48
1:B:85:PHE:HB2	1:B:109:ARG:CZ	2.44	0.48
1:B:97:GLU:O	1:B:101:ALA:HB2	2.14	0.48
1:C:181:VAL:HG22	1:C:234:ILE:HB	1.94	0.48
1:H:160:ARG:HH22	1:H:170:GLY:H	1.62	0.48
1:B:157:ALA:O	1:B:161:VAL:HG23	2.14	0.48
1:C:339:LEU:HG	1:D:172:VAL:HG22	1.95	0.48
1:G:166:TYR:HD2	1:H:300:LEU:O	1.95	0.48
1:B:39:CYS:SG	1:B:83:VAL:HG13	2.53	0.48
1:D:267:SER:HB3	2:D:1000:NAD:O2D	2.14	0.48
1:D:50:LEU:O	1:D:53:PRO:HD2	2.13	0.48
1:F:356:ALA:O	1:F:359:VAL:HG12	2.13	0.48
1:G:108:LEU:HB2	1:G:130:ARG:CB	2.44	0.48
1:C:39:CYS:SG	1:C:109:ARG:HD2	2.54	0.48
1:C:95:ILE:O	1:C:99:ALA:HB2	2.13	0.48
1:F:64:VAL:CG1	1:F:66:PRO:HG2	2.43	0.48
1:H:335:HIS:ND1	3:H:1101:HOH:O	2.12	0.48
1:B:186:THR:HG23	1:B:186:THR:O	2.12	0.48
1:D:25:THR:HG21	1:D:29:ALA:CA	2.44	0.48
1:B:294:TYR:O	1:B:297:GLU:HG3	2.14	0.47
1:C:174:VAL:HG13	1:C:179:LYS:NZ	2.29	0.47
1:C:26:PRO:HB2	1:C:28:GLU:CD	2.34	0.47
1:H:98:LEU:O	1:H:103:VAL:HG22	2.14	0.47
1:H:186:THR:HG21	1:H:222:TYR:CZ	2.49	0.47
1:A:42:THR:HG22	1:A:47:LYS:HG3	1.96	0.47
1:A:91:ASP:O	1:A:95:ILE:HD12	2.13	0.47
1:B:83:VAL:HA	1:B:107:ALA:O	2.13	0.47
1:A:340:THR:HG21	1:B:175:GLU:HG3	1.95	0.47
1:G:39:CYS:CA	1:G:83:VAL:HG13	2.43	0.47
1:G:92:ALA:HA	1:G:120:ALA:CB	2.44	0.47
1:D:95:ILE:HG22	1:D:124:HIS:ND1	2.29	0.47
1:D:27:GLN:C	1:D:29:ALA:N	2.68	0.47
1:E:257:MET:CE	1:E:261:VAL:HG11	2.44	0.47
1:G:104:LYS:O	1:G:126:VAL:HA	2.14	0.47
1:G:64:VAL:CG1	1:G:66:PRO:HG2	2.45	0.47
1:H:268:ARG:HG2	2:H:1000:NAD:O2D	2.14	0.47
1:D:30:ALA:O	1:D:34:THR:HG23	2.15	0.47
1:C:137:GLU:HG2	1:D:177:ARG:HD2	1.97	0.47
1:D:242:LEU:O	1:D:246:ARG:HG3	2.15	0.47
1:G:108:LEU:HB2	1:G:130:ARG:HB2	1.96	0.47
1:H:247:GLN:HG2	1:H:273:ASP:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:PHE:CE2	1:A:334:PRO:HA	2.49	0.47
1:C:118:LEU:HD23	1:C:128:VAL:HG21	1.96	0.47
1:C:297:GLU:OE1	3:C:1101:HOH:O	2.20	0.47
1:D:189:ILE:HD12	2:D:1000:NAD:O5D	2.14	0.47
1:E:144:VAL:HG21	1:E:196:ILE:HG21	1.95	0.47
1:F:159:ILE:O	1:F:163:MET:HG3	2.15	0.47
1:G:128:VAL:HG21	1:G:368:VAL:CG1	2.44	0.47
1:B:106:ILE:CG1	1:B:128:VAL:HA	2.45	0.47
1:C:108:LEU:HB2	1:C:130:ARG:CB	2.44	0.47
1:C:36:ARG:HH11	1:C:78:GLY:C	2.17	0.47
1:C:72:THR:HA	1:C:75:LEU:CD1	2.40	0.47
1:A:329:GLN:OE1	1:A:329:GLN:N	2.42	0.47
1:D:223:VAL:CG1	1:D:224:SER:N	2.78	0.47
1:F:208:ASP:OD2	2:F:1000:NAD:H1B	2.15	0.47
1:H:85:PHE:CE1	1:H:110:CYS:HB3	2.50	0.47
1:C:94:VAL:HA	1:C:97:GLU:OE2	2.15	0.47
1:C:340:THR:HG21	1:D:175:GLU:HG3	1.96	0.47
1:E:181:VAL:HG11	1:E:197:LEU:HD13	1.97	0.47
1:F:250:ASN:HB2	3:F:1106:HOH:O	2.13	0.47
1:C:96:LYS:HG3	1:C:124:HIS:CD2	2.50	0.47
1:C:65:GLU:N	1:C:66:PRO:HD2	2.30	0.47
1:E:65:GLU:N	1:E:66:PRO:HD2	2.30	0.47
1:G:87:ASN:C	1:G:115:ARG:NH1	2.69	0.47
1:H:129:VAL:HG11	1:H:354:ASN:HB3	1.97	0.47
1:C:106:ILE:CG1	1:C:128:VAL:HA	2.45	0.46
1:C:96:LYS:O	1:C:99:ALA:HB3	2.14	0.46
1:D:182:GLY:HA3	1:D:228:LEU:HD21	1.97	0.46
1:E:37:CYS:SG	1:E:81:VAL:HG13	2.55	0.46
1:G:174:VAL:HG13	1:G:179:LYS:HZ2	1.79	0.46
1:G:65:GLU:N	1:G:66:PRO:HD2	2.30	0.46
1:A:134:TYR:HE2	2:A:1000:NAD:C5N	2.27	0.46
1:B:186:THR:HG23	1:B:212:ASN:HB2	1.97	0.46
1:B:252:GLU:N	1:B:252:GLU:OE1	2.47	0.46
1:B:297:GLU:HG2	1:B:301:PHE:CD1	2.50	0.46
1:F:95:ILE:CD1	1:F:121:CYS:SG	3.03	0.46
1:F:297:GLU:HB2	1:F:301:PHE:CG	2.50	0.46
1:A:317:TRP:CE2	1:A:322:ARG:HG3	2.50	0.46
1:B:39:CYS:HB2	1:B:83:VAL:CG1	2.45	0.46
1:E:84:LEU:HD12	1:E:106:ILE:HG23	1.97	0.46
1:F:238:HIS:HA	1:F:267:SER:OG	2.16	0.46
1:B:240:PRO:HD3	2:B:1000:NAD:H52A	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:VAL:O	1:D:84:LEU:HD12	2.16	0.46
1:D:89:ARG:CG	1:D:115:ARG:HH21	2.29	0.46
1:G:187:GLY:HA3	2:G:1000:NAD:O5B	2.15	0.46
1:A:240:PRO:HD3	2:A:1000:NAD:C5B	2.42	0.46
1:D:90:ALA:HB1	1:D:95:ILE:HD11	1.97	0.46
1:B:70:LYS:HA	1:B:94:VAL:HG12	1.98	0.46
1:B:160:ARG:HD3	3:B:1110:HOH:O	2.14	0.46
1:C:172:VAL:HG22	1:D:339:LEU:HG	1.97	0.46
1:F:32:VAL:HG22	1:F:359:VAL:CG1	2.46	0.46
1:G:118:LEU:HD21	1:G:368:VAL:CG1	2.39	0.46
1:A:85:PHE:CE1	1:A:110:CYS:HB3	2.50	0.46
1:F:38:ILE:HD13	1:F:76:ALA:HA	1.98	0.46
1:H:345:ASN:O	1:H:349:THR:HG23	2.15	0.46
1:A:340:THR:HG22	1:A:342:GLU:N	2.30	0.46
1:A:99:ALA:HB2	1:A:124:HIS:HB3	1.98	0.46
1:B:105:LEU:HD22	1:B:358:TYR:CD2	2.51	0.46
1:B:331:LEU:HD12	1:B:332:VAL:N	2.30	0.46
1:E:129:VAL:HG11	1:E:354:ASN:HB3	1.98	0.46
1:A:90:ALA:CB	1:A:116:VAL:HG23	2.45	0.45
1:D:208:ASP:OD1	1:D:209:ILE:N	2.49	0.45
1:E:250:ASN:O	1:E:254:ILE:HG13	2.16	0.45
1:C:228:LEU:HD23	1:C:228:LEU:C	2.36	0.45
1:D:294:TYR:O	1:D:297:GLU:HG3	2.15	0.45
1:F:205:PHE:CD2	1:F:231:MET:HE1	2.51	0.45
1:B:163:MET:HB2	1:B:163:MET:HE2	1.65	0.45
1:E:84:LEU:HD12	1:E:106:ILE:HG21	1.97	0.45
1:F:297:GLU:HB2	1:F:301:PHE:CD1	2.51	0.45
1:F:92:ALA:HA	1:F:95:ILE:CG2	2.46	0.45
1:C:318:ASP:O	1:C:322:ARG:HG2	2.15	0.45
1:H:103:VAL:O	1:H:103:VAL:HG23	2.16	0.45
1:H:223:VAL:CG1	1:H:224:SER:N	2.80	0.45
1:A:40:TYR:HA	1:A:64:VAL:CG2	2.46	0.45
1:D:175:GLU:O	1:D:179:LYS:HE2	2.16	0.45
1:E:340:THR:HG23	1:E:342:GLU:OE1	2.15	0.45
1:B:310:PRO:O	1:B:314:MET:HG2	2.17	0.45
1:G:46:VAL:HG22	1:G:109:ARG:NH2	2.32	0.45
1:G:83:VAL:CG2	1:G:109:ARG:HG3	2.47	0.45
1:A:214:ALA:O	1:A:218:MET:HG3	2.16	0.45
1:A:25:THR:HG22	1:A:25:THR:O	2.17	0.45
1:C:205:PHE:CD2	1:C:221:PRO:HG2	2.52	0.45
1:C:84:LEU:HB2	1:C:108:LEU:CD2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:LEU:HB2	1:D:332:VAL:HG22	1.97	0.45
1:D:91:ASP:O	1:D:95:ILE:HD12	2.17	0.45
1:E:168:LEU:HD11	1:F:302:PHE:CE1	2.52	0.45
1:A:331:LEU:HD12	1:A:332:VAL:H	1.79	0.45
1:G:64:VAL:CG1	1:G:66:PRO:HD2	2.47	0.45
1:H:90:ALA:O	1:H:116:VAL:HA	2.16	0.45
1:B:128:VAL:O	1:B:128:VAL:HG23	2.16	0.45
1:D:129:VAL:HG22	1:D:130:ARG:H	1.82	0.45
1:E:70:LYS:CB	1:E:71:ASP:CB	2.80	0.45
1:E:85:PHE:HB2	1:E:109:ARG:NH1	2.31	0.45
1:H:331:LEU:C	1:H:331:LEU:HD12	2.35	0.45
1:C:345:ASN:O	1:C:349:THR:HG23	2.17	0.45
1:C:50:LEU:O	1:C:53:PRO:HD2	2.17	0.45
1:C:83:VAL:HA	1:C:107:ALA:O	2.17	0.45
1:D:27:GLN:C	1:D:29:ALA:H	2.20	0.45
1:F:77:ARG:HA	1:F:101:ALA:O	2.17	0.45
1:G:128:VAL:CG2	1:G:368:VAL:CG1	2.95	0.45
1:H:115:ARG:HH22	1:H:298:GLY:HA2	1.82	0.45
1:A:105:LEU:HD12	1:A:127:ARG:O	2.17	0.44
1:G:177:ARG:O	1:G:201:GLY:O	2.35	0.44
1:A:58:PHE:HB2	1:A:61:THR:HG23	1.99	0.44
1:C:92:ALA:HB1	1:C:120:ALA:HB2	1.99	0.44
1:E:69:ASP:OD1	1:E:72:THR:HG22	2.16	0.44
1:E:152:ARG:NH2	1:F:337:ALA:O	2.45	0.44
1:G:68:LEU:HB3	1:G:88:ASP:HB3	1.98	0.44
1:C:137:GLU:O	1:C:141:GLU:HG3	2.18	0.44
1:F:128:VAL:O	1:F:367:GLU:HA	2.18	0.44
1:B:208:ASP:OD1	1:B:209:ILE:N	2.50	0.44
1:C:96:LYS:HB2	1:C:124:HIS:NE2	2.33	0.44
1:D:129:VAL:HG22	1:D:130:ARG:N	2.31	0.44
1:E:127:ARG:NH2	1:E:364:LEU:HD12	2.33	0.44
1:F:58:PHE:CZ	1:F:355:ILE:HG21	2.53	0.44
1:H:76:ALA:C	1:H:101:ALA:HB1	2.38	0.44
1:B:118:LEU:HD23	1:B:128:VAL:HG11	1.98	0.44
1:B:238:HIS:HA	1:B:267:SER:OG	2.18	0.44
1:D:340:THR:HG22	1:D:342:GLU:N	2.32	0.44
1:D:58:PHE:CE1	1:D:355:ILE:HG21	2.53	0.44
1:E:142:HIS:CG	1:E:337:ALA:HA	2.53	0.44
1:F:137:GLU:O	1:F:141:GLU:HG3	2.16	0.44
1:G:113:PHE:O	1:G:116:VAL:HG12	2.16	0.44
1:G:129:VAL:HG22	1:G:130:ARG:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:HG23	1:A:342:GLU:OE1	2.17	0.44
1:C:239:CYS:HB2	1:C:240:PRO:HD2	1.98	0.44
1:D:148:PHE:CZ	1:D:176:MET:CE	3.00	0.44
1:G:307:LYS:HE3	1:G:308:PHE:CZ	2.52	0.44
1:B:340:THR:HG22	1:B:342:GLU:N	2.32	0.44
1:C:113:PHE:CD2	1:C:118:LEU:HD11	2.53	0.44
1:G:223:VAL:HG21	1:G:231:MET:HE1	1.97	0.44
1:G:68:LEU:HD12	1:G:72:THR:O	2.18	0.44
1:A:93:SER:HB3	1:H:247:GLN:OE1	2.18	0.44
1:D:148:PHE:CE2	1:D:176:MET:HE1	2.53	0.44
1:E:194:ALA:HB1	1:E:220:ILE:HD13	2.00	0.44
1:F:77:ARG:HA	1:F:101:ALA:CB	2.45	0.44
1:F:83:VAL:CG2	1:F:109:ARG:HG3	2.48	0.44
1:A:49:PHE:CD1	1:A:344:LEU:HB3	2.51	0.44
1:A:59:THR:HG23	1:A:60:ASP:N	2.33	0.44
1:C:62:TYR:HB2	1:C:79:TYR:OH	2.18	0.44
1:E:95:ILE:HG21	1:E:120:ALA:HB1	2.00	0.44
1:H:129:VAL:HG12	1:H:354:ASN:ND2	2.33	0.44
1:A:304:ASP:O	1:A:307:LYS:HG2	2.18	0.43
1:B:36:ARG:CZ	3:B:1104:HOH:O	2.66	0.43
1:G:99:ALA:HB2	1:G:124:HIS:HB3	2.00	0.43
1:A:151:ASN:HD22	1:A:176:MET:HE2	1.82	0.43
1:A:209:ILE:HG13	1:F:246:ARG:NH2	2.32	0.43
1:B:215:VAL:HA	1:B:218:MET:CE	2.48	0.43
1:C:49:PHE:CD1	1:C:344:LEU:HB3	2.53	0.43
1:E:340:THR:HG22	1:E:343:ALA:N	2.25	0.43
1:F:236:THR:HG23	1:F:236:THR:O	2.18	0.43
1:G:160:ARG:HH22	1:G:169:SER:C	2.19	0.43
1:G:351:THR:O	1:G:355:ILE:HG12	2.18	0.43
1:H:68:LEU:CD2	1:H:84:LEU:HD21	2.48	0.43
1:A:244:SER:HA	1:F:296:ASN:ND2	2.34	0.43
1:C:157:ALA:O	1:C:161:VAL:HG23	2.19	0.43
1:D:238:HIS:HA	1:D:267:SER:OG	2.19	0.43
1:D:65:GLU:N	1:D:66:PRO:HD2	2.33	0.43
1:E:174:VAL:HG13	1:E:179:LYS:NZ	2.32	0.43
1:H:274:SER:HB2	1:H:295:GLU:OE2	2.17	0.43
1:A:142:HIS:O	1:A:145:ALA:HB3	2.18	0.43
1:B:267:SER:HB3	2:B:1000:NAD:O2D	2.18	0.43
1:C:148:PHE:CD2	1:C:176:MET:HE1	2.54	0.43
1:C:73:ALA:HB1	1:C:98:LEU:HD23	2.00	0.43
1:E:340:THR:HG22	1:E:342:GLU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:LEU:HA	1:E:72:THR:HG21	1.98	0.43
1:E:160:ARG:NH2	1:G:306:THR:O	2.50	0.43
1:G:91:ASP:N	1:G:94:VAL:HG22	2.33	0.43
1:H:42:THR:HG22	1:H:47:LYS:HG3	2.00	0.43
1:A:113:PHE:CE2	1:A:368:VAL:HG21	2.53	0.43
1:B:106:ILE:CD1	1:B:128:VAL:HA	2.49	0.43
1:B:317:TRP:CE2	1:B:322:ARG:HG3	2.54	0.43
1:B:323:THR:O	1:B:326:SER:CB	2.67	0.43
1:E:62:TYR:HB2	1:E:79:TYR:CZ	2.54	0.43
1:F:105:LEU:HD12	1:F:127:ARG:O	2.19	0.43
1:A:160:ARG:NH2	1:C:306:THR:O	2.51	0.43
1:B:106:ILE:HD12	1:B:106:ILE:O	2.18	0.43
1:C:229:LEU:O	1:C:257:MET:HA	2.19	0.43
1:B:282:GLU:CD	1:D:319:ARG:HH21	2.20	0.43
1:F:223:VAL:HG13	1:F:224:SER:O	2.18	0.43
1:A:84:LEU:HD22	1:A:106:ILE:CG2	2.49	0.43
1:B:229:LEU:O	1:B:257:MET:HA	2.19	0.43
1:D:163:MET:HE3	1:D:163:MET:HB2	1.67	0.43
1:E:226:ASP:OD1	1:E:256:LYS:NZ	2.32	0.43
1:F:177:ARG:O	1:F:201:GLY:O	2.36	0.43
1:F:228:LEU:HA	1:F:231:MET:CE	2.49	0.43
1:D:209:ILE:HG13	1:D:210:LYS:N	2.34	0.43
1:F:148:PHE:CZ	1:F:176:MET:CE	2.98	0.43
1:G:240:PRO:HA	2:G:1000:NAD:O3D	2.19	0.43
1:G:39:CYS:HB3	1:G:63:PHE:HD1	1.80	0.43
1:A:228:LEU:HD23	1:A:228:LEU:C	2.39	0.43
1:B:294:TYR:OH	1:B:320:GLN:HG3	2.19	0.43
1:A:152:ARG:NH2	1:B:337:ALA:O	2.46	0.43
1:C:208:ASP:OD1	1:C:209:ILE:N	2.52	0.43
1:D:23:GLU:CD	1:D:24:LEU:H	2.21	0.43
1:F:215:VAL:HA	1:F:218:MET:HE3	2.01	0.43
1:C:30:ALA:O	1:C:34:THR:HG23	2.18	0.43
1:C:91:ASP:H	1:C:94:VAL:CG2	2.32	0.43
1:E:323:THR:HG22	1:G:323:THR:CG2	2.44	0.43
1:G:89:ARG:NE	1:G:115:ARG:NH2	2.66	0.43
1:G:205:PHE:CD2	1:G:231:MET:HE1	2.54	0.43
1:A:148:PHE:CE1	1:A:176:MET:HE3	2.54	0.42
1:B:148:PHE:CZ	1:B:176:MET:CE	3.00	0.42
1:C:107:ALA:HA	1:C:129:VAL:HG12	2.01	0.42
1:C:96:LYS:O	1:C:100:LYS:N	2.46	0.42
1:H:186:THR:HG21	1:H:222:TYR:OH	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MET:HE3	1:A:163:MET:HB2	1.62	0.42
1:B:340:THR:HG23	1:B:342:GLU:OE1	2.20	0.42
1:F:83:VAL:HA	1:F:107:ALA:O	2.18	0.42
1:A:174:VAL:HG13	1:A:179:LYS:NZ	2.34	0.42
1:B:250:ASN:HB2	3:B:1106:HOH:O	2.19	0.42
1:B:39:CYS:HB3	1:B:63:PHE:HD1	1.84	0.42
1:B:81:VAL:HG21	1:B:355:ILE:CD1	2.46	0.42
1:E:95:ILE:HD13	1:E:120:ALA:O	2.19	0.42
1:G:163:MET:HE2	1:G:163:MET:HB2	1.63	0.42
1:H:163:MET:HE3	1:H:163:MET:HB2	1.71	0.42
1:H:40:TYR:HA	1:H:64:VAL:HG22	2.01	0.42
1:A:189:ILE:HD12	2:A:1000:NAD:O5D	2.20	0.42
1:B:338:PHE:HB3	2:B:1000:NAD:N7N	2.34	0.42
1:B:70:LYS:N	1:B:94:VAL:HG12	2.33	0.42
1:C:103:VAL:O	1:C:103:VAL:HG23	2.20	0.42
1:D:105:LEU:HA	1:D:127:ARG:O	2.19	0.42
1:D:35:THR:O	3:D:1102:HOH:O	2.21	0.42
1:G:362:ARG:HB3	1:G:363:PRO:HD2	2.02	0.42
1:A:242:LEU:H	1:A:245:THR:HG1	1.63	0.42
1:A:360:LEU:HD23	1:A:360:LEU:HA	1.80	0.42
1:B:87:ASN:HA	1:B:115:ARG:NH1	2.34	0.42
1:B:241:LEU:HD11	1:B:246:ARG:HG2	2.01	0.42
1:B:285:GLN:HA	1:B:285:GLN:OE1	2.18	0.42
1:C:264:ILE:HD13	1:C:290:GLY:H	1.85	0.42
1:H:176:MET:HE2	1:H:176:MET:HB2	1.73	0.42
1:B:108:LEU:HB2	1:B:130:ARG:HB2	2.00	0.42
1:B:148:PHE:CD2	1:B:176:MET:HE1	2.55	0.42
1:C:250:ASN:O	1:C:254:ILE:HG13	2.20	0.42
1:C:62:TYR:HB2	1:C:79:TYR:CE2	2.54	0.42
1:E:166:TYR:HD2	1:F:300:LEU:O	2.03	0.42
1:G:81:VAL:CG2	1:G:105:LEU:HD23	2.49	0.42
1:H:90:ALA:CB	1:H:116:VAL:HG23	2.46	0.42
1:A:92:ALA:CB	1:H:247:GLN:HE22	2.23	0.42
1:A:99:ALA:CB	1:A:124:HIS:HB3	2.50	0.42
1:A:59:THR:CG2	1:A:60:ASP:N	2.83	0.42
1:C:233:ASP:OD1	1:C:258:LYS:NZ	2.32	0.42
1:F:163:MET:HB2	1:F:163:MET:HE2	1.67	0.42
1:A:121:CYS:HB3	1:A:126:VAL:O	2.20	0.42
1:B:253:SER:HA	1:B:256:LYS:HE2	2.02	0.42
1:B:39:CYS:HB3	1:B:63:PHE:CD1	2.55	0.42
1:C:325:LEU:HB3	1:D:162:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ILE:HG22	1:C:124:HIS:HB2	2.00	0.42
1:D:28:GLU:O	1:D:31:LYS:HB3	2.19	0.42
1:A:25:THR:N	1:A:26:PRO:HD3	2.35	0.41
1:E:223:VAL:HG21	1:E:231:MET:CE	2.50	0.41
1:G:41:SER:OG	1:G:67:PRO:HA	2.20	0.41
1:A:209:ILE:HA	1:A:209:ILE:HD12	1.74	0.41
1:E:331:LEU:HD12	1:E:331:LEU:C	2.40	0.41
1:G:331:LEU:HD12	1:G:332:VAL:N	2.35	0.41
1:G:39:CYS:HB2	1:G:83:VAL:CG1	2.50	0.41
1:B:69:ASP:C	1:B:94:VAL:HG12	2.41	0.41
1:C:209:ILE:HG22	1:C:210:LYS:HD2	2.02	0.41
1:D:148:PHE:CZ	1:D:176:MET:HE1	2.55	0.41
1:F:329:GLN:N	1:F:329:GLN:OE1	2.36	0.41
1:F:92:ALA:C	1:F:95:ILE:HG22	2.40	0.41
1:G:282:GLU:OE1	1:G:327:TYR:OH	2.33	0.41
1:G:51:ALA:HA	1:G:63:PHE:CZ	2.55	0.41
1:A:90:ALA:O	1:A:116:VAL:HA	2.20	0.41
1:A:58:PHE:HB2	1:A:61:THR:CG2	2.50	0.41
1:B:154:LEU:HA	1:B:154:LEU:HD23	1.75	0.41
1:C:38:ILE:HD11	1:C:64:VAL:CG2	2.51	0.41
1:G:137:GLU:HG2	1:H:177:ARG:HD2	2.03	0.41
1:B:51:ALA:HA	1:B:63:PHE:CZ	2.55	0.41
1:C:149:ALA:HA	1:C:154:LEU:HD12	2.02	0.41
1:E:268:ARG:HG2	2:E:1000:NAD:O2D	2.20	0.41
1:E:58:PHE:HB2	1:E:61:THR:CG2	2.50	0.41
1:F:38:ILE:CD1	1:F:76:ALA:CB	2.95	0.41
1:G:146:LEU:HD23	1:G:146:LEU:HA	1.87	0.41
1:G:152:ARG:NH2	1:H:142:HIS:HB2	2.35	0.41
1:C:182:GLY:CA	1:C:228:LEU:HD11	2.51	0.41
1:G:128:VAL:CG1	1:G:368:VAL:CG1	2.99	0.41
1:G:176:MET:HB2	1:G:176:MET:HE2	1.76	0.41
1:A:35:THR:HB	1:A:58:PHE:CD1	2.56	0.41
1:B:70:LYS:CA	1:B:94:VAL:HG12	2.50	0.41
1:C:57:VAL:CG1	1:C:58:PHE:CE1	3.04	0.41
1:D:90:ALA:O	1:D:116:VAL:HA	2.21	0.41
1:D:37:CYS:SG	1:D:81:VAL:CG1	3.08	0.41
1:E:89:ARG:HG2	1:E:115:ARG:HD3	2.03	0.41
1:E:96:LYS:HB3	1:E:124:HIS:NE2	2.35	0.41
1:F:37:CYS:SG	1:F:81:VAL:HG13	2.60	0.41
1:G:92:ALA:HA	1:G:120:ALA:HB2	2.02	0.41
1:G:74:GLN:CD	1:G:74:GLN:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:PHE:CE1	1:D:110:CYS:HB3	2.56	0.41
1:E:111:ALA:HB2	1:E:131:VAL:O	2.21	0.41
1:F:81:VAL:HG23	1:F:105:LEU:O	2.21	0.41
1:G:89:ARG:HE	1:G:115:ARG:NH2	2.19	0.41
1:F:38:ILE:HG13	1:F:38:ILE:O	2.20	0.41
1:H:28:GLU:HB3	1:H:360:LEU:HD21	2.03	0.41
1:C:208:ASP:OD2	2:C:1000:NAD:H1B	2.20	0.41
1:D:72:THR:O	1:D:75:LEU:HB2	2.21	0.41
1:H:109:ARG:HB3	3:H:1104:HOH:O	2.19	0.41
1:A:321:PHE:CE2	1:A:325:LEU:HD11	2.56	0.41
1:B:178:HIS:N	3:B:1101:HOH:O	2.05	0.41
1:B:62:TYR:C	1:B:62:TYR:CD1	2.95	0.41
1:C:76:ALA:O	1:C:101:ALA:HB1	2.21	0.41
1:D:68:LEU:N	1:D:88:ASP:OD1	2.52	0.41
1:A:32:VAL:HA	1:A:359:VAL:HG11	2.02	0.40
1:B:160:ARG:HH11	1:B:160:ARG:HD3	1.72	0.40
1:B:72:THR:O	1:B:75:LEU:HD13	2.21	0.40
1:B:76:ALA:CB	1:B:98:LEU:CD2	2.99	0.40
1:C:158:TYR:CD1	1:D:331:LEU:HD13	2.55	0.40
1:E:223:VAL:HG21	1:E:231:MET:HE2	2.03	0.40
1:E:92:ALA:HA	1:E:120:ALA:HB1	2.03	0.40
1:F:68:LEU:HD22	1:F:84:LEU:HD21	2.02	0.40
1:G:86:VAL:HG13	1:G:110:CYS:SG	2.62	0.40
1:A:242:LEU:HD12	2:A:1000:NAD:N7A	2.37	0.40
1:B:148:PHE:CE2	1:B:176:MET:CE	3.04	0.40
1:B:290:GLY:O	1:B:291:LEU:HD23	2.21	0.40
1:B:72:THR:CA	1:B:75:LEU:HD13	2.51	0.40
1:C:215:VAL:HA	1:C:218:MET:CE	2.51	0.40
1:D:25:THR:HG22	1:D:28:GLU:CB	2.41	0.40
1:G:53:PRO:O	1:G:56:LYS:HE2	2.21	0.40
1:A:229:LEU:O	1:A:257:MET:HA	2.20	0.40
1:B:247:GLN:CG	1:B:273:ASP:HB2	2.50	0.40
1:C:163:MET:HB2	1:C:163:MET:HE2	1.62	0.40
1:D:324:LEU:HD12	1:D:324:LEU:HA	1.62	0.40
1:E:70:LYS:HD3	1:E:71:ASP:CG	2.41	0.40
1:G:340:THR:HG23	1:G:342:GLU:OE1	2.22	0.40
1:D:250:ASN:O	1:D:254:ILE:HG13	2.22	0.40
1:E:105:LEU:HD11	1:E:129:VAL:HB	2.04	0.40
1:E:158:TYR:OH	1:E:162:ARG:NH1	2.52	0.40
1:F:274:SER:HB2	1:F:295:GLU:OE2	2.21	0.40
1:F:160:ARG:HD3	1:F:160:ARG:HH11	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:VAL:HG21	1:G:231:MET:HE2	2.03	0.40
1:H:242:LEU:H	1:H:245:THR:HG1	1.68	0.40

There are no symmetry-related clashes.

## 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	344/386 (89%)	336 (98%)	8 (2%)	0	100	100
1	B	336/386 (87%)	329 (98%)	7 (2%)	0	100	100
1	C	340/386 (88%)	331 (97%)	9 (3%)	0	100	100
1	D	344/386 (89%)	335 (97%)	7 (2%)	2 (1%)	25	29
1	E	342/386 (89%)	333 (97%)	9 (3%)	0	100	100
1	F	341/386 (88%)	335 (98%)	6 (2%)	0	100	100
1	G	341/386 (88%)	331 (97%)	10 (3%)	0	100	100
1	H	341/386 (88%)	334 (98%)	5 (2%)	2 (1%)	25	29
All	All	2729/3088 (88%)	2664 (98%)	61 (2%)	4 (0%)	51	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	24	LEU
1	H	27	GLN
1	H	26	PRO
1	D	26	PRO

### 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	287/318 (90%)	285 (99%)	2 (1%)	84	90
1	B	280/318 (88%)	275 (98%)	5 (2%)	59	71
1	C	284/318 (89%)	281 (99%)	3 (1%)	73	82
1	D	288/318 (91%)	281 (98%)	7 (2%)	49	61
1	E	286/318 (90%)	279 (98%)	7 (2%)	49	61
1	F	285/318 (90%)	279 (98%)	6 (2%)	53	66
1	G	285/318 (90%)	281 (99%)	4 (1%)	67	77
1	H	285/318 (90%)	282 (99%)	3 (1%)	73	82
All	All	2280/2544 (90%)	2243 (98%)	37 (2%)	62	74

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	VAL
1	A	340	THR
1	B	49	PHE
1	B	62	TYR
1	B	174	VAL
1	B	186	THR
1	B	340	THR
1	C	81	VAL
1	C	129	VAL
1	C	169	SER
1	D	23	GLU
1	D	69	ASP
1	D	174	VAL
1	D	223	VAL
1	D	236	THR
1	D	306	THR
1	D	340	THR
1	E	49	PHE
1	E	69	ASP

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Mol	Chain	Res	Type
1	E	81	VAL
1	E	129	VAL
1	E	244	SER
1	E	340	THR
1	E	349	THR
1	F	49	PHE
1	F	62	TYR
1	F	83	VAL
1	F	169	SER
1	F	223	VAL
1	F	246	ARG
1	G	49	PHE
1	G	93	SER
1	G	320	GLN
1	G	340	THR
1	H	27	GLN
1	H	49	PHE
1	H	340	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	B	151	ASN
1	B	354	ASN
1	B	366	ASN
1	F	151	ASN
1	G	151	ASN
1	H	247	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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAD	D	1000	-	42,48,48	2.58	17 (40%)	50,73,73	1.60	8 (16%)
2	NAD	F	1000	-	42,48,48	2.59	17 (40%)	50,73,73	1.59	8 (16%)
2	NAD	H	1000	-	42,48,48	2.62	17 (40%)	50,73,73	1.55	10 (20%)
2	NAD	A	1000	-	42,48,48	2.62	17 (40%)	50,73,73	1.55	11 (22%)
2	NAD	C	1000	-	42,48,48	2.60	18 (42%)	50,73,73	1.56	9 (18%)
2	NAD	E	1000	-	42,48,48	2.63	17 (40%)	50,73,73	1.58	11 (22%)
2	NAD	G	1000	-	42,48,48	2.55	17 (40%)	50,73,73	1.68	11 (22%)
2	NAD	B	1000	-	42,48,48	2.57	17 (40%)	50,73,73	1.52	9 (18%)

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
2	NAD	D	1000	-	-	14/26/62/62	0/5/5/5
2	NAD	F	1000	-	-	11/26/62/62	0/5/5/5
2	NAD	H	1000	-	-	13/26/62/62	0/5/5/5
2	NAD	A	1000	-	-	12/26/62/62	0/5/5/5
2	NAD	C	1000	-	-	14/26/62/62	0/5/5/5
2	NAD	E	1000	-	-	14/26/62/62	0/5/5/5
2	NAD	G	1000	-	-	8/26/62/62	0/5/5/5
2	NAD	B	1000	-	-	11/26/62/62	0/5/5/5



All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	NAD	O4B-C1B	6.60	1.50	1.41
2	H	1000	NAD	O4B-C1B	6.39	1.50	1.41
2	E	1000	NAD	O4B-C1B	6.30	1.49	1.41
2	D	1000	NAD	O4B-C1B	6.27	1.49	1.41
2	F	1000	NAD	O4B-C1B	6.21	1.49	1.41
2	H	1000	NAD	C2A-N1A	-6.20	1.22	1.33
2	G	1000	NAD	O4B-C1B	6.19	1.49	1.41
2	C	1000	NAD	C2A-N1A	-6.14	1.22	1.33
2	E	1000	NAD	C2A-N1A	-6.13	1.22	1.33
2	B	1000	NAD	C2A-N1A	-6.12	1.22	1.33
2	A	1000	NAD	C2A-N1A	-6.07	1.22	1.33
2	C	1000	NAD	O4B-C1B	6.07	1.49	1.41
2	D	1000	NAD	C2A-N1A	-6.05	1.22	1.33
2	F	1000	NAD	C2A-N1A	-6.05	1.22	1.33
2	G	1000	NAD	C2A-N1A	-6.00	1.22	1.33
2	B	1000	NAD	O4B-C1B	5.85	1.49	1.41
2	H	1000	NAD	C2N-N1N	5.80	1.42	1.35
2	A	1000	NAD	C2N-N1N	5.73	1.41	1.35
2	E	1000	NAD	C2N-N1N	5.60	1.41	1.35
2	C	1000	NAD	C2N-N1N	5.45	1.41	1.35
2	B	1000	NAD	O4D-C1D	5.44	1.48	1.41
2	E	1000	NAD	O4D-C1D	5.42	1.48	1.41
2	F	1000	NAD	C2N-N1N	5.41	1.41	1.35
2	C	1000	NAD	O4D-C1D	5.30	1.48	1.41
2	B	1000	NAD	C2N-N1N	5.27	1.41	1.35
2	A	1000	NAD	O4D-C1D	5.20	1.48	1.41
2	F	1000	NAD	O4D-C1D	5.20	1.48	1.41
2	H	1000	NAD	O4D-C1D	5.09	1.48	1.41
2	G	1000	NAD	C2N-N1N	5.01	1.41	1.35
2	D	1000	NAD	C2N-N1N	5.00	1.41	1.35
2	C	1000	NAD	C7N-N7N	4.97	1.42	1.33
2	G	1000	NAD	C7N-N7N	4.97	1.42	1.33
2	B	1000	NAD	C7N-N7N	4.95	1.42	1.33
2	F	1000	NAD	C7N-N7N	4.93	1.42	1.33
2	E	1000	NAD	C7N-N7N	4.92	1.42	1.33
2	H	1000	NAD	C7N-N7N	4.90	1.42	1.33
2	A	1000	NAD	C7N-N7N	4.90	1.42	1.33
2	D	1000	NAD	C7N-N7N	4.84	1.42	1.33
2	G	1000	NAD	O4D-C1D	4.83	1.47	1.41
2	D	1000	NAD	O4D-C1D	4.81	1.47	1.41
2	C	1000	NAD	C2B-C1B	-4.09	1.47	1.53
2	F	1000	NAD	C4A-N3A	3.90	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1000	NAD	C4A-N3A	3.88	1.41	1.35
2	A	1000	NAD	C4A-N3A	3.78	1.40	1.35
2	B	1000	NAD	C4A-N3A	3.78	1.40	1.35
2	H	1000	NAD	C4A-N3A	3.78	1.40	1.35
2	G	1000	NAD	C4A-N3A	3.73	1.40	1.35
2	D	1000	NAD	C2D-C1D	-3.69	1.48	1.53
2	D	1000	NAD	C8A-N7A	3.69	1.41	1.34
2	E	1000	NAD	C2B-C1B	-3.67	1.48	1.53
2	G	1000	NAD	C2D-C1D	-3.61	1.48	1.53
2	E	1000	NAD	C8A-N7A	3.61	1.41	1.34
2	B	1000	NAD	C2B-C1B	-3.61	1.48	1.53
2	D	1000	NAD	C4A-N3A	3.58	1.40	1.35
2	G	1000	NAD	C8A-N7A	3.55	1.41	1.34
2	A	1000	NAD	C2B-C1B	-3.55	1.48	1.53
2	F	1000	NAD	C2B-C1B	-3.55	1.48	1.53
2	C	1000	NAD	C4A-N3A	3.54	1.40	1.35
2	C	1000	NAD	C8A-N7A	3.51	1.41	1.34
2	A	1000	NAD	C8A-N7A	3.51	1.40	1.34
2	F	1000	NAD	C8A-N7A	3.50	1.40	1.34
2	D	1000	NAD	C2B-C1B	-3.50	1.48	1.53
2	B	1000	NAD	C8A-N7A	3.50	1.40	1.34
2	H	1000	NAD	C8A-N7A	3.46	1.40	1.34
2	B	1000	NAD	C2D-C1D	-3.42	1.48	1.53
2	C	1000	NAD	C2D-C1D	-3.40	1.48	1.53
2	H	1000	NAD	C2D-C1D	-3.24	1.48	1.53
2	H	1000	NAD	C2B-C1B	-3.21	1.48	1.53
2	E	1000	NAD	C2D-C1D	-3.20	1.48	1.53
2	F	1000	NAD	C2D-C1D	-3.18	1.48	1.53
2	A	1000	NAD	C2D-C1D	-3.17	1.49	1.53
2	D	1000	NAD	C2D-C3D	-3.11	1.44	1.53
2	G	1000	NAD	C2B-C1B	-3.06	1.49	1.53
2	D	1000	NAD	C6N-N1N	2.83	1.42	1.35
2	G	1000	NAD	C2D-C3D	-2.79	1.45	1.53
2	E	1000	NAD	C6N-N1N	2.77	1.42	1.35
2	F	1000	NAD	C2D-C3D	-2.75	1.45	1.53
2	C	1000	NAD	C2D-C3D	-2.73	1.45	1.53
2	H	1000	NAD	C2D-C3D	-2.73	1.45	1.53
2	B	1000	NAD	C6N-N1N	2.67	1.41	1.35
2	H	1000	NAD	C6N-N1N	2.66	1.41	1.35
2	G	1000	NAD	C2B-C3B	-2.63	1.46	1.53
2	C	1000	NAD	C2B-C3B	-2.62	1.46	1.53
2	A	1000	NAD	C5A-C4A	2.62	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1000	NAD	C2B-C3B	-2.62	1.46	1.53
2	G	1000	NAD	C5A-C4A	2.61	1.47	1.40
2	H	1000	NAD	C2B-C3B	-2.60	1.46	1.53
2	E	1000	NAD	C2D-C3D	-2.59	1.46	1.53
2	D	1000	NAD	C5A-C4A	2.58	1.47	1.40
2	H	1000	NAD	C6A-N1A	-2.57	1.25	1.37
2	F	1000	NAD	C6N-N1N	2.57	1.41	1.35
2	A	1000	NAD	C2B-C3B	-2.57	1.46	1.53
2	A	1000	NAD	C6N-N1N	2.56	1.41	1.35
2	B	1000	NAD	C2B-C3B	-2.56	1.46	1.53
2	E	1000	NAD	C5A-C4A	2.55	1.47	1.40
2	C	1000	NAD	C6N-N1N	2.54	1.41	1.35
2	D	1000	NAD	C6A-N1A	-2.54	1.26	1.37
2	A	1000	NAD	C6A-N1A	-2.51	1.26	1.37
2	E	1000	NAD	C6A-N1A	-2.51	1.26	1.37
2	C	1000	NAD	C6A-N1A	-2.50	1.26	1.37
2	B	1000	NAD	C2D-C3D	-2.50	1.46	1.53
2	F	1000	NAD	C2B-C3B	-2.49	1.46	1.53
2	H	1000	NAD	O4B-C4B	2.49	1.50	1.45
2	D	1000	NAD	C2B-C3B	-2.49	1.46	1.53
2	H	1000	NAD	C5A-C4A	2.49	1.47	1.40
2	A	1000	NAD	C2D-C3D	-2.48	1.46	1.53
2	G	1000	NAD	C6A-N1A	-2.48	1.26	1.37
2	F	1000	NAD	C6A-N1A	-2.46	1.26	1.37
2	A	1000	NAD	O4B-C4B	2.46	1.50	1.45
2	B	1000	NAD	C6A-N1A	-2.46	1.26	1.37
2	G	1000	NAD	C6N-N1N	2.45	1.41	1.35
2	B	1000	NAD	C5A-C4A	2.44	1.47	1.40
2	F	1000	NAD	C5A-C4A	2.44	1.47	1.40
2	F	1000	NAD	C3D-C4D	-2.43	1.46	1.53
2	C	1000	NAD	C5A-C4A	2.40	1.47	1.40
2	D	1000	NAD	O4B-C4B	2.39	1.50	1.45
2	D	1000	NAD	C3D-C4D	-2.36	1.46	1.53
2	E	1000	NAD	O4B-C4B	2.36	1.50	1.45
2	H	1000	NAD	C3D-C4D	-2.29	1.47	1.53
2	A	1000	NAD	C3D-C4D	-2.24	1.47	1.53
2	A	1000	NAD	C6A-N6A	2.22	1.42	1.34
2	F	1000	NAD	C6A-N6A	2.22	1.42	1.34
2	C	1000	NAD	O4B-C4B	2.19	1.49	1.45
2	G	1000	NAD	C6A-N6A	2.18	1.42	1.34
2	G	1000	NAD	O4B-C4B	2.18	1.49	1.45
2	C	1000	NAD	C6A-N6A	2.16	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1000	NAD	O4B-C4B	2.16	1.49	1.45
2	E	1000	NAD	C6A-N6A	2.15	1.41	1.34
2	B	1000	NAD	C6A-N6A	2.15	1.41	1.34
2	E	1000	NAD	C3D-C4D	-2.15	1.47	1.53
2	D	1000	NAD	C6A-N6A	2.14	1.41	1.34
2	B	1000	NAD	C3D-C4D	-2.14	1.47	1.53
2	C	1000	NAD	C3D-C4D	-2.13	1.47	1.53
2	H	1000	NAD	C6A-N6A	2.12	1.41	1.34
2	B	1000	NAD	O4B-C4B	2.09	1.49	1.45
2	C	1000	NAD	C2A-N3A	-2.01	1.28	1.32
2	G	1000	NAD	C3D-C4D	-2.00	1.47	1.53

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1000	NAD	C2A-N1A-C6A	5.48	128.13	118.75
2	C	1000	NAD	C2A-N1A-C6A	5.48	128.13	118.75
2	B	1000	NAD	C2A-N1A-C6A	5.45	128.08	118.75
2	E	1000	NAD	C2A-N1A-C6A	5.31	127.83	118.75
2	G	1000	NAD	C2A-N1A-C6A	5.28	127.79	118.75
2	A	1000	NAD	C2A-N1A-C6A	5.24	127.72	118.75
2	D	1000	NAD	C2A-N1A-C6A	5.18	127.61	118.75
2	H	1000	NAD	C2A-N1A-C6A	5.16	127.58	118.75
2	B	1000	NAD	N3A-C2A-N1A	-4.34	121.89	128.68
2	F	1000	NAD	N3A-C2A-N1A	-4.33	121.91	128.68
2	C	1000	NAD	N3A-C2A-N1A	-4.23	122.07	128.68
2	G	1000	NAD	C3N-C7N-N7N	4.13	122.71	117.75
2	E	1000	NAD	N3A-C2A-N1A	-4.12	122.23	128.68
2	G	1000	NAD	N3A-C2A-N1A	-4.10	122.27	128.68
2	H	1000	NAD	N3A-C2A-N1A	-4.10	122.27	128.68
2	A	1000	NAD	N3A-C2A-N1A	-3.98	122.46	128.68
2	D	1000	NAD	N3A-C2A-N1A	-3.92	122.55	128.68
2	A	1000	NAD	C3D-C2D-C1D	3.70	106.55	100.98
2	H	1000	NAD	C3D-C2D-C1D	3.59	106.38	100.98
2	F	1000	NAD	C3D-C2D-C1D	3.58	106.37	100.98
2	C	1000	NAD	C3D-C2D-C1D	3.50	106.24	100.98
2	E	1000	NAD	C6N-N1N-C2N	-3.48	118.81	121.97
2	D	1000	NAD	C3D-C2D-C1D	3.29	105.93	100.98
2	D	1000	NAD	C6N-N1N-C2N	-3.29	118.98	121.97
2	E	1000	NAD	C3D-C2D-C1D	3.25	105.87	100.98
2	G	1000	NAD	C3D-C2D-C1D	3.24	105.86	100.98
2	B	1000	NAD	C3D-C2D-C1D	3.10	105.64	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1000	NAD	C6N-N1N-C2N	-3.06	119.19	121.97
2	H	1000	NAD	C6N-N1N-C2N	-3.00	119.24	121.97
2	C	1000	NAD	C6N-N1N-C2N	-2.99	119.25	121.97
2	B	1000	NAD	C6N-N1N-C2N	-2.98	119.25	121.97
2	G	1000	NAD	PN-O3-PA	-2.97	122.62	132.83
2	G	1000	NAD	C6N-N1N-C2N	-2.88	119.35	121.97
2	A	1000	NAD	C3B-C2B-C1B	2.81	105.20	100.98
2	E	1000	NAD	C3B-C2B-C1B	2.70	105.05	100.98
2	H	1000	NAD	O2A-PA-O1A	-2.66	99.07	112.24
2	A	1000	NAD	C6N-N1N-C2N	-2.61	119.60	121.97
2	G	1000	NAD	O7N-C7N-N7N	-2.58	118.91	122.58
2	D	1000	NAD	C3B-C2B-C1B	2.54	104.80	100.98
2	A	1000	NAD	O2A-PA-O1A	-2.51	99.83	112.24
2	H	1000	NAD	C3B-C2B-C1B	2.51	104.76	100.98
2	F	1000	NAD	PN-O3-PA	-2.49	124.27	132.83
2	E	1000	NAD	O2A-PA-O1A	-2.45	100.11	112.24
2	G	1000	NAD	C2B-C3B-C4B	2.43	107.36	102.64
2	D	1000	NAD	PN-O3-PA	-2.41	124.55	132.83
2	B	1000	NAD	C3B-C2B-C1B	2.41	104.61	100.98
2	A	1000	NAD	PN-O3-PA	-2.41	124.55	132.83
2	C	1000	NAD	PN-O3-PA	-2.41	124.56	132.83
2	D	1000	NAD	O2A-PA-O1A	-2.41	100.34	112.24
2	G	1000	NAD	O2N-PN-O1N	-2.40	100.37	112.24
2	A	1000	NAD	O7N-C7N-N7N	-2.39	119.18	122.58
2	D	1000	NAD	C2B-C3B-C4B	2.39	107.28	102.64
2	F	1000	NAD	C2B-C3B-C4B	2.36	107.22	102.64
2	E	1000	NAD	C2B-C3B-C4B	2.34	107.19	102.64
2	A	1000	NAD	C3N-C7N-N7N	2.34	120.56	117.75
2	C	1000	NAD	O2A-PA-O1A	-2.33	100.74	112.24
2	B	1000	NAD	C3N-C7N-N7N	2.28	120.49	117.75
2	F	1000	NAD	O2A-PA-O1A	-2.27	101.01	112.24
2	H	1000	NAD	C3N-C7N-N7N	2.26	120.46	117.75
2	C	1000	NAD	O2N-PN-O1N	-2.24	101.15	112.24
2	B	1000	NAD	O2A-PA-O1A	-2.22	101.27	112.24
2	H	1000	NAD	O2N-PN-O1N	-2.21	101.31	112.24
2	F	1000	NAD	C3B-C2B-C1B	2.18	104.27	100.98
2	H	1000	NAD	O7N-C7N-N7N	-2.15	119.53	122.58
2	E	1000	NAD	O2N-PN-O1N	-2.15	101.63	112.24
2	C	1000	NAD	C2B-C3B-C4B	2.14	106.81	102.64
2	C	1000	NAD	C1B-N9A-C4A	-2.13	122.90	126.64
2	B	1000	NAD	O2N-PN-O1N	-2.11	101.81	112.24
2	H	1000	NAD	C2B-C3B-C4B	2.08	106.69	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	NAD	C2B-C3B-C4B	2.08	106.69	102.64
2	B	1000	NAD	C2B-C3B-C4B	2.08	106.68	102.64
2	G	1000	NAD	C3B-C2B-C1B	2.07	104.10	100.98
2	E	1000	NAD	C3N-C7N-N7N	2.07	120.23	117.75
2	E	1000	NAD	PN-O3-PA	-2.06	125.75	132.83
2	E	1000	NAD	O7N-C7N-N7N	-2.05	119.66	122.58
2	G	1000	NAD	O2A-PA-O1A	-2.05	102.12	112.24
2	A	1000	NAD	O2N-PN-O1N	-2.02	102.27	112.24

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1000	NAD	C5D-O5D-PN-O1N
2	D	1000	NAD	O4D-C1D-N1N-C2N
2	D	1000	NAD	O4D-C1D-N1N-C6N
2	D	1000	NAD	C2D-C1D-N1N-C2N
2	D	1000	NAD	C2D-C1D-N1N-C6N
2	D	1000	NAD	C2N-C3N-C7N-O7N
2	D	1000	NAD	C2N-C3N-C7N-N7N
2	F	1000	NAD	C5B-O5B-PA-O1A
2	F	1000	NAD	C3D-C4D-C5D-O5D
2	F	1000	NAD	O4D-C1D-N1N-C2N
2	F	1000	NAD	O4D-C1D-N1N-C6N
2	H	1000	NAD	O4B-C4B-C5B-O5B
2	H	1000	NAD	C5D-O5D-PN-O1N
2	H	1000	NAD	O4D-C1D-N1N-C2N
2	H	1000	NAD	O4D-C1D-N1N-C6N
2	H	1000	NAD	C2D-C1D-N1N-C2N
2	H	1000	NAD	C2D-C1D-N1N-C6N
2	A	1000	NAD	O4B-C4B-C5B-O5B
2	A	1000	NAD	O4D-C1D-N1N-C2N
2	A	1000	NAD	O4D-C1D-N1N-C6N
2	C	1000	NAD	O4B-C4B-C5B-O5B
2	C	1000	NAD	C5D-O5D-PN-O1N
2	C	1000	NAD	O4D-C1D-N1N-C2N
2	C	1000	NAD	O4D-C1D-N1N-C6N
2	C	1000	NAD	C2D-C1D-N1N-C2N
2	C	1000	NAD	C2D-C1D-N1N-C6N
2	E	1000	NAD	C3D-C4D-C5D-O5D
2	E	1000	NAD	O4D-C1D-N1N-C2N
2	E	1000	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	E	1000	NAD	C2D-C1D-N1N-C2N
2	E	1000	NAD	C2D-C1D-N1N-C6N
2	E	1000	NAD	C2N-C3N-C7N-O7N
2	E	1000	NAD	C2N-C3N-C7N-N7N
2	G	1000	NAD	C5D-O5D-PN-O3
2	G	1000	NAD	C5D-O5D-PN-O1N
2	G	1000	NAD	O4D-C1D-N1N-C2N
2	G	1000	NAD	O4D-C1D-N1N-C6N
2	G	1000	NAD	C2D-C1D-N1N-C2N
2	G	1000	NAD	C2D-C1D-N1N-C6N
2	B	1000	NAD	C5D-O5D-PN-O1N
2	B	1000	NAD	O4D-C1D-N1N-C2N
2	B	1000	NAD	O4D-C1D-N1N-C6N
2	B	1000	NAD	C2D-C1D-N1N-C2N
2	B	1000	NAD	C2D-C1D-N1N-C6N
2	E	1000	NAD	C4N-C3N-C7N-N7N
2	E	1000	NAD	C4N-C3N-C7N-O7N
2	D	1000	NAD	O4B-C4B-C5B-O5B
2	C	1000	NAD	C3B-C4B-C5B-O5B
2	D	1000	NAD	C4N-C3N-C7N-N7N
2	D	1000	NAD	C4N-C3N-C7N-O7N
2	H	1000	NAD	C3B-C4B-C5B-O5B
2	A	1000	NAD	C3B-C4B-C5B-O5B
2	B	1000	NAD	C2N-C3N-C7N-N7N
2	D	1000	NAD	C3B-C4B-C5B-O5B
2	B	1000	NAD	C2N-C3N-C7N-O7N
2	F	1000	NAD	O4D-C4D-C5D-O5D
2	E	1000	NAD	O4D-C4D-C5D-O5D
2	B	1000	NAD	C4N-C3N-C7N-O7N
2	B	1000	NAD	C4N-C3N-C7N-N7N
2	A	1000	NAD	PN-O3-PA-O5B
2	E	1000	NAD	PN-O3-PA-O5B
2	G	1000	NAD	O4B-C4B-C5B-O5B
2	D	1000	NAD	C5D-O5D-PN-O3
2	H	1000	NAD	C5B-O5B-PA-O3
2	A	1000	NAD	C5B-O5B-PA-O3
2	A	1000	NAD	PA-O3-PN-O2N
2	D	1000	NAD	C5B-O5B-PA-O2A
2	H	1000	NAD	C5B-O5B-PA-O2A
2	A	1000	NAD	C5B-O5B-PA-O1A
2	A	1000	NAD	C5B-O5B-PA-O2A
2	C	1000	NAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	F	1000	NAD	C2N-C3N-C7N-N7N
2	F	1000	NAD	C2N-C3N-C7N-O7N
2	C	1000	NAD	C2N-C3N-C7N-O7N
2	H	1000	NAD	PA-O3-PN-O2N
2	C	1000	NAD	PA-O3-PN-O2N
2	C	1000	NAD	C2N-C3N-C7N-N7N
2	H	1000	NAD	C2N-C3N-C7N-O7N
2	B	1000	NAD	O4B-C4B-C5B-O5B
2	H	1000	NAD	C2N-C3N-C7N-N7N
2	F	1000	NAD	C4N-C3N-C7N-N7N
2	F	1000	NAD	C4N-C3N-C7N-O7N
2	F	1000	NAD	C2D-C1D-N1N-C2N
2	A	1000	NAD	C2D-C1D-N1N-C2N
2	A	1000	NAD	C2D-C1D-N1N-C6N
2	C	1000	NAD	C5B-O5B-PA-O3
2	C	1000	NAD	C4N-C3N-C7N-O7N
2	F	1000	NAD	O4B-C4B-C5B-O5B
2	E	1000	NAD	O4B-C4B-C5B-O5B
2	D	1000	NAD	PA-O3-PN-O2N
2	E	1000	NAD	PA-O3-PN-O2N
2	C	1000	NAD	C4N-C3N-C7N-N7N
2	A	1000	NAD	C5D-O5D-PN-O1N
2	E	1000	NAD	C5D-O5D-PN-O1N
2	G	1000	NAD	C3B-C4B-C5B-O5B
2	H	1000	NAD	C4N-C3N-C7N-O7N
2	B	1000	NAD	C3D-C4D-C5D-O5D

There are no ring outliers.

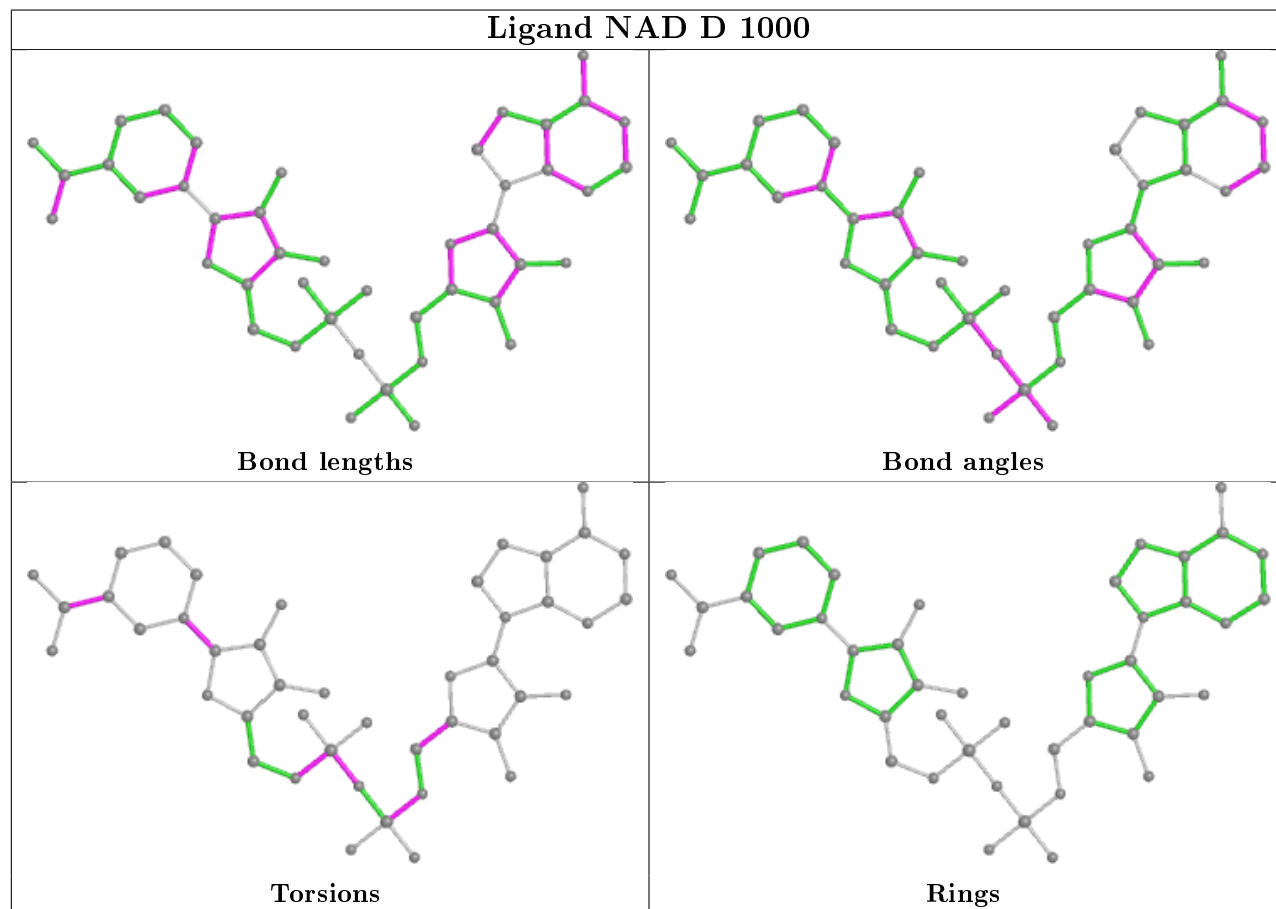
8 monomers are involved in 46 short contacts:

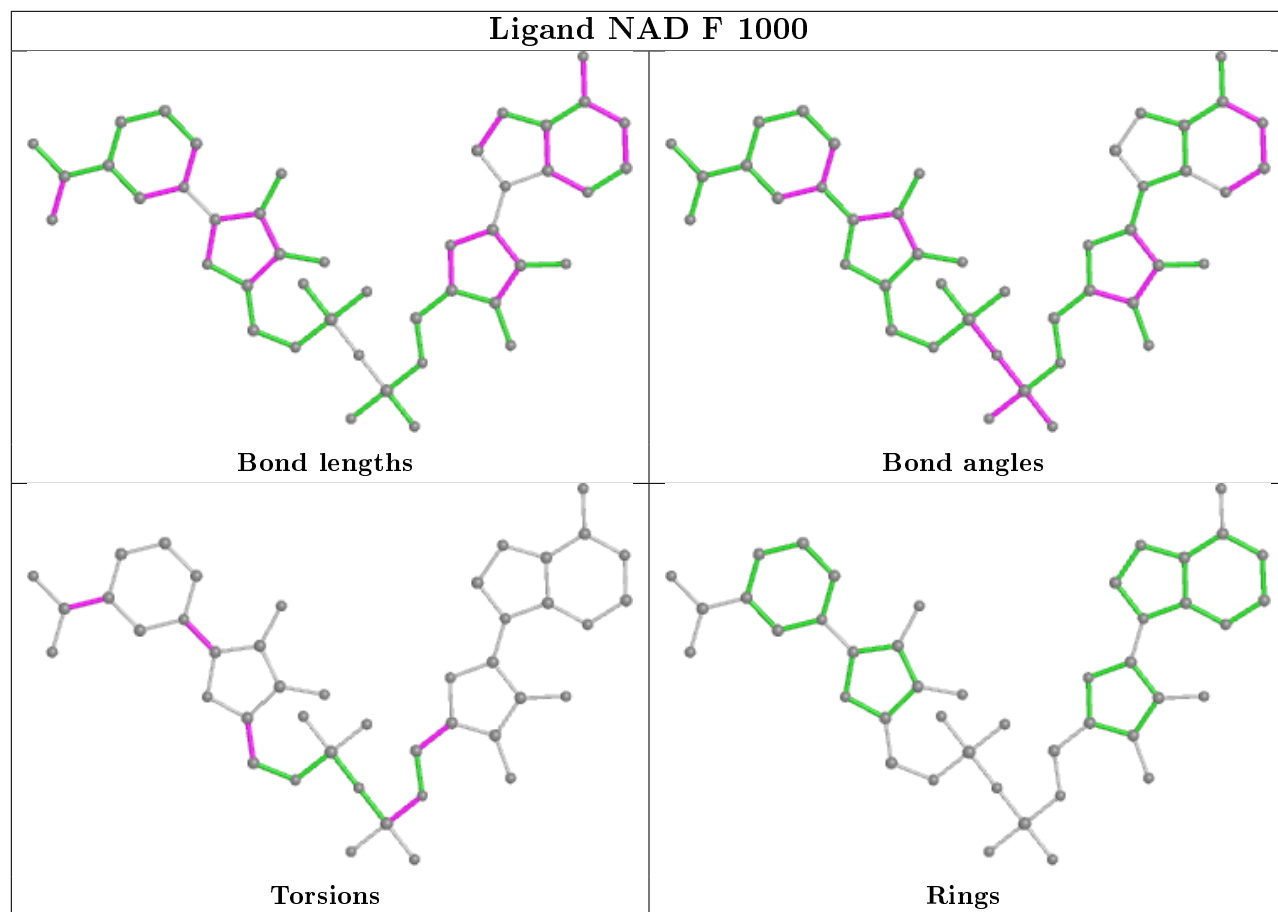
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1000	NAD	5	0
2	F	1000	NAD	4	0
2	H	1000	NAD	5	0
2	A	1000	NAD	6	0
2	C	1000	NAD	6	0
2	E	1000	NAD	3	0
2	G	1000	NAD	9	0
2	B	1000	NAD	8	0

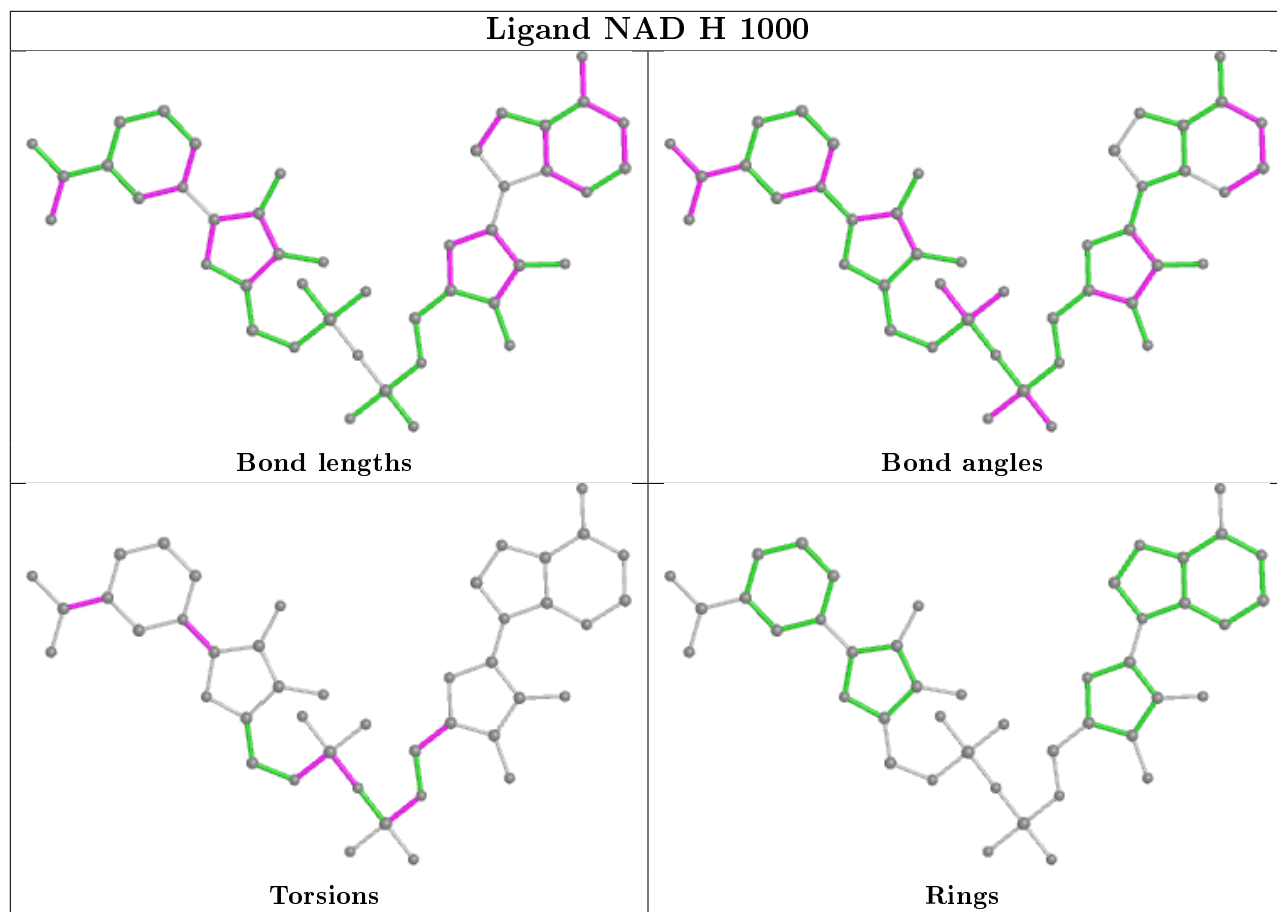
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

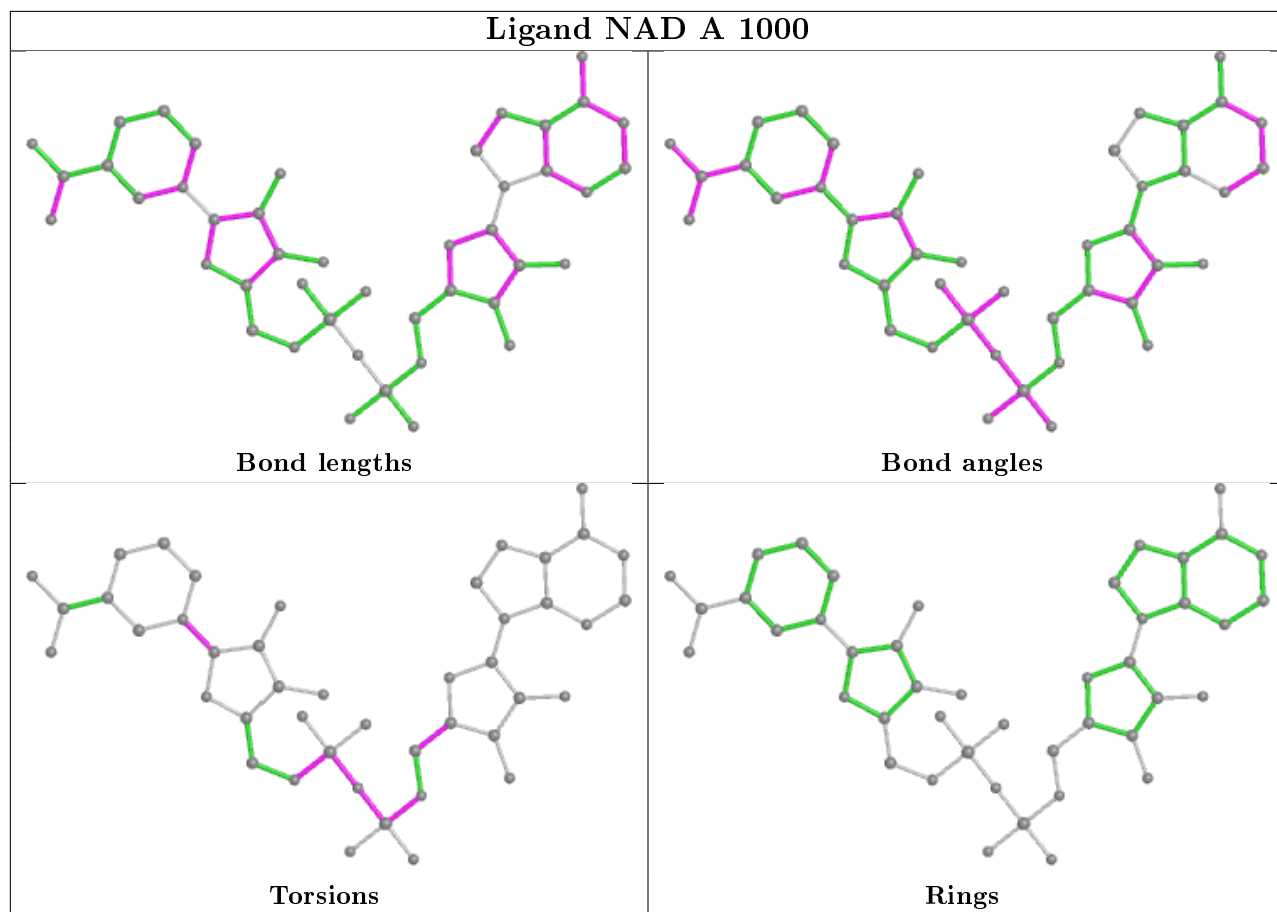


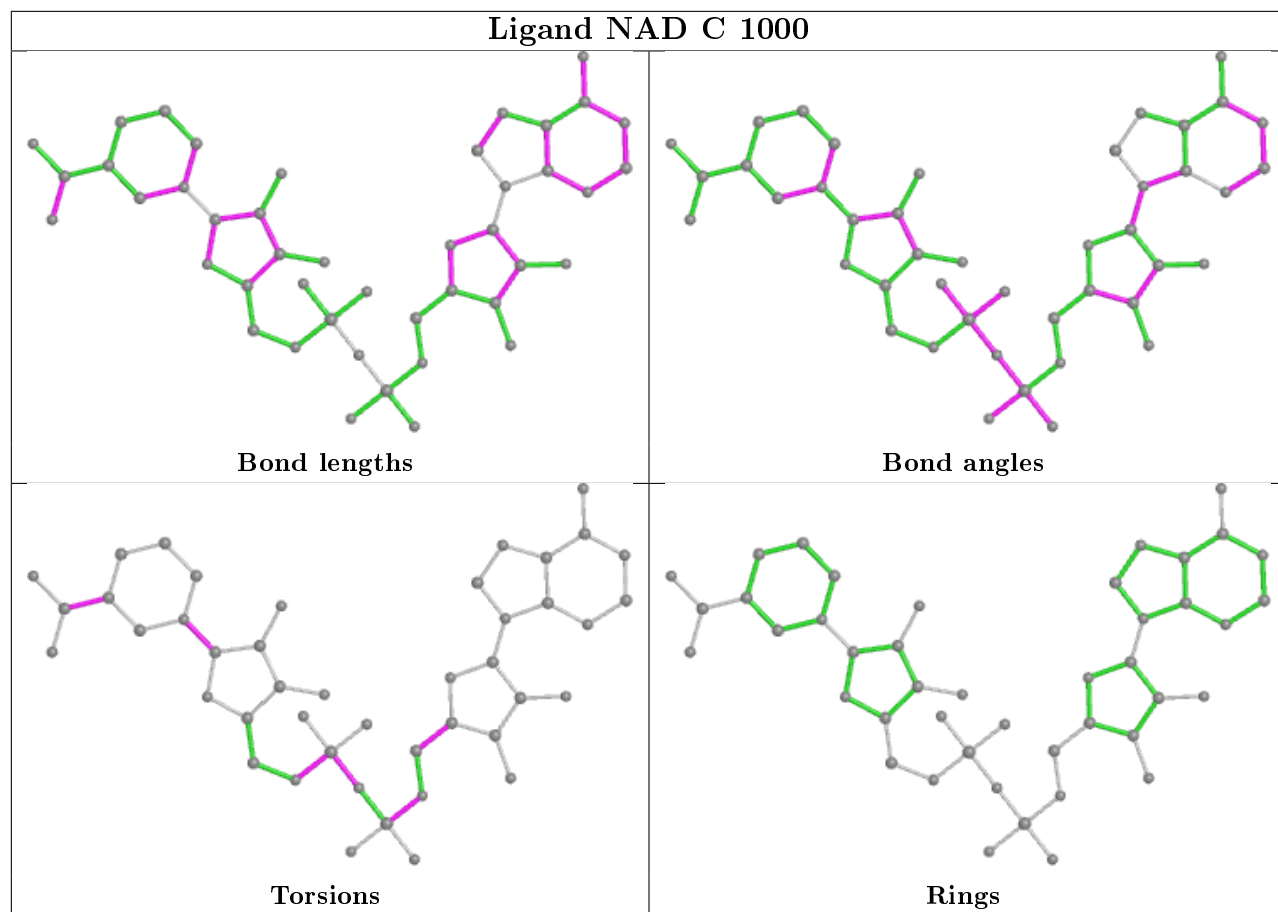
addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

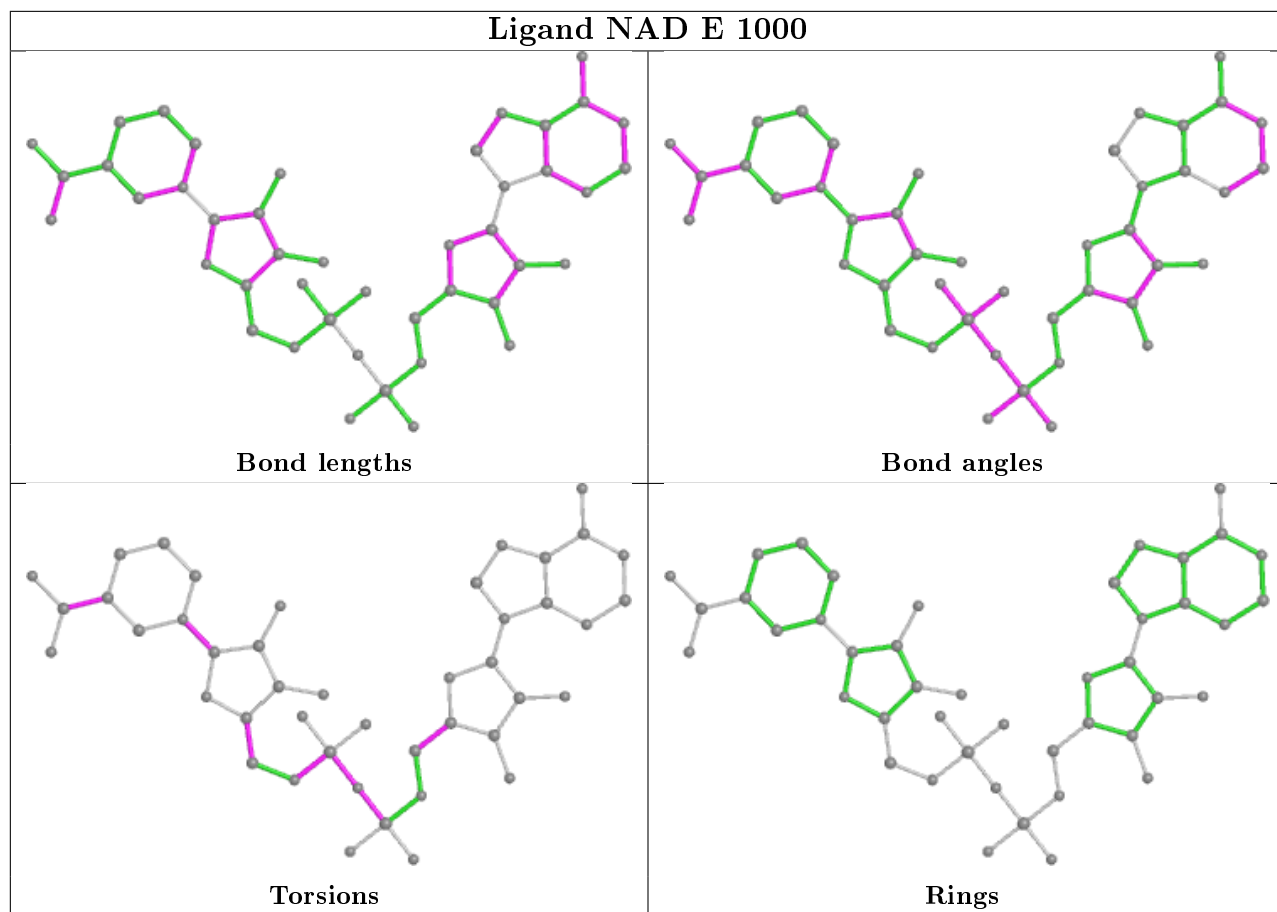


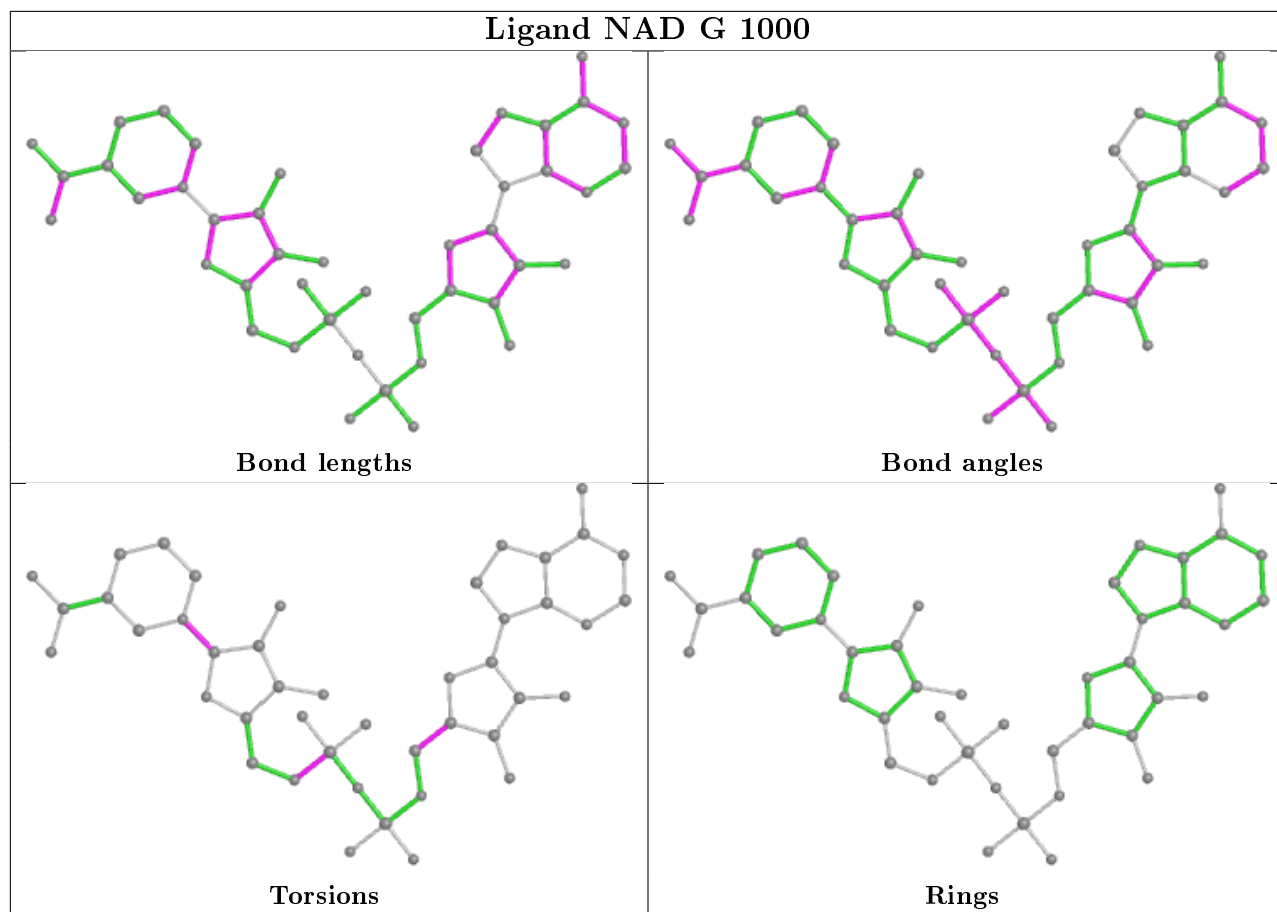


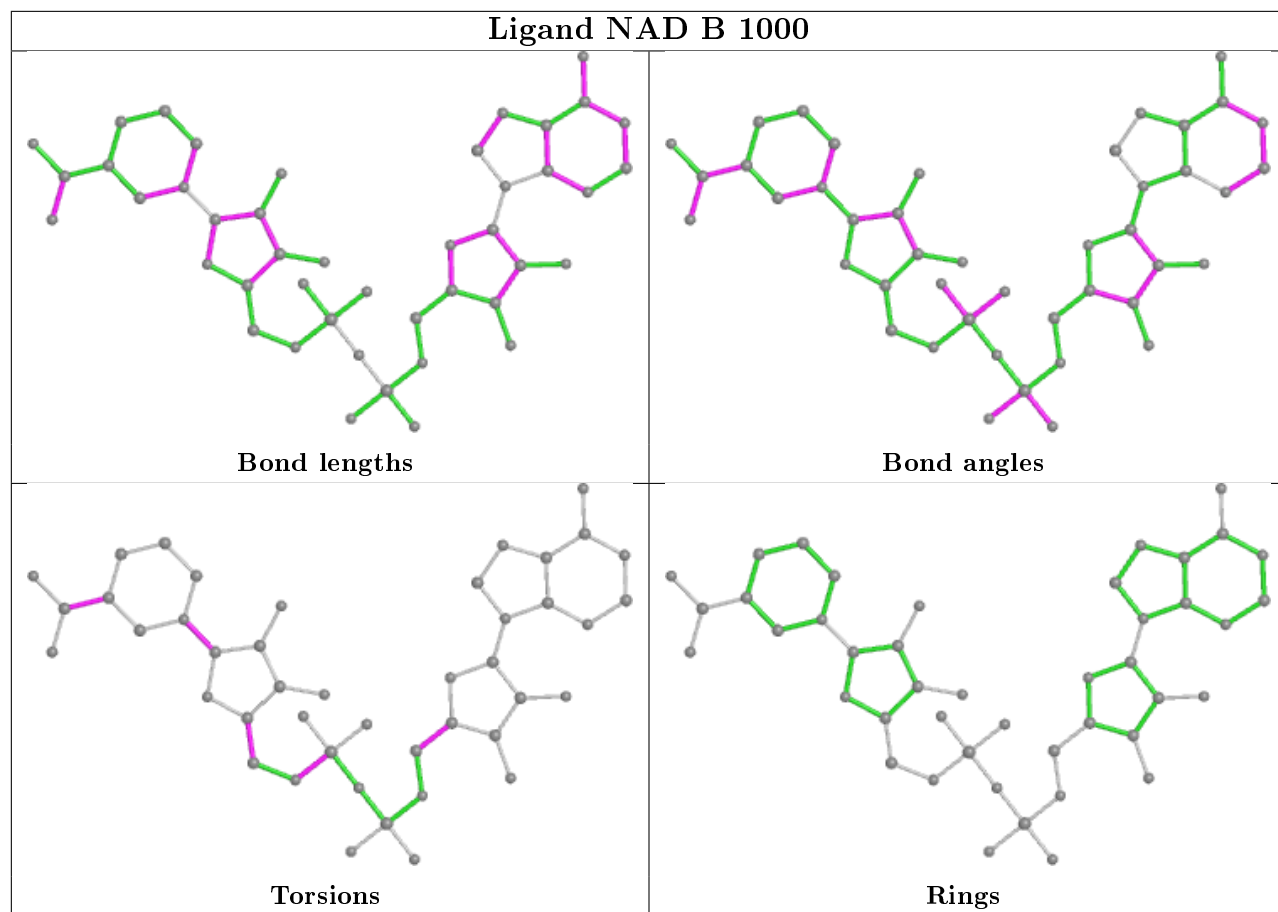












## 5.7 Other polymers [i](#)

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	346/386 (89%)	0.00	4 (1%) 79 77	30, 57, 95, 134	0
1	B	338/386 (87%)	0.58	50 (14%) 2 1	27, 61, 146, 199	0
1	C	342/386 (88%)	0.53	45 (13%) 3 2	32, 61, 160, 208	0
1	D	346/386 (89%)	0.21	23 (6%) 18 14	31, 58, 120, 175	0
1	E	344/386 (89%)	0.22	26 (7%) 13 10	30, 63, 133, 165	0
1	F	343/386 (88%)	0.43	40 (11%) 4 3	30, 58, 128, 170	0
1	G	343/386 (88%)	0.48	29 (8%) 10 8	29, 58, 163, 203	0
1	H	343/386 (88%)	0.36	25 (7%) 15 11	28, 59, 124, 173	0
All	All	2745/3088 (88%)	0.35	242 (8%) 10 7	27, 59, 138, 208	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	121	CYS	12.3
1	C	98	LEU	10.4
1	G	98	LEU	9.1
1	G	94	VAL	8.0
1	B	93	SER	7.9
1	B	121	CYS	7.6
1	C	103	VAL	6.9
1	C	113	PHE	6.6
1	B	98	LEU	6.3
1	E	126	VAL	6.3
1	C	116	VAL	6.1
1	D	126	VAL	6.1
1	C	84	LEU	6.0
1	H	126	VAL	5.8
1	G	99	ALA	5.8
1	G	40	TYR	5.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	117	ASP	5.6
1	B	95	ILE	5.6
1	H	118	LEU	5.5
1	C	126	VAL	5.5
1	B	94	VAL	5.4
1	G	116	VAL	5.3
1	D	22	VAL	5.2
1	C	40	TYR	5.2
1	B	38	ILE	5.1
1	G	84	LEU	5.0
1	B	113	PHE	5.0
1	F	116	VAL	4.8
1	G	100	LYS	4.7
1	F	126	VAL	4.7
1	C	104	LYS	4.6
1	B	92	ALA	4.6
1	B	40	TYR	4.5
1	C	39	CYS	4.5
1	C	38	ILE	4.5
1	F	98	LEU	4.5
1	E	118	LEU	4.4
1	B	118	LEU	4.4
1	B	117	ASP	4.4
1	F	93	SER	4.4
1	F	26	PRO	4.4
1	C	94	VAL	4.4
1	G	76	ALA	4.3
1	F	117	ASP	4.3
1	B	84	LEU	4.3
1	G	113	PHE	4.3
1	C	72	THR	4.3
1	G	122	ALA	4.2
1	B	39	CYS	4.2
1	D	25	THR	4.2
1	D	116	VAL	4.2
1	C	114	ASP	4.2
1	H	70	LYS	4.1
1	B	76	ALA	4.1
1	G	124	HIS	4.1
1	C	121	CYS	4.1
1	C	119	HIS	4.1
1	C	102	GLY	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	103	VAL	4.1
1	E	24	LEU	4.0
1	C	96	LYS	4.0
1	H	121	CYS	4.0
1	D	23	GLU	4.0
1	C	122	ALA	4.0
1	E	84	LEU	3.9
1	G	126	VAL	3.9
1	H	123	GLU	3.9
1	B	105	LEU	3.9
1	H	40	TYR	3.8
1	G	103	VAL	3.8
1	C	35	THR	3.8
1	B	126	VAL	3.8
1	F	38	ILE	3.7
1	F	32	VAL	3.7
1	B	122	ALA	3.7
1	D	24	LEU	3.7
1	F	70	LYS	3.6
1	B	62	TYR	3.6
1	B	116	VAL	3.6
1	B	100	LYS	3.6
1	C	80	ASP	3.6
1	C	100	LYS	3.6
1	F	119	HIS	3.6
1	B	119	HIS	3.5
1	H	124	HIS	3.5
1	E	77	ARG	3.5
1	H	119	HIS	3.5
1	F	368	VAL	3.5
1	C	117	ASP	3.4
1	F	94	VAL	3.4
1	B	115	ARG	3.4
1	C	71	ASP	3.4
1	D	98	LEU	3.3
1	F	125	GLY	3.3
1	C	77	ARG	3.3
1	B	81	VAL	3.2
1	D	81	VAL	3.2
1	B	123	GLU	3.2
1	H	120	ALA	3.2
1	G	77	ARG	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	355	ILE	3.1
1	H	125	GLY	3.1
1	D	77	ARG	3.1
1	F	121	CYS	3.1
1	B	82	ALA	3.1
1	E	25	THR	3.1
1	G	104	LYS	3.0
1	B	89	ARG	3.0
1	H	116	VAL	3.0
1	E	119	HIS	3.0
1	G	102	GLY	3.0
1	B	90	ALA	3.0
1	D	90	ALA	3.0
1	E	106	ILE	3.0
1	E	72	THR	3.0
1	D	94	VAL	2.9
1	F	40	TYR	2.9
1	G	364	LEU	2.9
1	C	358	TYR	2.9
1	H	89	ARG	2.9
1	G	119	HIS	2.9
1	A	126	VAL	2.9
1	C	125	GLY	2.9
1	C	118	LEU	2.8
1	F	55	GLN	2.8
1	B	70	LYS	2.8
1	B	125	GLY	2.8
1	C	92	ALA	2.8
1	E	74	GLN	2.8
1	F	122	ALA	2.8
1	H	74	GLN	2.7
1	H	100	LYS	2.7
1	F	92	ALA	2.7
1	B	91	ASP	2.7
1	B	77	ARG	2.7
1	E	62	TYR	2.7
1	F	113	PHE	2.7
1	F	96	LYS	2.7
1	E	116	VAL	2.7
1	B	104	LYS	2.7
1	E	71	ASP	2.7
1	G	96	LYS	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	129	VAL	2.7
1	A	27	GLN	2.7
1	D	118	LEU	2.7
1	D	297	GLU	2.7
1	B	58	PHE	2.7
1	B	96	LYS	2.7
1	G	125	GLY	2.7
1	G	118	LEU	2.6
1	C	130	ARG	2.6
1	F	54	MET	2.6
1	B	72	THR	2.6
1	F	28	GLU	2.6
1	E	100	LYS	2.6
1	F	104	LYS	2.6
1	C	76	ALA	2.6
1	F	99	ALA	2.6
1	C	70	LYS	2.6
1	H	113	PHE	2.5
1	C	69	ASP	2.5
1	E	82	ALA	2.5
1	F	355	ILE	2.5
1	H	358	TYR	2.5
1	F	89	ARG	2.5
1	C	93	SER	2.5
1	B	50	LEU	2.5
1	F	129	VAL	2.5
1	H	84	LEU	2.5
1	B	37	CYS	2.5
1	B	103	VAL	2.5
1	C	105	LEU	2.5
1	E	69	ASP	2.5
1	B	114	ASP	2.4
1	H	71	ASP	2.4
1	G	105	LEU	2.4
1	E	70	LYS	2.4
1	A	100	LYS	2.4
1	B	120	ALA	2.4
1	C	99	ALA	2.4
1	D	76	ALA	2.4
1	D	70	LYS	2.4
1	E	96	LYS	2.4
1	F	29	ALA	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	71	ASP	2.4
1	A	115	ARG	2.4
1	B	74	GLN	2.4
1	F	84	LEU	2.4
1	C	83	VAL	2.4
1	C	123	GLU	2.4
1	D	106	ILE	2.4
1	B	63	PHE	2.3
1	C	89	ARG	2.3
1	C	124	HIS	2.3
1	B	80	ASP	2.3
1	D	359	VAL	2.3
1	F	106	ILE	2.3
1	E	115	ARG	2.3
1	F	359	VAL	2.3
1	C	107	ALA	2.3
1	D	101	ALA	2.3
1	C	59	THR	2.3
1	D	28	GLU	2.3
1	H	104	LYS	2.2
1	H	72	THR	2.2
1	H	96	LYS	2.2
1	C	363	PRO	2.2
1	C	86	VAL	2.2
1	D	121	CYS	2.2
1	F	85	PHE	2.2
1	D	38	ILE	2.2
1	F	82	ALA	2.2
1	E	85	PHE	2.2
1	G	129	VAL	2.2
1	C	97	GLU	2.2
1	F	53	PRO	2.2
1	G	120	ALA	2.2
1	B	61	THR	2.2
1	E	355	ILE	2.2
1	G	130	ARG	2.2
1	B	71	ASP	2.1
1	B	107	ALA	2.1
1	E	89	ARG	2.1
1	D	95	ILE	2.1
1	H	32	VAL	2.1
1	F	100	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	98	LEU	2.1
1	C	129	VAL	2.1
1	H	355	ILE	2.1
1	E	75	LEU	2.1
1	F	118	LEU	2.1
1	E	246	ARG	2.1
1	F	90	ALA	2.1
1	B	124	HIS	2.1
1	G	71	ASP	2.1
1	G	85	PHE	2.1
1	B	112	GLY	2.1
1	H	73	ALA	2.0
1	D	124	HIS	2.0
1	E	124	HIS	2.0
1	H	106	ILE	2.0
1	F	363	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

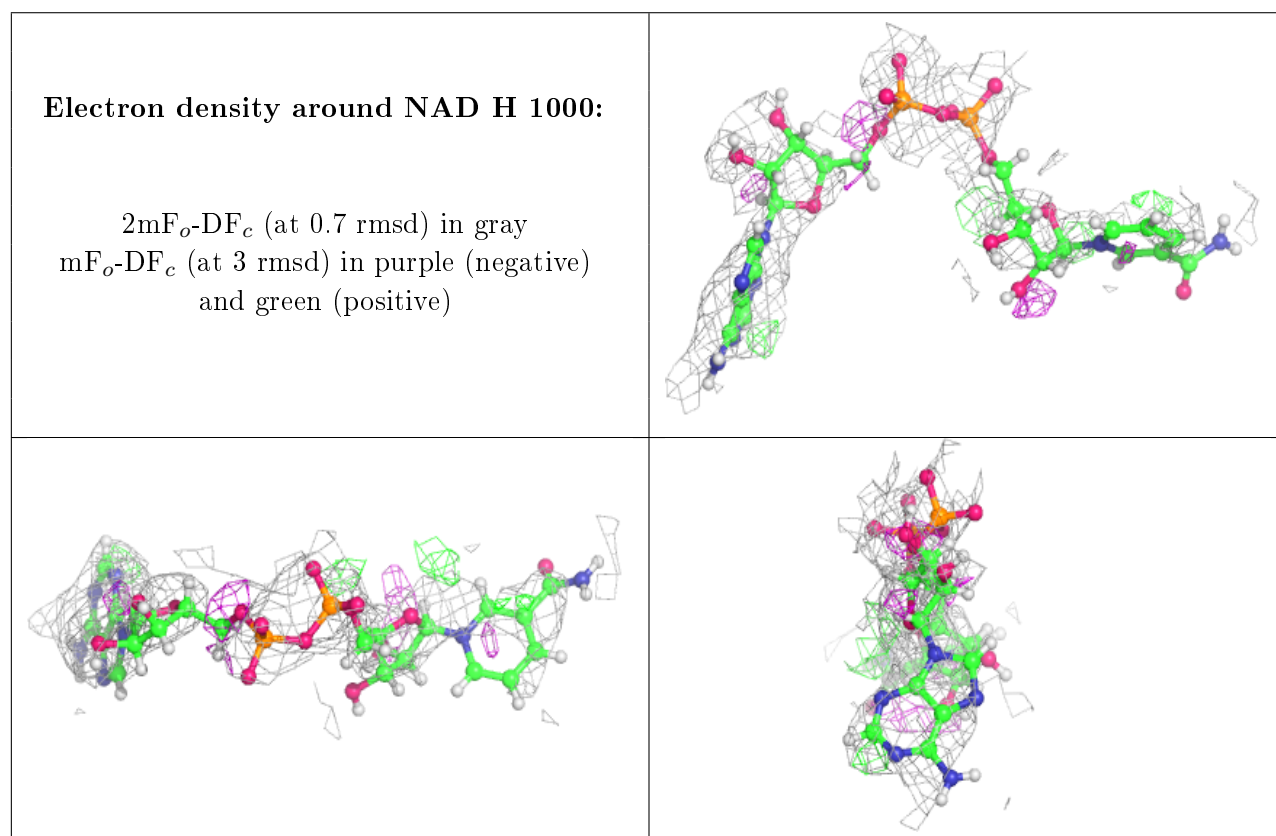
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAD	H	1000	44/44	0.63	0.42	161,163,197,199	0
2	NAD	B	1000	44/44	0.70	0.41	169,174,209,214	0
2	NAD	F	1000	44/44	0.73	0.43	172,177,213,216	0
2	NAD	E	1000	44/44	0.75	0.35	153,176,211,218	0
2	NAD	D	1000	44/44	0.75	0.38	156,163,195,204	0
2	NAD	C	1000	44/44	0.76	0.52	205,211,254,256	0
2	NAD	A	1000	44/44	0.77	0.36	157,163,196,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	G	1000	44/44	0.86	0.28	112,128,155,161	0

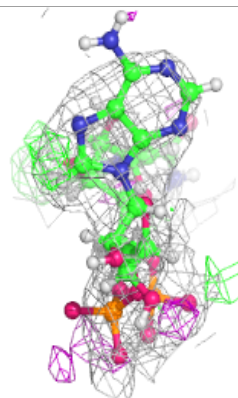
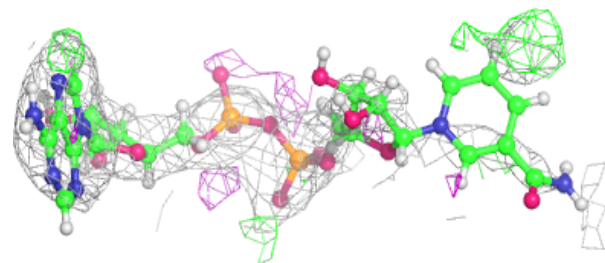
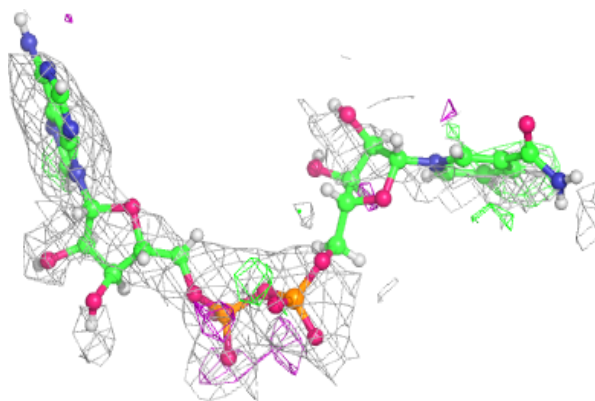
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



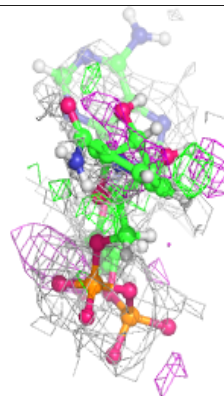
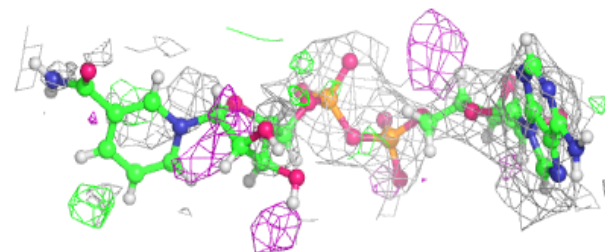
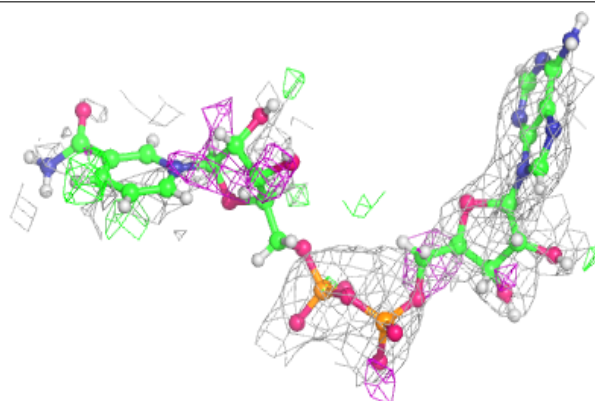


**Electron density around NAD B 1000:**

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

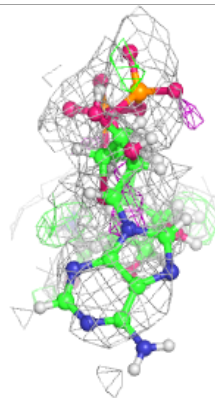
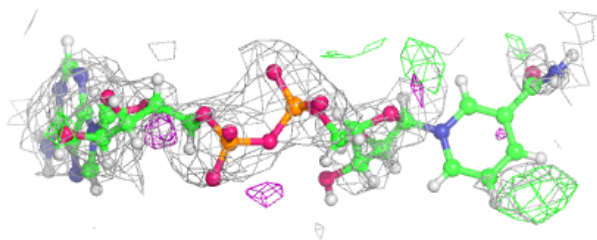
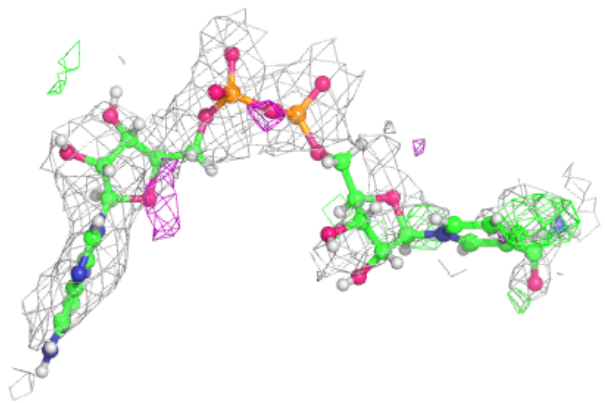
**Electron density around NAD F 1000:**

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

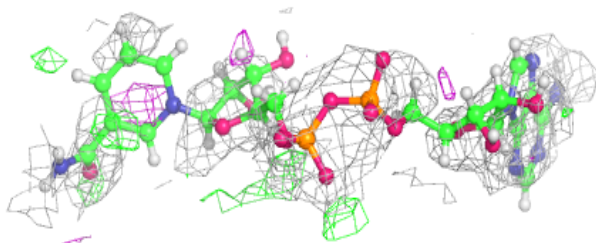
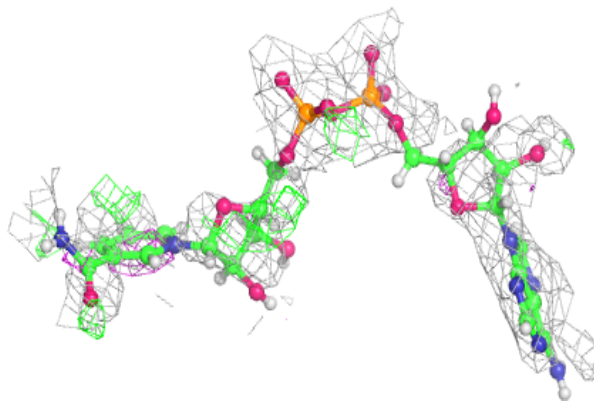


**Electron density around NAD E 1000:**

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

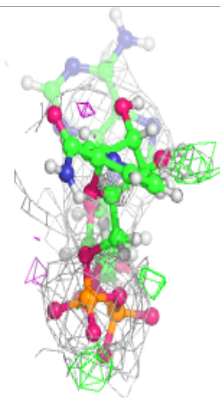
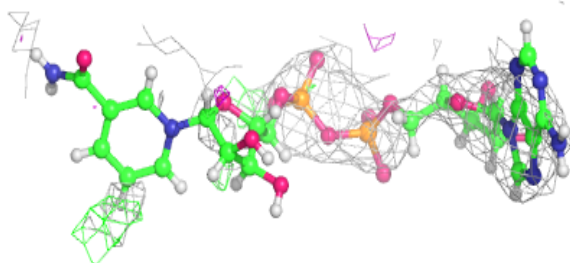
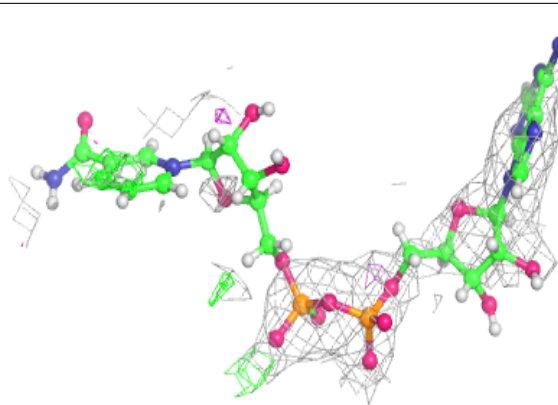
**Electron density around NAD D 1000:**

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

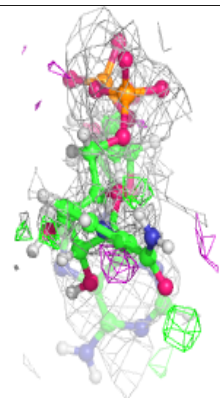
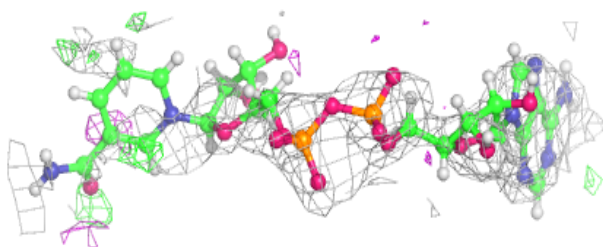
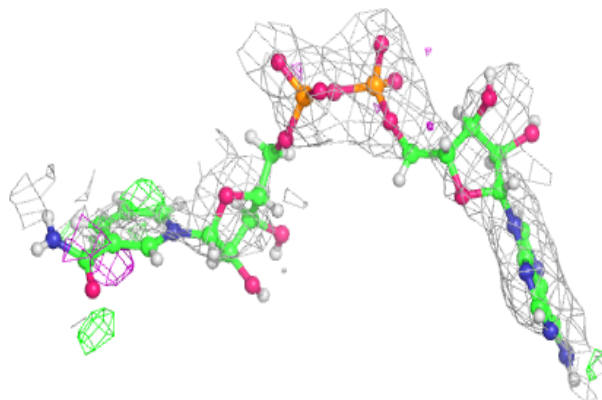


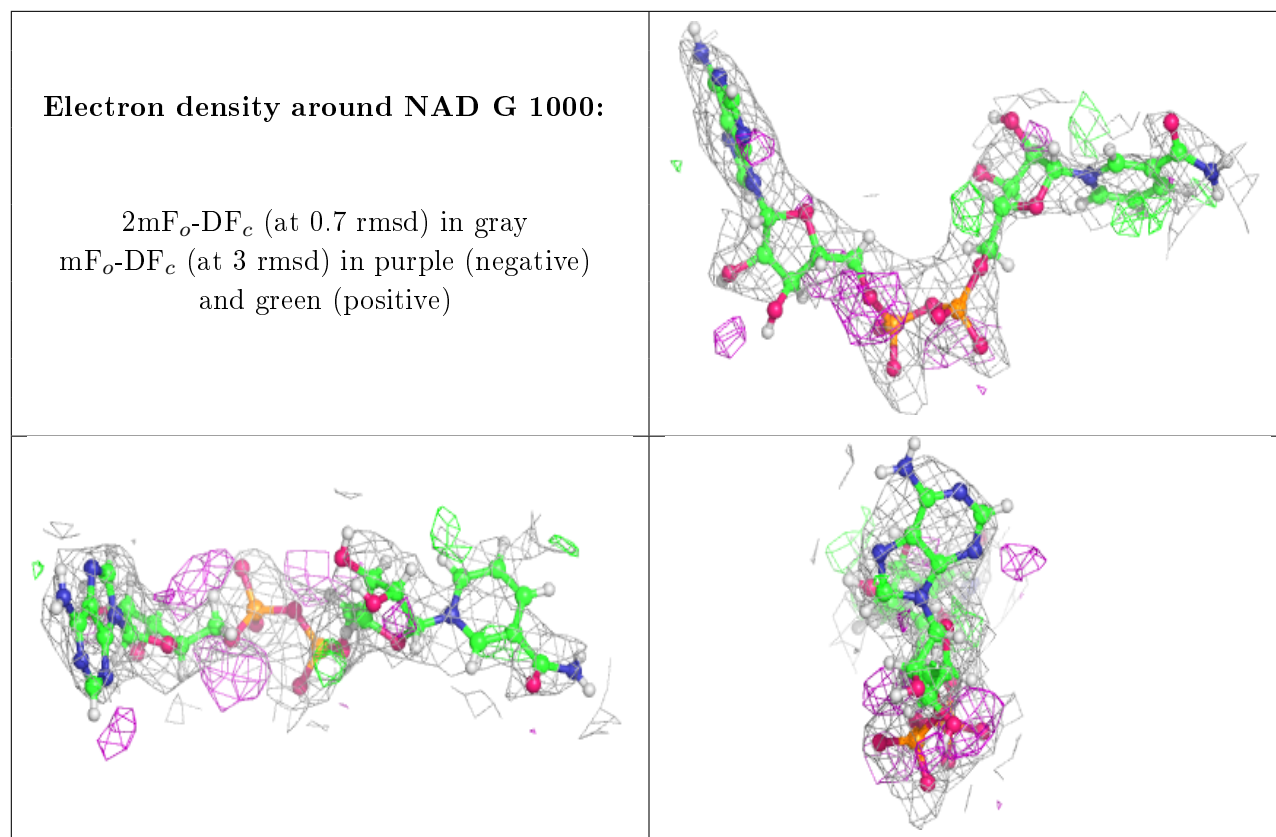
**Electron density around NAD C 1000:**

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

**Electron density around NAD A 1000:**

$2mF_o-DF_c$  (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.