



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:00 pm BST

PDB ID : 4GO4  
Title : Crystal structure of PnpE in complex with Nicotinamide adenine dinucleotide  
Authors : Su, J.; Zhang, C.; Liu, S.; Zhu, D.; Gu, L.  
Deposited on : 2012-08-18  
Resolution : 3.10 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

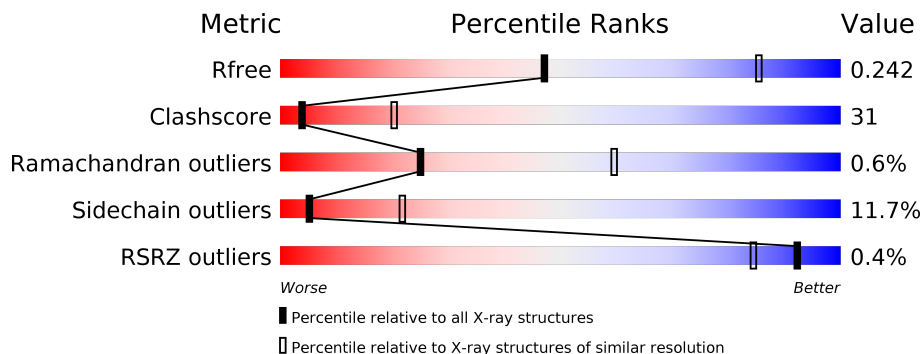
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	495	
1	B	495	
1	C	495	
1	D	495	
1	E	495	
1	F	495	

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Mol	Chain	Length	Quality of chain
1	G	495	 55% 37% 6%
1	H	495	 55% 37% 6%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30071 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 Putative gamma-hydroxymuconic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3698	2341	657	684	16	0	1	0
1	B	487	3698	2341	657	684	16	0	1	0
1	C	487	3698	2341	657	684	16	0	1	0
1	D	487	3698	2341	657	684	16	0	1	0
1	E	487	3698	2341	657	684	16	0	1	0
1	F	487	3698	2341	657	684	16	0	1	0
1	G	487	3698	2341	657	684	16	0	1	0
1	H	487	3698	2341	657	684	16	0	1	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
A	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
A	488	LEU	-	EXPRESSION TAG	UNP C1I208
A	489	GLY	-	EXPRESSION TAG	UNP C1I208
A	490	HIS	-	EXPRESSION TAG	UNP C1I208
A	491	HIS	-	EXPRESSION TAG	UNP C1I208
A	492	HIS	-	EXPRESSION TAG	UNP C1I208
A	493	HIS	-	EXPRESSION TAG	UNP C1I208
A	494	HIS	-	EXPRESSION TAG	UNP C1I208
A	495	HIS	-	EXPRESSION TAG	UNP C1I208
B	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
B	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
B	488	LEU	-	EXPRESSION TAG	UNP C1I208

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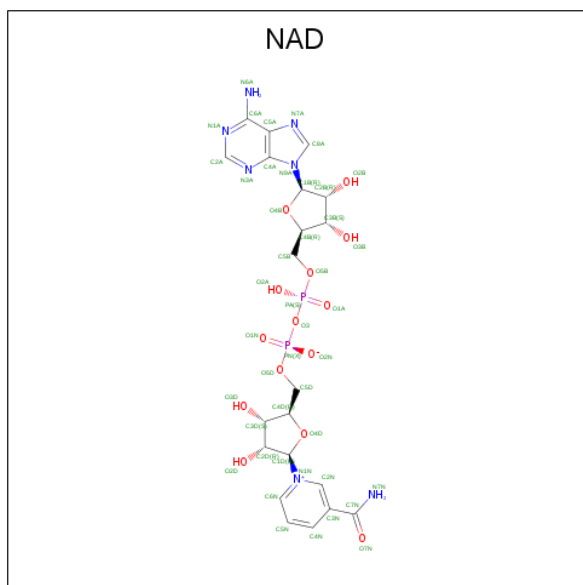
Chain	Residue	Modelled	Actual	Comment	Reference
B	489	GLY	-	EXPRESSION TAG	UNP C1I208
B	490	HIS	-	EXPRESSION TAG	UNP C1I208
B	491	HIS	-	EXPRESSION TAG	UNP C1I208
B	492	HIS	-	EXPRESSION TAG	UNP C1I208
B	493	HIS	-	EXPRESSION TAG	UNP C1I208
B	494	HIS	-	EXPRESSION TAG	UNP C1I208
B	495	HIS	-	EXPRESSION TAG	UNP C1I208
C	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
C	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
C	488	LEU	-	EXPRESSION TAG	UNP C1I208
C	489	GLY	-	EXPRESSION TAG	UNP C1I208
C	490	HIS	-	EXPRESSION TAG	UNP C1I208
C	491	HIS	-	EXPRESSION TAG	UNP C1I208
C	492	HIS	-	EXPRESSION TAG	UNP C1I208
C	493	HIS	-	EXPRESSION TAG	UNP C1I208
C	494	HIS	-	EXPRESSION TAG	UNP C1I208
C	495	HIS	-	EXPRESSION TAG	UNP C1I208
D	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
D	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
D	488	LEU	-	EXPRESSION TAG	UNP C1I208
D	489	GLY	-	EXPRESSION TAG	UNP C1I208
D	490	HIS	-	EXPRESSION TAG	UNP C1I208
D	491	HIS	-	EXPRESSION TAG	UNP C1I208
D	492	HIS	-	EXPRESSION TAG	UNP C1I208
D	493	HIS	-	EXPRESSION TAG	UNP C1I208
D	494	HIS	-	EXPRESSION TAG	UNP C1I208
D	495	HIS	-	EXPRESSION TAG	UNP C1I208
E	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
E	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
E	488	LEU	-	EXPRESSION TAG	UNP C1I208
E	489	GLY	-	EXPRESSION TAG	UNP C1I208
E	490	HIS	-	EXPRESSION TAG	UNP C1I208
E	491	HIS	-	EXPRESSION TAG	UNP C1I208
E	492	HIS	-	EXPRESSION TAG	UNP C1I208
E	493	HIS	-	EXPRESSION TAG	UNP C1I208
E	494	HIS	-	EXPRESSION TAG	UNP C1I208
E	495	HIS	-	EXPRESSION TAG	UNP C1I208
F	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
F	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
F	488	LEU	-	EXPRESSION TAG	UNP C1I208
F	489	GLY	-	EXPRESSION TAG	UNP C1I208
F	490	HIS	-	EXPRESSION TAG	UNP C1I208

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Chain	Residue	Modelled	Actual	Comment	Reference
F	491	HIS	-	EXPRESSION TAG	UNP C1I208
F	492	HIS	-	EXPRESSION TAG	UNP C1I208
F	493	HIS	-	EXPRESSION TAG	UNP C1I208
F	494	HIS	-	EXPRESSION TAG	UNP C1I208
F	495	HIS	-	EXPRESSION TAG	UNP C1I208
G	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
G	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
G	488	LEU	-	EXPRESSION TAG	UNP C1I208
G	489	GLY	-	EXPRESSION TAG	UNP C1I208
G	490	HIS	-	EXPRESSION TAG	UNP C1I208
G	491	HIS	-	EXPRESSION TAG	UNP C1I208
G	492	HIS	-	EXPRESSION TAG	UNP C1I208
G	493	HIS	-	EXPRESSION TAG	UNP C1I208
G	494	HIS	-	EXPRESSION TAG	UNP C1I208
G	495	HIS	-	EXPRESSION TAG	UNP C1I208
H	426	HIS	SER	ENGINEERED MUTATION	UNP C1I208
H	484	HIS	TYR	ENGINEERED MUTATION	UNP C1I208
H	488	LEU	-	EXPRESSION TAG	UNP C1I208
H	489	GLY	-	EXPRESSION TAG	UNP C1I208
H	490	HIS	-	EXPRESSION TAG	UNP C1I208
H	491	HIS	-	EXPRESSION TAG	UNP C1I208
H	492	HIS	-	EXPRESSION TAG	UNP C1I208
H	493	HIS	-	EXPRESSION TAG	UNP C1I208
H	494	HIS	-	EXPRESSION TAG	UNP C1I208
H	495	HIS	-	EXPRESSION TAG	UNP C1I208

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	20	Total	O	0	0
			20	20		
3	C	20	Total	O	0	0
			20	20		
3	D	15	Total	O	0	0
			15	15		

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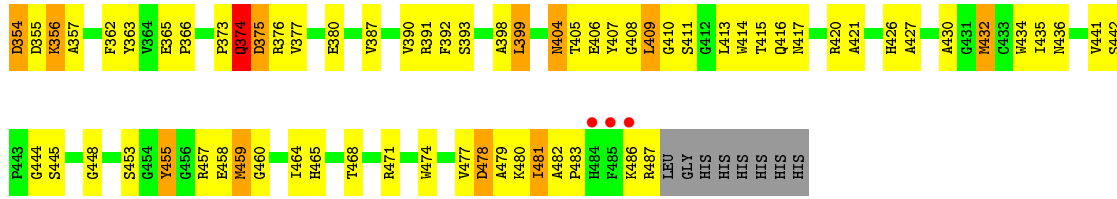
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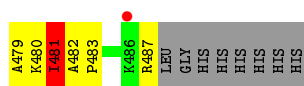
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	E	26	Total 26	O 26	0	0
3	F	12	Total 12	O 12	0	0
3	G	13	Total 13	O 13	0	0
3	H	15	Total 15	O 15	0	0





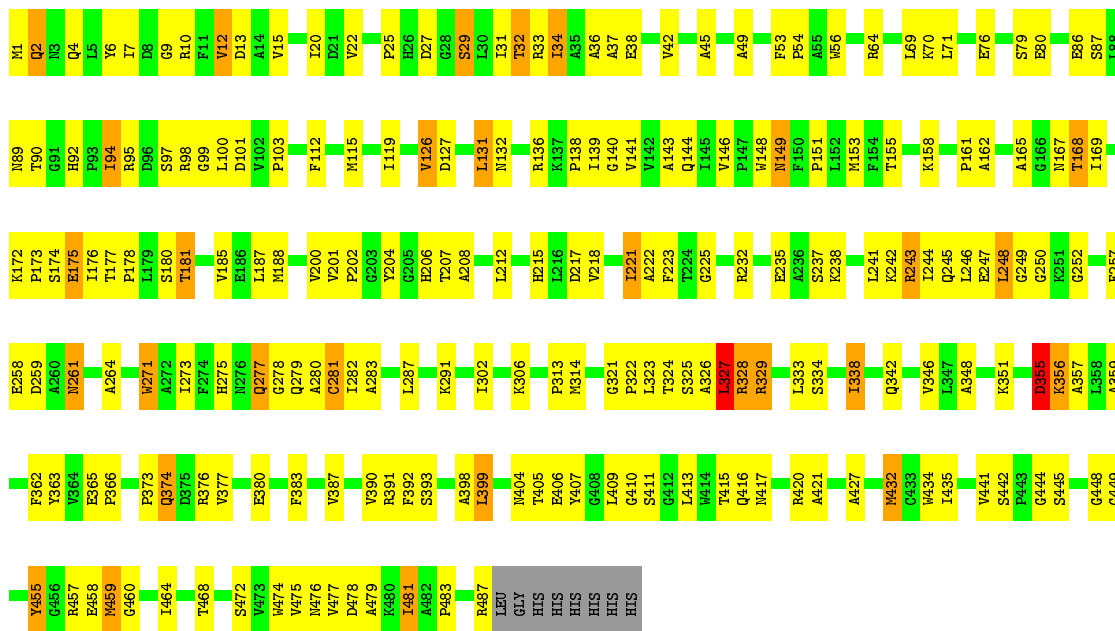






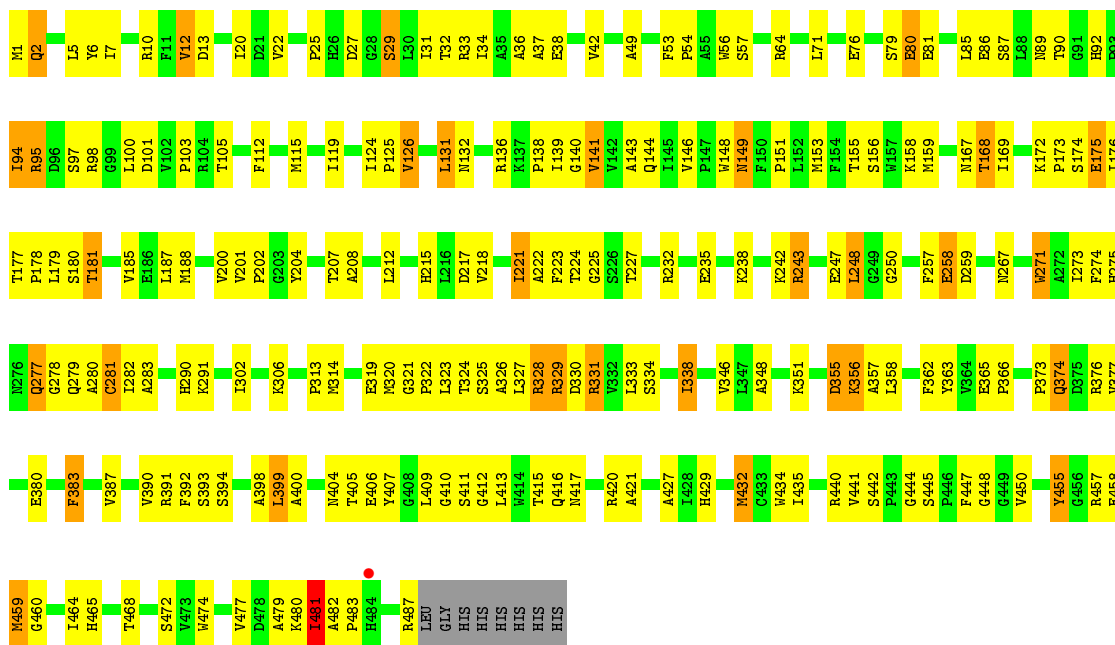
● Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain G: 55% 37% 6%



● Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain H: 55% 37% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.91Å 154.54Å 143.44Å 90.00° 95.24° 90.00°	Depositor
Resolution (Å)	37.24 – 3.10 48.46 – 3.10	Depositor EDS
% Data completeness (in resolution range)	88.6 (37.24-3.10) 92.1 (48.46-3.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.207 , 0.251 0.201 , 0.242	Depositor DCC
$R_{free}$ test set	1825 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.6	Xtrriage
Anisotropy	0.266	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	30071	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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:  
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	0.47	0/3775	0.71	10/5119 (0.2%)
1	B	0.46	0/3775	0.60	2/5119 (0.0%)
1	C	0.46	0/3775	0.63	2/5119 (0.0%)
1	D	0.54	0/3775	0.67	6/5119 (0.1%)
1	E	0.49	0/3775	0.64	4/5119 (0.1%)
1	F	0.46	0/3775	0.63	2/5119 (0.0%)
1	G	0.47	0/3775	0.61	2/5119 (0.0%)
1	H	0.45	0/3775	0.62	3/5119 (0.1%)
All	All	0.48	0/30200	0.64	31/40952 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ASP	CB-CA-C	-10.77	88.85	110.40
1	F	459	MET	CB-CA-C	-9.81	90.79	110.40
1	D	478	ASP	CB-CA-C	-9.65	91.11	110.40
1	D	479	ALA	N-CA-CB	-9.28	97.11	110.10
1	A	330	ASP	N-CA-C	9.12	135.62	111.00
1	C	459	MET	CB-CA-C	-8.94	92.53	110.40
1	E	459	MET	CB-CA-C	-8.12	94.17	110.40
1	A	283	ALA	N-CA-C	-7.78	90.00	111.00
1	A	282	ILE	N-CA-C	-7.56	90.58	111.00
1	A	282	ILE	CB-CA-C	-7.48	96.65	111.60
1	A	283	ALA	N-CA-CB	7.37	120.42	110.10
1	D	248	LEU	CA-CB-CG	-7.15	98.86	115.30
1	D	374	GLN	CB-CA-C	-7.12	96.15	110.40
1	G	411	SER	N-CA-CB	-6.96	100.06	110.50
1	H	459	MET	CB-CA-C	-6.69	97.02	110.40
1	A	459	MET	CB-CA-C	-6.58	97.24	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	LEU	N-CA-C	6.51	128.57	111.00
1	C	459	MET	N-CA-C	6.31	128.05	111.00
1	F	459	MET	N-CA-C	6.23	127.81	111.00
1	B	407	TYR	CB-CA-C	-6.15	98.10	110.40
1	G	248	LEU	CA-CB-CG	-6.15	101.16	115.30
1	H	248	LEU	N-CA-C	-5.97	94.87	111.00
1	E	459	MET	N-CA-C	5.90	126.92	111.00
1	A	248	LEU	CA-CB-CG	-5.86	101.82	115.30
1	A	459	MET	N-CA-C	5.70	126.40	111.00
1	E	374	GLN	CB-CA-C	-5.58	99.23	110.40
1	D	409	LEU	N-CA-C	5.47	125.76	111.00
1	B	411	SER	N-CA-CB	-5.43	102.35	110.50
1	E	248	LEU	CA-CB-CG	-5.38	102.92	115.30
1	D	375	ASP	N-CA-C	-5.28	96.73	111.00
1	H	459	MET	N-CA-C	5.26	125.21	111.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3698	0	3691	257	0
1	B	3698	0	3691	246	0
1	C	3698	0	3690	248	0
1	D	3698	0	3691	262	0
1	E	3698	0	3691	235	0
1	F	3698	0	3691	239	0
1	G	3698	0	3691	249	0
1	H	3698	0	3691	238	0
2	A	44	0	26	11	0
2	B	44	0	26	7	0
2	C	44	0	26	14	0
2	D	44	0	25	8	0
2	E	44	0	26	7	0
2	F	44	0	26	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	44	0	26	7	0
2	H	44	0	26	7	0
3	A	14	0	0	4	0
3	B	20	0	0	2	0
3	C	20	0	0	4	0
3	D	15	0	0	3	0
3	E	26	0	0	4	0
3	F	12	0	0	1	0
3	G	13	0	0	5	0
3	H	15	0	0	6	0
All	All	30071	0	29734	1824	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 31.

All (1824) 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:G:247:GLU:C	1:G:248:LEU:HD23	1.41	1.41
1:B:281:CYS:SG	1:B:409:LEU:HD21	1.61	1.39
1:F:325:SER:OG	1:F:328:ARG:CG	1.71	1.38
1:B:281:CYS:SG	1:B:409:LEU:CD2	2.14	1.35
1:G:325:SER:HB3	1:G:328:ARG:CZ	1.64	1.27
1:G:325:SER:HB3	1:G:328:ARG:NH2	1.49	1.26
1:G:245:GLN:O	1:G:246:LEU:HD23	1.31	1.24
1:E:328:ARG:NH1	1:E:331:ARG:HD2	1.51	1.23
1:D:247:GLU:C	1:D:248:LEU:HD23	1.58	1.23
1:A:481:ILE:CD1	1:A:481:ILE:H	1.51	1.22
1:A:481:ILE:N	1:A:481:ILE:HD12	1.56	1.17
1:E:328:ARG:NH1	1:E:331:ARG:HH11	1.43	1.17
1:B:248:LEU:N	1:B:248:LEU:HD23	1.52	1.16
1:F:444:GLY:N	1:F:459:MET:O	1.78	1.15
1:D:247:GLU:O	1:D:248:LEU:HD23	1.44	1.14
1:A:415:THR:HG22	1:A:417:ASN:H	1.13	1.14
1:B:245:GLN:C	1:B:246:LEU:HD23	1.66	1.14
1:B:2:GLN:HA	1:B:2:GLN:HE21	1.06	1.13
1:A:444:GLY:N	1:A:459:MET:O	1.81	1.13
1:A:248:LEU:HD23	1:A:248:LEU:N	1.61	1.13
1:E:444:GLY:N	1:E:459:MET:O	1.82	1.12
1:D:374:GLN:O	1:D:374:GLN:HG2	1.48	1.12
1:C:415:THR:HG22	1:C:417:ASN:H	1.15	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:415:THR:HG22	1:F:417:ASN:H	1.09	1.11
1:C:444:GLY:N	1:C:459:MET:O	1.83	1.11
1:G:247:GLU:O	1:G:248:LEU:HD23	1.47	1.11
1:H:95:ARG:HH21	1:H:319:GLU:HG2	1.07	1.10
1:D:415:THR:HG22	1:D:417:ASN:H	1.13	1.10
1:F:325:SER:OG	1:F:328:ARG:CD	1.99	1.10
1:H:415:THR:HG22	1:H:417:ASN:H	1.14	1.10
1:H:444:GLY:N	1:H:459:MET:O	1.82	1.09
1:D:374:GLN:CG	1:D:374:GLN:O	1.99	1.09
1:F:325:SER:OG	1:F:328:ARG:HG2	1.32	1.09
1:E:415:THR:HG22	1:E:417:ASN:H	1.11	1.09
1:F:376:ARG:CZ	1:G:206:HIS:NE2	2.15	1.09
1:C:94:ILE:HD11	1:C:314:MET:O	1.52	1.09
1:G:329:ARG:HH11	1:G:329:ARG:HG2	1.16	1.08
1:E:329:ARG:HH11	1:E:329:ARG:HG2	1.15	1.08
1:G:415:THR:HG22	1:G:417:ASN:H	1.11	1.08
1:D:356:LYS:HD3	1:D:356:LYS:H	1.19	1.07
1:E:356:LYS:H	1:E:356:LYS:HD3	1.17	1.07
1:B:329:ARG:HG2	1:B:329:ARG:NH1	1.52	1.07
1:B:415:THR:HG22	1:B:417:ASN:H	1.15	1.06
3:C:708:HOH:O	1:D:471:ARG:HD3	1.54	1.05
1:A:282:ILE:HD11	1:A:447:PHE:CE1	1.91	1.05
1:H:328:ARG:HH11	1:H:328:ARG:CG	1.70	1.05
1:C:94:ILE:HD11	1:C:314:MET:C	1.76	1.05
1:E:328:ARG:HH21	1:E:383:PHE:CB	1.68	1.04
1:G:325:SER:HB3	1:G:328:ARG:NH1	1.69	1.04
1:B:405:THR:HG22	1:B:407:TYR:H	1.19	1.04
1:D:329:ARG:HG2	1:D:329:ARG:HH11	1.18	1.04
1:F:329:ARG:HH11	1:F:329:ARG:HG2	0.88	1.04
1:F:329:ARG:NH1	1:F:329:ARG:HG2	1.63	1.04
1:B:329:ARG:CG	1:B:329:ARG:HH11	1.68	1.04
1:C:329:ARG:HG2	1:C:329:ARG:HH11	1.22	1.02
1:D:356:LYS:HE2	1:D:357:ALA:H	1.18	1.02
1:E:356:LYS:HE2	1:E:357:ALA:H	1.25	1.01
1:H:247:GLU:OE1	2:H:601:NAD:N7N	1.94	1.01
1:H:328:ARG:HG2	1:H:328:ARG:HH11	0.85	1.01
1:A:329:ARG:HH11	1:A:329:ARG:CG	1.73	1.01
1:H:328:ARG:HG2	1:H:328:ARG:NH1	1.67	1.01
1:A:329:ARG:HG2	1:A:329:ARG:HH11	0.85	1.00
1:C:325:SER:OG	1:C:328:ARG:CG	2.09	1.00
1:H:356:LYS:HE2	1:H:357:ALA:H	1.25	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:325:SER:OG	1:H:328:ARG:HG3	1.62	1.00
1:G:261:ASN:HD22	1:G:261:ASN:C	1.64	0.99
1:H:328:ARG:HH21	1:H:383:PHE:HB3	1.22	0.99
1:C:356:LYS:HE2	1:C:357:ALA:H	1.27	0.99
1:C:10[B]:ARG:HH11	1:C:10[B]:ARG:HG3	1.28	0.99
1:F:405:THR:HG22	1:F:407:TYR:H	1.27	0.99
1:G:356:LYS:HE2	1:G:357:ALA:H	1.26	0.99
1:C:356:LYS:H	1:C:356:LYS:HD3	1.23	0.98
1:D:356:LYS:H	1:D:356:LYS:CD	1.72	0.98
1:C:327:LEU:HD21	1:C:331:ARG:NH2	1.77	0.98
1:A:329:ARG:HG2	1:A:329:ARG:NH1	1.57	0.97
1:H:7:ILE:HG13	3:H:714:HOH:O	1.64	0.97
1:A:10[B]:ARG:HG3	1:A:10[B]:ARG:HH11	1.30	0.97
1:A:356:LYS:HE2	1:A:357:ALA:H	1.28	0.97
1:C:325:SER:OG	1:C:328:ARG:HG3	1.63	0.97
1:F:249:GLY:HA2	2:F:601:NAD:O2D	1.60	0.97
1:F:261:ASN:C	1:F:261:ASN:HD22	1.64	0.97
1:D:405:THR:HG22	1:D:407:TYR:H	1.28	0.96
1:G:405:THR:HG22	1:G:407:TYR:H	1.29	0.96
1:F:356:LYS:HE2	1:F:357:ALA:H	1.27	0.96
1:C:281:CYS:SG	2:C:601:NAD:C4N	2.53	0.96
1:E:405:THR:HG22	1:E:407:TYR:H	1.29	0.96
1:G:247:GLU:C	1:G:248:LEU:CD2	2.34	0.96
1:H:405:THR:HG22	1:H:407:TYR:H	1.29	0.96
1:B:90:THR:O	1:B:324:THR:HG22	1.65	0.96
1:F:325:SER:HG	1:F:328:ARG:HG2	1.31	0.96
1:G:10[B]:ARG:HH11	1:G:10[B]:ARG:HG3	1.31	0.96
1:H:329:ARG:CB	1:H:329:ARG:HH11	1.78	0.95
1:A:94:ILE:HD11	1:A:314:MET:C	1.87	0.95
1:F:10[B]:ARG:HH11	1:F:10[B]:ARG:HG3	1.32	0.95
1:F:329:ARG:HH11	1:F:329:ARG:CG	1.79	0.95
1:D:223:PHE:HZ	1:D:229:THR:HG21	1.31	0.95
1:E:328:ARG:HH12	1:E:331:ARG:HH11	1.06	0.94
1:A:90:THR:O	1:A:324:THR:HG22	1.68	0.94
1:C:405:THR:HG22	1:C:407:TYR:H	1.31	0.94
1:D:10[B]:ARG:HH11	1:D:10[B]:ARG:HG3	1.32	0.94
1:C:90:THR:O	1:C:324:THR:HG22	1.68	0.94
1:A:405:THR:HG22	1:A:407:TYR:H	1.30	0.93
1:H:10[B]:ARG:HH11	1:H:10[B]:ARG:HG3	1.32	0.93
1:D:223:PHE:CZ	1:D:229:THR:HG23	2.03	0.93
1:E:356:LYS:CD	1:E:356:LYS:H	1.74	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10[B]:ARG:HG3	1:E:10[B]:ARG:HH11	1.33	0.93
1:H:329:ARG:HH11	1:H:329:ARG:HB3	1.34	0.93
1:D:223:PHE:CZ	1:D:229:THR:CG2	2.52	0.93
1:B:94:ILE:HD11	1:B:314:MET:O	1.69	0.93
1:G:325:SER:CB	1:G:328:ARG:NH1	2.33	0.92
1:B:248:LEU:N	1:B:248:LEU:CD2	2.32	0.92
1:A:94:ILE:HD11	1:A:314:MET:O	1.67	0.92
1:B:244:ILE:CG2	1:B:246:LEU:HD21	1.99	0.91
1:E:328:ARG:HH21	1:E:383:PHE:HB2	1.35	0.91
1:B:10[B]:ARG:HG3	1:B:10[B]:ARG:HH11	1.35	0.91
1:E:328:ARG:HH12	1:E:331:ARG:CD	1.81	0.91
1:G:325:SER:CB	1:G:328:ARG:NH2	2.34	0.91
1:H:328:ARG:NH2	1:H:383:PHE:HB3	1.84	0.91
1:C:281:CYS:SG	2:C:601:NAD:C5N	2.59	0.91
1:G:281:CYS:SG	1:G:409:LEU:CD2	2.59	0.91
1:F:249:GLY:CA	2:F:601:NAD:O2D	2.19	0.91
1:G:139:ILE:H	1:G:167:ASN:HD21	1.19	0.91
1:G:90:THR:O	1:G:324:THR:HG22	1.71	0.91
1:G:325:SER:HB3	1:G:328:ARG:HH22	1.26	0.91
1:A:356:LYS:H	1:A:356:LYS:HD3	1.30	0.90
1:B:244:ILE:HG22	1:B:246:LEU:HD21	1.53	0.90
1:D:223:PHE:HZ	1:D:229:THR:CG2	1.82	0.90
1:A:4:GLN:HG3	3:A:703:HOH:O	1.69	0.90
1:D:90:THR:O	1:D:324:THR:HG22	1.71	0.90
1:G:325:SER:CB	1:G:328:ARG:HH12	1.83	0.90
1:C:356:LYS:CD	1:C:356:LYS:H	1.82	0.90
1:G:356:LYS:HD3	1:G:356:LYS:H	1.34	0.90
1:H:90:THR:O	1:H:324:THR:HG22	1.70	0.90
1:G:248:LEU:N	1:G:248:LEU:HD23	1.72	0.90
1:F:356:LYS:H	1:F:356:LYS:HD3	1.36	0.90
1:G:325:SER:CB	1:G:328:ARG:HH22	1.85	0.90
1:B:2:GLN:HA	1:B:2:GLN:NE2	1.87	0.89
1:H:356:LYS:H	1:H:356:LYS:HD3	1.36	0.89
1:B:148:TRP:HD1	1:B:174:SER:HG	1.19	0.89
1:E:139:ILE:H	1:E:167:ASN:HD21	1.19	0.89
1:E:328:ARG:HH21	1:E:383:PHE:HB3	1.38	0.89
1:E:328:ARG:HH12	1:E:331:ARG:HD2	1.15	0.88
1:D:247:GLU:C	1:D:248:LEU:CD2	2.42	0.88
1:E:90:THR:O	1:E:324:THR:HG22	1.73	0.87
1:H:139:ILE:H	1:H:167:ASN:HD21	1.22	0.87
1:A:408:GLY:O	1:A:430:ALA:HA	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:THR:O	1:F:324:THR:HG22	1.73	0.87
1:D:380:GLU:CD	1:E:376:ARG:HH12	1.76	0.87
1:A:122:SER:HA	1:C:122:SER:HA	1.57	0.86
1:G:328:ARG:HB2	1:G:328:ARG:CZ	2.04	0.86
1:H:329:ARG:CG	1:H:329:ARG:HH11	1.89	0.86
1:D:139:ILE:H	1:D:167:ASN:HD21	1.21	0.86
1:A:356:LYS:H	1:A:356:LYS:CD	1.85	0.85
1:A:281:CYS:SG	2:A:601:NAD:C4N	2.64	0.85
1:C:139:ILE:H	1:C:167:ASN:HD21	1.25	0.85
1:B:245:GLN:O	1:B:246:LEU:HD23	1.77	0.85
1:B:405:THR:HG22	1:B:407:TYR:N	1.91	0.84
1:C:374:GLN:HG2	1:C:374:GLN:O	1.74	0.84
1:E:273:ILE:HG12	1:E:387:VAL:HG22	1.60	0.84
1:F:356:LYS:H	1:F:356:LYS:CD	1.90	0.84
1:C:248:LEU:CD1	1:D:241:LEU:HD13	2.07	0.84
1:D:376:ARG:HH12	1:E:380:GLU:CD	1.81	0.84
1:F:139:ILE:H	1:F:167:ASN:HD21	1.21	0.84
1:D:273:ILE:HG12	1:D:387:VAL:HG22	1.59	0.84
1:F:273:ILE:HG12	1:F:387:VAL:HG22	1.60	0.84
1:B:227:THR:HA	1:B:248:LEU:HD13	1.60	0.84
1:E:248:LEU:N	1:E:248:LEU:HD23	1.92	0.83
1:G:356:LYS:CD	1:G:356:LYS:H	1.89	0.83
1:A:481:ILE:HD12	1:A:481:ILE:H	0.71	0.83
1:H:49:ALA:HB1	1:H:168:THR:HG23	1.59	0.83
1:B:246:LEU:N	1:B:246:LEU:HD23	1.89	0.83
1:C:374:GLN:CG	1:C:374:GLN:O	2.22	0.83
1:D:299:GLU:OE1	1:H:400:ALA:HB1	1.79	0.83
1:B:329:ARG:HG2	1:B:329:ARG:HH11	0.75	0.82
1:E:139:ILE:H	1:E:167:ASN:ND2	1.77	0.82
1:B:49:ALA:HB1	1:B:168:THR:HG23	1.60	0.82
1:B:244:ILE:HG22	1:B:246:LEU:CD2	2.10	0.82
1:E:328:ARG:NH1	1:E:331:ARG:NH1	2.26	0.81
1:F:415:THR:HG22	1:F:417:ASN:N	1.94	0.81
1:B:248:LEU:H	1:B:248:LEU:HD23	1.45	0.81
1:B:281:CYS:SG	1:B:409:LEU:HD22	2.19	0.81
1:F:149:ASN:HD21	2:F:601:NAD:H6N	1.45	0.81
1:C:476:ASN:OD1	1:C:479:ALA:HB3	1.81	0.81
1:C:249:GLY:HA3	2:C:601:NAD:O2D	1.79	0.81
1:A:484:HIS:O	1:B:95:ARG:NH2	2.14	0.80
1:A:458:GLU:O	1:A:459:MET:HB2	1.81	0.80
1:A:49:ALA:HB1	1:A:168:THR:HG23	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:ARG:NH2	1:H:319:GLU:HG2	1.92	0.80
1:F:49:ALA:HB1	1:F:168:THR:HG23	1.64	0.80
1:H:356:LYS:CD	1:H:356:LYS:H	1.92	0.80
1:F:325:SER:OG	1:F:328:ARG:HD2	1.80	0.80
1:H:273:ILE:HG12	1:H:387:VAL:HG22	1.64	0.80
1:C:49:ALA:HB1	1:C:168:THR:HG23	1.62	0.80
1:D:329:ARG:CG	1:D:329:ARG:HH11	1.96	0.79
1:D:408:GLY:O	1:D:430:ALA:HA	1.82	0.79
1:B:282:ILE:O	1:B:282:ILE:CG2	2.31	0.79
1:G:329:ARG:CG	1:G:329:ARG:HH11	1.96	0.79
1:A:139:ILE:H	1:A:167:ASN:HD21	1.29	0.78
1:E:329:ARG:HH11	1:E:329:ARG:CG	1.93	0.78
1:D:299:GLU:OE1	1:H:400:ALA:CB	2.31	0.78
1:C:137:LYS:HZ1	1:D:426:HIS:CD2	2.00	0.78
1:C:325:SER:OG	1:C:328:ARG:HG2	1.83	0.78
1:D:481:ILE:HD13	1:D:481:ILE:N	1.97	0.78
1:E:373:PRO:O	1:E:374:GLN:CG	2.32	0.78
1:G:49:ALA:HB1	1:G:168:THR:HG23	1.66	0.78
1:E:458:GLU:O	1:E:459:MET:HB2	1.83	0.78
1:F:376:ARG:NH1	1:G:206:HIS:NE2	2.31	0.78
1:E:328:ARG:HH12	1:E:331:ARG:NH1	1.81	0.78
1:C:458:GLU:O	1:C:459:MET:HB2	1.82	0.77
1:E:49:ALA:HB1	1:E:168:THR:HG23	1.66	0.77
1:D:380:GLU:CD	1:E:376:ARG:NH1	2.37	0.77
1:A:273:ILE:HG12	1:A:387:VAL:HG22	1.67	0.77
1:H:415:THR:HG22	1:H:416:GLN:N	1.99	0.77
1:D:49:ALA:HB1	1:D:168:THR:HG23	1.66	0.77
1:G:261:ASN:C	1:G:261:ASN:ND2	2.37	0.77
1:G:281:CYS:SG	1:G:409:LEU:HD22	2.25	0.77
1:B:374:GLN:CG	1:B:374:GLN:O	2.33	0.77
1:F:261:ASN:C	1:F:261:ASN:ND2	2.38	0.77
1:B:273:ILE:HG12	1:B:387:VAL:HG22	1.65	0.77
1:A:257:PHE:CE1	1:A:420:ARG:HD3	2.18	0.77
1:G:273:ILE:HG12	1:G:387:VAL:HG22	1.65	0.77
1:H:458:GLU:O	1:H:459:MET:HB2	1.83	0.77
1:A:415:THR:HG22	1:A:416:GLN:N	2.00	0.76
1:C:273:ILE:HG12	1:C:387:VAL:HG22	1.66	0.76
1:F:331:ARG:NH2	1:F:335:TYR:CE1	2.53	0.76
1:B:245:GLN:O	1:B:246:LEU:CD2	2.33	0.76
1:G:325:SER:N	1:G:328:ARG:NH2	2.33	0.76
1:A:282:ILE:CD1	1:A:447:PHE:CE1	2.69	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:LYS:HZ1	1:G:10[A]:ARG:HD2	1.50	0.76
1:A:27:ASP:OD1	1:A:29:SER:HB3	1.86	0.76
1:A:415:THR:HG22	1:A:417:ASN:N	1.97	0.76
1:D:376:ARG:NH1	1:E:380:GLU:CD	2.40	0.76
1:A:328:ARG:HH21	1:A:383:PHE:H	1.32	0.75
1:D:247:GLU:O	1:D:248:LEU:CD2	2.31	0.75
1:G:326:ALA:O	1:G:329:ARG:N	2.19	0.75
1:B:94:ILE:HD11	1:B:314:MET:C	2.07	0.75
1:B:2:GLN:CA	1:B:2:GLN:HE21	1.90	0.75
1:F:149:ASN:HD21	2:F:601:NAD:C6N	1.98	0.75
1:F:458:GLU:O	1:F:459:MET:HB2	1.87	0.75
1:A:148:TRP:HD1	1:A:174:SER:HG	1.31	0.75
1:G:476:ASN:OD1	1:G:479:ALA:HB3	1.86	0.75
1:D:458:GLU:O	1:D:459:MET:HB2	1.85	0.75
1:G:329:ARG:HG2	1:G:329:ARG:NH1	1.97	0.75
1:G:458:GLU:O	1:G:459:MET:HB2	1.87	0.74
1:H:148:TRP:CH2	1:H:328:ARG:HD2	2.21	0.74
1:G:405:THR:HG22	1:G:407:TYR:N	2.03	0.74
1:C:329:ARG:CG	1:C:329:ARG:HH11	1.98	0.74
1:B:374:GLN:O	1:B:374:GLN:HG2	1.86	0.74
1:A:245:GLN:O	1:A:246:LEU:HD23	1.87	0.74
1:A:282:ILE:HD11	1:A:447:PHE:HE1	1.51	0.74
1:C:415:THR:HG22	1:C:416:GLN:N	2.03	0.74
1:F:259:ASP:OD1	1:F:415:THR:HG23	1.88	0.74
1:G:325:SER:N	1:G:328:ARG:HH22	1.85	0.74
1:C:415:THR:HG22	1:C:417:ASN:N	1.99	0.74
1:B:458:GLU:O	1:B:459:MET:HB2	1.86	0.74
1:E:328:ARG:NH2	1:E:383:PHE:HB3	2.02	0.74
1:H:149:ASN:HD21	2:H:601:NAD:H5N	1.53	0.74
1:C:27:ASP:OD1	1:C:29:SER:HB3	1.88	0.74
1:A:405:THR:HG22	1:A:407:TYR:N	2.03	0.73
1:E:149:ASN:HD21	2:E:601:NAD:H6N	1.51	0.73
1:F:415:THR:CG2	1:F:417:ASN:H	1.97	0.73
1:D:356:LYS:HG2	1:G:12:VAL:HG21	1.69	0.73
1:H:215:HIS:HD2	1:H:217:ASP:H	1.35	0.73
1:B:415:THR:HG22	1:B:417:ASN:N	1.99	0.73
1:F:27:ASP:OD1	1:F:29:SER:HB3	1.89	0.73
1:F:95:ARG:NH2	1:F:319:GLU:HG2	2.04	0.73
1:H:415:THR:HG22	1:H:417:ASN:N	1.98	0.73
1:C:201:VAL:HG12	1:C:201:VAL:O	1.89	0.73
1:D:405:THR:HG22	1:D:407:TYR:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:SER:CB	1:F:328:ARG:HG2	2.18	0.73
1:H:149:ASN:HD21	2:H:601:NAD:C5N	2.02	0.73
1:A:248:LEU:CD1	1:B:241:LEU:HD13	2.18	0.73
1:F:376:ARG:NH2	1:G:206:HIS:CD2	2.56	0.73
1:C:282:ILE:HD11	1:C:439:LYS:HG2	1.71	0.73
1:D:149:ASN:HD21	2:D:601:NAD:C6N	2.01	0.73
1:E:374:GLN:CG	1:E:374:GLN:O	2.34	0.72
1:A:426:HIS:CD2	1:B:137:LYS:NZ	2.57	0.72
1:G:313:PRO:HB2	1:G:314:MET:HE2	1.71	0.72
1:D:415:THR:HG22	1:D:416:GLN:N	2.03	0.72
1:E:201:VAL:O	1:E:201:VAL:HG12	1.88	0.72
1:E:415:THR:HG22	1:E:417:ASN:N	1.96	0.72
1:D:281:CYS:SG	1:D:409:LEU:HD22	2.30	0.72
1:E:405:THR:HG22	1:E:407:TYR:N	2.05	0.72
1:C:476:ASN:CG	1:C:479:ALA:HB3	2.09	0.72
1:G:415:THR:HG22	1:G:416:GLN:N	2.05	0.72
1:E:328:ARG:NH2	1:E:383:PHE:CB	2.50	0.72
1:F:273:ILE:HB	1:F:284:GLY:O	1.90	0.72
1:G:27:ASP:OD1	1:G:29:SER:HB3	1.90	0.72
1:E:56:TRP:CZ2	1:E:64:ARG:HG2	2.25	0.71
1:H:405:THR:HG22	1:H:407:TYR:N	2.03	0.71
1:D:351:LYS:O	1:D:365:GLU:HG2	1.89	0.71
1:B:201:VAL:O	1:B:201:VAL:HG12	1.90	0.71
1:C:248:LEU:HD11	1:D:241:LEU:HD13	1.71	0.71
1:D:201:VAL:O	1:D:201:VAL:HG12	1.90	0.71
1:B:415:THR:HG22	1:B:416:GLN:N	2.04	0.71
1:C:351:LYS:O	1:C:365:GLU:HG2	1.90	0.71
1:D:149:ASN:HD21	2:D:601:NAD:H6N	1.55	0.71
1:E:27:ASP:OD1	1:E:29:SER:HB3	1.90	0.71
1:G:281:CYS:SG	1:G:409:LEU:HD21	2.29	0.71
1:H:49:ALA:HB1	1:H:168:THR:CG2	2.19	0.71
1:A:185:VAL:HG21	1:A:200:VAL:HG21	1.73	0.71
1:E:250:GLY:HA3	1:E:407:TYR:HB3	1.71	0.71
1:D:149:ASN:HD21	2:D:601:NAD:C5N	2.04	0.71
1:F:325:SER:H	1:F:328:ARG:HG3	1.56	0.71
1:F:328:ARG:O	1:F:331:ARG:HB2	1.90	0.71
1:E:415:THR:HG22	1:E:416:GLN:N	2.06	0.71
1:F:329:ARG:NH1	1:F:329:ARG:CG	2.47	0.71
1:B:1:MET:HG3	1:B:2:GLN:N	2.05	0.71
1:A:351:LYS:O	1:A:365:GLU:HG2	1.91	0.71
1:C:445:SER:HB2	1:D:132:ASN:ND2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:ILE:H	1:H:167:ASN:ND2	1.89	0.70
1:E:281:CYS:HB3	2:E:601:NAD:C5N	2.20	0.70
1:F:415:THR:HG22	1:F:416:GLN:N	2.06	0.70
1:E:328:ARG:NH1	1:E:331:ARG:CD	2.41	0.70
1:G:415:THR:HG22	1:G:417:ASN:N	1.96	0.70
1:B:185:VAL:HG21	1:B:200:VAL:HG21	1.73	0.70
1:C:455:TYR:HB3	1:D:243:ARG:HD2	1.73	0.70
1:D:350:GLY:O	1:D:351:LYS:HG2	1.91	0.70
1:D:356:LYS:HE2	1:D:357:ALA:N	2.00	0.70
1:D:18:GLY:HA2	1:E:33:ARG:HH21	1.56	0.70
1:G:247:GLU:HB3	2:G:601:NAD:N7N	2.07	0.70
1:H:27:ASP:OD1	1:H:29:SER:HB3	1.90	0.70
1:B:415:THR:CG2	1:B:417:ASN:H	2.01	0.70
1:C:137:LYS:NZ	1:D:426:HIS:CD2	2.59	0.70
1:D:139:ILE:H	1:D:167:ASN:ND2	1.88	0.70
1:E:132:ASN:ND2	1:F:445:SER:HB2	2.05	0.70
1:C:200:VAL:HG12	1:C:202:PRO:HD3	1.73	0.70
1:F:49:ALA:HB1	1:F:168:THR:CG2	2.21	0.70
1:E:10[B]:ARG:HG3	1:E:10[B]:ARG:NH1	2.07	0.69
1:G:247:GLU:O	1:G:248:LEU:CD2	2.34	0.69
1:D:27:ASP:OD1	1:D:29:SER:HB3	1.92	0.69
1:B:154:PHE:HZ	2:B:601:NAD:H5N	1.58	0.69
1:A:49:ALA:HB1	1:A:168:THR:CG2	2.22	0.69
1:B:329:ARG:CG	1:B:329:ARG:NH1	2.39	0.69
1:C:238:LYS:HE3	1:E:351:LYS:NZ	2.07	0.69
1:F:141:VAL:HG12	1:F:218:VAL:HA	1.74	0.69
1:D:89:ASN:HD21	1:D:177:THR:HA	1.58	0.69
1:D:248:LEU:HD23	1:D:248:LEU:N	1.82	0.69
1:H:279:GLN:HE22	1:H:324:THR:H	1.40	0.69
1:B:118:LYS:HE3	1:C:111:TYR:CE1	2.27	0.69
1:A:125:PRO:HG3	1:C:119:ILE:O	1.93	0.69
1:C:149:ASN:HD21	2:C:601:NAD:H6N	1.56	0.69
1:D:415:THR:HG22	1:D:417:ASN:N	1.98	0.69
1:D:148:TRP:HD1	1:D:174:SER:HG	1.39	0.69
1:G:215:HIS:HD2	1:G:217:ASP:H	1.40	0.69
1:F:280:ALA:HB3	1:F:283:ALA:HB2	1.74	0.69
1:A:426:HIS:NE2	1:B:137:LYS:HE3	2.08	0.69
1:D:356:LYS:HE3	1:G:12:VAL:HG11	1.74	0.69
1:G:200:VAL:HG12	1:G:202:PRO:HD3	1.75	0.69
1:B:49:ALA:HB1	1:B:168:THR:CG2	2.23	0.68
1:E:373:PRO:O	1:E:374:GLN:HG2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:THR:CG2	1:A:417:ASN:H	2.00	0.68
1:B:351:LYS:O	1:B:365:GLU:HG2	1.93	0.68
1:C:94:ILE:CD1	1:C:314:MET:O	2.36	0.68
1:C:405:THR:HG22	1:C:407:TYR:N	2.06	0.68
1:F:405:THR:HG22	1:F:407:TYR:N	2.03	0.68
1:H:280:ALA:HB3	1:H:283:ALA:HB2	1.76	0.68
1:A:185:VAL:HG21	1:A:200:VAL:CG2	2.23	0.68
1:A:455:TYR:HB3	1:B:243:ARG:HD2	1.75	0.68
1:B:27:ASP:OD1	1:B:29:SER:HB3	1.93	0.68
1:C:313:PRO:HB2	1:C:314:MET:HE2	1.74	0.68
1:D:94:ILE:HD11	1:D:314:MET:O	1.93	0.68
1:H:201:VAL:O	1:H:201:VAL:HG12	1.93	0.68
1:H:329:ARG:NH1	1:H:329:ARG:HB3	2.07	0.68
1:C:49:ALA:HB1	1:C:168:THR:CG2	2.23	0.68
1:C:279:GLN:HE22	1:C:324:THR:H	1.39	0.68
1:E:351:LYS:O	1:E:365:GLU:HG2	1.93	0.68
1:D:56:TRP:CZ2	1:D:64:ARG:HG2	2.29	0.68
1:G:10[B]:ARG:NH1	1:G:10[B]:ARG:HG3	2.05	0.68
1:E:200:VAL:HG12	1:E:202:PRO:HD3	1.74	0.68
1:G:280:ALA:HB3	1:G:283:ALA:HB2	1.75	0.68
1:G:351:LYS:O	1:G:365:GLU:HG2	1.94	0.68
1:A:374:GLN:CG	1:A:374:GLN:O	2.42	0.67
1:D:250:GLY:HA2	1:D:407:TYR:HB3	1.76	0.67
1:F:351:LYS:O	1:F:365:GLU:HG2	1.93	0.67
1:H:415:THR:CG2	1:H:417:ASN:H	2.01	0.67
1:A:10[B]:ARG:NH1	1:A:10[B]:ARG:HG3	2.04	0.67
1:A:279:GLN:HE22	1:A:324:THR:H	1.39	0.67
1:E:328:ARG:HE	1:E:383:PHE:HB3	1.59	0.67
1:D:481:ILE:CD1	1:D:481:ILE:N	2.57	0.67
1:F:279:GLN:HE22	1:F:324:THR:H	1.40	0.67
1:G:201:VAL:HG12	1:G:201:VAL:O	1.95	0.67
1:G:238:LYS:HD2	1:H:235:GLU:OE2	1.93	0.67
1:A:426:HIS:CD2	1:B:137:LYS:HZ1	2.12	0.67
1:G:291:LYS:HE3	1:G:391:ARG:HB3	1.77	0.67
1:C:215:HIS:HD2	1:C:217:ASP:H	1.42	0.67
1:D:356:LYS:HD3	1:D:356:LYS:N	2.04	0.67
1:D:481:ILE:H	1:D:481:ILE:HD13	1.60	0.67
1:A:313:PRO:HB2	1:A:314:MET:HE2	1.75	0.67
1:H:87:SER:HB2	1:H:92:HIS:O	1.95	0.67
1:A:332:VAL:HG12	1:A:333:LEU:N	2.09	0.67
1:C:329:ARG:NH1	1:C:329:ARG:HG2	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ASN:HD21	2:E:601:NAD:C6N	2.07	0.66
1:E:372:LYS:O	1:E:375:ASP:HB2	1.94	0.66
1:F:10[B]:ARG:NH1	1:F:10[B]:ARG:HG3	2.07	0.66
1:G:185:VAL:HG21	1:G:200:VAL:HG21	1.77	0.66
1:H:351:LYS:O	1:H:365:GLU:HG2	1.95	0.66
1:B:279:GLN:HE22	1:B:324:THR:H	1.43	0.66
1:H:323:LEU:HD12	1:H:329:ARG:HA	1.76	0.66
1:B:94:ILE:CD1	1:B:314:MET:O	2.43	0.66
1:B:111:TYR:CE1	1:C:118:LYS:HE3	2.31	0.66
1:C:282:ILE:CG1	1:C:282:ILE:O	2.43	0.66
1:B:313:PRO:HB2	1:B:314:MET:HE2	1.78	0.66
1:C:49:ALA:O	1:C:168:THR:HG21	1.96	0.66
1:F:313:PRO:HB2	1:F:314:MET:HE2	1.77	0.66
1:G:356:LYS:HD3	1:G:356:LYS:N	2.09	0.66
1:B:10[B]:ARG:NH1	1:B:10[B]:ARG:HG3	2.09	0.66
1:E:137:LYS:NZ	1:F:426:HIS:CD2	2.63	0.66
1:F:139:ILE:H	1:F:167:ASN:ND2	1.93	0.66
1:G:245:GLN:C	1:G:246:LEU:HD23	2.13	0.66
1:H:248:LEU:HD23	1:H:248:LEU:N	2.11	0.66
1:B:277:GLN:NE2	1:B:321:GLY:H	1.94	0.66
1:E:373:PRO:O	1:E:374:GLN:CD	2.34	0.66
1:H:1:MET:HG3	1:H:2:GLN:N	2.10	0.66
1:H:185:VAL:HG21	1:H:200:VAL:HG21	1.76	0.66
1:G:374:GLN:CG	1:G:374:GLN:O	2.43	0.66
1:A:90:THR:HG22	1:A:177:THR:HG21	1.78	0.66
1:A:215:HIS:HD2	1:A:217:ASP:H	1.42	0.66
1:A:257:PHE:CD1	1:A:420:ARG:HD3	2.30	0.66
1:A:329:ARG:HG3	1:A:330:ASP:N	2.08	0.66
1:D:149:ASN:HD21	2:D:601:NAD:H5N	1.61	0.66
1:G:261:ASN:ND2	1:G:264:ALA:H	1.93	0.66
1:A:282:ILE:HD11	1:A:447:PHE:CZ	2.31	0.65
1:D:356:LYS:HG2	1:G:12:VAL:CG2	2.25	0.65
1:B:149:ASN:HD21	2:B:601:NAD:C6N	2.09	0.65
1:C:100:LEU:O	1:C:103:PRO:HD2	1.96	0.65
1:F:356:LYS:HE2	1:F:357:ALA:N	2.08	0.65
1:D:279:GLN:HE22	1:D:324:THR:H	1.44	0.65
1:G:476:ASN:CG	1:G:479:ALA:HB3	2.15	0.65
1:H:22:VAL:CG2	1:H:34:ILE:HG12	2.27	0.65
1:D:380:GLU:OE2	1:E:376:ARG:NH1	2.30	0.65
1:H:313:PRO:HB2	1:H:314:MET:HE2	1.78	0.65
1:C:325:SER:O	1:C:328:ARG:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:ILE:HD11	1:E:314:MET:O	1.96	0.65
1:F:139:ILE:N	1:F:167:ASN:HD21	1.94	0.65
1:B:149:ASN:HD21	2:B:601:NAD:C5N	2.09	0.65
1:C:185:VAL:HG21	1:C:200:VAL:HG21	1.77	0.65
1:H:277:GLN:NE2	1:H:321:GLY:H	1.95	0.65
1:B:185:VAL:HG21	1:B:200:VAL:CG2	2.26	0.65
1:C:10[B]:ARG:HG3	1:C:10[B]:ARG:NH1	2.04	0.65
1:G:22:VAL:CG2	1:G:34:ILE:HG12	2.27	0.65
1:G:356:LYS:HE2	1:G:357:ALA:N	2.08	0.65
1:B:327:LEU:O	1:B:330:ASP:HB2	1.96	0.65
1:F:215:HIS:HD2	1:F:217:ASP:H	1.44	0.65
1:F:325:SER:HG	1:F:328:ARG:HD2	1.59	0.65
1:E:356:LYS:CD	1:E:356:LYS:N	2.56	0.64
1:E:356:LYS:HE2	1:E:357:ALA:N	2.07	0.64
1:A:56:TRP:CZ2	1:A:64:ARG:HG2	2.31	0.64
1:E:185:VAL:HG21	1:E:200:VAL:HG21	1.77	0.64
1:G:359:ALA:HB2	3:G:711:HOH:O	1.98	0.64
1:A:238:LYS:HD2	1:B:235:GLU:OE2	1.97	0.64
1:D:185:VAL:HG21	1:D:200:VAL:HG21	1.78	0.64
1:C:248:LEU:HD13	1:D:241:LEU:HD13	1.78	0.64
1:E:329:ARG:NH1	1:E:329:ARG:HG2	1.97	0.64
1:E:426:HIS:CD2	1:F:137:LYS:NZ	2.65	0.64
1:H:94:ILE:HD11	1:H:314:MET:O	1.98	0.64
1:A:273:ILE:HG21	1:A:387:VAL:CG2	2.27	0.64
1:B:139:ILE:HD11	1:B:243:ARG:NH2	2.12	0.64
1:C:238:LYS:HE3	1:E:351:LYS:HZ3	1.63	0.64
1:D:18:GLY:HA2	1:E:33:ARG:NH2	2.13	0.64
1:D:356:LYS:HZ2	1:G:10[A]:ARG:CZ	2.11	0.64
1:E:49:ALA:O	1:E:168:THR:HG21	1.97	0.64
1:F:185:VAL:HG21	1:F:200:VAL:HG21	1.80	0.64
1:F:261:ASN:ND2	1:F:264:ALA:H	1.96	0.64
1:G:481:ILE:H	1:G:481:ILE:HD13	1.62	0.64
1:D:399:LEU:HD11	1:D:427:ALA:HB1	1.78	0.64
1:E:373:PRO:O	1:E:374:GLN:NE2	2.31	0.64
1:E:426:HIS:CD2	1:F:137:LYS:HZ1	2.15	0.64
1:H:329:ARG:NH1	1:H:330:ASP:OD1	2.30	0.64
1:B:245:GLN:C	1:B:246:LEU:CD2	2.55	0.64
1:G:139:ILE:H	1:G:167:ASN:ND2	1.91	0.64
1:E:399:LEU:HD11	1:E:427:ALA:HB1	1.80	0.64
1:A:172:LYS:NZ	1:A:173:PRO:O	2.30	0.64
1:F:261:ASN:ND2	1:F:261:ASN:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:479:ALA:HB1	1:F:481:ILE:HD13	1.78	0.64
1:H:479:ALA:HB1	1:H:481:ILE:HD13	1.80	0.64
1:B:399:LEU:HD11	1:B:427:ALA:HB1	1.81	0.63
1:C:154:PHE:HZ	2:C:601:NAD:H5N	1.62	0.63
1:D:262:ILE:N	1:D:262:ILE:CD1	2.62	0.63
1:F:258:GLU:OE1	1:F:258:GLU:N	2.30	0.63
1:A:135:GLN:HE22	1:B:426:HIS:CE1	2.16	0.63
1:B:174:SER:O	1:B:176:ILE:N	2.32	0.63
1:B:71:LEU:HD22	1:B:188:MET:HG2	1.80	0.63
1:G:326:ALA:O	1:G:328:ARG:N	2.32	0.63
1:B:87:SER:HB2	1:B:92:HIS:O	1.99	0.63
1:F:93:PRO:HB2	1:F:95:ARG:HG2	1.80	0.63
1:G:279:GLN:HE22	1:G:324:THR:H	1.47	0.63
1:G:356:LYS:CD	1:G:356:LYS:N	2.62	0.63
1:A:227:THR:HA	1:A:248:LEU:HD13	1.79	0.63
1:D:22:VAL:CG2	1:D:34:ILE:HG12	2.29	0.63
1:G:49:ALA:HB1	1:G:168:THR:CG2	2.27	0.63
1:A:243:ARG:HD2	1:B:455:TYR:HB3	1.80	0.63
1:C:282:ILE:HG12	1:C:282:ILE:O	1.95	0.63
1:C:56:TRP:CZ2	1:C:64:ARG:HG2	2.33	0.63
1:H:185:VAL:HG21	1:H:200:VAL:CG2	2.29	0.63
1:H:49:ALA:O	1:H:168:THR:HG21	1.98	0.63
1:G:34:ILE:HG13	1:G:178:PRO:HG2	1.81	0.63
1:D:226:SER:O	1:D:229:THR:HG22	1.99	0.63
1:B:185:VAL:CG2	1:B:200:VAL:HG21	2.28	0.63
1:C:185:VAL:HG21	1:C:200:VAL:CG2	2.28	0.63
1:H:356:LYS:N	1:H:356:LYS:HD3	2.12	0.63
1:H:399:LEU:HD11	1:H:427:ALA:HB1	1.80	0.63
1:A:200:VAL:HG12	1:A:202:PRO:HD3	1.80	0.63
1:B:441:VAL:HG12	1:B:442:SER:H	1.63	0.63
1:D:215:HIS:HD2	1:D:217:ASP:H	1.46	0.63
1:A:441:VAL:HG12	1:A:442:SER:H	1.64	0.62
1:B:313:PRO:HB2	1:B:314:MET:CE	2.29	0.62
1:C:408:GLY:O	1:C:430:ALA:HA	1.98	0.62
1:F:100:LEU:O	1:F:103:PRO:HD2	1.99	0.62
1:F:481:ILE:HG22	1:F:481:ILE:O	1.99	0.62
1:H:200:VAL:HG12	1:H:202:PRO:HD3	1.81	0.62
1:C:87:SER:HB2	1:C:92:HIS:O	1.99	0.62
1:D:329:ARG:NH1	1:D:329:ARG:HG2	1.99	0.62
1:E:374:GLN:HG2	1:E:374:GLN:O	1.90	0.62
1:G:261:ASN:ND2	1:G:261:ASN:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:ASN:ND2	2:H:601:NAD:H5N	2.13	0.62
1:A:34:ILE:HG13	1:A:178:PRO:HG2	1.81	0.62
1:B:90:THR:HG22	1:B:177:THR:HG21	1.80	0.62
1:B:282:ILE:HG22	1:B:282:ILE:O	1.98	0.62
1:E:137:LYS:HZ1	1:F:426:HIS:CD2	2.17	0.62
1:F:201:VAL:O	1:F:201:VAL:HG12	1.99	0.62
1:G:326:ALA:O	1:G:327:LEU:C	2.36	0.62
1:A:185:VAL:CG2	1:A:200:VAL:HG21	2.29	0.62
1:C:421:ALA:HB1	1:C:435:ILE:HD13	1.81	0.62
1:F:273:ILE:HG21	1:F:387:VAL:CG2	2.29	0.62
1:C:415:THR:CG2	1:C:417:ASN:H	2.03	0.62
1:E:247:GLU:HB3	2:E:601:NAD:N7N	2.14	0.62
1:F:399:LEU:HD11	1:F:427:ALA:HB1	1.81	0.62
1:F:87:SER:HB2	1:F:92:HIS:O	1.99	0.62
1:C:140:GLY:H	1:C:167:ASN:HD22	1.48	0.62
1:D:49:ALA:HB1	1:D:168:THR:CG2	2.29	0.62
1:E:279:GLN:HE22	1:E:324:THR:H	1.47	0.62
1:A:258:GLU:HG2	1:A:259:ASP:N	2.13	0.62
1:B:215:HIS:HD2	1:B:217:ASP:H	1.48	0.62
1:E:49:ALA:HB1	1:E:168:THR:CG2	2.29	0.62
1:G:140:GLY:H	1:G:167:ASN:HD22	1.45	0.62
1:G:94:ILE:HD11	1:G:314:MET:O	1.99	0.62
1:G:241:LEU:HD13	1:H:248:LEU:HD11	1.81	0.62
1:H:34:ILE:HG13	1:H:178:PRO:HG2	1.80	0.62
1:B:175:GLU:OE2	1:B:175:GLU:N	2.31	0.62
1:G:374:GLN:HG2	1:G:374:GLN:O	1.98	0.62
1:E:415:THR:CG2	1:E:417:ASN:H	1.99	0.62
1:F:95:ARG:HD3	1:F:319:GLU:HA	1.80	0.62
1:F:22:VAL:CG2	1:F:34:ILE:HG12	2.30	0.62
1:G:238:LYS:HD2	1:H:235:GLU:HG3	1.81	0.62
1:G:472:SER:O	1:H:432:MET:HA	1.99	0.62
1:C:426:HIS:CD2	1:D:137:LYS:NZ	2.68	0.61
1:E:441:VAL:HG12	1:E:442:SER:H	1.63	0.61
1:G:1:MET:HG3	1:G:2:GLN:N	2.15	0.61
1:G:185:VAL:CG2	1:G:200:VAL:HG21	2.30	0.61
1:G:273:ILE:HG21	1:G:387:VAL:CG2	2.29	0.61
1:G:238:LYS:CD	1:H:235:GLU:HG3	2.30	0.61
1:G:235:GLU:HG3	1:H:238:LYS:HD2	1.81	0.61
1:F:444:GLY:HA2	1:F:460:GLY:HA2	1.82	0.61
1:H:329:ARG:HG2	1:H:329:ARG:NH1	2.14	0.61
1:A:87:SER:HB2	1:A:92:HIS:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ALA:HB3	1:B:283:ALA:HB2	1.82	0.61
1:E:185:VAL:HG21	1:E:200:VAL:CG2	2.30	0.61
1:D:356:LYS:HZ1	1:G:10[A]:ARG:CD	2.12	0.61
1:H:273:ILE:HG21	1:H:387:VAL:CG2	2.31	0.61
1:H:481:ILE:O	1:H:481:ILE:HG22	2.01	0.61
1:B:4:GLN:HG3	3:B:705:HOH:O	2.00	0.61
1:C:185:VAL:CG2	1:C:200:VAL:HG21	2.31	0.61
1:D:421:ALA:HB1	1:D:435:ILE:HD13	1.82	0.61
1:E:34:ILE:HG13	1:E:178:PRO:HG2	1.83	0.61
1:F:250:GLY:HA2	1:F:407:TYR:HB3	1.82	0.61
1:G:235:GLU:HG3	1:H:238:LYS:CD	2.29	0.61
1:H:10[B]:ARG:NH1	1:H:10[B]:ARG:HG3	2.05	0.61
1:A:252:GLY:HA2	1:A:410:GLY:O	2.01	0.61
1:A:399:LEU:HD11	1:A:427:ALA:HB1	1.83	0.61
1:E:486:LYS:HG2	1:F:95:ARG:HH12	1.65	0.61
1:F:329:ARG:CG	1:F:330:ASP:N	2.62	0.61
1:A:94:ILE:CD1	1:A:314:MET:HA	2.30	0.61
1:C:476:ASN:OD1	1:C:479:ALA:CB	2.48	0.61
1:G:277:GLN:NE2	1:G:321:GLY:H	1.99	0.61
1:A:241:LEU:HD13	1:B:248:LEU:HD11	1.81	0.61
1:B:34:ILE:HG13	1:B:178:PRO:HG2	1.82	0.61
1:G:441:VAL:HG12	1:G:442:SER:H	1.66	0.61
1:B:172:LYS:NZ	1:B:173:PRO:O	2.25	0.61
1:E:185:VAL:CG2	1:E:200:VAL:HG21	2.31	0.61
1:B:174:SER:C	1:B:176:ILE:H	2.03	0.61
1:B:281:CYS:SG	1:B:409:LEU:HD23	2.34	0.61
1:D:129:GLY:HA3	1:D:478:ASP:O	2.01	0.61
1:D:281:CYS:SG	1:D:282:ILE:N	2.71	0.61
1:E:273:ILE:HG21	1:E:387:VAL:CG2	2.31	0.61
1:E:479:ALA:HB1	1:E:481:ILE:HD13	1.82	0.61
1:D:277:GLN:NE2	1:D:321:GLY:H	1.99	0.60
1:F:1:MET:HG3	1:F:2:GLN:N	2.16	0.60
1:G:185:VAL:HG21	1:G:200:VAL:CG2	2.31	0.60
1:A:352:ALA:C	1:A:353:PRO:O	2.33	0.60
1:B:174:SER:C	1:B:176:ILE:N	2.54	0.60
1:D:376:ARG:NH1	1:E:380:GLU:OE2	2.34	0.60
1:F:185:VAL:HG21	1:F:200:VAL:CG2	2.31	0.60
1:G:476:ASN:OD1	1:G:479:ALA:CB	2.48	0.60
1:C:273:ILE:HG21	1:C:387:VAL:CG2	2.31	0.60
1:D:280:ALA:HB3	1:D:283:ALA:HB2	1.83	0.60
1:D:441:VAL:HG12	1:D:442:SER:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:GLN:OE1	1:G:158:LYS:HB3	2.01	0.60
1:A:421:ALA:HB1	1:A:435:ILE:HD13	1.83	0.60
1:D:415:THR:CG2	1:D:417:ASN:H	2.02	0.60
1:E:1:MET:HG3	1:E:2:GLN:N	2.16	0.60
1:F:273:ILE:HG21	1:F:387:VAL:HG21	1.82	0.60
1:G:248:LEU:CD2	1:G:248:LEU:N	2.41	0.60
1:B:421:ALA:HB1	1:B:435:ILE:HD13	1.83	0.60
1:C:277:GLN:NE2	1:C:321:GLY:H	1.98	0.60
1:D:140:GLY:H	1:D:167:ASN:HD22	1.49	0.60
1:F:34:ILE:HG13	1:F:178:PRO:HG2	1.82	0.60
1:F:444:GLY:CA	1:F:459:MET:O	2.49	0.60
1:A:248:LEU:HD11	1:B:241:LEU:HD13	1.83	0.60
1:D:49:ALA:O	1:D:168:THR:HG21	2.02	0.60
1:E:277:GLN:NE2	1:E:321:GLY:H	2.00	0.60
1:G:87:SER:HB2	1:G:92:HIS:O	2.02	0.60
1:H:374:GLN:CG	1:H:374:GLN:O	2.48	0.60
1:A:1:MET:HG3	1:A:2:GLN:N	2.17	0.60
1:A:322:PRO:HG3	1:A:363:TYR:CZ	2.37	0.60
1:C:282:ILE:HD13	1:C:282:ILE:O	2.02	0.60
1:E:421:ALA:HB1	1:E:435:ILE:HD13	1.84	0.60
1:G:56:TRP:CZ2	1:G:64:ARG:HG2	2.37	0.60
1:H:329:ARG:HG2	1:H:329:ARG:HH11	1.66	0.60
1:G:481:ILE:HG21	1:H:440:ARG:NH1	2.16	0.60
1:C:281:CYS:HB3	2:C:601:NAD:C6N	2.32	0.60
1:D:1:MET:HG3	1:D:2:GLN:N	2.16	0.60
1:E:313:PRO:HB2	1:E:314:MET:HE2	1.84	0.60
1:G:399:LEU:HD11	1:G:427:ALA:HB1	1.82	0.60
1:H:185:VAL:CG2	1:H:200:VAL:HG21	2.30	0.60
1:H:444:GLY:CA	1:H:459:MET:O	2.49	0.60
1:A:327:LEU:O	1:A:327:LEU:HD22	2.01	0.60
1:A:22:VAL:CG2	1:A:34:ILE:HG12	2.32	0.60
1:C:258:GLU:HG2	1:C:259:ASP:N	2.16	0.60
1:D:10[B]:ARG:HG3	1:D:10[B]:ARG:NH1	2.07	0.60
1:D:341:GLU:OE2	1:E:231:ARG:NH2	2.35	0.60
1:E:280:ALA:HB3	1:E:283:ALA:HB2	1.84	0.60
1:A:174:SER:O	1:A:177:THR:N	2.33	0.60
1:A:354:ASP:OD1	1:A:354:ASP:N	2.35	0.60
1:D:175:GLU:N	1:D:175:GLU:OE1	2.30	0.60
1:A:154:PHE:HZ	2:A:601:NAD:H5N	1.67	0.59
1:B:353:PRO:CB	1:B:358:LEU:HD23	2.32	0.59
1:C:4:GLN:HG3	3:C:705:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:ALA:O	1:G:168:THR:HG21	2.02	0.59
1:C:149:ASN:HD21	2:C:601:NAD:C6N	2.15	0.59
1:C:1:MET:HG3	1:C:2:GLN:N	2.17	0.59
1:F:149:ASN:HD21	2:F:601:NAD:C5N	2.15	0.59
1:D:200:VAL:HG12	1:D:202:PRO:HD3	1.84	0.59
1:F:277:GLN:NE2	1:F:321:GLY:H	2.00	0.59
1:G:89:ASN:HD21	1:G:177:THR:HA	1.67	0.59
1:H:356:LYS:N	1:H:356:LYS:CD	2.65	0.59
1:A:71:LEU:HD22	1:A:188:MET:HG2	1.83	0.59
1:B:273:ILE:HG21	1:B:387:VAL:CG2	2.32	0.59
1:E:481:ILE:O	1:E:481:ILE:HG22	2.01	0.59
1:F:22:VAL:HG21	1:F:34:ILE:HG12	1.85	0.59
1:F:325:SER:N	1:F:328:ARG:HG3	2.18	0.59
1:A:94:ILE:HD11	1:A:314:MET:CA	2.32	0.59
1:B:138:PRO:HG3	1:B:165:ALA:O	2.02	0.59
1:B:200:VAL:HG12	1:B:202:PRO:HD3	1.85	0.59
1:B:310:LEU:HD23	1:B:358:LEU:HD21	1.84	0.59
1:D:185:VAL:CG2	1:D:200:VAL:HG21	2.32	0.59
1:D:56:TRP:CH2	1:D:64:ARG:HG2	2.38	0.59
1:H:149:ASN:HD21	2:H:601:NAD:C6N	2.16	0.59
1:C:313:PRO:HB2	1:C:314:MET:CE	2.33	0.59
1:E:325:SER:OG	1:E:328:ARG:HB2	2.02	0.59
1:F:56:TRP:CZ2	1:F:64:ARG:HG2	2.38	0.59
1:A:444:GLY:HA2	1:A:460:GLY:HA2	1.85	0.59
1:B:326:ALA:HB2	1:B:362:PHE:CE1	2.38	0.59
1:C:174:SER:C	1:C:176:ILE:H	2.06	0.59
1:A:326:ALA:HB2	1:A:362:PHE:CE1	2.38	0.59
1:E:22:VAL:CG2	1:E:34:ILE:HG12	2.33	0.59
1:B:3:ASN:HB2	1:B:34:ILE:HD13	1.85	0.59
1:C:259:ASP:OD1	1:C:415:THR:HG23	2.02	0.59
1:E:56:TRP:CH2	1:E:64:ARG:HG2	2.37	0.59
1:F:257:PHE:CD1	1:F:420:ARG:HD3	2.38	0.59
1:A:356:LYS:N	1:A:356:LYS:CD	2.64	0.58
1:A:444:GLY:CA	1:A:459:MET:O	2.50	0.58
1:C:441:VAL:HG12	1:C:442:SER:H	1.68	0.58
1:C:95:ARG:NH1	1:C:318:THR:O	2.32	0.58
1:D:273:ILE:HG21	1:D:387:VAL:CG2	2.32	0.58
1:F:136:ARG:HG3	1:F:468:THR:OG1	2.02	0.58
1:F:185:VAL:CG2	1:F:200:VAL:HG21	2.33	0.58
1:C:22:VAL:CG2	1:C:34:ILE:HG12	2.33	0.58
1:B:56:TRP:CZ2	1:B:64:ARG:HG2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:MET:HB2	1:D:118:LYS:HE2	1.85	0.58
1:D:71:LEU:HD22	1:D:188:MET:HG2	1.86	0.58
1:E:356:LYS:N	1:E:356:LYS:HD3	2.02	0.58
1:A:235:GLU:OE2	1:B:238:LYS:HD2	2.02	0.58
1:B:22:VAL:CG2	1:B:34:ILE:HG12	2.33	0.58
1:C:34:ILE:HG13	1:C:178:PRO:HG2	1.85	0.58
1:C:338:ILE:N	1:C:338:ILE:HD13	2.18	0.58
1:C:399:LEU:HD11	1:C:427:ALA:HB1	1.84	0.58
1:D:185:VAL:HG21	1:D:200:VAL:CG2	2.34	0.58
1:G:415:THR:CG2	1:G:417:ASN:H	1.99	0.58
1:E:135:GLN:HE22	1:F:426:HIS:CE1	2.21	0.58
1:G:149:ASN:HD21	2:G:601:NAD:C5N	2.17	0.58
1:A:201:VAL:HG12	1:A:201:VAL:O	2.03	0.58
1:C:250:GLY:HA2	1:C:407:TYR:HB3	1.84	0.58
1:C:482:ALA:O	1:C:483:PRO:C	2.42	0.58
1:C:94:ILE:HG12	1:C:313:PRO:O	2.04	0.58
1:H:250:GLY:HA3	1:H:407:TYR:HB3	1.86	0.58
1:C:243:ARG:HD2	1:D:455:TYR:HB3	1.85	0.58
1:C:94:ILE:HD11	1:C:314:MET:CA	2.34	0.58
1:C:445:SER:HB2	1:D:132:ASN:HD21	1.67	0.58
1:G:417:ASN:HD22	1:G:420:ARG:HB2	1.68	0.58
1:E:215:HIS:HD2	1:E:217:ASP:H	1.52	0.58
1:E:373:PRO:C	1:E:375:ASP:N	2.55	0.58
1:E:328:ARG:NH2	1:E:383:PHE:HB2	2.13	0.58
1:G:235:GLU:OE2	1:H:238:LYS:HD2	2.03	0.58
1:H:444:GLY:HA2	1:H:460:GLY:HA2	1.86	0.58
1:A:280:ALA:HB3	1:A:283:ALA:HB2	1.86	0.58
1:A:49:ALA:O	1:A:168:THR:HG21	2.04	0.58
1:D:374:GLN:O	1:D:374:GLN:HG3	2.00	0.58
1:D:229:THR:HG21	2:D:601:NAD:O1A	2.04	0.58
1:H:22:VAL:HG21	1:H:34:ILE:HG12	1.86	0.58
1:A:374:GLN:O	1:A:374:GLN:HG2	2.01	0.57
1:F:376:ARG:CZ	1:G:206:HIS:CD2	2.87	0.57
1:H:441:VAL:HG12	1:H:442:SER:H	1.69	0.57
1:A:281:CYS:SG	2:A:601:NAD:C5N	2.91	0.57
1:B:139:ILE:HD11	1:B:243:ARG:CZ	2.33	0.57
1:D:480:LYS:O	1:D:481:ILE:C	2.42	0.57
1:F:322:PRO:HG3	1:F:363:TYR:CZ	2.39	0.57
1:G:172:LYS:NZ	1:G:173:PRO:O	2.32	0.57
1:B:100:LEU:O	1:B:103:PRO:HD2	2.04	0.57
1:D:282:ILE:HD13	1:D:434:TRP:CH2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:ALA:C	1:G:328:ARG:N	2.56	0.57
1:H:329:ARG:NH1	1:H:329:ARG:CG	2.54	0.57
1:H:71:LEU:HD22	1:H:188:MET:HG2	1.86	0.57
1:D:313:PRO:HB2	1:D:314:MET:CE	2.35	0.57
1:D:356:LYS:HZ2	1:G:10[A]:ARG:NH1	2.00	0.57
1:F:257:PHE:CE1	1:F:420:ARG:HD3	2.40	0.57
1:F:441:VAL:HG12	1:F:442:SER:H	1.70	0.57
1:G:257:PHE:CE1	1:G:420:ARG:HD3	2.39	0.57
1:G:476:ASN:ND2	1:G:479:ALA:HB3	2.19	0.57
1:H:421:ALA:HB1	1:H:435:ILE:HD13	1.86	0.57
1:A:356:LYS:HE2	1:A:357:ALA:N	2.09	0.57
1:A:259:ASP:OD1	1:A:415:THR:HG23	2.05	0.57
1:C:444:GLY:HA2	1:C:460:GLY:HA2	1.86	0.57
1:E:273:ILE:HG21	1:E:387:VAL:HG21	1.87	0.57
1:F:282:ILE:HD13	1:F:434:TRP:CH2	2.39	0.57
1:G:313:PRO:HB2	1:G:314:MET:CE	2.35	0.57
1:H:56:TRP:CZ2	1:H:64:ARG:HG2	2.40	0.57
1:B:89:ASN:HD21	1:B:177:THR:HA	1.69	0.57
1:D:22:VAL:HG21	1:D:34:ILE:HG12	1.86	0.57
1:F:376:ARG:NH2	1:G:206:HIS:NE2	2.53	0.57
1:D:273:ILE:HG21	1:D:387:VAL:HG21	1.87	0.57
1:F:172:LYS:NZ	1:F:173:PRO:O	2.32	0.57
1:A:172:LYS:HE2	2:A:601:NAD:O2B	2.04	0.57
1:D:139:ILE:HD11	1:D:243:ARG:CZ	2.35	0.57
1:E:484:HIS:O	1:F:95:ARG:NH1	2.37	0.57
1:A:56:TRP:CH2	1:A:64:ARG:HG2	2.40	0.57
1:G:257:PHE:CD1	1:G:420:ARG:HD3	2.40	0.57
1:H:328:ARG:NH1	1:H:331:ARG:HH21	2.03	0.57
1:A:174:SER:O	1:A:176:ILE:N	2.38	0.56
1:C:325:SER:HG	1:C:328:ARG:HG2	1.68	0.56
1:C:87:SER:CB	1:C:92:HIS:O	2.53	0.56
1:G:139:ILE:N	1:G:167:ASN:HD21	1.97	0.56
1:G:22:VAL:HG21	1:G:34:ILE:HG12	1.86	0.56
1:C:139:ILE:N	1:C:167:ASN:HD21	1.99	0.56
1:E:132:ASN:HD21	1:F:445:SER:HB2	1.69	0.56
1:H:356:LYS:HE2	1:H:357:ALA:N	2.07	0.56
1:A:277:GLN:NE2	1:A:321:GLY:H	2.03	0.56
1:C:139:ILE:H	1:C:167:ASN:ND2	1.99	0.56
1:D:231:ARG:HD2	1:E:337:ASP:OD2	2.05	0.56
1:E:139:ILE:N	1:E:167:ASN:HD21	1.95	0.56
1:G:273:ILE:HG21	1:G:387:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HB	1:C:121:GLY:HA3	1.87	0.56
1:A:313:PRO:HB2	1:A:314:MET:CE	2.35	0.56
1:E:180:SER:CB	3:E:720:HOH:O	2.53	0.56
1:H:259:ASP:OD1	1:H:415:THR:HG23	2.05	0.56
1:C:476:ASN:ND2	1:C:479:ALA:HB3	2.21	0.56
1:D:87:SER:HB2	1:D:92:HIS:O	2.05	0.56
1:E:149:ASN:OD1	1:E:149:ASN:N	2.38	0.56
1:E:89:ASN:HD21	1:E:177:THR:HA	1.70	0.56
1:E:243:ARG:HD2	1:F:455:TYR:HB3	1.86	0.56
1:E:328:ARG:NE	1:E:383:PHE:HB3	2.21	0.56
1:E:444:GLY:HA2	1:E:460:GLY:HA2	1.86	0.56
1:E:445:SER:HB2	1:F:132:ASN:ND2	2.21	0.56
1:G:249:GLY:HA2	2:G:601:NAD:O2D	2.05	0.56
1:A:149:ASN:OD1	1:A:149:ASN:N	2.39	0.56
1:A:476:ASN:OD1	1:A:479:ALA:HB3	2.05	0.56
1:C:56:TRP:CH2	1:C:64:ARG:HG2	2.41	0.56
1:A:100:LEU:O	1:A:103:PRO:HD2	2.06	0.56
1:B:282:ILE:O	1:B:282:ILE:HG23	2.05	0.56
1:C:444:GLY:CA	1:C:459:MET:O	2.53	0.56
1:D:231:ARG:NH2	1:E:341:GLU:OE2	2.39	0.56
1:G:149:ASN:HD21	2:G:601:NAD:H5N	1.71	0.56
1:G:475:VAL:HG22	1:H:435:ILE:HD12	1.87	0.56
1:C:22:VAL:HG21	1:C:34:ILE:HG12	1.87	0.56
1:G:421:ALA:HB1	1:G:435:ILE:HD13	1.88	0.55
1:G:136:ARG:HG3	1:G:468:THR:OG1	2.06	0.55
1:H:136:ARG:HG3	1:H:468:THR:OG1	2.06	0.55
1:A:282:ILE:CD1	1:A:447:PHE:CZ	2.90	0.55
1:D:223:PHE:CZ	1:D:229:THR:HG21	2.21	0.55
1:A:20:ILE:HG13	1:A:36:ALA:HB2	1.89	0.55
1:A:282:ILE:CD1	1:A:447:PHE:HE1	2.13	0.55
1:A:149:ASN:HD21	2:A:601:NAD:C5N	2.20	0.55
1:B:259:ASP:OD1	1:B:415:THR:HG23	2.07	0.55
1:B:282:ILE:HD13	1:B:434:TRP:CH2	2.41	0.55
1:C:426:HIS:CE1	1:D:135:GLN:HE22	2.24	0.55
1:E:373:PRO:C	1:E:375:ASP:H	2.10	0.55
1:F:10[B]:ARG:HH11	1:F:10[B]:ARG:CG	2.13	0.55
1:F:281:CYS:SG	1:F:409:LEU:HD22	2.47	0.55
1:G:148:TRP:CH2	1:G:328:ARG:CD	2.90	0.55
1:D:262:ILE:N	1:D:262:ILE:HD12	2.21	0.55
1:H:328:ARG:NH1	1:H:328:ARG:CG	2.41	0.55
1:H:322:PRO:HG3	1:H:363:TYR:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ASP:OD1	1:D:415:THR:HG23	2.07	0.55
1:G:100:LEU:O	1:G:103:PRO:HD2	2.07	0.55
1:H:313:PRO:HB2	1:H:314:MET:CE	2.36	0.55
1:A:356:LYS:N	1:A:356:LYS:HD3	2.12	0.55
1:A:136:ARG:HG3	1:A:468:THR:OG1	2.06	0.55
1:C:356:LYS:HE2	1:C:357:ALA:N	2.10	0.55
1:D:33:ARG:HH21	1:E:18:GLY:HA2	1.72	0.55
1:C:136:ARG:HG3	1:C:468:THR:OG1	2.07	0.55
1:D:313:PRO:HB2	1:D:314:MET:HE2	1.88	0.55
1:F:421:ALA:HB1	1:F:435:ILE:HD13	1.87	0.55
1:A:328:ARG:NH1	1:A:331:ARG:HD3	2.22	0.55
1:A:353:PRO:CD	1:A:353:PRO:O	2.52	0.55
1:B:149:ASN:HD21	2:B:601:NAD:H6N	1.71	0.55
1:C:282:ILE:CD1	1:C:282:ILE:O	2.54	0.55
1:D:356:LYS:HE3	1:G:12:VAL:CG1	2.35	0.55
1:H:325:SER:O	1:H:328:ARG:HB2	2.05	0.55
1:H:417:ASN:HD22	1:H:420:ARG:HB2	1.71	0.55
1:A:455:TYR:HB3	1:B:243:ARG:CD	2.37	0.55
1:B:417:ASN:HD22	1:B:420:ARG:HB2	1.72	0.55
1:C:417:ASN:HD22	1:C:420:ARG:HB2	1.71	0.55
1:E:139:ILE:HB	1:E:167:ASN:HD21	1.72	0.55
1:G:53:PHE:HB3	1:G:54:PRO:HD3	1.89	0.55
1:H:374:GLN:HG2	1:H:374:GLN:O	2.02	0.55
1:H:5:LEU:CB	3:H:714:HOH:O	2.54	0.55
1:A:332:VAL:O	1:A:335:TYR:N	2.39	0.55
1:B:323:LEU:HD12	1:B:329:ARG:HA	1.89	0.55
1:D:223:PHE:CE2	1:D:229:THR:HG23	2.40	0.55
1:H:415:THR:CG2	1:H:416:GLN:N	2.68	0.55
1:C:415:THR:CG2	1:C:416:GLN:N	2.70	0.54
1:H:20:ILE:HG13	1:H:36:ALA:HB2	1.88	0.54
1:E:259:ASP:OD1	1:E:415:THR:HG23	2.07	0.54
1:F:141:VAL:O	1:F:141:VAL:HG12	2.07	0.54
1:G:322:PRO:HG3	1:G:363:TYR:CZ	2.42	0.54
1:H:144:GLN:OE1	1:H:158:LYS:HB3	2.07	0.54
1:G:481:ILE:HG21	1:H:440:ARG:HH12	1.73	0.54
1:A:415:THR:CG2	1:A:416:GLN:N	2.68	0.54
1:B:415:THR:CG2	1:B:416:GLN:N	2.71	0.54
1:C:273:ILE:HG21	1:C:387:VAL:HG21	1.90	0.54
1:C:248:LEU:HD13	1:D:241:LEU:CD1	2.38	0.54
1:D:260:ALA:O	1:D:262:ILE:CD1	2.55	0.54
1:H:273:ILE:HG21	1:H:387:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:432:MET:HA	1:H:472:SER:O	2.06	0.54
1:A:22:VAL:HG21	1:A:34:ILE:HG12	1.89	0.54
1:C:27:ASP:CG	1:C:29:SER:HB3	2.28	0.54
1:C:249:GLY:CA	2:C:601:NAD:O2D	2.52	0.54
1:G:149:ASN:HD21	2:G:601:NAD:C6N	2.21	0.54
1:G:282:ILE:HD13	1:G:434:TRP:CH2	2.42	0.54
1:F:25:PRO:HA	1:F:362:PHE:CE2	2.43	0.54
1:F:17:GLY:HA3	1:H:376:ARG:NH1	2.22	0.54
1:A:90:THR:HG22	1:A:177:THR:CG2	2.37	0.54
1:A:87:SER:CB	1:A:92:HIS:O	2.56	0.54
1:B:273:ILE:HG21	1:B:387:VAL:HG21	1.90	0.54
1:D:149:ASN:ND2	2:D:601:NAD:H5N	2.23	0.54
1:F:325:SER:OG	1:F:328:ARG:HG3	1.91	0.54
1:H:273:ILE:O	1:H:278:GLY:HA2	2.07	0.54
1:A:273:ILE:HG21	1:A:387:VAL:HG21	1.87	0.54
1:B:136:ARG:HG3	1:B:468:THR:OG1	2.08	0.54
1:D:90:THR:HG22	1:D:177:THR:HG21	1.89	0.54
1:D:417:ASN:HD22	1:D:420:ARG:HB2	1.72	0.54
1:E:455:TYR:HB3	1:F:243:ARG:HD2	1.90	0.54
1:G:215:HIS:CD2	1:G:217:ASP:H	2.24	0.54
1:D:100:LEU:O	1:D:103:PRO:HD2	2.08	0.54
1:E:155:THR:CG2	1:E:181:THR:HB	2.38	0.54
1:E:248:LEU:CD1	1:F:241:LEU:HD13	2.38	0.54
1:F:415:THR:CG2	1:F:416:GLN:N	2.71	0.54
1:F:87:SER:CB	1:F:92:HIS:O	2.55	0.54
1:H:326:ALA:HB2	1:H:362:PHE:CE1	2.43	0.54
1:A:408:GLY:O	1:A:430:ALA:CA	2.50	0.54
1:C:258:GLU:OE2	1:C:420:ARG:NH2	2.41	0.54
1:C:458:GLU:O	1:C:459:MET:CB	2.56	0.54
1:H:10[B]:ARG:HH11	1:H:10[B]:ARG:CG	2.14	0.54
1:H:257:PHE:CD1	1:H:420:ARG:HD3	2.42	0.54
1:H:87:SER:CB	1:H:92:HIS:O	2.56	0.54
1:A:89:ASN:HD21	1:A:177:THR:HA	1.73	0.54
1:B:353:PRO:HB3	1:B:358:LEU:HD23	1.91	0.54
1:D:140:GLY:H	1:D:167:ASN:ND2	2.06	0.54
1:F:149:ASN:OD1	1:F:149:ASN:N	2.40	0.54
1:A:280:ALA:HB1	1:A:282:ILE:O	2.08	0.53
1:F:313:PRO:HB2	1:F:314:MET:CE	2.38	0.53
1:H:31:ILE:HG22	1:H:32:THR:HG22	1.90	0.53
1:B:444:GLY:HA2	1:B:460:GLY:HA2	1.90	0.53
1:H:100:LEU:O	1:H:103:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:O	1:B:242:LYS:HE3	2.09	0.53
1:C:154:PHE:HZ	2:C:601:NAD:C5N	2.21	0.53
1:D:238:LYS:NZ	3:D:703:HOH:O	2.41	0.53
1:D:326:ALA:HB2	1:D:362:PHE:CE1	2.44	0.53
1:D:53:PHE:HB3	1:D:54:PRO:HD3	1.90	0.53
1:F:200:VAL:HG12	1:F:202:PRO:HD3	1.90	0.53
1:F:31:ILE:HG22	1:F:32:THR:HG22	1.89	0.53
1:G:27:ASP:CG	1:G:29:SER:HB3	2.29	0.53
1:G:415:THR:CG2	1:G:416:GLN:N	2.72	0.53
1:H:27:ASP:CG	1:H:29:SER:HB3	2.28	0.53
1:A:445:SER:HB2	1:B:132:ASN:ND2	2.24	0.53
1:B:257:PHE:CD1	1:B:420:ARG:HD3	2.43	0.53
1:C:426:HIS:CD2	1:D:137:LYS:HZ2	2.25	0.53
1:D:247:GLU:HB3	2:D:601:NAD:N7N	2.23	0.53
1:D:257:PHE:CD1	1:D:420:ARG:HD3	2.44	0.53
1:D:258:GLU:HG3	1:D:290:HIS:CG	2.42	0.53
1:E:10[B]:ARG:HH11	1:E:10[B]:ARG:CG	2.15	0.53
1:E:444:GLY:CA	1:E:459:MET:O	2.55	0.53
1:H:227:THR:HA	1:H:248:LEU:HD13	1.89	0.53
1:H:365:GLU:HB2	1:H:366:PRO:HD2	1.91	0.53
1:H:411:SER:O	1:H:434:TRP:HE3	1.91	0.53
1:A:25:PRO:HA	1:A:362:PHE:CE2	2.43	0.53
1:A:302:ILE:O	1:A:306:LYS:HG3	2.08	0.53
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.90	0.53
1:D:27:ASP:CG	1:D:29:SER:HB3	2.28	0.53
1:D:355:ASP:HB3	1:D:356:LYS:HD3	1.91	0.53
1:E:180:SER:HB2	3:E:720:HOH:O	2.08	0.53
1:E:22:VAL:HG21	1:E:34:ILE:HG12	1.91	0.53
1:E:87:SER:HB2	1:E:92:HIS:O	2.08	0.53
1:G:259:ASP:OD1	1:G:415:THR:HG23	2.09	0.53
1:H:405:THR:HG22	1:H:406:GLU:N	2.22	0.53
1:B:154:PHE:HZ	2:B:601:NAD:C5N	2.21	0.53
1:C:148:TRP:CH2	1:C:328:ARG:HD3	2.44	0.53
1:D:261:ASN:OD1	1:D:261:ASN:C	2.45	0.53
1:E:136:ARG:HG3	1:E:468:THR:OG1	2.09	0.53
1:E:281:CYS:SG	1:E:409:LEU:HD22	2.48	0.53
1:B:22:VAL:HG21	1:B:34:ILE:HG12	1.89	0.53
1:B:87:SER:CB	1:B:92:HIS:O	2.57	0.53
1:C:149:ASN:OD1	1:C:149:ASN:N	2.41	0.53
1:B:273:ILE:O	1:B:278:GLY:HA2	2.09	0.53
1:D:444:GLY:HA2	1:D:460:GLY:HA2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:PRO:HB2	1:E:314:MET:CE	2.38	0.53
1:E:80:GLU:OE1	1:E:98:ARG:NE	2.42	0.53
1:F:94:ILE:HD11	1:F:314:MET:O	2.08	0.53
1:H:80:GLU:OE1	1:H:98:ARG:NE	2.41	0.53
1:A:144:GLN:OE1	1:A:158:LYS:HB3	2.09	0.53
1:B:373:PRO:HG3	1:B:390:VAL:HG11	1.91	0.53
1:B:49:ALA:O	1:B:168:THR:HG21	2.09	0.53
1:F:141:VAL:HG23	1:F:168:THR:CG2	2.39	0.53
1:A:455:TYR:CB	1:B:243:ARG:HD2	2.39	0.52
1:C:25:PRO:HA	1:C:362:PHE:CE2	2.43	0.52
1:D:415:THR:CG2	1:D:416:GLN:N	2.71	0.52
1:H:139:ILE:HG22	1:H:140:GLY:N	2.24	0.52
1:H:149:ASN:N	1:H:149:ASN:OD1	2.42	0.52
1:H:282:ILE:HD13	1:H:434:TRP:CH2	2.45	0.52
1:D:257:PHE:CE1	1:D:420:ARG:HD3	2.44	0.52
1:D:323:LEU:HB3	1:D:328:ARG:HG2	1.91	0.52
1:F:144:GLN:OE1	1:F:158:LYS:HB3	2.09	0.52
1:F:49:ALA:O	1:F:168:THR:HG21	2.09	0.52
1:H:281:CYS:SG	1:H:409:LEU:HD22	2.49	0.52
1:A:334:SER:O	1:A:338:ILE:HD13	2.10	0.52
1:B:477:VAL:CG2	1:B:478:ASP:N	2.72	0.52
1:D:262:ILE:CD1	1:D:262:ILE:H	2.22	0.52
1:A:365:GLU:HB2	1:A:366:PRO:HD2	1.91	0.52
1:F:365:GLU:HB2	1:F:366:PRO:HD2	1.91	0.52
1:H:175:GLU:N	1:H:175:GLU:OE2	2.40	0.52
1:E:100:LEU:O	1:E:103:PRO:HD2	2.09	0.52
1:E:415:THR:CG2	1:E:416:GLN:N	2.73	0.52
1:B:144:GLN:OE1	1:B:158:LYS:HB3	2.10	0.52
1:D:354:ASP:N	1:D:354:ASP:OD2	2.42	0.52
1:D:356:LYS:NZ	1:G:10[A]:ARG:CZ	2.72	0.52
1:F:405:THR:HG22	1:F:406:GLU:N	2.24	0.52
1:H:215:HIS:CD2	1:H:217:ASP:H	2.21	0.52
1:H:257:PHE:CE1	1:H:420:ARG:HD3	2.45	0.52
1:H:415:THR:HG22	1:H:416:GLN:H	1.73	0.52
1:A:221:ILE:HD13	1:A:222:ALA:N	2.25	0.52
1:E:53:PHE:HB3	1:E:54:PRO:HD3	1.91	0.52
1:F:89:ASN:HD21	1:F:177:THR:HA	1.75	0.52
1:F:325:SER:CB	1:F:328:ARG:CG	2.79	0.52
1:A:273:ILE:O	1:A:278:GLY:HA2	2.10	0.52
1:A:94:ILE:HD11	1:A:314:MET:HA	1.92	0.52
1:B:141:VAL:HA	1:B:168:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:GLY:H	1:C:167:ASN:ND2	2.07	0.52
1:C:415:THR:HG22	1:C:416:GLN:H	1.75	0.52
1:D:356:LYS:N	1:D:356:LYS:CD	2.55	0.52
1:E:282:ILE:HD13	1:E:434:TRP:CH2	2.44	0.52
1:G:258:GLU:HG2	1:G:259:ASP:N	2.23	0.52
1:G:22:VAL:HG23	1:G:34:ILE:HG12	1.92	0.52
1:C:282:ILE:HG13	1:C:434:TRP:CH2	2.45	0.52
1:E:126:VAL:HG21	1:E:474:TRP:CH2	2.44	0.52
1:F:131:LEU:HD22	1:F:131:LEU:C	2.30	0.52
1:F:356:LYS:CD	1:F:356:LYS:N	2.67	0.52
1:G:31:ILE:HG22	1:G:32:THR:HG22	1.92	0.52
1:H:411:SER:O	1:H:434:TRP:CE3	2.63	0.52
1:A:27:ASP:CG	1:A:29:SER:HB3	2.29	0.52
1:B:328:ARG:O	1:B:329:ARG:C	2.48	0.52
1:E:149:ASN:HD21	2:E:601:NAD:C5N	2.23	0.52
1:G:155:THR:CG2	1:G:181:THR:HB	2.41	0.52
1:G:325:SER:CA	1:G:328:ARG:HH22	2.22	0.52
1:G:365:GLU:HB2	1:G:366:PRO:HD2	1.92	0.52
1:G:444:GLY:HA2	1:G:460:GLY:HA2	1.91	0.52
1:H:333:LEU:HD22	1:H:351:LYS:HD3	1.90	0.52
1:C:484:HIS:N	3:C:704:HOH:O	2.42	0.51
1:F:302:ILE:HG23	1:F:348:ALA:HB2	1.92	0.51
1:G:334:SER:O	1:G:338:ILE:HD13	2.10	0.51
1:H:76:GLU:O	1:H:79:SER:HB2	2.10	0.51
1:A:417:ASN:HD22	1:A:420:ARG:HB2	1.74	0.51
1:B:365:GLU:HB2	1:B:366:PRO:HD2	1.92	0.51
1:C:144:GLN:OE1	1:C:158:LYS:HB3	2.10	0.51
1:F:356:LYS:HD3	1:F:356:LYS:N	2.14	0.51
1:A:94:ILE:HG12	1:A:313:PRO:O	2.10	0.51
1:E:27:ASP:CG	1:E:29:SER:HB3	2.30	0.51
1:H:325:SER:HG	1:H:328:ARG:HG3	1.74	0.51
1:H:22:VAL:HG23	1:H:34:ILE:HG12	1.92	0.51
1:A:415:THR:HG22	1:A:416:GLN:H	1.76	0.51
1:F:273:ILE:O	1:F:278:GLY:HA2	2.11	0.51
1:F:334:SER:O	1:F:338:ILE:HD13	2.10	0.51
1:A:215:HIS:CD2	1:A:217:ASP:H	2.25	0.51
1:C:322:PRO:HG3	1:C:363:TYR:CZ	2.46	0.51
1:E:71:LEU:HD22	1:E:188:MET:HG2	1.92	0.51
1:G:4:GLN:HG3	3:G:703:HOH:O	2.10	0.51
1:H:221:ILE:HD13	1:H:222:ALA:N	2.25	0.51
1:H:56:TRP:CH2	1:H:64:ARG:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:NZ	3:A:706:HOH:O	2.32	0.51
1:B:148:TRP:HD1	1:B:174:SER:OG	1.88	0.51
1:C:326:ALA:HB2	1:C:362:PHE:CE1	2.46	0.51
1:D:322:PRO:HG3	1:D:363:TYR:CZ	2.45	0.51
1:D:136:ARG:HG3	1:D:468:THR:OG1	2.10	0.51
1:H:87:SER:HB3	1:H:97:SER:OG	2.10	0.51
1:B:405:THR:HG22	1:B:406:GLU:N	2.25	0.51
1:B:221:ILE:HD13	1:B:222:ALA:N	2.26	0.51
1:B:459:MET:HE2	1:B:459:MET:HA	1.93	0.51
1:C:215:HIS:CD2	1:C:217:ASP:H	2.25	0.51
1:D:273:ILE:HG12	1:D:387:VAL:CG2	2.37	0.51
1:E:144:GLN:OE1	1:E:158:LYS:HB3	2.10	0.51
1:E:302:ILE:O	1:E:306:LYS:HG3	2.11	0.51
1:E:322:PRO:HG3	1:E:363:TYR:CZ	2.46	0.51
1:G:245:GLN:O	1:G:246:LEU:CD2	2.27	0.51
1:G:455:TYR:HB3	1:H:243:ARG:HD2	1.91	0.51
1:A:328:ARG:NH1	1:A:331:ARG:CD	2.74	0.51
1:C:10[B]:ARG:HH11	1:C:10[B]:ARG:CG	2.10	0.51
1:D:148:TRP:HD1	1:D:174:SER:OG	1.94	0.51
1:D:365:GLU:HB2	1:D:366:PRO:HD2	1.93	0.51
1:D:88:LEU:HA	1:D:314:MET:HE1	1.93	0.51
1:E:12:VAL:HG23	1:E:13:ASP:O	2.11	0.51
1:E:417:ASN:HD22	1:E:420:ARG:HB2	1.76	0.51
1:F:325:SER:O	1:F:328:ARG:HB2	2.11	0.51
1:F:56:TRP:CH2	1:F:64:ARG:HG2	2.46	0.51
1:H:141:VAL:HG12	1:H:141:VAL:O	2.09	0.51
1:C:174:SER:C	1:C:176:ILE:N	2.63	0.51
1:C:32:THR:OG1	1:C:33:ARG:N	2.44	0.51
1:E:140:GLY:H	1:E:167:ASN:HD22	1.57	0.51
1:G:148:TRP:CH2	1:G:328:ARG:HD2	2.46	0.51
1:H:174:SER:O	1:H:176:ILE:N	2.43	0.51
1:A:149:ASN:HD21	2:A:601:NAD:C6N	2.24	0.50
1:C:247:GLU:HB3	2:C:601:NAD:C7N	2.41	0.50
1:C:273:ILE:O	1:C:278:GLY:HA2	2.11	0.50
1:C:302:ILE:HG23	1:C:348:ALA:HB2	1.92	0.50
1:G:149:ASN:HD21	2:G:601:NAD:H6N	1.76	0.50
1:H:224:THR:HA	1:H:247:GLU:HB2	1.93	0.50
1:A:126:VAL:HG21	1:A:474:TRP:CH2	2.46	0.50
1:A:333:LEU:HD22	1:A:351:LYS:HD3	1.93	0.50
1:B:227:THR:HA	1:B:248:LEU:CD1	2.39	0.50
1:F:215:HIS:CD2	1:F:217:ASP:H	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ILE:HG12	1:C:464:ILE:HG21	1.92	0.50
1:D:262:ILE:HD13	1:D:262:ILE:H	1.76	0.50
1:F:20:ILE:HD11	1:F:204:TYR:CE2	2.46	0.50
1:A:282:ILE:HG22	1:A:282:ILE:O	2.09	0.50
1:C:221:ILE:HD13	1:C:222:ALA:N	2.26	0.50
1:B:162:ALA:O	1:B:167:ASN:HB2	2.12	0.50
1:B:257:PHE:CE1	1:B:420:ARG:HD3	2.47	0.50
1:D:231:ARG:CD	1:E:337:ASP:OD2	2.59	0.50
1:D:248:LEU:O	1:D:249:GLY:O	2.30	0.50
1:E:263:GLU:HG3	1:E:300:ARG:HH12	1.76	0.50
1:H:131:LEU:HD22	1:H:131:LEU:C	2.31	0.50
1:D:291:LYS:HE3	1:D:391:ARG:HB3	1.93	0.50
1:E:261:ASN:C	1:E:261:ASN:OD1	2.49	0.50
1:G:56:TRP:CH2	1:G:64:ARG:HG2	2.47	0.50
1:B:334:SER:O	1:B:338:ILE:HD13	2.10	0.50
1:C:155:THR:CG2	1:C:181:THR:HB	2.40	0.50
1:C:323:LEU:HD12	1:C:329:ARG:HA	1.93	0.50
1:C:291:LYS:HE3	1:C:391:ARG:HB3	1.94	0.50
1:D:146:VAL:HG23	1:D:147:PRO:O	2.11	0.50
1:D:459:MET:HE2	1:D:459:MET:HA	1.94	0.50
1:F:141:VAL:CG2	1:F:168:THR:HG22	2.42	0.50
1:G:355:ASP:O	3:G:711:HOH:O	2.19	0.50
1:G:291:LYS:HE3	1:G:391:ARG:CB	2.42	0.50
1:C:20:ILE:HG13	1:C:36:ALA:HB2	1.94	0.50
1:F:27:ASP:CG	1:F:29:SER:HB3	2.32	0.50
1:G:481:ILE:H	1:G:481:ILE:CD1	2.20	0.50
1:G:132:ASN:ND2	1:H:445:SER:HB2	2.27	0.50
1:A:121:GLY:HA3	1:C:123:VAL:HB	1.93	0.50
1:A:174:SER:O	1:A:175:GLU:C	2.49	0.50
1:A:400:ALA:HB2	3:A:704:HOH:O	2.11	0.50
1:D:89:ASN:ND2	1:D:177:THR:HA	2.25	0.50
1:D:261:ASN:O	1:D:261:ASN:OD1	2.30	0.50
1:E:328:ARG:CZ	1:E:383:PHE:HB3	2.42	0.50
1:G:140:GLY:H	1:G:167:ASN:ND2	2.08	0.50
1:A:248:LEU:CD2	1:A:248:LEU:N	2.32	0.49
1:C:334:SER:O	1:C:338:ILE:HG12	2.11	0.49
1:A:248:LEU:CD2	1:A:248:LEU:H	2.22	0.49
1:F:326:ALA:HB2	1:F:362:PHE:CE1	2.46	0.49
1:G:149:ASN:OD1	1:G:149:ASN:N	2.43	0.49
1:G:445:SER:HB2	1:H:132:ASN:ND2	2.27	0.49
1:H:140:GLY:H	1:H:167:ASN:HD22	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:THR:CG2	1:A:181:THR:HB	2.41	0.49
1:B:248:LEU:H	1:B:248:LEU:CD2	2.12	0.49
1:C:132:ASN:ND2	1:D:445:SER:HB2	2.28	0.49
1:E:139:ILE:HD11	1:E:243:ARG:CZ	2.43	0.49
1:F:325:SER:O	1:F:328:ARG:CG	2.61	0.49
1:G:250:GLY:HA2	1:G:407:TYR:HB3	1.94	0.49
1:B:458:GLU:O	1:B:459:MET:CB	2.60	0.49
1:D:432:MET:HE3	3:D:701:HOH:O	2.12	0.49
1:E:257:PHE:CE1	1:E:420:ARG:HD3	2.47	0.49
1:E:273:ILE:O	1:E:278:GLY:HA2	2.11	0.49
1:A:139:ILE:H	1:A:167:ASN:ND2	2.03	0.49
1:B:322:PRO:HG3	1:B:363:TYR:CZ	2.48	0.49
1:C:148:TRP:HB2	1:C:177:THR:HG21	1.94	0.49
1:E:257:PHE:CD1	1:E:420:ARG:HD3	2.47	0.49
1:D:356:LYS:NZ	1:G:10[A]:ARG:HD2	2.25	0.49
1:G:273:ILE:O	1:G:278:GLY:HA2	2.12	0.49
1:A:328:ARG:O	1:A:329:ARG:C	2.50	0.49
1:A:352:ALA:O	1:A:353:PRO:C	2.49	0.49
1:B:149:ASN:N	1:B:149:ASN:OD1	2.45	0.49
1:C:177:THR:N	1:C:178:PRO:HD3	2.26	0.49
1:C:411:SER:O	1:C:434:TRP:CE3	2.66	0.49
1:C:96:ASP:O	1:C:97:SER:C	2.50	0.49
1:G:175:GLU:N	1:G:175:GLU:OE2	2.41	0.49
1:G:71:LEU:HD22	1:G:188:MET:HG2	1.93	0.49
1:C:87:SER:HB3	1:C:97:SER:OG	2.12	0.49
1:G:87:SER:CB	1:G:92:HIS:O	2.60	0.49
1:H:86:GLU:OE2	1:H:180:SER:HB2	2.13	0.49
1:B:149:ASN:HD21	2:B:601:NAD:H5N	1.76	0.49
1:C:365:GLU:HB2	1:C:366:PRO:HD2	1.95	0.49
1:C:445:SER:CB	1:D:132:ASN:HD21	2.25	0.49
1:D:273:ILE:O	1:D:278:GLY:HA2	2.12	0.49
1:F:80:GLU:OE1	1:F:98:ARG:NE	2.45	0.49
1:A:118:LYS:HE2	1:D:115:MET:HB2	1.95	0.49
1:A:247:GLU:C	1:A:248:LEU:HD23	2.29	0.49
1:B:37:ALA:CB	1:B:201:VAL:HG13	2.43	0.49
1:C:96:ASP:O	1:C:98:ARG:N	2.46	0.49
1:D:392:PHE:CD1	1:D:398:ALA:HB2	2.47	0.49
1:F:71:LEU:HD22	1:F:188:MET:HG2	1.95	0.49
1:H:174:SER:C	1:H:176:ILE:N	2.65	0.49
1:A:174:SER:C	1:A:176:ILE:N	2.64	0.48
1:A:373:PRO:HG3	1:A:390:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:HD3	1:A:70:LYS:HA	1.62	0.48
1:A:248:LEU:HD12	1:B:241:LEU:HD13	1.92	0.48
1:B:311:GLY:HA2	1:B:358:LEU:HD11	1.95	0.48
1:C:10[B]:ARG:CG	1:C:10[B]:ARG:NH1	2.72	0.48
1:E:20:ILE:HG13	1:E:36:ALA:HB2	1.95	0.48
1:F:17:GLY:HA3	1:H:376:ARG:HH11	1.78	0.48
1:F:325:SER:HG	1:F:328:ARG:CD	2.06	0.48
1:H:126:VAL:HG21	1:H:474:TRP:CH2	2.48	0.48
1:A:261:ASN:O	1:A:261:ASN:OD1	2.31	0.48
1:B:90:THR:HG22	1:B:177:THR:CG2	2.41	0.48
1:G:302:ILE:HG23	1:G:348:ALA:HB2	1.95	0.48
1:H:291:LYS:HE3	1:H:391:ARG:HB3	1.94	0.48
1:B:333:LEU:HD22	1:B:351:LYS:HD3	1.94	0.48
1:B:53:PHE:HB3	1:B:54:PRO:HD3	1.94	0.48
1:C:141:VAL:HG22	1:C:168:THR:HG22	1.96	0.48
1:C:302:ILE:O	1:C:306:LYS:HG3	2.13	0.48
1:D:144:GLN:OE1	1:D:158:LYS:HB3	2.13	0.48
1:A:426:HIS:HD2	1:B:137:LYS:NZ	2.11	0.48
1:B:155:THR:CG2	1:B:181:THR:HB	2.43	0.48
1:B:27:ASP:CG	1:B:29:SER:HB3	2.34	0.48
1:B:56:TRP:CH2	1:B:64:ARG:HG2	2.48	0.48
1:C:373:PRO:HG3	1:C:390:VAL:HG11	1.95	0.48
1:E:365:GLU:HB2	1:E:366:PRO:HD2	1.95	0.48
1:E:405:THR:HG22	1:E:406:GLU:N	2.27	0.48
1:F:374:GLN:O	1:F:374:GLN:CG	2.60	0.48
1:G:99:GLY:O	1:G:100:LEU:HD12	2.14	0.48
1:A:302:ILE:HG23	1:A:348:ALA:HB2	1.95	0.48
1:E:291:LYS:HE3	1:E:391:ARG:HB3	1.95	0.48
1:E:326:ALA:HB2	1:E:362:PHE:CE1	2.49	0.48
1:F:291:LYS:HE3	1:F:391:ARG:HB3	1.96	0.48
1:H:149:ASN:HD21	2:H:601:NAD:H6N	1.76	0.48
1:A:248:LEU:CD1	1:B:241:LEU:CD1	2.91	0.48
1:A:327:LEU:O	1:A:327:LEU:CD2	2.61	0.48
1:A:241:LEU:HD13	1:B:248:LEU:CD1	2.43	0.48
1:C:281:CYS:HB3	2:C:601:NAD:N1N	2.29	0.48
1:D:149:ASN:OD1	1:D:149:ASN:N	2.44	0.48
1:D:177:THR:N	1:D:178:PRO:HD3	2.29	0.48
1:D:37:ALA:CB	1:D:201:VAL:HG13	2.44	0.48
1:D:87:SER:CB	1:D:92:HIS:O	2.62	0.48
1:G:333:LEU:HD22	1:G:351:LYS:HD3	1.95	0.48
1:G:448:GLY:HA3	1:G:457:ARG:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:223:PHE:CZ	1:H:225:GLY:HA3	2.49	0.48
1:A:172:LYS:CE	2:A:601:NAD:O2B	2.62	0.48
1:A:291:LYS:HE3	1:A:391:ARG:HB3	1.95	0.48
1:B:215:HIS:CD2	1:B:217:ASP:H	2.29	0.48
1:D:302:ILE:HG23	1:D:348:ALA:HB2	1.96	0.48
1:E:328:ARG:HG2	1:E:328:ARG:HH11	1.78	0.48
1:F:333:LEU:HD22	1:F:351:LYS:HD3	1.95	0.48
1:F:119:ILE:HG12	1:F:464:ILE:HG21	1.95	0.48
1:G:126:VAL:HG21	1:G:474:TRP:CH2	2.49	0.48
1:G:325:SER:H	1:G:328:ARG:NH2	2.11	0.48
1:B:223:PHE:CZ	1:B:225:GLY:HA3	2.49	0.48
1:B:94:ILE:CD1	1:B:314:MET:C	2.81	0.48
1:E:329:ARG:NH1	1:E:329:ARG:CG	2.62	0.48
1:E:57:SER:HB2	1:E:138:PRO:HG2	1.96	0.48
1:G:373:PRO:HG3	1:G:390:VAL:HG11	1.96	0.48
1:H:89:ASN:HD21	1:H:177:THR:HA	1.78	0.48
1:A:223:PHE:CZ	1:A:225:GLY:HA3	2.48	0.48
1:B:25:PRO:HA	1:B:362:PHE:CE2	2.49	0.48
1:C:119:ILE:HD11	1:C:464:ILE:HD12	1.95	0.48
1:D:334:SER:O	1:D:338:ILE:HD13	2.13	0.48
1:E:141:VAL:HG22	1:E:168:THR:CG2	2.43	0.48
1:C:141:VAL:HG22	1:C:168:THR:CG2	2.44	0.48
1:C:89:ASN:HD21	1:C:177:THR:HA	1.79	0.48
1:C:37:ALA:CB	1:C:201:VAL:HG13	2.44	0.48
1:D:12:VAL:HG23	1:D:13:ASP:O	2.13	0.48
1:D:215:HIS:CD2	1:D:217:ASP:H	2.28	0.48
1:E:146:VAL:HG22	1:E:173:PRO:HA	1.95	0.48
1:F:458:GLU:O	1:F:459:MET:CB	2.61	0.48
1:F:376:ARG:NH1	1:G:204:TYR:CD2	2.82	0.48
1:A:352:ALA:O	1:A:353:PRO:O	2.32	0.47
1:D:31:ILE:HG22	1:D:32:THR:HG22	1.96	0.47
1:D:405:THR:HG22	1:D:406:GLU:N	2.29	0.47
1:E:97:SER:HA	1:E:101:ASP:HB2	1.96	0.47
1:F:37:ALA:CB	1:F:201:VAL:HG13	2.44	0.47
1:A:32:THR:OG1	1:A:33:ARG:N	2.47	0.47
1:A:243:ARG:CD	1:B:455:TYR:HB3	2.44	0.47
1:G:97:SER:HA	1:G:101:ASP:HB2	1.95	0.47
1:C:148:TRP:HB2	1:C:177:THR:CG2	2.44	0.47
1:C:329:ARG:NH1	1:C:329:ARG:CG	2.67	0.47
1:D:126:VAL:HG21	1:D:474:TRP:CH2	2.50	0.47
1:D:338:ILE:N	1:D:338:ILE:HD13	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10[B]:ARG:CG	1:G:10[B]:ARG:NH1	2.74	0.47
1:H:53:PHE:HB3	1:H:54:PRO:HD3	1.96	0.47
1:A:172:LYS:HD2	1:A:208:ALA:HB3	1.95	0.47
1:C:126:VAL:HG21	1:C:474:TRP:CH2	2.49	0.47
1:C:405:THR:HG22	1:C:406:GLU:N	2.28	0.47
1:G:146:VAL:HG22	1:G:173:PRO:HA	1.97	0.47
1:G:405:THR:HG22	1:G:406:GLU:N	2.29	0.47
1:H:373:PRO:HG3	1:H:390:VAL:HG11	1.95	0.47
1:A:413:LEU:O	1:A:413:LEU:HD12	2.15	0.47
1:E:131:LEU:C	1:E:131:LEU:HD22	2.35	0.47
1:G:12:VAL:HG23	1:G:13:ASP:O	2.14	0.47
1:A:243:ARG:HD2	1:B:455:TYR:CB	2.44	0.47
1:C:413:LEU:HD11	1:C:435:ILE:HG12	1.97	0.47
1:A:281:CYS:SG	2:A:601:NAD:C3N	3.02	0.47
1:B:80:GLU:OE1	1:B:98:ARG:NE	2.47	0.47
1:E:132:ASN:HD21	1:F:445:SER:CB	2.27	0.47
1:E:135:GLN:HE22	1:F:426:HIS:HE1	1.59	0.47
1:E:215:HIS:CD2	1:E:217:ASP:H	2.33	0.47
1:E:334:SER:O	1:E:338:ILE:HD13	2.15	0.47
1:E:373:PRO:O	1:E:375:ASP:N	2.48	0.47
1:F:218:VAL:O	1:F:242:LYS:HE3	2.14	0.47
1:H:480:LYS:O	1:H:481:ILE:C	2.53	0.47
1:A:139:ILE:N	1:A:167:ASN:HD21	2.05	0.47
1:A:37:ALA:CB	1:A:201:VAL:HG13	2.45	0.47
1:B:87:SER:HB3	1:B:97:SER:OG	2.14	0.47
1:C:249:GLY:HA3	2:C:601:NAD:HO2N	1.78	0.47
1:F:95:ARG:CD	1:F:319:GLU:HA	2.45	0.47
1:F:329:ARG:O	1:F:330:ASP:C	2.53	0.47
1:F:417:ASN:HD22	1:F:420:ARG:HB2	1.79	0.47
1:G:323:LEU:HD12	1:G:329:ARG:HA	1.97	0.47
1:A:273:ILE:HG21	1:A:387:VAL:HG22	1.97	0.47
1:B:315:ASP:HB3	1:B:318:THR:OG1	2.14	0.47
1:C:131:LEU:HD22	1:C:131:LEU:C	2.34	0.47
1:E:155:THR:HG21	1:E:181:THR:HB	1.97	0.47
1:G:80:GLU:OE1	1:G:98:ARG:NE	2.48	0.47
1:B:118:LYS:HE3	1:C:111:TYR:CZ	2.50	0.47
1:C:2:GLN:CA	1:C:2:GLN:HE21	2.28	0.47
1:D:139:ILE:N	1:D:167:ASN:HD21	2.00	0.47
1:D:187:LEU:HD23	1:D:187:LEU:HA	1.77	0.47
1:D:201:VAL:CG1	1:D:201:VAL:O	2.61	0.47
1:G:138:PRO:HG3	1:G:165:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:PRO:HB3	1:B:267:ASN:CG	2.35	0.47
1:D:143:ALA:HB1	1:D:212:LEU:HG	1.97	0.47
1:D:18:GLY:HA3	3:D:709:HOH:O	2.15	0.47
1:E:19:THR:HG23	3:E:704:HOH:O	2.15	0.47
1:F:141:VAL:HG23	1:F:168:THR:HG22	1.96	0.47
1:G:218:VAL:O	1:G:242:LYS:HE3	2.14	0.47
1:H:155:THR:CG2	1:H:181:THR:HB	2.45	0.47
1:D:374:GLN:HB3	1:D:374:GLN:HE21	1.57	0.46
1:F:53:PHE:HB3	1:F:54:PRO:HD3	1.98	0.46
1:A:235:GLU:HG3	1:B:238:LYS:CD	2.44	0.46
1:A:149:ASN:HD21	2:A:601:NAD:H5N	1.80	0.46
1:A:94:ILE:H	1:A:94:ILE:HG12	1.42	0.46
1:B:131:LEU:HD22	1:B:131:LEU:C	2.36	0.46
1:B:27:ASP:C	1:B:360:ASN:O	2.54	0.46
1:C:105:THR:OG1	1:C:153:MET:HA	2.16	0.46
1:G:174:SER:O	1:G:176:ILE:N	2.47	0.46
1:H:302:ILE:O	1:H:306:LYS:HG3	2.16	0.46
1:H:25:PRO:HA	1:H:362:PHE:CE2	2.50	0.46
1:H:405:THR:CG2	1:H:406:GLU:N	2.78	0.46
1:B:252:GLY:HA2	1:B:410:GLY:O	2.15	0.46
1:B:76:GLU:O	1:B:79:SER:HB2	2.15	0.46
1:D:448:GLY:HA3	1:D:457:ARG:HD3	1.97	0.46
1:F:1:MET:CG	1:F:2:GLN:N	2.79	0.46
1:G:302:ILE:O	1:G:306:LYS:HG3	2.15	0.46
1:H:334:SER:O	1:H:338:ILE:HD13	2.15	0.46
1:B:10[B]:ARG:NH1	1:B:10[B]:ARG:CG	2.77	0.46
1:B:126:VAL:HG21	1:B:474:TRP:CH2	2.50	0.46
1:B:172:LYS:HD2	1:B:208:ALA:HB3	1.97	0.46
1:B:310:LEU:CD2	1:B:358:LEU:HD21	2.46	0.46
1:C:80:GLU:O	1:C:81:GLU:C	2.49	0.46
1:D:100:LEU:O	1:D:101:ASP:C	2.54	0.46
1:A:10[B]:ARG:CG	1:A:10[B]:ARG:NH1	2.73	0.46
1:A:119:ILE:O	1:C:125:PRO:HG3	2.16	0.46
1:A:31:ILE:HG22	1:A:32:THR:HG22	1.97	0.46
1:C:172:LYS:NZ	1:C:173:PRO:O	2.37	0.46
1:E:323:LEU:HD12	1:E:329:ARG:HA	1.97	0.46
1:H:302:ILE:HG23	1:H:348:ALA:HB2	1.98	0.46
1:A:218:VAL:O	1:A:242:LYS:HE3	2.16	0.46
1:B:86:GLU:OE2	1:B:180:SER:HB2	2.16	0.46
1:F:221:ILE:HD13	1:F:222:ALA:N	2.30	0.46
1:E:137:LYS:HZ2	1:F:426:HIS:CD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:PHE:CZ	1:G:225:GLY:HA3	2.50	0.46
1:A:145:ILE:HG21	2:A:601:NAD:H1B	1.97	0.46
1:D:90:THR:HG22	1:D:177:THR:CG2	2.45	0.46
1:F:249:GLY:HA3	2:F:601:NAD:O2D	2.09	0.46
1:G:328:ARG:NH2	1:G:328:ARG:HB2	2.27	0.46
1:A:162:ALA:HB3	1:A:169:ILE:HD11	1.97	0.46
1:A:328:ARG:HH12	1:A:331:ARG:HD3	1.80	0.46
1:C:135:GLN:HE22	1:D:426:HIS:CE1	2.33	0.46
1:C:70:LYS:HD3	1:C:70:LYS:HA	1.64	0.46
1:F:273:ILE:HG12	1:F:387:VAL:CG2	2.38	0.46
1:G:32:THR:OG1	1:G:33:ARG:N	2.49	0.46
1:A:328:ARG:HD2	1:A:328:ARG:HA	1.46	0.46
1:A:429:HIS:CD2	1:A:450:VAL:CG1	2.99	0.46
1:B:111:TYR:CZ	1:C:118:LYS:HE3	2.50	0.46
1:E:392:PHE:CD1	1:E:398:ALA:HB2	2.51	0.46
1:E:480:LYS:O	1:E:481:ILE:C	2.54	0.46
1:E:487:ARG:C	3:F:709:HOH:O	2.55	0.46
1:F:287:LEU:HA	1:F:287:LEU:HD23	1.79	0.46
1:G:25:PRO:HA	1:G:362:PHE:CE2	2.50	0.46
1:A:459:MET:HE2	1:A:459:MET:HA	1.98	0.46
1:B:477:VAL:HG23	1:B:478:ASP:HB2	1.98	0.46
1:D:148:TRP:HB3	1:D:174:SER:CB	2.45	0.46
1:E:459:MET:HE2	1:E:459:MET:HA	1.98	0.46
1:E:87:SER:CB	1:E:92:HIS:O	2.64	0.46
1:F:86:GLU:OE2	1:F:180:SER:HB2	2.16	0.46
1:G:172:LYS:HD2	1:G:208:ALA:HB3	1.98	0.46
1:G:392:PHE:CD1	1:G:398:ALA:HB2	2.51	0.46
1:G:252:GLY:HA2	1:G:410:GLY:O	2.15	0.46
1:H:5:LEU:HB2	3:H:714:HOH:O	2.16	0.46
1:A:94:ILE:HD13	1:A:314:MET:HA	1.98	0.45
1:C:12:VAL:HG23	1:C:13:ASP:O	2.16	0.45
1:E:37:ALA:CB	1:E:201:VAL:HG13	2.46	0.45
1:H:143:ALA:HB1	1:H:212:LEU:HG	1.98	0.45
1:G:483:PRO:HB3	1:H:267:ASN:CG	2.36	0.45
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.81	0.45
1:A:392:PHE:CD1	1:A:398:ALA:HB2	2.50	0.45
1:D:155:THR:CG2	1:D:181:THR:HB	2.47	0.45
1:D:33:ARG:NH2	1:E:18:GLY:HA2	2.31	0.45
1:D:80:GLU:OE1	1:D:98:ARG:NE	2.49	0.45
1:H:413:LEU:O	1:H:413:LEU:HD12	2.17	0.45
1:H:465:HIS:O	1:H:468:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LEU:HD12	1:A:329:ARG:HA	1.98	0.45
1:A:353:PRO:HD2	1:A:353:PRO:O	2.16	0.45
1:C:218:VAL:O	1:C:242:LYS:HE3	2.17	0.45
1:E:105:THR:OG1	1:E:153:MET:HA	2.16	0.45
1:E:302:ILE:HG23	1:E:348:ALA:HB2	1.97	0.45
1:E:333:LEU:HD22	1:E:351:LYS:HD3	1.98	0.45
1:F:57:SER:HB2	1:F:138:PRO:HG2	1.97	0.45
1:F:155:THR:CG2	1:F:181:THR:HB	2.46	0.45
1:G:70:LYS:HD3	1:G:70:LYS:HA	1.63	0.45
1:A:405:THR:HG22	1:A:406:GLU:N	2.31	0.45
1:A:448:GLY:HA3	1:A:457:ARG:HD3	1.98	0.45
1:B:146:VAL:HG22	1:B:173:PRO:HA	1.98	0.45
1:B:332:VAL:HG12	1:B:333:LEU:N	2.32	0.45
1:B:405:THR:CG2	1:B:406:GLU:N	2.80	0.45
1:C:287:LEU:HA	1:C:287:LEU:HD23	1.77	0.45
1:E:439:LYS:NZ	3:E:706:HOH:O	2.48	0.45
1:F:329:ARG:HG3	1:F:330:ASP:N	2.31	0.45
1:F:331:ARG:HB3	1:F:331:ARG:HE	1.41	0.45
1:F:373:PRO:HG3	1:F:390:VAL:HG11	1.97	0.45
1:G:243:ARG:HD2	1:H:455:TYR:HB3	1.98	0.45
1:A:140:GLY:H	1:A:167:ASN:HD22	1.65	0.45
1:B:302:ILE:HG23	1:B:348:ALA:HB2	1.98	0.45
1:C:247:GLU:HB3	2:C:601:NAD:N7N	2.32	0.45
1:C:392:PHE:CD1	1:C:398:ALA:HB2	2.51	0.45
1:C:411:SER:O	1:C:434:TRP:HE3	1.97	0.45
1:D:260:ALA:O	1:D:262:ILE:HD13	2.17	0.45
1:D:22:VAL:HG23	1:D:34:ILE:HG12	1.96	0.45
1:F:374:GLN:HE21	1:F:374:GLN:HB3	1.56	0.45
1:F:429:HIS:CD2	1:F:450:VAL:CG1	3.00	0.45
1:H:37:ALA:CB	1:H:201:VAL:HG13	2.46	0.45
1:B:46:VAL:HG11	1:B:215:HIS:CD2	2.52	0.45
1:C:97:SER:HA	1:C:101:ASP:HB2	1.97	0.45
1:C:327:LEU:HD21	1:C:331:ARG:CZ	2.44	0.45
1:C:455:TYR:HB3	1:D:243:ARG:CD	2.44	0.45
1:D:57:SER:HB2	1:D:138:PRO:HG2	1.99	0.45
1:D:149:ASN:ND2	2:D:601:NAD:H6N	2.27	0.45
1:E:162:ALA:HB3	1:E:169:ILE:HD11	1.99	0.45
1:E:248:LEU:HB2	1:E:453:SER:HA	1.98	0.45
1:E:76:GLU:O	1:E:79:SER:HB2	2.16	0.45
1:F:131:LEU:HD22	1:F:132:ASN:N	2.32	0.45
1:D:356:LYS:NZ	1:G:10[A]:ARG:NH1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ASN:CG	1:A:479:ALA:HB3	2.37	0.45
1:A:80:GLU:OE1	1:A:98:ARG:NE	2.50	0.45
1:D:32:THR:OG1	1:D:33:ARG:N	2.50	0.45
1:D:248:LEU:HB2	1:D:453:SER:HA	1.99	0.45
1:F:146:VAL:HG22	1:F:173:PRO:HA	1.99	0.45
1:F:140:GLY:H	1:F:167:ASN:ND2	2.14	0.45
1:F:141:VAL:CG2	1:F:168:THR:CG2	2.95	0.45
1:F:249:GLY:HA2	2:F:601:NAD:HO2N	1.71	0.45
1:F:302:ILE:O	1:F:306:LYS:HG3	2.16	0.45
1:A:22:VAL:HG23	1:A:34:ILE:HG12	1.99	0.45
1:D:162:ALA:HB3	1:D:169:ILE:HD11	1.99	0.45
1:D:86:GLU:OE2	1:D:180:SER:HB2	2.16	0.45
1:D:373:PRO:HG3	1:D:390:VAL:HG11	1.99	0.45
1:E:140:GLY:H	1:E:167:ASN:ND2	2.14	0.45
1:E:258:GLU:OE2	1:E:258:GLU:N	2.31	0.45
1:H:187:LEU:HA	1:H:187:LEU:HD23	1.75	0.45
1:H:374:GLN:HB3	1:H:374:GLN:HE21	1.53	0.45
1:A:12:VAL:HG23	1:A:13:ASP:O	2.17	0.45
1:A:86:GLU:OE2	1:A:180:SER:HB2	2.17	0.45
1:F:258:GLU:HB3	1:F:290:HIS:CD2	2.52	0.45
1:F:149:ASN:ND2	2:F:601:NAD:H6N	2.23	0.45
1:G:139:ILE:HB	1:G:167:ASN:HD21	1.82	0.45
1:G:221:ILE:HD13	1:G:222:ALA:N	2.32	0.45
1:G:1:MET:CG	1:G:2:GLN:N	2.80	0.45
1:G:119:ILE:HG12	1:G:464:ILE:HG21	1.99	0.45
1:H:6:TYR:N	3:H:714:HOH:O	2.49	0.45
1:B:105:THR:HG23	1:B:156:SER:HB3	1.98	0.45
1:D:296:GLN:NE2	1:H:394:SER:OG	2.50	0.45
1:F:105:THR:HG23	1:F:156:SER:HB3	1.99	0.45
1:F:390:VAL:HG12	1:F:391:ARG:N	2.32	0.45
1:G:459:MET:HE2	1:G:459:MET:HA	1.99	0.45
1:H:201:VAL:O	1:H:201:VAL:CG1	2.65	0.45
1:H:480:LYS:O	1:H:482:ALA:N	2.50	0.45
1:A:105:THR:HG23	1:A:156:SER:HB3	1.99	0.44
1:A:397:GLU:O	1:A:401:ILE:HG13	2.17	0.44
1:B:258:GLU:HG3	1:B:258:GLU:H	1.41	0.44
1:A:137:LYS:NZ	1:B:426:HIS:CD2	2.85	0.44
1:D:15:VAL:CG1	1:D:16:ALA:N	2.79	0.44
1:D:302:ILE:O	1:D:306:LYS:HG3	2.17	0.44
1:F:154:PHE:HZ	2:F:601:NAD:H5N	1.81	0.44
1:D:1:MET:CG	1:D:2:GLN:N	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LYS:HD3	1:D:70:LYS:HA	1.65	0.44
1:E:86:GLU:OE2	1:E:180:SER:HB2	2.17	0.44
1:F:405:THR:CG2	1:F:406:GLU:N	2.80	0.44
1:F:448:GLY:HA3	1:F:457:ARG:HD3	2.00	0.44
1:G:325:SER:CA	1:G:328:ARG:NH2	2.78	0.44
1:G:417:ASN:ND2	1:G:420:ARG:H	2.15	0.44
1:G:455:TYR:HB3	1:H:243:ARG:CD	2.48	0.44
1:H:100:LEU:O	1:H:101:ASP:C	2.55	0.44
1:H:5:LEU:C	3:H:714:HOH:O	2.56	0.44
1:A:253:ALA:HB2	1:A:286:ARG:NH2	2.33	0.44
1:A:329:ARG:CG	1:A:330:ASP:N	2.77	0.44
1:C:448:GLY:HA3	1:C:457:ARG:HD3	1.99	0.44
1:C:76:GLU:O	1:C:79:SER:HB2	2.17	0.44
1:B:417:ASN:HA	1:D:416:GLN:O	2.17	0.44
1:E:22:VAL:HG23	1:E:34:ILE:HG12	1.99	0.44
1:E:88:LEU:N	1:E:314:MET:HE1	2.32	0.44
1:F:177:THR:N	1:F:178:PRO:HD3	2.32	0.44
1:G:2:GLN:NE2	3:G:703:HOH:O	2.51	0.44
1:H:323:LEU:HD12	1:H:329:ARG:CA	2.44	0.44
1:C:100:LEU:O	1:C:101:ASP:C	2.56	0.44
1:C:80:GLU:OE1	1:C:98:ARG:NE	2.51	0.44
1:F:415:THR:HG22	1:F:416:GLN:H	1.81	0.44
1:G:174:SER:C	1:G:176:ILE:N	2.71	0.44
1:A:376:ARG:O	1:A:380:GLU:HG3	2.17	0.44
1:A:426:HIS:NE2	1:B:137:LYS:CE	2.80	0.44
1:B:237:SER:OG	1:B:244:ILE:HD11	2.17	0.44
1:B:32:THR:OG1	1:B:33:ARG:N	2.49	0.44
1:H:329:ARG:CZ	1:H:330:ASP:OD1	2.66	0.44
1:B:329:ARG:NE	1:B:362:PHE:HA	2.32	0.44
1:C:327:LEU:CD2	1:C:331:ARG:NH2	2.65	0.44
1:C:426:HIS:CD2	1:D:137:LYS:HZ1	2.36	0.44
1:D:172:LYS:HD2	1:D:208:ALA:HB3	2.00	0.44
1:E:390:VAL:HG12	1:E:391:ARG:N	2.32	0.44
1:E:480:LYS:O	1:E:482:ALA:N	2.50	0.44
1:G:149:ASN:ND2	2:G:601:NAD:H5N	2.33	0.44
1:H:328:ARG:HH12	1:H:331:ARG:HH21	1.66	0.44
1:A:105:THR:OG1	1:A:153:MET:HA	2.18	0.44
1:A:486:LYS:NZ	1:B:95:ARG:HH12	2.15	0.44
1:C:143:ALA:HB1	1:C:212:LEU:HG	1.99	0.44
1:C:412:GLY:HA2	1:C:434:TRP:O	2.17	0.44
1:D:274:PHE:HB3	1:D:320:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:481:ILE:HA	1:E:481:ILE:HD12	1.81	0.44
1:F:126:VAL:HG21	1:F:474:TRP:CH2	2.53	0.44
1:G:238:LYS:HD2	1:H:235:GLU:CG	2.48	0.44
1:H:328:ARG:NH1	1:H:331:ARG:NH2	2.65	0.44
1:H:392:PHE:CD1	1:H:398:ALA:HB2	2.53	0.44
1:A:119:ILE:HG12	1:A:464:ILE:HG21	1.98	0.44
1:A:6:TYR:CE2	1:A:9:GLY:HA2	2.53	0.44
1:C:333:LEU:HD22	1:C:351:LYS:HD3	1.98	0.44
1:C:257:PHE:CD2	1:C:415:THR:OG1	2.71	0.44
1:G:37:ALA:CB	1:G:201:VAL:HG13	2.48	0.44
1:G:20:ILE:HG13	1:G:36:ALA:HB2	2.00	0.44
1:H:172:LYS:NZ	1:H:173:PRO:O	2.37	0.44
1:H:376:ARG:O	1:H:380:GLU:HG3	2.17	0.44
1:H:85:LEU:HD11	1:H:179:LEU:HB3	2.00	0.44
1:A:112:PHE:HA	1:A:115:MET:HB3	2.00	0.44
1:D:131:LEU:C	1:D:131:LEU:HD22	2.39	0.44
1:D:218:VAL:O	1:D:242:LYS:HE3	2.18	0.44
1:D:376:ARG:O	1:D:380:GLU:HG3	2.18	0.44
1:E:143:ALA:HB1	1:E:212:LEU:HG	2.00	0.44
1:F:154:PHE:HZ	2:F:601:NAD:C5N	2.31	0.44
1:F:20:ILE:HD11	1:F:204:TYR:CD2	2.52	0.44
1:H:10[B]:ARG:NH1	1:H:10[B]:ARG:CG	2.74	0.44
1:H:273:ILE:HG12	1:H:387:VAL:CG2	2.43	0.44
1:H:1:MET:CG	1:H:2:GLN:N	2.78	0.44
1:A:235:GLU:HG3	1:B:238:LYS:HD2	1.98	0.43
1:B:244:ILE:HG22	1:B:246:LEU:HD23	1.97	0.43
1:B:31:ILE:HG22	1:B:32:THR:HG22	1.99	0.43
1:C:86:GLU:OE2	1:C:180:SER:HB2	2.18	0.43
1:C:271:TRP:O	1:C:275:HIS:HB3	2.18	0.43
1:D:404:ASN:CG	1:D:404:ASN:O	2.56	0.43
1:E:223:PHE:CZ	1:E:225:GLY:HA3	2.53	0.43
1:F:97:SER:HA	1:F:101:ASP:HB2	1.99	0.43
1:F:37:ALA:HB1	1:F:201:VAL:HG13	1.99	0.43
1:G:143:ALA:HB1	1:G:212:LEU:HG	1.99	0.43
1:G:237:SER:OG	1:G:244:ILE:HD11	2.17	0.43
1:H:282:ILE:HD11	1:H:447:PHE:CE1	2.53	0.43
1:A:159:MET:HE3	1:A:169:ILE:HG21	2.00	0.43
1:B:246:LEU:HD22	1:B:246:LEU:HA	1.73	0.43
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.72	0.43
1:G:112:PHE:CZ	1:G:161:PRO:HG3	2.53	0.43
1:H:412:GLY:HA2	1:H:434:TRP:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:SER:HB2	1:A:138:PRO:HG2	2.01	0.43
1:B:12:VAL:HG23	1:B:13:ASP:O	2.18	0.43
1:A:472:SER:O	1:B:432:MET:HA	2.18	0.43
1:B:97:SER:HA	1:B:101:ASP:HB2	2.01	0.43
1:D:37:ALA:HB1	1:D:201:VAL:HG13	2.00	0.43
1:E:10[B]:ARG:CG	1:E:10[B]:ARG:NH1	2.76	0.43
1:F:248:LEU:O	1:F:249:GLY:O	2.36	0.43
1:G:201:VAL:CG1	1:G:201:VAL:O	2.66	0.43
1:G:6:TYR:CE2	1:G:9:GLY:HA2	2.54	0.43
1:A:148:TRP:HD1	1:A:174:SER:OG	1.98	0.43
1:B:183:ARG:NH1	1:B:186:GLU:OE1	2.51	0.43
1:D:253:ALA:HB2	1:D:286:ARG:NH2	2.34	0.43
1:E:221:ILE:HD13	1:E:222:ALA:N	2.34	0.43
1:E:32:THR:OG1	1:E:33:ARG:N	2.51	0.43
1:E:376:ARG:O	1:E:380:GLU:HG3	2.19	0.43
1:F:139:ILE:HB	1:F:167:ASN:HD21	1.84	0.43
1:F:482:ALA:O	1:F:483:PRO:C	2.56	0.43
1:A:429:HIS:CD2	1:A:450:VAL:HG11	2.53	0.43
1:A:432:MET:HA	1:B:472:SER:O	2.18	0.43
1:B:302:ILE:O	1:B:306:LYS:HG3	2.18	0.43
1:B:330:ASP:O	1:B:331:ARG:C	2.56	0.43
1:B:405:THR:HG21	1:B:407:TYR:HB2	2.01	0.43
1:B:6:TYR:CE2	1:B:9:GLY:HA2	2.54	0.43
1:C:338:ILE:N	1:C:338:ILE:CD1	2.81	0.43
1:E:218:VAL:O	1:E:242:LYS:HE3	2.18	0.43
1:A:97:SER:HA	1:A:101:ASP:HB2	2.00	0.43
1:B:37:ALA:HB1	1:B:201:VAL:HG13	2.00	0.43
1:B:413:LEU:HD11	1:B:435:ILE:HG12	2.00	0.43
1:C:235:GLU:OE2	1:D:238:LYS:HD2	2.18	0.43
1:C:314:MET:O	1:C:316:PRO:HD3	2.19	0.43
1:D:323:LEU:HD12	1:D:329:ARG:HA	2.00	0.43
1:F:325:SER:O	1:F:328:ARG:CB	2.67	0.43
1:F:22:VAL:HG23	1:F:34:ILE:HG12	1.99	0.43
1:G:464:ILE:O	1:G:468:THR:HG22	2.18	0.43
1:B:115:MET:HB2	1:C:118:LYS:HE2	1.99	0.43
1:B:390:VAL:HG12	1:B:391:ARG:N	2.34	0.43
1:C:356:LYS:N	1:C:356:LYS:CD	2.63	0.43
1:C:53:PHE:HB3	1:C:54:PRO:HD3	2.01	0.43
1:D:273:ILE:HB	1:D:284:GLY:O	2.18	0.43
1:D:95:ARG:HG3	1:D:96:ASP:N	2.32	0.43
1:F:175:GLU:N	1:F:175:GLU:OE2	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:LEU:HD11	1:F:179:LEU:HB3	2.00	0.43
1:F:480:LYS:O	1:F:481:ILE:C	2.57	0.43
1:G:86:GLU:OE2	1:G:180:SER:HB2	2.19	0.43
1:G:415:THR:HG22	1:G:416:GLN:H	1.82	0.43
1:H:174:SER:C	1:H:176:ILE:H	2.21	0.43
1:H:34:ILE:HD13	1:H:34:ILE:HA	1.78	0.43
1:H:390:VAL:HG12	1:H:391:ARG:N	2.33	0.43
1:H:413:LEU:HD11	1:H:435:ILE:HG12	2.01	0.43
1:B:328:ARG:HE	1:B:383:PHE:HB3	1.84	0.43
1:C:459:MET:HE2	1:C:459:MET:HA	2.00	0.43
1:E:247:GLU:HB3	2:E:601:NAD:H72N	1.81	0.43
1:F:76:GLU:O	1:F:79:SER:HB2	2.19	0.43
1:H:172:LYS:HD2	1:H:208:ALA:HB3	2.01	0.43
1:A:88:LEU:N	1:A:314:MET:HE1	2.34	0.43
1:B:112:PHE:HA	1:B:115:MET:HB3	2.01	0.43
1:B:413:LEU:O	1:B:413:LEU:HD12	2.18	0.43
1:D:10[B]:ARG:CG	1:D:10[B]:ARG:NH1	2.75	0.43
1:D:25:PRO:HA	1:D:362:PHE:CE2	2.54	0.43
1:D:6:TYR:CE2	1:D:9:GLY:HA2	2.54	0.43
1:E:248:LEU:CD2	1:E:248:LEU:N	2.56	0.43
1:F:271:TRP:O	1:F:275:HIS:HB3	2.19	0.43
1:H:204:TYR:HB2	1:H:207:THR:OG1	2.19	0.43
1:A:148:TRP:HB3	1:A:174:SER:CB	2.49	0.42
1:A:76:GLU:O	1:A:79:SER:HB2	2.19	0.42
1:B:329:ARG:HE	1:B:362:PHE:HA	1.83	0.42
1:C:176:ILE:C	1:C:178:PRO:HD3	2.39	0.42
1:D:246:LEU:HD12	1:D:455:TYR:CE2	2.53	0.42
1:E:15:VAL:CG1	1:E:16:ALA:N	2.81	0.42
1:E:441:VAL:HG12	1:E:442:SER:N	2.31	0.42
1:F:162:ALA:HB3	1:F:169:ILE:HD11	2.01	0.42
1:F:429:HIS:CD2	1:F:450:VAL:HG11	2.54	0.42
1:G:76:GLU:O	1:G:79:SER:HB2	2.19	0.42
1:H:57:SER:HB2	1:H:138:PRO:HG2	2.01	0.42
1:A:143:ALA:HB1	1:A:212:LEU:HG	2.01	0.42
1:B:122:SER:HA	1:D:122:SER:HA	2.02	0.42
1:B:329:ARG:O	1:B:330:ASP:C	2.57	0.42
1:B:448:GLY:HA3	1:B:457:ARG:HD3	2.00	0.42
1:D:112:PHE:CZ	1:D:161:PRO:HG3	2.54	0.42
1:C:132:ASN:HD21	1:D:445:SER:HB2	1.84	0.42
1:H:97:SER:HA	1:H:101:ASP:HB2	2.01	0.42
1:H:12:VAL:HG23	1:H:13:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:THR:OG1	1:H:33:ARG:N	2.51	0.42
1:A:185:VAL:CG2	1:A:200:VAL:CG2	2.92	0.42
1:B:392:PHE:CD1	1:B:398:ALA:HB2	2.54	0.42
1:C:250:GLY:HA2	1:C:407:TYR:CB	2.49	0.42
1:E:100:LEU:O	1:E:101:ASP:C	2.58	0.42
1:E:338:ILE:N	1:E:338:ILE:HD13	2.35	0.42
1:F:148:TRP:HD1	1:F:174:SER:OG	2.02	0.42
1:F:87:SER:HB3	1:F:97:SER:OG	2.18	0.42
1:G:287:LEU:HA	1:G:287:LEU:HD23	1.89	0.42
1:G:325:SER:HB2	1:G:328:ARG:HH12	1.76	0.42
1:H:328:ARG:HH12	1:H:331:ARG:NH2	2.17	0.42
1:A:131:LEU:HD22	1:A:131:LEU:C	2.39	0.42
1:B:119:ILE:HD11	1:B:464:ILE:HD12	2.00	0.42
1:B:397:GLU:O	1:B:401:ILE:HG13	2.19	0.42
1:B:429:HIS:CD2	1:B:450:VAL:CG1	3.02	0.42
1:C:57:SER:HB2	1:C:138:PRO:HG2	2.02	0.42
1:D:465:HIS:O	1:D:468:THR:HG22	2.20	0.42
1:E:486:LYS:HG2	1:E:486:LYS:H	1.73	0.42
1:H:410:GLY:O	1:H:411:SER:HB3	2.19	0.42
1:C:112:PHE:HA	1:C:115:MET:HB3	2.02	0.42
1:D:76:GLU:O	1:D:79:SER:HB2	2.20	0.42
1:E:426:HIS:CD2	1:F:137:LYS:HZ2	2.37	0.42
1:E:149:ASN:ND2	2:E:601:NAD:H6N	2.25	0.42
1:E:69:LEU:HD23	1:E:69:LEU:HA	1.87	0.42
1:F:172:LYS:HD2	1:F:208:ALA:HB3	2.00	0.42
1:F:413:LEU:O	1:F:413:LEU:HD12	2.18	0.42
1:E:250:GLY:HA3	1:E:407:TYR:CB	2.44	0.42
1:E:31:ILE:HG22	1:E:32:THR:HG22	2.02	0.42
1:F:12:VAL:HG23	1:F:13:ASP:O	2.20	0.42
1:F:444:GLY:CA	1:F:460:GLY:HA2	2.49	0.42
1:F:6:TYR:CE2	1:F:9:GLY:HA2	2.55	0.42
1:H:105:THR:HG23	1:H:156:SER:HB3	2.00	0.42
1:A:100:LEU:O	1:A:101:ASP:C	2.58	0.42
1:A:149:ASN:HD21	2:A:601:NAD:H6N	1.84	0.42
1:B:149:ASN:ND2	2:B:601:NAD:H5N	2.34	0.42
1:C:151:PRO:HG3	1:C:177:THR:OG1	2.20	0.42
1:D:223:PHE:CZ	1:D:225:GLY:HA3	2.55	0.42
1:F:143:ALA:HB1	1:F:212:LEU:HG	2.01	0.42
1:F:105:THR:OG1	1:F:153:MET:HA	2.19	0.42
1:G:455:TYR:CB	1:H:243:ARG:HD2	2.50	0.42
1:A:171:ILE:O	1:A:173:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:PRO:C	1:A:375:ASP:N	2.72	0.42
1:B:338:ILE:N	1:B:338:ILE:HD13	2.34	0.42
1:B:119:ILE:HG12	1:B:464:ILE:HG21	2.01	0.42
1:C:273:ILE:HG21	1:C:387:VAL:HG22	2.02	0.42
1:D:390:VAL:HG12	1:D:391:ARG:N	2.34	0.42
1:D:415:THR:HG22	1:D:416:GLN:H	1.79	0.42
1:D:464:ILE:HA	1:D:464:ILE:HD13	1.87	0.42
1:E:429:HIS:CD2	1:E:450:VAL:CG1	3.03	0.42
1:F:376:ARG:O	1:F:380:GLU:HG3	2.19	0.42
1:F:464:ILE:HD13	1:F:464:ILE:HA	1.83	0.42
1:G:342:GLN:HE22	1:G:376:ARG:HB2	1.85	0.42
1:A:338:ILE:HD13	1:A:338:ILE:N	2.35	0.42
1:B:358:LEU:HD12	1:B:358:LEU:HA	1.83	0.42
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.87	0.42
1:F:149:ASN:HD21	2:F:601:NAD:H5N	1.84	0.42
1:F:17:GLY:C	1:H:376:ARG:NH1	2.74	0.42
1:H:159:MET:HE3	1:H:169:ILE:HG21	2.02	0.42
1:H:338:ILE:N	1:H:338:ILE:HD13	2.35	0.42
1:H:119:ILE:HG12	1:H:464:ILE:HG21	2.00	0.42
1:H:5:LEU:HB3	3:H:714:HOH:O	2.19	0.42
1:A:314:MET:O	1:A:316:PRO:HD3	2.20	0.42
1:C:414:TRP:CE3	1:C:436:ASN:HA	2.55	0.42
1:D:314:MET:O	1:D:316:PRO:HD3	2.19	0.42
1:E:141:VAL:HG22	1:E:168:THR:HG22	2.02	0.42
1:E:315:ASP:HB3	1:E:318:THR:OG1	2.19	0.42
1:E:405:THR:CG2	1:E:406:GLU:N	2.82	0.42
1:E:413:LEU:HD11	1:E:435:ILE:HG12	2.02	0.42
1:G:329:ARG:CG	1:G:329:ARG:NH1	2.65	0.42
1:G:458:GLU:O	1:G:459:MET:CB	2.61	0.42
1:H:429:HIS:CD2	1:H:450:VAL:CG1	3.03	0.42
1:A:141:VAL:HG22	1:A:168:THR:CG2	2.50	0.41
1:A:2:GLN:CA	1:A:2:GLN:HE21	2.31	0.41
1:C:231:ARG:HG2	1:D:241:LEU:HD21	2.02	0.41
1:D:410:GLY:O	1:D:411:SER:HB3	2.19	0.41
1:H:247:GLU:OE1	2:H:601:NAD:C7N	2.67	0.41
1:B:22:VAL:HG23	1:B:34:ILE:HG12	1.99	0.41
1:C:258:GLU:HG2	1:C:259:ASP:H	1.85	0.41
1:C:31:ILE:HG22	1:C:32:THR:HG22	2.02	0.41
1:C:404:ASN:CG	1:C:404:ASN:O	2.59	0.41
1:C:410:GLY:O	1:C:411:SER:HB3	2.20	0.41
1:D:414:TRP:CE3	1:D:436:ASN:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:141:VAL:HG22	1:G:168:THR:CG2	2.50	0.41
1:G:187:LEU:HD23	1:G:187:LEU:HA	1.82	0.41
1:G:413:LEU:O	1:G:413:LEU:HD12	2.20	0.41
1:A:132:ASN:ND2	1:B:445:SER:HB2	2.35	0.41
1:A:69:LEU:HA	1:A:69:LEU:HD23	1.82	0.41
1:B:2:GLN:NE2	3:B:705:HOH:O	2.52	0.41
1:C:223:PHE:CZ	1:C:225:GLY:HA3	2.55	0.41
1:C:274:PHE:HB3	1:C:320:MET:CE	2.50	0.41
1:C:22:VAL:HG23	1:C:34:ILE:HG12	2.02	0.41
1:C:405:THR:CG2	1:C:406:GLU:N	2.83	0.41
1:D:221:ILE:O	1:D:221:ILE:HG23	2.20	0.41
1:E:274:PHE:HB3	1:E:320:MET:CE	2.50	0.41
1:E:412:GLY:HA2	1:E:434:TRP:O	2.19	0.41
1:E:464:ILE:HD13	1:E:464:ILE:HA	1.87	0.41
1:E:482:ALA:O	1:E:483:PRO:C	2.57	0.41
1:G:185:VAL:CG2	1:G:200:VAL:CG2	2.97	0.41
1:H:458:GLU:O	1:H:459:MET:CB	2.59	0.41
1:H:464:ILE:HA	1:H:464:ILE:HD13	1.82	0.41
1:A:412:GLY:HA2	1:A:434:TRP:O	2.19	0.41
1:B:271:TRP:O	1:B:275:HIS:HB3	2.19	0.41
1:B:291:LYS:HE3	1:B:391:ARG:HB3	2.03	0.41
1:B:88:LEU:HA	1:B:314:MET:HE1	2.02	0.41
1:C:282:ILE:HD11	1:C:439:LYS:CG	2.45	0.41
1:D:482:ALA:O	1:D:483:PRO:C	2.58	0.41
1:E:2:GLN:CA	1:E:2:GLN:HE21	2.33	0.41
1:G:69:LEU:HA	1:G:69:LEU:HD23	1.82	0.41
1:B:245:GLN:O	1:B:246:LEU:HD22	2.18	0.41
1:B:405:THR:CG2	1:B:407:TYR:HB2	2.51	0.41
1:C:37:ALA:HB1	1:C:201:VAL:HG13	2.02	0.41
1:C:1:MET:CG	1:C:2:GLN:N	2.82	0.41
1:D:405:THR:CG2	1:D:406:GLU:N	2.83	0.41
1:E:194:PRO:HB2	1:E:197:VAL:HG23	2.01	0.41
1:E:70:LYS:HD3	1:E:70:LYS:HA	1.67	0.41
1:G:112:PHE:HA	1:G:115:MET:HB3	2.01	0.41
1:G:483:PRO:HB3	1:H:267:ASN:OD1	2.20	0.41
1:A:426:HIS:CD2	1:B:137:LYS:CE	3.04	0.41
1:B:177:THR:N	1:B:178:PRO:HD3	2.35	0.41
1:C:185:VAL:CG2	1:C:200:VAL:CG2	2.95	0.41
1:D:88:LEU:N	1:D:314:MET:HE1	2.35	0.41
1:H:271:TRP:O	1:H:275:HIS:HB3	2.21	0.41
1:B:124:ILE:HA	1:B:125:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ALA:HB3	1:B:169:ILE:HD11	2.01	0.41
1:B:477:VAL:HG23	1:B:478:ASP:N	2.34	0.41
1:C:247:GLU:OE1	2:C:601:NAD:O7N	2.39	0.41
1:D:413:LEU:HD11	1:D:435:ILE:HG12	2.03	0.41
1:D:87:SER:HB3	1:D:97:SER:OG	2.20	0.41
1:E:231:ARG:HG2	1:F:241:LEU:HD21	2.02	0.41
1:E:413:LEU:O	1:E:413:LEU:HD12	2.20	0.41
1:F:410:GLY:O	1:F:411:SER:HB3	2.20	0.41
1:F:465:HIS:O	1:F:468:THR:HG22	2.20	0.41
1:F:93:PRO:CB	1:F:95:ARG:HG2	2.49	0.41
1:G:174:SER:O	1:G:175:GLU:C	2.59	0.41
1:G:273:ILE:HG21	1:G:387:VAL:HG22	2.01	0.41
1:H:124:ILE:HA	1:H:125:PRO:HD3	1.91	0.41
1:H:136:ARG:NH1	1:H:136:ARG:HG2	2.36	0.41
1:H:139:ILE:HB	1:H:167:ASN:HD21	1.84	0.41
1:H:429:HIS:CD2	1:H:450:VAL:HG11	2.56	0.41
1:B:148:TRP:HB3	1:B:174:SER:CB	2.51	0.41
1:B:411:SER:O	1:B:433:CYS:HA	2.19	0.41
1:C:155:THR:HG21	1:C:181:THR:HB	2.02	0.41
1:C:71:LEU:HD22	1:C:188:MET:HG2	2.02	0.41
1:C:426:HIS:CE1	1:D:135:GLN:NE2	2.88	0.41
1:D:338:ILE:CD1	1:D:338:ILE:N	2.82	0.41
1:D:441:VAL:HG12	1:D:442:SER:N	2.34	0.41
1:F:2:GLN:HE21	1:F:2:GLN:CA	2.33	0.41
1:G:10[A]:ARG:NE	3:G:702:HOH:O	2.27	0.41
1:G:271:TRP:O	1:G:275:HIS:HB3	2.21	0.41
1:F:17:GLY:C	1:H:376:ARG:HH12	2.24	0.41
1:H:459:MET:HE2	1:H:459:MET:HA	2.03	0.41
1:B:174:SER:O	1:B:177:THR:N	2.50	0.41
1:C:64:ARG:HD3	1:C:166:GLY:HA2	2.03	0.41
1:E:414:TRP:CE3	1:E:436:ASN:HA	2.55	0.41
1:E:465:HIS:O	1:E:468:THR:HG22	2.21	0.41
1:F:10[B]:ARG:NH1	1:F:10[B]:ARG:CG	2.74	0.41
1:F:15:VAL:CG1	1:F:16:ALA:N	2.83	0.41
1:F:412:GLY:HA2	1:F:434:TRP:O	2.20	0.41
1:G:204:TYR:HB2	1:G:207:THR:OG1	2.21	0.41
1:G:481:ILE:N	1:G:481:ILE:HD13	2.32	0.41
1:H:141:VAL:HG22	1:H:168:THR:CG2	2.51	0.41
1:H:146:VAL:HG22	1:H:173:PRO:HA	2.03	0.41
1:H:185:VAL:CG2	1:H:200:VAL:CG2	2.97	0.41
1:H:258:GLU:HG3	1:H:290:HIS:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:481:ILE:HA	1:H:481:ILE:HD12	1.81	0.41
1:A:2:GLN:NE2	3:A:703:HOH:O	2.54	0.41
1:A:37:ALA:HB1	1:A:201:VAL:HG13	2.02	0.41
1:B:20:ILE:HG13	1:B:36:ALA:HB2	2.03	0.41
1:C:10[B]:ARG:NH2	3:C:709:HOH:O	2.54	0.41
1:C:15:VAL:CG1	1:C:16:ALA:N	2.84	0.41
1:C:172:LYS:HD2	1:C:208:ALA:HB3	2.02	0.41
1:D:112:PHE:HA	1:D:115:MET:HB3	2.02	0.41
1:D:246:LEU:HD12	1:D:455:TYR:CZ	2.56	0.41
1:B:416:GLN:O	1:D:417:ASN:HA	2.21	0.41
1:E:290:HIS:HD2	1:E:292:ASP:H	1.69	0.41
1:F:159:MET:HE3	1:F:169:ILE:HG21	2.02	0.41
1:F:282:ILE:HD13	1:F:434:TRP:HH2	1.85	0.41
1:F:390:VAL:HG12	1:F:391:ARG:H	1.86	0.41
1:F:404:ASN:CG	1:F:404:ASN:O	2.57	0.41
1:G:338:ILE:HD13	1:G:338:ILE:N	2.36	0.41
1:G:405:THR:CG2	1:G:406:GLU:N	2.83	0.41
1:H:218:VAL:O	1:H:242:LYS:HE3	2.20	0.41
1:B:143:ALA:HB1	1:B:212:LEU:HG	2.02	0.41
1:C:331:ARG:HA	1:C:331:ARG:HD3	1.73	0.41
1:D:46:VAL:HG11	1:D:215:HIS:CD2	2.56	0.41
1:D:237:SER:OG	1:D:244:ILE:HD11	2.21	0.41
1:D:271:TRP:O	1:D:275:HIS:HB3	2.21	0.41
1:E:131:LEU:HD22	1:E:132:ASN:N	2.36	0.41
1:E:273:ILE:HG12	1:E:387:VAL:CG2	2.40	0.41
1:F:325:SER:HG	1:F:328:ARG:CG	1.92	0.41
1:F:327:LEU:O	1:F:331:ARG:CG	2.69	0.41
1:F:459:MET:HE2	1:F:459:MET:HA	2.03	0.41
1:F:480:LYS:O	1:F:482:ALA:N	2.53	0.41
1:H:448:GLY:HA3	1:H:457:ARG:HD3	2.03	0.41
1:H:49:ALA:HB1	1:H:141:VAL:HG22	2.03	0.41
1:A:147:PRO:HD2	1:A:154:PHE:CE2	2.55	0.40
1:A:329:ARG:NH1	1:A:329:ARG:CG	2.42	0.40
1:C:146:VAL:HG22	1:C:173:PRO:HA	2.03	0.40
1:C:25:PRO:HA	1:C:362:PHE:CD2	2.57	0.40
1:D:282:ILE:O	1:D:282:ILE:CG2	2.68	0.40
1:D:2:GLN:CA	1:D:2:GLN:HE21	2.34	0.40
1:E:147:PRO:HD2	1:E:154:PHE:CE2	2.56	0.40
1:G:151:PRO:HG3	1:G:177:THR:OG1	2.21	0.40
1:B:34:ILE:HD13	1:B:34:ILE:HA	1.76	0.40
1:B:376:ARG:O	1:B:380:GLU:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LEU:HD22	1:C:132:ASN:N	2.35	0.40
1:C:376:ARG:O	1:C:380:GLU:HG3	2.21	0.40
1:C:390:VAL:HG12	1:C:391:ARG:N	2.36	0.40
1:D:136:ARG:HG2	1:D:136:ARG:NH1	2.35	0.40
1:E:174:SER:C	1:E:176:ILE:N	2.75	0.40
1:F:187:LEU:HA	1:F:187:LEU:HD23	1.72	0.40
1:F:70:LYS:HA	1:F:70:LYS:HD3	1.66	0.40
1:G:126:VAL:O	1:G:127:ASP:C	2.60	0.40
1:G:376:ARG:O	1:G:380:GLU:HG3	2.20	0.40
1:G:409:LEU:HD12	1:G:449:GLY:CA	2.52	0.40
1:G:7:ILE:HG23	1:G:45:ALA:HA	2.03	0.40
1:H:37:ALA:HB1	1:H:201:VAL:HG13	2.02	0.40
1:H:274:PHE:HB3	1:H:320:MET:CE	2.51	0.40
1:A:141:VAL:HG22	1:A:168:THR:HG22	2.03	0.40
1:C:429:HIS:CD2	1:C:450:VAL:CG1	3.05	0.40
1:C:94:ILE:HD11	1:C:314:MET:HA	2.01	0.40
1:F:32:THR:OG1	1:F:33:ARG:N	2.54	0.40
1:G:131:LEU:HD22	1:G:131:LEU:C	2.41	0.40
1:H:151:PRO:HG3	1:H:177:THR:OG1	2.21	0.40
1:H:248:LEU:CD2	1:H:248:LEU:N	2.72	0.40
1:H:482:ALA:O	1:H:483:PRO:C	2.57	0.40
1:A:99:GLY:O	1:A:100:LEU:HD12	2.21	0.40
1:A:426:HIS:HD2	1:B:137:LYS:HZ2	1.69	0.40
1:B:277:GLN:HE22	1:B:321:GLY:H	1.69	0.40
1:B:332:VAL:O	1:B:335:TYR:N	2.54	0.40
1:G:162:ALA:HB3	1:G:169:ILE:HD11	2.03	0.40
1:G:243:ARG:CD	1:H:455:TYR:HB3	2.52	0.40
1:G:464:ILE:HA	1:G:464:ILE:HD13	1.78	0.40
1:H:112:PHE:HA	1:H:115:MET:HB3	2.04	0.40
1:H:140:GLY:H	1:H:167:ASN:ND2	2.20	0.40
1:A:245:GLN:C	1:A:246:LEU:HD23	2.41	0.40
1:A:271:TRP:O	1:A:275:HIS:HB3	2.22	0.40
1:C:174:SER:O	1:C:176:ILE:N	2.55	0.40
1:C:94:ILE:CD1	1:C:314:MET:HA	2.51	0.40
1:E:1:MET:HG3	1:E:2:GLN:H	1.87	0.40
1:E:271:TRP:O	1:E:275:HIS:HB3	2.21	0.40
1:E:445:SER:HB2	1:F:132:ASN:HD21	1.84	0.40
1:G:177:THR:N	1:G:178:PRO:HD3	2.36	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	486/495 (98%)	446 (92%)	36 (7%)	4 (1%)	19	54
1	B	486/495 (98%)	443 (91%)	41 (8%)	2 (0%)	34	69
1	C	486/495 (98%)	445 (92%)	40 (8%)	1 (0%)	47	79
1	D	486/495 (98%)	448 (92%)	35 (7%)	3 (1%)	25	59
1	E	486/495 (98%)	450 (93%)	34 (7%)	2 (0%)	34	69
1	F	486/495 (98%)	444 (91%)	39 (8%)	3 (1%)	25	59
1	G	486/495 (98%)	447 (92%)	35 (7%)	4 (1%)	19	54
1	H	486/495 (98%)	446 (92%)	37 (8%)	3 (1%)	25	59
All	All	3888/3960 (98%)	3569 (92%)	297 (8%)	22 (1%)	25	59

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	459	MET
1	E	481	ILE
1	F	481	ILE
1	G	459	MET
1	H	481	ILE
1	B	175	GLU
1	D	459	MET
1	G	175	GLU
1	H	175	GLU
1	A	175	GLU
1	C	97	SER
1	G	327	LEU
1	G	355	ASP
1	H	355	ASP
1	F	101	ASP
1	D	486	LYS
1	F	249	GLY

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Mol	Chain	Res	Type
1	D	178	PRO
1	A	332	VAL
1	A	147	PRO
1	E	147	PRO
1	A	178	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	377/383 (98%)	335 (89%)	42 (11%)	6 24
1	B	377/383 (98%)	331 (88%)	46 (12%)	5 19
1	C	377/383 (98%)	332 (88%)	45 (12%)	5 20
1	D	377/383 (98%)	329 (87%)	48 (13%)	4 18
1	E	377/383 (98%)	333 (88%)	44 (12%)	5 22
1	F	377/383 (98%)	335 (89%)	42 (11%)	6 24
1	G	377/383 (98%)	335 (89%)	42 (11%)	6 24
1	H	377/383 (98%)	334 (89%)	43 (11%)	5 23
All	All	3016/3064 (98%)	2664 (88%)	352 (12%)	5 22

All (352) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	12	VAL
1	A	29	SER
1	A	32	THR
1	A	34	ILE
1	A	38	GLU
1	A	42	VAL
1	A	81	GLU
1	A	94	ILE
1	A	95	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	126	VAL
1	A	131	LEU
1	A	149	ASN
1	A	168	THR
1	A	172	LYS
1	A	181	THR
1	A	221	ILE
1	A	232	ARG
1	A	243	ARG
1	A	251	LYS
1	A	271	TRP
1	A	277	GLN
1	A	281	CYS
1	A	327	LEU
1	A	328	ARG
1	A	329	ARG
1	A	331	ARG
1	A	338	ILE
1	A	346	VAL
1	A	354	ASP
1	A	355	ASP
1	A	356	LYS
1	A	374	GLN
1	A	377	VAL
1	A	393	SER
1	A	399	LEU
1	A	404	ASN
1	A	432	MET
1	A	455	TYR
1	A	477	VAL
1	A	481	ILE
1	A	487	ARG
1	B	1	MET
1	B	2	GLN
1	B	15	VAL
1	B	29	SER
1	B	32	THR
1	B	38	GLU
1	B	42	VAL
1	B	81	GLU
1	B	94	ILE
1	B	95	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	126	VAL
1	B	131	LEU
1	B	149	ASN
1	B	153	MET
1	B	168	THR
1	B	181	THR
1	B	185	VAL
1	B	221	ILE
1	B	232	ARG
1	B	243	ARG
1	B	246	LEU
1	B	248	LEU
1	B	251	LYS
1	B	258	GLU
1	B	271	TRP
1	B	277	GLN
1	B	281	CYS
1	B	327	LEU
1	B	329	ARG
1	B	331	ARG
1	B	338	ILE
1	B	346	VAL
1	B	356	LYS
1	B	358	LEU
1	B	374	GLN
1	B	377	VAL
1	B	393	SER
1	B	399	LEU
1	B	404	ASN
1	B	432	MET
1	B	455	TYR
1	B	477	VAL
1	B	478	ASP
1	B	480	LYS
1	B	481	ILE
1	B	487	ARG
1	C	2	GLN
1	C	15	VAL
1	C	29	SER
1	C	32	THR
1	C	34	ILE
1	C	38	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	42	VAL
1	C	80	GLU
1	C	92	HIS
1	C	94	ILE
1	C	126	VAL
1	C	131	LEU
1	C	149	ASN
1	C	153	MET
1	C	168	THR
1	C	181	THR
1	C	221	ILE
1	C	232	ARG
1	C	251	LYS
1	C	258	GLU
1	C	259	ASP
1	C	261	ASN
1	C	271	TRP
1	C	277	GLN
1	C	281	CYS
1	C	282	ILE
1	C	327	LEU
1	C	328	ARG
1	C	329	ARG
1	C	331	ARG
1	C	338	ILE
1	C	346	VAL
1	C	355	ASP
1	C	356	LYS
1	C	358	LEU
1	C	374	GLN
1	C	393	SER
1	C	399	LEU
1	C	404	ASN
1	C	455	TYR
1	C	477	VAL
1	C	478	ASP
1	C	480	LYS
1	C	481	ILE
1	C	487	ARG
1	D	2	GLN
1	D	12	VAL
1	D	29	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	34	ILE
1	D	38	GLU
1	D	42	VAL
1	D	80	GLU
1	D	94	ILE
1	D	95	ARG
1	D	126	VAL
1	D	131	LEU
1	D	139	ILE
1	D	146	VAL
1	D	149	ASN
1	D	153	MET
1	D	168	THR
1	D	174	SER
1	D	181	THR
1	D	185	VAL
1	D	221	ILE
1	D	232	ARG
1	D	243	ARG
1	D	251	LYS
1	D	258	GLU
1	D	262	ILE
1	D	271	TRP
1	D	277	GLN
1	D	281	CYS
1	D	327	LEU
1	D	328	ARG
1	D	329	ARG
1	D	331	ARG
1	D	338	ILE
1	D	346	VAL
1	D	351	LYS
1	D	354	ASP
1	D	356	LYS
1	D	374	GLN
1	D	375	ASP
1	D	377	VAL
1	D	393	SER
1	D	399	LEU
1	D	404	ASN
1	D	432	MET
1	D	455	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	477	VAL
1	D	481	ILE
1	D	487	ARG
1	E	2	GLN
1	E	12	VAL
1	E	29	SER
1	E	34	ILE
1	E	38	GLU
1	E	42	VAL
1	E	80	GLU
1	E	81	GLU
1	E	94	ILE
1	E	95	ARG
1	E	126	VAL
1	E	131	LEU
1	E	149	ASN
1	E	153	MET
1	E	168	THR
1	E	181	THR
1	E	185	VAL
1	E	221	ILE
1	E	232	ARG
1	E	251	LYS
1	E	271	TRP
1	E	277	GLN
1	E	281	CYS
1	E	327	LEU
1	E	328	ARG
1	E	329	ARG
1	E	338	ILE
1	E	346	VAL
1	E	355	ASP
1	E	356	LYS
1	E	358	LEU
1	E	374	GLN
1	E	375	ASP
1	E	377	VAL
1	E	383	PHE
1	E	393	SER
1	E	399	LEU
1	E	404	ASN
1	E	432	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	441	VAL
1	E	455	TYR
1	E	477	VAL
1	E	481	ILE
1	E	487	ARG
1	F	2	GLN
1	F	29	SER
1	F	32	THR
1	F	38	GLU
1	F	42	VAL
1	F	80	GLU
1	F	81	GLU
1	F	94	ILE
1	F	126	VAL
1	F	131	LEU
1	F	149	ASN
1	F	153	MET
1	F	168	THR
1	F	174	SER
1	F	181	THR
1	F	221	ILE
1	F	232	ARG
1	F	251	LYS
1	F	259	ASP
1	F	261	ASN
1	F	271	TRP
1	F	277	GLN
1	F	281	CYS
1	F	327	LEU
1	F	328	ARG
1	F	329	ARG
1	F	331	ARG
1	F	338	ILE
1	F	346	VAL
1	F	355	ASP
1	F	356	LYS
1	F	358	LEU
1	F	374	GLN
1	F	377	VAL
1	F	393	SER
1	F	399	LEU
1	F	404	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	432	MET
1	F	455	TYR
1	F	477	VAL
1	F	481	ILE
1	F	487	ARG
1	G	2	GLN
1	G	12	VAL
1	G	15	VAL
1	G	29	SER
1	G	32	THR
1	G	34	ILE
1	G	38	GLU
1	G	42	VAL
1	G	94	ILE
1	G	95	ARG
1	G	126	VAL
1	G	131	LEU
1	G	149	ASN
1	G	153	MET
1	G	168	THR
1	G	181	THR
1	G	221	ILE
1	G	232	ARG
1	G	243	ARG
1	G	261	ASN
1	G	271	TRP
1	G	277	GLN
1	G	281	CYS
1	G	327	LEU
1	G	328	ARG
1	G	329	ARG
1	G	338	ILE
1	G	346	VAL
1	G	355	ASP
1	G	356	LYS
1	G	374	GLN
1	G	377	VAL
1	G	383	PHE
1	G	393	SER
1	G	399	LEU
1	G	404	ASN
1	G	432	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	455	TYR
1	G	477	VAL
1	G	478	ASP
1	G	481	ILE
1	G	487	ARG
1	H	2	GLN
1	H	12	VAL
1	H	29	SER
1	H	38	GLU
1	H	42	VAL
1	H	80	GLU
1	H	81	GLU
1	H	94	ILE
1	H	95	ARG
1	H	126	VAL
1	H	131	LEU
1	H	141	VAL
1	H	149	ASN
1	H	153	MET
1	H	168	THR
1	H	181	THR
1	H	221	ILE
1	H	232	ARG
1	H	243	ARG
1	H	258	GLU
1	H	271	TRP
1	H	277	GLN
1	H	281	CYS
1	H	327	LEU
1	H	328	ARG
1	H	329	ARG
1	H	331	ARG
1	H	338	ILE
1	H	346	VAL
1	H	355	ASP
1	H	356	LYS
1	H	358	LEU
1	H	374	GLN
1	H	377	VAL
1	H	383	PHE
1	H	393	SER
1	H	399	LEU

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Mol	Chain	Res	Type
1	H	404	ASN
1	H	432	MET
1	H	455	TYR
1	H	477	VAL
1	H	481	ILE
1	H	487	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	89	ASN
1	A	132	ASN
1	A	167	ASN
1	A	215	HIS
1	A	277	GLN
1	A	279	GLN
1	A	290	HIS
1	A	374	GLN
1	A	379	GLN
1	A	404	ASN
1	A	417	ASN
1	A	426	HIS
1	B	2	GLN
1	B	89	ASN
1	B	132	ASN
1	B	215	HIS
1	B	277	GLN
1	B	279	GLN
1	B	290	HIS
1	B	374	GLN
1	B	379	GLN
1	B	404	ASN
1	B	416	GLN
1	B	417	ASN
1	B	426	HIS
1	C	2	GLN
1	C	89	ASN
1	C	132	ASN
1	C	167	ASN
1	C	215	HIS
1	C	261	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	277	GLN
1	C	279	GLN
1	C	290	HIS
1	C	374	GLN
1	C	379	GLN
1	C	404	ASN
1	C	417	ASN
1	C	426	HIS
1	D	2	GLN
1	D	89	ASN
1	D	132	ASN
1	D	167	ASN
1	D	215	HIS
1	D	277	GLN
1	D	279	GLN
1	D	290	HIS
1	D	296	GLN
1	D	374	GLN
1	D	379	GLN
1	D	404	ASN
1	D	416	GLN
1	D	417	ASN
1	D	426	HIS
1	E	2	GLN
1	E	89	ASN
1	E	132	ASN
1	E	167	ASN
1	E	215	HIS
1	E	277	GLN
1	E	279	GLN
1	E	290	HIS
1	E	374	GLN
1	E	379	GLN
1	E	404	ASN
1	E	417	ASN
1	E	426	HIS
1	E	484	HIS
1	F	2	GLN
1	F	89	ASN
1	F	132	ASN
1	F	167	ASN
1	F	215	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	261	ASN
1	F	277	GLN
1	F	279	GLN
1	F	290	HIS
1	F	374	GLN
1	F	379	GLN
1	F	404	ASN
1	F	417	ASN
1	F	426	HIS
1	G	2	GLN
1	G	89	ASN
1	G	132	ASN
1	G	167	ASN
1	G	215	HIS
1	G	261	ASN
1	G	277	GLN
1	G	279	GLN
1	G	290	HIS
1	G	374	GLN
1	G	379	GLN
1	G	404	ASN
1	G	417	ASN
1	G	426	HIS
1	G	465	HIS
1	H	2	GLN
1	H	89	ASN
1	H	132	ASN
1	H	135	GLN
1	H	167	ASN
1	H	215	HIS
1	H	277	GLN
1	H	279	GLN
1	H	290	HIS
1	H	374	GLN
1	H	379	GLN
1	H	404	ASN
1	H	417	ASN
1	H	429	HIS
1	H	465	HIS

### 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	C	601	-	42,48,48	2.73	12 (28%)	50,73,73	2.03	18 (36%)
2	NAD	E	601	-	42,48,48	2.88	17 (40%)	50,73,73	1.99	19 (38%)
2	NAD	G	601	-	42,48,48	2.78	17 (40%)	50,73,73	2.16	21 (42%)
2	NAD	H	601	-	42,48,48	2.72	17 (40%)	50,73,73	2.20	17 (34%)
2	NAD	A	601	-	42,48,48	2.74	17 (40%)	50,73,73	2.23	22 (44%)
2	NAD	B	601	-	42,48,48	2.60	16 (38%)	50,73,73	2.03	18 (36%)
2	NAD	D	601	-	42,48,48	2.84	13 (30%)	50,73,73	2.10	15 (30%)
2	NAD	F	601	-	42,48,48	2.62	14 (33%)	50,73,73	2.16	20 (40%)

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	C	601	-	-	10/26/62/62	0/5/5/5
2	NAD	E	601	-	-	7/26/62/62	0/5/5/5
2	NAD	G	601	-	-	11/26/62/62	0/5/5/5
2	NAD	H	601	-	-	12/26/62/62	0/5/5/5
2	NAD	A	601	-	-	11/26/62/62	0/5/5/5
2	NAD	B	601	-	-	9/26/62/62	0/5/5/5
2	NAD	D	601	-	-	9/26/62/62	0/5/5/5
2	NAD	F	601	-	-	13/26/62/62	0/5/5/5

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAD	C7N-N7N	9.57	1.51	1.33
2	E	601	NAD	C2N-N1N	8.92	1.45	1.35
2	G	601	NAD	C2N-N1N	8.80	1.45	1.35
2	A	601	NAD	C2N-N1N	8.65	1.45	1.35
2	H	601	NAD	C2N-N1N	8.51	1.45	1.35
2	C	601	NAD	C2N-N1N	8.45	1.45	1.35
2	E	601	NAD	C2N-C3N	8.23	1.51	1.39
2	F	601	NAD	C2N-N1N	7.84	1.44	1.35
2	C	601	NAD	C2N-C3N	7.80	1.51	1.39
2	H	601	NAD	C2N-C3N	7.76	1.51	1.39
2	B	601	NAD	C2N-N1N	7.75	1.44	1.35
2	G	601	NAD	C2N-C3N	7.71	1.50	1.39
2	A	601	NAD	C2N-C3N	7.33	1.50	1.39
2	F	601	NAD	C2N-C3N	7.04	1.49	1.39
2	B	601	NAD	C2N-C3N	6.99	1.49	1.39
2	D	601	NAD	C2A-N3A	6.86	1.43	1.32
2	C	601	NAD	C7N-N7N	6.21	1.44	1.33
2	E	601	NAD	C7N-N7N	6.21	1.44	1.33
2	G	601	NAD	C7N-N7N	6.02	1.44	1.33
2	F	601	NAD	C7N-N7N	5.97	1.44	1.33
2	B	601	NAD	C7N-N7N	5.90	1.44	1.33
2	H	601	NAD	C7N-N7N	5.87	1.44	1.33
2	D	601	NAD	C6N-N1N	5.85	1.49	1.35
2	A	601	NAD	C7N-N7N	5.53	1.43	1.33
2	D	601	NAD	PN-O1N	4.61	1.67	1.50
2	B	601	NAD	O4D-C1D	4.61	1.47	1.41
2	C	601	NAD	O4D-C1D	4.52	1.47	1.41
2	A	601	NAD	O4D-C1D	4.42	1.47	1.41
2	D	601	NAD	C2N-C3N	4.36	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	NAD	O4D-C1D	4.15	1.46	1.41
2	F	601	NAD	O4D-C1D	4.14	1.46	1.41
2	E	601	NAD	C4N-C3N	4.02	1.46	1.39
2	D	601	NAD	PA-O1A	3.98	1.65	1.50
2	E	601	NAD	O4D-C1D	3.93	1.46	1.41
2	D	601	NAD	C8A-N7A	3.91	1.41	1.34
2	G	601	NAD	O4D-C1D	3.88	1.46	1.41
2	D	601	NAD	C2N-N1N	3.87	1.39	1.35
2	G	601	NAD	C2A-N3A	3.86	1.38	1.32
2	F	601	NAD	C2B-C1B	-3.84	1.47	1.53
2	E	601	NAD	C6N-C5N	3.83	1.47	1.38
2	H	601	NAD	C2B-C1B	-3.83	1.48	1.53
2	G	601	NAD	C4N-C3N	3.70	1.45	1.39
2	A	601	NAD	C6A-N6A	3.66	1.47	1.34
2	C	601	NAD	C6N-C5N	3.60	1.46	1.38
2	D	601	NAD	C6A-N6A	3.58	1.47	1.34
2	G	601	NAD	C2B-C3B	-3.58	1.43	1.53
2	F	601	NAD	C6A-N6A	3.55	1.47	1.34
2	C	601	NAD	C6A-N6A	3.50	1.46	1.34
2	A	601	NAD	C2A-N3A	3.47	1.37	1.32
2	D	601	NAD	C3D-C4D	3.47	1.61	1.53
2	A	601	NAD	C4N-C3N	3.45	1.45	1.39
2	H	601	NAD	C6A-N6A	3.44	1.46	1.34
2	B	601	NAD	C6A-N6A	3.40	1.46	1.34
2	C	601	NAD	C2A-N3A	3.38	1.37	1.32
2	F	601	NAD	C4N-C3N	3.38	1.45	1.39
2	E	601	NAD	C6A-N6A	3.35	1.46	1.34
2	G	601	NAD	C6A-N6A	3.33	1.46	1.34
2	B	601	NAD	C6N-C5N	3.32	1.46	1.38
2	E	601	NAD	C2A-N3A	3.32	1.37	1.32
2	C	601	NAD	C4N-C3N	3.30	1.45	1.39
2	G	601	NAD	C6N-C5N	3.29	1.45	1.38
2	E	601	NAD	C4A-N3A	3.29	1.40	1.35
2	F	601	NAD	C6N-C5N	3.29	1.45	1.38
2	A	601	NAD	C6N-C5N	3.20	1.45	1.38
2	A	601	NAD	C4A-N3A	3.18	1.40	1.35
2	H	601	NAD	C6N-C5N	3.16	1.45	1.38
2	E	601	NAD	C2B-C3B	-3.14	1.44	1.53
2	F	601	NAD	C2B-C3B	-3.13	1.44	1.53
2	C	601	NAD	C4A-N3A	3.13	1.40	1.35
2	H	601	NAD	C4N-C3N	3.09	1.44	1.39
2	C	601	NAD	C2B-C3B	-3.09	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	NAD	C5N-C4N	3.05	1.45	1.38
2	B	601	NAD	C2A-N3A	3.05	1.37	1.32
2	E	601	NAD	C5N-C4N	3.04	1.45	1.38
2	G	601	NAD	C4A-N3A	3.03	1.39	1.35
2	H	601	NAD	C2A-N3A	3.02	1.37	1.32
2	C	601	NAD	C5N-C4N	3.01	1.45	1.38
2	A	601	NAD	C5N-C4N	3.00	1.45	1.38
2	A	601	NAD	C2B-C1B	-2.98	1.49	1.53
2	B	601	NAD	C2B-C1B	-2.96	1.49	1.53
2	A	601	NAD	C2B-C3B	-2.95	1.45	1.53
2	B	601	NAD	C4N-C3N	2.94	1.44	1.39
2	E	601	NAD	C2B-C1B	-2.92	1.49	1.53
2	B	601	NAD	C2B-C3B	-2.89	1.45	1.53
2	F	601	NAD	C4A-N3A	2.84	1.39	1.35
2	F	601	NAD	C2A-N3A	2.76	1.36	1.32
2	H	601	NAD	C2B-C3B	-2.76	1.45	1.53
2	D	601	NAD	C5N-C4N	2.75	1.44	1.38
2	H	601	NAD	C4A-N3A	2.74	1.39	1.35
2	B	601	NAD	C4A-N3A	2.74	1.39	1.35
2	A	601	NAD	C2A-N1A	2.74	1.39	1.33
2	B	601	NAD	C5N-C4N	2.72	1.44	1.38
2	F	601	NAD	C5N-C4N	2.66	1.44	1.38
2	C	601	NAD	C2A-N1A	2.56	1.38	1.33
2	H	601	NAD	C5N-C4N	2.53	1.44	1.38
2	G	601	NAD	C2A-N1A	2.52	1.38	1.33
2	G	601	NAD	C2B-C1B	-2.47	1.50	1.53
2	A	601	NAD	PN-O1N	2.38	1.59	1.50
2	F	601	NAD	PN-O1N	2.37	1.59	1.50
2	E	601	NAD	C2A-N1A	2.36	1.38	1.33
2	H	601	NAD	PN-O1N	2.34	1.59	1.50
2	D	601	NAD	PA-O5B	2.33	1.68	1.59
2	E	601	NAD	C3N-C7N	2.33	1.54	1.50
2	E	601	NAD	PN-O1N	2.26	1.58	1.50
2	B	601	NAD	C2A-N1A	2.26	1.38	1.33
2	D	601	NAD	PN-O5D	2.24	1.68	1.59
2	E	601	NAD	PA-O1A	2.23	1.58	1.50
2	A	601	NAD	PA-O1A	2.20	1.58	1.50
2	G	601	NAD	C5B-C4B	2.16	1.58	1.51
2	G	601	NAD	O4D-C4D	2.15	1.49	1.45
2	G	601	NAD	PN-O1N	2.15	1.58	1.50
2	A	601	NAD	O4D-C4D	2.14	1.49	1.45
2	F	601	NAD	C2A-N1A	2.14	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAD	PN-O1N	2.11	1.58	1.50
2	H	601	NAD	C6N-N1N	-2.10	1.30	1.35
2	H	601	NAD	C2A-N1A	2.10	1.37	1.33
2	H	601	NAD	O4D-C4D	2.08	1.49	1.45
2	G	601	NAD	PA-O1A	2.07	1.58	1.50
2	E	601	NAD	C5B-C4B	2.03	1.57	1.51
2	B	601	NAD	PA-O1A	2.02	1.58	1.50
2	B	601	NAD	O4D-C4D	2.01	1.49	1.45
2	H	601	NAD	O4B-C4B	-2.00	1.40	1.45
2	A	601	NAD	C5B-C4B	2.00	1.57	1.51

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	NAD	N3A-C2A-N1A	-5.70	119.77	128.68
2	A	601	NAD	C3N-C2N-N1N	-5.69	114.87	120.43
2	D	601	NAD	PN-O3-PA	-5.62	113.53	132.83
2	B	601	NAD	C3N-C2N-N1N	-5.48	115.07	120.43
2	E	601	NAD	N3A-C2A-N1A	-5.44	120.17	128.68
2	F	601	NAD	C3N-C2N-N1N	-5.35	115.19	120.43
2	G	601	NAD	C3N-C2N-N1N	-5.35	115.20	120.43
2	D	601	NAD	N3A-C2A-N1A	-5.28	120.43	128.68
2	H	601	NAD	C3N-C2N-N1N	-5.18	115.37	120.43
2	H	601	NAD	N3A-C2A-N1A	-5.17	120.60	128.68
2	C	601	NAD	N3A-C2A-N1A	-5.04	120.79	128.68
2	A	601	NAD	N3A-C2A-N1A	-4.86	121.08	128.68
2	G	601	NAD	C3N-C7N-N7N	4.63	123.31	117.75
2	H	601	NAD	C3N-C7N-N7N	4.63	123.31	117.75
2	B	601	NAD	N3A-C2A-N1A	-4.50	121.65	128.68
2	C	601	NAD	C3N-C2N-N1N	-4.22	116.30	120.43
2	E	601	NAD	C3N-C7N-N7N	4.15	122.73	117.75
2	H	601	NAD	PN-O3-PA	-4.09	118.78	132.83
2	G	601	NAD	N3A-C2A-N1A	-4.09	122.29	128.68
2	B	601	NAD	C2N-N1N-C1D	-3.99	110.24	119.14
2	H	601	NAD	O5D-C5D-C4D	3.87	122.30	108.99
2	B	601	NAD	O5D-C5D-C4D	3.82	122.15	108.99
2	F	601	NAD	O4D-C1D-C2D	-3.73	101.48	106.93
2	E	601	NAD	C2N-N1N-C1D	-3.69	110.92	119.14
2	F	601	NAD	C2N-N1N-C1D	-3.68	110.93	119.14
2	D	601	NAD	C2B-C3B-C4B	-3.64	95.57	102.64
2	D	601	NAD	C3B-C2B-C1B	-3.59	95.58	100.98
2	G	601	NAD	C2N-N1N-C1D	-3.53	111.27	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NAD	O4B-C4B-C5B	3.53	120.99	109.37
2	A	601	NAD	C2N-N1N-C1D	-3.53	111.28	119.14
2	G	601	NAD	O4D-C1D-C2D	-3.51	101.80	106.93
2	D	601	NAD	O2B-C2B-C1B	3.46	123.62	110.85
2	C	601	NAD	C2N-N1N-C1D	-3.38	111.61	119.14
2	F	601	NAD	O4B-C1B-C2B	-3.37	102.00	106.93
2	A	601	NAD	O5D-C5D-C4D	3.36	120.55	108.99
2	C	601	NAD	O4D-C1D-C2D	-3.27	102.14	106.93
2	D	601	NAD	O3D-C3D-C4D	3.26	120.47	111.05
2	B	601	NAD	C4A-C5A-N7A	-3.23	106.04	109.40
2	A	601	NAD	C3N-C7N-N7N	3.20	121.59	117.75
2	D	601	NAD	O4D-C4D-C5D	3.19	119.86	109.37
2	G	601	NAD	O4B-C4B-C5B	3.19	119.86	109.37
2	F	601	NAD	O2B-C2B-C3B	3.18	122.10	111.82
2	D	601	NAD	O2D-C2D-C3D	3.17	122.07	111.82
2	H	601	NAD	C4A-C5A-N7A	-3.14	106.12	109.40
2	A	601	NAD	O2B-C2B-C3B	3.13	121.96	111.82
2	G	601	NAD	C6N-N1N-C2N	3.13	124.83	121.97
2	F	601	NAD	C3N-C7N-N7N	3.13	121.50	117.75
2	C	601	NAD	C5N-C6N-N1N	3.10	124.85	120.40
2	G	601	NAD	C4A-C5A-N7A	-3.10	106.17	109.40
2	A	601	NAD	PN-O3-PA	-3.08	122.24	132.83
2	E	601	NAD	C3N-C2N-N1N	-3.07	117.43	120.43
2	A	601	NAD	O2D-C2D-C3D	3.05	121.69	111.82
2	D	601	NAD	O3D-C3D-C2D	3.05	121.69	111.82
2	D	601	NAD	O2D-C2D-C1D	3.03	122.03	110.85
2	E	601	NAD	O5D-C5D-C4D	3.02	119.38	108.99
2	H	601	NAD	C3D-C2D-C1D	3.01	105.51	100.98
2	A	601	NAD	C3B-C2B-C1B	2.96	105.43	100.98
2	G	601	NAD	O4B-C1B-C2B	-2.95	102.62	106.93
2	D	601	NAD	O5B-C5B-C4B	2.95	119.13	108.99
2	B	601	NAD	O2B-C2B-C3B	2.92	121.28	111.82
2	C	601	NAD	O5D-C5D-C4D	2.92	119.03	108.99
2	C	601	NAD	C4A-C5A-N7A	-2.91	106.37	109.40
2	A	601	NAD	O3D-C3D-C4D	2.91	119.45	111.05
2	F	601	NAD	O7N-C7N-C3N	-2.89	116.18	119.63
2	G	601	NAD	O5D-C5D-C4D	2.88	118.90	108.99
2	F	601	NAD	PN-O3-PA	-2.88	122.95	132.83
2	B	601	NAD	C2N-C3N-C4N	2.87	121.51	118.26
2	D	601	NAD	C6N-N1N-C2N	-2.86	119.36	121.97
2	E	601	NAD	O3B-C3B-C4B	2.85	119.29	111.05
2	G	601	NAD	O2D-C2D-C3D	2.83	120.99	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAD	O5B-C5B-C4B	2.82	118.69	108.99
2	C	601	NAD	C3N-C7N-N7N	2.81	121.13	117.75
2	E	601	NAD	C2D-C3D-C4D	2.80	108.08	102.64
2	F	601	NAD	O5D-C5D-C4D	2.79	118.58	108.99
2	E	601	NAD	O2B-C2B-C3B	2.78	120.83	111.82
2	A	601	NAD	C4A-C5A-N7A	-2.78	106.50	109.40
2	E	601	NAD	C5N-C6N-N1N	2.77	124.38	120.40
2	E	601	NAD	C5A-C6A-N6A	-2.77	116.15	120.35
2	H	601	NAD	O2B-C2B-C3B	2.75	120.71	111.82
2	G	601	NAD	O3D-C3D-C4D	2.74	118.97	111.05
2	E	601	NAD	O3D-C3D-C4D	2.73	118.95	111.05
2	H	601	NAD	C2N-N1N-C1D	-2.73	113.06	119.14
2	A	601	NAD	O3B-C3B-C4B	2.71	118.89	111.05
2	G	601	NAD	O5B-C5B-C4B	2.70	118.28	108.99
2	C	601	NAD	O3B-C3B-C4B	2.70	118.85	111.05
2	H	601	NAD	O3D-C3D-C4D	2.69	118.83	111.05
2	H	601	NAD	C5N-C6N-N1N	2.68	124.24	120.40
2	H	601	NAD	O7N-C7N-C3N	-2.67	116.44	119.63
2	A	601	NAD	O4B-C1B-C2B	-2.66	103.04	106.93
2	G	601	NAD	C5A-C6A-N6A	-2.64	116.34	120.35
2	C	601	NAD	O7N-C7N-C3N	-2.63	116.48	119.63
2	H	601	NAD	O5B-C5B-C4B	2.62	118.01	108.99
2	C	601	NAD	O3D-C3D-C2D	2.61	120.27	111.82
2	F	601	NAD	O3D-C3D-C4D	2.61	118.59	111.05
2	F	601	NAD	C5N-C6N-N1N	2.59	124.12	120.40
2	E	601	NAD	C3D-C2D-C1D	2.59	104.87	100.98
2	B	601	NAD	O3D-C3D-C4D	2.58	118.52	111.05
2	E	601	NAD	O5B-C5B-C4B	2.58	117.87	108.99
2	B	601	NAD	O2D-C2D-C3D	2.56	120.10	111.82
2	E	601	NAD	C4A-C5A-N7A	-2.53	106.77	109.40
2	C	601	NAD	O4B-C1B-C2B	-2.52	103.24	106.93
2	B	601	NAD	O3B-C3B-C4B	2.50	118.27	111.05
2	G	601	NAD	O2D-C2D-C1D	2.46	119.94	110.85
2	A	601	NAD	C5N-C6N-N1N	2.46	123.92	120.40
2	D	601	NAD	O4D-C1D-C2D	-2.45	103.34	106.93
2	E	601	NAD	O7N-C7N-N7N	-2.43	119.12	122.58
2	C	601	NAD	O2D-C2D-C3D	2.42	119.64	111.82
2	F	601	NAD	C4A-C5A-N7A	-2.41	106.88	109.40
2	B	601	NAD	O7N-C7N-C3N	-2.40	116.76	119.63
2	A	601	NAD	O2D-C2D-C1D	2.39	119.67	110.85
2	E	601	NAD	O5B-PA-O1A	2.36	118.27	109.07
2	H	601	NAD	C2B-C3B-C4B	2.36	107.22	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	NAD	O4D-C1D-C2D	-2.35	103.48	106.93
2	A	601	NAD	O4D-C1D-C2D	-2.35	103.49	106.93
2	F	601	NAD	C2N-C3N-C4N	2.34	120.92	118.26
2	E	601	NAD	C5D-C4D-C3D	2.34	123.95	115.18
2	C	601	NAD	C2N-C3N-C4N	2.33	120.89	118.26
2	E	601	NAD	PN-O3-PA	-2.30	124.92	132.83
2	B	601	NAD	C5N-C6N-N1N	2.30	123.70	120.40
2	A	601	NAD	C5D-C4D-C3D	2.29	123.76	115.18
2	H	601	NAD	C2D-C3D-C4D	2.28	107.08	102.64
2	F	601	NAD	O3D-C3D-C2D	2.28	119.19	111.82
2	B	601	NAD	O3B-C3B-C2B	2.26	119.13	111.82
2	F	601	NAD	C5A-C6A-N6A	-2.25	116.94	120.35
2	G	601	NAD	O3D-C3D-C2D	2.25	119.09	111.82
2	A	601	NAD	O3D-C3D-C2D	2.22	119.01	111.82
2	A	601	NAD	C6N-N1N-C2N	2.21	123.99	121.97
2	G	601	NAD	O7N-C7N-N7N	-2.21	119.44	122.58
2	F	601	NAD	O2D-C2D-C3D	2.20	118.94	111.82
2	C	601	NAD	O3B-C3B-C2B	2.19	118.90	111.82
2	F	601	NAD	O5B-C5B-C4B	2.18	116.50	108.99
2	B	601	NAD	O5B-C5B-C4B	2.18	116.48	108.99
2	B	601	NAD	C3N-C7N-N7N	2.17	120.36	117.75
2	G	601	NAD	O2B-C2B-C3B	2.16	118.79	111.82
2	G	601	NAD	C1B-N9A-C4A	2.15	130.41	126.64
2	C	601	NAD	PN-O3-PA	-2.13	125.51	132.83
2	C	601	NAD	O5B-C5B-C4B	2.13	116.32	108.99
2	B	601	NAD	C3B-C2B-C1B	2.12	104.18	100.98
2	A	601	NAD	O4D-C4D-C5D	2.12	116.36	109.37
2	D	601	NAD	O5D-C5D-C4D	2.12	116.30	108.99
2	B	601	NAD	C5D-C4D-C3D	2.12	123.13	115.18
2	H	601	NAD	O2D-C2D-C3D	2.11	118.65	111.82
2	F	601	NAD	O4D-C4D-C5D	2.10	116.29	109.37
2	E	601	NAD	O2D-C2D-C1D	2.08	118.53	110.85
2	G	601	NAD	C5D-C4D-C3D	2.06	122.92	115.18
2	F	601	NAD	O2D-C2D-C1D	2.03	118.34	110.85
2	C	601	NAD	O4D-C4D-C5D	2.02	116.03	109.37
2	A	601	NAD	N6A-C6A-N1A	2.02	122.77	118.57
2	G	601	NAD	O7N-C7N-C3N	-2.02	117.22	119.63
2	B	601	NAD	O3D-C3D-C2D	2.01	118.33	111.82

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	NAD	C5D-O5D-PN-O1N
2	C	601	NAD	C3D-C4D-C5D-O5D
2	E	601	NAD	C4D-C5D-O5D-PN
2	E	601	NAD	C3D-C4D-C5D-O5D
2	G	601	NAD	C5D-O5D-PN-O1N
2	G	601	NAD	C5D-O5D-PN-O2N
2	G	601	NAD	C3D-C4D-C5D-O5D
2	H	601	NAD	C5B-O5B-PA-O1A
2	H	601	NAD	C5B-O5B-PA-O2A
2	H	601	NAD	C5B-O5B-PA-O3
2	H	601	NAD	PA-O3-PN-O5D
2	H	601	NAD	C5D-O5D-PN-O3
2	H	601	NAD	C5D-O5D-PN-O1N
2	H	601	NAD	C5D-O5D-PN-O2N
2	H	601	NAD	C3D-C4D-C5D-O5D
2	A	601	NAD	C5B-O5B-PA-O1A
2	A	601	NAD	C5B-O5B-PA-O2A
2	A	601	NAD	C5D-O5D-PN-O1N
2	A	601	NAD	C5D-O5D-PN-O2N
2	D	601	NAD	PN-O3-PA-O5B
2	D	601	NAD	C5D-O5D-PN-O1N
2	D	601	NAD	C3D-C4D-C5D-O5D
2	F	601	NAD	C5D-O5D-PN-O1N
2	F	601	NAD	C3D-C4D-C5D-O5D
2	A	601	NAD	C3D-C4D-C5D-O5D
2	B	601	NAD	C3D-C4D-C5D-O5D
2	E	601	NAD	O4D-C4D-C5D-O5D
2	G	601	NAD	O4D-C4D-C5D-O5D
2	H	601	NAD	O4D-C4D-C5D-O5D
2	F	601	NAD	O4D-C4D-C5D-O5D
2	B	601	NAD	PA-O3-PN-O1N
2	G	601	NAD	C4B-C5B-O5B-PA
2	D	601	NAD	C4D-C5D-O5D-PN
2	C	601	NAD	PN-O3-PA-O5B
2	E	601	NAD	PN-O3-PA-O5B
2	G	601	NAD	PN-O3-PA-O5B
2	H	601	NAD	PN-O3-PA-O5B
2	A	601	NAD	PN-O3-PA-O5B
2	B	601	NAD	PN-O3-PA-O5B
2	F	601	NAD	PN-O3-PA-O5B
2	B	601	NAD	C4D-C5D-O5D-PN
2	F	601	NAD	C4B-C5B-O5B-PA
2	F	601	NAD	C4D-C5D-O5D-PN

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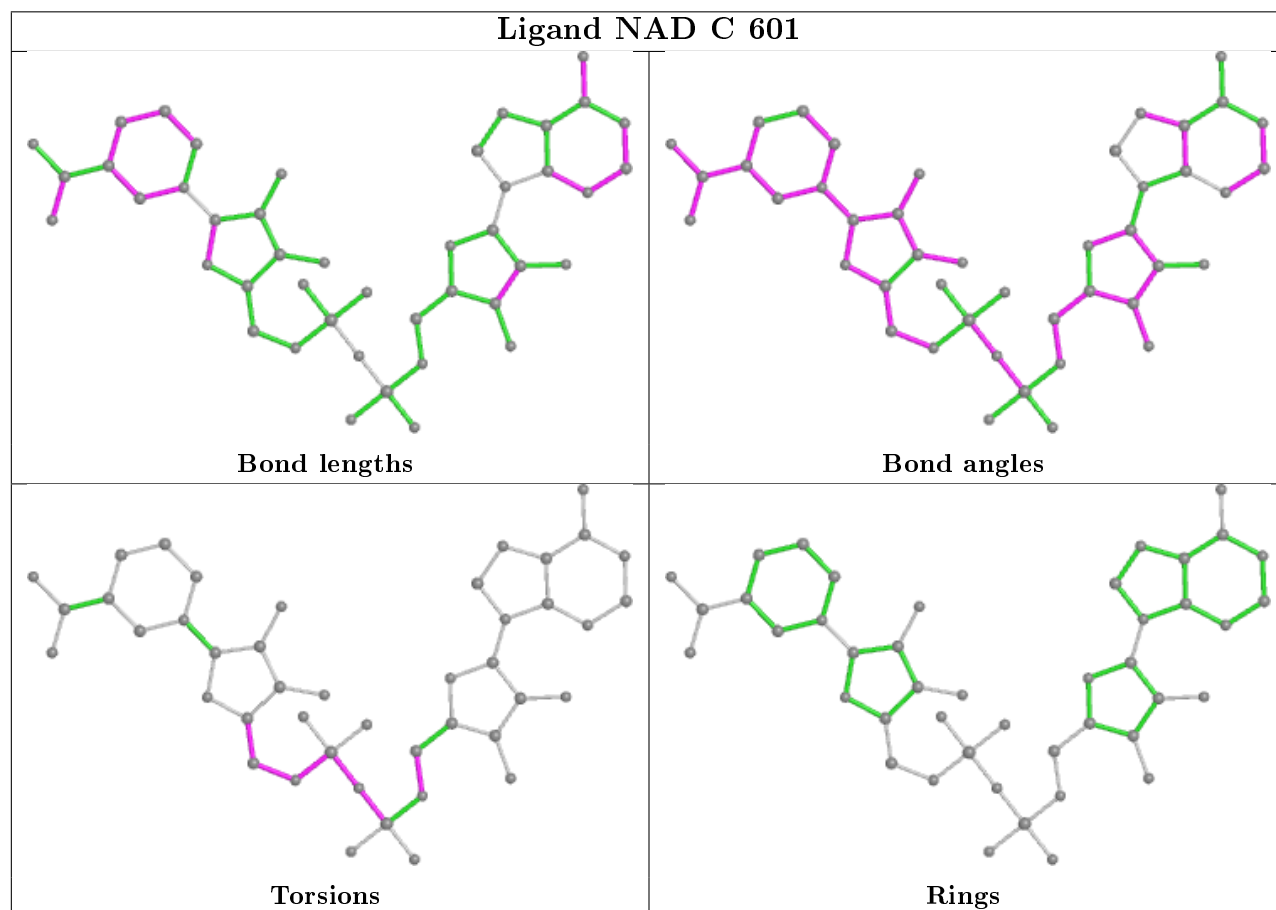
Mol	Chain	Res	Type	Atoms
2	C	601	NAD	C5D-O5D-PN-O3
2	E	601	NAD	C5D-O5D-PN-O3
2	G	601	NAD	C5B-O5B-PA-O3
2	B	601	NAD	C5B-O5B-PA-O3
2	B	601	NAD	C5D-O5D-PN-O3
2	D	601	NAD	C5D-O5D-PN-O3
2	F	601	NAD	C5B-O5B-PA-O3
2	F	601	NAD	C5D-O5D-PN-O3
2	E	601	NAD	PA-O3-PN-O1N
2	G	601	NAD	PN-O3-PA-O1A
2	C	601	NAD	C4D-C5D-O5D-PN
2	G	601	NAD	C4D-C5D-O5D-PN
2	H	601	NAD	C4B-C5B-O5B-PA
2	A	601	NAD	C4B-C5B-O5B-PA
2	C	601	NAD	C5D-O5D-PN-O2N
2	E	601	NAD	C5D-O5D-PN-O2N
2	G	601	NAD	C5B-O5B-PA-O2A
2	B	601	NAD	C5D-O5D-PN-O2N
2	D	601	NAD	C5D-O5D-PN-O2N
2	F	601	NAD	C5B-O5B-PA-O1A
2	F	601	NAD	C5B-O5B-PA-O2A
2	F	601	NAD	C5D-O5D-PN-O2N
2	C	601	NAD	C4B-C5B-O5B-PA
2	D	601	NAD	PA-O3-PN-O2N
2	F	601	NAD	PN-O3-PA-O1A
2	H	601	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	C4D-C5D-O5D-PN
2	C	601	NAD	PA-O3-PN-O1N
2	B	601	NAD	PN-O3-PA-O1A
2	F	601	NAD	PA-O3-PN-O1N
2	G	601	NAD	C5D-O5D-PN-O3
2	A	601	NAD	C5B-O5B-PA-O3
2	A	601	NAD	C5D-O5D-PN-O3
2	D	601	NAD	C4B-C5B-O5B-PA
2	C	601	NAD	PA-O3-PN-O2N
2	A	601	NAD	PN-O3-PA-O1A
2	D	601	NAD	PA-O3-PN-O1N
2	B	601	NAD	C5B-O5B-PA-O2A
2	C	601	NAD	O4D-C4D-C5D-O5D

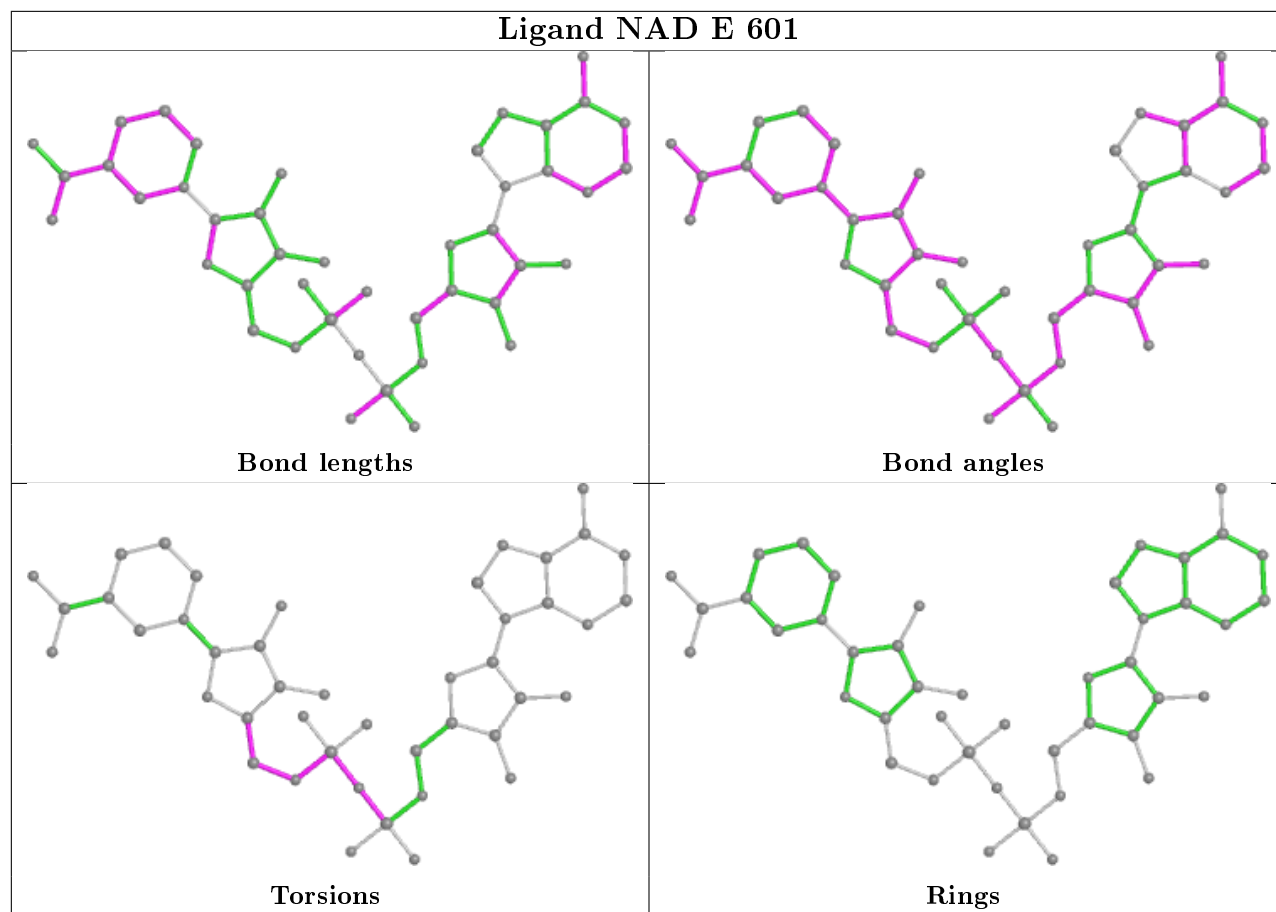
There are no ring outliers.

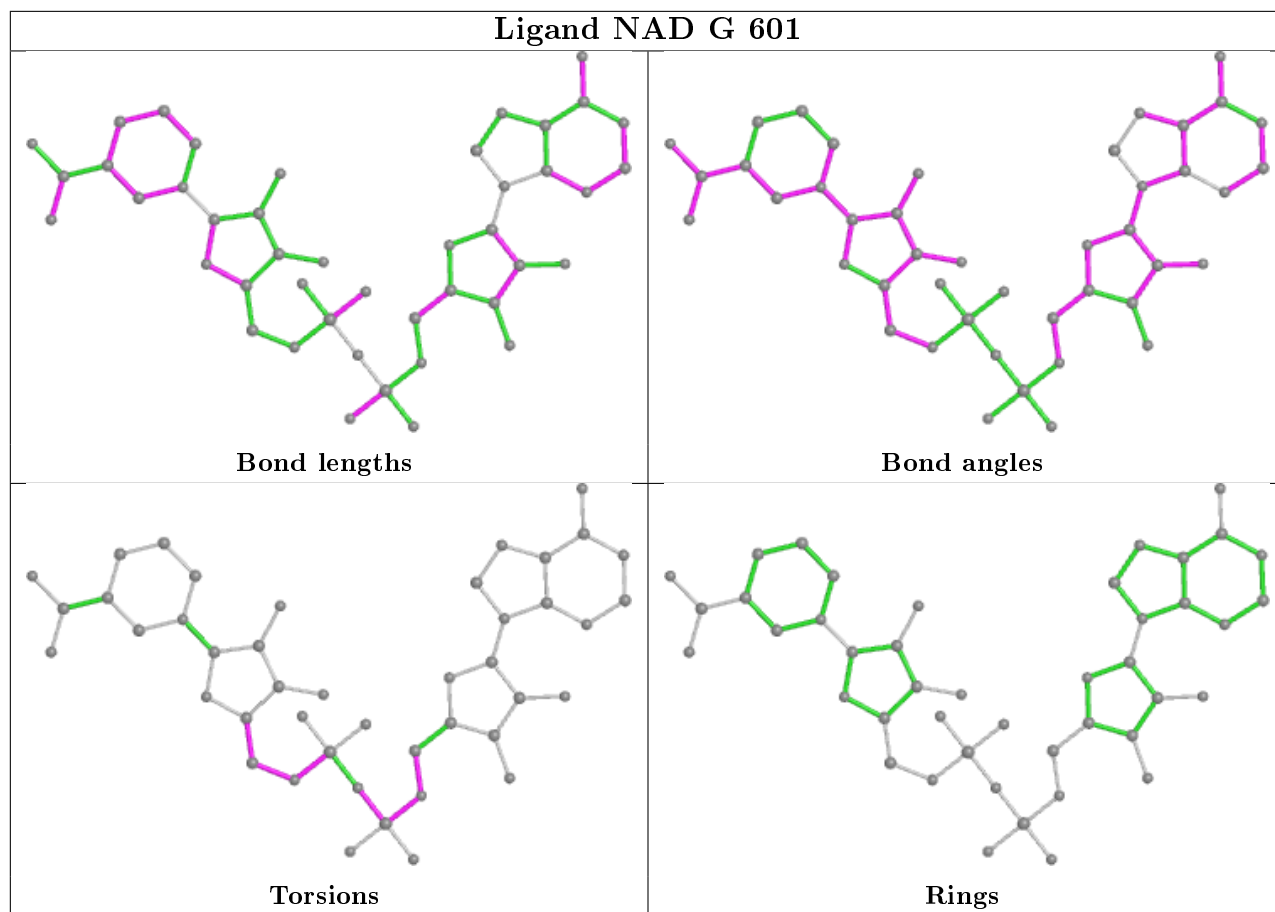
8 monomers are involved in 72 short contacts:

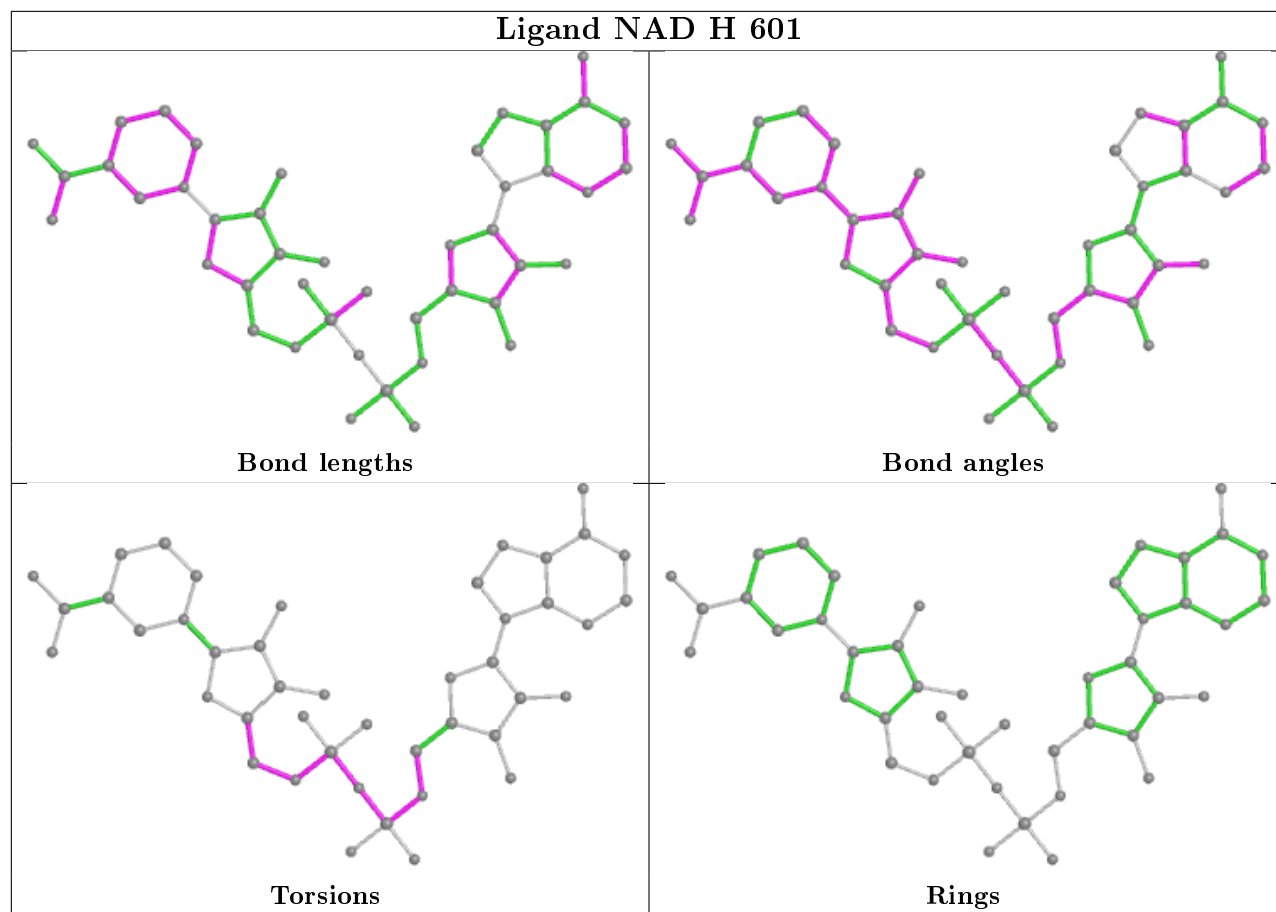
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	NAD	14	0
2	E	601	NAD	7	0
2	G	601	NAD	7	0
2	H	601	NAD	7	0
2	A	601	NAD	11	0
2	B	601	NAD	7	0
2	D	601	NAD	8	0
2	F	601	NAD	11	0

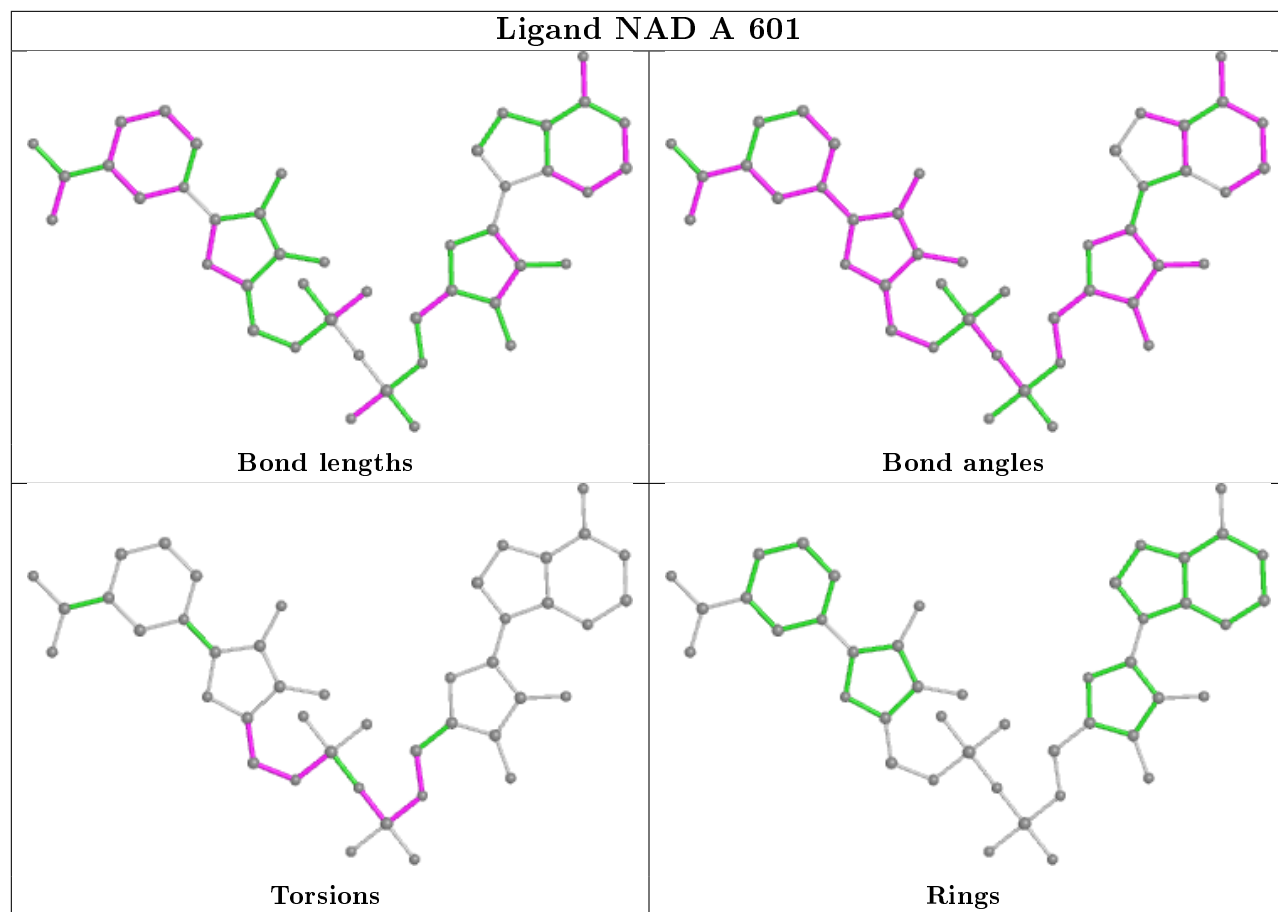
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



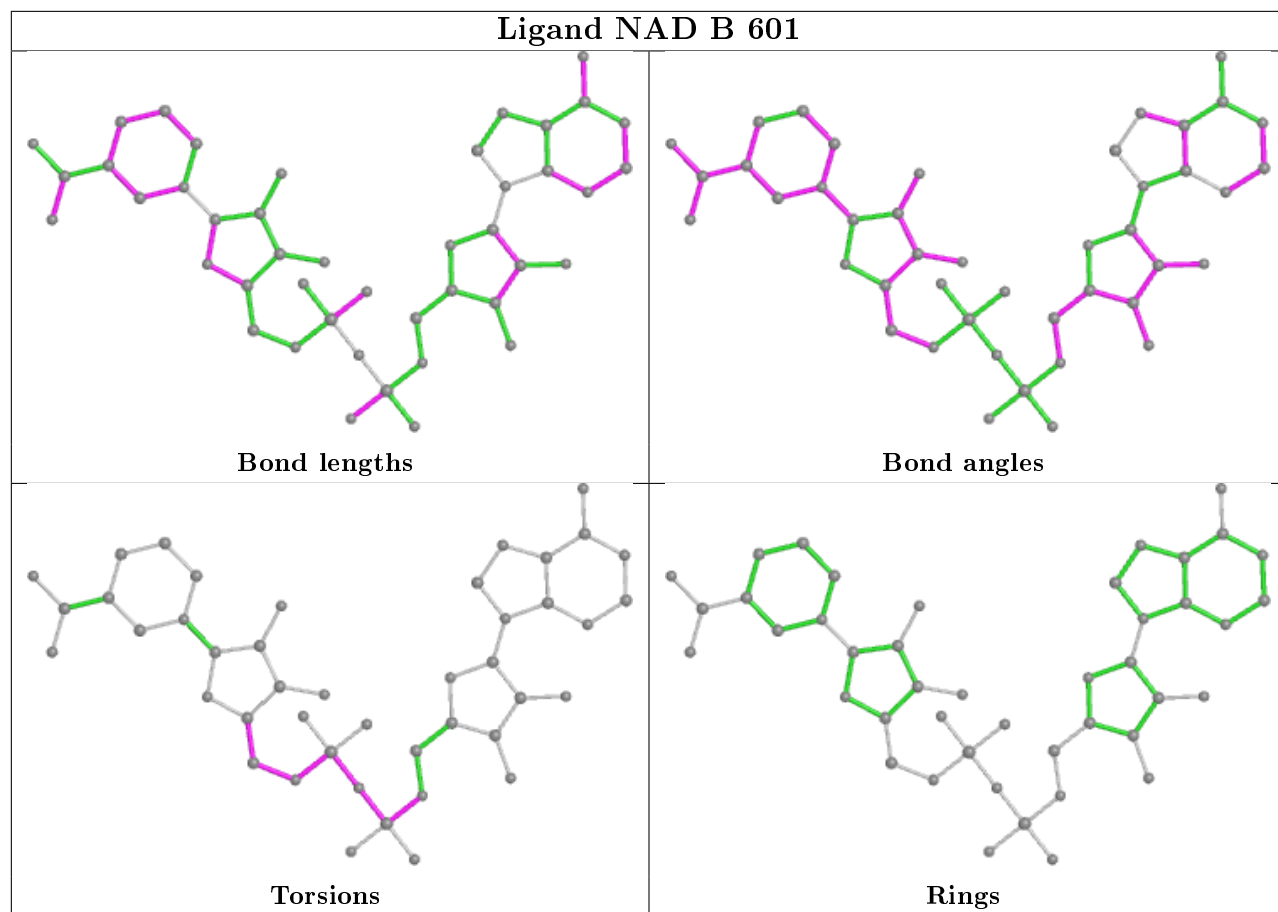


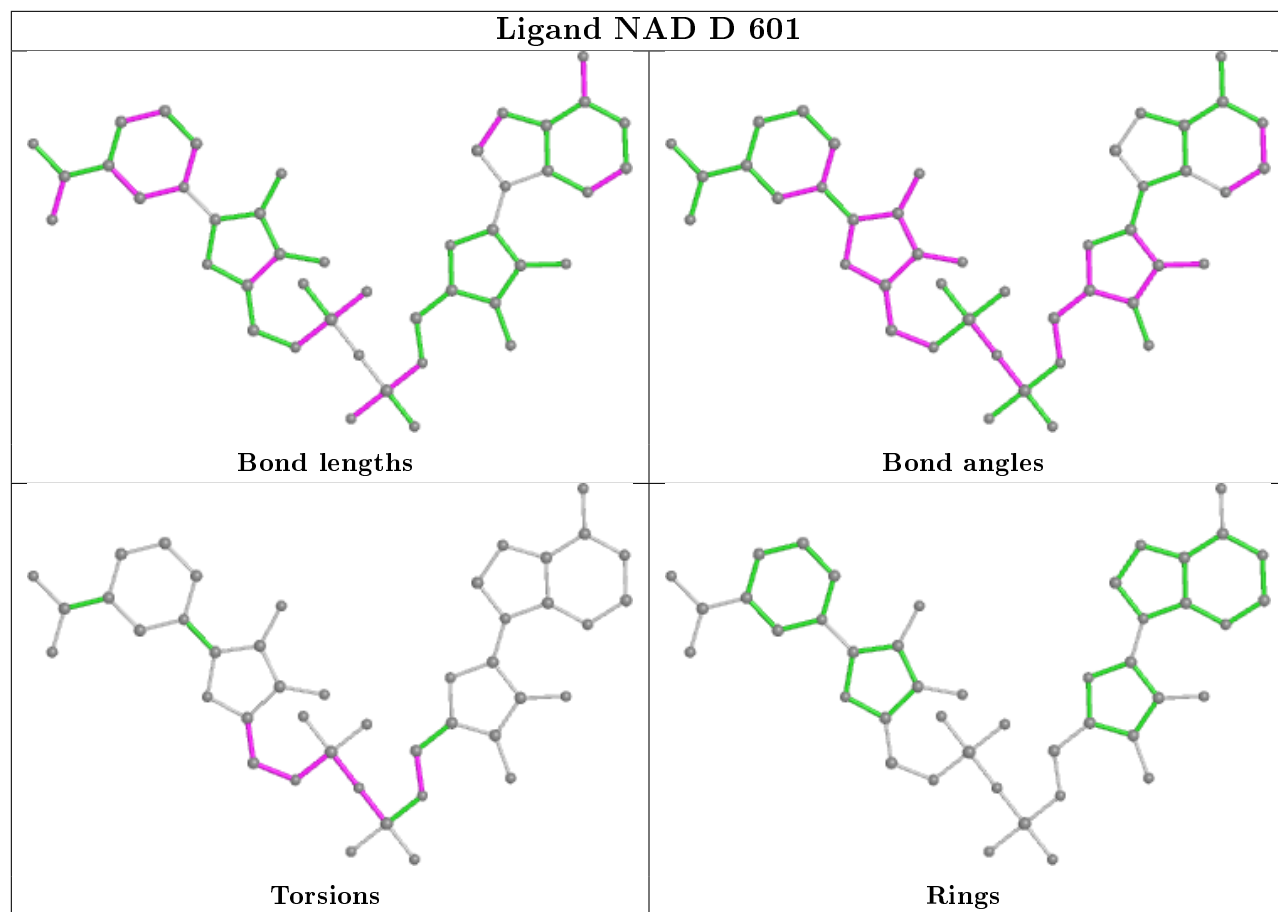


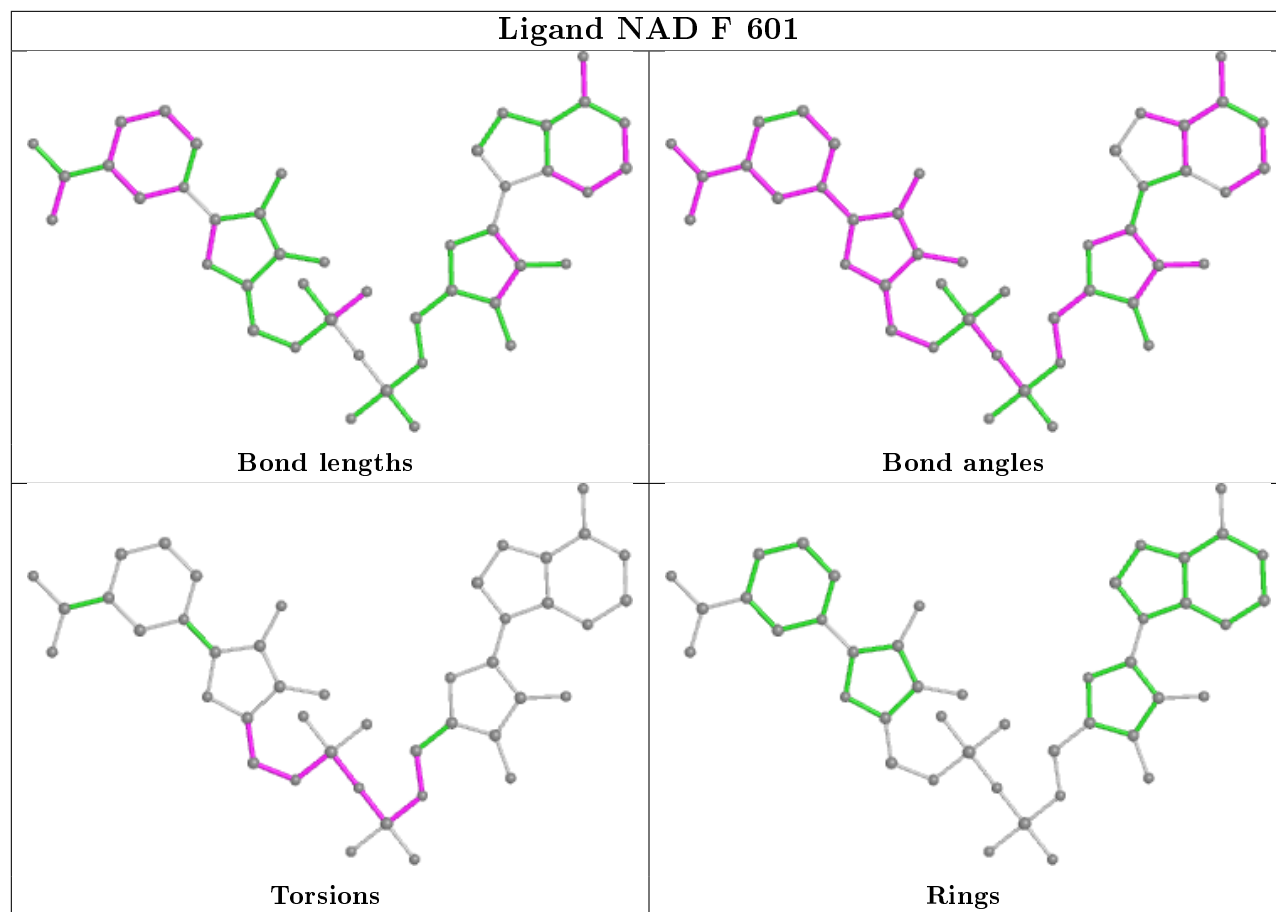












## 5.7 Other polymers [i](#)

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	487/495 (98%)	-0.17	2 (0%) 92 84	33, 61, 91, 111	0
1	B	487/495 (98%)	-0.12	4 (0%) 86 72	38, 60, 91, 115	0
1	C	487/495 (98%)	-0.30	0 100 100	31, 57, 90, 116	0
1	D	487/495 (98%)	-0.38	3 (0%) 89 78	30, 50, 83, 118	0
1	E	487/495 (98%)	-0.34	4 (0%) 86 72	32, 50, 85, 123	0
1	F	487/495 (98%)	-0.23	3 (0%) 89 78	29, 62, 91, 120	0
1	G	487/495 (98%)	-0.23	0 100 100	29, 58, 89, 120	0
1	H	487/495 (98%)	-0.15	1 (0%) 95 90	36, 62, 90, 124	0
All	All	3896/3960 (98%)	-0.24	17 (0%) 92 84	29, 57, 90, 124	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	486	LYS	3.2
1	D	484	HIS	3.0
1	F	376	ARG	2.9
1	E	378	CYS	2.9
1	B	324	THR	2.8
1	D	485	PHE	2.8
1	E	485	PHE	2.7
1	B	25	PRO	2.6
1	E	486	LYS	2.5
1	H	484	HIS	2.4
1	E	484	HIS	2.3
1	F	486	LYS	2.3
1	A	346	VAL	2.2
1	B	34	ILE	2.1
1	B	335	TYR	2.0
1	F	276	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	379	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

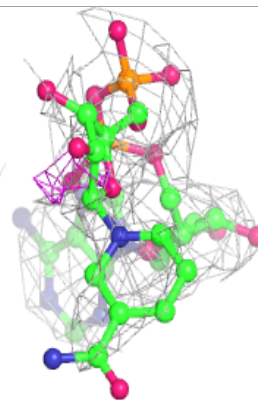
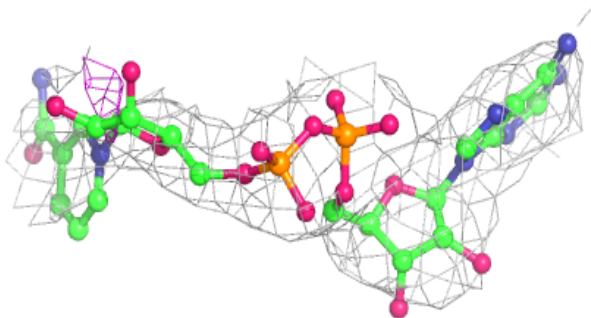
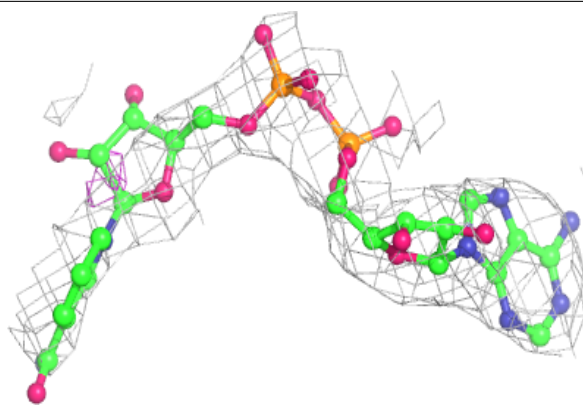
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAD	A	601	44/44	0.90	0.23	48,77,102,113	0
2	NAD	G	601	44/44	0.92	0.24	48,74,90,103	0
2	NAD	E	601	44/44	0.92	0.22	37,60,82,85	0
2	NAD	D	601	44/44	0.92	0.23	45,66,90,95	0
2	NAD	H	601	44/44	0.93	0.21	54,75,91,108	0
2	NAD	B	601	44/44	0.94	0.21	45,67,89,100	0
2	NAD	C	601	44/44	0.94	0.21	38,55,82,90	0
2	NAD	F	601	44/44	0.94	0.21	49,68,83,101	0

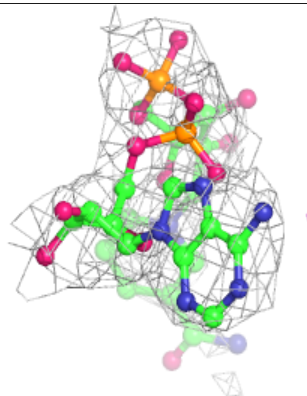
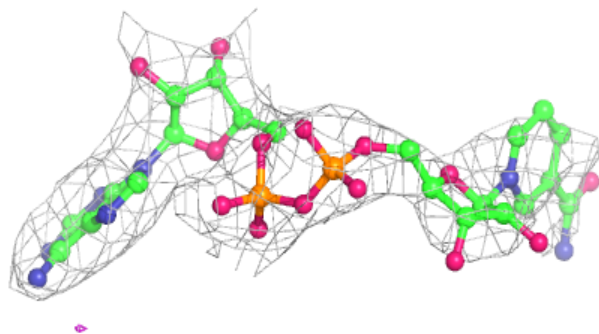
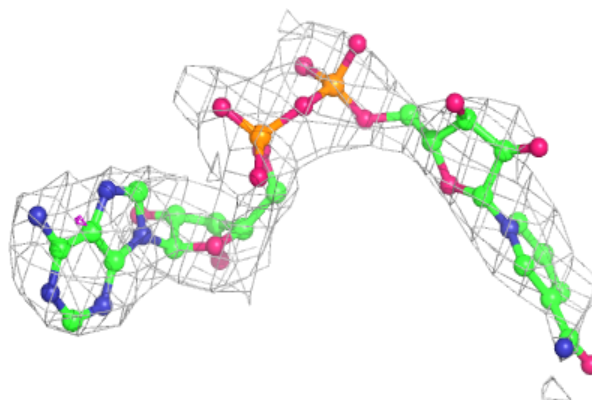
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD A 601:**

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

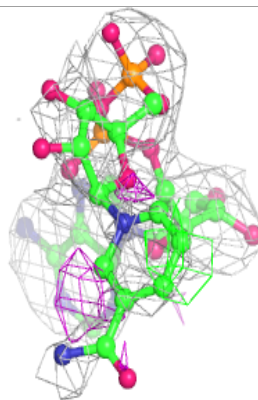
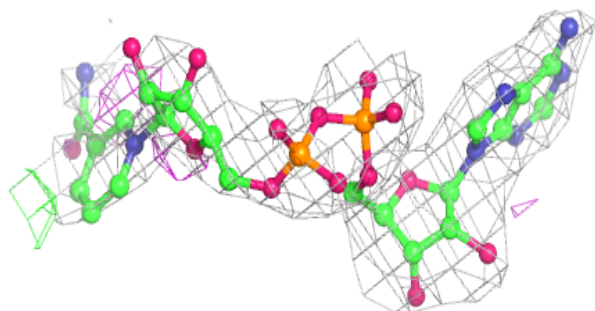
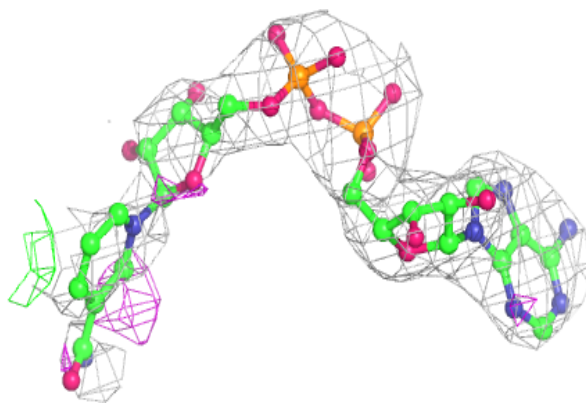
**Electron density around NAD G 601:**

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

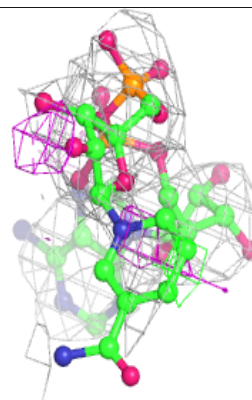
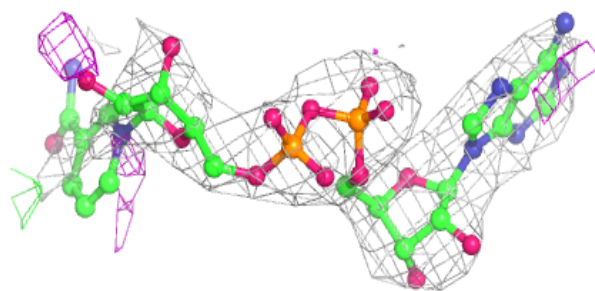
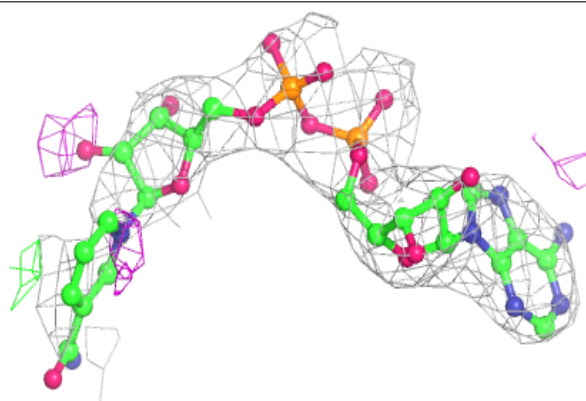


**Electron density around NAD E 601:**

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

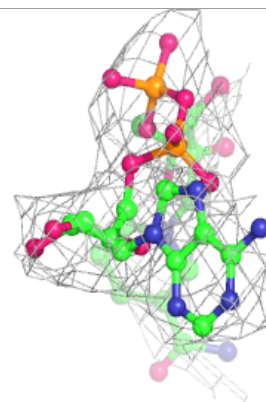
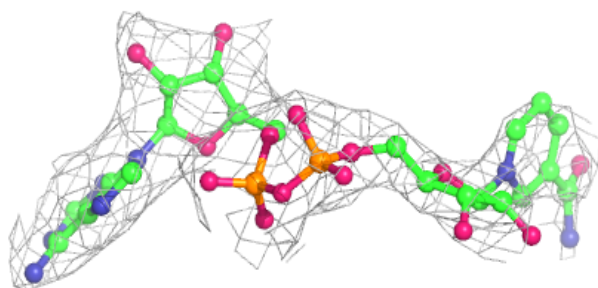
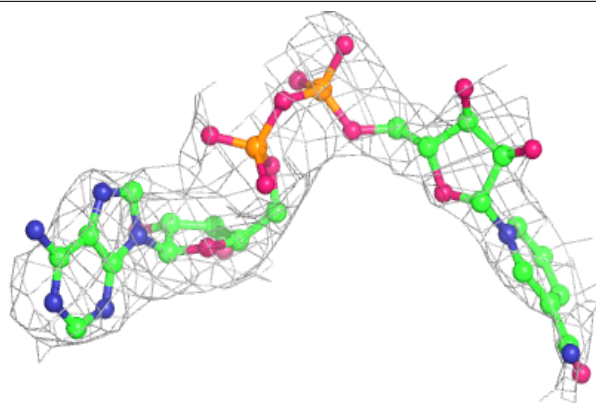
**Electron density around NAD D 601:**

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

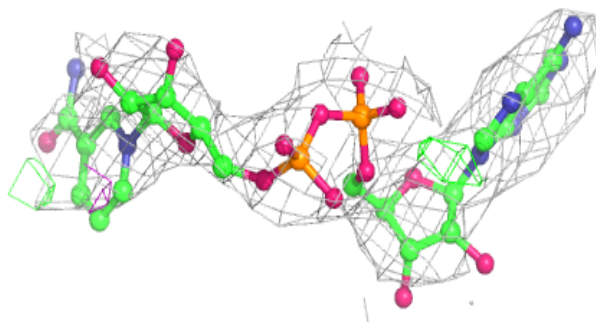
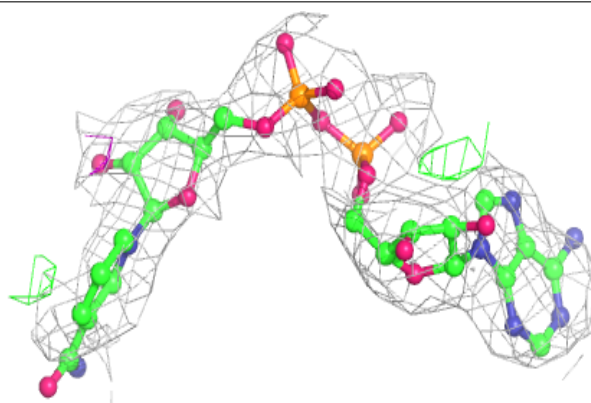


**Electron density around NAD H 601:**

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

**Electron density around NAD B 601:**

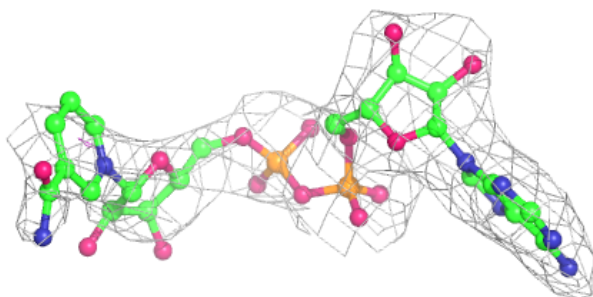
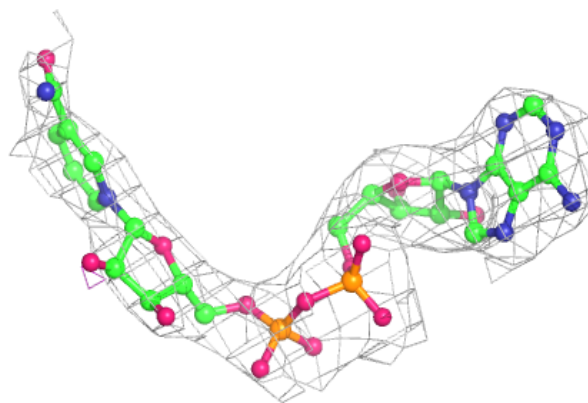
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



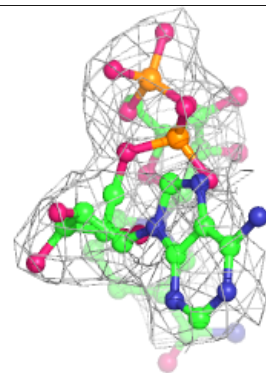
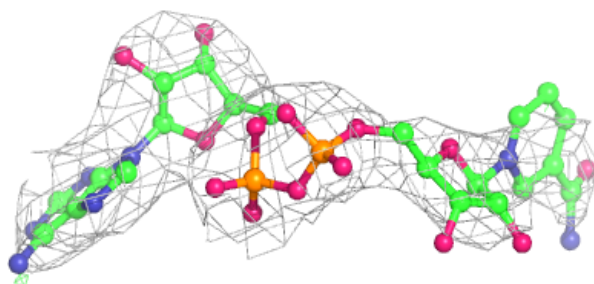
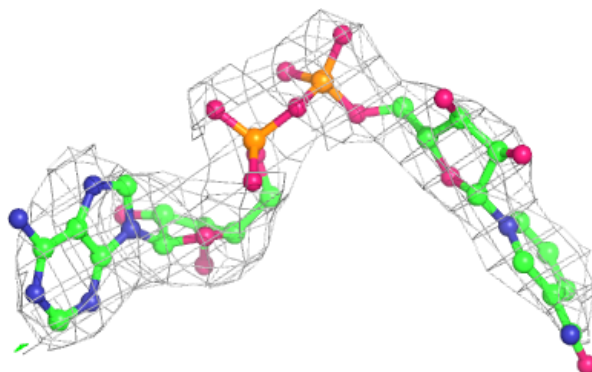


**Electron density around NAD C 601:**

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

**Electron density around NAD F 601:**

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



## 6.5 Other polymers

There are no such residues in this entry.