



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:53 AM UTC

PDB ID : 4GO4 / pdb_00004go4
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

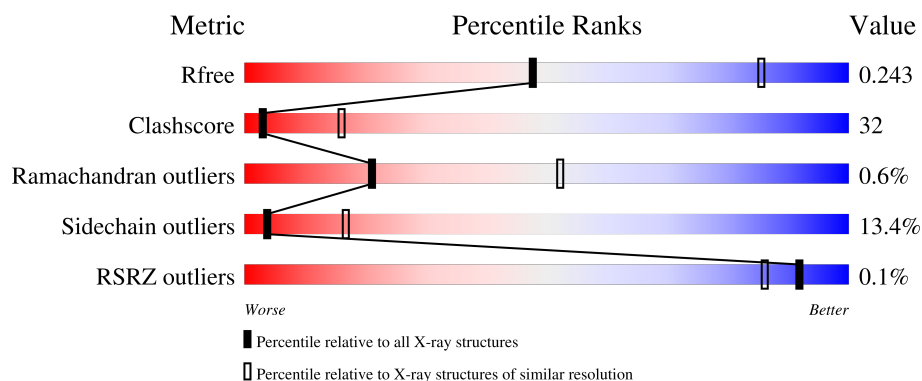
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	

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Mol	Chain	Length	Quality of chain
1	F	495	 55% 36% 8% .
1	G	495	 53% 37% 8% .
1	H	495	 53% 37% 7% ..

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
1	A	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	B	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	C	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	D	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	E	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	F	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	G	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			
1	H	487	Total	C	N	O	S	0	1	0
			3698	2341	657	684	16			

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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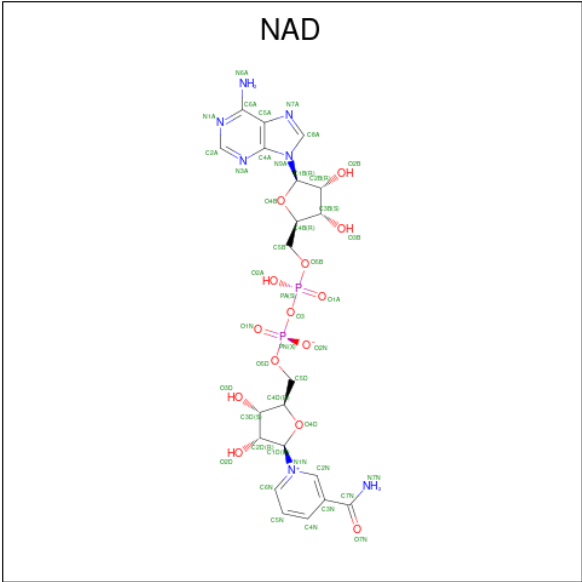
Chain	Residue	Modelled	Actual	Comment	Reference
B	489	GLY	-	expression tag	UNP C1I208
B	490	HIS	-	expression tag	UNP C1I208
B	491	HIS	-	expression tag	UNP C1I208
B	492	HIS	-	expression tag	UNP C1I208
B	493	HIS	-	expression tag	UNP C1I208
B	494	HIS	-	expression tag	UNP C1I208
B	495	HIS	-	expression tag	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 (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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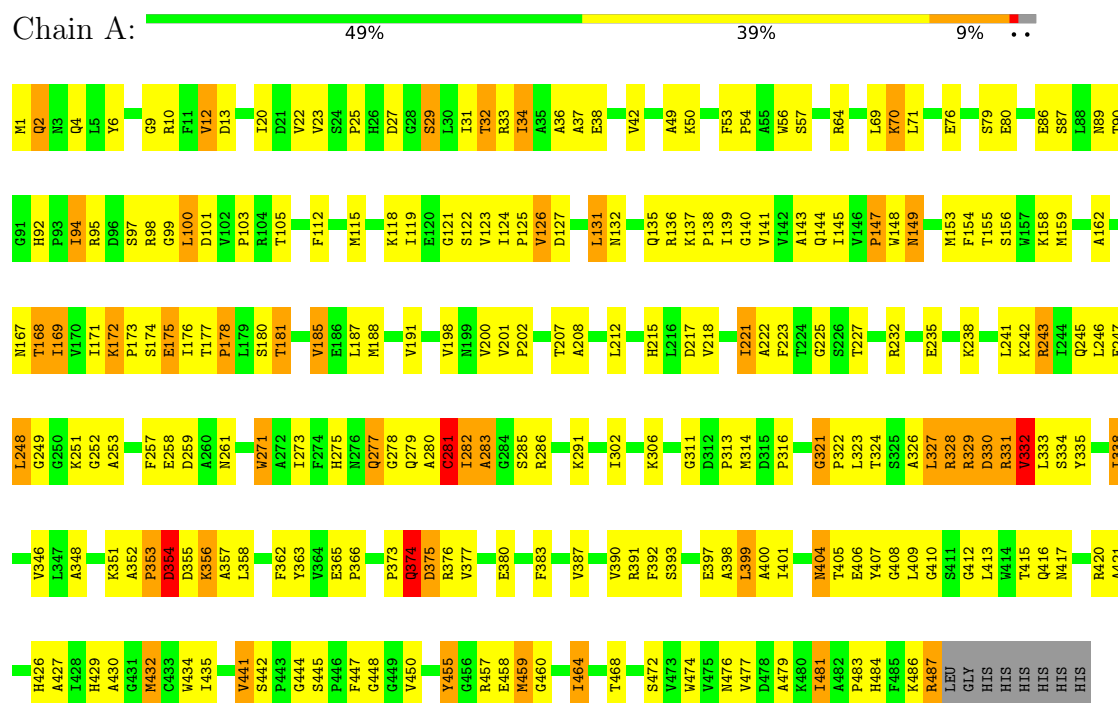
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	26	Total 26	O 26	0	0
3	F	12	Total 12	O 12	0	0
3	G	13	Total 13	O 13	0	0
3	H	15	Total 15	O 15	0	0

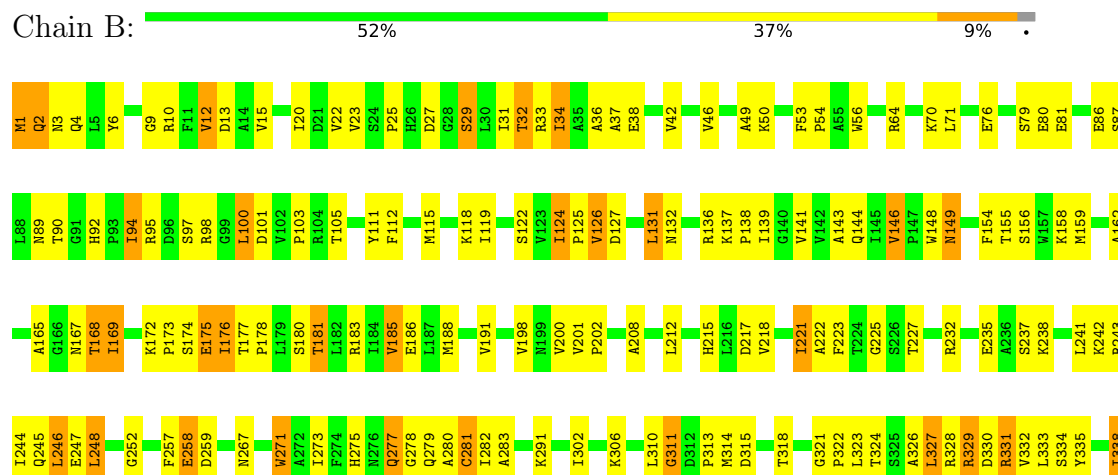
3 Residue-property plots [i](#)

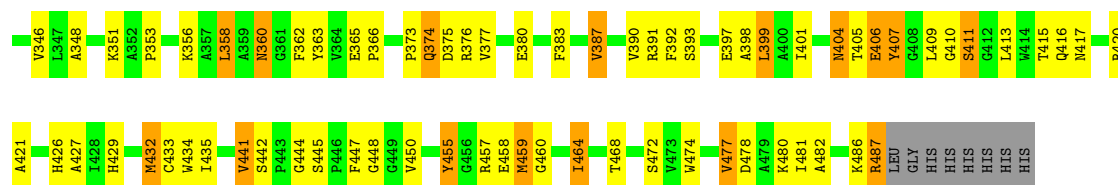
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase



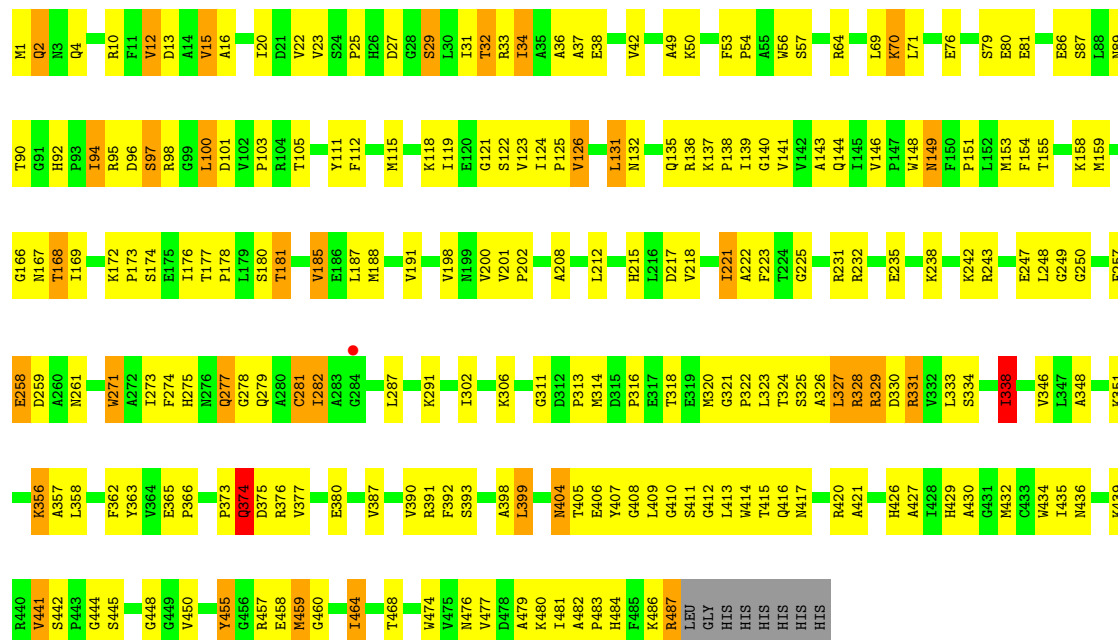
- Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase





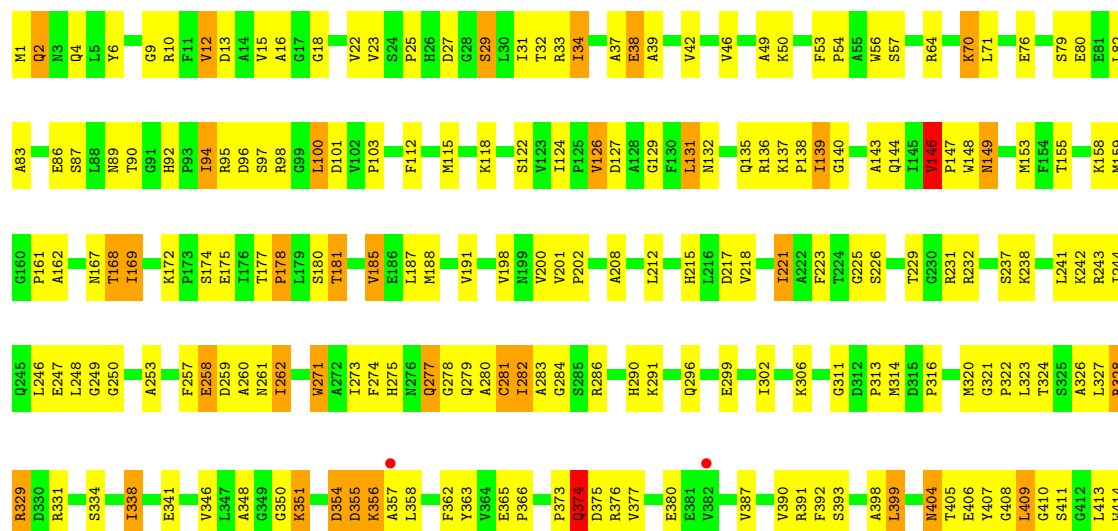
• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

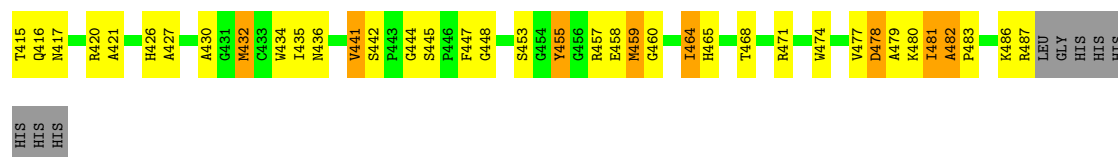
Chain C: 52% 39% 7%



• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

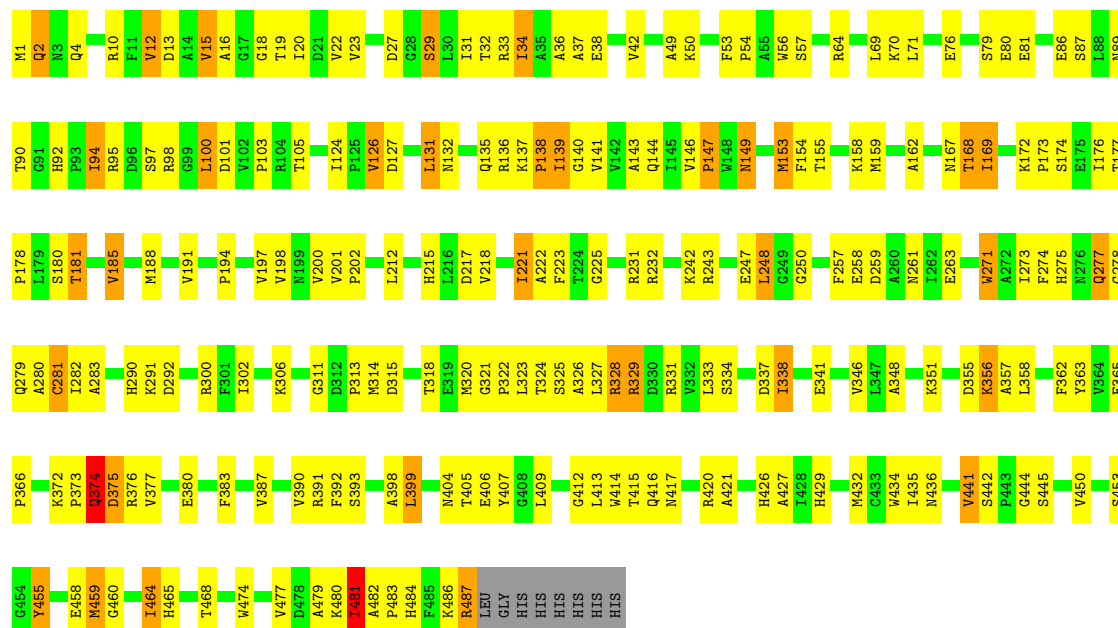
Chain D: 50% 39% 8%





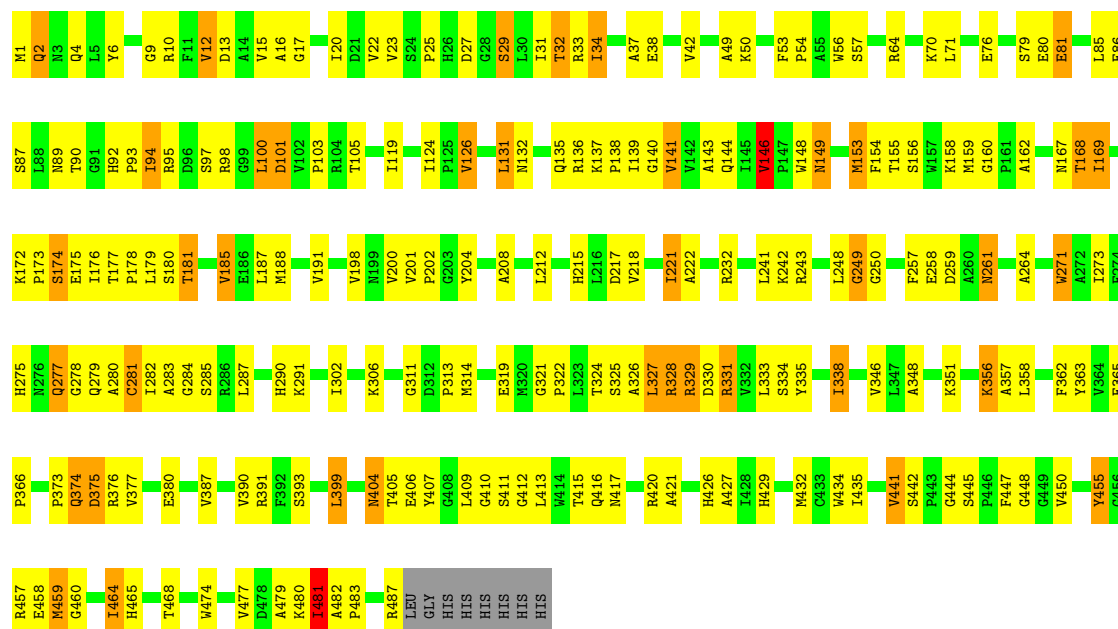
- Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain E: 54% 37% 7% .

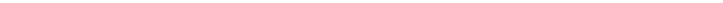


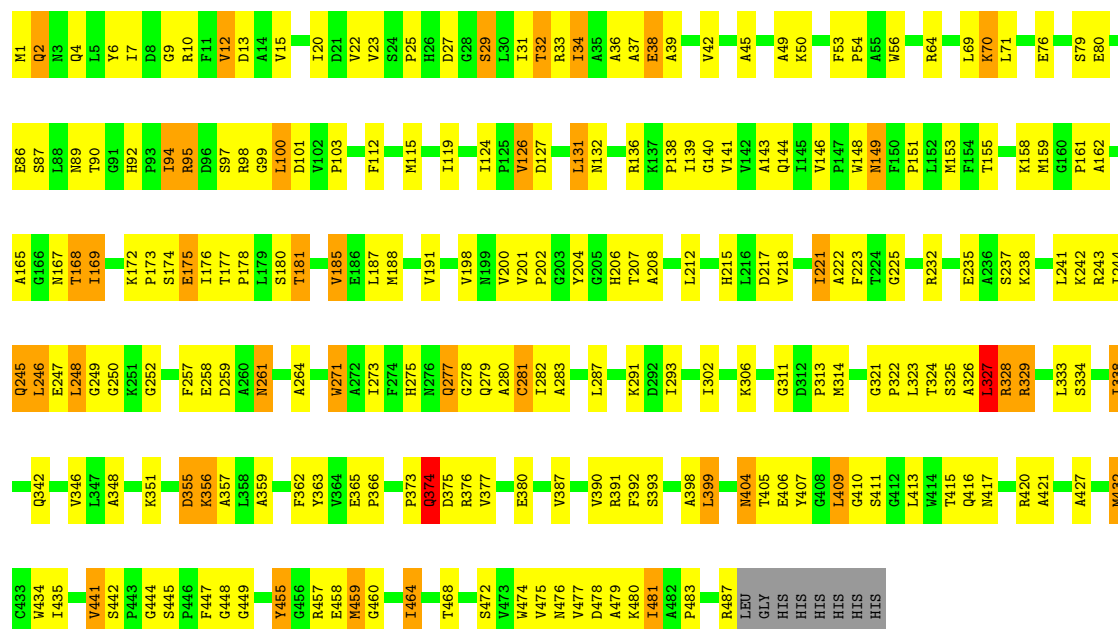
- Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain F: 55% 36% 8% .

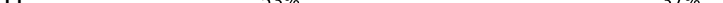


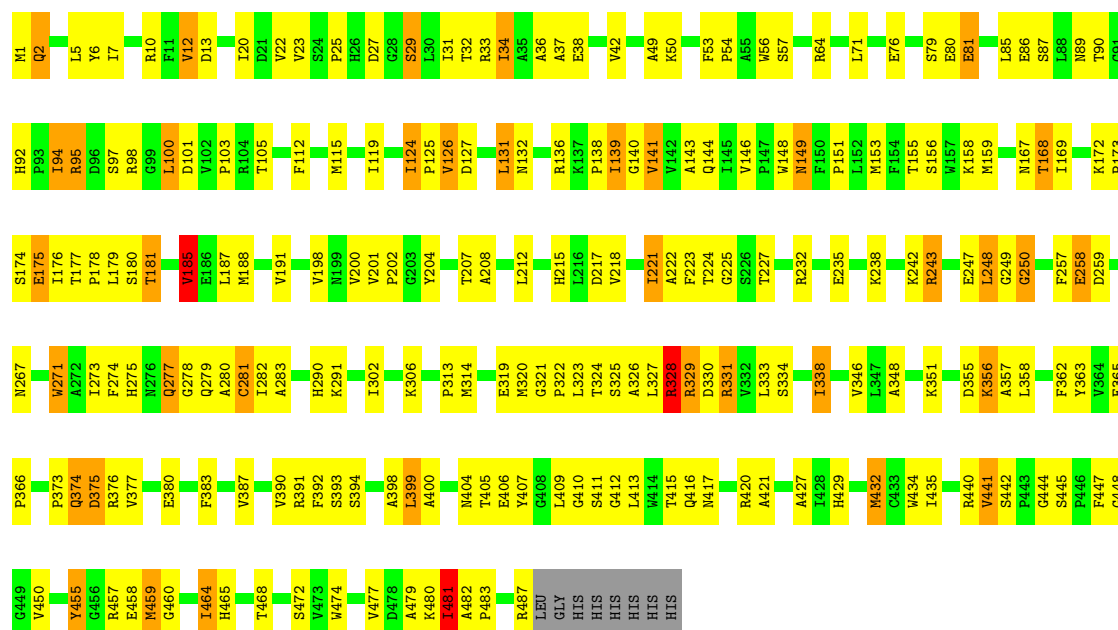
- Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain G:  53% 37% 8% .



- Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain H:  53% 37% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.91Å 154.54Å 143.44Å 90.00° 95.24° 90.00°	Depositor
Resolution (Å)	37.24 – 3.10 37.24 – 3.10	Depositor EDS
% Data completeness (in resolution range)	88.6 (37.24-3.10) 92.0 (37.24-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.207 , 0.251 0.201 , 0.243	Depositor DCC
R_{free} test set	1825 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30071	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.64	1/3775 (0.0%)	1.08	21/5119 (0.4%)
1	B	0.59	0/3775	0.94	10/5119 (0.2%)
1	C	0.60	0/3775	0.94	9/5119 (0.2%)
1	D	0.70	2/3775 (0.1%)	0.97	11/5119 (0.2%)
1	E	0.65	0/3775	0.96	12/5119 (0.2%)
1	F	0.57	0/3775	0.94	10/5119 (0.2%)
1	G	0.63	0/3775	0.91	7/5119 (0.1%)
1	H	0.58	0/3775	0.95	12/5119 (0.2%)
All	All	0.62	3/30200 (0.0%)	0.96	92/40952 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	146	VAL	C-O	-6.02	1.18	1.24
1	D	146	VAL	CA-CB	-5.83	1.48	1.55
1	A	283	ALA	CA-C	-5.79	1.45	1.52

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ASP	N-CA-C	22.33	135.62	111.28
1	A	409	LEU	N-CA-C	14.44	128.57	111.82
1	A	282	ILE	CB-CA-C	-13.50	96.65	111.23
1	F	459	MET	CB-CA-C	-13.38	90.79	110.06
1	A	330	ASP	CB-CA-C	-13.22	88.85	110.79
1	D	478	ASP	CB-CA-C	-12.36	91.11	110.14
1	C	459	MET	CB-CA-C	-12.17	92.53	110.06
1	A	282	ILE	N-CA-C	-11.52	90.58	107.98
1	A	283	ALA	N-CA-C	-11.45	90.00	108.55
1	E	459	MET	CB-CA-C	-11.04	94.17	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	328	ARG	N-CA-C	10.93	123.16	111.03
1	D	374	GLN	CB-CA-C	-9.88	96.15	111.66
1	H	248	LEU	N-CA-C	-9.67	94.87	109.86
1	D	409	LEU	N-CA-C	9.58	125.76	112.45
1	D	479	ALA	N-CA-CB	-9.51	97.11	111.56
1	C	459	MET	N-CA-C	9.41	128.05	113.28
1	F	459	MET	N-CA-C	9.26	127.81	113.28
1	D	375	ASP	N-CA-C	-8.83	96.73	110.42
1	E	459	MET	N-CA-C	8.69	126.92	113.28
1	H	459	MET	CB-CA-C	-8.62	97.02	110.04
1	A	459	MET	CB-CA-C	-8.48	97.24	110.04
1	B	360	ASN	N-CA-C	-7.72	103.19	114.39
1	A	124	ILE	N-CA-C	7.62	115.18	108.63
1	H	124	ILE	N-CA-C	7.56	115.13	108.63
1	C	124	ILE	N-CA-C	7.51	115.09	108.63
1	G	411	SER	N-CA-CB	-7.42	100.06	111.56
1	F	124	ILE	N-CA-C	7.26	114.88	108.63
1	C	375	ASP	N-CA-C	-7.01	100.15	110.52
1	B	482	ALA	N-CA-C	-6.96	98.78	109.64
1	E	375	ASP	N-CA-C	-6.96	98.34	109.76
1	G	124	ILE	N-CA-C	6.85	114.52	108.63
1	B	169	ILE	N-CA-C	6.72	118.15	108.48
1	A	354	ASP	CB-CA-C	-6.71	100.67	111.28
1	C	374	GLN	CB-CA-C	-6.55	101.06	111.48
1	H	250	GLY	N-CA-C	6.50	120.81	111.12
1	C	169	ILE	N-CA-C	6.45	118.79	108.85
1	B	406	GLU	N-CA-C	-6.44	105.00	112.92
1	B	407	TYR	CB-CA-C	-6.41	98.10	109.70
1	H	328	ARG	CB-CA-C	-6.39	101.05	110.95
1	E	124	ILE	N-CA-C	6.35	114.09	108.63
1	A	459	MET	N-CA-C	6.35	126.40	113.20
1	H	169	ILE	N-CA-C	6.33	117.60	108.48
1	F	169	ILE	N-CA-C	6.17	117.36	108.48
1	B	375	ASP	N-CA-C	-6.11	101.48	110.52
1	E	248	LEU	CA-C-N	-6.10	116.34	122.69
1	E	248	LEU	C-N-CA	-6.10	116.34	122.69
1	E	169	ILE	N-CA-C	6.08	117.24	108.48
1	A	353	PRO	N-CA-C	-6.07	99.97	112.47
1	B	411	SER	N-CA-CB	-6.06	102.35	111.56
1	A	311	GLY	N-CA-C	6.05	119.02	110.74
1	G	375	ASP	N-CA-C	-6.01	101.62	110.52
1	D	169	ILE	N-CA-C	5.94	117.03	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	311	GLY	N-CA-C	5.87	118.78	110.74
1	F	311	GLY	N-CA-C	5.84	118.75	110.74
1	G	169	ILE	N-CA-C	5.82	116.86	108.48
1	A	374	GLN	CB-CA-C	-5.79	101.80	111.23
1	H	459	MET	N-CA-C	5.77	125.21	113.20
1	H	375	ASP	N-CA-C	-5.72	102.83	110.55
1	G	311	GLY	N-CA-C	5.68	118.52	110.74
1	A	169	ILE	N-CA-C	5.64	117.54	108.85
1	F	285	SER	N-CA-C	-5.64	105.08	112.41
1	E	374	GLN	CB-CA-C	-5.62	99.23	110.42
1	D	124	ILE	N-CA-C	5.61	113.45	108.63
1	A	321	GLY	CA-C-N	5.58	126.05	120.52
1	A	321	GLY	C-N-CA	5.58	126.05	120.52
1	A	375	ASP	N-CA-C	-5.53	102.34	110.52
1	F	375	ASP	N-CA-C	-5.52	103.09	110.55
1	A	281	CYS	CB-CA-C	-5.43	102.35	110.88
1	D	482	ALA	N-CA-C	-5.43	98.91	108.69
1	F	160	GLY	CA-C-N	5.43	124.62	118.97
1	F	160	GLY	C-N-CA	5.43	124.62	118.97
1	E	311	GLY	N-CA-C	5.37	118.09	110.74
1	A	283	ALA	N-CA-CB	5.33	120.42	110.99
1	C	311	GLY	N-CA-C	5.29	117.98	110.74
1	E	248	LEU	N-CA-C	-5.29	103.16	110.35
1	D	311	GLY	N-CA-C	5.28	117.98	110.74
1	E	138	PRO	CB-CA-C	-5.28	102.86	111.56
1	H	249	GLY	CA-C-N	-5.27	115.29	122.03
1	H	249	GLY	C-N-CA	-5.27	115.29	122.03
1	F	146	VAL	N-CA-C	5.25	113.67	107.84
1	A	374	GLN	N-CA-C	-5.23	107.26	113.38
1	G	245	GLN	N-CA-C	-5.21	101.38	109.72
1	B	124	ILE	N-CA-C	5.20	113.10	108.63
1	H	185	VAL	CB-CA-C	-5.15	105.18	112.14
1	G	374	GLN	CB-CA-C	-5.13	102.86	111.23
1	C	409	LEU	N-CA-C	5.13	119.42	112.04
1	E	355	ASP	N-CA-C	5.11	117.13	110.43
1	A	249	GLY	N-CA-C	5.08	120.02	112.41
1	D	355	ASP	CA-C-N	5.07	128.50	120.89
1	D	355	ASP	C-N-CA	5.07	128.50	120.89
1	B	387	VAL	CB-CA-C	-5.04	103.17	110.63
1	C	338	ILE	CB-CA-C	-5.03	105.28	112.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	268	0
1	B	3698	0	3691	260	0
1	C	3698	0	3690	258	0
1	D	3698	0	3691	271	0
1	E	3698	0	3691	242	0
1	F	3698	0	3691	248	0
1	G	3698	0	3691	259	0
1	H	3698	0	3691	245	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
2	G	44	0	26	8	0
2	H	44	0	26	7	0
3	A	14	0	0	3	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	3	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	1899	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 32.

All (1899) 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	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:247:GLU:C	1:D:248:LEU:HD23	1.58	1.28
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:A:481:ILE:H	1:A:481:ILE:CD1	1.51	1.22
1:B:245:GLN:C	1:B:246:LEU:HD23	1.66	1.18
1:A:481:ILE:HD12	1:A:481:ILE:N	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:2:GLN:HE21	1:B:2:GLN:HA	1.06	1.13
1:A:444:GLY:N	1:A:459:MET:O	1.81	1.13
1:A:248:LEU:N	1:A:248:LEU:HD23	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
1:C:444:GLY:N	1:C:459:MET:O	1.83	1.11
1:F:415:THR:HG22	1:F:417:ASN:H	1.09	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:C:94:ILE:HD11	1:C:314:MET:C	1.76	1.09
1:D:374:GLN:O	1:D:374:GLN:CG	1.99	1.09
1:F:325:SER:OG	1:F:328:ARG:HG2	1.32	1.09
1:H:444:GLY:N	1:H:459:MET:O	1.82	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:E:329:ARG:HG2	1:E:329:ARG:HH11	1.15	1.08
1:G:329:ARG:HG2	1:G:329:ARG:HH11	1.16	1.08
1:G:415:THR:HG22	1:G:417:ASN:H	1.11	1.08
1:D:356:LYS:H	1:D:356:LYS:HD3	1.19	1.07
1:E:356:LYS:HD3	1:E:356:LYS:H	1.17	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:NH1	1:B:329:ARG:HG2	1.52	1.07
1:B:415:THR:HG22	1:B:417:ASN:H	1.15	1.06
1:A:282:ILE:HD11	1:A:447:PHE:CE1	1.91	1.05
3:C:708:HOH:O	1:D:471:ARG:HD3	1.54	1.05
1:H:328:ARG:HH11	1:H:328:ARG:CG	1.70	1.05
1:E:328:ARG:HH21	1:E:383:PHE:CB	1.68	1.04
1:B:405:THR:HG22	1:B:407:TYR:H	1.19	1.04
1:G:261:ASN:C	1:G:261:ASN:HD22	1.64	1.04
1:G:325:SER:HB3	1:G:328:ARG:NH1	1.69	1.04
1:D:329:ARG:HG2	1:D:329:ARG:HH11	1.18	1.04
1:F:329:ARG:HG2	1:F:329:ARG:HH11	0.88	1.04
1:F:329:ARG:HG2	1:F:329:ARG:NH1	1.63	1.04
1:B:329:ARG:HH11	1:B:329:ARG:CG	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:F:261:ASN:HD22	1:F:261:ASN:C	1.64	1.01
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:A:329:ARG:HH11	1:A:329:ARG:CG	1.73	1.01
1:H:328:ARG:HH11	1:H:328:ARG:HG2	0.85	1.01
1:H:328:ARG:HG2	1:H:328:ARG:NH1	1.67	1.01
1:A:329:ARG:HH11	1:A:329:ARG:HG2	0.85	1.00
1:C:325:SER:OG	1:C:328:ARG:CG	2.09	1.00
1:G:247:GLU:C	1:G:248:LEU:CD2	2.34	1.00
1:H:356:LYS:HE2	1:H:357:ALA:H	1.25	1.00
1:H:325:SER:OG	1:H:328:ARG:HG3	1.62	1.00
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:A:94:ILE:HD11	1:A:314:MET:C	1.87	0.98
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:10[B]:ARG:HG3	1:F:10[B]:ARG:HH11	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:H	1:E:356:LYS:CD	1.74	0.93
1:E:10[B]:ARG:HH11	1:E:10[B]:ARG:HG3	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:D:247:GLU:C	1:D:248:LEU:CD2	2.42	0.92
1:A:94:ILE:HD11	1:A:314:MET:O	1.67	0.92
1:D:380:GLU:CD	1:E:376:ARG:HH12	1.76	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:HH11	1:B:10[B]:ARG:HG3	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:90:THR:O	1:G:324:THR:HG22	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:ILE:H	1:G:167:ASN:HD21	1.19	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:H	1:C:356:LYS:CD	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:HD23	1:G:248:LEU:N	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: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:D:376:ARG:HH12	1:E:380:GLU:CD	1.81	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: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
1:F:90:THR:O	1:F:324:THR:HG22	1.73	0.87
1:A:122:SER:HA	1:C:122:SER:HA	1.57	0.86
1:G:328:ARG:CZ	1:G:328:ARG:HB2	2.04	0.86
1:H:329:ARG:HH11	1:H:329:ARG:CG	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:O	1:C:374:GLN:HG2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:LEU:N	1:E:248:LEU:HD23	1.92	0.83
1:G:356:LYS:H	1:G:356:LYS:CD	1.89	0.83
1:A:481:ILE:H	1:A:481:ILE:HD12	0.71	0.83
1:H:49:ALA:HB1	1:H:168:THR:HG23	1.59	0.83
1:B:246:LEU:HD23	1:B:246:LEU:N	1.89	0.83
1:C:374:GLN:O	1:C:374:GLN:CG	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:B:2:GLN:HA	1:B:2:GLN:NE2	1.87	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:D:380:GLU:CD	1:E:376:ARG:NH1	2.37	0.82
1:E:328:ARG:NH1	1:E:331:ARG:NH1	2.26	0.81
1:B:148:TRP:CD1	1:B:174:SER:HG	1.97	0.81
1:F:415:THR:HG22	1:F:417:ASN:N	1.94	0.81
1:B:248:LEU:HD23	1:B:248:LEU:H	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:249:GLY:HA3	2:C:601:NAD:O2D	1.79	0.81
1:C:476:ASN:OD1	1:C:479:ALA:HB3	1.81	0.81
1:A:484:HIS:O	1:B:95:ARG:NH2	2.14	0.80
1:F:261:ASN:C	1:F:261:ASN:ND2	2.38	0.80
1:D:376:ARG:NH1	1:E:380:GLU:CD	2.40	0.80
1:A:49:ALA:HB1	1:A:168:THR:HG23	1.64	0.80
1:A:458:GLU:O	1:A:459:MET:HB2	1.81	0.80
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:H	1:H:356:LYS:CD	1.92	0.80
1:B:94:ILE:HD11	1:B:314:MET:C	2.07	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:HH11	1:D:329:ARG:CG	1.96	0.79
1:B:313:PRO:HB2	1:B:314:MET:HE2	1.64	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:HH11	1:G:329:ARG:CG	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:B:245:GLN:C	1:B:246:LEU:CD2	2.55	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:GLU:OE1	1:H:400:ALA:CB	2.31	0.78
1:G:261:ASN:C	1:G:261:ASN:ND2	2.37	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:A:273:ILE:HG12	1:A:387:VAL:HG22	1.67	0.77
1:D:313:PRO:HB2	1:D:314:MET:HE2	1.66	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: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: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:C:476:ASN:CG	1:C:479:ALA:HB3	2.09	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
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:G:313:PRO:HB2	1:G:314:MET:HE2	1.67	0.76
1:H:313:PRO:HB2	1:H:314:MET:HE2	1.66	0.76
1:A:328:ARG:HH21	1:A:383:PHE:H	1.32	0.75
1:G:326:ALA:O	1:G:329:ARG:N	2.19	0.75
1:B:2:GLN:HE21	1:B:2:GLN:CA	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:247:GLU:O	1:D:248:LEU:CD2	2.31	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:313:PRO:HB2	1:E:314:MET:HE2	1.68	0.74
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:HH11	1:C:329:ARG:CG	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:D:356:LYS:HZ1	1:G:10[A]:ARG:HD2	1.52	0.74
1:A:405:THR:HG22	1:A:407:TYR:N	2.03	0.73
1:D:356:LYS:HG2	1:G:12:VAL:HG21	1.69	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: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:A:313:PRO:HB2	1:A:314:MET:HE2	1.71	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:THR:HG22	1:E:417:ASN:N	1.96	0.72
1:A:148:TRP:CD1	1:A:174:SER:HG	2.08	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: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:C:313:PRO:HB2	1:C:314:MET:HE2	1.72	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
1:G:245:GLN:C	1:G:246:LEU:HD23	2.13	0.70
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:E:373:PRO:O	1:E:374:GLN:CD	2.34	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:18:GLY:HA2	1:E:33:ARG:HH21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:247:GLU:HB3	2:G:601:NAD:N7N	2.07	0.70
1:G:476:ASN:CG	1:G:479:ALA:HB3	2.15	0.70
1:F:313:PRO:HB2	1:F:314:MET:HE2	1.73	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:NH1	1:B:329:ARG:CG	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:A:125:PRO:HG3	1:C:119:ILE:O	1.93	0.69
1:B:118:LYS:HE3	1:C:111:TYR:CE1	2.27	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HB3	1:H:329:ARG:NH1	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:HG3	1:G:10[B]:ARG:NH1	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:HG3	1:A:10[B]:ARG:NH1	2.04	0.67
1:A:279:GLN:HE22	1:A:324:THR:H	1.39	0.67
1:D:356:LYS:HZ2	1:G:10[A]:ARG:CZ	2.07	0.67
1:E:328:ARG:HE	1:E:383:PHE:HB3	1.59	0.67
1:D:481:ILE:N	1:D:481:ILE:CD1	2.57	0.67
1:F:279:GLN:HE22	1:F:324:THR:H	1.40	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:G:326:ALA:O	1:G:327:LEU:C	2.36	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:HD13	1:D:481:ILE:H	1.60	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:HG2	1:C:329:ARG:NH1	2.03	0.67
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:HG3	1:F:10[B]:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:TYR:CE1	1:C:118:LYS:HE3	2.31	0.66
1:C:282:ILE:O	1:C:282:ILE:CG1	2.43	0.66
1:C:49:ALA:O	1:C:168:THR:HG21	1.96	0.66
1:G:356:LYS:HD3	1:G:356:LYS:N	2.09	0.66
1:B:10[B]:ARG:HG3	1:B:10[B]:ARG:NH1	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:H:248:LEU:N	1:H:248:LEU:HD23	2.11	0.66
1:B:277:GLN:NE2	1:B:321:GLY:H	1.94	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:201:VAL:O	1:G:201:VAL:HG12	1.95	0.66
1:G:374:GLN:O	1:G:374:GLN:CG	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:B:174:SER:C	1:B:176:ILE:H	2.03	0.65
1:D:279:GLN:HE22	1:D:324:THR:H	1.44	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:C:325:SER:O	1:C:328:ARG:HB2	1.96	0.65
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:A:352:ALA:C	1:A:353:PRO:O	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:SER:HG	1:F:328:ARG:HD2	1.59	0.65
1:E:356:LYS:HE2	1:E:357:ALA:N	2.07	0.64
1:E:356:LYS:CD	1:E:356:LYS:N	2.56	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:C:248:LEU:HD13	1:D:241:LEU:HD13	1.78	0.64
1:D:185:VAL:HG21	1:D:200:VAL:HG21	1.78	0.64
1:E:329:ARG:HG2	1:E:329:ARG:NH1	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:D:18:GLY:HA2	1:E:33:ARG:NH2	2.13	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:HD13	1:G:481:ILE:H	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: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
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:CD1	1:D:262:ILE:N	2.62	0.63
1:F:258:GLU:N	1:F:258:GLU:OE1	2.30	0.63
1:A:135:GLN:HE22	1:B:426:HIS:CE1	2.16	0.63
1:B:71:LEU:HD22	1:B:188:MET:HG2	1.80	0.63
1:B:174:SER:O	1:B:176:ILE:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:TRP:CZ2	1:C:64:ARG:HG2	2.33	0.63
1:C:282:ILE:O	1:C:282:ILE:HG12	1.95	0.63
1:H:49:ALA:O	1:H:168:THR:HG21	1.98	0.63
1:H:185:VAL:HG21	1:H:200:VAL:CG2	2.29	0.63
1:G:34:ILE:HG13	1:G:178:PRO:HG2	1.81	0.63
1:C:174:SER:C	1:C:176:ILE:H	2.06	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:C:482:ALA:O	1:C:483:PRO:C	2.42	0.63
1:H:356:LYS:HD3	1:H:356:LYS:N	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:O	1:F:481:ILE:HG22	1.99	0.62
1:H:200:VAL:HG12	1:H:202:PRO:HD3	1.81	0.62
1:B:174:SER:C	1:B:176:ILE:N	2.54	0.62
1:C:87:SER:HB2	1:C:92:HIS:O	1.99	0.62
1:D:329:ARG:HG2	1:D:329:ARG:NH1	1.99	0.62
1:E:373:PRO:C	1:E:375:ASP:N	2.55	0.62
1:G:261:ASN:ND2	1:G:261:ASN:O	2.32	0.62
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:O	1:B:282:ILE:HG22	1.98	0.62
1:F:201:VAL:O	1:F:201:VAL:HG12	1.99	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:D:480:LYS:O	1:D:481:ILE:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:SER:HB2	1:F:92:HIS:O	1.99	0.62
1:F:399:LEU:HD11	1:F:427:ALA:HB1	1.81	0.62
1:G:326:ALA:C	1:G:328:ARG:N	2.56	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:94:ILE:HD11	1:G:314:MET:O	1.99	0.62
1:G:140:GLY:H	1:G:167:ASN:HD22	1.45	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:E:415:THR:CG2	1:E:417:ASN:H	1.99	0.62
1:F:22:VAL:CG2	1:F:34:ILE:HG12	2.30	0.62
1:F:95:ARG:HD3	1:F:319:GLU:HA	1.80	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:235:GLU:HG3	1:H:238:LYS:HD2	1.81	0.61
1:G:238:LYS:CD	1:H:235:GLU:HG3	2.30	0.61
1:G:273:ILE:HG21	1:G:387:VAL:CG2	2.29	0.61
1:F:444:GLY:HA2	1:F:460:GLY:HA2	1.82	0.61
1:H:329:ARG:NH1	1:H:329:ARG:HG2	2.14	0.61
1:A:87:SER:HB2	1:A:92:HIS:O	2.00	0.61
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:H:273:ILE:HG21	1:H:387:VAL:CG2	2.31	0.61
1:H:481:ILE:HG22	1:H:481:ILE:O	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:HG3	1:H:10[B]:ARG:NH1	2.05	0.61
1:A:252:GLY:HA2	1:A:410:GLY:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:356:LYS:HZ2	1:G:10[A]:ARG:NH1	1.97	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:G:185:VAL:HG21	1:G:200:VAL:CG2	2.31	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
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:G:172:LYS:NZ	1:G:173:PRO:O	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:C:282:ILE:HD13	2.02	0.60
1:E:421:ALA:HB1	1:E:435:ILE:HD13	1.84	0.60
1:F:1:MET:HG3	1:F:2:GLN:N	2.16	0.60
1:G:56:TRP:CZ2	1:G:64:ARG:HG2	2.37	0.60
1:G:481:ILE:HG21	1:H:440:ARG:NH1	2.16	0.60
1:H:329:ARG:HH11	1:H:329:ARG:HG2	1.66	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: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:22:VAL:CG2	1:A:34:ILE:HG12	2.32	0.60
1:A:327:LEU:O	1:A:327:LEU:HD22	2.01	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:N	1:A:354:ASP:OD1	2.35	0.60
1:D:175:GLU:OE1	1:D:175:GLU:N	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
1:E:159:MET:HE1	1:E:198:VAL:CG1	2.32	0.59
1:E:373:PRO:C	1:E:375:ASP:H	2.10	0.59
1:G:49:ALA:O	1:G:168:THR:HG21	2.02	0.59
1:C:1:MET:HG3	1:C:2:GLN:N	2.17	0.59
1:C:149:ASN:HD21	2:C:601:NAD:C6N	2.15	0.59
1:D:376:ARG:NH1	1:E:380:GLU:OE2	2.34	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:CD	1:H:356:LYS:N	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:HG22	1:E:481:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:TRP:CH2	1:D:64:ARG:HG2	2.38	0.59
1:D:185:VAL:CG2	1:D:200:VAL:HG21	2.32	0.59
1:D:356:LYS:HZ1	1:G:10[A]:ARG:CD	2.14	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:27:ASP:CG	1:C:29:SER:HB3	2.28	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:CD	1:A:356:LYS:N	2.64	0.58
1:A:444:GLY:CA	1:A:459:MET:O	2.50	0.58
1:C:95:ARG:NH1	1:C:318:THR:O	2.32	0.58
1:C:441:VAL:HG12	1:C:442:SER:H	1.68	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:A:115:MET:HB2	1:D:118:LYS:HE2	1.85	0.58
1:B:56:TRP:CZ2	1:B:64:ARG:HG2	2.38	0.58
1:D:71:LEU:HD22	1:D:188:MET:HG2	1.86	0.58
1:E:137:LYS:HZ1	1:F:426:HIS:CD2	2.21	0.58
1:E:356:LYS:HD3	1:E:356:LYS:N	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:HD13	1:C:338:ILE:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:ASN:HD21	2:G:601:NAD:C5N	2.17	0.58
1:A:201:VAL:O	1:A:201:VAL:HG12	2.03	0.58
1:C:94:ILE:HG12	1:C:313:PRO:O	2.04	0.58
1:C:250:GLY:HA2	1:C:407:TYR:HB3	1.84	0.58
1:H:250:GLY:HA3	1:H:407:TYR:HB3	1.86	0.58
1:C:94:ILE:HD11	1:C:314:MET:CA	2.34	0.58
1:C:243:ARG:HD2	1:D:455:TYR:HB3	1.85	0.58
1:C:445:SER:HB2	1:D:132:ASN:HD21	1.67	0.58
1:G:27:ASP:CG	1:G:29:SER:HB3	2.29	0.58
1:G:417:ASN:HD22	1:G:420:ARG:HB2	1.68	0.58
1:C:238:LYS:HE3	1:E:351:LYS:HZ2	1.69	0.58
1:E:215:HIS:HD2	1:E:217:ASP:H	1.52	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:27:ASP:CG	1:H:29:SER:HB3	2.28	0.58
1:H:444:GLY:HA2	1:H:460:GLY:HA2	1.86	0.58
1:A:49:ALA:O	1:A:168:THR:HG21	2.04	0.58
1:A:280:ALA:HB3	1:A:283:ALA:HB2	1.86	0.58
1:D:27:ASP:CG	1:D:29:SER:HB3	2.28	0.58
1:D:229:THR:HG21	2:D:601:NAD:O1A	2.04	0.58
1:D:374:GLN:O	1:D:374:GLN:HG3	2.00	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:D:261:ASN:C	1:D:261:ASN:OD1	2.45	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:F:322:PRO:HG3	1:F:363:TYR:CZ	2.39	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
1:H:71:LEU:HD22	1:H:188:MET:HG2	1.86	0.57
1:H:329:ARG:CG	1:H:329:ARG:NH1	2.54	0.57
1:D:313:PRO:HB2	1:D:314:MET:CE	2.35	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:259:ASP:OD1	1:A:415:THR:HG23	2.05	0.57
1:A:356:LYS:HE2	1:A:357:ALA:N	2.09	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:87:SER:CB	1:C:92:HIS:O	2.53	0.56
1:C:325:SER:HG	1:C:328:ARG:HG2	1.68	0.56
1:E:27:ASP:CG	1:E:29:SER:HB3	2.30	0.56
1:G:22:VAL:HG21	1:G:34:ILE:HG12	1.86	0.56
1:G:139:ILE:N	1:G:167:ASN:HD21	1.97	0.56
1:A:27:ASP:CG	1:A:29:SER:HB3	2.29	0.56
1:A:277:GLN:NE2	1:A:321:GLY:H	2.03	0.56
1:B:328:ARG:O	1:B:329:ARG:C	2.48	0.56
1:C:139:ILE:H	1:C:167:ASN:ND2	1.99	0.56
1:C:139:ILE:N	1:C:167:ASN:HD21	1.99	0.56
1:C:249:GLY:HA3	2:C:601:NAD:HO2N	1.70	0.56
1:D:231:ARG:HD2	1:E:337:ASP:OD2	2.05	0.56
1:E:132:ASN:HD21	1:F:445:SER:HB2	1.69	0.56
1:E:139:ILE:N	1:E:167:ASN:HD21	1.95	0.56
1:F:131:LEU:HD22	1:F:131:LEU:C	2.30	0.56
1:G:273:ILE:HG21	1:G:387:VAL:HG21	1.88	0.56
1:H:356:LYS:HE2	1:H:357:ALA:N	2.07	0.56
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:89:ASN:HD21	1:E:177:THR:HA	1.70	0.56
1:E:149:ASN:OD1	1:E:149:ASN:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:136:ARG:HG3	1:G:468:THR:OG1	2.06	0.55
1:G:421:ALA:HB1	1:G:435:ILE:HD13	1.88	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:149:ASN:HD21	2:A:601:NAD:C5N	2.20	0.55
1:A:282:ILE:CD1	1:A:447:PHE:HE1	2.13	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: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:322:PRO:HG3	1:H:363:TYR:CZ	2.42	0.55
1:H:328:ARG:CG	1:H:328:ARG:NH1	2.41	0.55
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:136:ARG:HG3	1:A:468:THR:OG1	2.06	0.55
1:A:356:LYS:HD3	1:A:356:LYS:N	2.12	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:F:421:ALA:HB1	1:F:435:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:NH1	1:A:331:ARG:HD3	2.22	0.55
1:A:353:PRO:O	1:A:353:PRO:CD	2.52	0.55
1:B:149:ASN:HD21	2:B:601:NAD:H6N	1.71	0.55
1:C:282:ILE:O	1:C:282:ILE:CD1	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:E:261:ASN:C	1:E:261:ASN:OD1	2.49	0.55
1:G:53:PHE:HB3	1:G:54:PRO:HD3	1.89	0.55
1:H:5:LEU:CB	3:H:714:HOH:O	2.54	0.55
1:H:131:LEU:HD22	1:H:131:LEU:C	2.31	0.55
1:H:374:GLN:O	1:H:374:GLN:HG2	2.02	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:A:159:MET:HE1	1:A:198:VAL:HG13	1.89	0.54
1:C:415:THR:CG2	1:C:416:GLN:N	2.70	0.54
1:F:27:ASP:CG	1:F:29:SER:HB3	2.32	0.54
1:H:20:ILE:HG13	1:H:36:ALA:HB2	1.88	0.54
1:A:174:SER:O	1:A:175:GLU:C	2.49	0.54
1:E:259:ASP:OD1	1:E:415:THR:HG23	2.07	0.54
1:F:141:VAL:HG12	1:F:141:VAL:O	2.07	0.54
1:G:322:PRO:HG3	1:G:363:TYR:CZ	2.42	0.54
1:G:481:ILE:HG21	1:H:440:ARG:HH12	1.73	0.54
1:H:144:GLN:OE1	1:H:158:LYS:HB3	2.07	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:248:LEU:HD13	1:D:241:LEU:CD1	2.38	0.54
1:C:273:ILE:HG21	1:C:387:VAL:HG21	1.90	0.54
1:D:260:ALA:O	1:D:262:ILE:CD1	2.55	0.54
1:D:459:MET:HE2	1:D:459:MET:HA	1.90	0.54
1:G:432:MET:HA	1:H:472:SER:O	2.06	0.54
1:H:273:ILE:HG21	1:H:387:VAL:HG21	1.88	0.54
1:A:22:VAL:HG21	1:A:34:ILE:HG12	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:282:ILE:HD13	1:G:434:TRP:CH2	2.42	0.54
1:G:313:PRO:HB2	1:G:314:MET:CE	2.35	0.54
1:F:17:GLY:HA3	1:H:376:ARG:NH1	2.22	0.54
1:F:25:PRO:HA	1:F:362:PHE:CE2	2.43	0.54
1:A:87:SER:CB	1:A:92:HIS:O	2.56	0.54
1:A:90:THR:HG22	1:A:177:THR:CG2	2.37	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:A:352:ALA:O	1:A:353:PRO:C	2.49	0.54
1:C:96:ASP:O	1:C:97:SER:C	2.50	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:87:SER:CB	1:F:92:HIS:O	2.55	0.54
1:F:415:THR:CG2	1:F:416:GLN:N	2.71	0.54
1:H:326:ALA:HB2	1:H:362:PHE:CE1	2.43	0.54
1:A:328:ARG:O	1:A:329:ARG:C	2.50	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:87:SER:CB	1:H:92:HIS:O	2.56	0.54
1:H:172:LYS:NZ	1:H:173:PRO:O	2.37	0.54
1:H:257:PHE:CD1	1:H:420:ARG:HD3	2.42	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:C:459:MET:HE2	1:C:459:MET:HA	1.90	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:247:GLU:C	1:A:248:LEU:HD23	2.29	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:GLY:HA2	1:B:460:GLY:HA2	1.90	0.53
1:H:174:SER:C	1:H:176:ILE:N	2.65	0.53
1:H:100:LEU:O	1:H:103:PRO:HD2	2.08	0.53
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:53:PHE:HB3	1:D:54:PRO:HD3	1.90	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:F:31:ILE:HG22	1:F:32:THR:HG22	1.89	0.53
1:F:200:VAL:HG12	1:F:202:PRO:HD3	1.90	0.53
1:G:415:THR:CG2	1:G:416:GLN:N	2.72	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:53:PHE:HB3	1:A:54:PRO:HD3	1.90	0.53
1:A:302:ILE:O	1:A:306:LYS:HG3	2.08	0.53
1:B:27:ASP:CG	1:B:29:SER:HB3	2.34	0.53
1:D:355:ASP:HB3	1:D:356:LYS:HD3	1.91	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:E:180:SER:HB2	3:E:720:HOH: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: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:F:459:MET:HE2	1:F:459:MET:HA	1.91	0.53
1:G:159:MET:HE1	1:G:198:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:80:GLU:OE1	1:E:98:ARG:NE	2.42	0.53
1:E:313:PRO:HB2	1:E:314:MET:CE	2.38	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:49:ALA:O	1:B:168:THR:HG21	2.09	0.53
1:B:373:PRO:HG3	1:B:390:VAL:HG11	1.91	0.53
1:E:459:MET:HA	1:E:459:MET:HE2	1.91	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:OD1	1:H:149:ASN:N	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:49:ALA:O	1:F:168:THR:HG21	2.09	0.52
1:F:144:GLN:OE1	1:F:158:LYS:HB3	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:OE2	1:H:175:GLU:N	2.40	0.52
1:C:80:GLU:O	1:C:81:GLU:C	2.49	0.52
1:D:159:MET:HE1	1:D:198:VAL:HG13	1.92	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:F:249:GLY:CA	2:F:601:NAD:HO2N	2.22	0.52
1:B:144:GLN:OE1	1:B:158:LYS:HB3	2.10	0.52
1:D:354:ASP:OD2	1:D:354:ASP:N	2.42	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:174:SER:C	1:A:176:ILE:N	2.64	0.52
1:A:221:ILE:HD13	1:A:222:ALA:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:459:MET:HE2	1:G:459:MET:HA	1.92	0.52
1:A:94:ILE:HD11	1:A:314:MET:HA	1.92	0.52
1:A:273:ILE:O	1:A:278:GLY:HA2	2.10	0.52
1:B:141:VAL:HA	1:B:168:THR:HG22	1.90	0.52
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:CD	1:D:356:LYS:N	2.55	0.52
1:E:159:MET:HE1	1:E:198:VAL:HG13	1.90	0.52
1:E:282:ILE:HD13	1:E:434:TRP:CH2	2.44	0.52
1:G:22:VAL:HG23	1:G:34:ILE:HG12	1.92	0.52
1:G:258:GLU:HG2	1:G:259:ASP:N	2.23	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: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:H:480:LYS:O	1:H:481:ILE:C	2.53	0.52
1:C:174:SER:C	1:C:176:ILE:N	2.63	0.52
1:E:149:ASN:HD21	2:E:601:NAD:C5N	2.23	0.52
1:F:329:ARG:O	1:F:330:ASP:C	2.53	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:A:483:PRO:HB3	1:B:267:ASN:CG	2.35	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:B:459:MET:HA	1:B:459:MET:HE2	1.90	0.51
1:C:131:LEU:HD22	1:C:131:LEU:C	2.34	0.51
1:E:258:GLU:H	1:E:258:GLU:CD	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:22:VAL:HG23	1:H:34:ILE:HG12	1.92	0.51
1:H:325:SER:HG	1:H:328:ARG:HG3	1.74	0.51
1:A:415:THR:HG22	1:A:416:GLN:H	1.76	0.51
1:E:131:LEU:C	1:E:131:LEU:HD22	2.35	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:G:374:GLN:O	1:G:374:GLN:HG2	1.98	0.51
1:A:215:HIS:CD2	1:A:217:ASP:H	2.25	0.51
1:B:27:ASP:C	1:B:360:ASN:O	2.54	0.51
1:B:131:LEU:C	1:B:131:LEU:HD22	2.36	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:56:TRP:CH2	1:H:64:ARG:HG2	2.46	0.51
1:H:221:ILE:HD13	1:H:222:ALA:N	2.25	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:136:ARG:HG3	1:D:468:THR:OG1	2.10	0.51
1:D:322:PRO:HG3	1:D:363:TYR:CZ	2.45	0.51
1:H:87:SER:HB3	1:H:97:SER:OG	2.10	0.51
1:D:100:LEU:O	1:D:101:ASP:C	2.54	0.51
1:D:148:TRP:HD1	1:D:174:SER:OG	1.94	0.51
1:D:356:LYS:NZ	1:G:10[A]:ARG:CZ	2.72	0.51
1:B:221:ILE:HD13	1:B:222:ALA:N	2.26	0.51
1:B:405:THR:HG22	1:B:406:GLU:N	2.25	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:365:GLU:HB2	1:D:366:PRO:HD2	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:56:TRP:CH2	1:F:64:ARG:HG2	2.46	0.51
1:F:325:SER:O	1:F:328:ARG:HB2	2.11	0.51
1:H:141:VAL:O	1:H:141:VAL:HG12	2.09	0.51
1:E:140:GLY:H	1:E:167:ASN:HD22	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:480:LYS:O	1:E:481:ILE:C	2.54	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:E:487:ARG:C	3:F:709:HOH:O	2.55	0.50
1:F:215:HIS:CD2	1:F:217:ASP:H	2.27	0.50
1:C:32:THR:OG1	1:C:33:ARG:N	2.44	0.50
1:C:119:ILE:HG12	1:C:464:ILE:HG21	1.92	0.50
1:D:262:ILE:H	1:D:262:ILE:HD13	1.76	0.50
1:F:20:ILE:HD11	1:F:204:TYR:CE2	2.46	0.50
1:C:159:MET:HE1	1:C:198:VAL:CG1	2.42	0.50
1:C:221:ILE:HD13	1:C:222:ALA:N	2.26	0.50
1:G:483:PRO:HB3	1:H:267:ASN:CG	2.36	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:159:MET:HE1	1:D:198:VAL:CG1	2.41	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:D:291:LYS:HE3	1:D:391:ARG:HB3	1.93	0.50
1:E:374:GLN:O	1:E:374:GLN:HG2	1.90	0.50
1:G:56:TRP:CH2	1:G:64:ARG:HG2	2.47	0.50
1:B:94:ILE:CD1	1:B:314:MET:C	2.81	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:291:LYS:HE3	1:C:391:ARG:HB3	1.94	0.50
1:C:323:LEU:HD12	1:C:329:ARG:HA	1.93	0.50
1:D:146:VAL:HG23	1:D:147:PRO:O	2.11	0.50
1:F:141:VAL:CG2	1:F:168:THR:HG22	2.42	0.50
1:G:291:LYS:HE3	1:G:391:ARG:CB	2.42	0.50
1:G:355:ASP:O	3:G:711:HOH:O	2.19	0.50
1:C:20:ILE:HG13	1:C:36:ALA:HB2	1.94	0.50
1:E:137:LYS:HZ2	1:F:426:HIS:CD2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:ASN:ND2	1:H:445:SER:HB2	2.27	0.50
1:G:159:MET:HE1	1:G:198:VAL:CG1	2.42	0.50
1:G:481:ILE:H	1:G:481:ILE:CD1	2.20	0.50
1:A:121:GLY:HA3	1:C:123:VAL:HB	1.93	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:OD1	1:D:261:ASN:O	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:N	1:A:248:LEU:CD2	2.32	0.49
1:A:476:ASN:CG	1:A:479:ALA:HB3	2.37	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
1:A:155:THR:CG2	1:A:181:THR:HB	2.41	0.49
1:B:248:LEU:CD2	1:B:248:LEU:H	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:A:159:MET:HE1	1:A:198:VAL:CG1	2.43	0.49
1:B:458:GLU:O	1:B:459:MET:CB	2.60	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:H:5:LEU:C	3:H:714:HOH:O	2.56	0.49
1:H:159:MET:HE1	1:H:198:VAL:HG13	1.93	0.49
1:C:148:TRP:HB2	1:C:177:THR:HG21	1.94	0.49
1:D:356:LYS:NZ	1:G:10[A]:ARG:HD2	2.25	0.49
1:E:257:PHE:CD1	1:E:420:ARG:HD3	2.47	0.49
1:G:273:ILE:O	1:G:278:GLY:HA2	2.12	0.49
1:B:149:ASN:OD1	1:B:149:ASN:N	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:G:71:LEU:HD22	1:G:188:MET:HG2	1.93	0.49
1:G:175:GLU:OE2	1:G:175:GLU:N	2.41	0.49
1:B:159:MET:HE1	1:B:198:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:SER:HB3	1:C:97:SER:OG	2.12	0.49
1:C:100:LEU:O	1:C:101:ASP:C	2.56	0.49
1:G:87:SER:CB	1:G:92:HIS:O	2.60	0.49
1:G:174:SER:C	1:G:176:ILE:N	2.71	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: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:A:70:LYS:HA	1:A:70:LYS:HD3	1.62	0.48
1:A:248:LEU:HD12	1:B:241:LEU:HD13	1.92	0.48
1:A:373:PRO:HG3	1:A:390:VAL:HG11	1.95	0.48
1:B:311:GLY:HA2	1:B:358:LEU:HD11	1.95	0.48
1:C:10[B]:ARG:NH1	1:C:10[B]:ARG:CG	2.72	0.48
1:C:238:LYS:HE3	1:E:351:LYS:HZ3	1.78	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:OD1	1:A:261:ASN:O	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:53:PHE:HB3	1:B:54:PRO:HD3	1.94	0.48
1:B:333:LEU:HD22	1:B:351:LYS: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:H:159:MET:HE1	1:H:198:VAL:CG1	2.43	0.48
1:A:426:HIS:HD2	1:B:137:LYS:NZ	2.11	0.48
1:A:459:MET:HE2	1:A:459:MET:HA	1.96	0.48
1:B:56:TRP:CH2	1:B:64:ARG:HG2	2.48	0.48
1:B:155:THR:CG2	1:B:181:THR:HB	2.43	0.48
1:C:373:PRO:HG3	1:C:390:VAL:HG11	1.95	0.48
1:D:131:LEU:C	1:D:131:LEU:HD22	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:174:SER:C	1:H:176:ILE:H	2.21	0.48
1:A:241:LEU:HD13	1:B:248:LEU:CD1	2.43	0.48
1:A:248:LEU:CD1	1:B:241:LEU:CD1	2.91	0.48
1:A:282:ILE:O	1:A:282:ILE:HG22	2.09	0.48
1:A:327:LEU:O	1:A:327:LEU:CD2	2.61	0.48
1:C:281:CYS:HB3	2:C:601:NAD:N1N	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: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: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
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:D:404:ASN:O	1:D:404:ASN:CG	2.56	0.48
1:E:328:ARG:HG2	1:E:328:ARG:HH11	1.78	0.48
1:F:119:ILE:HG12	1:F:464:ILE:HG21	1.95	0.48
1:F:159:MET:HE1	1:F:198:VAL:HG13	1.95	0.48
1:F:249:GLY:HA3	2:F:601:NAD:HO2N	1.78	0.48
1:F:333:LEU:HD22	1:F:351:LYS:HD3	1.95	0.48
1:F:482:ALA:O	1:F:483:PRO:C	2.56	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:330:ASP:O	1:B:331:ARG:C	2.56	0.48
1:C:176:ILE:C	1:C:178:PRO:HD3	2.39	0.48
1:E:57:SER:HB2	1:E:138:PRO:HG2	1.96	0.48
1:E:329:ARG:CG	1:E:329:ARG:NH1	2.62	0.48
1:G:373:PRO:HG3	1:G:390:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:37:ALA:CB	1:C:201:VAL:HG13	2.44	0.48
1:C:89:ASN:HD21	1:C:177:THR:HA	1.79	0.48
1:C:141:VAL:HG22	1:C:168:THR:CG2	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:376:ARG:NH1	1:G:204:TYR:CD2	2.82	0.48
1:F:458:GLU:O	1:F:459:MET:CB	2.61	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:E:159:MET:HE1	1:E:198:VAL:HG11	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:CG	1:C:329:ARG:NH1	2.67	0.47
1:D:126:VAL:HG21	1:D:474:TRP:CH2	2.50	0.47
1:D:338:ILE:HD13	1:D:338:ILE:N	2.29	0.47
1:G:10[B]:ARG:NH1	1:G:10[B]:ARG:CG	2.74	0.47
1:H:53:PHE:HB3	1:H:54:PRO:HD3	1.96	0.47
1:H:100:LEU:O	1:H:101:ASP:C	2.55	0.47
1:A:172:LYS:HD2	1:A:208:ALA:HB3	1.95	0.47
1:A:486:LYS:HZ1	1:B:95:ARG:NH1	2.12	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:HD12	1:A:413:LEU:O	2.15	0.47
1:B:329:ARG:O	1:B:330:ASP:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:LEU:HD11	1:C:435:ILE:HG12	1.97	0.47
1:A:37:ALA:CB	1:A:201:VAL:HG13	2.45	0.47
1:A:131:LEU:C	1:A:131:LEU:HD22	2.39	0.47
1:A:139:ILE:N	1:A:167:ASN:HD21	2.05	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:B:87:SER:HB3	1:B:97:SER:OG	2.14	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:95:ARG:CD	1:F:319:GLU:HA	2.45	0.47
1:F:218:VAL:O	1:F:242:LYS:HE3	2.14	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: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:A:100:LEU:O	1:A:101:ASP:C	2.58	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:HA	1:D:187:LEU:HD23	1.77	0.47
1:D:201:VAL:O	1:D:201:VAL:CG1	2.61	0.47
1:E:100:LEU:O	1:E:101:ASP:C	2.58	0.47
1:G:138:PRO:HG3	1:G:165:ALA:O	2.14	0.47
1:D:18:GLY:HA3	3:D:709:HOH:O	2.15	0.47
1:D:143:ALA:HB1	1:D:212:LEU:HG	1.97	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:HE21	1:D:374:GLN:HB3	1.57	0.46
1:F:17:GLY:C	1:H:376:ARG:NH1	2.74	0.46
1:F:53:PHE:HB3	1:F:54:PRO:HD3	1.98	0.46
1:F:480:LYS:O	1:F:481:ILE:C	2.57	0.46
1:A:94:ILE:HG12	1:A:94:ILE:H	1.42	0.46
1:A:149:ASN:HD21	2:A:601:NAD:H5N	1.80	0.46
1:A:235:GLU:HG3	1:B:238:LYS:CD	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:25:PRO:HA	1:H:362:PHE:CE2	2.50	0.46
1:H:302:ILE:O	1:H:306:LYS:HG3	2.16	0.46
1:H:405:THR:CG2	1:H:406:GLU:N	2.78	0.46
1:B:76:GLU:O	1:B:79:SER:HB2	2.15	0.46
1:B:252:GLY:HA2	1:B:410:GLY:O	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:404:ASN:CG	1:C:404:ASN:O	2.59	0.46
1:A:10[B]:ARG:NH1	1:A:10[B]:ARG:CG	2.73	0.46
1:A:31:ILE:HG22	1:A:32:THR:HG22	1.97	0.46
1:A:119:ILE:O	1:C:125:PRO:HG3	2.16	0.46
1:C:172:LYS:NZ	1:C:173:PRO:O	2.37	0.46
1:D:482:ALA:O	1:D:483:PRO:C	2.58	0.46
1:E:323:LEU:HD12	1:E:329:ARG:HA	1.97	0.46
1:E:482:ALA:O	1:E:483:PRO:C	2.57	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:B:159:MET:HE1	1:B:198:VAL:CG1	2.46	0.46
1:F:221:ILE:HD13	1:F:222:ALA:N	2.30	0.46
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: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:70:LYS:HA	1:C:70:LYS:HD3	1.64	0.46
1:C:135:GLN:HE22	1:D:426:HIS:CE1	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:PHE:CD1	1:E:398:ALA:HB2	2.51	0.46
1:F:17:GLY:C	1:H:376:ARG:HH12	2.24	0.46
1:F:287:LEU:HD23	1:F:287:LEU:HA	1.79	0.46
1:G:25:PRO:HA	1:G:362:PHE:CE2	2.50	0.46
1:G:174:SER:O	1:G:175:GLU:C	2.59	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: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:131:LEU:C	1:G:131:LEU:HD22	2.41	0.46
1:G:172:LYS:HD2	1:G:208:ALA:HB3	1.98	0.46
1:G:252:GLY:HA2	1:G:410:GLY:O	2.15	0.46
1:G:392:PHE:CD1	1:G:398:ALA:HB2	2.51	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:A:187:LEU:HD23	1:A:187:LEU:HA	1.81	0.45
1:A:392:PHE:CD1	1:A:398:ALA:HB2	2.50	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:D:155:THR:CG2	1:D:181:THR:HB	2.47	0.45
1:F:404:ASN:CG	1:F:404:ASN:O	2.57	0.45
1:H:413:LEU:HD12	1:H:413:LEU:O	2.17	0.45
1:H:459:MET:HE2	1:H:459:MET:HA	1.98	0.45
1:H:465:HIS:O	1:H:468:THR:HG22	2.16	0.45
1:A:323:LEU:HD12	1:A:329:ARG:HA	1.98	0.45
1:A:353:PRO:O	1:A:353:PRO:HD2	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: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:C:287:LEU:HD23	1:C:287:LEU:HA	1.77	0.45
1:F:159:MET:HE1	1:F:198:VAL:CG1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:329:ARG:HG3	1:F:330:ASP:N	2.31	0.45
1:F:331:ARG:HE	1:F:331:ARG:HB3	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:22:VAL:HG23	1:D:34:ILE:HG12	1.96	0.45
1:D:260:ALA:O	1:D:262:ILE:HD13	2.17	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:G:126:VAL:O	1:G:127:ASP:C	2.60	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:76:GLU:O	1:E:79:SER:HB2	2.16	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:F:131:LEU:HD22	1:F:132:ASN:N	2.32	0.45
1:H:482:ALA:O	1:H:483:PRO:C	2.57	0.45
1:A:80:GLU:OE1	1:A:98:ARG:NE	2.50	0.45
1:A:245:GLN:C	1:A:246:LEU:HD23	2.41	0.45
1:B:405:THR:CG2	1:B:406:GLU:N	2.80	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: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:146:VAL:HG22	1:F:173:PRO:HA	1.99	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:86:GLU:OE2	1:D:180:SER:HB2	2.16	0.45
1:D:162:ALA:HB3	1:D:169:ILE:HD11	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:187:LEU:HD23	1:H:187:LEU:HA	1.75	0.45
1:H:374:GLN:HE21	1:H:374:GLN:HB3	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:A:221:ILE:HD13	1:A:221:ILE:C	2.42	0.45
1:D:94:ILE:O	1:D:95:ARG:C	2.60	0.45
1:E:126:VAL:O	1:E:127:ASP:C	2.60	0.45
1:F:149:ASN:ND2	2:F:601:NAD:H6N	2.23	0.45
1:F:258:GLU:HB3	1:F:290:HIS:CD2	2.52	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: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:H:6:TYR:N	3:H:714:HOH:O	2.49	0.45
1:A:405:THR:HG22	1:A:406:GLU:N	2.31	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: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:137:LYS:NZ	1:B:426:HIS:CD2	2.85	0.44
1:A:397:GLU:O	1:A:401:ILE:HG13	2.17	0.44
1:B:258:GLU:H	1:B:258:GLU:HG3	1.41	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:A:251:LYS:HZ2	1:A:285:SER:CB	2.30	0.44
1:D:1:MET:CG	1:D:2:GLN:N	2.79	0.44
1:D:70:LYS:HA	1:D:70:LYS:HD3	1.65	0.44
1:E:86:GLU:OE2	1:E:180:SER:HB2	2.17	0.44
1:F:404:ASN:C	1:F:404:ASN:ND2	2.74	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: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:B:417:ASN:HA	1:D:416:GLN:O	2.17	0.44
1:C:76:GLU:O	1:C:79:SER:HB2	2.17	0.44
1:C:448:GLY:HA3	1:C:457:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:VAL:HG23	1:E:34:ILE:HG12	1.99	0.44
1:F:177:THR:N	1:F:178:PRO:HD3	2.32	0.44
1:F:221:ILE:HD13	1:F:221:ILE:C	2.42	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:A:373:PRO:C	1:A:375:ASP:N	2.72	0.44
1:C:80:GLU:OE1	1:C:98:ARG:NE	2.51	0.44
1:D:126:VAL:O	1:D:127:ASP:C	2.60	0.44
1:F:405:THR:CG2	1:F:406:GLU:N	2.80	0.44
1:F:415:THR:HG22	1:F:416:GLN:H	1.81	0.44
1:H:221:ILE:HD13	1:H:221:ILE:C	2.42	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:32:THR:OG1	1:B:33:ARG:N	2.49	0.44
1:B:237:SER:OG	1:B:244:ILE:HD11	2.17	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:159:MET:HE1	1:C:198:VAL:HG13	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
1:D:356:LYS:NZ	1:G:10[A]:ARG:NH1	2.64	0.44
1:E:481:ILE:HD12	1:E:481:ILE:HA	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:126:VAL:O	1:H:127:ASP:C	2.60	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:6:TYR:CE2	1:A:9:GLY:HA2	2.53	0.44
1:A:119:ILE:HG12	1:A:464:ILE:HG21	1.98	0.44
1:C:257:PHE:CD2	1:C:415:THR:OG1	2.71	0.44
1:C:333:LEU:HD22	1:C:351:LYS:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:ILE:HG13	1:G:36:ALA:HB2	2.00	0.44
1:G:37:ALA:CB	1:G:201:VAL:HG13	2.48	0.44
1:H:85:LEU:HD11	1:H:179:LEU:HB3	2.00	0.44
1:H:376:ARG:O	1:H:380:GLU:HG3	2.17	0.44
1:A:112:PHE:HA	1:A:115:MET:HB3	2.00	0.44
1:B:404:ASN:O	1:B:404:ASN:CG	2.61	0.44
1:D:218:VAL:O	1:D:242:LYS:HE3	2.18	0.44
1:D:246:LEU:C	1:D:247:GLU:HG2	2.43	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:20:ILE:HD11	1:F:204:TYR:CD2	2.52	0.44
1:F:154:PHE:HZ	2:F:601:NAD:C5N	2.31	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:A:87:SER:C	1:A:314:MET:HE1	2.43	0.43
1:A:235:GLU:HG3	1:B:238:LYS:HD2	1.98	0.43
1:B:31:ILE:HG22	1:B:32:THR:HG22	1.99	0.43
1:B:244:ILE:HG22	1:B:246:LEU:HD23	1.97	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:E:223:PHE:CZ	1:E:225:GLY:HA3	2.53	0.43
1:F:37:ALA:HB1	1:F:201:VAL:HG13	1.99	0.43
1:F:97:SER:HA	1:F:101:ASP:HB2	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: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
1:A:57:SER:HB2	1:A:138:PRO:HG2	2.01	0.43
1:A:472:SER:O	1:B:432:MET:HA	2.18	0.43
1:B:12:VAL:HG23	1:B:13:ASP:O	2.18	0.43
1:B:97:SER:HA	1:B:101:ASP:HB2	2.01	0.43
1:D:15:VAL:CG1	1:D:16:ALA:N	2.79	0.43
1:D:37:ALA:HB1	1:D:201:VAL:HG13	2.00	0.43
1:E:10[B]:ARG:NH1	1:E:10[B]:ARG:CG	2.76	0.43
1:F:248:LEU:O	1:F:249:GLY:O	2.36	0.43
1:G:6:TYR:CE2	1:G:9:GLY:HA2	2.54	0.43
1:G:201:VAL:O	1:G:201:VAL:CG1	2.66	0.43
1:A:148:TRP:HD1	1:A:174:SER:OG	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:O	1:B:101:ASP:C	2.60	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:32:THR:OG1	1:E:33:ARG:N	2.51	0.43
1:E:221:ILE:HD13	1:E:222:ALA:N	2.34	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:A:373:PRO:C	1:A:375:ASP:H	2.26	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:6:TYR:CE2	1:B:9:GLY:HA2	2.54	0.43
1:B:302:ILE:O	1:B:306:LYS:HG3	2.18	0.43
1:B:405:THR:HG21	1:B:407:TYR:HB2	2.01	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:22:VAL:HG23	1:F:34:ILE:HG12	1.99	0.43
1:F:325:SER:O	1:F:328:ARG:CB	2.67	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:53:PHE:HB3	1:C:54:PRO:HD3	2.01	0.43
1:C:261:ASN:ND2	1:C:261:ASN:C	2.75	0.43
1:C:356:LYS:CD	1:C:356:LYS:N	2.63	0.43
1:D:273:ILE:HB	1:D:284:GLY:O	2.18	0.43
1:F:85:LEU:HD11	1:F:179:LEU:HB3	2.00	0.43
1:F:175:GLU:OE2	1:F:175:GLU:N	2.42	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:34:ILE:HD13	1:H:34:ILE:HA	1.78	0.43
1:H:247:GLU:C	1:H:248:LEU:HD23	2.44	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:404:ASN:C	1:C:404:ASN:ND2	2.76	0.43
1:D:404:ASN:ND2	1:D:404:ASN:C	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:112:PHE:HA	1:B:115:MET:HB3	2.01	0.43
1:B:413:LEU:HD12	1:B:413:LEU:O	2.18	0.43
1:D:6:TYR:CE2	1:D:9:GLY:HA2	2.54	0.43
1:D:10[B]:ARG:NH1	1:D:10[B]:ARG:CG	2.75	0.43
1:D:25:PRO:HA	1:D:362:PHE:CE2	2.54	0.43
1:E:248:LEU:N	1:E:248:LEU:CD2	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:76:GLU:O	1:A:79:SER:HB2	2.19	0.42
1:A:148:TRP:HB3	1:A:174:SER:CB	2.49	0.42
1:B:329:ARG:HE	1:B:362:PHE:HA	1.83	0.42
1:D:38:GLU:O	1:D:39:ALA:C	2.62	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:448:GLY:HA3	1:B:457:ARG:HD3	2.00	0.42
1:C:132:ASN:HD21	1:D:445:SER:HB2	1.84	0.42
1:D:112:PHE:CZ	1:D:161:PRO:HG3	2.54	0.42
1:H:12:VAL:HG23	1:H:13:ASP:O	2.19	0.42
1:H:32:THR:OG1	1:H:33:ARG:N	2.51	0.42
1:H:97:SER:HA	1:H:101:ASP:HB2	2.01	0.42
1:H:174:SER:O	1:H:175:GLU:C	2.62	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:C:259:ASP:O	1:C:259:ASP:CG	2.61	0.42
1:D:248:LEU:C	1:D:249:GLY:O	2.61	0.42
1:E:338:ILE:HD13	1:E:338:ILE:N	2.35	0.42
1:F:87:SER:HB3	1:F:97:SER:OG	2.18	0.42
1:F:148:TRP:HD1	1:F:174:SER:OG	2.02	0.42
1:F:373:PRO:C	1:F:375:ASP:H	2.26	0.42
1:G:287:LEU:HD23	1:G:287:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:172:LYS:NZ	1:E:173:PRO:O	2.41	0.42
1:E:486:LYS:HG2	1:E:486:LYS:H	1.73	0.42
1:G:447:PHE:C	1:G:447:PHE:CD2	2.97	0.42
1:H:447:PHE:C	1:H:447:PHE:CD2	2.97	0.42
1:A:126:VAL:O	1:A:127:ASP:C	2.63	0.42
1:B:126:VAL:O	1:B:127:ASP:C	2.61	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:69:LEU:HD23	1:E:69:LEU:HA	1.87	0.42
1:E:149:ASN:ND2	2:E:601:NAD:H6N	2.25	0.42
1:E:426:HIS:CD2	1:F:137:LYS:HZ2	2.37	0.42
1:F:80:GLU:O	1:F:81:GLU:C	2.62	0.42
1:F:172:LYS:HD2	1:F:208:ALA:HB3	2.00	0.42
1:F:413:LEU:HD12	1:F:413:LEU:O	2.18	0.42
1:B:247:GLU:C	1:B:248:LEU:HD23	2.33	0.42
1:C:221:ILE:HD13	1:C:221:ILE:C	2.44	0.42
1:D:95:ARG:HG3	1:D:96:ASP:N	2.32	0.42
1:E:31:ILE:HG22	1:E:32:THR:HG22	2.02	0.42
1:E:250:GLY:HA3	1:E:407:TYR:CB	2.44	0.42
1:F:6:TYR:CE2	1:F:9:GLY:HA2	2.55	0.42
1:F:12:VAL:HG23	1:F:13:ASP:O	2.20	0.42
1:F:325:SER:C	1:F:328:ARG:HG2	2.45	0.42
1:F:444:GLY:CA	1:F:460:GLY:HA2	2.49	0.42
1:H:105:THR:HG23	1:H:156:SER:HB3	2.00	0.42
1:A:149:ASN:HD21	2:A:601:NAD:H6N	1.84	0.42
1:A:447:PHE:C	1:A:447:PHE:CD2	2.98	0.42
1:B:149:ASN:ND2	2:B:601:NAD:H5N	2.34	0.42
1:B:447:PHE:CD2	1:B:447:PHE:C	2.98	0.42
1:C:151:PRO:HG3	1:C:177:THR:OG1	2.20	0.42
1:C:330:ASP:O	1:C:331:ARG:C	2.61	0.42
1:D:223:PHE:CZ	1:D:225:GLY:HA3	2.55	0.42
1:F:105:THR:OG1	1:F:153:MET:HA	2.19	0.42
1:F:143:ALA:HB1	1:F:212:LEU:HG	2.01	0.42
1:G:455:TYR:CB	1:H:243:ARG:HD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ILE:O	1:A:173:PRO:HD3	2.20	0.42
1:B:119:ILE:HG12	1:B:464:ILE:HG21	2.01	0.42
1:B:338:ILE:HD13	1:B:338:ILE:N	2.34	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:HD13	1:D:464:ILE:HA	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:D:459:MET:HE2	1:D:459:MET:CA	2.50	0.42
1:F:149:ASN:HD21	2:F:601:NAD:H5N	1.84	0.42
1:G:100:LEU:O	1:G:101:ASP:C	2.62	0.42
1:H:5:LEU:HB3	3:H:714:HOH:O	2.19	0.42
1:H:119:ILE:HG12	1:H:464:ILE:HG21	2.00	0.42
1:H:338:ILE:HD13	1:H:338:ILE:N	2.35	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:2:GLN:CA	1:A:2:GLN:HE21	2.31	0.41
1:A:141:VAL:HG22	1:A:168:THR:CG2	2.50	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:E:174:SER:C	1:E:176:ILE:N	2.75	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:B:327:LEU:C	1:B:327:LEU:CD2	2.93	0.41
1:C:31:ILE:HG22	1:C:32:THR:HG22	2.02	0.41
1:C:258:GLU:HG2	1:C:259:ASP:H	1.85	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:E:459:MET:HE2	1:E:459:MET:CA	2.50	0.41
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:69:LEU:HD23	1:A:69:LEU:HA	1.82	0.41
1:A:132:ASN:ND2	1:B:445:SER:HB2	2.35	0.41
1:B:2:GLN:NE2	3:B:705:HOH:O	2.52	0.41
1:C:22:VAL:HG23	1:C:34:ILE:HG12	2.02	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: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:F:447:PHE:C	1:F:447:PHE:CD2	2.99	0.41
1:G:185:VAL:CG2	1:G:200:VAL:CG2	2.97	0.41
1:H:464:ILE:HD13	1:H:464:ILE:HA	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:C:282:ILE:HD11	1:C:439:LYS:CG	2.45	0.41
1:C:486:LYS:O	1:C:487:ARG:C	2.63	0.41
1:D:274:PHE:HB3	1:D:320:MET:HE2	2.01	0.41
1:E:2:GLN:CA	1:E:2:GLN:HE21	2.33	0.41
1:G:69:LEU:HD23	1:G:69:LEU:HA	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:1:MET:CG	1:C:2:GLN:N	2.82	0.41
1:C:37:ALA:HB1	1:C:201:VAL:HG13	2.02	0.41
1:D:405:THR:CG2	1:D:406:GLU:N	2.83	0.41
1:E:70:LYS:HA	1:E:70:LYS:HD3	1.67	0.41
1:E:194:PRO:HB2	1:E:197:VAL:HG23	2.01	0.41
1:G:38:GLU:O	1:G:39:ALA:C	2.63	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:G:413:LEU:HD12	1:G:413:LEU:C	2.46	0.41
1:H:271:TRP:O	1:H:275:HIS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:373:PRO:C	1:H:375:ASP:H	2.28	0.41
1:B:124:ILE:HA	1:B:125:PRO:HD3	1.94	0.41
1:B:162:ALA:HB3	1:B:169:ILE:HD11	2.01	0.41
1:B:404:ASN:ND2	1:B:404:ASN:C	2.78	0.41
1:B:477:VAL:HG23	1:B:478:ASP:N	2.34	0.41
1:B:486:LYS:O	1:B:487:ARG:C	2.63	0.41
1:C:247:GLU:OE1	2:C:601:NAD:O7N	2.39	0.41
1:C:459:MET:HE2	1:C:459:MET:CA	2.50	0.41
1:D:82:LEU:O	1:D:83:ALA:C	2.63	0.41
1:D:87:SER:HB3	1:D:97:SER:OG	2.20	0.41
1:D:413:LEU:HD11	1:D:435:ILE:HG12	2.03	0.41
1:E:231:ARG:HG2	1:F:241:LEU:HD21	2.02	0.41
1:E:413:LEU:HD12	1:E:413:LEU:O	2.20	0.41
1:F:93:PRO:CB	1:F:95:ARG:HG2	2.49	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: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:HG2	1:H:136:ARG:NH1	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:221:ILE:HD13	1:B:221:ILE:C	2.46	0.41
1:B:411:SER:O	1:B:433:CYS:HA	2.19	0.41
1:C:71:LEU:HD22	1:C:188:MET:HG2	2.02	0.41
1:C:155:THR:HG21	1:C:181:THR:HB	2.02	0.41
1:C:426:HIS:CE1	1:D:135:GLN:NE2	2.88	0.41
1:D:338:ILE:N	1:D:338:ILE:CD1	2.82	0.41
1:D:432:MET:HE3	3:D:701:HOH:O	2.20	0.41
1:D:441:VAL:HG12	1:D:442:SER:N	2.34	0.41
1:F:2:GLN:CA	1:F:2:GLN:HE21	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: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:A:331:ARG:O	1:A:332:VAL:C	2.64	0.41
1:A:404:ASN:CG	1:A:404:ASN:O	2.64	0.41
1:A:413:LEU:HD12	1:A:413:LEU:C	2.46	0.41
1:A:486:LYS:O	1:A:487:ARG:C	2.64	0.41
1:B:20:ILE:HG13	1:B:36:ALA:HB2	2.03	0.41
1:B:174:SER:O	1:B:177:THR:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLN:O	1:D:417:ASN:HA	2.21	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:64:ARG:HD3	1:C:166:GLY:HA2	2.03	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:E:290:HIS:HD2	1:E:292:ASP:H	1.69	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: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:412:GLY:HA2	1:F:434:TRP:O	2.20	0.41
1:G:94:ILE:O	1:G:95:ARG:C	2.62	0.41
1:G:204:TYR:HB2	1:G:207:THR:OG1	2.21	0.41
1:G:338:ILE:HD13	1:G:338:ILE:N	2.36	0.41
1:G:404:ASN:O	1:G:404:ASN:CG	2.64	0.41
1:G:405:THR:CG2	1:G:406:GLU:N	2.83	0.41
1:G:481:ILE:HD13	1:G:481:ILE:N	2.32	0.41
1:H:80:GLU:O	1:H:81:GLU:C	2.62	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:218:VAL:O	1:H:242:LYS:HE3	2.20	0.41
1:H:258:GLU:HG3	1:H:290:HIS:CG	2.56	0.41
1:H:410:GLY:O	1:H:411:SER:HB3	2.19	0.41
1:H:481:ILE:HA	1:H:481:ILE:HD12	1.81	0.41
1:B:143:ALA:HB1	1:B:212:LEU:HG	2.02	0.41
1:B:174:SER:O	1:B:175:GLU:C	2.61	0.41
1:C:331:ARG:HA	1:C:331:ARG:HD3	1.73	0.41
1:C:410:GLY:O	1:C:411:SER:HB3	2.20	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:D:447:PHE:C	1:D:447:PHE:CD2	2.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:480:LYS:O	1:F:482:ALA:N	2.53	0.41
1:H:49:ALA:HB1	1:H:141:VAL:HG22	2.03	0.41
1:H:448:GLY:HA3	1:H:457:ARG:HD3	2.03	0.41
1:A:147:PRO:HD2	1:A:154:PHE:CE2	2.55	0.40
1:A:329:ARG:CG	1:A:329:ARG:NH1	2.42	0.40
1:C:25:PRO:HA	1:C:362:PHE:CD2	2.57	0.40
1:C:146:VAL:HG22	1:C:173:PRO:HA	2.03	0.40
1:D:2:GLN:CA	1:D:2:GLN:HE21	2.34	0.40
1:D:282:ILE:O	1:D:282:ILE:CG2	2.68	0.40
1:E:147:PRO:HD2	1:E:154:PHE:CE2	2.56	0.40
1:E:328:ARG:O	1:E:329:ARG:C	2.62	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
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:NH1	1:D:136:ARG:HG2	2.35	0.40
1:F:70:LYS:HA	1:F:70:LYS:HD3	1.66	0.40
1:F:187:LEU:HD23	1:F:187:LEU:HA	1.72	0.40
1:F:459:MET:HE2	1:F:459:MET:CA	2.51	0.40
1:G:7:ILE:HG23	1:G:45:ALA:HA	2.03	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: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:B:87:SER:C	1:B:314:MET:HE1	2.46	0.40
1:C:94:ILE:HD11	1:C:314:MET:HA	2.01	0.40
1:C:429:HIS:CD2	1:C:450:VAL:CG1	3.05	0.40
1:F:32:THR:OG1	1:F:33:ARG:N	2.54	0.40
1:H:151:PRO:HG3	1:H:177:THR:OG1	2.21	0.40
1:H:248:LEU:N	1:H:248:LEU:CD2	2.72	0.40
1:H:274:PHE:HB3	1:H:320:MET:HE2	2.04	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:F:174:SER:C	1:F:176:ILE:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:ILE:HD12	1:G:293:ILE:C	2.47	0.40
1:G:464:ILE:HD13	1:G:464:ILE:HA	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:271:TRP:O	1:A:275:HIS:HB3	2.22	0.40
1:C:94:ILE:CD1	1:C:314:MET:HA	2.51	0.40
1:C:174:SER:O	1:C:176:ILE:N	2.55	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:146:VAL:O	2:G:601:NAD:O3B	2.24	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%)	16	47
1	B	486/495 (98%)	443 (91%)	41 (8%)	2 (0%)	30	61
1	C	486/495 (98%)	445 (92%)	40 (8%)	1 (0%)	43	73
1	D	486/495 (98%)	448 (92%)	35 (7%)	3 (1%)	21	52
1	E	486/495 (98%)	450 (93%)	34 (7%)	2 (0%)	30	61
1	F	486/495 (98%)	444 (91%)	39 (8%)	3 (1%)	21	52
1	G	486/495 (98%)	447 (92%)	35 (7%)	4 (1%)	16	47
1	H	486/495 (98%)	446 (92%)	37 (8%)	3 (1%)	21	52
All	All	3888/3960 (98%)	3569 (92%)	297 (8%)	22 (1%)	21	52

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
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 ⓘ

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%)	325 (86%)	52 (14%)	3	15
1	B	377/383 (98%)	325 (86%)	52 (14%)	3	15
1	C	377/383 (98%)	329 (87%)	48 (13%)	4	18
1	D	377/383 (98%)	325 (86%)	52 (14%)	3	15
1	E	377/383 (98%)	330 (88%)	47 (12%)	4	19
1	F	377/383 (98%)	326 (86%)	51 (14%)	4	16
1	G	377/383 (98%)	326 (86%)	51 (14%)	4	16
1	H	377/383 (98%)	328 (87%)	49 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3016/3064 (98%)	2614 (87%)	402 (13%)	4 17

All (402) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	12	VAL
1	A	23	VAL
1	A	29	SER
1	A	32	THR
1	A	34	ILE
1	A	38	GLU
1	A	42	VAL
1	A	50	LYS
1	A	70	LYS
1	A	94	ILE
1	A	95	ARG
1	A	100	LEU
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	185	VAL
1	A	191	VAL
1	A	207	THR
1	A	221	ILE
1	A	232	ARG
1	A	243	ARG
1	A	248	LEU
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	332	VAL
1	A	338	ILE
1	A	346	VAL
1	A	354	ASP

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Mol	Chain	Res	Type
1	A	355	ASP
1	A	356	LYS
1	A	358	LEU
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	441	VAL
1	A	455	TYR
1	A	464	ILE
1	A	477	VAL
1	A	481	ILE
1	A	487	ARG
1	B	1	MET
1	B	2	GLN
1	B	12	VAL
1	B	15	VAL
1	B	23	VAL
1	B	29	SER
1	B	32	THR
1	B	34	ILE
1	B	38	GLU
1	B	42	VAL
1	B	50	LYS
1	B	70	LYS
1	B	81	GLU
1	B	94	ILE
1	B	100	LEU
1	B	126	VAL
1	B	131	LEU
1	B	146	VAL
1	B	149	ASN
1	B	168	THR
1	B	176	ILE
1	B	181	THR
1	B	185	VAL
1	B	191	VAL
1	B	221	ILE
1	B	232	ARG
1	B	246	LEU

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Mol	Chain	Res	Type
1	B	248	LEU
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	441	VAL
1	B	455	TYR
1	B	464	ILE
1	B	477	VAL
1	B	480	LYS
1	B	481	ILE
1	B	487	ARG
1	C	2	GLN
1	C	12	VAL
1	C	15	VAL
1	C	23	VAL
1	C	29	SER
1	C	32	THR
1	C	34	ILE
1	C	38	GLU
1	C	42	VAL
1	C	50	LYS
1	C	70	LYS
1	C	94	ILE
1	C	100	LEU
1	C	126	VAL
1	C	131	LEU
1	C	149	ASN
1	C	168	THR

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Mol	Chain	Res	Type
1	C	181	THR
1	C	185	VAL
1	C	191	VAL
1	C	221	ILE
1	C	232	ARG
1	C	258	GLU
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	356	LYS
1	C	358	LEU
1	C	374	GLN
1	C	377	VAL
1	C	393	SER
1	C	399	LEU
1	C	404	ASN
1	C	432	MET
1	C	441	VAL
1	C	455	TYR
1	C	464	ILE
1	C	477	VAL
1	C	480	LYS
1	C	481	ILE
1	C	487	ARG
1	D	2	GLN
1	D	4	GLN
1	D	12	VAL
1	D	23	VAL
1	D	29	SER
1	D	34	ILE
1	D	38	GLU
1	D	42	VAL
1	D	50	LYS
1	D	70	LYS
1	D	94	ILE

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Mol	Chain	Res	Type
1	D	100	LEU
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	181	THR
1	D	185	VAL
1	D	191	VAL
1	D	221	ILE
1	D	232	ARG
1	D	258	GLU
1	D	262	ILE
1	D	271	TRP
1	D	277	GLN
1	D	281	CYS
1	D	282	ILE
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	358	LEU
1	D	374	GLN
1	D	377	VAL
1	D	393	SER
1	D	399	LEU
1	D	404	ASN
1	D	432	MET
1	D	441	VAL
1	D	455	TYR
1	D	464	ILE
1	D	477	VAL
1	D	481	ILE
1	D	487	ARG
1	E	2	GLN

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Mol	Chain	Res	Type
1	E	4	GLN
1	E	12	VAL
1	E	15	VAL
1	E	23	VAL
1	E	29	SER
1	E	34	ILE
1	E	38	GLU
1	E	42	VAL
1	E	50	LYS
1	E	81	GLU
1	E	94	ILE
1	E	95	ARG
1	E	100	LEU
1	E	126	VAL
1	E	131	LEU
1	E	139	ILE
1	E	149	ASN
1	E	153	MET
1	E	168	THR
1	E	181	THR
1	E	185	VAL
1	E	191	VAL
1	E	221	ILE
1	E	232	ARG
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	356	LYS
1	E	358	LEU
1	E	374	GLN
1	E	377	VAL
1	E	393	SER
1	E	399	LEU
1	E	404	ASN
1	E	432	MET
1	E	441	VAL
1	E	455	TYR

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Mol	Chain	Res	Type
1	E	464	ILE
1	E	477	VAL
1	E	481	ILE
1	E	487	ARG
1	F	2	GLN
1	F	4	GLN
1	F	12	VAL
1	F	23	VAL
1	F	29	SER
1	F	32	THR
1	F	34	ILE
1	F	38	GLU
1	F	42	VAL
1	F	50	LYS
1	F	81	GLU
1	F	94	ILE
1	F	100	LEU
1	F	126	VAL
1	F	131	LEU
1	F	135	GLN
1	F	141	VAL
1	F	146	VAL
1	F	149	ASN
1	F	153	MET
1	F	168	THR
1	F	174	SER
1	F	181	THR
1	F	185	VAL
1	F	191	VAL
1	F	221	ILE
1	F	232	ARG
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	356	LYS

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Mol	Chain	Res	Type
1	F	358	LEU
1	F	374	GLN
1	F	377	VAL
1	F	393	SER
1	F	399	LEU
1	F	404	ASN
1	F	432	MET
1	F	441	VAL
1	F	455	TYR
1	F	464	ILE
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	23	VAL
1	G	29	SER
1	G	32	THR
1	G	34	ILE
1	G	38	GLU
1	G	42	VAL
1	G	50	LYS
1	G	70	LYS
1	G	94	ILE
1	G	95	ARG
1	G	100	LEU
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	185	VAL
1	G	191	VAL
1	G	221	ILE
1	G	232	ARG
1	G	246	LEU
1	G	248	LEU
1	G	261	ASN
1	G	271	TRP
1	G	277	GLN

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Mol	Chain	Res	Type
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	356	LYS
1	G	374	GLN
1	G	377	VAL
1	G	393	SER
1	G	399	LEU
1	G	404	ASN
1	G	409	LEU
1	G	432	MET
1	G	441	VAL
1	G	455	TYR
1	G	464	ILE
1	G	477	VAL
1	G	478	ASP
1	G	480	LYS
1	G	481	ILE
1	G	487	ARG
1	H	2	GLN
1	H	12	VAL
1	H	23	VAL
1	H	29	SER
1	H	34	ILE
1	H	38	GLU
1	H	42	VAL
1	H	50	LYS
1	H	81	GLU
1	H	94	ILE
1	H	95	ARG
1	H	100	LEU
1	H	126	VAL
1	H	131	LEU
1	H	139	ILE
1	H	141	VAL
1	H	149	ASN
1	H	153	MET
1	H	168	THR
1	H	181	THR

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Mol	Chain	Res	Type
1	H	185	VAL
1	H	191	VAL
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	356	LYS
1	H	358	LEU
1	H	374	GLN
1	H	377	VAL
1	H	393	SER
1	H	399	LEU
1	H	404	ASN
1	H	432	MET
1	H	441	VAL
1	H	455	TYR
1	H	464	ILE
1	H	477	VAL
1	H	481	ILE
1	H	487	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	89	ASN
1	A	132	ASN
1	A	135	GLN
1	A	167	ASN
1	A	215	HIS
1	A	277	GLN
1	A	279	GLN
1	A	290	HIS

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Mol	Chain	Res	Type
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	B	429	HIS
1	C	2	GLN
1	C	89	ASN
1	C	132	ASN
1	C	135	GLN
1	C	167	ASN
1	C	215	HIS
1	C	261	ASN
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	C	429	HIS
1	D	2	GLN
1	D	89	ASN
1	D	132	ASN
1	D	135	GLN
1	D	167	ASN
1	D	215	HIS
1	D	277	GLN

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Mol	Chain	Res	Type
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	417	ASN
1	D	426	HIS
1	E	2	GLN
1	E	89	ASN
1	E	132	ASN
1	E	135	GLN
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	465	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
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	F	429	HIS
1	G	2	GLN
1	G	89	ASN
1	G	132	ASN

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Mol	Chain	Res	Type
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	404	ASN
1	G	417	ASN
1	G	426	HIS
1	G	429	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	374	GLN
1	H	404	ASN
1	H	417	ASN
1	H	465	HIS
1	H	484	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	601	-	46,48,48	2.87	17 (36%)	64,73,73	2.34	25 (39%)
2	NAD	D	601	-	46,48,48	3.05	16 (34%)	64,73,73	2.15	20 (31%)
2	NAD	C	601	-	46,48,48	2.97	17 (36%)	64,73,73	2.33	26 (40%)
2	NAD	A	601	-	46,48,48	2.96	19 (41%)	64,73,73	2.39	26 (40%)
2	NAD	H	601	-	46,48,48	2.93	19 (41%)	64,73,73	2.31	23 (35%)
2	NAD	E	601	-	46,48,48	3.05	19 (41%)	64,73,73	2.38	24 (37%)
2	NAD	G	601	-	46,48,48	3.05	20 (43%)	64,73,73	2.42	23 (35%)
2	NAD	F	601	-	46,48,48	2.83	15 (32%)	64,73,73	2.33	24 (37%)

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	B	601	-	-	9/30/62/62	0/5/5/5
2	NAD	D	601	-	-	10/30/62/62	0/5/5/5
2	NAD	C	601	-	-	10/30/62/62	0/5/5/5
2	NAD	A	601	-	-	12/30/62/62	0/5/5/5
2	NAD	H	601	-	-	13/30/62/62	0/5/5/5
2	NAD	E	601	-	-	7/30/62/62	0/5/5/5
2	NAD	G	601	-	-	11/30/62/62	0/5/5/5
2	NAD	F	601	-	-	13/30/62/62	0/5/5/5

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAD	C7N-N7N	9.92	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NAD	C2N-N1N	9.87	1.45	1.35
2	G	601	NAD	C2N-N1N	9.74	1.45	1.35
2	A	601	NAD	C2N-N1N	9.58	1.45	1.35
2	H	601	NAD	C2N-N1N	9.42	1.45	1.35
2	C	601	NAD	C2N-N1N	9.35	1.45	1.35
2	F	601	NAD	C2N-N1N	8.68	1.44	1.35
2	B	601	NAD	C2N-N1N	8.58	1.44	1.35
2	E	601	NAD	C2N-C3N	8.06	1.51	1.39
2	C	601	NAD	C2N-C3N	7.64	1.51	1.39
2	H	601	NAD	C2N-C3N	7.60	1.51	1.39
2	G	601	NAD	C2N-C3N	7.55	1.50	1.39
2	G	601	NAD	PA-O3	7.37	1.67	1.59
2	B	601	NAD	PA-O3	7.23	1.67	1.59
2	A	601	NAD	C2N-C3N	7.18	1.50	1.39
2	F	601	NAD	C2N-C3N	6.90	1.49	1.39
2	H	601	NAD	PA-O3	6.89	1.66	1.59
2	B	601	NAD	C2N-C3N	6.84	1.49	1.39
2	F	601	NAD	PA-O3	6.70	1.66	1.59
2	A	601	NAD	PA-O3	6.68	1.66	1.59
2	C	601	NAD	PA-O3	6.58	1.66	1.59
2	C	601	NAD	C7N-N7N	6.44	1.44	1.33
2	E	601	NAD	C7N-N7N	6.44	1.44	1.33
2	D	601	NAD	C6N-N1N	6.30	1.49	1.35
2	G	601	NAD	C7N-N7N	6.25	1.44	1.33
2	F	601	NAD	C7N-N7N	6.19	1.44	1.33
2	B	601	NAD	C7N-N7N	6.12	1.44	1.33
2	H	601	NAD	C7N-N7N	6.09	1.44	1.33
2	A	601	NAD	C7N-N7N	5.74	1.43	1.33
2	E	601	NAD	PA-O3	5.67	1.65	1.59
2	D	601	NAD	C8A-N7A	5.20	1.41	1.31
2	D	601	NAD	C2A-N3A	5.19	1.43	1.33
2	A	601	NAD	C6A-N6A	5.17	1.47	1.34
2	D	601	NAD	C6A-N6A	5.06	1.47	1.34
2	B	601	NAD	O4D-C1D	5.05	1.47	1.40
2	F	601	NAD	C6A-N6A	5.01	1.47	1.34
2	C	601	NAD	O4D-C1D	4.95	1.47	1.40
2	C	601	NAD	C6A-N6A	4.94	1.46	1.34
2	H	601	NAD	C6A-N6A	4.85	1.46	1.34
2	A	601	NAD	O4D-C1D	4.84	1.47	1.40
2	B	601	NAD	C6A-N6A	4.80	1.46	1.34
2	D	601	NAD	PN-O1N	4.75	1.67	1.50
2	E	601	NAD	C6A-N6A	4.72	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	NAD	C6A-N6A	4.69	1.46	1.34
2	D	601	NAD	PA-O3	4.63	1.64	1.59
2	H	601	NAD	O4D-C1D	4.55	1.46	1.40
2	D	601	NAD	PN-O3	4.55	1.64	1.59
2	F	601	NAD	O4D-C1D	4.54	1.46	1.40
2	E	601	NAD	C4N-C3N	4.46	1.46	1.39
2	E	601	NAD	O4D-C1D	4.32	1.46	1.40
2	D	601	NAD	C2N-N1N	4.27	1.39	1.35
2	D	601	NAD	C2N-C3N	4.27	1.45	1.39
2	G	601	NAD	O4D-C1D	4.27	1.46	1.40
2	G	601	NAD	C4N-C3N	4.11	1.45	1.39
2	D	601	NAD	PA-O1A	4.10	1.65	1.50
2	E	601	NAD	C6N-C5N	4.09	1.47	1.38
2	C	601	NAD	C6N-C5N	3.85	1.46	1.38
2	A	601	NAD	C4N-C3N	3.82	1.45	1.39
2	D	601	NAD	C4A-N9A	3.77	1.45	1.37
2	G	601	NAD	C5N-C4N	3.77	1.45	1.38
2	E	601	NAD	C5N-C4N	3.76	1.45	1.38
2	F	601	NAD	C4N-C3N	3.74	1.45	1.39
2	C	601	NAD	C5N-C4N	3.72	1.45	1.38
2	A	601	NAD	C5N-C4N	3.71	1.45	1.38
2	C	601	NAD	C4N-C3N	3.66	1.45	1.39
2	G	601	NAD	C2B-C3B	-3.62	1.43	1.53
2	B	601	NAD	C6N-C5N	3.55	1.46	1.38
2	G	601	NAD	C6N-C5N	3.51	1.45	1.38
2	F	601	NAD	C6N-C5N	3.51	1.45	1.38
2	D	601	NAD	C3D-C4D	3.50	1.61	1.53
2	A	601	NAD	C6N-C5N	3.42	1.45	1.38
2	H	601	NAD	C4N-C3N	3.41	1.44	1.39
2	D	601	NAD	C5N-C4N	3.40	1.44	1.38
2	H	601	NAD	C6N-C5N	3.37	1.45	1.38
2	B	601	NAD	C5N-C4N	3.36	1.44	1.38
2	F	601	NAD	C5N-C4N	3.29	1.44	1.38
2	H	601	NAD	C8A-N7A	3.28	1.38	1.31
2	B	601	NAD	C4N-C3N	3.25	1.44	1.39
2	B	601	NAD	C8A-N7A	3.23	1.37	1.31
2	E	601	NAD	C2B-C3B	-3.18	1.44	1.53
2	F	601	NAD	C2B-C3B	-3.18	1.44	1.53
2	C	601	NAD	C2B-C3B	-3.13	1.44	1.53
2	H	601	NAD	C5N-C4N	3.13	1.44	1.38
2	E	601	NAD	C4A-N3A	3.09	1.40	1.34
2	A	601	NAD	C4A-N3A	3.01	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	C2B-C3B	-2.99	1.45	1.53
2	C	601	NAD	C4A-N3A	2.97	1.40	1.34
2	E	601	NAD	C8A-N7A	2.96	1.37	1.31
2	G	601	NAD	C8A-N7A	2.93	1.37	1.31
2	B	601	NAD	C2B-C3B	-2.93	1.45	1.53
2	G	601	NAD	C4A-N3A	2.90	1.39	1.34
2	C	601	NAD	C8A-N7A	2.89	1.37	1.31
2	F	601	NAD	C8A-N7A	2.86	1.37	1.31
2	A	601	NAD	C2A-N1A	2.85	1.39	1.33
2	H	601	NAD	C2B-C3B	-2.80	1.45	1.53
2	F	601	NAD	C4A-N3A	2.76	1.39	1.34
2	A	601	NAD	C8A-N7A	2.73	1.36	1.31
2	A	601	NAD	C5A-C4A	2.73	1.44	1.39
2	E	601	NAD	PN-O3	-2.70	1.56	1.59
2	H	601	NAD	C4A-N3A	2.68	1.39	1.34
2	B	601	NAD	C4A-N3A	2.68	1.39	1.34
2	C	601	NAD	C2A-N1A	2.66	1.38	1.33
2	G	601	NAD	C2A-N1A	2.62	1.38	1.33
2	C	601	NAD	C5A-C4A	2.51	1.43	1.39
2	G	601	NAD	C2A-N3A	2.47	1.38	1.33
2	A	601	NAD	PN-O1N	2.46	1.59	1.50
2	E	601	NAD	C2A-N1A	2.46	1.38	1.33
2	F	601	NAD	PN-O1N	2.45	1.59	1.50
2	G	601	NAD	C5A-C4A	2.44	1.43	1.39
2	H	601	NAD	PN-O1N	2.42	1.59	1.50
2	D	601	NAD	PA-O5B	2.39	1.68	1.59
2	H	601	NAD	C5A-C4A	2.38	1.43	1.39
2	B	601	NAD	C2A-N1A	2.35	1.38	1.33
2	E	601	NAD	PN-O1N	2.34	1.58	1.50
2	E	601	NAD	C3N-C7N	2.34	1.54	1.50
2	E	601	NAD	PA-O1A	2.30	1.58	1.50
2	D	601	NAD	PN-O5D	2.30	1.68	1.59
2	A	601	NAD	PA-O1A	2.28	1.58	1.50
2	B	601	NAD	C5A-C4A	2.27	1.43	1.39
2	G	601	NAD	C5B-C4B	2.26	1.58	1.51
2	E	601	NAD	C5A-C4A	2.24	1.43	1.39
2	G	601	NAD	PN-O1N	2.23	1.58	1.50
2	F	601	NAD	C2A-N1A	2.22	1.37	1.33
2	H	601	NAD	C6N-N1N	-2.21	1.30	1.35
2	H	601	NAD	C2A-N1A	2.18	1.37	1.33
2	B	601	NAD	PN-O1N	2.18	1.58	1.50
2	G	601	NAD	O4D-C4D	2.17	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	O4D-C4D	2.16	1.49	1.45
2	G	601	NAD	PA-O1A	2.14	1.58	1.50
2	A	601	NAD	C2A-N3A	2.12	1.37	1.33
2	E	601	NAD	C5B-C4B	2.11	1.57	1.51
2	G	601	NAD	C1B-N9A	2.10	1.52	1.46
2	H	601	NAD	O4D-C4D	2.10	1.49	1.45
2	B	601	NAD	PA-O1A	2.09	1.58	1.50
2	A	601	NAD	C5B-C4B	2.09	1.57	1.51
2	H	601	NAD	PA-O1A	2.07	1.58	1.50
2	C	601	NAD	PN-O1N	2.05	1.57	1.50
2	C	601	NAD	C2A-N3A	2.03	1.37	1.33
2	C	601	NAD	C5B-C4B	2.03	1.57	1.51
2	B	601	NAD	O4D-C4D	2.02	1.49	1.45
2	H	601	NAD	O4B-C4B	-2.01	1.40	1.45
2	F	601	NAD	C5A-C4A	2.00	1.42	1.39

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	NAD	C5A-C4A-N3A	-8.25	115.36	126.72
2	C	601	NAD	C5A-C4A-N3A	-7.39	116.54	126.72
2	E	601	NAD	C5A-C4A-N3A	-6.81	117.34	126.72
2	B	601	NAD	C5A-C4A-N3A	-6.68	117.52	126.72
2	A	601	NAD	C5A-C4A-N3A	-6.41	117.89	126.72
2	D	601	NAD	C5A-C4A-N3A	-6.36	117.97	126.72
2	F	601	NAD	C5A-C4A-N3A	-6.17	118.22	126.72
2	G	601	NAD	N3A-C4A-N9A	6.03	137.43	127.17
2	F	601	NAD	N3A-C2A-N1A	-5.82	119.77	128.58
2	H	601	NAD	C5A-C4A-N3A	-5.72	118.84	126.72
2	E	601	NAD	N3A-C2A-N1A	-5.56	120.17	128.58
2	C	601	NAD	N3A-C4A-N9A	5.51	136.54	127.17
2	D	601	NAD	N3A-C2A-N1A	-5.39	120.43	128.58
2	E	601	NAD	N3A-C4A-N9A	5.37	136.30	127.17
2	H	601	NAD	N3A-C2A-N1A	-5.27	120.60	128.58
2	C	601	NAD	N3A-C2A-N1A	-5.15	120.79	128.58
2	H	601	NAD	N9A-C8A-N7A	-5.11	106.69	113.94
2	B	601	NAD	N9A-C8A-N7A	-5.08	106.72	113.94
2	A	601	NAD	N3A-C4A-N9A	5.08	135.80	127.17
2	A	601	NAD	N3A-C2A-N1A	-4.96	121.08	128.58
2	B	601	NAD	N3A-C4A-N9A	4.93	135.55	127.17
2	F	601	NAD	N3A-C4A-N9A	4.82	135.37	127.17
2	F	601	NAD	N9A-C8A-N7A	-4.63	107.37	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAD	N3A-C2A-N1A	-4.58	121.65	128.58
2	E	601	NAD	C2A-N3A-C4A	4.54	122.92	111.83
2	G	601	NAD	C3N-C7N-N7N	4.52	123.31	117.74
2	C	601	NAD	C2A-N3A-C4A	4.52	122.87	111.83
2	H	601	NAD	C3N-C7N-N7N	4.52	123.31	117.74
2	B	601	NAD	C5A-N7A-C8A	4.49	110.50	103.45
2	E	601	NAD	N9A-C8A-N7A	-4.45	107.62	113.94
2	F	601	NAD	C2A-N3A-C4A	4.45	122.69	111.83
2	A	601	NAD	N9A-C8A-N7A	-4.41	107.68	113.94
2	G	601	NAD	C5A-N7A-C8A	4.40	110.37	103.45
2	G	601	NAD	C2A-N3A-C4A	4.38	122.54	111.83
2	H	601	NAD	C5A-N7A-C8A	4.35	110.29	103.45
2	A	601	NAD	C5A-N7A-C8A	4.29	110.20	103.45
2	B	601	NAD	C2A-N3A-C4A	4.26	122.23	111.83
2	C	601	NAD	C5A-N7A-C8A	4.26	110.14	103.45
2	H	601	NAD	C2A-N3A-C4A	4.18	122.04	111.83
2	G	601	NAD	N3A-C2A-N1A	-4.16	122.29	128.58
2	H	601	NAD	N3A-C4A-N9A	4.14	134.22	127.17
2	E	601	NAD	C3N-C7N-N7N	4.05	122.73	117.74
2	E	601	NAD	C5A-N7A-C8A	4.03	109.79	103.45
2	B	601	NAD	C2N-N1N-C1D	-4.03	110.24	119.13
2	H	601	NAD	C4A-N9A-C8A	4.01	109.95	105.74
2	C	601	NAD	N9A-C8A-N7A	-3.98	108.29	113.94
2	B	601	NAD	C4A-C5A-N7A	-3.98	106.04	110.58
2	F	601	NAD	C5A-N7A-C8A	3.96	109.67	103.45
2	A	601	NAD	C2A-N3A-C4A	3.95	121.47	111.83
2	D	601	NAD	N3A-C4A-N9A	3.93	133.85	127.17
2	D	601	NAD	O2B-C2B-C1B	3.92	123.62	110.10
2	A	601	NAD	C2B-C1B-N9A	-3.92	103.57	113.30
2	H	601	NAD	O5D-C5D-C4D	3.91	122.30	108.99
2	H	601	NAD	C4A-C5A-N7A	-3.90	106.12	110.58
2	B	601	NAD	C4A-N9A-C8A	3.88	109.82	105.74
2	B	601	NAD	O5D-C5D-C4D	3.86	122.15	108.99
2	G	601	NAD	C4A-C5A-N7A	-3.86	106.17	110.58
2	F	601	NAD	C4D-O4D-C1D	-3.85	106.40	109.92
2	G	601	NAD	N9A-C8A-N7A	-3.84	108.49	113.94
2	D	601	NAD	C2A-N3A-C4A	3.83	121.18	111.83
2	E	601	NAD	C6N-N1N-C1D	3.81	127.20	119.73
2	F	601	NAD	C4A-N9A-C8A	3.73	109.66	105.74
2	E	601	NAD	C2N-N1N-C1D	-3.72	110.92	119.13
2	F	601	NAD	C2N-N1N-C1D	-3.71	110.93	119.13
2	C	601	NAD	C4A-C5A-N7A	-3.69	106.37	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NAD	C2B-C3B-C4B	-3.64	95.57	102.61
2	D	601	NAD	O4B-C4B-C5B	3.64	120.99	109.33
2	A	601	NAD	C4A-C5A-N7A	-3.57	106.50	110.58
2	G	601	NAD	C2N-N1N-C1D	-3.56	111.27	119.13
2	A	601	NAD	C2N-N1N-C1D	-3.56	111.28	119.13
2	E	601	NAD	C4A-N9A-C8A	3.54	109.46	105.74
2	D	601	NAD	N9A-C8A-N7A	-3.52	108.94	113.94
2	G	601	NAD	C6N-N1N-C2N	3.47	124.83	121.88
2	C	601	NAD	C6N-N1N-C1D	3.45	126.49	119.73
2	C	601	NAD	C2N-N1N-C1D	-3.41	111.61	119.13
2	A	601	NAD	C4A-N9A-C8A	3.40	109.31	105.74
2	A	601	NAD	O5D-C5D-C4D	3.39	120.55	108.99
2	E	601	NAD	C4A-C5A-N7A	-3.34	106.77	110.58
2	B	601	NAD	C6N-N1N-C1D	3.32	126.23	119.73
2	D	601	NAD	O4D-C4D-C5D	3.29	119.86	109.33
2	G	601	NAD	O4B-C4B-C5B	3.28	119.86	109.33
2	C	601	NAD	C5N-C6N-N1N	3.27	124.85	120.38
2	D	601	NAD	O3D-C3D-C4D	3.27	120.47	111.08
2	F	601	NAD	C4A-C5A-N7A	-3.23	106.88	110.58
2	F	601	NAD	O2B-C2B-C3B	3.21	122.10	111.82
2	D	601	NAD	O2D-C2D-C3D	3.20	122.07	111.82
2	A	601	NAD	O2B-C2B-C3B	3.17	121.96	111.82
2	A	601	NAD	C3N-C7N-N7N	3.12	121.59	117.74
2	E	601	NAD	O4B-C1B-N9A	3.12	114.08	108.09
2	D	601	NAD	C3B-C2B-C1B	-3.11	95.58	101.46
2	A	601	NAD	O2D-C2D-C3D	3.08	121.69	111.82
2	D	601	NAD	O3D-C3D-C2D	3.08	121.69	111.82
2	F	601	NAD	C3N-C7N-N7N	3.05	121.50	117.74
2	E	601	NAD	O5D-C5D-C4D	3.05	119.38	108.99
2	D	601	NAD	C6A-C5A-C4A	2.99	121.25	117.18
2	D	601	NAD	O5B-C5B-C4B	2.98	119.13	108.99
2	F	601	NAD	C6N-N1N-C1D	2.97	125.56	119.73
2	D	601	NAD	C6N-N1N-C2N	-2.96	119.36	121.88
2	B	601	NAD	O2B-C2B-C3B	2.95	121.28	111.82
2	C	601	NAD	O5D-C5D-C4D	2.95	119.03	108.99
2	E	601	NAD	C5N-C6N-N1N	2.93	124.38	120.38
2	A	601	NAD	O3D-C3D-C4D	2.91	119.45	111.08
2	G	601	NAD	O5D-C5D-C4D	2.91	118.90	108.99
2	E	601	NAD	C5A-C6A-N6A	-2.88	116.15	123.29
2	G	601	NAD	O2D-C2D-C3D	2.86	120.99	111.82
2	E	601	NAD	O3B-C3B-C4B	2.86	119.29	111.08
2	A	601	NAD	O5B-C5B-C4B	2.85	118.69	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	NAD	C2D-C3D-C4D	2.83	108.08	102.61
2	H	601	NAD	C5N-C6N-N1N	2.83	124.24	120.38
2	F	601	NAD	O5D-C5D-C4D	2.82	118.58	108.99
2	E	601	NAD	O2B-C2B-C3B	2.81	120.83	111.82
2	G	601	NAD	C5A-C6A-N6A	-2.81	116.34	123.29
2	F	601	NAD	O7N-C7N-C3N	-2.80	116.18	119.60
2	B	601	NAD	C2N-C3N-C4N	2.80	121.51	118.26
2	H	601	NAD	O2B-C2B-C3B	2.77	120.71	111.82
2	H	601	NAD	C2N-N1N-C1D	-2.75	113.06	119.13
2	C	601	NAD	C3N-C7N-N7N	2.75	121.13	117.74
2	G	601	NAD	O3D-C3D-C4D	2.75	118.97	111.08
2	D	601	NAD	C5A-N7A-C8A	2.74	107.76	103.45
2	F	601	NAD	C5N-C6N-N1N	2.74	124.12	120.38
2	E	601	NAD	O3D-C3D-C4D	2.74	118.95	111.08
2	G	601	NAD	O5B-C5B-C4B	2.73	118.28	108.99
2	A	601	NAD	O3B-C3B-C4B	2.72	118.89	111.08
2	C	601	NAD	O3B-C3B-C4B	2.71	118.85	111.08
2	H	601	NAD	O3D-C3D-C4D	2.70	118.83	111.08
2	H	601	NAD	O5B-C5B-C4B	2.65	118.01	108.99
2	C	601	NAD	O3D-C3D-C2D	2.64	120.27	111.82
2	F	601	NAD	O3D-C3D-C4D	2.61	118.59	111.08
2	E	601	NAD	O5B-C5B-C4B	2.61	117.87	108.99
2	A	601	NAD	C5N-C6N-N1N	2.60	123.92	120.38
2	B	601	NAD	O3D-C3D-C4D	2.59	118.52	111.08
2	B	601	NAD	O2D-C2D-C3D	2.58	120.10	111.82
2	H	601	NAD	O7N-C7N-C3N	-2.58	116.44	119.60
2	F	601	NAD	C5A-C6A-N6A	-2.56	116.94	123.29
2	C	601	NAD	O7N-C7N-C3N	-2.55	116.48	119.60
2	A	601	NAD	C6N-N1N-C1D	2.54	124.72	119.73
2	B	601	NAD	O3B-C3B-C4B	2.50	118.27	111.08
2	A	601	NAD	C6N-N1N-C2N	2.49	123.99	121.88
2	H	601	NAD	C6A-C5A-N7A	2.46	136.82	132.09
2	C	601	NAD	O2D-C2D-C3D	2.44	119.64	111.82
2	B	601	NAD	C5N-C6N-N1N	2.43	123.70	120.38
2	C	601	NAD	C4A-N9A-C8A	2.43	108.29	105.74
2	E	601	NAD	C5D-C4D-C3D	2.43	123.95	115.21
2	E	601	NAD	O7N-C7N-N7N	-2.42	119.12	122.62
2	C	601	NAD	C5A-C6A-N6A	-2.41	117.32	123.29
2	A	601	NAD	C1B-N9A-C8A	-2.40	121.77	127.09
2	A	601	NAD	C5A-C6A-N6A	-2.39	117.37	123.29
2	H	601	NAD	C2B-C3B-C4B	2.39	107.22	102.61
2	A	601	NAD	C5D-C4D-C3D	2.37	123.76	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	NAD	C1B-N9A-C8A	-2.37	121.84	127.09
2	G	601	NAD	C6A-C5A-C4A	2.36	120.40	117.18
2	C	601	NAD	O2B-C2B-C1B	2.36	118.23	110.10
2	E	601	NAD	O5B-PA-O1A	2.36	118.27	108.94
2	B	601	NAD	O7N-C7N-C3N	-2.32	116.76	119.60
2	H	601	NAD	C2D-C3D-C4D	2.31	107.08	102.61
2	F	601	NAD	O3D-C3D-C2D	2.30	119.19	111.82
2	F	601	NAD	C2N-C3N-C4N	2.28	120.92	118.26
2	B	601	NAD	O3B-C3B-C2B	2.28	119.13	111.82
2	G	601	NAD	O3D-C3D-C2D	2.27	119.09	111.82
2	C	601	NAD	C2N-C3N-C4N	2.27	120.89	118.26
2	A	601	NAD	O3D-C3D-C2D	2.24	119.01	111.82
2	F	601	NAD	O2D-C2D-C3D	2.22	118.94	111.82
2	C	601	NAD	O3B-C3B-C2B	2.21	118.90	111.82
2	E	601	NAD	C4D-O4D-C1D	2.21	111.95	109.92
2	F	601	NAD	O5B-C5B-C4B	2.20	116.50	108.99
2	G	601	NAD	O7N-C7N-N7N	-2.20	119.44	122.62
2	B	601	NAD	C5D-C4D-C3D	2.20	123.13	115.21
2	B	601	NAD	O5B-C5B-C4B	2.20	116.48	108.99
2	B	601	NAD	C5A-C6A-N6A	-2.20	117.85	123.29
2	A	601	NAD	O4D-C4D-C5D	2.19	116.36	109.33
2	H	601	NAD	O2N-PN-O3	-2.19	101.36	107.27
2	G	601	NAD	O2B-C2B-C3B	2.18	118.79	111.82
2	D	601	NAD	C5A-C4A-N9A	2.17	108.18	105.81
2	F	601	NAD	O4D-C4D-C5D	2.17	116.29	109.33
2	C	601	NAD	C1B-N9A-C8A	-2.16	122.31	127.09
2	F	601	NAD	O4B-C1B-C2B	-2.16	102.00	106.62
2	C	601	NAD	O5B-C5B-C4B	2.15	116.32	108.99
2	D	601	NAD	O5D-C5D-C4D	2.15	116.30	108.99
2	G	601	NAD	C5D-C4D-C3D	2.14	122.92	115.21
2	H	601	NAD	O2D-C2D-C3D	2.13	118.65	111.82
2	B	601	NAD	C3N-C7N-N7N	2.13	120.36	117.74
2	G	601	NAD	C6N-N1N-C1D	2.13	123.90	119.73
2	A	601	NAD	C3B-C2B-C1B	2.10	105.43	101.46
2	C	601	NAD	O4D-C4D-C5D	2.09	116.03	109.33
2	H	601	NAD	O4B-C1B-N9A	-2.08	104.09	108.09
2	B	601	NAD	O3D-C3D-C2D	2.03	118.33	111.82
2	D	601	NAD	C4A-C5A-N7A	-2.03	108.26	110.58
2	H	601	NAD	C6N-N1N-C1D	2.03	123.72	119.73
2	C	601	NAD	C5N-C4N-C3N	-2.03	118.37	120.36
2	B	601	NAD	O4D-C4D-C5D	2.01	115.77	109.33
2	C	601	NAD	O2B-C2B-C3B	2.01	118.25	111.82

There are no chirality outliers.

All (85) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	A	601	NAD	PN-O3-PA-O5B
2	B	601	NAD	PN-O3-PA-O5B
2	C	601	NAD	PN-O3-PA-O5B
2	E	601	NAD	PN-O3-PA-O5B
2	F	601	NAD	PN-O3-PA-O5B
2	G	601	NAD	PN-O3-PA-O5B
2	H	601	NAD	PN-O3-PA-O5B
2	E	601	NAD	PA-O3-PN-O1N
2	G	601	NAD	PN-O3-PA-O1A
2	B	601	NAD	C4D-C5D-O5D-PN
2	F	601	NAD	C4B-C5B-O5B-PA
2	F	601	NAD	C4D-C5D-O5D-PN
2	H	601	NAD	C4B-C5B-O5B-PA
2	B	601	NAD	C5B-O5B-PA-O3
2	B	601	NAD	C5D-O5D-PN-O3
2	B	601	NAD	C5D-O5D-PN-O2N
2	C	601	NAD	C5D-O5D-PN-O2N
2	D	601	NAD	C5D-O5D-PN-O2N
2	E	601	NAD	C5D-O5D-PN-O3
2	E	601	NAD	C5D-O5D-PN-O2N
2	F	601	NAD	C5B-O5B-PA-O2A
2	F	601	NAD	C5D-O5D-PN-O2N
2	G	601	NAD	C5B-O5B-PA-O2A
2	G	601	NAD	C5B-O5B-PA-O3
2	A	601	NAD	C4B-C5B-O5B-PA
2	C	601	NAD	C4D-C5D-O5D-PN
2	G	601	NAD	C4B-C5B-O5B-PA
2	G	601	NAD	C4D-C5D-O5D-PN
2	D	601	NAD	PA-O3-PN-O2N
2	F	601	NAD	PN-O3-PA-O1A
2	B	601	NAD	C2B-C1B-N9A-C8A
2	C	601	NAD	C4B-C5B-O5B-PA
2	B	601	NAD	PN-O3-PA-O1A
2	C	601	NAD	PA-O3-PN-O1N
2	F	601	NAD	PA-O3-PN-O1N
2	A	601	NAD	C4D-C5D-O5D-PN
2	H	601	NAD	C4D-C5D-O5D-PN
2	D	601	NAD	C2B-C1B-N9A-C8A
2	A	601	NAD	PN-O3-PA-O1A
2	C	601	NAD	PA-O3-PN-O2N
2	D	601	NAD	PA-O3-PN-O1N
2	D	601	NAD	C4B-C5B-O5B-PA

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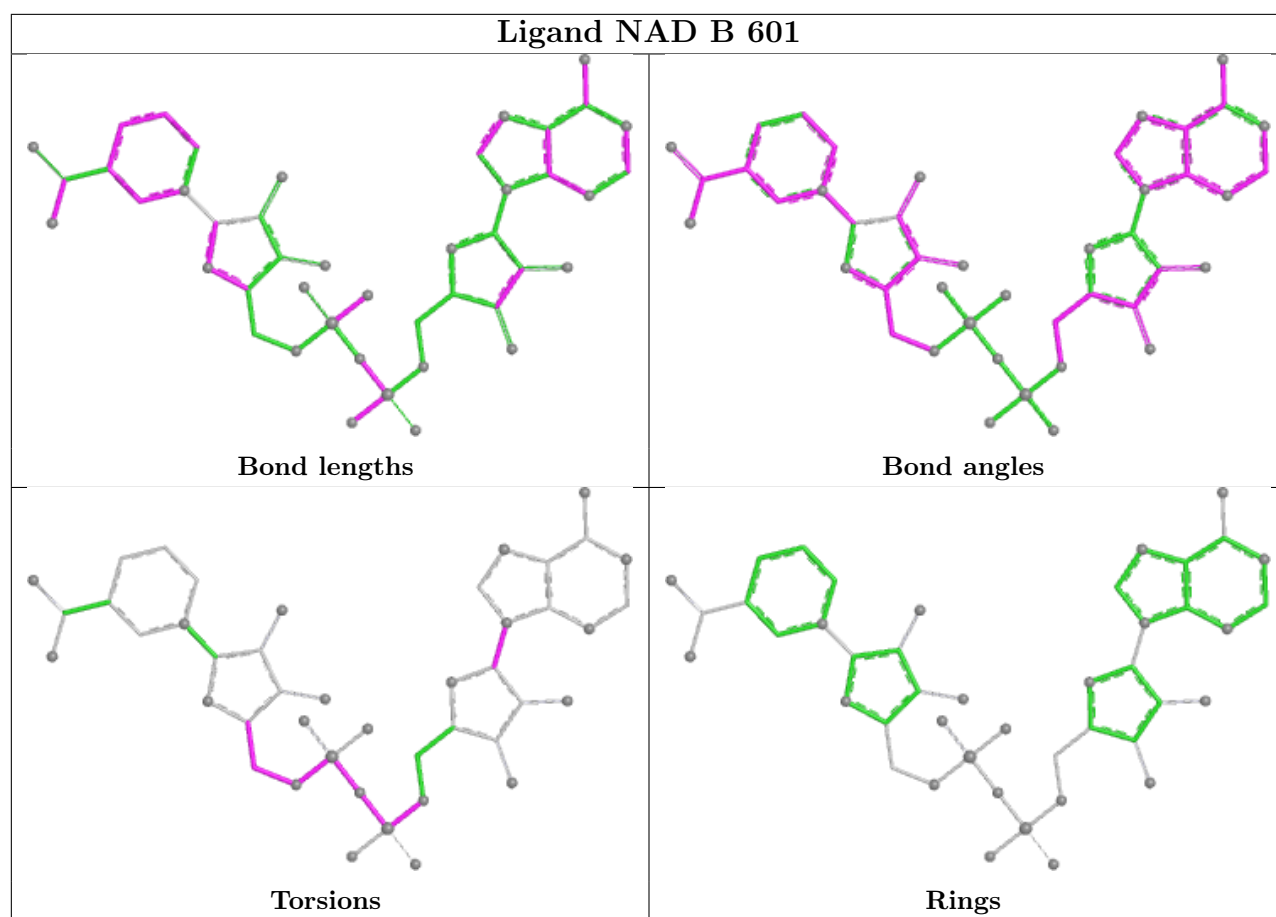
Mol	Chain	Res	Type	Atoms
2	A	601	NAD	PN-O3-PA-O2A
2	H	601	NAD	PN-O3-PA-O1A
2	C	601	NAD	O4D-C4D-C5D-O5D

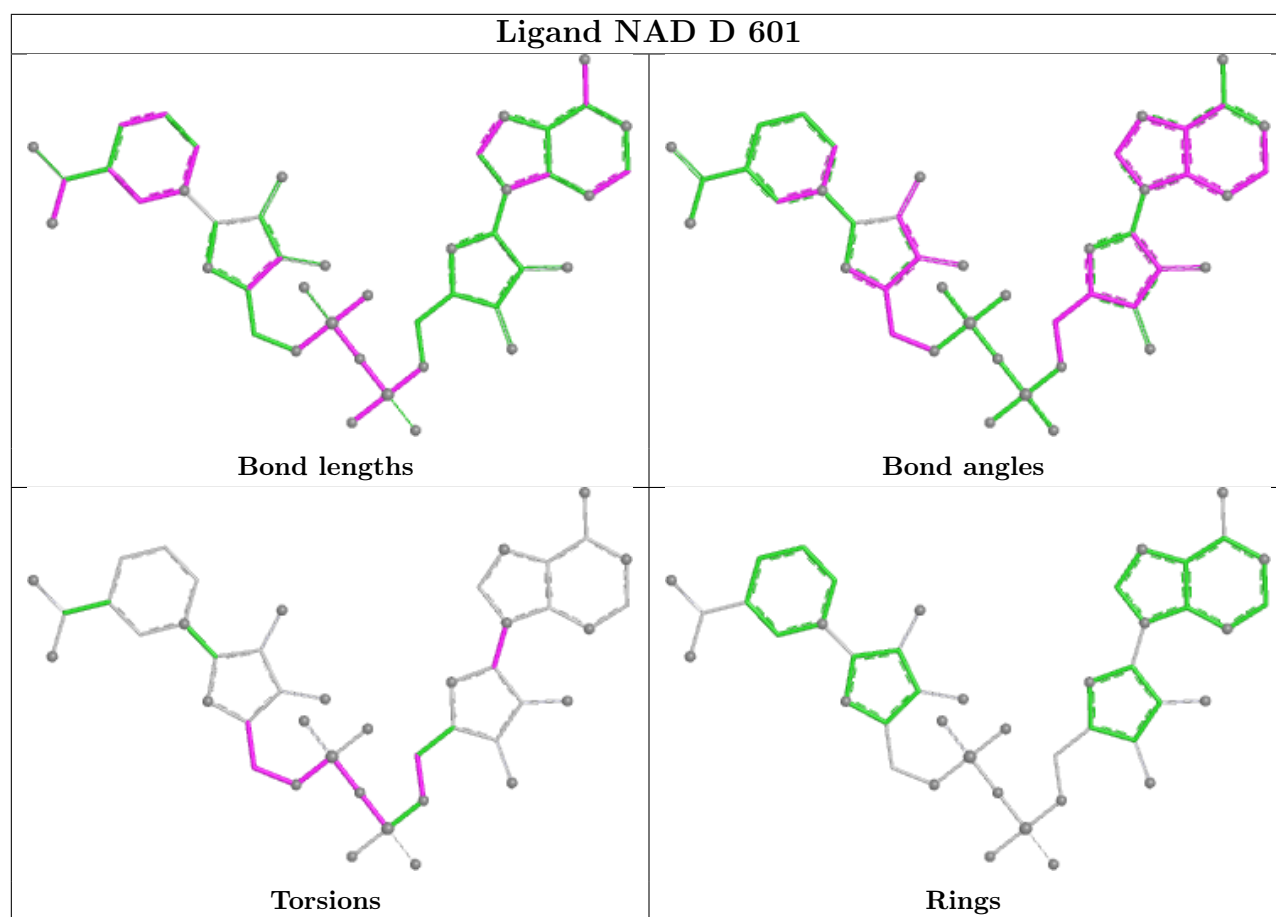
There are no ring outliers.

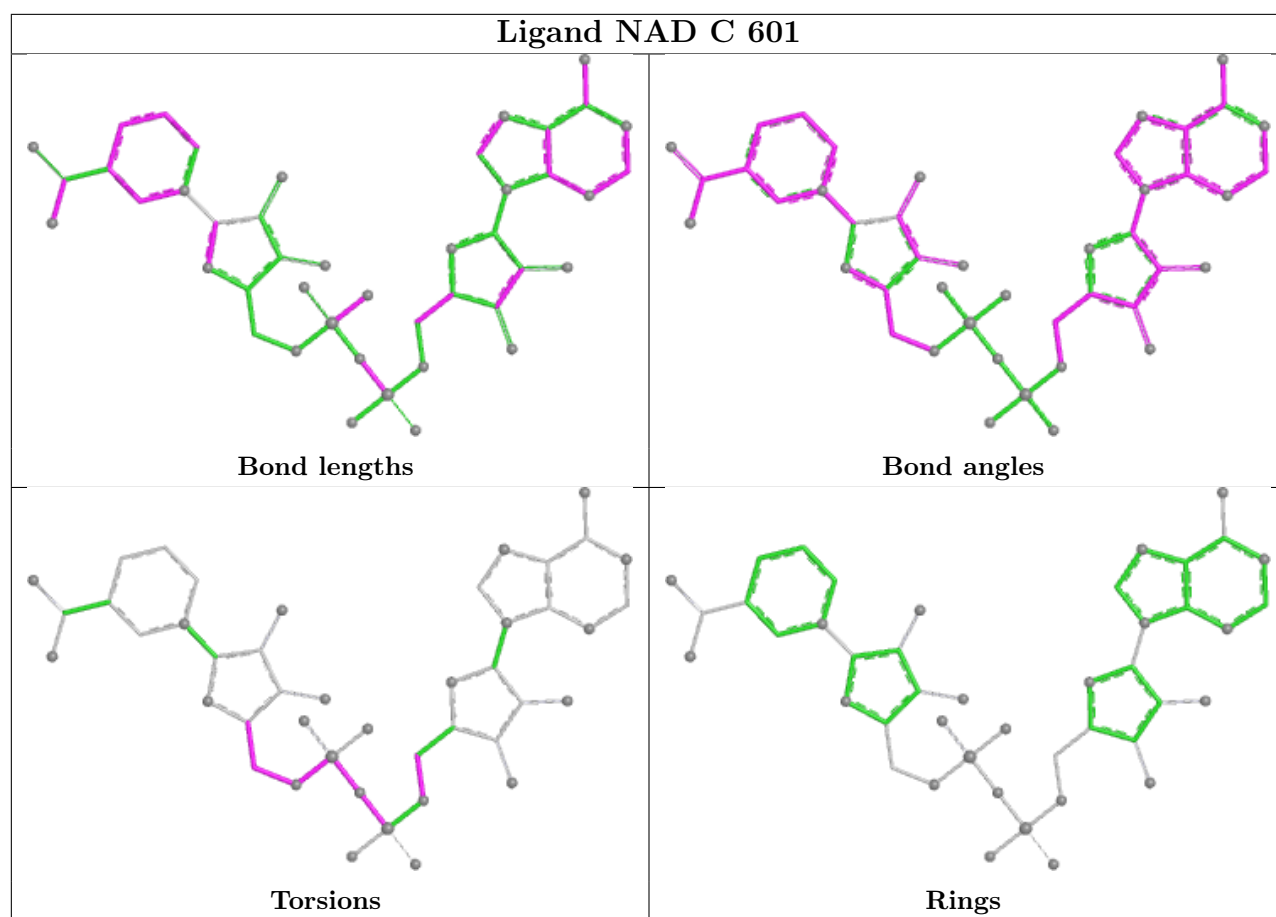
8 monomers are involved in 73 short contacts:

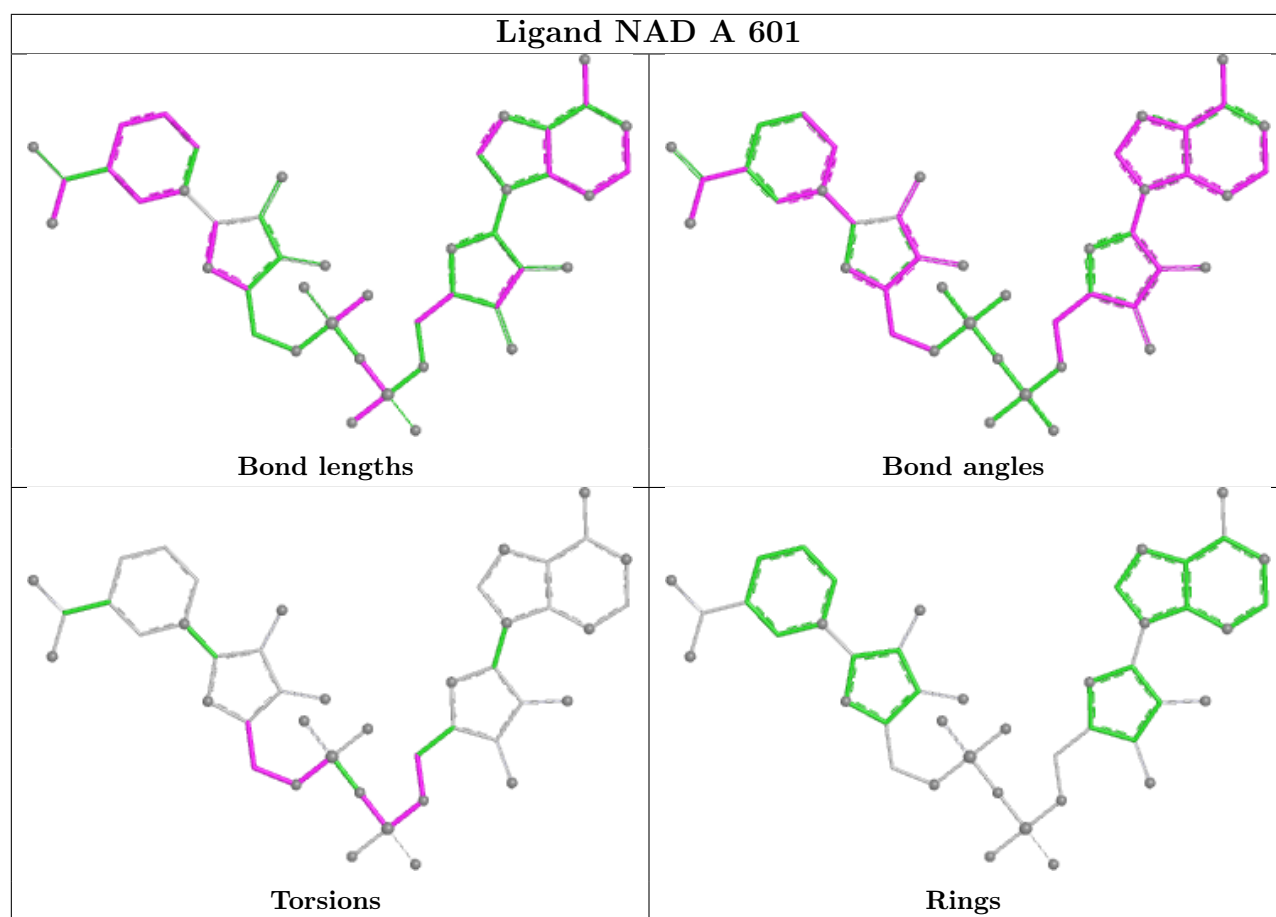
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	NAD	7	0
2	D	601	NAD	8	0
2	C	601	NAD	14	0
2	A	601	NAD	11	0
2	H	601	NAD	7	0
2	E	601	NAD	7	0
2	G	601	NAD	8	0
2	F	601	NAD	11	0

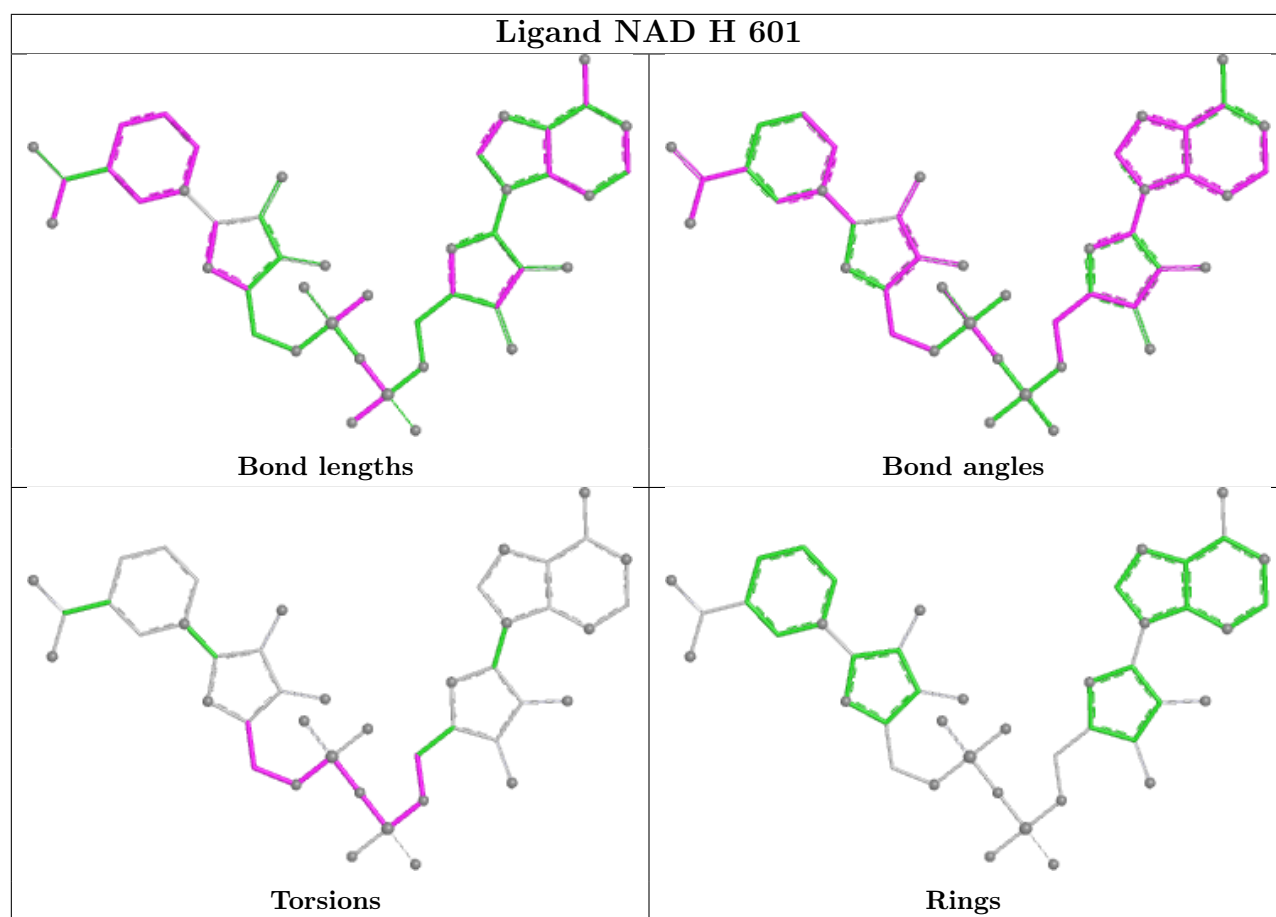
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

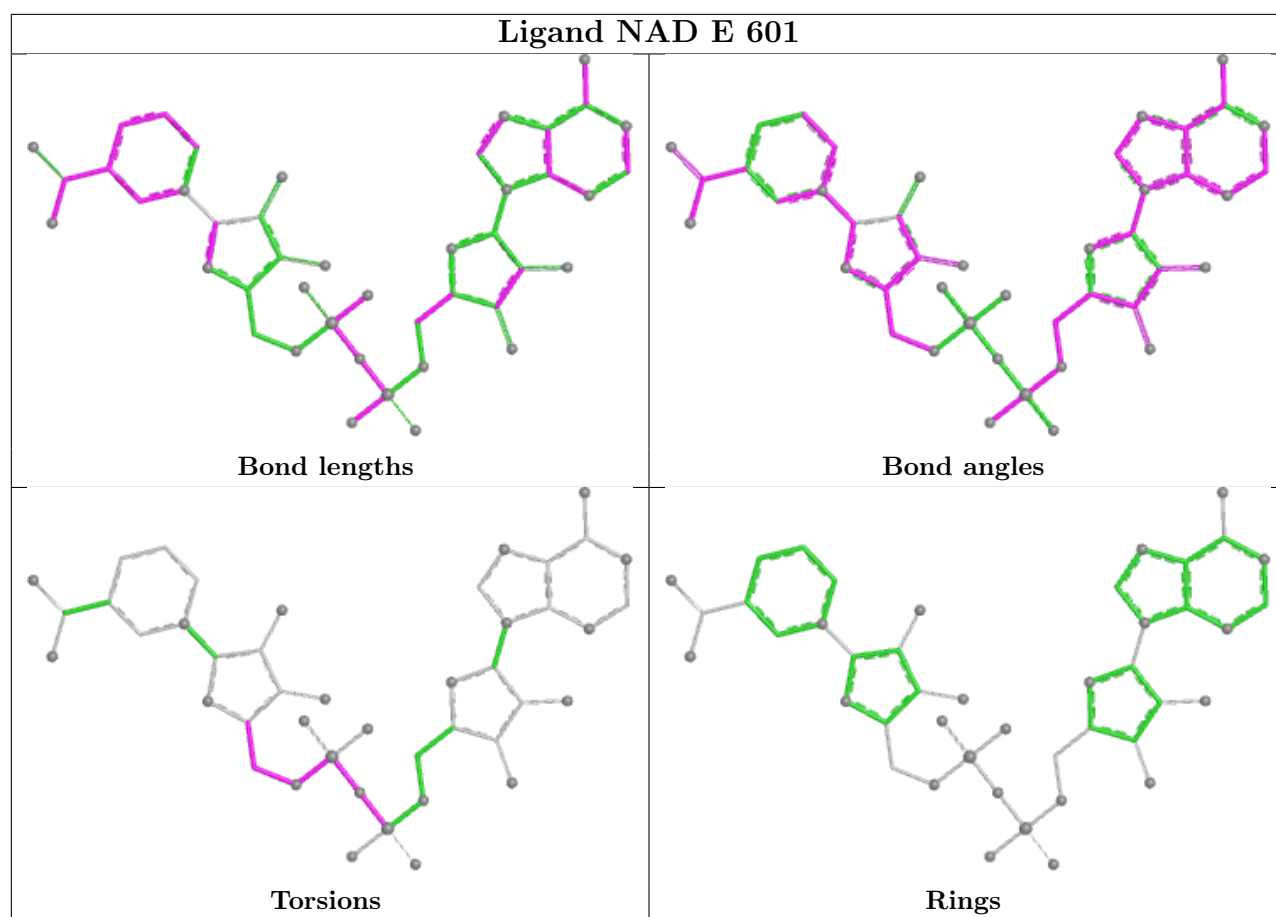


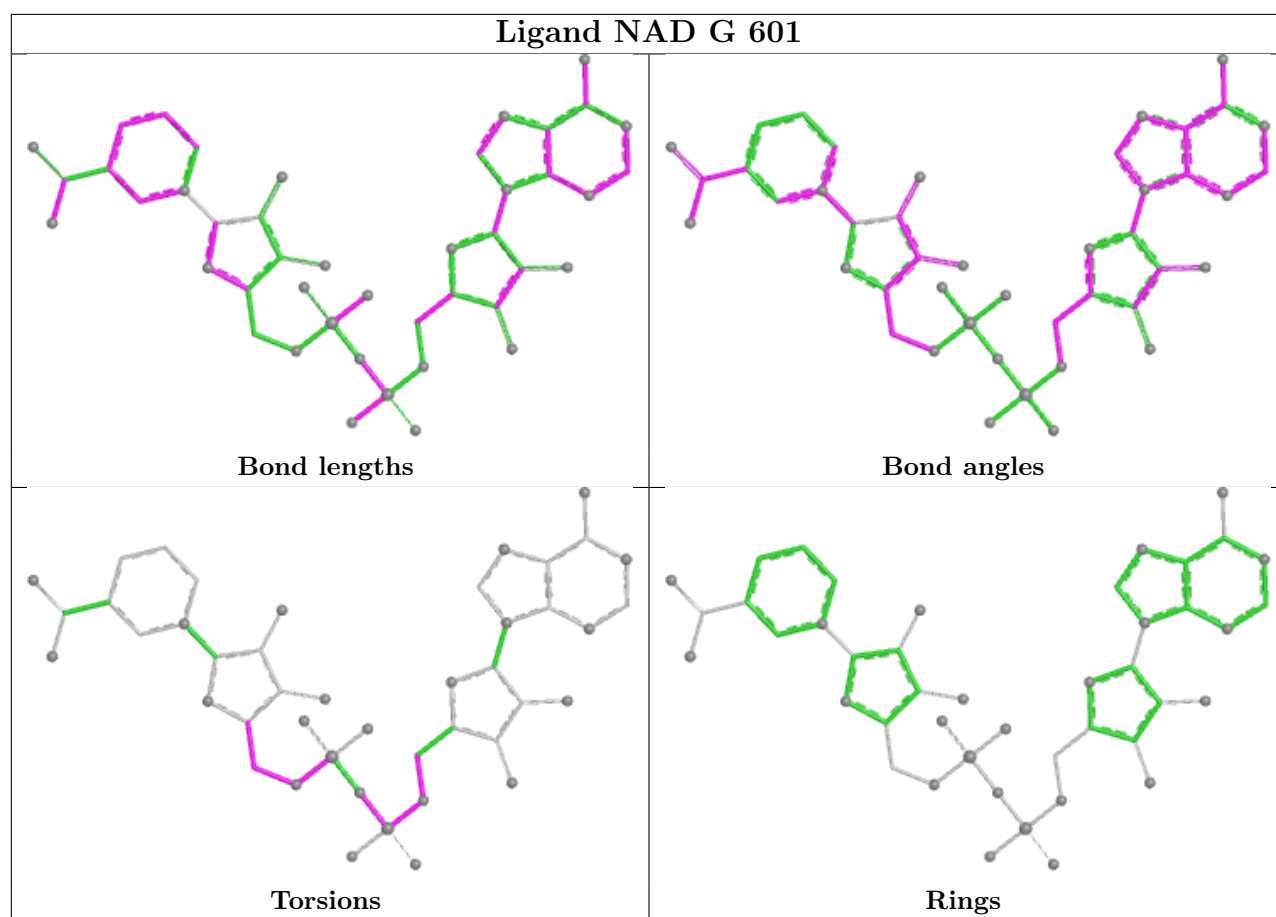


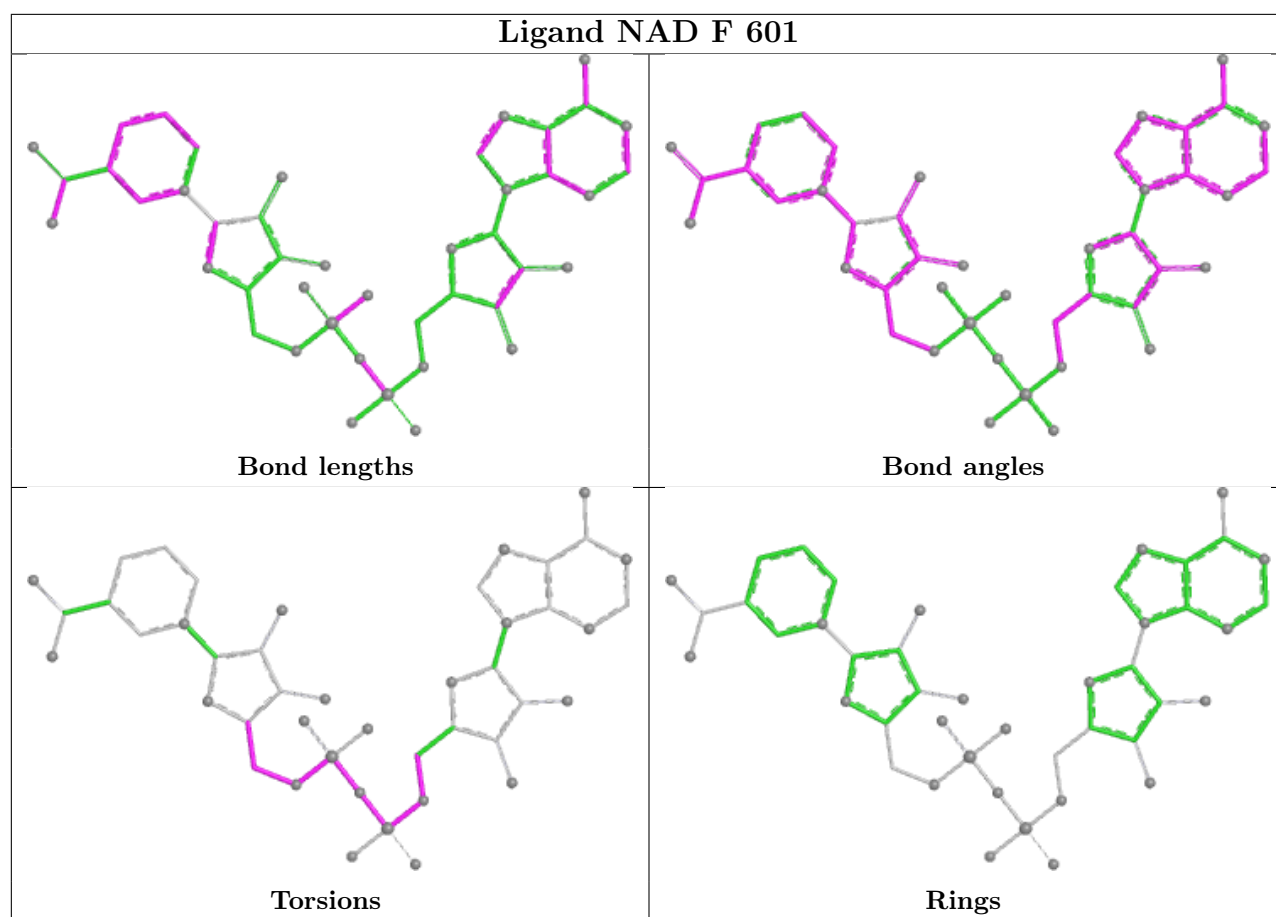












5.7 Other polymers [i](#)

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q < 0.9
1	A	487/495 (98%)	-0.27	0	100	100	30, 61, 91, 111	1 (0%)
1	B	487/495 (98%)	-0.25	0	100	100	30, 60, 91, 115	1 (0%)
1	C	487/495 (98%)	-0.29	1 (0%)	91	83	29, 57, 90, 116	1 (0%)
1	D	487/495 (98%)	-0.25	2 (0%)	88	76	30, 50, 83, 118	1 (0%)
1	E	487/495 (98%)	-0.22	0	100	100	30, 50, 85, 123	1 (0%)
1	F	487/495 (98%)	-0.28	0	100	100	29, 62, 91, 120	1 (0%)
1	G	487/495 (98%)	-0.30	0	100	100	29, 58, 89, 120	1 (0%)
1	H	487/495 (98%)	-0.20	0	100	100	30, 62, 90, 124	1 (0%)
All	All	3896/3960 (98%)	-0.26	3 (0%)	92	86	29, 57, 90, 124	8 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	357	ALA	2.5
1	C	284	GLY	2.5
1	D	382	VAL	2.1

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](#)

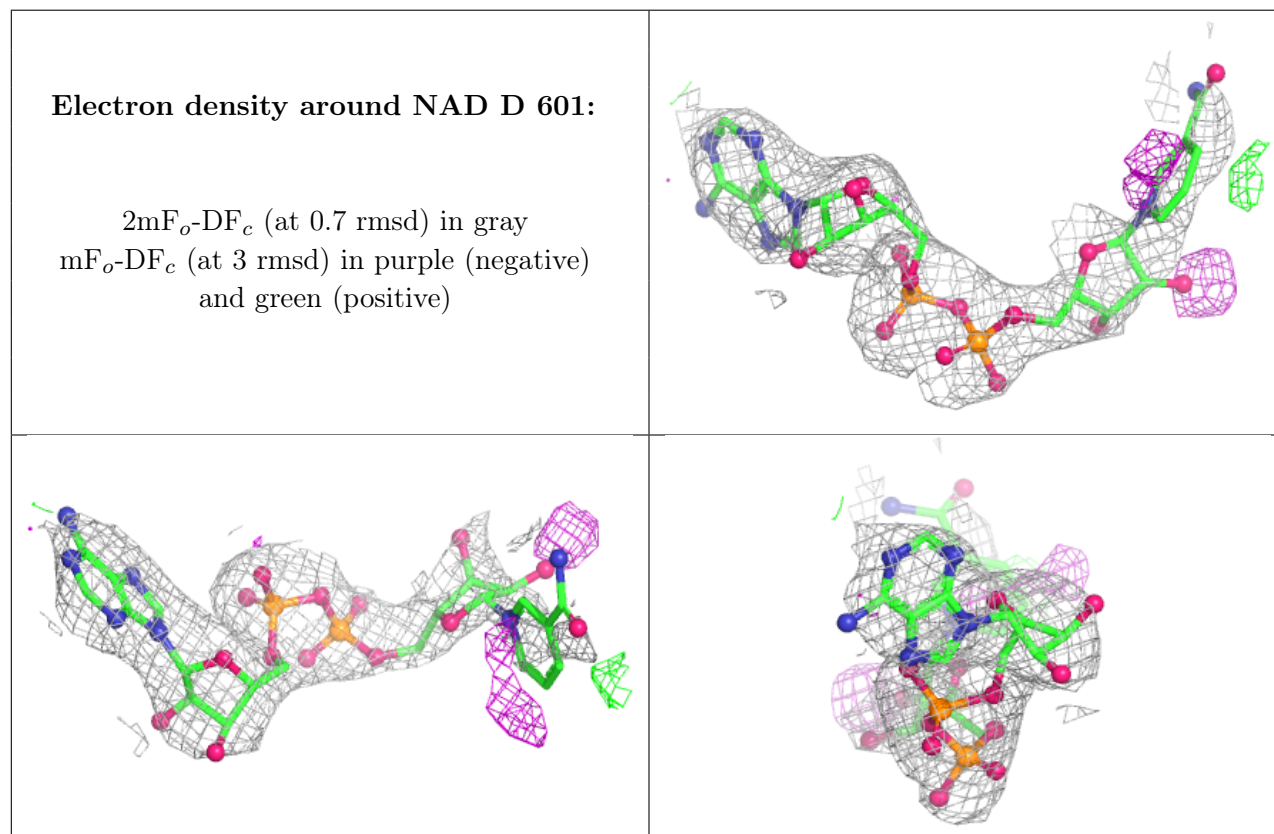
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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.

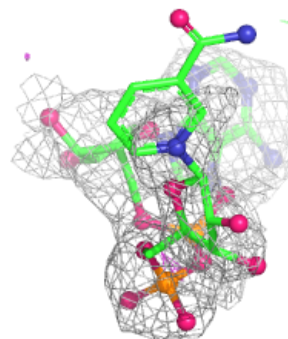
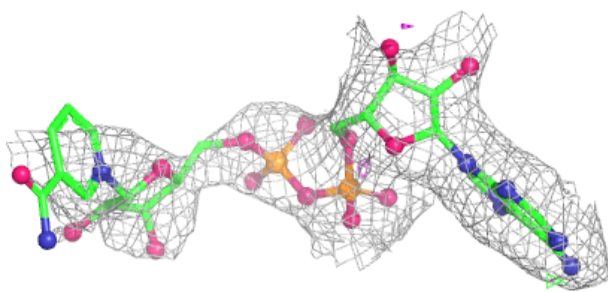
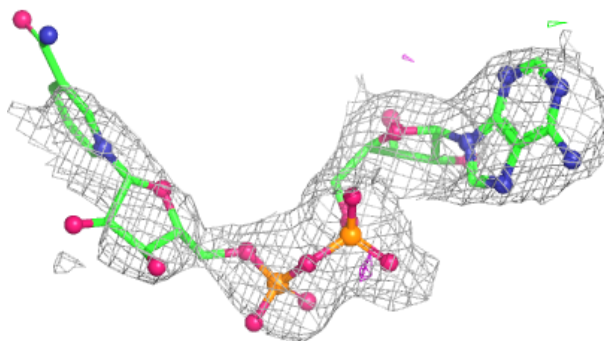
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	D	601	44/44	0.90	0.10	45,66,90,95	0
2	NAD	G	601	44/44	0.90	0.10	48,74,90,103	0
2	NAD	E	601	44/44	0.91	0.10	37,60,82,85	0
2	NAD	A	601	44/44	0.91	0.10	48,77,102,113	0
2	NAD	F	601	44/44	0.92	0.08	49,68,83,101	0
2	NAD	B	601	44/44	0.92	0.09	45,67,89,100	0
2	NAD	H	601	44/44	0.92	0.10	54,75,91,108	0
2	NAD	C	601	44/44	0.94	0.09	38,55,82,90	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.

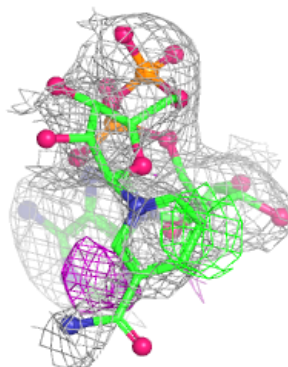
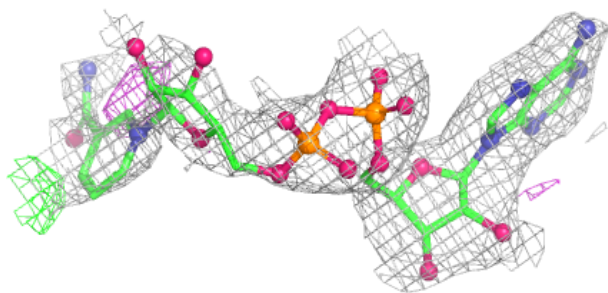
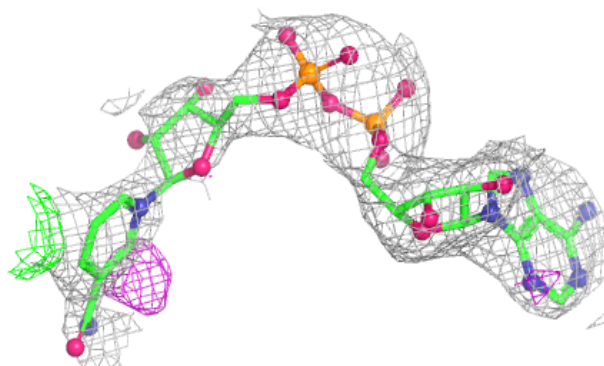


Electron density around NAD G 601:

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

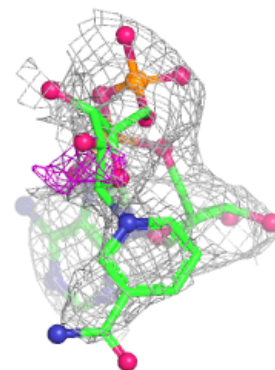
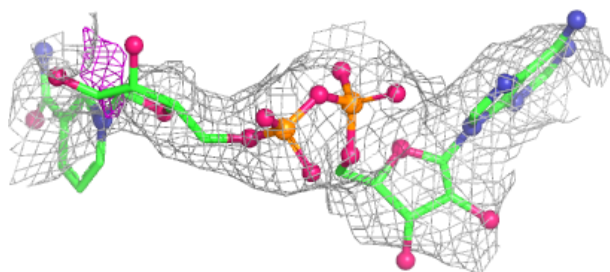
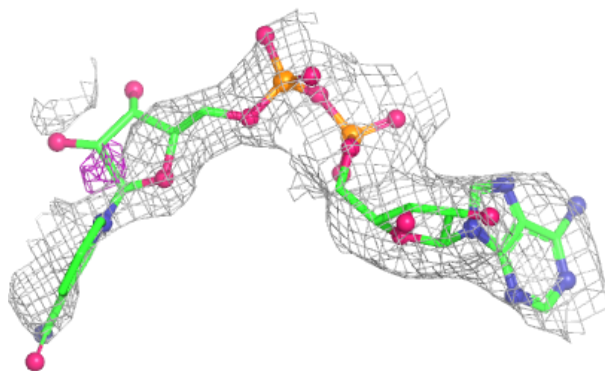
**Electron density around NAD E 601:**

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

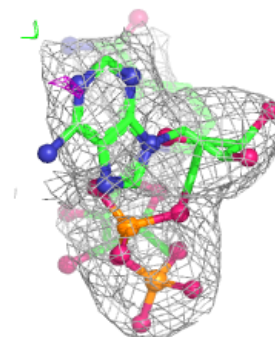
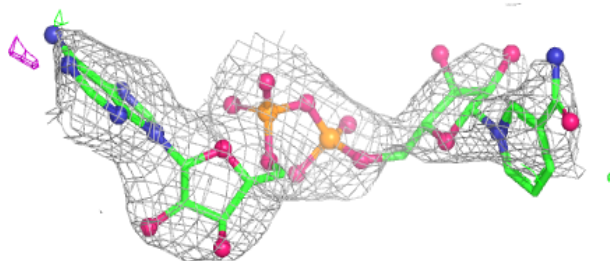
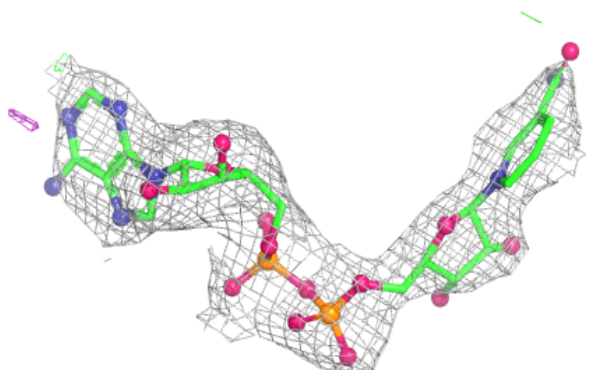


Electron density around NAD A 601:

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

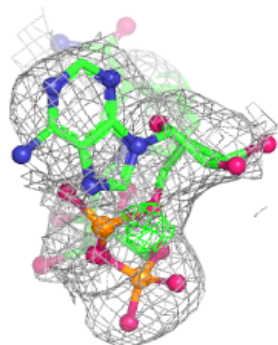
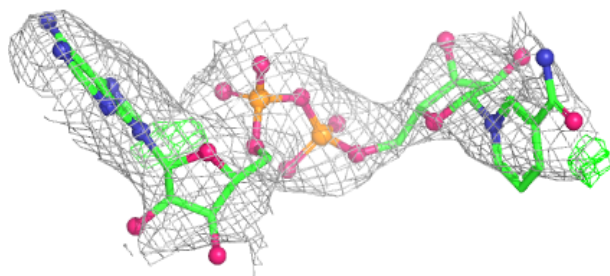
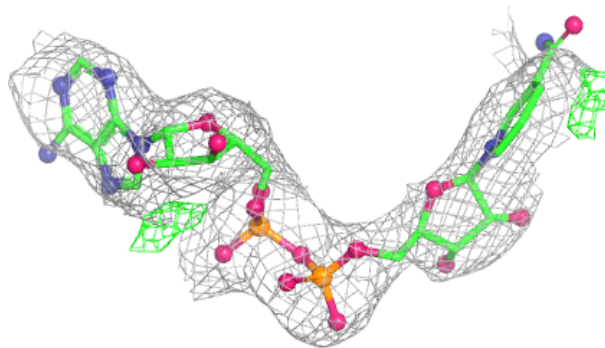
**Electron density around NAD F 601:**

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

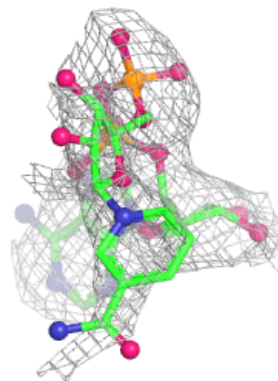
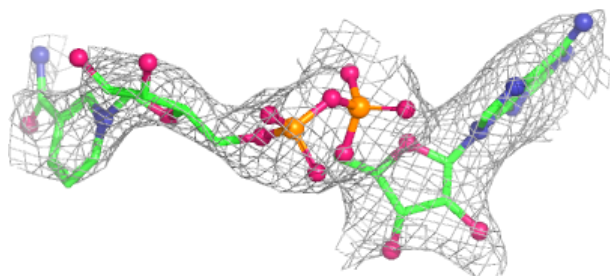
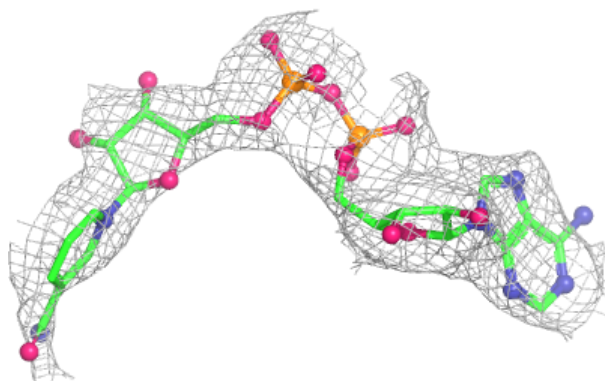


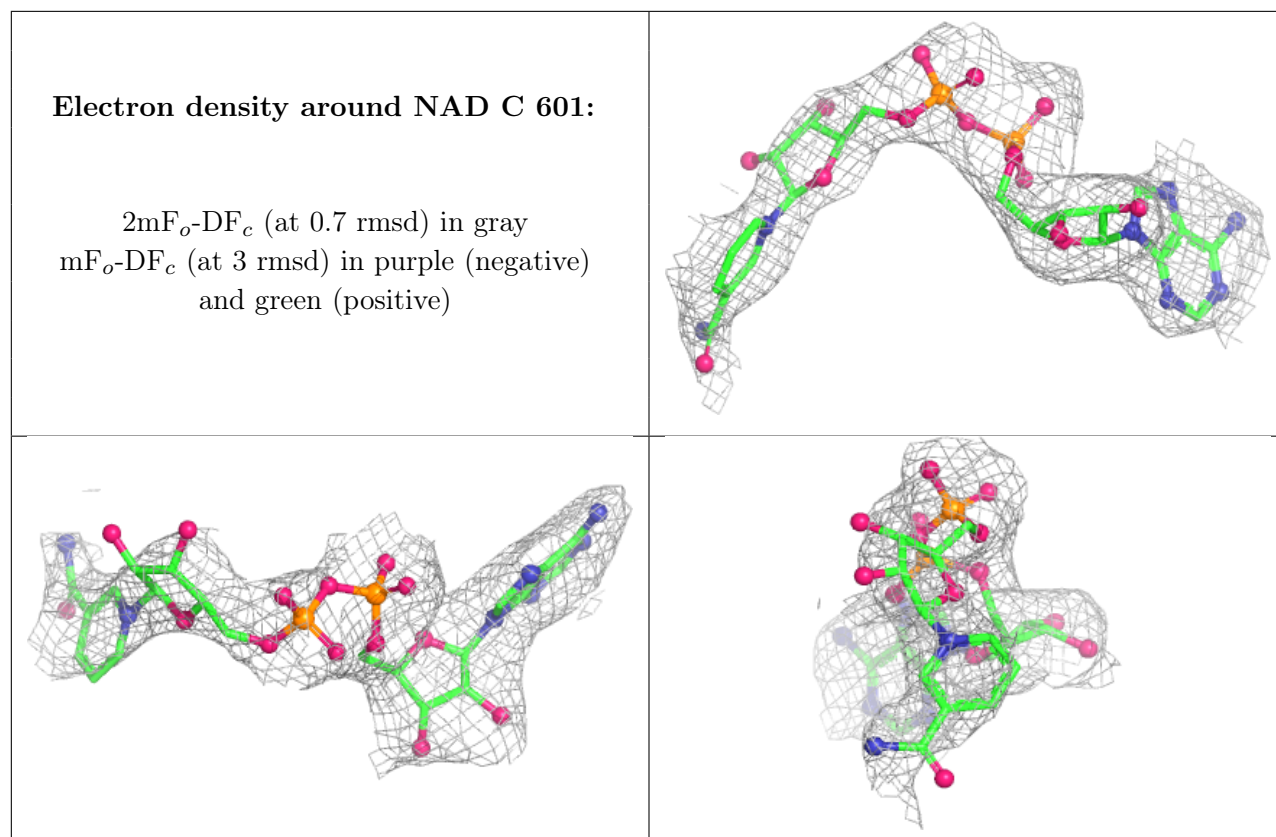
Electron density around NAD B 601:

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

**Electron density around NAD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.