



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:40 PM EDT

PDB ID : 1LDN / pdb_00001ldn
Title : STRUCTURE OF A TERNARY COMPLEX OF AN ALLOSTERIC LACTATE DEHYDROGENASE FROM BACILLUS STEAROTHERMOPHILUS AT 2.5 ANGSTROMS RESOLUTION
Authors : Wigley, D.B.; Gamblin, S.J.; Turkenburg, J.P.; Dodson, E.J.; Piontek, K.; Muirhead, H.; Holbrook, J.J.
Deposited on : 1991-11-19
Resolution : 2.50 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](#) ①) 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

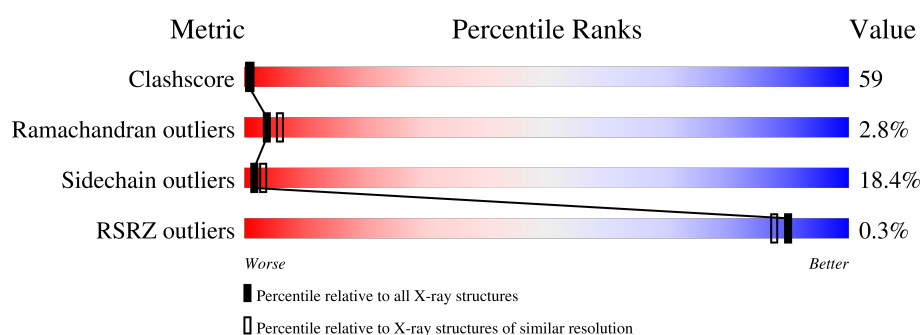
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	316	16% 42% 34% 7%
1	B	316	22% 43% 28% 6%
1	C	316	28% 38% 28% 7%
1	D	316	22% 42% 28% 8%
1	E	316	23% 42% 29% 6%
1	F	316	24% 41% 28% 8%
1	G	316	25% 39% 30% 6%

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Mol	Chain	Length	Quality of chain
1	H	316	% 17% 46% 28% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXM	A	351	-	X	X	-
3	OXM	B	351	-	X	X	-
3	OXM	C	351	-	-	X	-
3	OXM	E	351	-	-	X	-

2 Entry composition

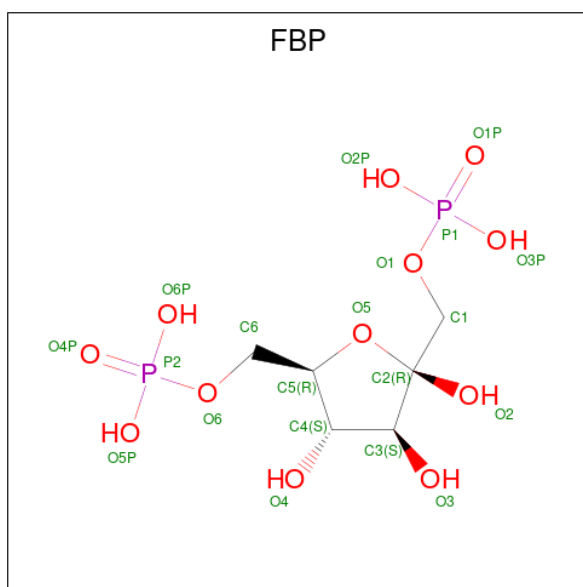
There are 5 unique types of molecules in this entry. The entry contains 20716 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-LACTATE DEHYDROGENASE.

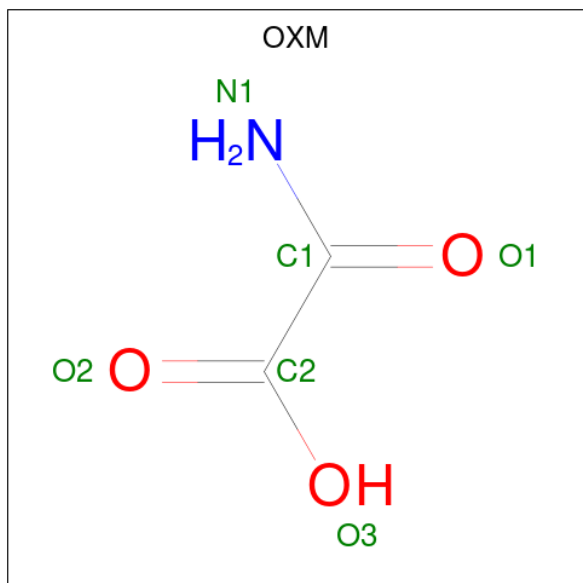
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	B	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	C	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	D	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	E	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	F	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	G	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	H	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).



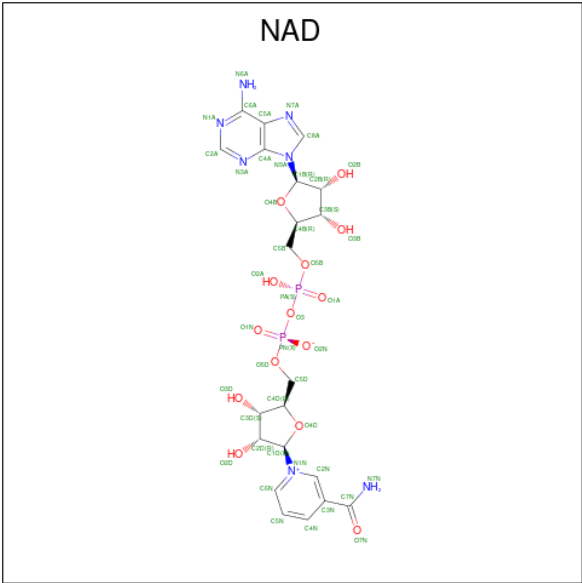
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	1
			40	12	24	4		
2	B	1	Total	C	O	P	0	1
			40	12	24	4		
2	E	1	Total	C	O	P	0	1
			40	12	24	4		
2	F	1	Total	C	O	P	0	1
			40	12	24	4		

- Molecule 3 is OXAMIC ACID (CCD ID: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	2	1	3		
3	B	1	Total	C	N	O	0	0
			6	2	1	3		
3	C	1	Total	C	N	O	0	0
			6	2	1	3		
3	D	1	Total	C	N	O	0	0
			6	2	1	3		
3	E	1	Total	C	N	O	0	0
			6	2	1	3		
3	F	1	Total	C	N	O	0	0
			6	2	1	3		
3	G	1	Total	C	N	O	0	0
			6	2	1	3		
3	H	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

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

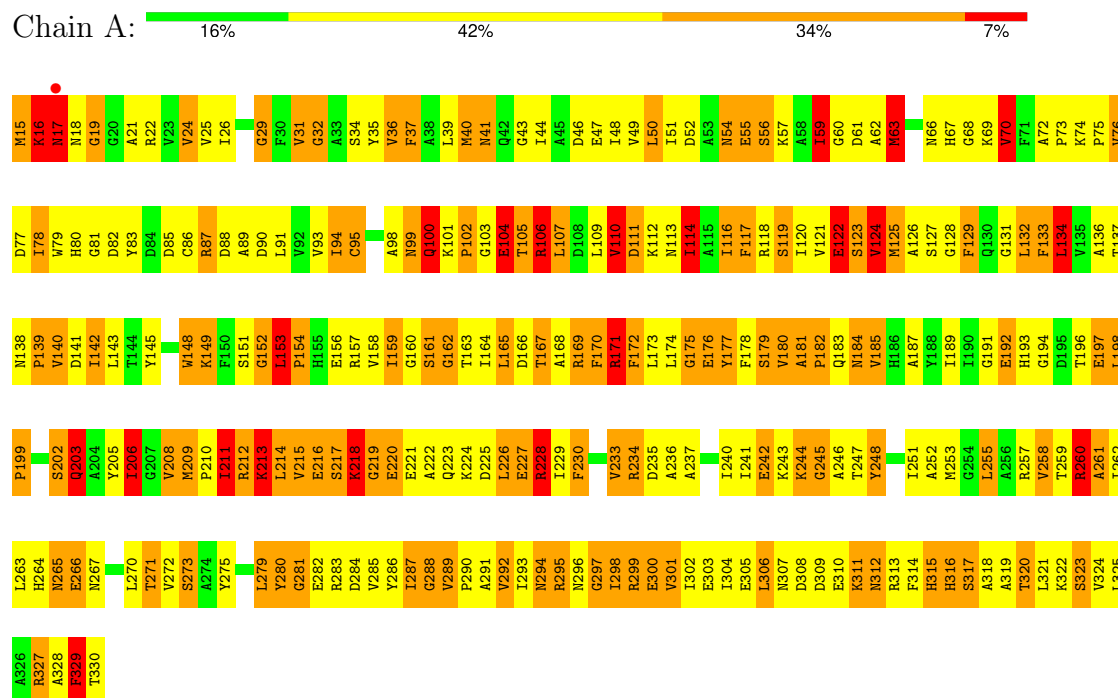
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	72	Total	O	0	0
			72	72		
5	C	69	Total	O	0	0
			69	69		
5	D	74	Total	O	0	0
			74	74		
5	E	70	Total	O	0	0
			70	70		
5	F	72	Total	O	0	0
			72	72		
5	G	70	Total	O	0	0
			70	70		
5	H	73	Total	O	0	0
			73	73		

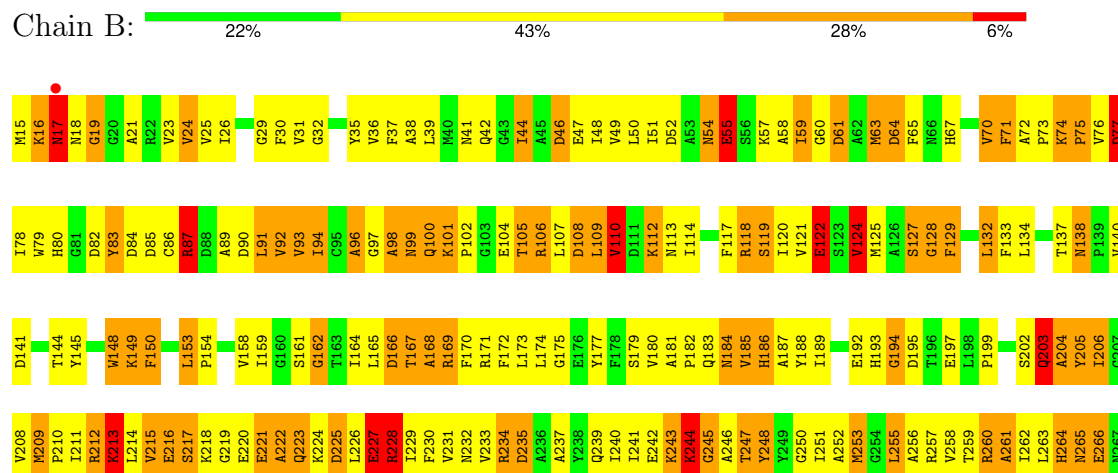
3 Residue-property plots

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: L-LACTATE DEHYDROGENASE



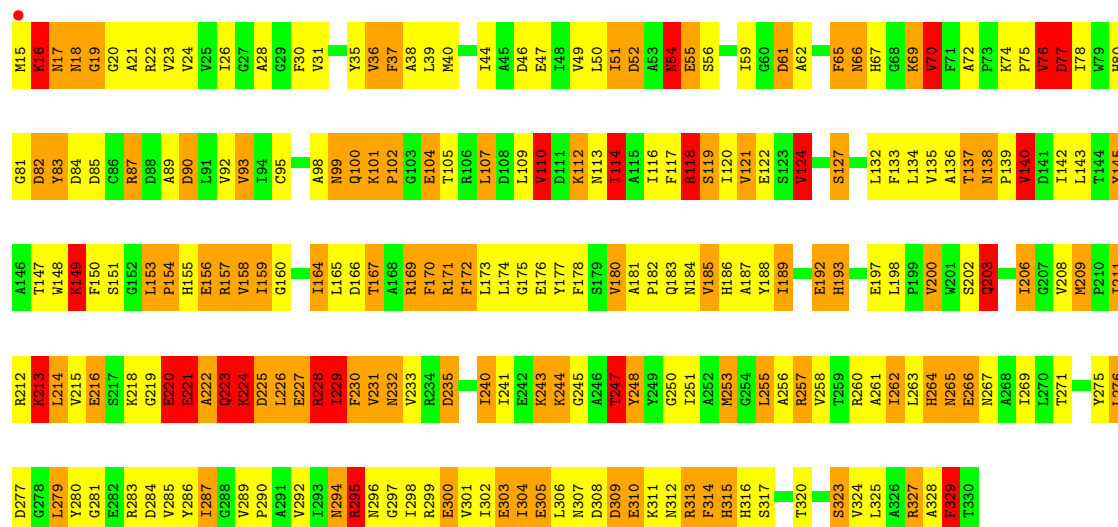
• Molecule 1: L-LACTATE DEHYDROGENASE





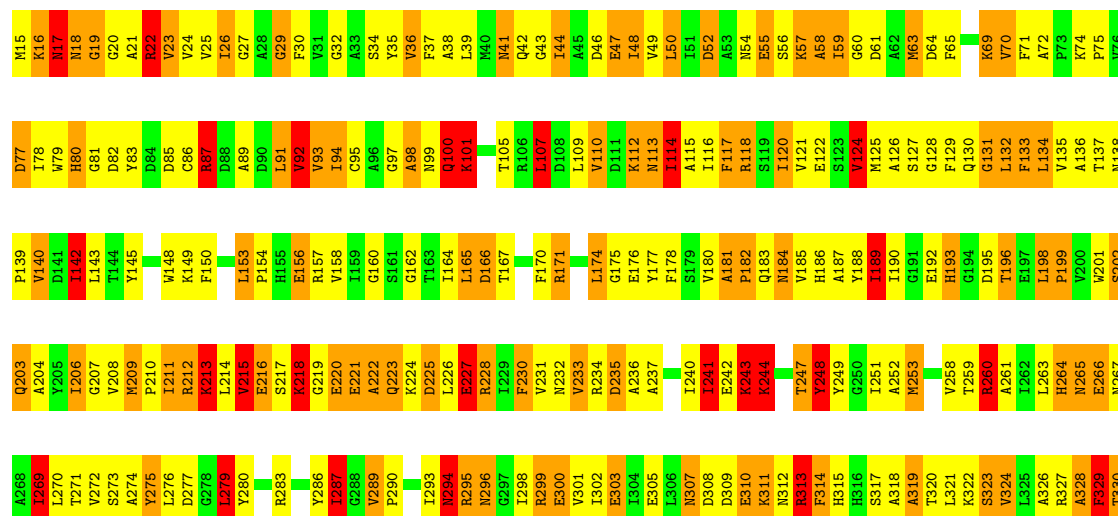
• Molecule 1: L-LACTATE DEHYDROGENASE

Chain C: 28% 38% 28% 7%



• Molecule 1: L-LACTATE DEHYDROGENASE

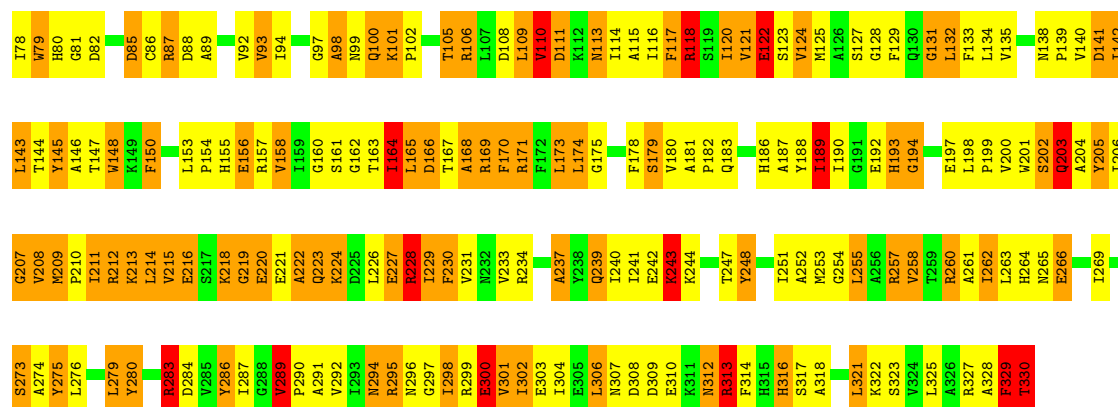
Chain D: 22% 42% 28% 8%



• Molecule 1: L-LACTATE DEHYDROGENASE

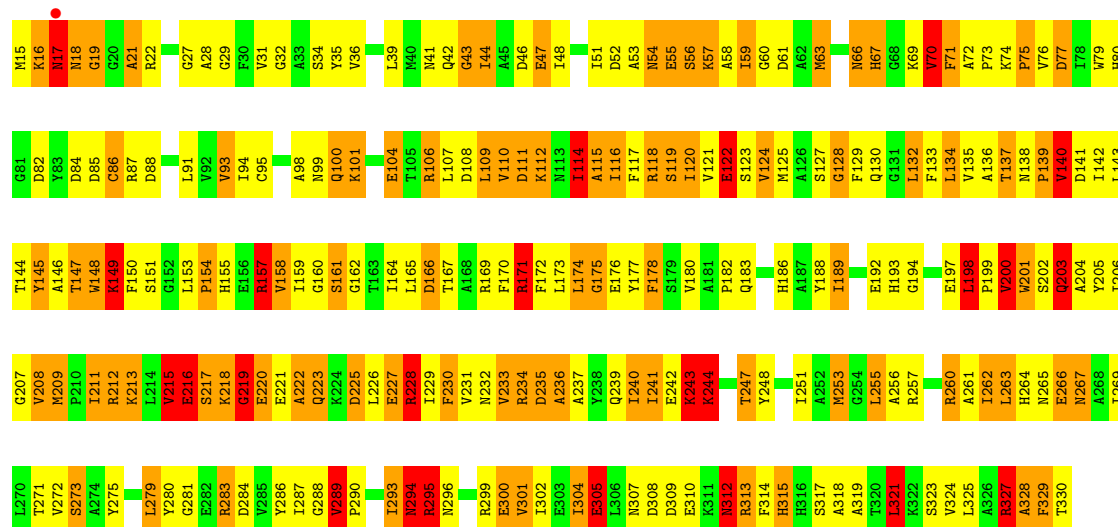
Chain E: 23% 42% 29% 6%





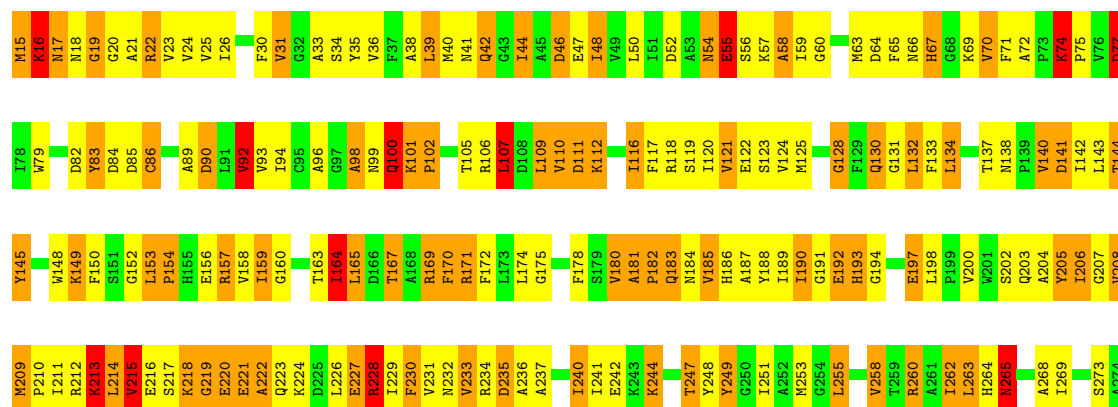
● Molecule 1: L-LACTATE DEHYDROGENASE

Chain F: 24% 41% 28% 8%



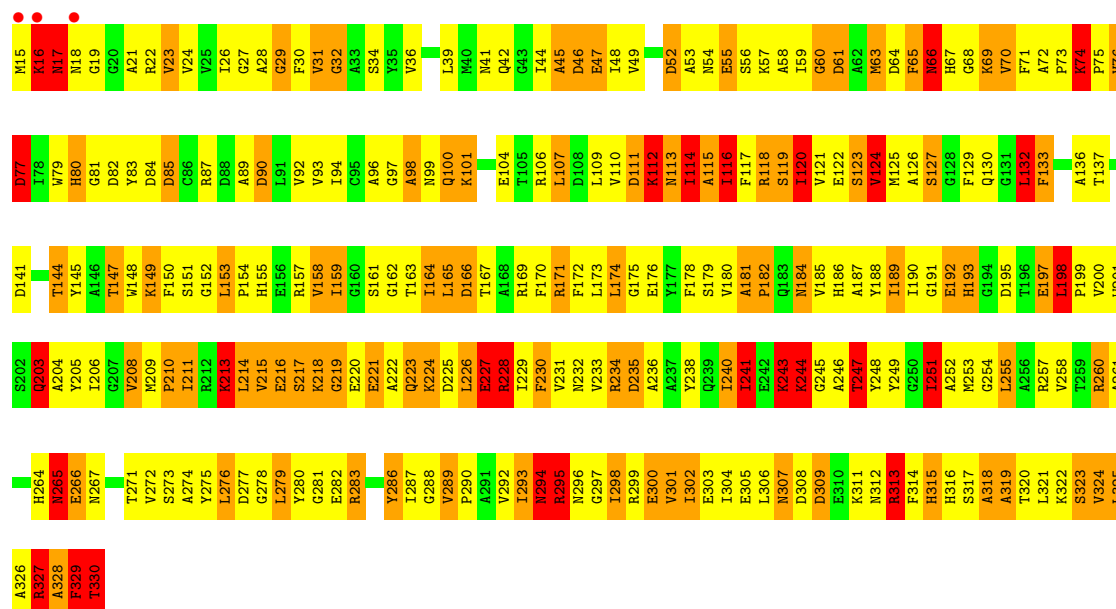
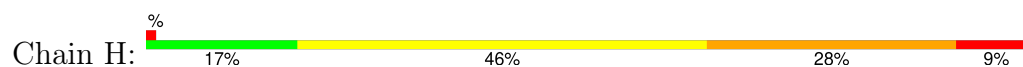
● Molecule 1: L-LACTATE DEHYDROGENASE

Chain G: 25% 39% 30% 6%





• Molecule 1: L-LACTATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.90Å 118.20Å 135.50Å 90.00° 96.07° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50 134.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50) 68.0 (134.74-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.81 (at 2.51Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.157 , (Not available) 0.146 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 168.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20716	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, FBP, OXM

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	1.07	1/2496 (0.0%)	2.63	209/3384 (6.2%)
1	B	1.07	1/2496 (0.0%)	2.66	189/3384 (5.6%)
1	C	1.02	0/2496	2.61	193/3384 (5.7%)
1	D	1.04	0/2496	2.61	199/3384 (5.9%)
1	E	1.04	0/2496	2.69	205/3384 (6.1%)
1	F	1.04	0/2496	2.70	224/3384 (6.6%)
1	G	1.04	0/2496	2.52	170/3384 (5.0%)
1	H	1.05	1/2496 (0.0%)	2.73	219/3384 (6.5%)
All	All	1.05	3/19968 (0.0%)	2.64	1608/27072 (5.9%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLY	N-CA	5.28	1.49	1.44
1	B	329	PHE	N-CA	5.14	1.52	1.46
1	H	163	THR	CA-CB	5.11	1.61	1.53

All (1608) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	171	ARG	CD-NE-CZ	39.46	179.65	124.40
1	B	327	ARG	CD-NE-CZ	31.84	168.97	124.40
1	H	228	ARG	CD-NE-CZ	24.42	158.59	124.40
1	F	327	ARG	CD-NE-CZ	24.05	158.07	124.40
1	B	99	ASN	CA-CB-CG	23.89	136.49	112.60
1	G	99	ASN	CA-CB-CG	23.58	136.18	112.60
1	E	82	ASP	CA-CB-CG	22.99	135.59	112.60
1	F	228	ARG	CD-NE-CZ	21.96	155.15	124.40
1	H	329	PHE	CA-CB-CG	-20.21	93.59	113.80
1	A	82	ASP	CA-CB-CG	17.20	129.80	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	329	PHE	CA-CB-CG	-16.63	97.17	113.80
1	C	98	ALA	CA-C-N	16.45	147.16	122.65
1	C	98	ALA	C-N-CA	16.45	147.16	122.65
1	C	212	ARG	CD-NE-CZ	16.34	147.27	124.40
1	H	329	PHE	CA-C-N	16.31	151.06	121.70
1	H	329	PHE	C-N-CA	16.31	151.06	121.70
1	C	222	ALA	N-CA-C	-15.93	92.16	112.23
1	D	82	ASP	CA-CB-CG	15.79	128.40	112.60
1	B	328	ALA	CA-C-N	-15.73	102.39	122.84
1	B	328	ALA	C-N-CA	-15.73	102.39	122.84
1	A	329	PHE	CA-CB-CG	-15.29	98.52	113.80
1	G	17	ASN	CA-CB-CG	-15.04	97.56	112.60
1	A	170	PHE	CA-CB-CG	14.83	128.63	113.80
1	D	315	HIS	CA-CB-CG	-14.78	99.02	113.80
1	F	99	ASN	CA-CB-CG	14.61	127.21	112.60
1	B	230	PHE	CA-CB-CG	-14.43	99.37	113.80
1	E	186	HIS	CA-CB-CG	-14.43	99.37	113.80
1	B	329	PHE	CA-CB-CG	-14.35	99.45	113.80
1	B	17	ASN	CA-CB-CG	-14.19	98.41	112.60
1	H	98	ALA	CA-C-N	14.04	141.58	121.50
1	H	98	ALA	C-N-CA	14.04	141.58	121.50
1	G	150	PHE	CA-CB-CG	13.90	127.70	113.80
1	G	329	PHE	CA-C-N	13.88	146.68	121.70
1	G	329	PHE	C-N-CA	13.88	146.68	121.70
1	B	85	ASP	CA-CB-CG	13.73	126.33	112.60
1	C	266	GLU	N-CA-C	13.23	125.79	111.36
1	C	295	ARG	CD-NE-CZ	13.04	142.66	124.40
1	D	184	ASN	CA-CB-CG	12.90	125.50	112.60
1	B	329	PHE	CA-C-N	12.86	144.84	121.70
1	B	329	PHE	C-N-CA	12.86	144.84	121.70
1	B	227	GLU	CB-CG-CD	12.82	134.39	112.60
1	A	175	GLY	N-CA-C	-12.77	97.68	112.50
1	H	16	LYS	N-CA-C	-12.72	97.27	112.92
1	A	185	VAL	CA-C-O	-12.61	106.84	120.59
1	G	300	GLU	O-C-N	12.50	134.66	123.41
1	D	133	PHE	CA-CB-CG	12.49	126.29	113.80
1	E	133	PHE	CA-CB-CG	12.35	126.15	113.80
1	E	100	GLN	CA-C-O	12.33	134.75	120.69
1	B	329	PHE	CA-C-O	12.32	133.35	120.54
1	C	16	LYS	N-CA-C	-12.30	98.30	113.18
1	D	232	ASN	OD1-CG-ND2	12.25	134.85	122.60
1	D	329	PHE	CA-C-O	12.24	134.20	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	329	PHE	CA-CB-CG	-12.14	101.66	113.80
1	D	329	PHE	CA-C-N	12.11	143.50	121.70
1	D	329	PHE	C-N-CA	12.11	143.50	121.70
1	C	153	LEU	O-C-N	12.09	129.84	121.14
1	A	329	PHE	CA-C-N	12.08	143.44	121.70
1	A	329	PHE	C-N-CA	12.08	143.44	121.70
1	F	234	ARG	CD-NE-CZ	12.08	141.31	124.40
1	H	266	GLU	N-CA-C	12.03	125.78	111.82
1	F	307	ASN	CA-CB-CG	11.94	124.54	112.60
1	E	222	ALA	N-CA-C	-11.92	98.36	111.36
1	G	222	ALA	N-CA-C	-11.91	96.49	111.02
1	D	16	LYS	N-CA-C	-11.90	98.86	113.50
1	A	309	ASP	CA-CB-CG	-11.90	100.70	112.60
1	B	71	PHE	CA-CB-CG	11.88	125.68	113.80
1	C	99	ASN	CA-CB-CG	11.85	124.45	112.60
1	E	16	LYS	N-CA-C	-11.74	98.93	113.01
1	C	305	GLU	CA-CB-CG	11.68	137.47	114.10
1	A	233	VAL	N-CA-C	-11.43	100.33	110.74
1	E	312	ASN	CA-CB-CG	-11.43	101.17	112.60
1	D	98	ALA	CA-C-N	11.38	138.93	122.09
1	D	98	ALA	C-N-CA	11.38	138.93	122.09
1	D	100	GLN	CA-C-O	11.38	133.66	120.69
1	D	171	ARG	CD-NE-CZ	11.31	140.24	124.40
1	D	99	ASN	CA-CB-CG	11.31	123.91	112.60
1	D	294	ASN	CA-CB-CG	11.26	123.86	112.60
1	C	186	HIS	CA-CB-CG	-11.24	102.56	113.80
1	D	186	HIS	CA-CB-CG	-11.22	102.58	113.80
1	E	312	ASN	OD1-CG-ND2	11.22	133.82	122.60
1	C	16	LYS	CA-C-O	11.21	133.46	119.11
1	G	16	LYS	CA-C-O	11.20	132.83	119.28
1	A	85	ASP	CA-CB-CG	11.18	123.78	112.60
1	H	133	PHE	CA-CB-CG	11.15	124.95	113.80
1	H	99	ASN	CA-CB-CG	11.11	123.71	112.60
1	F	294	ASN	CA-CB-CG	11.07	123.67	112.60
1	A	98	ALA	CA-C-O	11.01	132.98	120.54
1	E	214	LEU	N-CA-C	-10.96	99.64	113.23
1	H	32	GLY	N-CA-C	10.95	125.86	112.73
1	A	320	THR	N-CA-C	10.86	122.69	111.07
1	H	171	ARG	CD-NE-CZ	10.86	139.60	124.40
1	G	65	PHE	CA-CB-CG	10.85	124.65	113.80
1	B	44	ILE	N-CA-C	10.83	121.53	111.45
1	E	327	ARG	NE-CZ-NH1	-10.80	110.70	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	MET	O-C-N	10.79	133.25	122.03
1	D	232	ASN	CA-CB-CG	-10.79	101.81	112.60
1	F	222	ALA	N-CA-C	-10.75	97.90	111.02
1	F	66	ASN	OD1-CG-ND2	10.68	133.28	122.60
1	A	316	HIS	CA-CB-CG	-10.63	103.17	113.80
1	A	327	ARG	CA-CB-CG	10.58	135.26	114.10
1	C	206	ILE	N-CA-C	-10.57	90.47	107.28
1	E	99	ASN	CA-CB-CG	10.55	123.15	112.60
1	F	215	VAL	O-C-N	10.45	132.55	121.78
1	F	110	VAL	N-CA-C	10.44	121.08	110.23
1	B	206	ILE	O-C-N	10.39	132.69	122.30
1	F	180	VAL	CA-C-O	-10.38	111.07	121.45
1	F	44	ILE	N-CA-C	10.36	120.17	110.74
1	C	192	GLU	CB-CG-CD	10.32	130.15	112.60
1	E	22	ARG	CD-NE-CZ	-10.30	109.98	124.40
1	C	264	HIS	CA-CB-CG	-10.28	103.53	113.80
1	F	100	GLN	N-CA-CB	10.27	125.87	109.95
1	E	283	ARG	CD-NE-CZ	10.24	138.74	124.40
1	D	277	ASP	CA-CB-CG	10.19	122.79	112.60
1	B	289	VAL	N-CA-CB	-10.15	96.99	111.21
1	E	329	PHE	CA-CB-CG	-10.15	103.65	113.80
1	G	140	VAL	CA-C-O	-10.10	109.64	120.64
1	C	232	ASN	CA-CB-CG	-10.09	102.51	112.60
1	C	227	GLU	CB-CG-CD	10.07	129.73	112.60
1	G	184	ASN	CA-CB-CG	10.00	122.60	112.60
1	B	77	ASP	CA-CB-CG	9.97	122.57	112.60
1	C	214	LEU	N-CA-C	-9.97	101.25	113.41
1	F	234	ARG	NE-CZ-NH1	9.95	131.45	121.50
1	F	175	GLY	N-CA-C	-9.94	100.80	112.73
1	H	158	VAL	N-CA-CB	9.93	123.97	111.46
1	A	99	ASN	CA-CB-CG	9.91	122.51	112.60
1	E	266	GLU	N-CA-C	9.91	121.84	111.14
1	F	166	ASP	CA-CB-CG	9.88	122.48	112.60
1	C	329	PHE	CA-C-N	9.86	139.46	121.70
1	C	329	PHE	C-N-CA	9.86	139.46	121.70
1	E	316	HIS	CA-CB-CG	-9.86	103.94	113.80
1	A	212	ARG	CD-NE-CZ	9.84	138.18	124.40
1	G	170	PHE	CA-CB-CG	9.83	123.63	113.80
1	A	153	LEU	N-CA-C	-9.82	97.21	110.36
1	H	90	ASP	CA-C-O	9.80	130.31	119.24
1	H	240	ILE	O-C-N	9.79	131.92	121.83
1	H	98	ALA	CA-C-O	9.77	131.58	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	ILE	CA-C-O	-9.73	110.77	121.09
1	B	232	ASN	O-C-N	9.72	132.42	122.12
1	G	307	ASN	CA-CB-CG	9.71	122.31	112.60
1	B	244	LYS	CA-CB-CG	9.70	133.49	114.10
1	H	116	ILE	N-CA-C	9.64	120.45	110.72
1	E	85	ASP	CA-CB-CG	9.62	122.22	112.60
1	A	308	ASP	CA-CB-CG	9.59	122.19	112.60
1	A	44	ILE	N-CA-C	9.58	121.74	111.58
1	H	17	ASN	CA-CB-CG	-9.56	103.04	112.60
1	H	157	ARG	CD-NE-CZ	-9.53	111.06	124.40
1	F	283	ARG	NE-CZ-NH2	9.51	127.76	119.20
1	D	175	GLY	N-CA-C	-9.49	100.63	112.77
1	E	328	ALA	CA-C-N	-9.45	108.39	123.23
1	E	328	ALA	C-N-CA	-9.45	108.39	123.23
1	C	102	PRO	N-CA-C	-9.43	96.44	111.14
1	B	16	LYS	N-CA-C	-9.39	101.83	113.20
1	G	63	MET	O-C-N	9.33	132.06	122.08
1	G	214	LEU	N-CA-C	-9.32	102.04	113.50
1	B	245	GLY	N-CA-C	9.32	127.89	115.59
1	H	180	VAL	CA-C-O	-9.30	112.42	121.63
1	A	157	ARG	NE-CZ-NH2	9.28	127.56	119.20
1	A	122	GLU	CA-C-O	9.28	131.31	120.92
1	E	170	PHE	CA-C-N	9.25	133.02	120.54
1	E	170	PHE	C-N-CA	9.25	133.02	120.54
1	H	157	ARG	NE-CZ-NH1	-9.23	112.27	121.50
1	F	18	ASN	CA-CB-CG	9.22	121.82	112.60
1	C	279	LEU	CA-C-O	-9.21	111.42	120.90
1	A	170	PHE	N-CA-C	-9.18	100.96	110.97
1	D	214	LEU	N-CA-C	-9.15	102.12	113.38
1	G	295	ARG	CD-NE-CZ	9.15	137.21	124.40
1	A	98	ALA	CA-C-N	9.14	133.75	120.95
1	A	98	ALA	C-N-CA	9.14	133.75	120.95
1	A	106	ARG	CD-NE-CZ	9.14	137.19	124.40
1	F	328	ALA	CA-C-N	-9.14	110.27	122.42
1	F	328	ALA	C-N-CA	-9.14	110.27	122.42
1	G	279	LEU	CA-C-O	-9.13	110.74	120.42
1	G	122	GLU	O-C-N	9.12	131.88	122.03
1	A	215	VAL	O-C-N	9.12	131.32	122.20
1	F	70	VAL	N-CA-C	-9.10	99.85	112.50
1	D	140	VAL	CA-C-O	-9.10	111.59	121.05
1	F	120	ILE	O-C-N	9.05	130.78	121.91
1	G	102	PRO	CB-CA-C	9.04	121.42	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	329	PHE	CA-C-N	9.04	137.97	121.70
1	E	329	PHE	C-N-CA	9.04	137.97	121.70
1	C	307	ASN	CA-CB-CG	9.03	121.63	112.60
1	F	42	GLN	OE1-CD-NE2	8.97	131.57	122.60
1	F	111	ASP	CA-CB-CG	8.96	121.56	112.60
1	H	100	GLN	N-CA-CB	8.95	123.19	109.85
1	D	41	ASN	CA-CB-CG	-8.91	103.69	112.60
1	E	283	ARG	NE-CZ-NH1	8.90	130.40	121.50
1	H	297	GLY	CA-C-O	-8.88	110.64	121.83
1	D	222	ALA	N-CA-C	-8.85	96.85	111.37
1	B	328	ALA	CA-C-O	-8.84	107.87	120.51
1	F	157	ARG	NE-CZ-NH1	-8.83	112.67	121.50
1	E	189	ILE	N-CA-CB	8.81	126.72	111.39
1	E	255	LEU	CA-C-O	-8.79	111.10	120.42
1	G	327	ARG	CD-NE-CZ	8.79	136.70	124.40
1	B	188	TYR	CA-CB-CG	8.77	129.69	113.90
1	H	329	PHE	CA-C-O	8.77	130.04	120.92
1	H	170	PHE	CA-CB-CG	8.75	122.55	113.80
1	D	212	ARG	CD-NE-CZ	8.74	136.64	124.40
1	E	37	PHE	N-CA-C	-8.74	101.70	111.14
1	C	172	PHE	CA-CB-CG	-8.72	105.08	113.80
1	F	279	LEU	CA-C-O	-8.72	110.81	121.02
1	E	16	LYS	CA-C-O	8.71	130.37	119.05
1	B	208	VAL	N-CA-C	-8.70	104.66	113.10
1	H	132	LEU	CA-CB-CG	8.70	146.74	116.30
1	C	232	ASN	O-C-N	8.69	132.06	122.15
1	C	113	ASN	CA-C-O	-8.67	111.23	120.42
1	A	266	GLU	N-CA-C	8.67	120.81	111.36
1	D	117	PHE	CA-CB-CG	-8.63	105.17	113.80
1	C	150	PHE	CA-CB-CG	8.62	122.42	113.80
1	H	34	SER	N-CA-C	-8.61	101.81	111.71
1	D	234	ARG	CD-NE-CZ	8.60	136.44	124.40
1	E	228	ARG	CD-NE-CZ	8.59	136.42	124.40
1	C	277	ASP	CA-CB-CG	-8.59	104.02	112.60
1	D	329	PHE	N-CA-C	8.59	123.00	108.23
1	H	85	ASP	CA-CB-CG	-8.57	104.03	112.60
1	E	230	PHE	CA-CB-CG	-8.57	105.23	113.80
1	G	74	LYS	O-C-N	8.57	127.96	121.88
1	A	245	GLY	N-CA-C	8.57	126.90	115.59
1	B	264	HIS	CA-CB-CG	-8.57	105.23	113.80
1	C	315	HIS	CA-CB-CG	-8.54	105.26	113.80
1	E	207	GLY	N-CA-C	-8.54	95.15	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	30	PHE	O-C-N	8.54	131.25	122.03
1	F	16	LYS	CA-C-O	8.52	129.88	119.31
1	H	208	VAL	N-CA-C	-8.51	104.61	112.43
1	G	193	HIS	N-CA-CB	8.50	122.82	110.58
1	E	192	GLU	CB-CG-CD	8.50	127.04	112.60
1	F	203	GLN	N-CA-CB	-8.47	98.45	111.66
1	A	311	LYS	CA-C-N	8.46	132.31	120.29
1	A	311	LYS	C-N-CA	8.46	132.31	120.29
1	G	230	PHE	CA-CB-CG	-8.45	105.35	113.80
1	H	77	ASP	CA-C-O	-8.44	111.77	120.54
1	A	124	VAL	O-C-N	8.43	130.17	121.91
1	B	218	LYS	O-C-N	8.43	130.52	122.18
1	C	102	PRO	CB-CA-C	8.41	122.31	111.46
1	F	88	ASP	CA-CB-CG	-8.40	104.20	112.60
1	H	90	ASP	CA-CB-CG	8.39	120.99	112.60
1	H	235	ASP	CA-CB-CG	8.39	121.00	112.60
1	H	265	ASN	CA-CB-CG	8.39	120.99	112.60
1	C	235	ASP	N-CA-C	8.38	123.34	113.20
1	D	266	GLU	N-CA-C	8.38	122.79	112.23
1	C	230	PHE	CA-CB-CG	-8.36	105.44	113.80
1	D	92	VAL	CB-CA-C	8.36	121.86	110.99
1	D	17	ASN	CA-CB-CG	-8.32	104.28	112.60
1	E	106	ARG	CA-C-N	8.32	134.02	120.63
1	E	106	ARG	C-N-CA	8.32	134.02	120.63
1	A	181	ALA	CB-CA-C	8.31	122.66	109.52
1	B	106	ARG	CD-NE-CZ	-8.31	112.77	124.40
1	F	189	ILE	N-CA-C	-8.30	96.16	108.12
1	D	135	VAL	CB-CA-C	8.29	123.83	111.31
1	F	203	GLN	CA-CB-CG	8.29	130.67	114.10
1	C	153	LEU	CA-C-O	-8.26	113.73	121.08
1	F	234	ARG	NE-CZ-NH2	-8.26	111.76	119.20
1	G	42	GLN	N-CA-C	-8.26	102.99	113.23
1	G	228	ARG	CD-NE-CZ	8.26	135.96	124.40
1	F	215	VAL	N-CA-C	-8.24	105.28	113.20
1	D	289	VAL	N-CA-CB	-8.24	99.68	111.21
1	F	289	VAL	N-CA-CB	-8.23	99.69	111.21
1	G	175	GLY	N-CA-C	-8.21	102.56	112.49
1	B	101	LYS	N-CA-CB	8.20	118.75	109.49
1	C	329	PHE	CA-CB-CG	-8.17	105.63	113.80
1	G	283	ARG	CD-NE-CZ	8.17	135.84	124.40
1	H	171	ARG	O-C-N	8.16	130.77	122.12
1	B	185	VAL	CA-C-O	-8.15	111.11	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	31	VAL	CB-CA-C	8.15	122.41	111.97
1	B	307	ASN	CA-CB-CG	8.14	120.74	112.60
1	H	46	ASP	CA-CB-CG	-8.11	104.49	112.60
1	H	252	ALA	CA-C-N	8.11	131.81	120.29
1	H	252	ALA	C-N-CA	8.11	131.81	120.29
1	D	16	LYS	CA-C-O	8.11	128.06	119.14
1	D	267	ASN	CA-CB-CG	8.10	120.70	112.60
1	C	225	ASP	CA-CB-CG	8.09	120.69	112.60
1	C	66	ASN	CA-CB-CG	-8.09	104.51	112.60
1	G	242	GLU	CA-C-O	-8.06	112.00	120.55
1	F	71	PHE	CA-CB-CG	8.06	121.86	113.80
1	F	122	GLU	CB-CA-C	-8.06	97.92	110.81
1	E	198	LEU	O-C-N	8.06	127.60	121.88
1	E	298	ILE	N-CA-C	8.05	120.14	107.98
1	D	303	GLU	O-C-N	8.04	132.49	122.84
1	G	153	LEU	N-CA-C	-8.03	98.34	110.07
1	A	104	GLU	CB-CG-CD	8.02	126.23	112.60
1	F	98	ALA	CA-C-N	8.00	134.67	121.39
1	F	98	ALA	C-N-CA	8.00	134.67	121.39
1	C	329	PHE	CA-C-O	7.98	129.22	120.92
1	C	70	VAL	N-CA-C	-7.97	101.08	111.05
1	E	97	GLY	CA-C-N	7.97	133.28	121.72
1	E	97	GLY	C-N-CA	7.97	133.28	121.72
1	E	215	VAL	O-C-N	7.97	129.41	122.16
1	F	220	GLU	CA-C-O	7.97	131.35	122.03
1	F	266	GLU	N-CA-C	7.97	119.97	111.28
1	B	277	ASP	CA-CB-CG	-7.97	104.63	112.60
1	B	186	HIS	CA-CB-CG	-7.95	105.85	113.80
1	F	106	ARG	NE-CZ-NH2	7.94	126.35	119.20
1	E	212	ARG	CD-NE-CZ	7.93	135.50	124.40
1	B	222	ALA	N-CA-C	-7.92	102.59	111.07
1	B	113	ASN	CA-C-O	-7.92	110.86	119.97
1	H	261	ALA	N-CA-C	-7.92	102.60	111.07
1	B	313	ARG	O-C-N	7.91	132.51	122.23
1	H	315	HIS	CA-CB-CG	-7.91	105.89	113.80
1	A	279	LEU	CA-C-O	-7.90	109.22	120.51
1	E	182	PRO	N-CA-C	-7.90	102.99	113.65
1	C	206	ILE	CB-CA-C	7.89	121.25	110.99
1	E	211	ILE	O-C-N	7.88	130.10	121.90
1	D	167	THR	O-C-N	7.88	130.47	122.12
1	D	269	ILE	CB-CA-C	7.88	123.23	111.26
1	F	287	ILE	CB-CA-C	7.87	122.50	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	230	PHE	CA-CB-CG	-7.86	105.94	113.80
1	E	102	PRO	N-CA-C	-7.86	98.71	111.21
1	C	189	ILE	N-CA-CB	7.85	121.65	112.15
1	H	87	ARG	NE-CZ-NH2	-7.85	112.14	119.20
1	F	66	ASN	CA-CB-CG	-7.85	104.75	112.60
1	D	233	VAL	O-C-N	7.84	130.02	121.94
1	H	186	HIS	CA-CB-CG	-7.83	105.97	113.80
1	C	101	LYS	O-C-N	7.82	128.42	120.99
1	D	220	GLU	CA-C-N	7.81	136.46	121.54
1	D	220	GLU	C-N-CA	7.81	136.46	121.54
1	B	132	LEU	CA-CB-CG	7.81	143.63	116.30
1	F	104	GLU	CA-CB-CG	7.81	129.71	114.10
1	A	220	GLU	CA-C-N	7.80	136.44	121.54
1	A	220	GLU	C-N-CA	7.80	136.44	121.54
1	H	221	GLU	O-C-N	7.80	132.96	122.59
1	F	133	PHE	CA-CB-CG	7.79	121.59	113.80
1	E	321	LEU	O-C-N	7.79	130.50	122.09
1	H	66	ASN	CA-CB-CG	-7.77	104.83	112.60
1	F	228	ARG	CG-CD-NE	7.77	129.10	112.00
1	C	158	VAL	O-C-N	7.77	131.30	122.99
1	C	257	ARG	NE-CZ-NH1	-7.77	113.73	121.50
1	H	232	ASN	OD1-CG-ND2	7.76	130.37	122.60
1	B	252	ALA	CA-C-O	-7.75	111.06	119.97
1	E	34	SER	N-CA-C	-7.74	102.78	111.14
1	D	158	VAL	CB-CA-C	7.74	119.93	110.73
1	H	260	ARG	NE-CZ-NH1	-7.73	113.77	121.50
1	H	113	ASN	CA-C-O	-7.72	112.37	120.55
1	E	327	ARG	CA-CB-CG	7.71	129.53	114.10
1	F	101	LYS	O-C-N	7.70	131.35	121.34
1	C	54	ASN	CA-CB-CG	7.70	120.30	112.60
1	H	66	ASN	OD1-CG-ND2	7.69	130.29	122.60
1	D	167	THR	CA-C-O	-7.68	112.41	120.55
1	E	122	GLU	N-CA-C	7.67	120.61	111.33
1	G	121	VAL	CA-C-N	-7.67	110.20	120.63
1	G	121	VAL	C-N-CA	-7.67	110.20	120.63
1	E	22	ARG	NE-CZ-NH1	-7.67	113.83	121.50
1	G	55	GLU	O-C-N	7.67	129.97	122.07
1	C	325	LEU	N-CA-C	-7.66	102.87	111.07
1	E	170	PHE	CA-CB-CG	7.65	121.45	113.80
1	D	113	ASN	N-CA-C	7.65	120.73	111.40
1	C	170	PHE	CA-CB-CG	7.64	121.44	113.80
1	C	87	ARG	CD-NE-CZ	7.63	135.08	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ARG	NE-CZ-NH1	-7.61	113.89	121.50
1	A	314	PHE	CA-CB-CG	-7.61	106.19	113.80
1	B	97	GLY	N-CA-C	7.61	119.80	112.04
1	G	311	LYS	CA-C-O	7.61	128.72	120.20
1	H	221	GLU	N-CA-C	-7.60	94.60	110.80
1	A	208	VAL	N-CA-C	-7.60	105.44	112.43
1	D	192	GLU	CB-CG-CD	7.60	125.53	112.60
1	G	314	PHE	CA-CB-CG	-7.59	106.21	113.80
1	H	234	ARG	CD-NE-CZ	7.59	135.03	124.40
1	E	188	TYR	CA-CB-CG	7.59	127.56	113.90
1	F	76	VAL	CA-C-O	-7.58	114.12	121.63
1	G	330	THR	N-CA-CB	7.58	124.39	111.50
1	E	327	ARG	NE-CZ-NH2	7.58	126.02	119.20
1	A	16	LYS	N-CA-C	-7.57	104.07	113.38
1	G	235	ASP	CA-CB-CG	7.57	120.17	112.60
1	G	181	ALA	CB-CA-C	7.56	121.47	109.52
1	F	283	ARG	NE-CZ-NH1	-7.56	113.94	121.50
1	C	65	PHE	CA-CB-CG	-7.54	106.25	113.80
1	B	324	VAL	O-C-N	7.53	129.29	121.91
1	E	148	TRP	CA-C-N	7.53	130.59	120.65
1	E	148	TRP	C-N-CA	7.53	130.59	120.65
1	B	203	GLN	N-CA-CB	-7.53	99.92	111.66
1	F	289	VAL	CB-CA-C	7.53	125.06	111.36
1	C	212	ARG	NE-CZ-NH1	7.52	129.02	121.50
1	C	70	VAL	N-CA-CB	7.50	123.48	110.65
1	A	131	GLY	N-CA-C	-7.50	103.79	112.79
1	B	279	LEU	CA-C-O	-7.50	112.52	120.92
1	B	52	ASP	CA-CB-CG	-7.49	105.11	112.60
1	A	203	GLN	N-CA-CB	-7.49	100.43	111.51
1	B	194	GLY	O-C-N	7.48	130.01	123.80
1	B	205	TYR	CA-C-N	7.47	130.06	122.96
1	B	205	TYR	C-N-CA	7.47	130.06	122.96
1	H	44	ILE	CA-C-O	-7.46	112.18	120.46
1	A	281	GLY	N-CA-C	-7.46	102.84	115.08
1	C	82	ASP	CA-CB-CG	7.45	120.05	112.60
1	B	90	ASP	CA-CB-CG	-7.44	105.16	112.60
1	E	102	PRO	CB-CA-C	7.44	120.75	111.23
1	H	30	PHE	CA-CB-CG	-7.44	106.36	113.80
1	C	176	GLU	CB-CG-CD	7.41	125.20	112.60
1	H	116	ILE	CB-CA-C	-7.41	102.00	112.22
1	A	25	VAL	O-C-N	7.41	131.25	123.03
1	H	277	ASP	CB-CA-C	7.40	122.73	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ASP	CA-CB-CG	-7.40	105.20	112.60
1	E	227	GLU	CA-C-O	7.39	128.39	120.55
1	G	122	GLU	CA-CB-CG	-7.39	99.32	114.10
1	B	282	GLU	CA-CB-CG	7.38	128.87	114.10
1	A	208	VAL	O-C-N	7.38	130.13	122.09
1	C	265	ASN	OD1-CG-ND2	7.36	129.96	122.60
1	B	32	GLY	O-C-N	7.36	129.25	122.18
1	F	293	ILE	CA-C-O	-7.36	112.14	121.48
1	F	17	ASN	CA-CB-CG	-7.35	105.25	112.60
1	A	215	VAL	N-CA-C	-7.35	104.18	113.22
1	F	70	VAL	N-CA-CB	7.34	127.81	111.50
1	G	58	ALA	CA-C-N	7.34	129.84	120.88
1	G	58	ALA	C-N-CA	7.34	129.84	120.88
1	D	120	ILE	O-C-N	7.33	129.88	121.96
1	B	314	PHE	N-CA-C	-7.33	102.98	110.97
1	H	65	PHE	CA-CB-CG	7.33	121.13	113.80
1	D	156	GLU	CA-CB-CG	7.33	128.75	114.10
1	D	131	GLY	N-CA-C	-7.32	102.32	112.13
1	B	195	ASP	N-CA-C	7.32	119.26	111.28
1	D	193	HIS	N-CA-CB	7.32	120.85	110.46
1	D	206	ILE	N-CA-C	-7.31	95.65	107.28
1	B	72	ALA	N-CA-C	-7.31	99.43	110.39
1	A	271	THR	N-CA-CB	7.30	121.30	110.49
1	G	99	ASN	CB-CA-C	7.30	121.85	109.50
1	B	169	ARG	CD-NE-CZ	-7.29	114.19	124.40
1	G	284	ASP	N-CA-CB	-7.29	100.62	111.71
1	A	199	PRO	CA-C-N	7.29	128.50	121.65
1	A	199	PRO	C-N-CA	7.29	128.50	121.65
1	D	265	ASN	CA-CB-CG	7.29	119.89	112.60
1	G	283	ARG	O-C-N	7.27	131.46	123.10
1	A	16	LYS	CA-C-O	7.26	127.43	119.15
1	D	209	MET	CA-C-O	-7.26	114.57	119.29
1	F	203	GLN	CA-C-N	7.25	132.41	122.77
1	F	203	GLN	C-N-CA	7.25	132.41	122.77
1	E	229	ILE	N-CA-CB	7.24	119.53	110.47
1	A	286	TYR	N-CA-C	-7.24	97.44	109.46
1	B	170	PHE	CA-CB-CG	7.24	121.04	113.80
1	H	114	ILE	O-C-N	7.23	129.17	121.87
1	D	98	ALA	CA-C-O	7.23	128.93	120.69
1	D	25	VAL	O-C-N	7.23	132.51	122.97
1	F	260	ARG	O-C-N	7.21	131.99	122.33
1	G	16	LYS	N-CA-C	-7.21	104.22	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	150	PHE	O-C-N	7.20	131.75	122.39
1	G	191	GLY	N-CA-C	-7.20	99.86	112.53
1	D	211	ILE	CB-CA-C	-7.19	102.62	112.04
1	F	54	ASN	CA-CB-CG	7.19	119.79	112.60
1	B	313	ARG	CA-C-N	-7.18	111.17	120.65
1	B	313	ARG	C-N-CA	-7.18	111.17	120.65
1	E	118	ARG	O-C-N	7.18	129.73	122.12
1	E	283	ARG	NE-CZ-NH2	-7.17	112.75	119.20
1	C	37	PHE	CA-CB-CG	7.17	120.97	113.80
1	C	76	VAL	CA-C-O	-7.17	112.97	120.64
1	B	282	GLU	CB-CG-CD	7.17	124.78	112.60
1	G	289	VAL	N-CA-CB	-7.17	101.18	111.21
1	A	100	GLN	OE1-CD-NE2	7.16	129.76	122.60
1	H	55	GLU	CA-C-N	7.16	130.74	120.79
1	H	55	GLU	C-N-CA	7.16	130.74	120.79
1	C	310	GLU	CB-CG-CD	7.16	124.77	112.60
1	A	114	ILE	CA-C-O	7.15	128.49	121.05
1	D	176	GLU	CB-CG-CD	7.15	124.76	112.60
1	H	251	ILE	N-CA-C	-7.15	102.85	110.36
1	B	225	ASP	CA-CB-CG	-7.15	105.45	112.60
1	E	193	HIS	N-CA-CB	7.15	122.29	110.42
1	F	72	ALA	CA-C-N	7.14	126.67	119.24
1	F	72	ALA	C-N-CA	7.14	126.67	119.24
1	D	184	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	D	149	LYS	CB-CA-C	-7.13	99.63	110.90
1	F	108	ASP	CA-CB-CG	-7.13	105.47	112.60
1	F	114	ILE	N-CA-C	-7.12	103.84	110.53
1	F	150	PHE	CA-CB-CG	7.12	120.92	113.80
1	F	222	ALA	O-C-N	7.12	129.69	122.08
1	G	282	GLU	CA-C-O	7.12	129.74	121.49
1	C	137	THR	CA-C-O	-7.11	113.33	121.15
1	A	44	ILE	CA-C-O	-7.10	112.58	120.46
1	A	70	VAL	N-CA-C	-7.10	102.64	112.50
1	D	63	MET	N-CA-C	-7.10	103.23	110.97
1	G	77	ASP	CA-CB-CG	7.09	119.69	112.60
1	F	178	PHE	CA-CB-CG	-7.09	106.71	113.80
1	H	16	LYS	CA-C-O	7.08	127.85	119.56
1	H	301	VAL	N-CA-C	-7.06	98.29	108.53
1	A	234	ARG	NE-CZ-NH1	-7.05	114.45	121.50
1	D	64	ASP	CA-CB-CG	7.05	119.66	112.60
1	D	190	ILE	CB-CA-C	7.05	121.20	110.91
1	H	63	MET	N-CA-CB	7.05	120.56	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	ALA	CA-C-N	7.04	129.31	120.72
1	D	58	ALA	C-N-CA	7.04	129.31	120.72
1	E	190	ILE	CA-C-O	-7.04	114.74	121.64
1	D	308	ASP	O-C-N	7.04	129.58	122.12
1	A	37	PHE	CA-CB-CG	-7.03	106.77	113.80
1	B	184	ASN	CA-CB-CG	7.03	119.63	112.60
1	D	189	ILE	N-CA-C	-7.03	98.00	108.12
1	C	283	ARG	CA-C-O	7.03	128.86	120.99
1	E	317	SER	O-C-N	7.03	129.60	122.08
1	G	167	THR	O-C-N	7.02	129.56	122.12
1	F	93	VAL	CA-C-O	-7.01	113.07	120.57
1	H	203	GLN	CA-CB-CG	7.01	128.11	114.10
1	B	154	PRO	CB-CA-C	7.00	120.53	111.21
1	H	60	GLY	CA-C-N	7.00	129.54	120.44
1	H	60	GLY	C-N-CA	7.00	129.54	120.44
1	A	292	VAL	CB-CA-C	-7.00	103.72	111.35
1	D	234	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	H	141	ASP	CA-C-N	6.99	129.44	120.70
1	H	141	ASP	C-N-CA	6.99	129.44	120.70
1	C	100	GLN	CA-C-O	6.99	129.50	121.47
1	F	110	VAL	CA-C-O	-6.98	114.15	121.41
1	B	206	ILE	N-CA-C	-6.98	95.88	106.42
1	E	201	TRP	O-C-N	6.96	130.83	122.27
1	F	305	GLU	CA-CB-CG	6.95	128.01	114.10
1	E	280	TYR	CA-CB-CG	6.95	126.41	113.90
1	B	64	ASP	CB-CA-C	6.95	121.79	110.88
1	H	182	PRO	N-CA-C	-6.94	103.41	113.75
1	D	59	ILE	N-CA-C	6.93	116.94	110.42
1	G	304	ILE	N-CA-C	-6.93	102.50	110.05
1	H	319	ALA	N-CA-C	-6.93	102.57	111.02
1	H	124	VAL	O-C-N	6.92	130.38	121.94
1	E	300	GLU	CB-CA-C	-6.92	98.81	110.43
1	A	193	HIS	N-CA-CB	6.92	119.91	110.57
1	H	289	VAL	N-CA-CB	-6.91	104.24	111.64
1	A	134	LEU	CB-CA-C	6.91	121.05	110.62
1	B	17	ASN	OD1-CG-ND2	6.90	129.50	122.60
1	E	165	LEU	O-C-N	6.90	129.21	122.03
1	D	148	TRP	CA-C-N	6.89	129.81	120.44
1	D	148	TRP	C-N-CA	6.89	129.81	120.44
1	E	56	SER	O-C-N	6.89	129.45	122.08
1	H	313	ARG	NE-CZ-NH1	-6.88	114.62	121.50
1	E	108	ASP	N-CA-C	-6.88	104.75	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	ALA	CA-C-O	6.88	128.72	120.81
1	E	98	ALA	N-CA-C	6.88	119.78	109.25
1	H	215	VAL	N-CA-C	-6.88	105.64	112.17
1	C	158	VAL	CA-C-O	-6.88	112.92	120.48
1	C	314	PHE	N-CA-C	-6.88	103.40	111.03
1	C	101	LYS	CB-CA-C	6.87	120.27	109.96
1	D	180	VAL	CA-C-O	-6.87	114.83	121.63
1	C	17	ASN	CA-CB-CG	-6.87	105.73	112.60
1	H	23	VAL	CA-C-O	-6.86	113.18	120.39
1	H	300	GLU	CB-CA-C	-6.86	98.90	110.43
1	F	135	VAL	N-CA-C	6.86	118.17	108.36
1	G	193	HIS	N-CA-C	-6.86	96.59	108.52
1	A	211	ILE	O-C-N	6.85	129.03	121.90
1	C	80	HIS	CA-C-O	-6.85	113.25	120.58
1	H	198	LEU	O-C-N	6.85	126.10	121.71
1	F	70	VAL	O-C-N	6.85	131.57	122.12
1	B	98	ALA	CA-C-N	6.85	131.21	121.42
1	B	98	ALA	C-N-CA	6.85	131.21	121.42
1	A	226	LEU	CB-CA-C	6.84	123.21	110.70
1	F	208	VAL	O-C-N	6.84	131.00	122.11
1	E	239	GLN	CA-C-N	6.83	130.12	120.42
1	E	239	GLN	C-N-CA	6.83	130.12	120.42
1	E	289	VAL	CA-C-O	-6.82	110.81	119.95
1	D	215	VAL	CA-C-O	-6.82	112.26	120.78
1	D	314	PHE	N-CA-C	-6.82	103.78	111.07
1	C	133	PHE	CA-CB-CG	6.81	120.61	113.80
1	F	294	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	C	84	ASP	N-CA-C	-6.81	103.65	112.23
1	H	184	ASN	O-C-N	6.81	130.48	122.24
1	A	209	MET	CA-C-O	6.81	125.08	119.36
1	F	86	CYS	CA-C-N	-6.81	111.59	120.44
1	F	86	CYS	C-N-CA	-6.81	111.59	120.44
1	F	267	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	B	192	GLU	CB-CG-CD	6.80	124.16	112.60
1	D	36	VAL	CA-C-O	-6.80	114.20	121.27
1	E	169	ARG	CA-C-N	6.80	129.28	120.44
1	E	169	ARG	C-N-CA	6.80	129.28	120.44
1	D	97	GLY	N-CA-C	6.79	120.39	111.70
1	B	307	ASN	N-CA-C	-6.79	102.06	110.41
1	F	247	THR	CA-C-O	-6.79	113.22	121.36
1	D	248	TYR	CA-C-O	-6.77	110.82	120.51
1	A	306	LEU	O-C-N	6.77	132.19	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	243	LYS	N-CA-C	-6.77	103.92	112.93
1	C	193	HIS	N-CA-CB	6.77	120.44	110.49
1	D	189	ILE	N-CA-CB	6.77	121.40	111.52
1	C	54	ASN	O-C-N	6.76	131.80	123.01
1	B	72	ALA	CA-C-O	-6.75	113.32	120.88
1	H	213	LYS	CA-C-O	6.75	130.16	120.51
1	G	123	SER	CA-C-O	-6.75	112.64	120.20
1	E	106	ARG	NE-CZ-NH2	6.74	125.27	119.20
1	F	176	GLU	CB-CG-CD	6.74	124.06	112.60
1	A	194	GLY	CA-C-O	-6.74	115.72	121.04
1	G	102	PRO	N-CA-C	-6.73	99.94	110.50
1	A	214	LEU	CA-C-O	6.73	128.21	120.00
1	B	98	ALA	CA-C-O	6.72	128.54	120.81
1	H	276	LEU	N-CA-CB	-6.72	100.02	110.57
1	H	57	LYS	N-CA-C	-6.71	103.66	110.97
1	F	85	ASP	CA-CB-CG	6.70	119.30	112.60
1	G	249	TYR	N-CA-C	6.70	119.41	111.71
1	E	182	PRO	CB-CA-C	6.70	122.66	112.21
1	H	171	ARG	CA-CB-CG	-6.70	100.70	114.10
1	H	115	ALA	CA-C-O	-6.70	113.79	120.82
1	C	304	ILE	CA-C-O	-6.69	115.41	121.97
1	H	97	GLY	N-CA-C	6.69	123.41	112.84
1	E	297	GLY	N-CA-C	-6.69	100.58	112.22
1	F	299	ARG	N-CA-C	-6.69	103.92	111.14
1	D	44	ILE	CA-C-O	-6.69	112.42	120.78
1	B	237	ALA	CA-C-N	6.68	130.46	120.31
1	B	237	ALA	C-N-CA	6.68	130.46	120.31
1	B	82	ASP	CA-CB-CG	6.68	119.28	112.60
1	C	21	ALA	N-CA-C	-6.67	98.38	109.46
1	H	193	HIS	N-CA-CB	6.67	119.94	110.46
1	H	158	VAL	N-CA-C	-6.67	98.12	107.80
1	A	179	SER	CA-C-N	6.67	132.16	122.69
1	A	179	SER	C-N-CA	6.67	132.16	122.69
1	D	201	TRP	O-C-N	6.67	129.19	122.12
1	E	79	TRP	O-C-N	6.67	130.63	123.56
1	C	52	ASP	CA-C-O	-6.67	112.99	120.66
1	F	301	VAL	N-CA-CB	6.66	118.99	110.99
1	B	148	TRP	N-CA-C	-6.66	103.72	110.97
1	D	166	ASP	CA-CB-CG	6.66	119.25	112.60
1	G	192	GLU	CA-C-O	6.66	128.51	121.19
1	E	150	PHE	CA-C-N	6.65	131.99	120.68
1	E	150	PHE	C-N-CA	6.65	131.99	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	LEU	CA-C-O	-6.65	113.78	120.90
1	F	170	PHE	CA-C-N	6.65	129.19	120.28
1	F	170	PHE	C-N-CA	6.65	129.19	120.28
1	A	297	GLY	N-CA-C	-6.64	102.35	112.84
1	F	17	ASN	O-C-N	6.64	129.68	122.64
1	F	225	ASP	CA-CB-CG	-6.64	105.96	112.60
1	H	61	ASP	CA-C-O	-6.64	113.84	120.82
1	H	300	GLU	CA-CB-CG	6.64	127.38	114.10
1	F	200	VAL	CA-C-O	6.64	129.07	120.78
1	G	289	VAL	CB-CA-C	6.64	123.44	111.36
1	H	112	LYS	CA-C-N	6.63	129.17	120.28
1	H	112	LYS	C-N-CA	6.63	129.17	120.28
1	H	181	ALA	CA-C-O	-6.63	113.58	120.02
1	A	175	GLY	CA-C-O	-6.63	113.84	121.00
1	G	208	VAL	O-C-N	6.63	128.61	121.78
1	F	161	SER	CA-CB-OG	6.62	124.35	111.10
1	H	87	ARG	NE-CZ-NH1	6.62	128.12	121.50
1	H	276	LEU	N-CA-C	6.62	119.72	109.07
1	C	229	ILE	O-C-N	6.61	128.75	121.94
1	B	242	GLU	N-CA-C	6.61	119.48	111.82
1	F	100	GLN	CB-CA-C	-6.60	99.08	109.84
1	F	101	LYS	N-CA-C	-6.60	101.51	110.36
1	C	253	MET	N-CA-CB	6.60	120.03	110.20
1	E	37	PHE	CB-CA-C	6.60	121.33	110.90
1	H	80	HIS	CA-CB-CG	6.60	120.40	113.80
1	C	140	VAL	CA-C-O	-6.59	112.54	120.78
1	C	65	PHE	CA-C-N	6.58	129.40	120.38
1	C	65	PHE	C-N-CA	6.58	129.40	120.38
1	H	106	ARG	NE-CZ-NH1	-6.58	114.92	121.50
1	D	29	GLY	N-CA-C	-6.58	103.07	112.55
1	G	268	ALA	CA-C-N	-6.58	114.31	122.93
1	G	268	ALA	C-N-CA	-6.58	114.31	122.93
1	H	273	SER	N-CA-CB	6.58	119.78	110.24
1	H	247	THR	CB-CA-C	6.57	121.74	109.71
1	H	42	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	D	114	ILE	CA-C-N	6.57	129.92	120.79
1	D	114	ILE	C-N-CA	6.57	129.92	120.79
1	G	212	ARG	CA-CB-CG	6.57	127.23	114.10
1	A	125	MET	CA-CB-CG	6.57	127.23	114.10
1	A	133	PHE	N-CA-CB	6.56	121.26	110.69
1	F	189	ILE	N-CA-CB	6.56	121.10	111.52
1	B	239	GLN	N-CA-C	-6.55	104.22	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	312	ASN	CA-CB-CG	-6.55	106.05	112.60
1	F	88	ASP	O-C-N	6.55	130.75	122.37
1	D	260	ARG	NE-CZ-NH1	-6.54	114.95	121.50
1	A	206	ILE	CA-C-O	-6.54	113.90	120.31
1	A	100	GLN	N-CA-C	-6.54	100.60	110.28
1	C	157	ARG	CD-NE-CZ	-6.54	115.25	124.40
1	C	281	GLY	N-CA-C	-6.53	106.22	115.43
1	F	34	SER	N-CA-C	-6.53	104.20	111.71
1	F	100	GLN	OE1-CD-NE2	6.53	129.13	122.60
1	A	159	ILE	CA-C-O	-6.53	112.73	121.02
1	H	211	ILE	N-CA-CB	6.53	117.47	110.62
1	A	166	ASP	CA-CB-CG	6.52	119.12	112.60
1	D	52	ASP	CA-CB-CG	6.52	119.12	112.60
1	G	83	TYR	CA-CB-CG	-6.52	102.16	113.90
1	C	232	ASN	OD1-CG-ND2	6.50	129.10	122.60
1	F	321	LEU	CA-C-N	6.50	129.28	120.38
1	F	321	LEU	C-N-CA	6.50	129.28	120.38
1	C	327	ARG	CA-C-N	-6.49	112.04	122.62
1	C	327	ARG	C-N-CA	-6.49	112.04	122.62
1	A	212	ARG	O-C-N	6.49	130.95	122.38
1	D	37	PHE	CA-CB-CG	6.49	120.29	113.80
1	B	216	GLU	O-C-N	6.48	128.99	122.12
1	A	292	VAL	CA-C-O	-6.47	112.53	120.69
1	D	128	GLY	N-CA-C	-6.47	105.98	115.63
1	F	153	LEU	CA-C-O	-6.47	113.91	120.96
1	H	240	ILE	CB-CA-C	-6.46	103.30	112.22
1	H	283	ARG	CD-NE-CZ	6.45	133.44	124.40
1	E	307	ASN	N-CA-C	-6.45	100.97	110.52
1	F	267	ASN	CB-CA-C	6.45	123.25	110.42
1	H	170	PHE	CA-C-N	6.45	128.92	120.28
1	H	170	PHE	C-N-CA	6.45	128.92	120.28
1	B	247	THR	CB-CA-C	6.45	120.39	109.50
1	E	190	ILE	O-C-N	6.45	130.11	122.95
1	F	253	MET	N-CA-C	-6.45	104.33	111.36
1	G	21	ALA	CA-C-N	-6.44	114.04	123.05
1	G	21	ALA	C-N-CA	-6.44	114.04	123.05
1	F	313	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	A	161	SER	CA-C-O	6.43	127.28	119.31
1	G	117	PHE	O-C-N	6.43	129.04	122.09
1	D	307	ASN	N-CA-C	-6.43	101.27	110.59
1	E	260	ARG	CA-CB-CG	6.43	126.96	114.10
1	F	279	LEU	N-CA-C	6.43	121.92	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	244	LYS	CA-CB-CG	6.43	126.95	114.10
1	G	44	ILE	CA-C-O	-6.42	112.67	121.15
1	G	235	ASP	O-C-N	6.42	130.00	122.24
1	H	89	ALA	CB-CA-C	6.42	120.48	109.51
1	A	307	ASN	N-CA-C	-6.41	101.89	110.55
1	A	17	ASN	CA-CB-CG	-6.40	106.20	112.60
1	D	57	LYS	N-CA-C	-6.40	103.99	110.97
1	E	100	GLN	CA-C-N	6.40	130.41	120.68
1	E	100	GLN	C-N-CA	6.40	130.41	120.68
1	A	233	VAL	CB-CA-C	6.40	120.39	111.94
1	B	266	GLU	CA-CB-CG	6.39	126.89	114.10
1	A	281	GLY	O-C-N	6.39	129.91	122.30
1	H	85	ASP	O-C-N	6.39	129.70	122.22
1	F	201	TRP	O-C-N	6.39	128.99	122.09
1	A	289	VAL	N-CA-CB	-6.39	102.27	111.21
1	G	182	PRO	N-CA-C	-6.38	104.66	113.53
1	G	145	TYR	N-CA-C	-6.38	104.01	110.97
1	A	299	ARG	NH1-CZ-NH2	6.38	127.59	119.30
1	G	92	VAL	CB-CA-C	6.37	119.28	110.99
1	B	205	TYR	CA-CB-CG	-6.37	102.43	113.90
1	H	49	VAL	CA-C-O	-6.36	113.74	120.48
1	B	321	LEU	O-C-N	6.36	128.88	122.08
1	A	175	GLY	O-C-N	6.35	128.28	122.18
1	E	77	ASP	CA-CB-CG	6.35	118.95	112.60
1	H	165	LEU	CA-C-O	6.35	127.29	119.79
1	H	255	LEU	CB-CA-C	6.35	120.80	110.95
1	A	320	THR	CA-C-N	6.35	129.07	120.44
1	A	320	THR	C-N-CA	6.35	129.07	120.44
1	B	287	ILE	CA-C-O	6.34	128.71	120.78
1	E	312	ASN	N-CA-C	6.34	118.76	111.02
1	H	226	LEU	CB-CA-C	6.34	122.31	110.70
1	F	115	ALA	CA-C-N	6.34	129.14	120.46
1	F	115	ALA	C-N-CA	6.34	129.14	120.46
1	D	314	PHE	O-C-N	6.33	128.59	122.07
1	C	283	ARG	CD-NE-CZ	-6.33	115.54	124.40
1	F	271	THR	N-CA-CB	6.33	119.85	110.49
1	F	321	LEU	CB-CA-C	6.32	120.97	110.92
1	H	98	ALA	N-CA-C	6.32	119.95	109.46
1	G	33	ALA	O-C-N	6.32	131.12	122.46
1	F	211	ILE	N-CA-C	-6.32	104.17	110.30
1	A	302	ILE	N-CA-CB	6.31	118.59	111.21
1	B	128	GLY	N-CA-C	-6.31	98.23	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	69	LYS	N-CA-C	6.31	120.07	112.38
1	D	244	LYS	CA-CB-CG	6.30	126.70	114.10
1	A	88	ASP	N-CA-C	6.30	120.97	113.16
1	G	260	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	B	189	ILE	N-CA-CB	6.30	120.10	111.41
1	H	313	ARG	CG-CD-NE	-6.30	98.15	112.00
1	B	124	VAL	O-C-N	6.29	128.31	121.83
1	B	235	ASP	CA-CB-CG	6.29	118.89	112.60
1	F	283	ARG	CD-NE-CZ	-6.29	115.59	124.40
1	B	153	LEU	CA-CB-CG	6.28	138.29	116.30
1	H	23	VAL	O-C-N	6.28	130.04	123.26
1	A	129	PHE	CA-C-O	6.28	128.20	121.55
1	B	75	PRO	CA-C-N	6.27	131.60	122.69
1	B	75	PRO	C-N-CA	6.27	131.60	122.69
1	H	298	ILE	N-CA-C	6.27	117.12	108.84
1	C	189	ILE	CB-CG1-CD1	6.27	126.96	113.80
1	D	313	ARG	NE-CZ-NH1	-6.27	115.23	121.50
1	A	182	PRO	N-CA-C	-6.26	104.42	113.75
1	E	39	LEU	CA-C-O	6.26	127.39	120.63
1	E	299	ARG	CA-C-O	-6.26	114.25	120.70
1	E	329	PHE	CA-C-O	6.26	128.81	121.11
1	H	195	ASP	N-CA-C	6.26	118.11	111.28
1	A	312	ASN	N-CA-C	6.25	118.17	111.36
1	C	153	LEU	N-CA-C	-6.25	100.83	110.58
1	F	63	MET	CA-C-N	6.25	128.66	120.28
1	F	63	MET	C-N-CA	6.25	128.66	120.28
1	D	209	MET	CB-CA-C	6.25	117.27	110.08
1	F	261	ALA	O-C-N	6.25	128.50	122.07
1	D	312	ASN	N-CA-C	6.25	117.89	111.14
1	H	114	ILE	N-CA-C	-6.24	103.25	111.05
1	D	26	ILE	N-CA-CB	6.24	119.21	111.41
1	E	100	GLN	CA-CB-CG	6.23	126.56	114.10
1	G	180	VAL	CA-C-O	-6.23	115.46	121.63
1	C	52	ASP	O-C-N	6.23	130.87	123.27
1	B	169	ARG	NE-CZ-NH1	-6.22	115.28	121.50
1	H	84	ASP	CB-CA-C	6.22	123.32	110.31
1	D	160	GLY	CA-C-O	-6.22	114.84	120.94
1	F	227	GLU	CB-CG-CD	6.22	123.17	112.60
1	F	176	GLU	N-CA-CB	6.22	119.09	110.07
1	G	312	ASN	OD1-CG-ND2	6.22	128.82	122.60
1	E	166	ASP	CA-CB-CG	6.21	118.81	112.60
1	F	99	ASN	N-CA-CB	-6.21	100.84	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	GLY	N-CA-C	-6.21	102.04	111.42
1	F	18	ASN	N-CA-C	6.21	120.22	111.52
1	F	148	TRP	N-CA-C	-6.21	103.82	111.40
1	H	192	GLU	CB-CG-CD	6.21	123.15	112.60
1	A	205	TYR	CA-C-N	6.20	131.67	123.11
1	A	205	TYR	C-N-CA	6.20	131.67	123.11
1	H	313	ARG	O-C-N	6.20	128.69	122.12
1	G	96	ALA	O-C-N	6.20	130.00	123.06
1	A	18	ASN	O-C-N	6.20	130.89	123.33
1	B	317	SER	CA-C-O	6.20	127.33	120.82
1	B	87	ARG	NE-CZ-NH1	-6.19	115.31	121.50
1	B	175	GLY	N-CA-C	-6.19	105.04	113.27
1	E	189	ILE	N-CA-C	-6.19	99.56	108.48
1	F	145	TYR	CA-C-N	6.19	128.90	120.54
1	F	145	TYR	C-N-CA	6.19	128.90	120.54
1	D	100	GLN	CA-CB-CG	6.19	126.47	114.10
1	C	119	SER	O-C-N	6.18	128.77	122.09
1	H	328	ALA	CA-C-O	-6.18	114.77	121.20
1	H	241	ILE	CA-C-O	6.18	127.48	121.05
1	A	153	LEU	CB-CA-C	6.18	119.19	109.37
1	D	267	ASN	O-C-N	6.18	129.99	122.58
1	F	269	ILE	CA-C-O	-6.17	113.22	120.75
1	B	94	ILE	N-CA-C	6.17	117.36	107.73
1	G	183	GLN	CA-C-O	-6.17	112.02	119.49
1	A	185	VAL	O-C-N	6.17	131.11	122.97
1	A	299	ARG	NE-CZ-NH1	-6.17	115.33	121.50
1	C	265	ASN	N-CA-CB	-6.17	102.65	111.84
1	C	145	TYR	N-CA-C	-6.16	104.19	111.03
1	D	264	HIS	CA-CB-CG	-6.16	107.64	113.80
1	H	133	PHE	N-CA-CB	6.16	120.24	110.57
1	E	62	ALA	CA-C-N	6.16	128.53	120.28
1	E	62	ALA	C-N-CA	6.16	128.53	120.28
1	H	174	LEU	N-CA-C	-6.16	103.72	111.11
1	G	41	ASN	OD1-CG-ND2	6.15	128.75	122.60
1	H	157	ARG	N-CA-C	6.15	120.48	112.92
1	D	100	GLN	N-CA-CB	6.15	119.48	109.95
1	D	218	LYS	CA-C-N	6.15	133.46	121.41
1	D	218	LYS	C-N-CA	6.15	133.46	121.41
1	F	299	ARG	NE-CZ-NH1	-6.15	115.35	121.50
1	H	74	LYS	O-C-N	6.15	127.44	121.66
1	E	120	ILE	O-C-N	6.14	130.25	122.57
1	H	318	ALA	O-C-N	6.14	128.63	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	THR	CA-C-O	-6.14	112.55	119.79
1	F	327	ARG	CA-CB-CG	6.13	126.36	114.10
1	E	289	VAL	O-C-N	6.13	128.09	121.10
1	C	232	ASN	CA-C-O	-6.13	113.92	120.42
1	C	160	GLY	CA-C-O	-6.12	114.94	120.94
1	F	154	PRO	CB-CA-C	6.12	119.36	111.21
1	B	183	GLN	CA-C-O	-6.12	111.75	120.51
1	F	128	GLY	CA-C-O	6.12	125.57	118.96
1	G	307	ASN	CB-CA-C	6.12	120.54	109.83
1	D	112	LYS	CA-C-N	6.12	130.93	120.71
1	D	112	LYS	C-N-CA	6.12	130.93	120.71
1	F	70	VAL	CA-C-O	-6.11	112.18	119.58
1	F	211	ILE	O-C-N	6.11	128.23	121.94
1	G	117	PHE	CA-C-O	-6.11	114.41	120.70
1	H	210	PRO	CA-C-O	-6.11	114.66	121.32
1	A	309	ASP	O-C-N	6.11	128.38	122.03
1	C	87	ARG	O-C-N	6.11	128.59	122.12
1	H	84	ASP	CA-CB-CG	-6.11	106.49	112.60
1	H	163	THR	CB-CA-C	-6.11	100.25	110.81
1	G	164	ILE	CA-C-O	-6.10	114.60	120.95
1	A	124	VAL	CA-C-O	-6.10	114.71	121.17
1	F	295	ARG	CD-NE-CZ	6.10	132.94	124.40
1	D	153	LEU	N-CA-C	-6.10	103.12	110.13
1	E	209	MET	CA-C-O	6.09	124.15	119.46
1	F	120	ILE	CA-C-O	-6.09	114.71	121.17
1	G	55	GLU	N-CA-CB	6.09	118.84	110.01
1	H	297	GLY	O-C-N	6.09	128.77	122.86
1	A	63	MET	O-C-N	6.09	128.61	122.03
1	F	67	HIS	N-CA-CB	6.09	119.17	110.16
1	G	31	VAL	CB-CA-C	6.08	120.36	112.14
1	B	67	HIS	CA-CB-CG	-6.08	107.72	113.80
1	A	36	VAL	O-C-N	6.08	128.01	121.87
1	B	129	PHE	CA-CB-CG	-6.08	107.72	113.80
1	H	81	GLY	CA-C-N	6.08	131.84	121.87
1	H	81	GLY	C-N-CA	6.08	131.84	121.87
1	A	212	ARG	CA-C-O	-6.07	115.06	122.41
1	D	114	ILE	CB-CA-C	6.07	120.00	112.04
1	E	194	GLY	CA-C-N	6.07	133.14	121.54
1	E	194	GLY	C-N-CA	6.07	133.14	121.54
1	B	310	GLU	CB-CG-CD	6.07	122.92	112.60
1	F	149	LYS	O-C-N	6.07	130.66	122.59
1	C	310	GLU	CA-CB-CG	6.07	126.24	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	GLU	CA-C-O	6.07	129.19	120.51
1	H	240	ILE	N-CA-CB	6.07	119.68	110.58
1	F	158	VAL	O-C-N	6.07	130.15	122.57
1	C	245	GLY	N-CA-C	6.06	122.29	115.08
1	B	137	THR	CA-C-O	-6.06	114.49	121.15
1	E	93	VAL	CB-CA-C	6.05	118.28	110.96
1	E	156	GLU	CA-CB-CG	6.05	126.20	114.10
1	G	55	GLU	CB-CA-C	-6.05	101.38	110.88
1	C	287	ILE	CA-C-O	-6.04	115.41	121.45
1	A	163	THR	CA-C-O	-6.04	112.16	119.59
1	C	74	LYS	O-C-N	6.04	129.28	122.16
1	A	55	GLU	CA-C-O	-6.03	114.48	120.82
1	E	145	TYR	CA-C-N	6.03	129.19	120.38
1	E	145	TYR	C-N-CA	6.03	129.19	120.38
1	B	321	LEU	N-CA-C	-6.03	103.67	111.02
1	C	18	ASN	N-CA-CB	-6.02	102.13	111.65
1	B	283	ARG	CA-CB-CG	6.01	126.12	114.10
1	F	253	MET	CB-CA-C	6.01	121.07	110.85
1	G	222	ALA	CB-CA-C	6.01	120.47	110.92
1	A	123	SER	N-CA-C	-6.00	104.43	110.97
1	B	91	LEU	N-CA-CB	-6.00	100.42	110.80
1	A	102	PRO	O-C-N	6.00	130.74	122.64
1	H	255	LEU	N-CA-C	-6.00	104.37	111.03
1	C	185	VAL	CA-C-O	-6.00	113.94	120.71
1	C	231	VAL	CA-C-O	6.00	127.19	120.95
1	H	111	ASP	CB-CA-C	6.00	120.29	110.88
1	H	232	ASN	CA-CB-CG	-6.00	106.61	112.60
1	A	32	GLY	N-CA-C	5.99	119.45	112.50
1	F	140	VAL	CA-CB-CG1	5.99	120.59	110.40
1	H	277	ASP	CA-C-O	5.99	133.10	121.35
1	B	87	ARG	CD-NE-CZ	-5.99	116.01	124.40
1	C	44	ILE	N-CA-C	5.99	116.96	111.81
1	D	215	VAL	CB-CA-C	5.99	121.11	111.29
1	E	76	VAL	CB-CA-C	5.99	121.26	110.48
1	E	301	VAL	CA-C-N	-5.99	115.77	123.19
1	E	301	VAL	C-N-CA	-5.99	115.77	123.19
1	F	101	LYS	CA-C-O	-5.99	114.43	120.96
1	B	212	ARG	CA-CB-CG	5.99	126.07	114.10
1	F	53	ALA	N-CA-C	-5.99	105.24	112.54
1	A	63	MET	N-CA-CB	5.98	118.65	109.98
1	C	66	ASN	N-CA-C	5.98	118.56	111.33
1	G	157	ARG	NE-CZ-NH2	5.98	124.58	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ASP	CB-CA-C	5.97	120.37	110.81
1	C	83	TYR	N-CA-C	5.97	120.04	112.87
1	H	73	PRO	N-CA-C	-5.97	105.15	113.81
1	F	304	ILE	CA-C-O	-5.97	115.44	121.59
1	C	276	LEU	CA-C-O	5.96	126.93	120.43
1	H	300	GLU	O-C-N	5.96	129.36	123.46
1	B	72	ALA	O-C-N	5.96	128.21	121.53
1	C	92	VAL	CA-C-O	5.96	127.04	120.48
1	E	234	ARG	N-CA-C	5.96	117.78	111.28
1	A	165	LEU	CA-C-N	5.95	128.85	120.28
1	A	165	LEU	C-N-CA	5.95	128.85	120.28
1	E	109	LEU	N-CA-C	5.95	120.38	113.18
1	A	214	LEU	N-CA-C	-5.95	104.18	112.45
1	E	98	ALA	CA-C-N	5.95	130.58	122.19
1	E	98	ALA	C-N-CA	5.95	130.58	122.19
1	D	249	TYR	N-CA-CB	5.95	119.25	110.33
1	H	227	GLU	CB-CA-C	-5.94	100.92	110.79
1	F	209	MET	N-CA-C	5.94	118.91	109.64
1	F	312	ASN	OD1-CG-ND2	5.94	128.54	122.60
1	C	82	ASP	O-C-N	5.94	129.34	122.99
1	H	206	ILE	N-CA-C	-5.94	97.28	106.72
1	C	221	GLU	CB-CG-CD	5.94	122.69	112.60
1	D	94	ILE	N-CA-C	5.94	116.36	107.51
1	H	255	LEU	CA-C-N	5.94	128.52	120.38
1	H	255	LEU	C-N-CA	5.94	128.52	120.38
1	F	304	ILE	O-C-N	5.94	128.92	122.57
1	D	189	ILE	CA-C-N	-5.93	115.34	123.46
1	D	189	ILE	C-N-CA	-5.93	115.34	123.46
1	B	108	ASP	CA-CB-CG	-5.93	106.67	112.60
1	E	260	ARG	CD-NE-CZ	-5.93	116.10	124.40
1	H	313	ARG	CD-NE-CZ	-5.93	116.10	124.40
1	C	180	VAL	O-C-N	5.92	129.61	123.04
1	C	226	LEU	CA-C-N	5.92	128.21	120.28
1	C	226	LEU	C-N-CA	5.92	128.21	120.28
1	E	258	VAL	CA-C-N	5.92	129.02	120.38
1	E	258	VAL	C-N-CA	5.92	129.02	120.38
1	H	29	GLY	CA-C-O	-5.92	115.86	121.90
1	B	298	ILE	CB-CA-C	-5.92	104.16	111.08
1	E	54	ASN	CA-CB-CG	5.92	118.52	112.60
1	F	260	ARG	CD-NE-CZ	-5.92	116.12	124.40
1	G	105	THR	N-CA-C	-5.91	101.45	110.14
1	D	181	ALA	O-C-N	5.91	127.39	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	319	ALA	O-C-N	5.91	128.16	122.07
1	H	244	LYS	CA-CB-CG	5.91	125.92	114.10
1	A	69	LYS	N-CA-C	5.91	119.96	112.87
1	E	309	ASP	CA-CB-CG	-5.91	106.69	112.60
1	A	197	GLU	CA-C-O	-5.90	115.29	121.55
1	G	128	GLY	N-CA-C	-5.90	106.84	115.63
1	A	55	GLU	O-C-N	5.90	128.15	122.07
1	C	154	PRO	N-CA-C	-5.90	101.93	111.19
1	D	142	ILE	O-C-N	5.90	128.03	121.90
1	G	48	ILE	O-C-N	5.90	129.31	123.18
1	E	312	ASN	O-C-N	5.90	128.39	122.08
1	H	166	ASP	CA-CB-CG	-5.89	106.71	112.60
1	D	212	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	A	192	GLU	CG-CD-OE2	-5.88	104.88	118.40
1	C	283	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	A	171	ARG	O-C-N	5.88	128.87	122.11
1	E	302	ILE	CB-CA-C	5.88	119.59	110.83
1	A	298	ILE	N-CA-CB	-5.88	104.30	110.82
1	A	258	VAL	CA-C-O	5.88	128.12	120.78
1	A	308	ASP	O-C-N	5.87	128.86	122.11
1	E	150	PHE	CA-CB-CG	5.87	119.67	113.80
1	C	211	ILE	N-CA-CB	5.87	116.78	110.62
1	G	34	SER	N-CA-C	-5.87	104.24	111.40
1	G	189	ILE	N-CA-CB	5.87	119.27	111.64
1	F	116	ILE	N-CA-C	5.87	116.60	110.62
1	E	105	THR	CA-C-O	-5.86	114.28	121.78
1	B	314	PHE	CB-CA-C	5.86	119.99	110.96
1	G	182	PRO	O-C-N	5.86	129.26	122.23
1	G	282	GLU	CA-CB-CG	5.86	125.82	114.10
1	F	247	THR	CA-CB-OG1	-5.86	100.82	109.60
1	B	89	ALA	N-CA-C	5.85	118.74	109.96
1	B	227	GLU	CA-CB-CG	5.85	125.81	114.10
1	F	106	ARG	CA-CB-CG	5.85	125.80	114.10
1	B	46	ASP	CA-CB-CG	-5.85	106.75	112.60
1	H	21	ALA	CA-C-N	-5.85	114.75	122.99
1	H	21	ALA	C-N-CA	-5.85	114.75	122.99
1	F	317	SER	CA-C-N	5.84	128.91	120.79
1	F	317	SER	C-N-CA	5.84	128.91	120.79
1	A	171	ARG	CA-C-O	-5.84	114.38	120.92
1	G	90	ASP	CA-C-N	5.84	132.14	122.33
1	G	90	ASP	C-N-CA	5.84	132.14	122.33
1	D	153	LEU	CA-CB-CG	5.84	136.72	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	ALA	O-C-N	5.83	128.30	122.12
1	C	17	ASN	OD1-CG-ND2	5.83	128.43	122.60
1	F	21	ALA	CB-CA-C	5.83	119.63	110.19
1	F	84	ASP	O-C-N	5.83	130.24	122.43
1	B	234	ARG	CA-C-N	5.82	131.33	121.14
1	B	234	ARG	C-N-CA	5.82	131.33	121.14
1	F	329	PHE	CA-C-N	5.82	132.18	121.70
1	F	329	PHE	C-N-CA	5.82	132.18	121.70
1	D	249	TYR	O-C-N	5.82	130.62	122.36
1	D	299	ARG	CA-C-O	-5.82	114.71	120.82
1	G	248	TYR	CA-CB-CG	5.82	124.37	113.90
1	D	171	ARG	NE-CZ-NH1	5.82	127.31	121.50
1	C	200	VAL	CA-C-O	-5.81	113.51	120.78
1	E	124	VAL	O-C-N	5.80	127.50	121.87
1	F	206	ILE	CA-C-O	-5.80	114.10	120.48
1	C	189	ILE	CA-C-O	-5.80	113.15	120.69
1	F	119	SER	O-C-N	5.80	128.04	122.07
1	G	25	VAL	N-CA-CB	-5.80	104.37	111.67
1	B	216	GLU	CB-CA-C	-5.79	100.83	110.68
1	A	68	GLY	N-CA-C	5.79	121.17	114.16
1	D	243	LYS	CA-C-O	-5.79	113.81	120.24
1	B	221	GLU	N-CA-C	-5.79	98.47	110.80
1	C	253	MET	CA-CB-CG	5.79	125.67	114.10
1	G	265	ASN	CA-CB-CG	5.79	118.39	112.60
1	H	224	LYS	CA-C-N	5.78	128.50	120.29
1	H	224	LYS	C-N-CA	5.78	128.50	120.29
1	B	273	SER	N-CA-C	-5.78	99.77	108.96
1	G	117	PHE	CA-CB-CG	-5.78	108.02	113.80
1	A	24	VAL	N-CA-CB	-5.78	104.18	111.46
1	A	301	VAL	CA-C-O	-5.78	113.68	121.02
1	D	63	MET	N-CA-CB	5.78	118.35	109.91
1	G	107	LEU	CB-CA-C	5.78	121.91	110.42
1	G	154	PRO	CA-C-O	-5.78	114.62	121.67
1	H	295	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	B	109	LEU	N-CA-C	5.77	118.52	111.82
1	B	312	ASN	O-C-N	5.77	128.09	122.09
1	D	48	ILE	CA-C-O	-5.77	114.54	120.25
1	D	79	TRP	CA-CB-CG	5.77	124.57	113.60
1	F	111	ASP	CA-C-N	5.77	128.27	120.65
1	F	111	ASP	C-N-CA	5.77	128.27	120.65
1	B	306	LEU	CA-C-O	5.77	126.83	120.71
1	D	215	VAL	CA-CB-CG2	5.77	120.20	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	174	LEU	CA-C-O	5.77	126.59	119.79
1	A	197	GLU	CA-CB-CG	5.76	125.63	114.10
1	C	228	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	F	286	TYR	CA-C-N	-5.76	115.65	122.11
1	F	286	TYR	C-N-CA	-5.76	115.65	122.11
1	G	145	TYR	O-C-N	5.76	128.02	122.03
1	H	203	GLN	CA-C-O	-5.76	113.57	120.65
1	G	282	GLU	CB-CA-C	-5.76	99.02	111.11
1	H	163	THR	N-CA-C	5.76	119.38	112.93
1	D	272	VAL	O-C-N	5.75	129.76	122.57
1	A	228	ARG	NE-CZ-NH2	5.75	124.38	119.20
1	D	105	THR	N-CA-CB	5.75	119.29	110.49
1	G	15	MET	O-C-N	5.75	132.21	123.00
1	B	225	ASP	CA-C-N	5.75	127.99	120.28
1	B	225	ASP	C-N-CA	5.75	127.99	120.28
1	H	114	ILE	N-CA-CB	5.75	120.48	110.65
1	E	81	GLY	CA-C-N	5.75	132.48	122.82
1	E	81	GLY	C-N-CA	5.75	132.48	122.82
1	A	230	PHE	CA-CB-CG	-5.75	108.05	113.80
1	E	34	SER	O-C-N	5.75	128.30	122.09
1	A	171	ARG	CA-CB-CG	-5.75	102.61	114.10
1	A	216	GLU	CB-CA-C	-5.75	101.30	110.84
1	B	70	VAL	N-CA-C	-5.74	105.54	113.00
1	H	294	ASN	CA-CB-CG	5.74	118.34	112.60
1	B	279	LEU	CA-C-N	-5.74	114.63	123.17
1	B	279	LEU	C-N-CA	-5.74	114.63	123.17
1	C	136	ALA	O-C-N	5.74	128.69	121.64
1	D	248	TYR	O-C-N	5.74	130.22	122.59
1	B	138	ASN	CA-C-O	-5.73	115.38	120.19
1	F	157	ARG	CD-NE-CZ	-5.73	116.37	124.40
1	B	21	ALA	O-C-N	5.73	130.35	123.13
1	C	221	GLU	CA-C-O	5.73	128.70	120.51
1	F	216	GLU	CB-CG-CD	5.73	122.33	112.60
1	F	309	ASP	CA-CB-CG	-5.73	106.87	112.60
1	C	227	GLU	CA-CB-CG	5.73	125.55	114.10
1	C	169	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	D	195	ASP	CA-C-O	-5.72	113.63	120.10
1	G	205	TYR	CA-C-O	5.72	128.16	121.46
1	H	76	VAL	CB-CA-C	5.72	120.95	110.71
1	A	24	VAL	CB-CA-C	5.72	119.31	110.96
1	F	207	GLY	N-CA-C	-5.71	101.23	110.95
1	A	100	GLN	CB-CA-C	5.71	119.42	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	GLY	CA-C-O	5.71	125.37	118.86
1	B	266	GLU	N-CA-C	5.71	119.97	112.89
1	D	195	ASP	N-CA-C	5.71	118.27	111.71
1	B	74	LYS	N-CA-CB	-5.70	100.68	110.72
1	D	235	ASP	CA-C-O	5.70	126.32	119.59
1	E	300	GLU	CB-CG-CD	5.69	122.28	112.60
1	E	143	LEU	CA-C-O	-5.69	113.43	119.97
1	C	167	THR	O-C-N	5.69	128.15	122.12
1	E	55	GLU	CA-CB-CG	5.69	125.47	114.10
1	H	307	ASN	CA-CB-CG	5.69	118.29	112.60
1	D	328	ALA	CA-C-O	-5.68	112.88	119.59
1	H	31	VAL	CA-C-O	-5.68	115.15	121.17
1	C	317	SER	O-C-N	5.68	129.04	122.17
1	F	216	GLU	N-CA-C	-5.67	105.19	111.71
1	B	77	ASP	O-C-N	5.67	130.60	123.12
1	A	41	ASN	OD1-CG-ND2	5.67	128.27	122.60
1	A	121	VAL	CA-C-N	5.67	129.32	120.82
1	A	121	VAL	C-N-CA	5.67	129.32	120.82
1	G	313	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	F	208	VAL	N-CA-C	-5.67	105.88	111.77
1	B	268	ALA	CA-C-O	-5.66	115.04	121.72
1	F	47	GLU	CA-C-O	-5.66	112.56	120.21
1	F	171	ARG	CD-NE-CZ	5.66	132.32	124.40
1	A	203	GLN	OE1-CD-NE2	5.66	128.26	122.60
1	E	110	VAL	N-CA-C	5.66	121.11	109.34
1	A	50	LEU	O-C-N	5.66	130.58	123.23
1	F	281	GLY	N-CA-C	-5.66	105.09	114.48
1	G	25	VAL	CB-CA-C	5.66	119.05	111.19
1	C	186	HIS	CB-CA-C	-5.65	102.97	111.73
1	B	264	HIS	CA-C-N	-5.65	114.79	122.82
1	B	264	HIS	C-N-CA	-5.65	114.79	122.82
1	D	241	ILE	N-CA-C	-5.65	104.99	110.42
1	E	30	PHE	O-C-N	5.65	128.19	122.09
1	F	63	MET	CA-CB-CG	5.65	125.41	114.10
1	B	329	PHE	CB-CA-C	5.65	119.82	110.78
1	F	155	HIS	CA-CB-CG	5.65	119.45	113.80
1	C	265	ASN	CB-CG-ND2	-5.65	107.93	116.40
1	D	253	MET	O-C-N	5.65	128.59	122.15
1	G	105	THR	N-CA-CB	5.65	119.11	110.70
1	D	227	GLU	CA-C-N	5.64	127.78	120.44
1	D	227	GLU	C-N-CA	5.64	127.78	120.44
1	D	93	VAL	CB-CA-C	5.64	118.71	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ALA	CA-C-N	-5.64	115.51	122.84
1	A	21	ALA	C-N-CA	-5.64	115.51	122.84
1	D	107	LEU	CA-C-O	-5.64	113.73	120.10
1	E	227	GLU	CB-CG-CD	5.64	122.19	112.60
1	B	208	VAL	N-CA-CB	5.63	119.68	112.36
1	A	34	SER	N-CA-C	-5.63	105.14	111.28
1	B	204	ALA	CA-C-O	5.63	126.52	120.38
1	C	62	ALA	N-CA-C	-5.63	104.52	111.33
1	E	65	PHE	N-CA-C	-5.63	105.06	111.14
1	F	158	VAL	CA-C-O	-5.63	113.74	120.78
1	G	198	LEU	O-C-N	5.63	126.23	121.84
1	E	88	ASP	O-C-N	5.63	129.00	122.19
1	A	154	PRO	CB-CA-C	5.63	118.43	111.23
1	G	324	VAL	O-C-N	5.63	127.58	121.90
1	A	34	SER	O-C-N	5.63	128.09	122.12
1	A	327	ARG	N-CA-C	5.63	120.21	113.23
1	A	169	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	C	23	VAL	CA-C-O	-5.62	114.54	120.39
1	A	89	ALA	N-CA-C	5.62	119.41	109.96
1	D	253	MET	CA-C-N	5.62	126.07	119.94
1	D	253	MET	C-N-CA	5.62	126.07	119.94
1	D	271	THR	CA-C-O	-5.62	115.08	121.66
1	C	110	VAL	CB-CA-C	-5.62	102.07	111.29
1	G	221	GLU	CA-C-N	-5.62	112.98	120.79
1	G	221	GLU	C-N-CA	-5.62	112.98	120.79
1	B	127	SER	CA-C-O	5.61	126.69	120.63
1	C	225	ASP	O-C-N	5.61	127.85	122.07
1	D	55	GLU	CB-CG-CD	-5.61	103.06	112.60
1	C	138	ASN	OD1-CG-ND2	5.61	128.21	122.60
1	H	324	VAL	O-C-N	5.61	129.58	122.57
1	A	252	ALA	CB-CA-C	5.60	119.75	110.90
1	A	177	TYR	CA-CB-CG	5.60	123.99	113.90
1	B	107	LEU	N-CA-C	5.60	119.73	113.01
1	F	75	PRO	CA-C-O	-5.60	115.23	121.23
1	D	183	GLN	CA-C-O	-5.60	113.00	119.61
1	A	242	GLU	CG-CD-OE1	-5.60	105.53	118.40
1	C	149	LYS	CA-CB-CG	5.60	125.30	114.10
1	C	308	ASP	CA-CB-CG	5.60	118.20	112.60
1	D	287	ILE	CB-CA-C	5.60	119.29	111.40
1	G	44	ILE	N-CA-C	5.60	115.83	110.74
1	E	286	TYR	CA-C-O	-5.59	114.33	120.43
1	H	76	VAL	CA-C-O	-5.59	115.35	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	282	GLU	N-CA-C	5.59	117.12	109.18
1	H	203	GLN	CB-CG-CD	5.59	122.10	112.60
1	G	299	ARG	N-CA-CB	5.59	118.43	110.16
1	A	103	GLY	O-C-N	5.58	129.96	122.70
1	A	152	GLY	O-C-N	5.58	128.44	122.41
1	F	209	MET	CA-C-O	5.58	126.59	119.67
1	E	17	ASN	CA-CB-CG	-5.58	107.02	112.60
1	C	289	VAL	N-CA-CB	-5.58	103.40	111.21
1	E	208	VAL	CA-C-N	5.58	129.01	121.20
1	E	208	VAL	C-N-CA	5.58	129.01	121.20
1	B	137	THR	O-C-N	5.58	129.77	122.97
1	B	124	VAL	CA-C-O	-5.57	114.94	120.85
1	F	325	LEU	O-C-N	5.57	127.81	122.07
1	G	67	HIS	O-C-N	5.57	128.73	122.22
1	A	148	TRP	CA-C-N	5.56	127.99	120.65
1	A	148	TRP	C-N-CA	5.56	127.99	120.65
1	B	144	THR	CA-C-O	5.56	126.43	120.70
1	C	220	GLU	CA-C-O	5.56	128.46	120.51
1	D	324	VAL	O-C-N	5.56	127.50	121.94
1	C	247	THR	CB-CA-C	5.56	119.39	109.38
1	E	141	ASP	CA-CB-CG	-5.56	107.04	112.60
1	F	183	GLN	N-CA-C	-5.56	105.60	112.38
1	H	329	PHE	N-CA-C	5.56	117.78	107.99
1	B	314	PHE	CA-CB-CG	-5.56	108.24	113.80
1	G	258	VAL	N-CA-C	-5.56	105.31	110.53
1	C	285	VAL	CA-C-O	-5.55	116.30	120.96
1	F	198	LEU	O-C-N	5.55	125.82	121.88
1	A	319	ALA	CA-C-O	-5.55	114.96	120.90
1	B	113	ASN	CA-CB-CG	-5.55	107.05	112.60
1	D	209	MET	O-C-N	5.55	125.72	121.23
1	H	240	ILE	CA-C-O	-5.55	114.97	120.85
1	H	281	GLY	N-CA-C	-5.55	105.27	114.48
1	F	215	VAL	CA-C-O	-5.55	115.13	119.46
1	H	87	ARG	O-C-N	5.54	127.86	122.09
1	F	236	ALA	O-C-N	5.54	128.01	122.08
1	G	206	ILE	CA-C-O	-5.54	114.69	120.51
1	E	173	LEU	CA-C-O	-5.54	114.71	120.92
1	F	88	ASP	N-CA-C	5.54	119.14	112.93
1	A	234	ARG	O-C-N	5.54	128.51	122.20
1	F	147	THR	CA-C-O	-5.54	113.84	120.10
1	D	166	ASP	CA-C-O	-5.54	114.55	120.42
1	C	61	ASP	N-CA-C	5.54	118.50	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	183	GLN	N-CA-C	-5.54	105.63	112.38
1	E	266	GLU	CB-CA-C	-5.53	102.16	110.90
1	H	113	ASN	CA-CB-CG	5.53	118.13	112.60
1	E	115	ALA	CB-CA-C	5.53	119.71	110.92
1	G	286	TYR	N-CA-CB	5.53	119.46	110.17
1	A	116	ILE	O-C-N	5.53	127.45	121.87
1	D	199	PRO	CA-C-O	-5.53	114.50	120.97
1	E	147	THR	N-CA-CB	5.53	118.43	110.20
1	D	188	TYR	CA-CB-CG	5.52	123.84	113.90
1	C	110	VAL	N-CA-C	5.52	120.83	109.34
1	F	134	LEU	CA-C-O	-5.52	114.37	120.33
1	H	302	ILE	CA-C-O	-5.52	114.66	120.57
1	B	96	ALA	CA-C-O	-5.52	115.47	121.87
1	D	124	VAL	CA-CB-CG1	5.52	119.78	110.40
1	G	302	ILE	N-CA-CB	5.51	117.61	110.99
1	D	249	TYR	N-CA-C	-5.51	105.68	112.90
1	E	257	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	H	243	LYS	CA-C-O	-5.50	114.59	120.42
1	C	257	ARG	CB-CA-C	-5.50	102.24	110.88
1	F	57	LYS	N-CA-C	-5.50	104.31	111.02
1	H	152	GLY	O-C-N	5.50	128.15	122.54
1	C	84	ASP	CA-CB-CG	-5.50	107.10	112.60
1	E	237	ALA	CA-C-N	5.50	130.03	120.68
1	E	237	ALA	C-N-CA	5.50	130.03	120.68
1	E	239	GLN	CB-CG-CD	5.50	121.94	112.60
1	A	270	LEU	CB-CA-C	5.50	120.16	109.33
1	A	172	PHE	CA-C-N	5.49	127.58	120.44
1	A	172	PHE	C-N-CA	5.49	127.58	120.44
1	D	82	ASP	CA-C-N	5.49	128.19	120.28
1	D	82	ASP	C-N-CA	5.49	128.19	120.28
1	A	261	ALA	N-CA-C	-5.49	104.99	110.97
1	G	185	VAL	CB-CA-C	5.49	119.01	110.83
1	F	19	GLY	O-C-N	5.48	129.82	122.70
1	E	260	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	G	192	GLU	CB-CG-CD	5.48	121.91	112.60
1	A	318	ALA	N-CA-C	-5.48	105.39	111.36
1	E	300	GLU	CA-CB-CG	5.48	125.05	114.10
1	B	228	ARG	CD-NE-CZ	5.47	132.06	124.40
1	C	208	VAL	N-CA-C	-5.47	107.40	112.43
1	F	28	ALA	N-CA-C	-5.47	105.76	113.20
1	H	106	ARG	CD-NE-CZ	-5.47	116.74	124.40
1	C	209	MET	O-C-N	5.47	126.33	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	315	HIS	CA-CB-CG	-5.47	108.33	113.80
1	G	46	ASP	CA-CB-CG	-5.47	107.13	112.60
1	H	61	ASP	O-C-N	5.47	127.70	122.07
1	A	139	PRO	N-CD-CG	-5.47	97.24	103.80
1	G	48	ILE	CA-C-O	-5.47	114.75	120.27
1	A	225	ASP	O-C-N	5.46	130.00	122.46
1	F	157	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	E	205	TYR	CA-C-N	5.46	131.80	121.97
1	E	205	TYR	C-N-CA	5.46	131.80	121.97
1	C	104	GLU	O-C-N	5.46	129.01	122.79
1	A	280	TYR	CA-C-O	5.46	127.36	120.65
1	E	203	GLN	CA-CB-CG	5.45	125.01	114.10
1	G	260	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	H	101	LYS	N-CA-C	-5.45	103.05	110.36
1	G	303	GLU	CA-C-N	-5.45	113.16	120.95
1	G	303	GLU	C-N-CA	-5.45	113.16	120.95
1	H	221	GLU	CA-CB-CG	-5.45	103.20	114.10
1	B	125	MET	O-C-N	5.45	127.91	122.08
1	D	81	GLY	O-C-N	5.45	128.81	123.31
1	B	61	ASP	CA-CB-CG	-5.45	107.15	112.60
1	E	327	ARG	CD-NE-CZ	-5.45	116.77	124.40
1	B	166	ASP	N-CA-C	-5.45	104.74	111.33
1	E	46	ASP	CA-CB-CG	5.44	118.04	112.60
1	G	309	ASP	CA-C-O	-5.44	114.78	120.55
1	D	225	ASP	CA-C-O	-5.44	115.08	121.07
1	H	330	THR	CA-C-O	5.44	130.05	120.80
1	G	118	ARG	N-CA-CB	5.44	118.65	109.78
1	E	279	LEU	CA-C-N	-5.44	115.07	123.17
1	E	279	LEU	C-N-CA	-5.44	115.07	123.17
1	D	247	THR	CB-CA-C	5.43	120.03	109.33
1	C	76	VAL	O-C-N	5.43	129.28	123.03
1	B	67	HIS	O-C-N	5.43	127.88	122.12
1	B	150	PHE	CA-CB-CG	5.43	119.23	113.80
1	C	224	LYS	CA-C-N	5.42	127.49	120.44
1	C	224	LYS	C-N-CA	5.42	127.49	120.44
1	C	296	ASN	CA-CB-CG	-5.42	107.18	112.60
1	C	323	SER	O-C-N	5.42	127.86	122.12
1	E	113	ASN	CA-C-O	-5.42	115.13	120.82
1	E	117	PHE	CA-CB-CG	-5.41	108.39	113.80
1	B	232	ASN	CA-C-O	-5.41	114.81	120.55
1	D	307	ASN	CB-CA-C	5.41	120.73	110.51
1	D	80	HIS	CA-C-O	-5.41	114.53	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	307	ASN	CB-CA-C	5.41	119.29	109.83
1	F	175	GLY	CA-C-N	-5.41	113.09	120.44
1	F	175	GLY	C-N-CA	-5.41	113.09	120.44
1	D	252	ALA	CA-C-N	5.40	127.96	120.29
1	D	252	ALA	C-N-CA	5.40	127.96	120.29
1	H	93	VAL	CA-C-O	-5.40	114.75	120.53
1	G	313	ARG	CD-NE-CZ	-5.40	116.84	124.40
1	A	94	ILE	O-C-N	5.39	130.09	122.97
1	H	107	LEU	CB-CA-C	5.39	121.14	110.42
1	H	47	GLU	O-C-N	5.38	129.56	123.42
1	D	265	ASN	OD1-CG-ND2	5.38	127.98	122.60
1	E	23	VAL	CA-C-O	-5.38	114.84	120.27
1	D	174	LEU	CA-C-N	5.38	125.92	120.00
1	D	174	LEU	C-N-CA	5.38	125.92	120.00
1	F	240	ILE	CB-CA-C	-5.38	104.97	112.02
1	H	45	ALA	CA-C-O	-5.38	115.33	121.68
1	H	53	ALA	CA-C-O	5.38	126.44	120.63
1	E	39	LEU	N-CA-C	5.38	117.83	111.33
1	C	228	ARG	CD-NE-CZ	5.37	131.92	124.40
1	G	258	VAL	CA-CB-CG2	5.37	119.53	110.40
1	B	199	PRO	CA-C-O	-5.37	114.69	120.97
1	C	247	THR	CA-CB-CG2	5.37	119.63	110.50
1	C	223	GLN	CA-C-N	5.37	127.73	120.38
1	C	223	GLN	C-N-CA	5.37	127.73	120.38
1	G	169	ARG	O-C-N	5.37	127.81	122.12
1	H	123	SER	N-CA-C	5.37	118.05	111.82
1	G	116	ILE	CA-CB-CG2	5.37	119.62	110.50
1	B	24	VAL	CA-C-O	-5.36	114.61	120.72
1	D	232	ASN	O-C-N	5.36	127.81	122.12
1	E	313	ARG	CD-NE-CZ	5.36	131.91	124.40
1	B	185	VAL	N-CA-CB	-5.36	104.89	111.00
1	A	76	VAL	CB-CA-C	5.36	118.70	110.55
1	D	167	THR	CA-C-N	5.36	127.46	120.28
1	D	167	THR	C-N-CA	5.36	127.46	120.28
1	B	83	TYR	CA-CB-CG	-5.36	104.26	113.90
1	E	158	VAL	CA-C-N	5.35	130.00	123.10
1	E	158	VAL	C-N-CA	5.35	130.00	123.10
1	F	123	SER	CA-C-O	-5.35	114.75	120.42
1	F	327	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	192	GLU	CB-CG-CD	5.35	121.69	112.60
1	A	78	ILE	N-CA-CB	5.35	119.42	110.86
1	F	219	GLY	N-CA-C	5.35	125.85	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	GLU	O-C-N	5.35	128.67	122.20
1	B	283	ARG	CG-CD-NE	5.34	123.76	112.00
1	C	82	ASP	CA-C-O	-5.34	115.59	121.31
1	D	232	ASN	CB-CG-OD1	-5.34	110.11	120.80
1	F	67	HIS	CA-C-O	-5.34	114.76	120.42
1	A	76	VAL	N-CA-CB	-5.34	103.47	112.44
1	B	268	ALA	O-C-N	5.34	128.92	122.94
1	B	306	LEU	N-CA-C	5.34	118.18	109.59
1	G	279	LEU	N-CA-C	5.34	117.18	111.36
1	A	176	GLU	N-CA-C	5.33	116.78	110.97
1	F	208	VAL	CA-C-O	-5.33	114.39	120.26
1	B	112	LYS	O-C-N	5.33	127.78	122.08
1	H	87	ARG	CD-NE-CZ	5.33	131.86	124.40
1	B	122	GLU	N-CA-C	5.33	118.57	111.75
1	G	215	VAL	N-CA-C	-5.33	105.56	113.39
1	E	66	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	323	SER	CA-C-O	5.32	128.12	120.51
1	A	270	LEU	CA-C-O	-5.32	115.10	121.11
1	C	160	GLY	O-C-N	5.32	129.19	123.18
1	G	194	GLY	O-C-N	5.32	128.21	123.80
1	H	52	ASP	CA-CB-CG	-5.32	107.28	112.60
1	H	197	GLU	CA-C-O	-5.32	116.02	121.87
1	F	119	SER	N-CA-C	5.32	116.76	111.07
1	E	87	ARG	O-C-N	5.31	129.66	122.59
1	A	87	ARG	N-CA-CB	5.31	118.44	109.78
1	D	296	ASN	CA-CB-CG	5.31	117.91	112.60
1	B	46	ASP	N-CA-C	-5.31	107.35	113.88
1	F	59	ILE	CA-C-N	5.31	125.84	120.00
1	F	59	ILE	C-N-CA	5.31	125.84	120.00
1	A	15	MET	N-CA-CB	5.31	119.52	110.50
1	G	307	ASN	N-CA-C	-5.30	102.67	110.52
1	D	182	PRO	N-CA-C	-5.30	105.19	113.78
1	H	87	ARG	N-CA-CB	5.30	117.84	109.94
1	D	202	SER	O-C-N	5.30	128.24	122.20
1	F	211	ILE	N-CA-CB	5.30	116.39	110.62
1	B	158	VAL	CB-CA-C	5.29	116.97	111.09
1	E	298	ILE	N-CA-CB	-5.29	105.25	111.39
1	F	55	GLU	CA-CB-CG	5.29	124.69	114.10
1	G	111	ASP	CA-CB-CG	5.29	117.89	112.60
1	G	171	ARG	CA-C-N	5.29	127.69	120.54
1	G	171	ARG	C-N-CA	5.29	127.69	120.54
1	C	118	ARG	CD-NE-CZ	5.29	131.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	249	TYR	N-CA-CB	-5.29	102.07	110.22
1	H	327	ARG	CA-C-N	-5.29	112.91	122.54
1	H	327	ARG	C-N-CA	-5.29	112.91	122.54
1	D	115	ALA	O-C-N	5.29	127.74	122.08
1	H	206	ILE	CB-CA-C	5.29	117.72	111.32
1	A	309	ASP	CA-C-O	-5.29	115.45	121.00
1	C	257	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	E	329	PHE	N-CA-C	5.29	118.09	107.41
1	G	169	ARG	N-CA-C	-5.29	105.52	111.28
1	B	271	THR	N-CA-CB	5.28	118.22	110.35
1	G	318	ALA	CA-C-N	5.28	127.67	120.54
1	G	318	ALA	C-N-CA	5.28	127.67	120.54
1	C	180	VAL	CA-C-O	-5.28	116.13	121.67
1	F	314	PHE	N-CA-C	-5.27	105.61	111.36
1	C	28	ALA	CA-C-N	-5.27	116.00	122.75
1	C	28	ALA	C-N-CA	-5.27	116.00	122.75
1	C	36	VAL	N-CA-CB	5.27	117.31	110.57
1	C	235	ASP	CA-C-N	5.26	127.65	120.54
1	C	235	ASP	C-N-CA	5.26	127.65	120.54
1	G	221	GLU	N-CA-C	-5.26	99.58	110.80
1	D	199	PRO	O-C-N	5.26	128.98	123.03
1	G	144	THR	O-C-N	5.26	128.15	122.15
1	B	261	ALA	CB-CA-C	5.26	119.13	110.88
1	F	56	SER	O-C-N	5.26	127.77	122.09
1	D	176	GLU	CA-CB-CG	-5.25	103.59	114.10
1	B	110	VAL	CB-CA-C	-5.25	102.67	111.29
1	B	265	ASN	N-CA-C	-5.25	103.76	111.17
1	F	122	GLU	O-C-N	5.25	127.55	122.09
1	C	77	ASP	CA-C-O	-5.25	115.08	120.54
1	E	183	GLN	N-CA-CB	5.25	119.25	110.32
1	B	17	ASN	N-CA-C	5.25	118.64	107.67
1	F	327	ARG	N-CA-C	5.25	119.32	113.02
1	D	310	GLU	O-C-N	5.25	127.76	122.09
1	F	232	ASN	OD1-CG-ND2	5.25	127.84	122.60
1	E	101	LYS	N-CA-C	-5.24	102.84	110.08
1	D	260	ARG	CD-NE-CZ	-5.24	117.07	124.40
1	F	313	ARG	CD-NE-CZ	-5.24	117.07	124.40
1	A	181	ALA	N-CA-CB	-5.24	101.76	109.98
1	H	172	PHE	CA-CB-CG	5.24	119.04	113.80
1	H	198	LEU	CA-C-N	5.23	126.38	119.84
1	H	198	LEU	C-N-CA	5.23	126.38	119.84
1	C	309	ASP	O-C-N	5.23	128.11	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	309	ASP	CA-CB-CG	-5.23	107.37	112.60
1	A	157	ARG	CD-NE-CZ	-5.23	117.08	124.40
1	A	191	GLY	N-CA-C	-5.23	103.33	112.53
1	H	154	PRO	N-CA-C	-5.23	102.90	111.21
1	C	203	GLN	N-CA-CB	-5.23	103.96	111.54
1	D	22	ARG	CB-CA-C	5.23	118.66	110.19
1	F	180	VAL	O-C-N	5.23	128.52	122.82
1	C	118	ARG	CB-CA-C	-5.23	102.67	110.88
1	C	240	ILE	N-CA-CB	5.23	118.42	110.58
1	D	188	TYR	CB-CA-C	-5.23	99.52	109.66
1	E	223	GLN	O-C-N	5.23	127.66	122.12
1	C	113	ASN	CA-CB-CG	5.22	117.83	112.60
1	G	313	ARG	CA-C-O	5.22	125.97	119.97
1	C	271	THR	CA-C-N	5.22	130.03	122.77
1	C	271	THR	C-N-CA	5.22	130.03	122.77
1	E	17	ASN	O-C-N	5.22	129.88	122.83
1	E	108	ASP	CA-CB-CG	5.22	117.82	112.60
1	E	330	THR	CA-CB-CG2	5.22	119.37	110.50
1	F	186	HIS	CA-CB-CG	-5.22	108.58	113.80
1	H	133	PHE	O-C-N	5.22	129.45	123.29
1	H	188	TYR	CB-CA-C	-5.22	100.32	109.71
1	E	168	ALA	O-C-N	5.22	128.32	122.22
1	D	87	ARG	CD-NE-CZ	5.21	131.70	124.40
1	D	115	ALA	CA-C-N	5.21	127.88	120.53
1	D	115	ALA	C-N-CA	5.21	127.88	120.53
1	C	114	ILE	N-CA-CB	5.21	118.72	110.54
1	E	275	TYR	CA-C-O	5.21	126.43	120.54
1	G	96	ALA	N-CA-CB	5.21	118.91	110.41
1	C	159	ILE	O-C-N	5.21	128.81	123.18
1	H	215	VAL	N-CA-CB	-5.21	105.35	112.28
1	B	134	LEU	CB-CA-C	5.21	119.98	111.23
1	E	115	ALA	CA-C-N	5.21	128.70	120.47
1	E	115	ALA	C-N-CA	5.21	128.70	120.47
1	E	164	ILE	O-C-N	5.21	127.15	121.94
1	E	202	SER	CA-CB-OG	5.21	121.51	111.10
1	C	175	GLY	N-CA-C	-5.21	106.19	112.49
1	C	121	VAL	O-C-N	5.20	126.92	121.87
1	D	101	LYS	CB-CA-C	5.20	121.32	110.50
1	D	311	LYS	CA-C-O	5.20	126.75	120.92
1	A	125	MET	O-C-N	5.20	128.31	122.22
1	B	252	ALA	O-C-N	5.20	128.67	122.27
1	E	260	ARG	NE-CZ-NH1	-5.20	116.30	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	157	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	216	GLU	O-C-N	5.20	128.49	122.20
1	A	317	SER	O-C-N	5.20	127.42	122.07
1	E	61	ASP	CA-CB-CG	-5.20	107.40	112.60
1	G	279	LEU	CA-C-N	-5.20	114.32	122.79
1	G	279	LEU	C-N-CA	-5.20	114.32	122.79
1	B	93	VAL	CA-C-O	-5.20	114.41	120.75
1	D	181	ALA	CA-C-O	-5.20	114.77	120.17
1	F	233	VAL	N-CA-C	-5.20	106.01	110.74
1	F	240	ILE	N-CA-C	5.19	115.41	110.53
1	H	153	LEU	O-C-N	5.19	127.52	121.39
1	E	297	GLY	O-C-N	5.19	127.90	122.86
1	H	230	PHE	CA-CB-CG	-5.19	108.61	113.80
1	B	122	GLU	O-C-N	5.19	128.12	122.20
1	G	100	GLN	OE1-CD-NE2	5.19	127.79	122.60
1	G	206	ILE	N-CA-C	-5.19	97.38	106.61
1	H	79	TRP	CA-C-O	-5.19	115.68	121.23
1	B	168	ALA	N-CA-C	-5.18	105.63	111.28
1	F	212	ARG	CD-NE-CZ	5.18	131.66	124.40
1	G	192	GLU	N-CA-C	5.18	117.74	110.23
1	A	288	GLY	O-C-N	5.18	126.30	122.62
1	B	181	ALA	CB-CA-C	5.18	117.70	109.52
1	C	36	VAL	N-CA-C	-5.17	105.67	110.53
1	F	95	CYS	O-C-N	5.17	128.45	122.19
1	A	220	GLU	CB-CG-CD	5.17	121.39	112.60
1	E	289	VAL	N-CA-CB	-5.17	103.97	111.21
1	A	252	ALA	N-CA-C	-5.17	105.56	111.14
1	D	225	ASP	O-C-N	5.17	127.61	122.08
1	H	24	VAL	CA-C-O	5.17	125.76	120.39
1	H	286	TYR	CA-C-O	-5.16	115.26	120.84
1	E	269	ILE	CA-C-O	-5.16	114.75	120.74
1	D	230	PHE	CA-CB-CG	-5.16	108.64	113.80
1	F	109	LEU	N-CA-C	5.16	119.20	113.01
1	H	89	ALA	N-CA-C	-5.16	102.12	110.32
1	B	228	ARG	N-CA-C	-5.16	105.57	111.14
1	E	144	THR	N-CA-CB	5.16	118.27	110.28
1	A	29	GLY	N-CA-C	-5.15	100.97	113.18
1	D	265	ASN	N-CA-CB	-5.15	103.88	111.71
1	D	223	GLN	OE1-CD-NE2	5.15	127.75	122.60
1	E	135	VAL	N-CA-CB	-5.15	105.11	110.72
1	C	186	HIS	CA-C-O	-5.15	115.20	121.58
1	H	158	VAL	O-C-N	5.15	129.12	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	LYS	N-CA-CB	5.15	119.19	110.49
1	H	64	ASP	CA-C-O	-5.14	115.10	120.55
1	G	277	ASP	CB-CA-C	5.14	119.92	111.74
1	C	325	LEU	CB-CA-C	5.14	118.95	110.88
1	C	93	VAL	O-C-N	5.14	129.11	123.10
1	E	70	VAL	CA-C-N	5.14	130.43	122.26
1	E	70	VAL	C-N-CA	5.14	130.43	122.26
1	E	192	GLU	CG-CD-OE1	5.14	130.22	118.40
1	G	141	ASP	CA-CB-CG	-5.14	107.46	112.60
1	G	153	LEU	O-C-N	5.14	128.41	121.12
1	D	264	HIS	O-C-N	5.13	128.36	122.25
1	A	279	LEU	N-CA-C	5.13	121.73	110.80
1	F	300	GLU	CB-CA-C	-5.13	101.81	110.43
1	H	271	THR	CA-C-N	5.13	129.90	122.77
1	H	271	THR	C-N-CA	5.13	129.90	122.77
1	C	113	ASN	N-CA-C	5.13	116.95	111.36
1	C	304	ILE	CB-CA-C	5.13	117.64	111.13
1	D	47	GLU	CB-CG-CD	5.12	121.31	112.60
1	D	167	THR	N-CA-CB	5.12	117.65	110.12
1	A	234	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	G	298	ILE	N-CA-C	5.12	116.12	108.54
1	A	305	GLU	CA-C-N	-5.12	114.21	122.81
1	A	305	GLU	C-N-CA	-5.12	114.21	122.81
1	G	86	CYS	O-C-N	5.12	127.98	122.15
1	G	218	LYS	CA-C-N	5.12	131.44	121.41
1	G	218	LYS	C-N-CA	5.12	131.44	121.41
1	A	227	GLU	CB-CG-CD	5.11	121.29	112.60
1	C	279	LEU	CA-C-N	-5.11	114.50	122.73
1	C	279	LEU	C-N-CA	-5.11	114.50	122.73
1	B	330	THR	CA-CB-OG1	-5.11	101.94	109.60
1	F	17	ASN	OD1-CG-ND2	5.11	127.71	122.60
1	C	145	TYR	CA-C-O	-5.11	115.64	120.90
1	A	59	ILE	CA-C-O	-5.11	115.25	120.71
1	H	100	GLN	O-C-N	5.11	129.21	122.93
1	B	318	ALA	CA-C-O	5.10	125.96	120.55
1	D	87	ARG	NE-CZ-NH2	-5.10	114.61	119.20
1	E	291	ALA	N-CA-C	5.10	116.82	108.55
1	E	85	ASP	N-CA-CB	5.10	117.60	110.56
1	G	55	GLU	CG-CD-OE2	-5.10	106.67	118.40
1	F	235	ASP	O-C-N	5.10	128.41	122.24
1	H	217	SER	CA-C-O	-5.10	112.58	119.11
1	A	25	VAL	CA-C-O	-5.09	115.12	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	MET	N-CA-C	-5.09	105.38	111.03
1	A	184	ASN	CA-CB-CG	5.09	117.69	112.60
1	E	202	SER	N-CA-CB	5.09	117.61	110.12
1	A	85	ASP	N-CA-C	-5.09	106.33	112.54
1	G	328	ALA	CA-C-O	-5.09	115.33	121.34
1	F	47	GLU	O-C-N	5.09	129.70	123.44
1	G	163	THR	CA-CB-CG2	5.09	119.15	110.50
1	G	321	LEU	CA-C-O	-5.09	114.59	120.24
1	H	190	ILE	N-CA-CB	-5.09	106.75	112.45
1	A	178	PHE	N-CA-C	5.09	119.33	113.18
1	C	18	ASN	CA-CB-CG	5.09	117.69	112.60
1	E	77	ASP	O-C-N	5.09	129.65	123.14
1	B	77	ASP	CA-C-N	-5.08	115.28	122.34
1	B	77	ASP	C-N-CA	-5.08	115.28	122.34
1	E	327	ARG	N-CA-CB	5.08	117.89	110.47
1	F	43	GLY	CA-C-O	-5.08	113.94	119.88
1	F	312	ASN	O-C-N	5.08	127.94	122.15
1	H	279	LEU	N-CA-C	5.08	117.56	111.71
1	E	156	GLU	CA-C-N	-5.08	114.18	122.26
1	E	156	GLU	C-N-CA	-5.08	114.18	122.26
1	G	312	ASN	O-C-N	5.08	127.57	122.09
1	B	264	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	G	189	ILE	N-CA-C	-5.07	100.34	107.75
1	B	168	ALA	CB-CA-C	5.07	119.21	110.79
1	F	100	GLN	O-C-N	5.07	128.97	123.04
1	F	147	THR	CA-CB-OG1	-5.07	102.00	109.60
1	A	172	PHE	CA-CB-CG	-5.07	108.73	113.80
1	H	120	ILE	CB-CA-C	5.07	119.60	111.29
1	C	100	GLN	CA-C-N	-5.07	114.08	123.55
1	C	100	GLN	C-N-CA	-5.07	114.08	123.55
1	C	228	ARG	CG-CD-NE	5.07	123.14	112.00
1	E	44	ILE	CA-C-O	-5.07	114.45	120.78
1	A	117	PHE	CA-CB-CG	-5.06	108.74	113.80
1	B	167	THR	O-C-N	5.06	129.11	122.33
1	C	316	HIS	CA-C-O	5.06	125.61	119.38
1	E	275	TYR	CB-CA-C	5.06	118.10	109.80
1	C	303	GLU	O-C-N	5.06	128.00	122.64
1	H	147	THR	CA-C-O	5.06	125.81	120.10
1	B	253	MET	O-C-N	5.05	129.54	122.36
1	D	193	HIS	N-CA-C	-5.05	98.82	108.17
1	G	98	ALA	CA-C-O	5.05	127.42	121.36
1	A	260	ARG	O-C-N	5.05	129.20	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	GLU	CG-CD-OE1	5.05	130.01	118.40
1	D	287	ILE	N-CA-CB	-5.05	102.63	110.96
1	E	131	GLY	N-CA-C	-5.05	105.84	112.81
1	A	305	GLU	N-CA-CB	5.05	118.81	110.69
1	E	243	LYS	N-CA-CB	5.05	118.01	110.19
1	C	124	VAL	CA-C-O	-5.04	114.96	120.96
1	D	17	ASN	CB-CA-C	5.04	119.43	111.72
1	G	30	PHE	CB-CA-C	-5.04	103.14	110.95
1	H	115	ALA	CA-C-N	5.04	127.58	120.42
1	H	115	ALA	C-N-CA	5.04	127.58	120.42
1	D	192	GLU	CB-CA-C	-5.04	102.28	109.84
1	F	174	LEU	N-CA-C	-5.04	105.88	112.23
1	C	153	LEU	N-CA-CB	5.04	117.07	109.82
1	B	298	ILE	O-C-N	5.03	128.47	122.83
1	F	220	GLU	CA-C-N	5.03	131.15	121.54
1	F	220	GLU	C-N-CA	5.03	131.15	121.54
1	G	165	LEU	O-C-N	5.03	127.89	122.15
1	C	222	ALA	CA-C-O	5.03	125.73	119.79
1	B	98	ALA	N-CA-C	5.03	117.50	109.96
1	E	308	ASP	CA-CB-CG	5.03	117.63	112.60
1	H	302	ILE	O-C-N	5.03	128.62	123.03
1	F	212	ARG	CB-CA-C	5.03	119.55	111.05
1	A	217	SER	CA-C-O	-5.03	113.32	120.51
1	E	312	ASN	CA-C-O	-5.03	115.54	121.07
1	H	206	ILE	O-C-N	5.03	128.79	122.66
1	A	315	HIS	CA-CB-CG	-5.02	108.78	113.80
1	D	269	ILE	N-CA-C	-5.02	103.10	109.58
1	D	299	ARG	N-CA-CB	5.02	117.29	110.01
1	E	128	GLY	CA-C-O	5.02	124.30	118.98
1	A	167	THR	N-CA-C	-5.02	104.81	112.04
1	B	91	LEU	N-CA-C	5.02	117.24	108.76
1	H	174	LEU	CB-CA-C	5.02	118.84	110.81
1	D	149	LYS	N-CA-C	5.01	116.56	111.14
1	E	328	ALA	CA-C-O	-5.01	112.55	121.38
1	H	321	LEU	N-CA-C	5.01	116.74	111.28
1	A	285	VAL	O-C-N	5.01	128.83	122.57
1	A	316	HIS	CA-C-N	5.01	126.95	120.44
1	A	316	HIS	C-N-CA	5.01	126.95	120.44
1	C	320	THR	CA-CB-OG1	-5.01	102.09	109.60
1	F	329	PHE	CB-CA-C	5.01	119.07	110.81
1	G	99	ASN	CA-C-N	-5.01	114.68	122.09
1	G	99	ASN	C-N-CA	-5.01	114.68	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	137	THR	CA-CB-OG1	-5.00	102.09	109.60
1	H	179	SER	CA-C-O	-5.00	115.45	121.40

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	2448	0	2433	348	0
1	B	2448	0	2433	322	0
1	C	2448	0	2433	324	2
1	D	2448	0	2433	327	0
1	E	2448	0	2433	318	0
1	F	2448	0	2433	309	0
1	G	2448	0	2433	312	0
1	H	2448	0	2433	336	0
2	A	40	0	20	0	0
2	B	40	0	20	0	0
2	E	40	0	20	0	0
2	F	40	0	20	0	0
3	A	6	0	2	2	0
3	B	6	0	2	2	0
3	C	6	0	2	2	0
3	D	6	0	2	1	0
3	E	6	0	2	2	0
3	F	6	0	2	1	0
3	G	6	0	2	1	0
3	H	6	0	2	0	0
4	A	44	0	26	7	0
4	B	44	0	26	9	0
4	C	44	0	26	3	0
4	D	44	0	26	6	0
4	E	44	0	26	9	0
4	F	44	0	26	6	0
4	G	44	0	26	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	44	0	26	4	0
5	A	72	0	0	34	0
5	B	72	0	0	29	2
5	C	69	0	0	23	0
5	D	74	0	0	20	0
5	E	70	0	0	29	0
5	F	72	0	0	23	0
5	G	70	0	0	22	0
5	H	73	0	0	22	0
All	All	20716	0	19768	2348	2

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 59.

All (2348) 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:E:279:LEU:HB2	5:E:398:HOH:O	1.34	1.26
1:A:15:MET:HB2	1:A:19:GLY:CA	1.69	1.21
5:E:421:HOH:O	1:H:70:VAL:HG22	1.35	1.21
1:D:215:VAL:HG23	5:D:405:HOH:O	1.42	1.18
1:D:215:VAL:HB	1:D:222:ALA:CB	1.71	1.17
1:F:204:ALA:HB1	1:F:211:ILE:HD12	1.28	1.15
1:D:101:LYS:HD2	5:D:423:HOH:O	1.47	1.13
1:E:15:MET:HB2	1:E:19:GLY:N	1.64	1.12
1:H:215:VAL:HB	1:H:222:ALA:CB	1.80	1.11
1:A:15:MET:HB2	1:A:19:GLY:HA3	1.28	1.11
1:B:209:MET:HG2	1:B:214:LEU:HD21	1.28	1.11
1:B:215:VAL:HB	1:B:222:ALA:HB1	1.24	1.11
1:H:215:VAL:HB	1:H:222:ALA:HB1	1.17	1.11
1:D:221:GLU:HA	5:D:425:HOH:O	1.47	1.10
1:F:212:ARG:HH12	1:F:226:LEU:HB2	1.07	1.10
1:G:209:MET:HG2	1:G:214:LEU:HD21	1.20	1.09
1:E:215:VAL:HA	1:E:218:LYS:HD2	1.30	1.09
1:G:265:ASN:HB3	1:H:15:MET:HA	1.32	1.09
1:D:22:ARG:HG2	1:D:89:ALA:HA	1.30	1.08
1:B:149:LYS:HE2	1:B:149:LYS:HA	1.36	1.08
1:G:16:LYS:N	1:G:16:LYS:HD2	1.62	1.08
1:B:153:LEU:O	5:B:384:HOH:O	1.72	1.07
1:A:206:ILE:HD11	1:A:211:ILE:HD11	1.14	1.07
1:E:118:ARG:HB3	1:E:118:ARG:HH11	1.02	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:LEU:HB3	1:F:313:ARG:HD3	1.37	1.07
1:A:100:GLN:HB2	1:A:105:THR:O	1.54	1.06
1:F:146:ALA:HA	1:F:329:PHE:HZ	1.16	1.06
1:G:112:LYS:HE2	1:G:112:LYS:HA	1.37	1.05
1:H:112:LYS:O	1:H:115:ALA:HB3	1.56	1.05
1:H:114:ILE:HG21	1:H:330:THR:HA	1.35	1.05
1:H:118:ARG:HG2	1:H:150:PHE:CE2	1.91	1.05
1:H:210:PRO:HG2	1:H:213:LYS:HD3	1.14	1.05
1:G:215:VAL:HB	1:G:222:ALA:HB1	1.08	1.05
1:D:15:MET:N	5:D:359:HOH:O	1.87	1.04
1:G:265:ASN:CB	1:H:15:MET:HA	1.85	1.04
1:F:212:ARG:HH12	1:F:226:LEU:CB	1.68	1.04
1:H:209:MET:HG3	1:H:214:LEU:HD21	1.39	1.04
1:F:265:ASN:HD22	1:F:295:ARG:HB2	1.23	1.04
1:B:118:ARG:HH11	1:B:118:ARG:HB3	0.90	1.04
1:E:215:VAL:HB	1:E:222:ALA:HB1	1.37	1.03
1:E:240:ILE:HG12	1:H:63:MET:HE3	1.33	1.03
1:D:215:VAL:HG21	1:D:226:LEU:HD11	1.37	1.03
1:C:221:GLU:OE1	1:C:224:LYS:HG2	1.59	1.03
4:G:352:NAD:H2D	5:G:452:HOH:O	1.56	1.03
1:G:221:GLU:HA	5:G:501:HOH:O	1.57	1.02
1:C:221:GLU:HG2	1:C:223:GLN:HB2	1.40	1.02
1:F:212:ARG:HH11	1:F:226:LEU:HD12	1.23	1.02
1:A:182:PRO:HG3	5:A:389:HOH:O	1.60	1.02
1:A:295:ARG:HD2	1:B:15:MET:CG	1.90	1.02
1:F:125:MET:HA	1:F:125:MET:HE3	1.41	1.02
1:B:39:LEU:HD22	1:B:44:ILE:HB	1.41	1.02
1:A:101:LYS:HB3	1:A:102:PRO:HD2	1.40	1.01
1:E:15:MET:HA	1:F:265:ASN:HB2	1.38	1.01
1:E:218:LYS:HG3	1:E:222:ALA:HB2	1.42	1.01
1:H:15:MET:N	5:H:360:HOH:O	1.92	1.01
1:A:16:LYS:HD2	1:A:46:ASP:O	1.57	1.01
1:D:215:VAL:CB	1:D:222:ALA:HB1	1.90	1.01
1:A:265:ASN:HB2	1:B:15:MET:HA	1.43	1.01
1:D:215:VAL:HB	1:D:222:ALA:HB1	1.05	1.00
1:E:265:ASN:CB	1:F:15:MET:HA	1.91	1.00
1:H:221:GLU:OE1	1:H:221:GLU:HA	1.58	1.00
1:F:55:GLU:O	1:F:59:ILE:HG13	1.61	1.00
1:B:118:ARG:HB3	1:B:118:ARG:NH1	1.76	1.00
1:A:295:ARG:HD2	1:B:15:MET:HG3	1.43	1.00
1:C:221:GLU:HB3	1:C:224:LYS:HB2	1.39	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:VAL:HG13	1:D:142:ILE:HG21	1.43	0.99
1:B:234:ARG:NH1	1:B:235:ASP:OD1	1.94	0.99
1:D:209:MET:HA	1:D:209:MET:HE2	1.43	0.98
1:F:265:ASN:ND2	1:F:295:ARG:HB2	1.77	0.98
1:G:215:VAL:HB	1:G:222:ALA:CB	1.93	0.98
1:H:215:VAL:CB	1:H:222:ALA:HB1	1.94	0.98
1:E:215:VAL:HB	1:E:222:ALA:CB	1.95	0.97
1:F:145:TYR:CE1	1:F:149:LYS:HD3	2.00	0.97
1:E:264:HIS:HB3	1:F:16:LYS:HZ3	1.27	0.97
1:H:74:LYS:HD2	1:H:75:PRO:HD2	1.44	0.97
1:H:209:MET:CG	1:H:214:LEU:HD21	1.94	0.97
1:G:138:ASN:HB2	4:G:352:NAD:O2D	1.64	0.96
1:E:265:ASN:HB3	1:F:15:MET:HA	1.46	0.95
1:A:206:ILE:CD1	1:A:211:ILE:HD11	1.94	0.95
1:B:70:VAL:HG23	5:B:363:HOH:O	1.65	0.95
1:F:304:ILE:HA	1:H:209:MET:CE	1.97	0.95
1:H:83:TYR:O	1:H:127:SER:HB2	1.66	0.95
1:E:15:MET:HB2	1:E:19:GLY:CA	1.96	0.95
1:G:124:VAL:HG11	1:G:133:PHE:HZ	1.32	0.95
1:E:209:MET:HB3	1:E:214:LEU:HD21	1.49	0.95
1:F:87:ARG:HD3	1:F:127:SER:O	1.67	0.95
1:F:118:ARG:HB3	1:F:118:ARG:HH11	1.29	0.95
1:C:83:TYR:O	1:C:127:SER:HB2	1.67	0.94
1:E:294:ASN:C	1:E:294:ASN:HD22	1.75	0.94
1:G:209:MET:HE2	1:G:209:MET:HA	1.50	0.94
1:G:86:CYS:SG	1:G:124:VAL:HG23	2.07	0.94
1:E:251:ILE:HD13	4:E:352:NAD:O7N	1.66	0.94
1:C:16:LYS:HZ1	1:D:264:HIS:HB3	1.30	0.94
1:B:112:LYS:HD2	5:B:378:HOH:O	1.65	0.93
1:G:190:ILE:HD13	1:G:200:VAL:HG21	1.50	0.93
1:C:16:LYS:NZ	1:D:264:HIS:O	1.99	0.93
1:G:213:LYS:HA	1:G:216:GLU:HB3	1.49	0.93
1:F:145:TYR:CD1	1:F:329:PHE:HE2	1.85	0.93
1:A:70:VAL:HG13	1:D:182:PRO:HB2	1.50	0.93
1:B:87:ARG:HG3	1:B:127:SER:O	1.69	0.93
1:A:213:LYS:HA	1:A:216:GLU:HB2	1.49	0.93
1:E:16:LYS:HB2	5:F:355:HOH:O	1.67	0.93
1:H:118:ARG:HB3	1:H:118:ARG:HH11	1.31	0.93
1:G:215:VAL:CB	1:G:222:ALA:HB1	1.98	0.92
1:E:220:GLU:HA	1:E:223:GLN:HB2	1.51	0.92
1:G:16:LYS:HD2	1:G:16:LYS:H	1.28	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:LYS:O	1:H:104:GLU:HB2	1.69	0.92
1:F:215:VAL:HB	1:F:222:ALA:HB1	1.51	0.92
1:E:118:ARG:HB3	1:E:118:ARG:NH1	1.84	0.92
1:H:240:ILE:CG2	1:H:244:LYS:HD2	2.00	0.92
1:C:15:MET:HB2	1:C:19:GLY:N	1.85	0.92
1:A:54:ASN:HD22	1:A:54:ASN:C	1.75	0.92
1:D:74:LYS:HG2	1:D:75:PRO:HD2	1.52	0.92
1:D:22:ARG:CG	1:D:89:ALA:HA	2.00	0.91
1:B:265:ASN:HD22	1:B:295:ARG:H	1.19	0.91
1:G:74:LYS:HD2	1:G:75:PRO:HD2	1.49	0.91
1:F:234:ARG:HD2	1:F:235:ASP:OD1	1.70	0.91
1:B:118:ARG:HH11	1:B:118:ARG:CB	1.81	0.91
1:D:220:GLU:HA	1:D:223:GLN:HB2	1.51	0.91
1:G:213:LYS:HB2	1:G:213:LYS:NZ	1.86	0.91
1:F:166:ASP:OD1	5:F:387:HOH:O	1.89	0.90
1:B:149:LYS:HE2	1:B:149:LYS:CA	1.97	0.90
1:D:138:ASN:HB2	4:D:352:NAD:O2D	1.71	0.90
1:F:87:ARG:HG3	1:F:128:GLY:C	1.95	0.90
1:E:15:MET:HA	1:F:265:ASN:CB	2.01	0.90
1:H:309:ASP:O	1:H:313:ARG:HG3	1.71	0.90
1:F:204:ALA:CB	1:F:211:ILE:HD12	2.02	0.90
1:G:213:LYS:HB2	1:G:213:LYS:HZ3	1.35	0.90
1:D:16:LYS:HG3	1:D:46:ASP:O	1.72	0.90
1:E:204:ALA:HB1	1:E:211:ILE:HD12	1.49	0.90
1:A:294:ASN:HD22	1:A:294:ASN:C	1.79	0.90
1:B:36:VAL:HG21	1:B:50:LEU:HD21	1.54	0.89
1:B:215:VAL:HB	1:B:222:ALA:CB	2.01	0.89
1:C:118:ARG:HB3	1:C:118:ARG:HH11	1.38	0.89
1:G:209:MET:CG	1:G:214:LEU:HD21	2.02	0.89
1:A:15:MET:CB	1:A:19:GLY:HA3	2.01	0.89
1:F:146:ALA:HA	1:F:329:PHE:CZ	2.07	0.89
1:A:152:GLY:HA2	5:A:381:HOH:O	1.73	0.89
1:D:318:ALA:O	1:D:322:LYS:HG2	1.71	0.89
1:E:59:ILE:CG2	1:H:243:LYS:HD3	2.03	0.89
1:G:101:LYS:HB3	1:G:102:PRO:HD2	1.53	0.88
1:G:224:LYS:HB2	5:G:501:HOH:O	1.71	0.88
1:F:87:ARG:NH1	1:F:87:ARG:HB2	1.86	0.88
1:H:114:ILE:CG2	1:H:330:THR:HA	2.04	0.88
1:B:59:ILE:HG22	1:B:63:MET:HE2	1.53	0.88
1:D:223:GLN:OE1	1:D:223:GLN:HA	1.73	0.88
1:A:264:HIS:HB3	1:B:16:LYS:HZ3	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:GLU:HG2	1:C:223:GLN:CB	2.04	0.88
1:B:203:GLN:NE2	1:D:209:MET:HE1	1.88	0.88
1:F:198:LEU:CB	1:F:313:ARG:HD3	2.03	0.88
1:B:138:ASN:HB2	4:B:352:NAD:O2D	1.73	0.87
1:C:264:HIS:HB3	1:D:16:LYS:HZ3	1.35	0.87
1:E:40:MET:HE2	1:E:72:ALA:HB2	1.56	0.87
1:F:146:ALA:CA	1:F:329:PHE:HZ	1.86	0.87
1:G:209:MET:HG2	1:G:214:LEU:CD2	2.04	0.87
1:A:181:ALA:HB1	1:A:183:GLN:OE1	1.73	0.87
1:F:212:ARG:NH1	1:F:226:LEU:CD1	2.37	0.87
1:B:54:ASN:C	1:B:54:ASN:HD22	1.83	0.86
1:F:70:VAL:CG1	1:G:182:PRO:HB2	2.04	0.86
1:F:212:ARG:NH1	1:F:226:LEU:HD12	1.90	0.86
1:G:283:ARG:O	1:G:322:LYS:HE2	1.75	0.86
1:A:265:ASN:HB3	1:B:16:LYS:H	1.41	0.86
1:B:215:VAL:HG11	1:B:226:LEU:HD11	1.58	0.86
1:B:289:VAL:CG1	1:B:301:VAL:HG13	2.05	0.86
1:H:169:ARG:NH1	5:H:395:HOH:O	2.07	0.86
1:D:83:TYR:O	1:D:86:CYS:HB2	1.76	0.86
1:H:110:VAL:HG21	1:H:324:VAL:HG11	1.58	0.86
1:E:155:HIS:HD2	5:E:378:HOH:O	1.59	0.86
1:B:161:SER:O	1:B:164:ILE:HG22	1.76	0.85
1:H:55:GLU:C	1:H:59:ILE:HD12	2.02	0.85
1:C:117:PHE:O	1:C:121:VAL:HG23	1.77	0.85
1:A:264:HIS:CB	1:B:16:LYS:HZ3	1.90	0.85
1:D:94:ILE:HG21	1:D:117:PHE:CZ	2.12	0.84
1:C:215:VAL:HA	1:C:218:LYS:HG2	1.58	0.84
1:B:224:LYS:HB2	5:B:418:HOH:O	1.77	0.84
1:A:107:LEU:O	1:A:110:VAL:HG22	1.77	0.84
1:D:215:VAL:HG21	1:D:226:LEU:CD1	2.07	0.84
1:G:107:LEU:O	1:G:110:VAL:HG23	1.77	0.84
1:A:154:PRO:HA	5:A:380:HOH:O	1.78	0.84
1:B:101:LYS:HB3	1:B:102:PRO:HD2	1.58	0.84
1:B:220:GLU:HA	1:B:223:GLN:HB2	1.59	0.84
1:C:189:ILE:HD12	1:C:230:PHE:HE1	1.41	0.84
1:G:16:LYS:HB3	1:G:77:ASP:OD1	1.78	0.83
1:A:168:ALA:HA	1:D:70:VAL:HG21	1.57	0.83
1:G:215:VAL:HG23	5:G:479:HOH:O	1.76	0.83
1:E:36:VAL:HG21	1:E:50:LEU:HD21	1.58	0.83
1:H:118:ARG:HD2	1:H:330:THR:OG1	1.79	0.83
1:A:206:ILE:HD11	1:A:211:ILE:CD1	2.06	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:GLU:HA	5:E:416:HOH:O	1.77	0.83
1:F:212:ARG:HH11	1:F:226:LEU:CD1	1.91	0.83
1:A:264:HIS:HB3	1:B:16:LYS:NZ	1.93	0.83
1:E:70:VAL:HG23	5:E:360:HOH:O	1.77	0.83
1:A:15:MET:HB2	1:A:19:GLY:N	1.94	0.82
1:B:109:LEU:HD22	5:B:378:HOH:O	1.77	0.82
1:F:294:ASN:HD22	1:F:296:ASN:H	1.25	0.82
4:E:352:NAD:O7N	5:E:381:HOH:O	1.97	0.82
1:F:87:ARG:HG3	1:F:128:GLY:CA	2.09	0.82
1:D:209:MET:HE2	1:D:209:MET:CA	2.04	0.82
1:D:221:GLU:HA	1:D:221:GLU:OE1	1.79	0.82
1:E:265:ASN:HB2	1:E:295:ARG:HB2	1.61	0.82
1:D:218:LYS:HG3	1:D:222:ALA:HB2	1.60	0.82
1:C:15:MET:SD	1:C:19:GLY:HA3	2.20	0.82
1:E:118:ARG:HH11	1:E:118:ARG:CB	1.89	0.82
1:F:70:VAL:HG13	1:G:182:PRO:HB2	1.58	0.81
1:A:43:GLY:O	1:A:74:LYS:HD2	1.81	0.81
1:D:228:ARG:HB3	1:D:228:ARG:HH11	1.45	0.81
1:F:216:GLU:HA	5:F:398:HOH:O	1.78	0.81
1:H:144:THR:HG22	1:H:286:TYR:CD2	2.15	0.81
1:H:244:LYS:HD3	1:H:246:ALA:O	1.80	0.81
1:D:221:GLU:O	1:D:222:ALA:C	2.24	0.81
1:F:15:MET:N	5:F:354:HOH:O	2.13	0.81
1:G:218:LYS:HG3	1:G:222:ALA:HB2	1.60	0.81
1:B:15:MET:N	5:B:354:HOH:O	2.12	0.81
1:G:190:ILE:HD13	1:G:200:VAL:CG2	2.09	0.81
1:F:315:HIS:HB2	5:F:400:HOH:O	1.81	0.81
1:C:82:ASP:O	1:C:85:ASP:HB2	1.80	0.81
1:G:264:HIS:C	1:H:16:LYS:HZ3	1.87	0.81
1:A:40:MET:HE2	1:A:72:ALA:HB2	1.62	0.81
1:A:264:HIS:O	1:B:16:LYS:HD3	1.81	0.81
1:A:294:ASN:ND2	1:A:296:ASN:H	1.78	0.80
1:B:15:MET:HB2	1:B:19:GLY:N	1.96	0.80
1:F:212:ARG:NH1	1:F:226:LEU:HB2	1.91	0.80
1:H:220:GLU:HA	1:H:223:GLN:HB2	1.61	0.80
1:D:23:VAL:HG22	1:D:91:LEU:HD23	1.62	0.80
1:A:210:PRO:O	1:A:214:LEU:HG	1.81	0.80
1:A:295:ARG:HD3	1:B:15:MET:HE3	1.62	0.80
1:D:265:ASN:HB2	1:D:295:ARG:HB2	1.63	0.80
1:B:106:ARG:HB2	5:B:376:HOH:O	1.82	0.80
1:B:114:ILE:HG21	1:B:330:THR:HA	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:ARG:NH1	1:F:226:LEU:CB	2.42	0.80
1:C:215:VAL:HB	1:C:222:ALA:CB	2.12	0.80
1:D:107:LEU:O	1:D:110:VAL:HG23	1.82	0.80
1:G:145:TYR:CE1	1:G:329:PHE:HE2	2.00	0.80
1:G:315:HIS:HB2	5:G:482:HOH:O	1.81	0.80
1:A:104:GLU:O	1:A:105:THR:HG22	1.82	0.79
1:B:257:ARG:NH2	1:B:266:GLU:OE2	2.15	0.79
1:B:289:VAL:HG13	1:B:301:VAL:HG13	1.64	0.79
1:D:319:ALA:O	1:D:322:LYS:HB2	1.82	0.79
1:E:294:ASN:ND2	1:E:296:ASN:H	1.80	0.79
1:C:16:LYS:NZ	1:D:264:HIS:HB3	1.96	0.79
1:C:228:ARG:NH1	1:C:232:ASN:ND2	2.31	0.79
1:H:221:GLU:O	1:H:222:ALA:C	2.26	0.79
1:B:15:MET:HB2	1:B:19:GLY:CA	2.12	0.79
1:H:243:LYS:NZ	1:H:243:LYS:HB2	1.95	0.79
1:G:124:VAL:HG11	1:G:133:PHE:CZ	2.17	0.79
1:A:54:ASN:ND2	1:A:57:LYS:H	1.80	0.79
1:C:107:LEU:O	1:C:110:VAL:HG23	1.83	0.79
1:G:222:ALA:HB3	5:G:479:HOH:O	1.82	0.79
1:E:240:ILE:HG12	1:H:63:MET:CE	2.11	0.79
1:B:177:TYR:CE1	1:B:225:ASP:HB3	2.17	0.78
1:F:16:LYS:HB3	1:F:77:ASP:OD1	1.84	0.78
1:G:227:GLU:O	1:G:231:VAL:HG23	1.83	0.78
1:A:100:GLN:CB	1:A:105:THR:O	2.30	0.78
1:A:213:LYS:HE2	1:C:305:GLU:HG3	1.65	0.78
1:C:180:VAL:HG21	1:C:206:ILE:HG23	1.66	0.78
1:D:265:ASN:ND2	1:D:295:ARG:HB2	1.98	0.78
1:D:294:ASN:HD22	1:D:296:ASN:H	1.29	0.78
1:E:264:HIS:CB	1:F:16:LYS:HZ3	1.95	0.78
1:F:304:ILE:HA	1:H:209:MET:HE1	1.66	0.78
1:F:194:GLY:O	1:F:197:GLU:HG2	1.83	0.78
1:H:220:GLU:CA	1:H:223:GLN:HB2	2.12	0.78
1:A:265:ASN:CB	1:B:16:LYS:H	1.96	0.78
1:A:295:ARG:HB3	1:B:15:MET:HE2	1.66	0.78
1:B:221:GLU:CA	5:B:418:HOH:O	2.31	0.78
1:H:215:VAL:HA	1:H:218:LYS:HE3	1.65	0.78
1:C:221:GLU:HB3	1:C:224:LYS:H	1.49	0.77
1:F:145:TYR:CE1	1:F:329:PHE:HE2	2.02	0.77
1:A:120:ILE:O	1:A:124:VAL:HG13	1.84	0.77
1:C:16:LYS:HB3	1:C:77:ASP:OD1	1.83	0.77
5:E:423:HOH:O	1:H:71:PHE:HE2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:ASN:O	1:G:69:LYS:HG2	1.83	0.77
1:A:70:VAL:HG22	5:A:360:HOH:O	1.82	0.77
1:C:264:HIS:HB3	1:D:16:LYS:NZ	1.99	0.77
1:B:221:GLU:HA	5:B:418:HOH:O	1.84	0.77
1:A:251:ILE:O	1:A:255:LEU:HD22	1.85	0.77
1:B:61:ASP:HB3	1:B:65:PHE:CE2	2.20	0.77
1:B:87:ARG:HG3	1:B:127:SER:C	2.10	0.77
1:C:265:ASN:HD22	1:C:295:ARG:HB2	1.49	0.77
1:D:212:ARG:HH11	1:D:226:LEU:HD13	1.50	0.77
1:D:248:TYR:HA	1:D:251:ILE:HG22	1.67	0.77
1:F:304:ILE:HB	1:H:209:MET:HE1	1.66	0.76
1:A:35:TYR:CZ	1:A:39:LEU:HD11	2.19	0.76
4:G:352:NAD:H6N	5:G:450:HOH:O	1.84	0.76
1:A:221:GLU:HA	5:A:417:HOH:O	1.85	0.76
1:H:267:ASN:ND2	1:H:294:ASN:HB3	1.99	0.76
1:C:114:ILE:HD13	1:C:143:LEU:HD23	1.68	0.76
1:E:244:LYS:HE2	1:H:61:ASP:OD1	1.85	0.76
1:H:254:GLY:O	1:H:258:VAL:HG23	1.85	0.76
1:B:209:MET:HG2	1:B:214:LEU:CD2	2.11	0.76
1:D:265:ASN:HD22	1:D:295:ARG:HB2	1.48	0.76
1:A:91:LEU:HD21	1:A:134:LEU:HD23	1.67	0.76
1:C:189:ILE:HD12	1:C:230:PHE:CE1	2.21	0.76
1:E:59:ILE:HG21	1:H:243:LYS:HD3	1.67	0.76
1:E:295:ARG:HD2	1:F:15:MET:HG3	1.66	0.76
1:C:16:LYS:HZ3	1:D:264:HIS:C	1.93	0.76
1:G:15:MET:HB2	1:G:19:GLY:C	2.11	0.76
1:B:15:MET:SD	1:B:19:GLY:HA3	2.26	0.76
1:H:322:LYS:O	1:H:325:LEU:HB2	1.86	0.76
1:E:265:ASN:HB2	1:F:15:MET:HA	1.68	0.75
1:E:59:ILE:HG22	1:H:243:LYS:HD3	1.68	0.75
1:G:22:ARG:HG2	1:G:89:ALA:HA	1.68	0.75
1:H:75:PRO:HA	5:H:370:HOH:O	1.85	0.75
1:A:315:HIS:HB2	5:A:400:HOH:O	1.86	0.75
1:E:15:MET:HG3	1:F:295:ARG:HD2	1.68	0.75
1:G:215:VAL:HG11	1:G:226:LEU:HD11	1.69	0.75
1:B:227:GLU:O	1:B:231:VAL:HG23	1.86	0.75
1:C:264:HIS:CB	1:D:16:LYS:HZ3	1.99	0.75
1:F:125:MET:HA	1:F:125:MET:CE	2.16	0.75
1:C:174:LEU:HD23	1:C:229:ILE:HD13	1.67	0.75
1:E:194:GLY:O	1:E:197:GLU:HG2	1.86	0.75
1:H:309:ASP:O	1:H:313:ARG:CG	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLU:HG3	1:B:75:PRO:HG3	1.69	0.75
1:A:16:LYS:HE3	1:A:46:ASP:HA	1.66	0.75
1:A:192:GLU:O	1:A:197:GLU:HB3	1.87	0.75
1:B:243:LYS:HG2	1:C:56:SER:O	1.86	0.75
1:G:54:ASN:C	1:G:54:ASN:HD22	1.94	0.75
1:A:275:TYR:CE1	1:A:284:ASP:HA	2.22	0.75
1:H:55:GLU:O	1:H:59:ILE:HD12	1.87	0.75
1:H:144:THR:CG2	1:H:286:TYR:CD2	2.70	0.75
1:C:35:TYR:CZ	1:C:39:LEU:HD11	2.22	0.74
1:E:15:MET:CG	1:E:19:GLY:HA3	2.17	0.74
1:E:15:MET:HB3	1:E:17:ASN:C	2.12	0.74
1:G:210:PRO:O	1:G:213:LYS:HG2	1.88	0.74
1:B:315:HIS:HB2	5:B:402:HOH:O	1.86	0.74
4:C:352:NAD:O2D	5:C:373:HOH:O	2.05	0.74
1:E:15:MET:HB2	1:E:19:GLY:HA3	1.67	0.74
1:B:39:LEU:HD23	1:B:44:ILE:HD12	1.69	0.74
1:F:304:ILE:HA	1:H:209:MET:HE3	1.68	0.74
1:C:265:ASN:ND2	1:C:295:ARG:HB2	2.03	0.74
1:E:212:ARG:HH12	1:E:226:LEU:HD12	1.52	0.74
1:C:228:ARG:HH12	1:C:232:ASN:ND2	1.85	0.74
1:D:174:LEU:O	1:D:178:PHE:HD1	1.70	0.74
1:E:203:GLN:NE2	1:G:209:MET:HE1	2.02	0.74
1:H:39:LEU:HD12	1:H:48:ILE:HD13	1.69	0.74
1:F:132:LEU:HD12	1:F:157:ARG:HB3	1.69	0.74
1:B:64:ASP:OD2	1:C:244:LYS:CE	2.36	0.74
1:A:107:LEU:O	1:A:110:VAL:CG2	2.36	0.74
1:B:98:ALA:O	1:B:109:LEU:HD13	1.88	0.74
1:E:110:VAL:HG12	1:E:111:ASP:N	2.03	0.74
1:F:313:ARG:HG2	1:F:313:ARG:HH11	1.50	0.74
1:G:15:MET:HA	1:H:265:ASN:HB3	1.70	0.74
1:A:234:ARG:O	5:A:385:HOH:O	2.06	0.73
1:A:54:ASN:HD21	1:A:57:LYS:H	1.33	0.73
1:A:106:ARG:O	1:A:109:LEU:HG	1.88	0.73
1:C:309:ASP:O	1:C:312:ASN:HB3	1.88	0.73
1:E:16:LYS:H	1:F:265:ASN:HB3	1.53	0.73
1:G:283:ARG:O	1:G:322:LYS:CE	2.36	0.73
1:A:180:VAL:HG11	1:C:269:ILE:HD11	1.70	0.73
1:B:141:ASP:OD1	1:B:273:SER:OG	2.05	0.73
1:F:213:LYS:HA	1:F:216:GLU:HB3	1.71	0.73
1:H:15:MET:HB2	1:H:19:GLY:N	2.03	0.73
1:C:215:VAL:HB	1:C:222:ALA:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ASN:HB2	1:D:15:MET:HA	1.69	0.73
1:C:247:THR:HG21	3:C:351:OXM:O3	1.89	0.73
1:E:212:ARG:NH1	1:E:226:LEU:HD12	2.04	0.73
1:D:74:LYS:CG	1:D:75:PRO:HD2	2.18	0.73
1:E:218:LYS:CG	1:E:222:ALA:HB2	2.19	0.73
1:H:292:VAL:C	1:H:293:ILE:HD13	2.14	0.73
1:A:211:ILE:HA	1:A:214:LEU:HD12	1.68	0.73
1:C:167:THR:O	1:C:171:ARG:HG2	1.89	0.73
1:H:22:ARG:HA	1:H:47:GLU:O	1.89	0.73
1:H:210:PRO:CG	1:H:213:LYS:HD3	2.08	0.73
1:B:54:ASN:C	1:B:54:ASN:ND2	2.42	0.73
1:B:265:ASN:ND2	1:B:294:ASN:HB2	2.03	0.73
1:D:113:ASN:ND2	1:D:138:ASN:O	2.21	0.73
1:E:15:MET:HG3	1:E:19:GLY:HA3	1.71	0.72
1:E:213:LYS:HA	1:E:216:GLU:HB3	1.69	0.72
1:H:94:ILE:HG21	1:H:117:PHE:CZ	2.24	0.72
1:H:254:GLY:N	5:H:358:HOH:O	2.22	0.72
1:C:16:LYS:HB3	1:C:77:ASP:HB2	1.69	0.72
1:D:165:LEU:HD12	1:D:165:LEU:O	1.90	0.72
1:F:57:LYS:NZ	1:F:61:ASP:OD2	2.21	0.72
1:E:240:ILE:HD11	1:H:67:HIS:CE1	2.25	0.72
1:C:286:TYR:HB2	5:C:380:HOH:O	1.87	0.72
1:E:15:MET:N	5:E:417:HOH:O	2.22	0.72
1:F:43:GLY:HA2	5:F:361:HOH:O	1.90	0.72
1:G:145:TYR:HA	1:G:286:TYR:CD1	2.24	0.72
1:C:15:MET:CG	1:C:19:GLY:HA3	2.19	0.72
1:F:29:GLY:HA3	4:F:352:NAD:O5B	1.89	0.72
1:C:315:HIS:HB2	5:C:401:HOH:O	1.89	0.72
1:D:22:ARG:HG2	1:D:89:ALA:CA	2.17	0.72
1:G:221:GLU:O	1:G:222:ALA:C	2.33	0.72
1:B:213:LYS:HG3	1:B:213:LYS:O	1.84	0.72
5:B:421:HOH:O	1:C:70:VAL:HG22	1.89	0.72
1:D:110:VAL:CG1	1:D:142:ILE:HG21	2.18	0.72
1:D:164:ILE:HD11	1:D:270:LEU:HD22	1.72	0.72
1:H:80:HIS:NE2	5:H:368:HOH:O	2.23	0.72
1:E:41:ASN:O	1:E:73:PRO:CG	2.38	0.71
1:F:112:LYS:N	5:F:375:HOH:O	2.01	0.71
1:G:16:LYS:HB3	1:G:77:ASP:CG	2.15	0.71
1:A:15:MET:CG	1:A:19:GLY:HA3	2.20	0.71
1:A:54:ASN:C	1:A:54:ASN:ND2	2.48	0.71
1:H:240:ILE:HG22	1:H:244:LYS:HD2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:323:SER:O	1:H:324:VAL:C	2.32	0.71
1:E:74:LYS:HD2	1:E:75:PRO:HD2	1.72	0.71
1:E:59:ILE:HG22	1:H:243:LYS:CD	2.20	0.71
1:C:294:ASN:HD22	1:C:294:ASN:C	1.97	0.71
1:C:298:ILE:HD12	5:C:382:HOH:O	1.89	0.71
1:G:15:MET:SD	1:G:19:GLY:HA3	2.30	0.71
1:B:215:VAL:CB	1:B:222:ALA:HB1	2.12	0.71
5:B:362:HOH:O	1:C:253:MET:HE3	1.90	0.71
1:F:145:TYR:CD1	1:F:329:PHE:CE2	2.76	0.71
1:E:92:VAL:HG23	1:E:129:PHE:CZ	2.25	0.71
1:F:112:LYS:HE2	1:F:112:LYS:HA	1.72	0.71
1:H:294:ASN:ND2	1:H:296:ASN:H	1.89	0.71
1:A:55:GLU:C	1:A:59:ILE:HD12	2.16	0.71
1:A:206:ILE:HG13	1:A:214:LEU:CD1	2.21	0.71
1:A:212:ARG:HH11	1:A:226:LEU:HD12	1.56	0.71
1:A:294:ASN:HD22	1:A:296:ASN:H	1.37	0.71
1:E:289:VAL:HG22	1:E:290:PRO:HD2	1.73	0.71
1:F:294:ASN:ND2	1:F:296:ASN:H	1.88	0.71
1:H:228:ARG:NH1	1:H:228:ARG:O	2.24	0.71
1:D:107:LEU:HD13	1:D:324:VAL:HG21	1.72	0.70
1:E:75:PRO:HA	5:H:356:HOH:O	1.91	0.70
1:B:55:GLU:C	1:B:59:ILE:HD13	2.15	0.70
1:F:59:ILE:O	1:F:63:MET:HG3	1.91	0.70
1:B:258:VAL:O	1:B:261:ALA:N	2.25	0.70
1:D:110:VAL:HG22	1:D:139:PRO:HG2	1.74	0.70
1:F:87:ARG:CD	1:F:128:GLY:HA3	2.21	0.70
1:B:15:MET:CG	1:B:19:GLY:HA3	2.22	0.70
1:D:213:LYS:HG3	1:D:213:LYS:O	1.91	0.70
1:D:225:ASP:O	1:D:228:ARG:HB2	1.91	0.70
1:E:15:MET:CB	1:E:19:GLY:HA3	2.20	0.70
1:A:218:LYS:HG3	1:A:222:ALA:CB	2.21	0.70
1:B:55:GLU:HB3	1:B:59:ILE:HD11	1.73	0.70
1:C:116:ILE:CG2	1:C:120:ILE:HD12	2.21	0.70
1:G:138:ASN:CB	4:G:352:NAD:O2D	2.39	0.70
1:D:287:ILE:HG13	1:D:321:LEU:HD12	1.73	0.70
1:E:294:ASN:C	1:E:294:ASN:ND2	2.50	0.70
1:B:138:ASN:CG	4:B:352:NAD:HO2N	1.99	0.70
1:E:15:MET:HG3	1:F:295:ARG:CD	2.22	0.70
1:F:39:LEU:HD23	1:F:44:ILE:HD12	1.72	0.70
1:A:209:MET:HE3	1:C:304:ILE:HA	1.72	0.70
1:C:145:TYR:HD1	1:C:329:PHE:HZ	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:VAL:HA	1:E:79:TRP:O	1.91	0.70
1:F:66:ASN:O	1:F:69:LYS:HG2	1.91	0.70
1:G:101:LYS:HD2	5:G:499:HOH:O	1.92	0.70
1:H:45:ALA:O	1:H:76:VAL:HG23	1.92	0.70
1:B:114:ILE:HD11	1:B:328:ALA:HB1	1.73	0.70
1:C:240:ILE:CG2	1:C:244:LYS:HD3	2.22	0.70
1:F:215:VAL:HB	1:F:222:ALA:CB	2.21	0.70
1:F:304:ILE:CB	1:H:209:MET:HE1	2.22	0.70
1:H:240:ILE:CG2	1:H:244:LYS:CD	2.70	0.70
1:C:295:ARG:HB3	1:D:15:MET:HE2	1.73	0.70
1:D:209:MET:HA	1:D:209:MET:CE	2.15	0.70
1:H:167:THR:O	1:H:171:ARG:HG3	1.92	0.70
1:E:170:PHE:CE2	1:E:187:ALA:HB1	2.27	0.69
1:H:161:SER:OG	5:H:391:HOH:O	2.10	0.69
1:C:16:LYS:HB3	1:C:77:ASP:CG	2.17	0.69
1:C:229:ILE:HG22	1:C:230:PHE:N	2.08	0.69
1:E:274:ALA:O	1:E:286:TYR:HA	1.92	0.69
1:G:92:VAL:HG12	1:G:133:PHE:CE1	2.27	0.69
1:A:224:LYS:HB2	5:A:417:HOH:O	1.91	0.69
1:F:15:MET:HB2	1:F:19:GLY:C	2.16	0.69
1:F:15:MET:HB2	1:F:19:GLY:CA	2.21	0.69
1:F:323:SER:O	1:F:327:ARG:HG3	1.92	0.69
1:G:211:ILE:O	1:G:215:VAL:HG13	1.92	0.69
1:G:294:ASN:ND2	1:G:296:ASN:H	1.91	0.69
1:H:83:TYR:O	1:H:127:SER:CB	2.41	0.69
1:B:80:HIS:NE2	5:B:361:HOH:O	2.25	0.69
1:G:264:HIS:O	1:G:265:ASN:C	2.35	0.69
1:B:294:ASN:C	1:B:294:ASN:HD22	2.00	0.69
1:E:294:ASN:HD22	1:E:296:ASN:H	1.40	0.69
1:G:327:ARG:NH2	1:G:328:ALA:HB2	2.07	0.69
1:H:210:PRO:HB2	1:H:213:LYS:HB2	1.74	0.69
1:B:265:ASN:HB2	1:B:295:ARG:CG	2.22	0.69
1:B:287:ILE:HG13	1:B:321:LEU:HD11	1.72	0.69
1:G:299:ARG:NH2	1:G:300:GLU:OE2	2.25	0.69
1:A:145:TYR:CD1	1:A:329:PHE:HE2	2.11	0.69
1:E:145:TYR:CE1	1:E:329:PHE:HE2	2.11	0.69
1:F:87:ARG:HB2	1:F:87:ARG:HH11	1.53	0.69
1:G:124:VAL:CG1	1:G:133:PHE:HZ	2.04	0.69
1:G:309:ASP:O	1:G:313:ARG:HG3	1.92	0.69
1:B:221:GLU:O	5:B:418:HOH:O	2.11	0.68
1:C:145:TYR:HD1	1:C:329:PHE:CZ	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:ALA:CB	1:E:211:ILE:HD12	2.24	0.68
1:G:213:LYS:NZ	1:G:213:LYS:CB	2.56	0.68
1:G:237:ALA:O	1:G:241:ILE:HD12	1.93	0.68
1:A:295:ARG:CD	1:B:15:MET:HE3	2.22	0.68
1:B:138:ASN:CB	4:B:352:NAD:O2D	2.41	0.68
1:C:15:MET:HA	1:D:265:ASN:HB3	1.75	0.68
1:D:294:ASN:ND2	1:D:296:ASN:H	1.92	0.68
1:F:289:VAL:HG13	1:F:301:VAL:HG13	1.74	0.68
1:H:94:ILE:CG2	1:H:117:PHE:CZ	2.76	0.68
1:A:264:HIS:CA	1:B:16:LYS:HZ3	2.05	0.68
1:C:265:ASN:CB	1:D:15:MET:HA	2.23	0.68
1:E:43:GLY:HA2	5:E:357:HOH:O	1.94	0.68
1:A:41:ASN:O	1:A:73:PRO:HG3	1.92	0.68
1:A:215:VAL:HA	1:A:218:LYS:HD2	1.76	0.68
1:B:55:GLU:O	1:B:58:ALA:N	2.26	0.68
1:C:264:HIS:CE1	1:D:74:LYS:HD3	2.29	0.68
1:D:16:LYS:HB3	1:D:77:ASP:HB2	1.76	0.68
1:D:91:LEU:CD2	1:D:259:THR:HG23	2.23	0.68
1:F:256:ALA:HB3	5:F:420:HOH:O	1.92	0.68
1:D:54:ASN:HD21	1:D:56:SER:HB2	1.58	0.68
1:E:193:HIS:NE2	3:E:351:OXM:O1	2.24	0.68
1:E:265:ASN:CB	1:E:295:ARG:HB2	2.24	0.68
1:F:87:ARG:CD	1:F:127:SER:O	2.39	0.68
1:G:16:LYS:N	1:G:16:LYS:CD	2.49	0.68
1:H:222:ALA:HB3	5:H:405:HOH:O	1.94	0.68
1:D:210:PRO:HB3	5:D:403:HOH:O	1.92	0.68
1:H:238:TYR:CD1	5:H:380:HOH:O	2.47	0.68
1:B:299:ARG:NH2	1:B:300:GLU:OE2	2.26	0.68
1:D:295:ARG:O	1:D:295:ARG:HD3	1.93	0.68
1:G:264:HIS:O	1:H:16:LYS:NZ	2.28	0.67
1:H:209:MET:HG3	1:H:214:LEU:CD2	2.22	0.67
1:H:220:GLU:N	1:H:223:GLN:HB2	2.09	0.67
1:G:132:LEU:HD22	1:G:132:LEU:N	2.08	0.67
1:A:189:ILE:HD13	1:A:199:PRO:HA	1.76	0.67
1:G:22:ARG:CG	1:G:89:ALA:HA	2.24	0.67
1:C:16:LYS:CB	1:C:77:ASP:HB2	2.24	0.67
1:E:63:MET:CE	1:H:243:LYS:HD2	2.24	0.67
1:G:77:ASP:HB3	1:G:79:TRP:HZ3	1.58	0.67
1:C:260:ARG:HH22	1:D:75:PRO:CD	2.07	0.67
1:F:138:ASN:HD22	1:F:139:PRO:HA	1.60	0.67
1:A:247:THR:OG1	3:A:351:OXM:O3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:VAL:HG21	1:B:206:ILE:HG23	1.75	0.67
1:D:22:ARG:NH1	1:D:85:ASP:O	2.27	0.67
1:F:148:TRP:HB2	1:F:158:VAL:HG21	1.75	0.67
1:H:293:ILE:HD13	1:H:293:ILE:N	2.08	0.67
1:B:39:LEU:CD2	1:B:44:ILE:HB	2.23	0.67
1:C:279:LEU:HD23	1:C:301:VAL:HB	1.77	0.67
1:E:16:LYS:HD3	1:F:264:HIS:O	1.94	0.67
1:A:15:MET:HG2	1:B:295:ARG:HG3	1.76	0.67
1:C:116:ILE:HG22	1:C:120:ILE:HD12	1.76	0.67
1:F:290:PRO:HG2	1:F:304:ILE:HG23	1.77	0.67
1:A:55:GLU:O	1:A:59:ILE:HD12	1.94	0.67
1:C:218:LYS:HG3	1:C:222:ALA:HB2	1.77	0.67
1:D:253:MET:HE3	5:D:354:HOH:O	1.94	0.67
1:E:237:ALA:O	1:E:241:ILE:HG13	1.95	0.67
1:F:141:ASP:OD1	1:F:273:SER:OG	2.13	0.67
1:A:35:TYR:OH	1:A:39:LEU:HD11	1.95	0.67
1:B:316:HIS:O	1:B:319:ALA:HB3	1.95	0.67
1:D:114:ILE:HG22	5:D:415:HOH:O	1.94	0.67
1:F:244:LYS:HG2	1:F:244:LYS:O	1.93	0.67
1:H:276:LEU:CD2	1:H:279:LEU:HB3	2.25	0.67
1:A:212:ARG:HH12	1:A:226:LEU:HB3	1.59	0.66
1:B:109:LEU:O	1:B:112:LYS:HB2	1.94	0.66
1:F:16:LYS:NZ	1:F:46:ASP:OD1	2.26	0.66
1:H:294:ASN:C	1:H:294:ASN:HD22	2.03	0.66
1:E:15:MET:HB2	1:E:18:ASN:C	2.19	0.66
1:F:87:ARG:O	5:F:367:HOH:O	2.13	0.66
1:H:162:GLY:O	5:H:391:HOH:O	2.13	0.66
1:E:117:PHE:O	1:E:121:VAL:HG23	1.95	0.66
1:E:244:LYS:HD2	1:H:60:GLY:HA3	1.77	0.66
1:F:55:GLU:O	1:F:59:ILE:CG1	2.40	0.66
1:E:203:GLN:HE21	1:G:209:MET:HE1	1.60	0.66
1:E:265:ASN:HB3	1:F:16:LYS:H	1.58	0.66
1:F:188:TYR:O	1:F:189:ILE:HD13	1.95	0.66
1:A:212:ARG:HH12	1:A:226:LEU:CB	2.08	0.66
1:B:26:ILE:HG21	1:B:120:ILE:CG2	2.26	0.66
1:B:279:LEU:HD23	1:B:301:VAL:HB	1.77	0.66
1:E:141:ASP:OD1	1:E:273:SER:OG	2.13	0.66
1:F:145:TYR:CE1	1:F:149:LYS:CD	2.77	0.66
1:G:164:ILE:HD12	1:G:258:VAL:HG23	1.78	0.66
1:H:167:THR:O	1:H:171:ARG:CG	2.43	0.66
1:A:251:ILE:HG13	1:A:255:LEU:CD2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:HD22	1:A:295:ARG:N	1.94	0.66
1:C:40:MET:CE	1:C:69:LYS:HB3	2.25	0.66
1:G:170:PHE:CE2	1:G:187:ALA:HB1	2.31	0.66
1:A:16:LYS:HE2	1:A:75:PRO:O	1.95	0.66
1:C:15:MET:O	1:C:47:GLU:OE2	2.13	0.66
1:C:221:GLU:CB	1:C:224:LYS:HB2	2.21	0.66
1:H:227:GLU:O	1:H:231:VAL:HG23	1.95	0.66
1:B:304:ILE:HB	1:D:209:MET:HE3	1.76	0.66
1:E:15:MET:C	1:E:17:ASN:N	2.47	0.66
1:F:114:ILE:CG2	1:F:330:THR:HA	2.25	0.66
1:F:329:PHE:HD1	1:F:330:THR:N	1.93	0.66
1:H:299:ARG:NH2	1:H:300:GLU:OE2	2.28	0.66
1:B:202:SER:HB3	1:B:310:GLU:OE2	1.96	0.66
1:D:199:PRO:HG3	1:D:230:PHE:CD1	2.31	0.66
1:F:251:ILE:O	1:F:255:LEU:HD22	1.96	0.66
1:F:257:ARG:HG2	1:G:71:PHE:CD1	2.31	0.66
1:H:229:ILE:O	1:H:233:VAL:HG23	1.95	0.66
1:D:170:PHE:CD2	1:D:189:ILE:CD1	2.79	0.66
1:E:16:LYS:NZ	1:E:46:ASP:OD1	2.28	0.66
1:B:289:VAL:HG11	1:B:301:VAL:HG13	1.79	0.65
1:E:66:ASN:O	1:E:69:LYS:HG2	1.94	0.65
1:B:264:HIS:O	1:B:265:ASN:C	2.36	0.65
1:C:16:LYS:N	1:C:16:LYS:HD3	2.11	0.65
1:G:209:MET:HA	1:G:209:MET:CE	2.25	0.65
1:H:294:ASN:HD22	1:H:296:ASN:H	1.43	0.65
1:A:213:LYS:HG3	1:A:213:LYS:O	1.95	0.65
1:E:94:ILE:HG21	1:E:117:PHE:CE2	2.32	0.65
1:A:295:ARG:O	1:A:295:ARG:HG2	1.96	0.65
1:B:243:LYS:HG3	1:C:56:SER:HB3	1.79	0.65
1:G:74:LYS:CD	1:G:75:PRO:HD2	2.26	0.65
1:H:54:ASN:C	1:H:54:ASN:HD22	2.03	0.65
1:A:91:LEU:HD11	1:A:134:LEU:HB2	1.79	0.65
1:A:109:LEU:HB3	1:A:113:ASN:ND2	2.12	0.65
1:B:70:VAL:HG22	1:C:182:PRO:HB3	1.78	0.65
1:C:260:ARG:HH22	1:D:75:PRO:HD3	1.61	0.65
1:E:54:ASN:ND2	1:E:57:LYS:H	1.94	0.65
1:E:116:ILE:HG22	1:E:120:ILE:HD11	1.76	0.65
1:G:228:ARG:O	1:G:228:ARG:HD3	1.96	0.65
1:H:218:LYS:CG	1:H:218:LYS:O	2.43	0.65
1:A:16:LYS:HE3	1:A:46:ASP:CA	2.27	0.65
1:E:132:LEU:HD22	1:E:132:LEU:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:PHE:HE2	1:E:187:ALA:HB1	1.60	0.65
1:E:304:ILE:HG13	1:E:306:LEU:CD2	2.27	0.65
1:F:145:TYR:HD1	1:F:329:PHE:HE2	1.40	0.65
1:F:87:ARG:CB	1:F:87:ARG:CZ	2.73	0.65
1:G:138:ASN:HB2	4:G:352:NAD:HO2N	1.58	0.65
1:A:266:GLU:CG	1:B:75:PRO:HG3	2.26	0.65
1:C:35:TYR:CD1	1:C:255:LEU:HB3	2.31	0.65
1:E:253:MET:SD	1:H:41:ASN:OD1	2.54	0.65
1:F:313:ARG:HG2	1:F:313:ARG:NH1	2.11	0.65
1:A:313:ARG:O	1:A:316:HIS:HB3	1.97	0.65
1:E:40:MET:O	5:E:358:HOH:O	2.14	0.65
1:H:54:ASN:C	1:H:54:ASN:ND2	2.55	0.65
1:E:41:ASN:O	1:E:73:PRO:HG3	1.96	0.65
1:F:87:ARG:NH1	1:F:87:ARG:CB	2.60	0.65
1:G:159:ILE:HD13	1:G:298:ILE:HG12	1.79	0.65
1:G:213:LYS:CA	1:G:216:GLU:HB3	2.26	0.65
1:C:101:LYS:NZ	1:C:101:LYS:HB3	2.12	0.64
1:E:220:GLU:CA	1:E:223:GLN:HB2	2.26	0.64
1:G:291:ALA:HB1	1:G:298:ILE:HG23	1.79	0.64
1:A:151:SER:HB2	1:A:153:LEU:HD12	1.79	0.64
1:B:209:MET:HE1	1:D:305:GLU:H	1.63	0.64
1:C:117:PHE:HD2	1:C:147:THR:OG1	1.81	0.64
1:C:148:TRP:HA	1:C:158:VAL:HG21	1.77	0.64
1:C:221:GLU:OE1	1:C:224:LYS:CG	2.41	0.64
1:D:228:ARG:HH11	1:D:228:ARG:CB	2.10	0.64
1:E:215:VAL:HA	1:E:218:LYS:CD	2.17	0.64
1:F:147:THR:O	1:F:151:SER:HB3	1.96	0.64
1:G:237:ALA:C	1:G:241:ILE:HD12	2.23	0.64
1:F:162:GLY:O	1:F:193:HIS:HB2	1.98	0.64
1:D:224:LYS:HB2	5:D:425:HOH:O	1.96	0.64
1:G:36:VAL:HG21	1:G:50:LEU:HD21	1.78	0.64
1:H:243:LYS:HB2	1:H:243:LYS:HZ3	1.61	0.64
1:A:257:ARG:O	1:A:260:ARG:HG3	1.98	0.64
1:F:100:GLN:HG3	5:F:371:HOH:O	1.97	0.64
1:A:221:GLU:CA	5:A:417:HOH:O	2.43	0.64
5:A:419:HOH:O	1:B:295:ARG:CG	2.45	0.64
1:C:101:LYS:HB3	1:C:102:PRO:HD2	1.80	0.64
1:G:299:ARG:O	1:G:300:GLU:HG3	1.97	0.64
1:A:148:TRP:CZ3	1:A:149:LYS:NZ	2.60	0.64
1:A:213:LYS:CA	1:A:216:GLU:HB2	2.24	0.64
1:E:98:ALA:HB1	5:E:374:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:LYS:HB3	1:G:102:PRO:CD	2.27	0.64
1:D:32:GLY:O	1:D:35:TYR:HB3	1.97	0.64
1:B:265:ASN:HB2	1:B:295:ARG:HG3	1.79	0.63
1:C:16:LYS:HB3	1:C:77:ASP:CB	2.26	0.63
1:C:147:THR:O	1:C:151:SER:HB3	1.99	0.63
1:F:87:ARG:HG3	1:F:128:GLY:HA3	1.79	0.63
1:A:295:ARG:HD2	1:B:15:MET:HG2	1.77	0.63
1:B:100:GLN:HG3	5:B:373:HOH:O	1.98	0.63
1:B:215:VAL:HG23	5:B:399:HOH:O	1.97	0.63
1:A:119:SER:O	1:A:122:GLU:HB2	1.99	0.63
1:F:15:MET:SD	1:F:19:GLY:HA3	2.38	0.63
1:F:167:THR:O	1:F:171:ARG:HG3	1.98	0.63
1:G:15:MET:HA	1:H:265:ASN:CB	2.27	0.63
1:A:219:GLY:O	1:A:221:GLU:HG2	1.98	0.63
1:C:324:VAL:HG13	1:C:327:ARG:NH1	2.14	0.63
5:C:420:HOH:O	1:D:295:ARG:HG2	1.99	0.63
1:D:274:ALA:HB3	1:D:289:VAL:CG1	2.28	0.63
1:E:161:SER:O	1:E:164:ILE:HG22	1.98	0.63
1:F:120:ILE:O	1:F:124:VAL:HG12	1.99	0.63
1:G:98:ALA:O	4:G:352:NAD:H3D	1.98	0.63
1:H:220:GLU:HA	1:H:223:GLN:CB	2.28	0.63
1:A:104:GLU:C	1:A:105:THR:CG2	2.71	0.63
1:C:215:VAL:HA	1:C:218:LYS:CG	2.28	0.63
1:E:295:ARG:HG3	1:F:15:MET:CG	2.28	0.63
1:F:188:TYR:CE2	1:F:290:PRO:HG3	2.34	0.63
1:H:74:LYS:CD	1:H:75:PRO:HD2	2.22	0.63
1:A:159:ILE:HD11	1:A:297:GLY:HA2	1.81	0.63
1:C:16:LYS:CE	1:D:264:HIS:O	2.46	0.63
1:C:181:ALA:O	1:C:182:PRO:C	2.41	0.63
1:A:148:TRP:HA	1:A:158:VAL:HG21	1.81	0.63
1:F:136:ALA:O	4:F:352:NAD:H2N	1.97	0.63
1:G:31:VAL:HG23	4:G:352:NAD:PN	2.39	0.63
1:H:265:ASN:HD22	1:H:295:ARG:H	1.46	0.63
1:C:145:TYR:CD1	1:C:329:PHE:CZ	2.87	0.63
1:C:311:LYS:CB	5:C:402:HOH:O	2.47	0.63
1:D:199:PRO:HG3	1:D:230:PHE:CG	2.34	0.63
1:F:114:ILE:HG21	1:F:330:THR:HA	1.81	0.63
1:H:110:VAL:HG21	1:H:324:VAL:CG1	2.28	0.63
1:B:29:GLY:HA3	4:B:352:NAD:O5B	1.98	0.63
1:F:215:VAL:CB	1:F:222:ALA:HB1	2.27	0.63
1:A:234:ARG:O	1:A:234:ARG:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:166:ASP:OD1	1:H:193:HIS:ND1	2.30	0.62
1:A:31:VAL:HG12	1:A:95:CYS:HB3	1.80	0.62
5:A:419:HOH:O	1:B:295:ARG:HD2	1.98	0.62
1:B:101:LYS:O	1:B:104:GLU:HB2	1.99	0.62
1:B:241:ILE:O	1:B:245:GLY:HA2	1.99	0.62
1:C:309:ASP:O	1:C:313:ARG:CG	2.47	0.62
1:F:304:ILE:CA	1:H:209:MET:HE1	2.28	0.62
1:G:152:GLY:HA2	5:G:463:HOH:O	1.99	0.62
1:D:223:GLN:OE1	1:D:223:GLN:CA	2.42	0.62
1:A:63:MET:HE1	1:D:243:LYS:HD3	1.81	0.62
1:A:70:VAL:CG2	5:A:360:HOH:O	2.45	0.62
1:A:291:ALA:HB1	1:A:298:ILE:HG23	1.81	0.62
1:B:265:ASN:ND2	1:B:295:ARG:HB2	2.13	0.62
1:F:228:ARG:NH2	1:F:231:VAL:HG11	2.14	0.62
1:A:101:LYS:CB	1:A:102:PRO:HD2	2.23	0.62
1:B:39:LEU:HD22	1:B:44:ILE:CB	2.23	0.62
1:C:87:ARG:NH1	1:C:87:ARG:HB2	2.15	0.62
1:E:15:MET:SD	1:E:18:ASN:O	2.58	0.62
1:E:222:ALA:HB3	5:E:396:HOH:O	1.98	0.62
1:G:218:LYS:CG	1:G:222:ALA:HB2	2.27	0.62
1:G:236:ALA:O	1:G:240:ILE:HG13	2.00	0.62
1:H:118:ARG:HB3	1:H:118:ARG:NH1	2.10	0.62
1:A:59:ILE:O	1:A:63:MET:HG2	2.00	0.62
1:A:93:VAL:HA	1:A:134:LEU:O	1.99	0.62
1:A:208:VAL:O	1:C:203:GLN:HG3	2.00	0.62
1:A:215:VAL:HG23	5:A:398:HOH:O	1.99	0.62
1:C:36:VAL:HG21	1:C:50:LEU:HD21	1.81	0.62
1:G:93:VAL:HA	1:G:134:LEU:O	2.00	0.62
1:A:220:GLU:HA	1:A:223:GLN:HB2	1.82	0.62
1:C:299:ARG:C	1:C:300:GLU:HG3	2.24	0.62
1:E:69:LYS:C	1:E:71:PHE:N	2.54	0.62
1:E:200:VAL:HG12	1:E:203:GLN:HB2	1.80	0.62
1:G:112:LYS:HE2	1:G:112:LYS:CA	2.21	0.62
1:H:121:VAL:O	1:H:125:MET:HG2	1.98	0.62
1:B:64:ASP:OD2	1:C:244:LYS:HE3	2.00	0.62
1:D:218:LYS:CG	1:D:222:ALA:HB2	2.30	0.62
1:G:170:PHE:HE2	1:G:187:ALA:HB1	1.64	0.62
1:G:209:MET:HE2	1:G:209:MET:CA	2.27	0.62
1:H:238:TYR:HD1	5:H:380:HOH:O	1.83	0.62
1:C:311:LYS:HB3	5:C:402:HOH:O	2.00	0.61
1:F:253:MET:HE2	1:G:40:MET:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:ILE:O	1:G:60:GLY:C	2.41	0.61
1:B:26:ILE:HG21	1:B:120:ILE:HG21	1.82	0.61
1:E:150:PHE:HZ	1:E:330:THR:HB	1.65	0.61
1:E:200:VAL:CG1	1:E:203:GLN:HB2	2.30	0.61
1:G:186:HIS:O	1:G:204:ALA:HA	2.00	0.61
1:A:209:MET:HE1	1:C:305:GLU:H	1.64	0.61
1:B:194:GLY:O	1:B:197:GLU:HG2	2.00	0.61
1:C:66:ASN:O	1:C:69:LYS:HG2	2.01	0.61
1:H:114:ILE:HD12	1:H:328:ALA:O	1.99	0.61
1:A:101:LYS:HB3	1:A:102:PRO:CD	2.23	0.61
1:C:15:MET:HE3	1:D:295:ARG:HB3	1.80	0.61
1:E:298:ILE:O	1:E:298:ILE:HG22	1.99	0.61
1:F:145:TYR:CE1	1:F:329:PHE:CE2	2.87	0.61
1:G:183:GLN:NE2	5:G:369:HOH:O	2.03	0.61
1:G:211:ILE:HA	1:G:214:LEU:HD12	1.82	0.61
1:H:31:VAL:HG22	1:H:251:ILE:HG21	1.81	0.61
1:C:145:TYR:CE1	1:C:329:PHE:CE2	2.89	0.61
1:C:209:MET:CG	1:C:214:LEU:HD21	2.30	0.61
1:G:77:ASP:HB3	1:G:79:TRP:CZ3	2.36	0.61
1:H:219:GLY:HA2	5:H:405:HOH:O	1.98	0.61
5:A:423:HOH:O	1:D:75:PRO:HA	2.00	0.61
1:E:294:ASN:HD22	1:E:295:ARG:N	1.99	0.61
1:G:145:TYR:CE1	1:G:329:PHE:CE2	2.87	0.61
1:B:94:ILE:HG21	1:B:117:PHE:CZ	2.36	0.61
1:C:209:MET:HE2	1:C:209:MET:CA	2.29	0.61
1:E:15:MET:C	1:E:17:ASN:H	2.01	0.61
1:E:138:ASN:HB2	4:E:352:NAD:O2D	2.01	0.61
1:H:29:GLY:HA3	4:H:352:NAD:O5B	2.01	0.61
1:H:82:ASP:O	1:H:85:ASP:HB2	2.01	0.61
1:H:116:ILE:H	1:H:116:ILE:HD12	1.66	0.61
1:H:215:VAL:HB	1:H:222:ALA:HB2	1.78	0.61
1:A:94:ILE:HG21	1:A:117:PHE:CE2	2.35	0.61
1:A:230:PHE:O	1:A:233:VAL:HB	2.00	0.61
1:D:171:ARG:HD2	1:D:185:VAL:O	2.00	0.61
1:A:234:ARG:HD2	1:A:235:ASP:OD1	2.01	0.61
1:F:117:PHE:O	1:F:118:ARG:C	2.44	0.61
1:H:257:ARG:NH2	1:H:266:GLU:OE2	2.31	0.61
1:A:228:ARG:HB3	1:A:228:ARG:HH11	1.66	0.60
1:B:63:MET:HE3	1:C:243:LYS:HD2	1.81	0.60
1:D:202:SER:HB3	1:D:310:GLU:OE2	2.01	0.60
1:B:86:CYS:O	1:B:129:PHE:HD1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:LEU:O	1:C:303:GLU:OE2	2.20	0.60
1:E:150:PHE:CZ	1:E:330:THR:HB	2.37	0.60
1:F:74:LYS:HD3	5:F:418:HOH:O	2.01	0.60
1:G:186:HIS:O	1:G:205:TYR:N	2.30	0.60
1:B:221:GLU:C	5:B:418:HOH:O	2.43	0.60
1:C:215:VAL:HB	1:C:222:ALA:HB1	1.82	0.60
1:C:295:ARG:HG3	1:D:15:MET:HG2	1.82	0.60
1:F:211:ILE:HG22	1:F:212:ARG:HG2	1.81	0.60
1:A:287:ILE:HG13	1:A:321:LEU:HD13	1.83	0.60
1:F:204:ALA:HB1	1:F:211:ILE:CD1	2.18	0.60
1:A:36:VAL:HG21	1:A:50:LEU:HD21	1.83	0.60
1:B:114:ILE:CD1	1:B:328:ALA:HB1	2.30	0.60
1:D:116:ILE:HG22	1:D:120:ILE:CD1	2.31	0.60
1:E:169:ARG:O	1:E:173:LEU:HG	2.01	0.60
1:E:295:ARG:CG	1:F:15:MET:HG2	2.31	0.60
1:F:213:LYS:HE2	1:H:305:GLU:OE2	2.01	0.60
1:A:49:VAL:HG22	1:A:79:TRP:CE2	2.36	0.60
1:A:176:GLU:O	1:A:177:TYR:C	2.44	0.60
1:B:101:LYS:CB	1:B:102:PRO:HD2	2.30	0.60
1:H:313:ARG:O	5:H:402:HOH:O	2.16	0.60
1:F:87:ARG:CG	1:F:128:GLY:HA3	2.31	0.60
1:F:243:LYS:HG2	1:G:56:SER:O	2.02	0.60
1:H:280:TYR:CE1	1:H:289:VAL:HG21	2.37	0.60
1:A:218:LYS:HG3	1:A:222:ALA:HB2	1.83	0.60
1:E:116:ILE:HG23	4:E:352:NAD:N6A	2.16	0.60
1:F:169:ARG:HG2	1:G:67:HIS:CG	2.37	0.60
1:A:15:MET:HA	1:B:265:ASN:CB	2.30	0.60
1:A:212:ARG:NH1	1:A:226:LEU:CB	2.65	0.60
1:B:121:VAL:HG11	1:B:150:PHE:HB2	1.84	0.60
1:B:244:LYS:HD3	1:B:246:ALA:O	2.02	0.60
1:H:112:LYS:CA	1:H:112:LYS:HE2	2.29	0.60
1:E:210:PRO:O	1:E:214:LEU:HG	2.02	0.59
1:F:43:GLY:O	1:F:74:LYS:HD2	2.01	0.59
1:G:132:LEU:N	1:G:132:LEU:CD2	2.65	0.59
1:G:234:ARG:NH1	1:G:235:ASP:OD1	2.34	0.59
1:D:38:ALA:O	1:D:42:GLN:HB2	2.02	0.59
1:F:272:VAL:O	1:F:288:GLY:HA2	2.01	0.59
1:G:308:ASP:O	1:G:312:ASN:HB2	2.01	0.59
1:A:125:MET:HE1	1:A:153:LEU:HD11	1.83	0.59
1:A:209:MET:CG	1:A:214:LEU:HD21	2.33	0.59
1:D:39:LEU:HD22	1:D:44:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:LYS:HE2	1:F:112:LYS:CA	2.31	0.59
1:E:41:ASN:O	1:E:73:PRO:HG2	2.02	0.59
1:G:26:ILE:HG21	1:G:120:ILE:CG2	2.32	0.59
1:B:280:TYR:OH	1:B:302:ILE:O	2.15	0.59
1:D:228:ARG:NH1	1:D:228:ARG:CA	2.66	0.59
1:F:218:LYS:HG3	1:F:222:ALA:HB2	1.85	0.59
1:F:329:PHE:HD1	1:F:329:PHE:C	2.11	0.59
1:G:279:LEU:HD23	1:G:301:VAL:HB	1.84	0.59
1:A:159:ILE:HD12	1:A:262:ILE:HD11	1.85	0.59
1:D:269:ILE:CG2	1:D:302:ILE:HD12	2.33	0.59
1:G:22:ARG:O	1:G:22:ARG:HG3	2.03	0.59
1:A:22:ARG:NH2	1:A:47:GLU:OE1	2.33	0.59
5:A:419:HOH:O	1:B:295:ARG:HG2	2.01	0.59
1:C:202:SER:OG	1:C:310:GLU:OE1	2.21	0.59
1:C:309:ASP:O	1:C:313:ARG:HG3	2.02	0.59
1:D:290:PRO:HB2	1:D:302:ILE:HB	1.83	0.59
1:F:251:ILE:HG13	1:F:255:LEU:CD2	2.32	0.59
1:G:264:HIS:C	1:H:16:LYS:NZ	2.60	0.59
1:H:149:LYS:N	1:H:149:LYS:HD2	2.17	0.59
1:A:165:LEU:O	1:A:169:ARG:HG3	2.03	0.59
1:B:224:LYS:CB	5:B:418:HOH:O	2.45	0.59
1:H:215:VAL:CG2	1:H:222:ALA:HB1	2.33	0.59
1:B:193:HIS:NE2	3:B:351:OXM:O1	2.36	0.59
1:D:280:TYR:CE1	1:D:289:VAL:CG2	2.86	0.59
1:E:29:GLY:HA3	4:E:352:NAD:O5B	2.03	0.59
1:E:138:ASN:HD21	1:E:193:HIS:HD2	1.50	0.59
1:F:132:LEU:CD1	1:F:157:ARG:HB3	2.33	0.59
1:A:264:HIS:CB	1:B:16:LYS:NZ	2.59	0.58
1:B:105:THR:HG23	1:B:108:ASP:OD2	2.03	0.58
1:E:21:ALA:CB	1:E:263:LEU:HD13	2.33	0.58
1:E:164:ILE:HD12	1:E:258:VAL:HG23	1.85	0.58
1:F:146:ALA:CA	1:F:329:PHE:CZ	2.78	0.58
1:G:192:GLU:O	1:G:197:GLU:HB3	2.04	0.58
1:B:35:TYR:CE2	1:B:93:VAL:HG21	2.37	0.58
1:B:169:ARG:NH1	5:B:389:HOH:O	2.35	0.58
1:C:209:MET:HG2	1:C:214:LEU:HD21	1.85	0.58
1:C:228:ARG:HH12	1:C:232:ASN:CG	2.11	0.58
1:C:240:ILE:HG23	1:C:244:LYS:HD3	1.85	0.58
1:D:261:ALA:HA	1:D:266:GLU:HB2	1.85	0.58
1:E:80:HIS:NE2	5:E:359:HOH:O	2.26	0.58
1:F:205:TYR:HE1	1:H:208:VAL:HB	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:262:ILE:O	1:G:264:HIS:N	2.35	0.58
1:G:275:TYR:CE1	1:G:284:ASP:HA	2.38	0.58
1:A:218:LYS:HG3	1:A:222:ALA:HB3	1.83	0.58
1:B:16:LYS:HB3	1:B:77:ASP:OD1	2.03	0.58
1:F:209:MET:HE1	1:H:305:GLU:H	1.68	0.58
1:G:295:ARG:HG3	1:H:15:MET:HG3	1.85	0.58
1:A:15:MET:HA	1:B:295:ARG:HG3	1.84	0.58
1:A:60:GLY:HA2	1:A:63:MET:HG3	1.85	0.58
1:A:267:ASN:HD22	1:A:292:VAL:CG1	2.17	0.58
1:B:203:GLN:HE21	1:D:209:MET:HE1	1.68	0.58
1:C:101:LYS:H	1:C:104:GLU:HB2	1.68	0.58
1:E:244:LYS:CE	1:H:61:ASP:OD1	2.50	0.58
1:F:289:VAL:CG1	1:F:301:VAL:HG13	2.34	0.58
1:G:82:ASP:O	1:G:85:ASP:HB2	2.04	0.58
1:G:220:GLU:HA	1:G:223:GLN:HB2	1.85	0.58
1:D:221:GLU:O	1:D:222:ALA:O	2.22	0.58
1:E:205:TYR:O	1:E:206:ILE:HD13	2.02	0.58
1:G:40:MET:CE	1:G:69:LYS:HA	2.33	0.58
1:A:151:SER:CB	1:A:153:LEU:HD12	2.34	0.58
1:D:177:TYR:HD2	1:D:178:PHE:CE1	2.21	0.58
1:E:138:ASN:HD22	1:E:140:VAL:H	1.50	0.58
1:A:125:MET:SD	1:A:151:SER:HB2	2.44	0.58
1:A:212:ARG:NH1	1:A:226:LEU:HB3	2.19	0.58
1:C:228:ARG:NH1	1:C:228:ARG:O	2.37	0.58
1:D:258:VAL:HG22	1:D:270:LEU:HD13	1.86	0.58
1:E:205:TYR:C	1:E:206:ILE:HG12	2.29	0.58
1:F:208:VAL:HG23	1:H:203:GLN:HG3	1.84	0.58
1:H:189:ILE:HD13	1:H:230:PHE:HE1	1.69	0.58
1:H:315:HIS:HB2	5:H:408:HOH:O	2.02	0.58
1:B:265:ASN:HD22	1:B:295:ARG:N	1.94	0.58
1:H:209:MET:HG2	1:H:214:LEU:HD21	1.84	0.58
1:C:153:LEU:HB3	1:C:154:PRO:HD2	1.86	0.58
1:E:215:VAL:HG23	5:E:396:HOH:O	2.02	0.58
1:F:275:TYR:CE1	1:F:284:ASP:HA	2.38	0.58
1:G:149:LYS:HE2	1:G:149:LYS:HA	1.86	0.58
1:G:265:ASN:HB2	1:G:295:ARG:HB2	1.86	0.58
1:G:306:LEU:HB2	1:G:311:LYS:HG2	1.86	0.58
1:H:311:LYS:HG2	5:H:409:HOH:O	2.02	0.58
1:A:16:LYS:NZ	1:B:264:HIS:O	2.36	0.57
1:A:294:ASN:C	1:A:294:ASN:ND2	2.52	0.57
1:C:181:ALA:HB3	5:C:417:HOH:O	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:VAL:HG22	1:C:206:ILE:HD13	1.86	0.57
1:D:24:VAL:HG22	1:D:49:VAL:HB	1.86	0.57
1:D:129:PHE:CZ	1:D:131:GLY:N	2.72	0.57
1:E:132:LEU:N	1:E:132:LEU:CD2	2.67	0.57
1:B:15:MET:C	1:B:17:ASN:H	2.05	0.57
1:B:118:ARG:NE	1:B:330:THR:OG1	2.37	0.57
1:C:264:HIS:CB	1:D:16:LYS:NZ	2.63	0.57
1:C:324:VAL:HA	1:C:327:ARG:HG3	1.87	0.57
1:D:265:ASN:CB	1:D:295:ARG:HB2	2.33	0.57
1:E:64:ASP:OD2	1:H:244:LYS:HE3	2.03	0.57
1:G:54:ASN:C	1:G:54:ASN:ND2	2.63	0.57
1:H:201:TRP:CH2	1:H:226:LEU:HB3	2.40	0.57
1:A:83:TYR:O	1:A:127:SER:HB2	2.04	0.57
1:A:138:ASN:HD22	1:A:140:VAL:H	1.51	0.57
1:B:59:ILE:HD12	1:B:59:ILE:N	2.18	0.57
1:C:138:ASN:OD1	4:C:352:NAD:O2D	2.11	0.57
1:G:16:LYS:HG3	1:G:46:ASP:O	2.05	0.57
1:G:174:LEU:O	1:G:178:PHE:HD2	1.87	0.57
1:G:315:HIS:O	1:G:319:ALA:HB2	2.05	0.57
1:H:159:ILE:HG23	1:H:298:ILE:HD11	1.85	0.57
1:C:75:PRO:HG3	1:D:266:GLU:HG2	1.86	0.57
1:C:215:VAL:HG11	1:C:226:LEU:HD11	1.85	0.57
1:D:118:ARG:NE	1:D:330:THR:OG1	2.37	0.57
1:G:15:MET:HB2	1:G:19:GLY:CA	2.34	0.57
1:G:138:ASN:HD22	1:G:140:VAL:H	1.50	0.57
1:G:216:GLU:CG	1:G:217:SER:N	2.67	0.57
1:H:200:VAL:HG12	1:H:203:GLN:HB2	1.87	0.57
1:H:210:PRO:HG2	1:H:213:LYS:CD	2.09	0.57
4:A:352:NAD:H6N	5:A:368:HOH:O	2.04	0.57
1:B:165:LEU:HD11	1:B:250:GLY:HA3	1.85	0.57
1:C:16:LYS:HB2	5:D:360:HOH:O	2.05	0.57
1:C:200:VAL:HG21	1:C:304:ILE:HD11	1.86	0.57
1:E:93:VAL:HA	1:E:134:LEU:O	2.04	0.57
1:E:169:ARG:NH1	5:E:385:HOH:O	2.27	0.57
1:G:130:GLN:O	1:G:157:ARG:NH1	2.37	0.57
1:G:215:VAL:HG23	1:G:222:ALA:HB3	1.86	0.57
1:B:36:VAL:HG21	1:B:50:LEU:CD2	2.31	0.57
1:B:96:ALA:HB1	4:B:352:NAD:C4A	2.34	0.57
1:C:118:ARG:O	1:C:122:GLU:HG3	2.05	0.57
1:D:15:MET:HG3	1:D:19:GLY:HA3	1.87	0.57
1:D:29:GLY:HA3	4:D:352:NAD:O1A	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:GLN:HG3	1:G:208:VAL:CG2	2.34	0.57
1:E:266:GLU:CG	1:F:75:PRO:HG3	2.35	0.57
1:G:67:HIS:ND1	5:G:444:HOH:O	2.12	0.57
1:A:168:ALA:HB1	1:D:70:VAL:HG23	1.87	0.57
1:A:251:ILE:HG13	1:A:255:LEU:HD22	1.86	0.57
1:D:230:PHE:O	1:D:233:VAL:HB	2.05	0.57
1:D:265:ASN:HD22	1:D:295:ARG:H	1.53	0.57
1:E:18:ASN:HA	5:E:355:HOH:O	2.04	0.57
1:E:173:LEU:HB3	1:E:229:ILE:HG23	1.87	0.57
1:E:295:ARG:HG3	1:F:15:MET:HG2	1.85	0.57
1:F:107:LEU:O	1:F:110:VAL:HG23	2.05	0.57
1:H:15:MET:HB2	1:H:19:GLY:H	1.68	0.57
1:C:15:MET:HB2	1:C:19:GLY:CA	2.35	0.57
1:E:251:ILE:CD1	4:E:352:NAD:O7N	2.49	0.57
1:F:240:ILE:CG2	1:F:244:LYS:HD3	2.35	0.57
1:G:309:ASP:O	1:G:313:ARG:CG	2.52	0.57
1:H:149:LYS:HA	1:H:149:LYS:HE2	1.87	0.57
1:H:276:LEU:HD12	1:H:287:ILE:HG22	1.87	0.57
1:A:275:TYR:HE1	1:A:284:ASP:HA	1.69	0.57
1:B:101:LYS:HB3	1:B:102:PRO:CD	2.28	0.57
1:F:172:PHE:CE1	1:G:66:ASN:HB3	2.40	0.57
1:A:107:LEU:HA	1:A:139:PRO:HG3	1.86	0.56
1:C:95:CYS:O	5:C:361:HOH:O	2.17	0.56
1:C:221:GLU:HB3	1:C:224:LYS:CB	2.26	0.56
1:D:55:GLU:C	1:D:59:ILE:HD12	2.30	0.56
1:E:15:MET:HB3	1:E:17:ASN:O	2.04	0.56
1:E:26:ILE:HG21	1:E:120:ILE:HG23	1.87	0.56
1:E:279:LEU:O	1:E:303:GLU:HG3	2.05	0.56
1:G:22:ARG:HB2	1:G:47:GLU:HB2	1.87	0.56
1:D:206:ILE:HG12	1:D:211:ILE:HG12	1.87	0.56
1:E:279:LEU:CB	5:E:398:HOH:O	2.16	0.56
1:F:119:SER:O	1:F:122:GLU:HB2	2.04	0.56
1:F:242:GLU:HG2	1:F:242:GLU:O	2.03	0.56
1:G:209:MET:CE	1:G:209:MET:CA	2.82	0.56
1:H:98:ALA:O	1:H:109:LEU:HD13	2.05	0.56
1:C:218:LYS:HG3	1:C:222:ALA:CB	2.35	0.56
4:C:352:NAD:H6N	5:C:371:HOH:O	2.05	0.56
1:D:132:LEU:CD2	1:D:132:LEU:N	2.68	0.56
1:E:165:LEU:O	1:E:168:ALA:HB3	2.05	0.56
1:E:202:SER:OG	1:E:310:GLU:OE1	2.23	0.56
1:E:265:ASN:HB3	1:F:15:MET:CA	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:VAL:HG21	1:F:293:ILE:HD11	1.86	0.56
1:G:294:ASN:HD22	1:G:296:ASN:H	1.53	0.56
1:A:138:ASN:HB2	4:A:352:NAD:O2D	2.06	0.56
1:A:184:ASN:HB3	1:C:269:ILE:HD12	1.87	0.56
1:B:211:ILE:HA	1:B:214:LEU:HD12	1.86	0.56
1:E:54:ASN:C	1:E:54:ASN:HD22	2.14	0.56
1:G:215:VAL:CB	1:G:222:ALA:CB	2.71	0.56
1:H:274:ALA:HB3	1:H:289:VAL:HG12	1.87	0.56
1:C:138:ASN:HD22	1:C:140:VAL:H	1.54	0.56
1:D:39:LEU:O	1:D:43:GLY:N	2.39	0.56
1:D:212:ARG:HH11	1:D:226:LEU:CD1	2.18	0.56
1:E:167:THR:O	1:E:171:ARG:CG	2.53	0.56
1:E:295:ARG:HD2	1:F:15:MET:CG	2.36	0.56
1:H:117:PHE:O	1:H:121:VAL:HG23	2.06	0.56
1:A:177:TYR:OH	1:A:222:ALA:HA	2.05	0.56
1:B:99:ASN:HA	4:B:352:NAD:H3D	1.87	0.56
1:D:118:ARG:HH11	1:D:118:ARG:CG	2.19	0.56
1:D:215:VAL:CG2	1:D:222:ALA:HB1	2.35	0.56
1:E:18:ASN:N	1:E:47:GLU:OE2	2.38	0.56
1:F:27:GLY:O	1:F:32:GLY:HA3	2.06	0.56
1:H:222:ALA:O	1:H:225:ASP:HB2	2.05	0.56
1:A:32:GLY:O	1:A:36:VAL:HG23	2.05	0.56
1:A:49:VAL:HG22	1:A:79:TRP:CZ2	2.41	0.56
1:A:203:GLN:HA	5:A:395:HOH:O	2.06	0.56
1:F:313:ARG:HH11	1:F:313:ARG:CG	2.13	0.56
1:G:159:ILE:HD13	1:G:298:ILE:CG1	2.36	0.56
1:G:186:HIS:HD2	1:G:207:GLY:O	1.89	0.56
1:H:189:ILE:CD1	1:H:230:PHE:HE1	2.18	0.56
1:H:219:GLY:O	1:H:221:GLU:HG2	2.05	0.56
1:A:100:GLN:HA	1:A:109:LEU:HD21	1.87	0.56
1:A:304:ILE:HB	1:C:209:MET:HE1	1.88	0.56
1:B:166:ASP:OD1	1:B:193:HIS:ND1	2.31	0.56
1:C:15:MET:HG3	1:C:19:GLY:HA3	1.88	0.56
1:C:166:ASP:HB3	1:C:189:ILE:HG21	1.88	0.56
1:C:260:ARG:NH2	1:D:75:PRO:CD	2.69	0.56
1:E:16:LYS:HB3	1:E:77:ASP:OD1	2.05	0.56
1:F:209:MET:HE3	1:H:304:ILE:HA	1.86	0.56
1:H:240:ILE:HG22	1:H:244:LYS:CD	2.35	0.56
1:C:185:VAL:HG22	1:C:206:ILE:CD1	2.36	0.56
1:D:283:ARG:O	1:D:322:LYS:HE2	2.05	0.56
1:E:69:LYS:C	1:E:71:PHE:H	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:MET:CB	1:E:214:LEU:HD21	2.30	0.56
1:E:209:MET:CE	1:G:305:GLU:H	2.19	0.56
1:H:182:PRO:O	1:H:185:VAL:HB	2.06	0.56
1:A:83:TYR:CE2	1:A:124:VAL:HG12	2.40	0.56
1:D:307:ASN:O	1:D:311:LYS:HG2	2.06	0.56
1:G:264:HIS:O	1:H:16:LYS:HE2	2.06	0.56
1:H:218:LYS:HG2	1:H:222:ALA:HB2	1.87	0.56
1:A:15:MET:CG	1:B:295:ARG:HG3	2.36	0.55
1:A:16:LYS:CD	1:A:46:ASP:O	2.42	0.55
1:A:142:ILE:HD12	1:A:325:LEU:CD2	2.36	0.55
1:A:280:TYR:CE1	1:A:289:VAL:CG2	2.89	0.55
1:G:228:ARG:HD3	1:G:228:ARG:C	2.30	0.55
1:A:242:GLU:CG	1:A:242:GLU:O	2.49	0.55
1:B:121:VAL:HG11	1:B:150:PHE:CB	2.36	0.55
1:B:222:ALA:O	1:B:226:LEU:HG	2.06	0.55
1:C:295:ARG:NH1	1:C:295:ARG:O	2.39	0.55
1:E:264:HIS:O	1:E:265:ASN:C	2.49	0.55
1:F:228:ARG:HH22	1:F:231:VAL:HG11	1.71	0.55
1:B:31:VAL:HG13	1:B:251:ILE:HG23	1.88	0.55
1:D:15:MET:N	1:D:20:GLY:CA	2.70	0.55
1:G:15:MET:HB2	1:G:20:GLY:N	2.20	0.55
1:G:92:VAL:CG1	1:G:133:PHE:CE1	2.89	0.55
1:G:142:ILE:HG13	1:G:324:VAL:HG11	1.87	0.55
1:A:86:CYS:O	1:A:87:ARG:C	2.49	0.55
1:A:243:LYS:HD3	1:D:59:ILE:CG2	2.36	0.55
1:B:118:ARG:O	1:B:122:GLU:HB2	2.06	0.55
1:C:189:ILE:HD11	1:C:233:VAL:HG11	1.88	0.55
1:D:55:GLU:O	1:D:59:ILE:HG13	2.07	0.55
1:D:94:ILE:CG2	1:D:117:PHE:CZ	2.85	0.55
1:D:269:ILE:HG23	1:D:302:ILE:HD12	1.89	0.55
1:D:309:ASP:O	1:D:313:ARG:HG2	2.07	0.55
1:E:15:MET:O	1:E:47:GLU:OE2	2.23	0.55
1:E:109:LEU:HD23	5:E:374:HOH:O	2.05	0.55
1:F:209:MET:CE	1:H:304:ILE:HA	2.36	0.55
1:G:18:ASN:N	1:G:18:ASN:OD1	2.40	0.55
1:H:107:LEU:HD11	1:H:192:GLU:OE2	2.07	0.55
1:H:113:ASN:HA	1:H:116:ILE:HD13	1.89	0.55
1:H:148:TRP:HA	1:H:158:VAL:HG21	1.88	0.55
1:A:136:ALA:O	4:A:352:NAD:H2N	2.06	0.55
1:A:209:MET:CE	1:C:304:ILE:HA	2.37	0.55
1:B:61:ASP:HB3	1:B:65:PHE:HE2	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:TYR:CE1	1:E:302:ILE:O	2.60	0.55
1:H:187:ALA:HB2	1:H:204:ALA:HB1	1.89	0.55
1:H:240:ILE:HG23	1:H:244:LYS:HD2	1.84	0.55
1:B:299:ARG:NE	1:B:300:GLU:OE2	2.39	0.55
1:E:16:LYS:N	1:E:16:LYS:HD2	2.21	0.55
1:F:71:PHE:HE2	5:G:373:HOH:O	1.89	0.55
1:F:114:ILE:HD12	1:F:328:ALA:O	2.07	0.55
1:H:65:PHE:O	1:H:68:GLY:N	2.36	0.55
1:A:15:MET:HB2	1:A:19:GLY:C	2.32	0.55
1:B:322:LYS:HG2	5:B:408:HOH:O	2.06	0.55
1:F:305:GLU:OE1	1:H:213:LYS:HD2	2.07	0.55
1:G:299:ARG:C	1:G:300:GLU:HG3	2.32	0.55
1:B:55:GLU:O	1:B:58:ALA:HB3	2.06	0.55
1:D:100:GLN:HG3	5:D:378:HOH:O	2.07	0.55
1:E:155:HIS:HB2	1:E:286:TYR:OH	2.06	0.55
1:E:174:LEU:O	1:E:178:PHE:HD1	1.89	0.55
1:E:209:MET:HE3	1:G:305:GLU:H	1.71	0.55
1:H:220:GLU:H	1:H:223:GLN:HB2	1.71	0.55
1:A:100:GLN:HB3	1:A:109:LEU:HD11	1.89	0.55
1:C:93:VAL:HA	1:C:134:LEU:O	2.07	0.55
1:C:184:ASN:OD1	5:C:417:HOH:O	2.17	0.55
1:A:63:MET:CE	1:D:243:LYS:HD3	2.36	0.55
1:A:170:PHE:CE2	1:A:187:ALA:HB1	2.42	0.55
1:A:304:ILE:HG22	1:C:209:MET:HE3	1.89	0.55
1:B:74:LYS:HD2	1:B:75:PRO:O	2.07	0.55
1:B:187:ALA:HB2	1:B:204:ALA:HB1	1.89	0.55
1:C:327:ARG:CZ	1:C:328:ALA:HB2	2.37	0.55
1:E:203:GLN:HG3	1:G:208:VAL:HG23	1.89	0.55
4:E:352:NAD:H6N	5:E:367:HOH:O	2.07	0.55
1:G:39:LEU:HD22	1:G:44:ILE:HB	1.89	0.55
1:G:86:CYS:HG	1:G:124:VAL:HG23	1.68	0.55
1:H:114:ILE:HD13	1:H:329:PHE:CE1	2.41	0.55
1:A:280:TYR:CE1	1:A:289:VAL:HG21	2.42	0.54
1:B:15:MET:C	1:B:17:ASN:N	2.62	0.54
1:D:209:MET:CA	1:D:209:MET:CE	2.80	0.54
1:E:265:ASN:HB3	1:F:16:LYS:N	2.22	0.54
1:E:276:LEU:O	1:E:283:ARG:HA	2.07	0.54
1:E:290:PRO:HG3	1:E:304:ILE:CG2	2.36	0.54
1:H:205:TYR:N	1:H:205:TYR:CD1	2.74	0.54
1:C:153:LEU:HB3	1:C:154:PRO:CD	2.36	0.54
1:E:148:TRP:HA	1:E:158:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:VAL:HG13	1:E:301:VAL:HG13	1.88	0.54
1:E:295:ARG:CB	1:F:15:MET:HG2	2.37	0.54
1:G:52:ASP:OD1	1:G:54:ASN:N	2.34	0.54
1:G:249:TYR:O	1:G:253:MET:HG2	2.06	0.54
1:B:70:VAL:HG22	1:C:182:PRO:CB	2.37	0.54
1:C:189:ILE:CD1	1:C:230:PHE:CE1	2.90	0.54
1:C:221:GLU:CB	1:C:224:LYS:H	2.20	0.54
1:E:116:ILE:HG22	1:E:120:ILE:CD1	2.38	0.54
1:E:240:ILE:HD11	1:H:67:HIS:HE1	1.72	0.54
1:G:282:GLU:HG3	1:G:318:ALA:HB1	1.89	0.54
1:H:150:PHE:HZ	1:H:330:THR:HB	1.73	0.54
1:A:74:LYS:HG2	5:A:418:HOH:O	2.07	0.54
1:B:87:ARG:CZ	1:B:87:ARG:HB3	2.37	0.54
1:B:211:ILE:O	1:B:213:LYS:N	2.41	0.54
5:B:363:HOH:O	1:C:172:PHE:HB2	2.07	0.54
1:C:75:PRO:HG3	1:D:266:GLU:CG	2.37	0.54
1:C:167:THR:O	1:C:171:ARG:CG	2.56	0.54
1:D:220:GLU:CA	1:D:223:GLN:HB2	2.31	0.54
1:F:220:GLU:HA	1:F:223:GLN:HB2	1.88	0.54
1:G:218:LYS:HD2	1:G:222:ALA:HB2	1.89	0.54
1:H:248:TYR:O	1:H:251:ILE:HG22	2.07	0.54
1:B:87:ARG:CG	1:B:127:SER:O	2.51	0.54
1:B:265:ASN:HD22	1:B:294:ASN:HB2	1.71	0.54
1:E:265:ASN:OD1	1:F:17:ASN:N	2.37	0.54
1:E:295:ARG:O	1:E:295:ARG:HD3	2.08	0.54
1:G:232:ASN:O	1:G:236:ALA:HB2	2.07	0.54
1:G:278:GLY:N	1:G:282:GLU:O	2.35	0.54
1:H:216:GLU:HG2	1:H:217:SER:N	2.22	0.54
1:A:104:GLU:C	1:A:105:THR:HG22	2.31	0.54
1:C:15:MET:HB2	1:C:19:GLY:H	1.68	0.54
1:D:94:ILE:HG21	1:D:117:PHE:CE2	2.42	0.54
1:D:109:LEU:O	1:D:112:LYS:HB2	2.08	0.54
1:F:212:ARG:CD	1:F:223:GLN:HE22	2.20	0.54
1:G:57:LYS:HG2	5:G:492:HOH:O	2.07	0.54
1:G:145:TYR:CD1	1:G:329:PHE:CE2	2.96	0.54
1:G:190:ILE:CD1	1:G:200:VAL:HG21	2.30	0.54
1:A:173:LEU:HD12	1:A:233:VAL:CG2	2.38	0.54
1:B:54:ASN:ND2	1:B:57:LYS:H	2.05	0.54
1:B:114:ILE:CG2	1:B:330:THR:HA	2.37	0.54
1:C:240:ILE:HG22	1:C:244:LYS:HD3	1.88	0.54
1:F:265:ASN:HA	1:F:295:ARG:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:GLN:HA	1:G:109:LEU:HD21	1.90	0.54
1:H:276:LEU:HD22	1:H:279:LEU:HB3	1.89	0.54
1:A:265:ASN:OD1	1:B:17:ASN:CB	2.56	0.54
1:B:59:ILE:HB	1:C:243:LYS:HD3	1.88	0.54
1:B:76:VAL:HB	5:B:359:HOH:O	2.08	0.54
1:D:118:ARG:HG2	1:D:118:ARG:NH1	2.23	0.54
1:D:240:ILE:HG22	1:D:244:LYS:HD3	1.90	0.54
1:F:87:ARG:CG	1:F:127:SER:O	2.55	0.54
1:F:139:PRO:HD2	1:F:143:LEU:HD12	1.90	0.54
1:G:317:SER:O	1:G:318:ALA:C	2.51	0.54
1:B:138:ASN:CB	4:B:352:NAD:HO2N	2.21	0.54
1:E:215:VAL:HG21	1:E:226:LEU:HD11	1.90	0.54
1:G:315:HIS:O	1:G:319:ALA:CB	2.56	0.54
1:A:142:ILE:HD12	1:A:325:LEU:HD21	1.88	0.54
1:B:37:PHE:HD2	1:C:37:PHE:HD2	1.56	0.54
1:C:55:GLU:O	1:C:56:SER:C	2.51	0.54
1:C:280:TYR:OH	1:C:304:ILE:HG12	2.08	0.54
1:D:21:ALA:H	1:D:46:ASP:HB2	1.73	0.54
1:D:110:VAL:HG12	1:D:114:ILE:HD12	1.89	0.54
1:F:77:ASP:HB3	1:F:79:TRP:HZ3	1.73	0.54
1:G:16:LYS:O	1:G:77:ASP:OD2	2.26	0.54
1:H:112:LYS:HE2	1:H:112:LYS:HA	1.89	0.54
1:H:280:TYR:O	1:H:282:GLU:HG2	2.08	0.54
1:A:87:ARG:HB2	1:A:127:SER:O	2.08	0.53
1:F:145:TYR:HD1	1:F:329:PHE:CE2	2.19	0.53
1:A:306:LEU:O	1:A:311:LYS:HE2	2.08	0.53
1:B:54:ASN:ND2	1:B:54:ASN:O	2.40	0.53
1:D:15:MET:HB2	1:D:19:GLY:N	2.24	0.53
1:E:70:VAL:HG22	1:H:182:PRO:HB2	1.88	0.53
1:H:120:ILE:O	1:H:124:VAL:HG12	2.08	0.53
1:H:218:LYS:O	1:H:218:LYS:HG2	2.07	0.53
1:A:15:MET:HG3	1:A:19:GLY:HA3	1.91	0.53
1:A:279:LEU:HD23	1:A:301:VAL:CG1	2.38	0.53
1:B:149:LYS:HA	1:B:149:LYS:CE	2.25	0.53
1:C:117:PHE:CD2	1:C:147:THR:OG1	2.60	0.53
1:C:145:TYR:CD1	1:C:329:PHE:CE2	2.97	0.53
1:C:215:VAL:CA	1:C:218:LYS:HG2	2.36	0.53
1:C:264:HIS:CA	1:D:16:LYS:HZ3	2.21	0.53
1:D:22:ARG:HB2	1:D:47:GLU:HB2	1.89	0.53
1:D:222:ALA:HB3	5:D:405:HOH:O	2.07	0.53
1:G:221:GLU:HA	1:G:221:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:ASN:HD22	1:G:294:ASN:C	2.17	0.53
1:G:299:ARG:NE	1:G:300:GLU:OE2	2.41	0.53
1:H:228:ARG:O	1:H:231:VAL:HB	2.07	0.53
1:A:247:THR:OG1	4:A:352:NAD:H5N	2.08	0.53
1:B:203:GLN:HE22	1:B:305:GLU:HB3	1.74	0.53
1:B:241:ILE:O	1:B:245:GLY:CA	2.57	0.53
1:C:257:ARG:HG3	1:C:257:ARG:O	2.00	0.53
1:D:309:ASP:O	1:D:313:ARG:CG	2.57	0.53
1:E:212:ARG:NH1	1:E:226:LEU:CD1	2.72	0.53
1:A:168:ALA:CA	1:D:70:VAL:HG21	2.32	0.53
1:A:202:SER:OG	1:A:310:GLU:OE1	2.26	0.53
1:B:162:GLY:O	1:B:193:HIS:HB2	2.08	0.53
1:E:224:LYS:NZ	1:E:224:LYS:HB3	2.24	0.53
1:F:219:GLY:HA2	5:F:397:HOH:O	2.07	0.53
1:G:16:LYS:NZ	1:H:264:HIS:O	2.33	0.53
1:H:147:THR:O	1:H:151:SER:HB3	2.08	0.53
1:A:61:ASP:OD1	1:D:244:LYS:HE2	2.09	0.53
1:A:264:HIS:O	1:B:16:LYS:CD	2.54	0.53
1:C:24:VAL:CG1	1:C:51:ILE:HD11	2.38	0.53
1:D:27:GLY:O	1:D:95:CYS:HB2	2.09	0.53
1:D:165:LEU:HD12	1:D:165:LEU:C	2.31	0.53
1:D:216:GLU:HA	5:D:406:HOH:O	2.09	0.53
1:E:56:SER:O	1:H:243:LYS:HG2	2.07	0.53
1:E:110:VAL:CG1	1:E:111:ASP:N	2.69	0.53
1:E:207:GLY:HA3	5:E:395:HOH:O	2.08	0.53
1:A:234:ARG:HG2	5:A:385:HOH:O	2.07	0.53
1:B:15:MET:HB2	1:B:19:GLY:HA3	1.89	0.53
1:C:118:ARG:HH11	1:C:118:ARG:CB	2.16	0.53
1:C:209:MET:HE2	1:C:209:MET:HA	1.89	0.53
1:D:17:ASN:HA	5:D:419:HOH:O	2.09	0.53
1:D:329:PHE:HD1	1:D:330:THR:N	2.07	0.53
1:F:112:LYS:O	1:F:115:ALA:HB3	2.08	0.53
1:F:217:SER:O	1:F:218:LYS:HB3	2.08	0.53
1:A:15:MET:HA	1:B:265:ASN:HB2	1.91	0.53
1:C:15:MET:CG	1:D:295:ARG:HG3	2.39	0.53
1:C:87:ARG:CB	1:C:87:ARG:CZ	2.86	0.53
1:D:280:TYR:CZ	1:D:303:GLU:HA	2.44	0.53
1:F:174:LEU:HD23	1:F:229:ILE:HD13	1.91	0.53
1:G:137:THR:HG23	4:G:352:NAD:O3D	2.08	0.53
1:H:307:ASN:O	1:H:311:LYS:HG3	2.09	0.53
1:A:173:LEU:HD12	1:A:233:VAL:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:PHE:HB3	1:E:248:TYR:CD2	2.44	0.53
1:E:162:GLY:C	5:E:377:HOH:O	2.51	0.53
1:F:138:ASN:HA	1:F:140:VAL:H	1.74	0.53
1:G:264:HIS:O	1:H:16:LYS:CE	2.56	0.53
1:A:55:GLU:HB3	1:A:59:ILE:HD11	1.89	0.52
1:A:114:ILE:HD12	1:A:328:ALA:O	2.09	0.52
1:A:159:ILE:HG12	1:A:298:ILE:HD11	1.90	0.52
1:A:160:GLY:HA3	1:A:273:SER:HB3	1.91	0.52
1:G:288:GLY:O	1:G:289:VAL:HB	2.08	0.52
1:H:112:LYS:O	1:H:115:ALA:CB	2.43	0.52
1:D:52:ASP:OD1	4:D:352:NAD:O2B	2.27	0.52
1:E:295:ARG:CG	1:F:15:MET:CG	2.86	0.52
1:E:304:ILE:HG13	1:E:306:LEU:HD21	1.89	0.52
1:E:313:ARG:HA	1:E:316:HIS:HB3	1.90	0.52
1:G:145:TYR:CD1	1:G:329:PHE:HE2	2.26	0.52
1:G:219:GLY:O	1:G:221:GLU:N	2.42	0.52
1:B:243:LYS:CD	1:C:59:ILE:HG22	2.39	0.52
1:C:220:GLU:O	1:C:221:GLU:C	2.52	0.52
1:D:295:ARG:HD3	1:D:295:ARG:C	2.34	0.52
1:D:323:SER:O	1:D:326:ALA:HB3	2.09	0.52
1:D:324:VAL:O	1:D:328:ALA:CB	2.57	0.52
1:E:118:ARG:O	1:E:122:GLU:HB2	2.10	0.52
1:E:167:THR:O	1:E:171:ARG:HG2	2.09	0.52
1:H:228:ARG:HH11	1:H:228:ARG:C	2.17	0.52
1:B:276:LEU:O	1:B:283:ARG:HA	2.09	0.52
1:D:56:SER:HA	1:D:59:ILE:HD12	1.90	0.52
1:E:215:VAL:O	1:E:218:LYS:HG2	2.09	0.52
1:F:145:TYR:HE1	1:F:149:LYS:HD3	1.65	0.52
1:A:86:CYS:HB2	1:A:127:SER:CB	2.39	0.52
1:A:215:VAL:HG11	1:A:226:LEU:HD11	1.90	0.52
1:B:55:GLU:HB3	1:B:59:ILE:CD1	2.38	0.52
1:B:114:ILE:HD13	1:B:328:ALA:O	2.10	0.52
1:D:138:ASN:HD22	1:D:140:VAL:H	1.55	0.52
1:D:218:LYS:O	1:D:221:GLU:HB2	2.09	0.52
1:F:161:SER:O	1:F:162:GLY:C	2.51	0.52
1:F:203:GLN:HG2	1:H:208:VAL:HG23	1.91	0.52
1:H:218:LYS:O	1:H:221:GLU:HB2	2.10	0.52
1:H:276:LEU:HD21	1:H:279:LEU:HB3	1.91	0.52
1:A:145:TYR:HE1	1:A:149:LYS:HD2	1.75	0.52
1:A:156:GLU:O	1:A:297:GLY:HA3	2.10	0.52
1:B:256:ALA:O	1:B:260:ARG:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:LEU:HD22	1:D:279:LEU:HB3	1.92	0.52
1:E:161:SER:O	1:E:164:ILE:CG2	2.57	0.52
1:B:71:PHE:HE2	5:C:356:HOH:O	1.93	0.52
1:C:145:TYR:CE1	1:C:329:PHE:HE2	2.27	0.52
1:C:250:GLY:N	5:C:355:HOH:O	2.41	0.52
1:D:39:LEU:HD22	1:D:44:ILE:CG2	2.39	0.52
1:D:71:PHE:HB3	5:D:368:HOH:O	2.09	0.52
1:G:16:LYS:NZ	1:H:264:HIS:HB3	2.24	0.52
1:G:54:ASN:HD21	1:G:56:SER:HB2	1.75	0.52
1:B:94:ILE:CG2	1:B:117:PHE:CZ	2.92	0.52
1:F:86:CYS:O	1:F:129:PHE:HD1	1.93	0.52
1:F:149:LYS:CE	1:F:149:LYS:HA	2.39	0.52
1:A:75:PRO:HG3	1:B:266:GLU:HG3	1.92	0.52
1:A:145:TYR:CE1	1:A:149:LYS:HD2	2.45	0.52
1:A:243:LYS:HD3	1:D:59:ILE:HG22	1.92	0.52
1:B:174:LEU:HB2	1:B:185:VAL:HG11	1.91	0.52
1:B:243:LYS:HG3	1:C:56:SER:CB	2.40	0.52
1:C:192:GLU:O	1:C:197:GLU:HB3	2.09	0.52
1:H:94:ILE:HG22	1:H:117:PHE:CZ	2.45	0.52
1:H:313:ARG:O	1:H:314:PHE:C	2.53	0.52
1:C:15:MET:HA	1:D:265:ASN:OD1	2.10	0.52
1:C:69:LYS:HA	1:C:72:ALA:HB2	1.92	0.52
1:C:266:GLU:HG2	1:D:75:PRO:HG3	1.91	0.52
1:G:101:LYS:CB	1:G:102:PRO:CD	2.88	0.52
1:G:112:LYS:HA	1:G:112:LYS:CE	2.16	0.52
1:A:137:THR:HB	1:A:143:LEU:HD13	1.91	0.51
1:B:64:ASP:OD2	1:C:244:LYS:HE2	2.10	0.51
1:B:289:VAL:HG11	1:B:301:VAL:CG1	2.39	0.51
1:C:178:PHE:HZ	1:C:215:VAL:CG1	2.22	0.51
1:C:265:ASN:HD22	1:C:295:ARG:H	1.58	0.51
1:E:71:PHE:CD1	1:H:257:ARG:HG2	2.45	0.51
5:E:423:HOH:O	1:H:71:PHE:CE2	2.50	0.51
1:F:57:LYS:HG2	5:F:409:HOH:O	2.09	0.51
1:C:87:ARG:HB2	1:C:87:ARG:HH11	1.74	0.51
1:C:116:ILE:HG23	1:C:120:ILE:HD12	1.92	0.51
1:D:65:PHE:HB3	1:D:78:ILE:HD13	1.92	0.51
1:D:187:ALA:HA	5:D:399:HOH:O	2.09	0.51
1:E:199:PRO:HG3	1:E:230:PHE:CD1	2.46	0.51
1:F:223:GLN:HG2	5:F:397:HOH:O	2.10	0.51
1:H:125:MET:CE	1:H:125:MET:HA	2.37	0.51
1:H:197:GLU:OE2	1:H:234:ARG:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:O	1:A:322:LYS:HE2	2.09	0.51
5:A:422:HOH:O	1:D:70:VAL:HG22	2.08	0.51
1:F:198:LEU:CB	1:F:313:ARG:CD	2.84	0.51
1:F:213:LYS:CA	1:F:216:GLU:HB3	2.38	0.51
1:F:215:VAL:O	1:F:215:VAL:HG23	2.10	0.51
1:A:258:VAL:O	1:A:261:ALA:N	2.43	0.51
1:A:299:ARG:C	1:A:300:GLU:HG3	2.34	0.51
1:E:228:ARG:HH22	1:E:231:VAL:HG11	1.74	0.51
1:F:294:ASN:HD22	1:F:296:ASN:N	2.02	0.51
1:G:26:ILE:HG21	1:G:120:ILE:HG23	1.92	0.51
1:G:185:VAL:HG13	1:G:206:ILE:HD13	1.92	0.51
1:B:26:ILE:HG21	1:B:120:ILE:HG23	1.93	0.51
1:B:76:VAL:HG13	1:B:78:ILE:HD12	1.92	0.51
1:D:22:ARG:CG	1:D:89:ALA:CA	2.82	0.51
1:D:170:PHE:CD2	1:D:189:ILE:HD13	2.44	0.51
1:H:66:ASN:O	1:H:69:LYS:HG2	2.11	0.51
1:A:167:THR:O	1:A:168:ALA:C	2.53	0.51
1:B:15:MET:CB	1:B:19:GLY:HA3	2.41	0.51
1:E:153:LEU:HB3	1:E:154:PRO:HD2	1.93	0.51
1:H:15:MET:HB3	1:H:17:ASN:H	1.75	0.51
1:H:251:ILE:HG12	4:H:352:NAD:C4N	2.39	0.51
1:A:208:VAL:HB	1:C:203:GLN:HG3	1.92	0.51
1:B:87:ARG:NH1	1:B:87:ARG:CB	2.74	0.51
1:C:132:LEU:HD12	1:C:157:ARG:HA	1.93	0.51
1:A:52:ASP:OD1	1:A:54:ASN:N	2.33	0.51
1:A:223:GLN:NE2	5:A:398:HOH:O	2.44	0.51
1:C:101:LYS:NZ	1:C:101:LYS:CB	2.73	0.51
1:C:112:LYS:HE2	1:C:112:LYS:HA	1.92	0.51
1:D:21:ALA:HB1	1:D:263:LEU:HD13	1.93	0.51
1:E:24:VAL:HG22	1:E:49:VAL:HB	1.91	0.51
1:G:187:ALA:HA	5:G:473:HOH:O	2.09	0.51
1:H:118:ARG:HG2	1:H:150:PHE:CZ	2.45	0.51
1:H:241:ILE:HG12	1:H:247:THR:HG22	1.91	0.51
1:A:208:VAL:HG22	1:C:188:TYR:CE2	2.46	0.51
1:C:260:ARG:NH2	1:D:75:PRO:HD2	2.25	0.51
1:C:280:TYR:OH	1:C:304:ILE:N	2.43	0.51
1:E:63:MET:HE2	1:H:243:LYS:HD2	1.93	0.51
1:F:280:TYR:OH	1:F:302:ILE:O	2.19	0.51
1:H:215:VAL:HG23	5:H:406:HOH:O	2.10	0.51
1:A:63:MET:HE1	1:D:243:LYS:CD	2.41	0.51
1:H:116:ILE:HD12	1:H:116:ILE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:TYR:CD1	1:A:329:PHE:CE2	2.97	0.50
1:C:117:PHE:O	1:C:121:VAL:CG2	2.54	0.50
1:D:36:VAL:HG21	1:D:50:LEU:HD21	1.92	0.50
1:E:24:VAL:HG13	1:E:51:ILE:HD12	1.93	0.50
1:G:55:GLU:O	1:G:58:ALA:HB3	2.11	0.50
1:H:248:TYR:C	1:H:251:ILE:HG22	2.35	0.50
1:B:24:VAL:CG1	1:B:51:ILE:CD1	2.88	0.50
1:B:63:MET:CE	1:C:243:LYS:HD2	2.41	0.50
1:C:311:LYS:CA	5:C:402:HOH:O	2.59	0.50
1:F:118:ARG:HB3	1:F:118:ARG:NH1	2.12	0.50
1:G:101:LYS:CB	1:G:102:PRO:HD2	2.32	0.50
1:H:293:ILE:HD12	1:H:298:ILE:HG13	1.93	0.50
1:C:16:LYS:CA	1:C:77:ASP:HB2	2.41	0.50
1:C:169:ARG:NH1	5:C:389:HOH:O	2.25	0.50
1:C:327:ARG:NH2	1:C:328:ALA:HB2	2.26	0.50
1:D:265:ASN:HB2	1:D:295:ARG:CB	2.37	0.50
1:F:114:ILE:HG22	1:F:115:ALA:N	2.24	0.50
1:F:159:ILE:HG22	1:F:160:GLY:N	2.27	0.50
1:F:169:ARG:HG2	1:G:67:HIS:CD2	2.46	0.50
1:F:264:HIS:O	1:F:265:ASN:C	2.54	0.50
1:A:15:MET:SD	1:A:17:ASN:O	2.70	0.50
1:B:307:ASN:OD1	1:B:310:GLU:HG3	2.11	0.50
1:D:91:LEU:HD22	1:D:259:THR:HG23	1.93	0.50
1:D:228:ARG:CB	1:D:228:ARG:NH1	2.75	0.50
1:E:30:PHE:HB3	1:E:248:TYR:CG	2.46	0.50
1:E:69:LYS:HA	1:E:72:ALA:H	1.75	0.50
1:F:125:MET:HE3	1:F:125:MET:CA	2.26	0.50
1:F:172:PHE:HA	5:F:390:HOH:O	2.10	0.50
1:F:251:ILE:HG13	1:F:255:LEU:HD21	1.94	0.50
1:G:265:ASN:HB2	1:H:15:MET:HA	1.87	0.50
1:H:257:ARG:HD2	1:H:257:ARG:O	2.11	0.50
1:A:320:THR:O	1:A:323:SER:HB2	2.11	0.50
1:B:23:VAL:CG1	1:B:91:LEU:HD23	2.42	0.50
1:B:59:ILE:CG2	1:B:63:MET:HE2	2.33	0.50
1:B:167:THR:O	1:B:171:ARG:HG3	2.12	0.50
1:B:209:MET:CE	1:D:203:GLN:NE2	2.75	0.50
1:C:40:MET:O	5:C:363:HOH:O	2.20	0.50
1:E:215:VAL:CB	1:E:222:ALA:HB1	2.26	0.50
1:F:145:TYR:CZ	1:F:149:LYS:HD3	2.46	0.50
1:F:174:LEU:HD23	1:F:229:ILE:CD1	2.42	0.50
1:H:221:GLU:OE1	1:H:221:GLU:CA	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:PHE:HZ	1:C:215:VAL:HG12	1.77	0.50
1:E:164:ILE:HD11	1:E:254:GLY:O	2.11	0.50
1:E:266:GLU:HG3	1:F:75:PRO:HG3	1.91	0.50
1:F:189:ILE:HD13	1:F:199:PRO:HA	1.92	0.50
1:A:31:VAL:HG22	1:A:251:ILE:HG21	1.93	0.50
1:A:132:LEU:HD22	1:A:132:LEU:N	2.27	0.50
1:D:228:ARG:NH1	1:D:228:ARG:O	2.45	0.50
1:D:287:ILE:HD13	1:D:314:PHE:CE1	2.47	0.50
1:E:69:LYS:O	1:E:70:VAL:C	2.53	0.50
1:G:148:TRP:HA	1:G:158:VAL:HG21	1.93	0.50
1:G:207:GLY:HA3	5:G:478:HOH:O	2.10	0.50
1:G:219:GLY:C	1:G:221:GLU:N	2.69	0.50
1:H:90:ASP:HB3	1:H:295:ARG:HH22	1.76	0.50
1:A:215:VAL:HB	1:A:222:ALA:HB1	1.94	0.50
1:B:59:ILE:CG2	1:C:243:LYS:HD3	2.42	0.50
1:C:20:GLY:HA3	1:C:46:ASP:HB2	1.94	0.50
1:D:269:ILE:HD13	1:D:302:ILE:CD1	2.42	0.50
1:E:71:PHE:CD2	5:H:358:HOH:O	2.64	0.50
1:E:118:ARG:NE	1:E:330:THR:OG1	2.43	0.50
1:E:146:ALA:HA	1:E:329:PHE:HZ	1.75	0.50
1:F:116:ILE:O	1:F:120:ILE:HG13	2.12	0.50
1:A:141:ASP:OD1	1:A:273:SER:OG	2.30	0.50
1:A:162:GLY:CA	5:A:378:HOH:O	2.59	0.50
1:A:162:GLY:HA2	5:A:378:HOH:O	2.12	0.50
1:D:57:LYS:NZ	1:D:61:ASP:OD2	2.41	0.50
1:E:110:VAL:HG12	1:E:111:ASP:OD1	2.12	0.50
1:H:118:ARG:O	1:H:122:GLU:HB2	2.12	0.50
1:H:248:TYR:HA	1:H:251:ILE:HG22	1.93	0.50
1:A:91:LEU:HA	1:A:132:LEU:O	2.12	0.49
5:A:422:HOH:O	1:D:70:VAL:CG2	2.59	0.49
1:D:116:ILE:HG22	1:D:120:ILE:HD11	1.95	0.49
1:D:166:ASP:OD1	1:D:193:HIS:ND1	2.35	0.49
1:E:61:ASP:O	1:E:65:PHE:CD2	2.65	0.49
1:G:148:TRP:O	1:G:148:TRP:CD1	2.65	0.49
1:G:169:ARG:NH1	5:G:468:HOH:O	2.44	0.49
1:G:221:GLU:O	1:G:222:ALA:O	2.30	0.49
1:H:32:GLY:O	1:H:36:VAL:HG23	2.12	0.49
1:H:272:VAL:O	1:H:288:GLY:HA2	2.12	0.49
1:B:186:HIS:N	1:B:205:TYR:O	2.40	0.49
1:B:240:ILE:O	1:B:241:ILE:C	2.54	0.49
1:C:241:ILE:HD13	5:C:374:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:LYS:HB2	5:G:456:HOH:O	2.13	0.49
1:B:287:ILE:HG13	1:B:321:LEU:CD1	2.41	0.49
1:D:114:ILE:CG2	5:D:415:HOH:O	2.58	0.49
1:D:124:VAL:O	1:D:127:SER:OG	2.20	0.49
1:D:196:THR:HB	1:D:317:SER:HB2	1.92	0.49
1:D:264:HIS:O	1:D:265:ASN:C	2.55	0.49
1:E:180:VAL:O	1:E:181:ALA:C	2.54	0.49
1:E:265:ASN:HB2	1:E:295:ARG:CB	2.38	0.49
1:A:15:MET:HG2	1:B:295:ARG:CG	2.43	0.49
1:A:26:ILE:HA	1:A:51:ILE:O	2.13	0.49
1:B:268:ALA:O	1:B:292:VAL:HA	2.12	0.49
1:E:265:ASN:OD1	1:F:16:LYS:N	2.45	0.49
1:F:35:TYR:CZ	1:F:39:LEU:HD11	2.48	0.49
1:G:22:ARG:HA	1:G:47:GLU:O	2.13	0.49
1:A:206:ILE:CG1	1:A:211:ILE:HD11	2.42	0.49
1:B:18:ASN:HA	5:B:357:HOH:O	2.11	0.49
1:B:216:GLU:CG	1:B:217:SER:N	2.75	0.49
1:C:138:ASN:HA	1:C:140:VAL:N	2.27	0.49
1:D:116:ILE:HG22	1:D:120:ILE:HD12	1.95	0.49
1:E:44:ILE:HD13	1:E:260:ARG:HB3	1.95	0.49
1:E:63:MET:O	1:E:67:HIS:CG	2.66	0.49
1:E:264:HIS:CA	1:F:16:LYS:HZ3	2.24	0.49
1:A:174:LEU:HB2	1:A:185:VAL:HG11	1.94	0.49
1:C:222:ALA:O	1:C:226:LEU:HG	2.12	0.49
1:D:164:ILE:CD1	1:D:270:LEU:HD22	2.41	0.49
1:E:68:GLY:HA3	1:H:253:MET:HG3	1.95	0.49
1:F:139:PRO:O	1:F:140:VAL:C	2.56	0.49
1:F:145:TYR:CD1	1:F:145:TYR:C	2.90	0.49
1:H:178:PHE:CZ	1:H:211:ILE:HG23	2.47	0.49
1:H:319:ALA:O	1:H:320:THR:C	2.54	0.49
1:A:22:ARG:HG2	1:A:24:VAL:HG23	1.95	0.49
1:D:235:ASP:O	1:D:236:ALA:C	2.56	0.49
1:E:94:ILE:HD13	1:E:120:ILE:HG21	1.94	0.49
1:G:193:HIS:CE1	3:G:351:OXM:O2	2.65	0.49
1:H:175:GLY:HA2	1:H:185:VAL:HG21	1.94	0.49
1:A:209:MET:HG2	1:A:214:LEU:CD2	2.43	0.49
1:B:59:ILE:HG22	1:B:63:MET:CE	2.35	0.49
1:C:22:ARG:HB3	1:C:89:ALA:HA	1.93	0.49
1:E:40:MET:O	1:E:73:PRO:HD2	2.12	0.49
1:G:190:ILE:CD1	1:G:200:VAL:CG2	2.86	0.49
1:H:124:VAL:CG2	1:H:129:PHE:CD2	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:MET:N	5:A:419:HOH:O	2.45	0.49
1:A:215:VAL:O	1:A:218:LYS:HG2	2.12	0.49
1:B:87:ARG:HG2	1:B:128:GLY:O	2.13	0.49
1:C:90:ASP:HB3	1:C:295:ARG:HH22	1.77	0.49
1:C:114:ILE:HD13	1:C:143:LEU:CD2	2.39	0.49
1:C:140:VAL:CG1	1:C:193:HIS:HB3	2.43	0.49
1:C:148:TRP:CD1	1:C:153:LEU:O	2.66	0.49
1:C:247:THR:CG2	3:C:351:OXM:O3	2.57	0.49
1:C:261:ALA:HA	1:C:266:GLU:HB2	1.95	0.49
1:C:275:TYR:HB2	1:C:286:TYR:CE2	2.47	0.49
1:D:21:ALA:N	1:D:46:ASP:HB2	2.28	0.49
1:F:329:PHE:C	1:F:329:PHE:CD1	2.89	0.49
1:A:279:LEU:HD23	1:A:301:VAL:HG12	1.95	0.49
1:B:92:VAL:HG12	1:B:133:PHE:CD1	2.48	0.49
1:C:31:VAL:CG1	1:C:95:CYS:HB3	2.43	0.49
1:C:31:VAL:HG12	1:C:95:CYS:HB3	1.95	0.49
1:G:24:VAL:HB	1:G:92:VAL:HG22	1.95	0.49
1:G:218:LYS:CD	1:G:222:ALA:HB2	2.42	0.49
1:A:83:TYR:O	1:A:127:SER:CB	2.61	0.48
1:B:222:ALA:HB3	5:B:399:HOH:O	2.12	0.48
1:C:213:LYS:HA	1:C:216:GLU:CB	2.42	0.48
1:E:170:PHE:O	1:E:174:LEU:HD12	2.13	0.48
1:E:212:ARG:HH12	1:E:226:LEU:CD1	2.25	0.48
1:F:192:GLU:O	1:F:197:GLU:HB3	2.13	0.48
1:G:220:GLU:CA	1:G:223:GLN:HB2	2.43	0.48
1:H:289:VAL:CG2	1:H:290:PRO:HD2	2.42	0.48
1:A:206:ILE:HG13	1:A:214:LEU:HD13	1.94	0.48
1:C:101:LYS:HB3	1:C:101:LYS:HZ2	1.78	0.48
1:D:216:GLU:CD	1:G:327:ARG:HB2	2.38	0.48
1:F:139:PRO:O	1:F:141:ASP:N	2.45	0.48
1:G:40:MET:HE3	1:G:69:LYS:HA	1.95	0.48
1:C:15:MET:C	1:C:17:ASN:N	2.57	0.48
1:D:39:LEU:CD2	1:D:44:ILE:HB	2.44	0.48
1:E:145:TYR:CD1	1:E:329:PHE:HE2	2.31	0.48
1:E:221:GLU:CA	5:E:416:HOH:O	2.49	0.48
1:G:240:ILE:HG22	1:G:244:LYS:CD	2.43	0.48
1:A:236:ALA:O	1:A:240:ILE:HG13	2.12	0.48
1:C:26:ILE:HA	1:C:51:ILE:O	2.12	0.48
1:C:90:ASP:HB3	1:C:295:ARG:NH2	2.29	0.48
1:F:112:LYS:HA	1:F:112:LYS:CE	2.41	0.48
1:H:16:LYS:O	1:H:77:ASP:OD2	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:LYS:O	1:H:77:ASP:CG	2.56	0.48
1:A:67:HIS:CE1	1:D:240:ILE:HD11	2.49	0.48
1:B:23:VAL:HG13	1:B:91:LEU:HD23	1.94	0.48
1:B:212:ARG:HH11	1:B:226:LEU:HD12	1.78	0.48
1:D:117:PHE:O	1:D:121:VAL:HG23	2.13	0.48
1:F:262:ILE:O	1:F:264:HIS:N	2.46	0.48
1:G:213:LYS:CB	1:G:213:LYS:HZ2	2.26	0.48
1:A:100:GLN:CG	1:A:105:THR:O	2.61	0.48
1:A:106:ARG:O	1:A:109:LEU:CG	2.59	0.48
1:A:122:GLU:O	1:A:126:ALA:HB2	2.14	0.48
1:A:241:ILE:O	1:A:245:GLY:HA2	2.13	0.48
1:B:166:ASP:OD2	1:B:197:GLU:OE1	2.32	0.48
1:C:15:MET:C	1:C:17:ASN:H	2.00	0.48
1:C:26:ILE:HG12	1:C:51:ILE:HD12	1.94	0.48
1:C:264:HIS:ND1	1:D:74:LYS:HD3	2.28	0.48
1:D:15:MET:O	1:D:47:GLU:OE2	2.32	0.48
1:D:293:ILE:CD1	1:D:298:ILE:HD13	2.43	0.48
1:E:175:GLY:O	1:E:179:SER:N	2.47	0.48
1:F:182:PRO:HB2	1:G:70:VAL:CG1	2.43	0.48
1:G:24:VAL:CG2	1:G:89:ALA:HB2	2.44	0.48
1:G:141:ASP:HB3	1:G:286:TYR:O	2.13	0.48
1:H:164:ILE:HD12	1:H:258:VAL:CG2	2.43	0.48
1:H:278:GLY:N	1:H:282:GLU:O	2.44	0.48
1:B:145:TYR:C	1:B:145:TYR:CD1	2.92	0.48
1:C:174:LEU:CD2	1:C:229:ILE:HD13	2.41	0.48
1:D:204:ALA:O	5:D:403:HOH:O	2.20	0.48
1:E:290:PRO:HG3	1:E:304:ILE:HG23	1.95	0.48
1:G:26:ILE:HG21	1:G:120:ILE:HG21	1.95	0.48
1:G:90:ASP:O	1:G:131:GLY:HA3	2.13	0.48
1:G:134:LEU:HA	1:G:159:ILE:O	2.13	0.48
1:G:260:ARG:HE	1:G:260:ARG:HB3	1.51	0.48
1:A:161:SER:OG	5:A:382:HOH:O	2.15	0.48
1:A:258:VAL:O	1:A:259:THR:C	2.56	0.48
1:B:124:VAL:CG2	1:B:129:PHE:CB	2.92	0.48
1:B:215:VAL:CB	1:B:222:ALA:CB	2.82	0.48
1:B:322:LYS:HE3	5:B:408:HOH:O	2.13	0.48
1:D:280:TYR:OH	1:D:303:GLU:HA	2.14	0.48
1:F:39:LEU:CD2	1:F:44:ILE:HD12	2.42	0.48
1:F:67:HIS:CD2	1:G:169:ARG:HG2	2.49	0.48
1:F:118:ARG:NE	1:F:330:THR:OG1	2.47	0.48
1:F:142:ILE:CD1	1:F:321:LEU:HD22	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:ASP:O	1:F:239:GLN:HG3	2.13	0.48
1:G:19:GLY:N	5:G:433:HOH:O	2.47	0.48
1:G:167:THR:O	1:G:171:ARG:HG3	2.14	0.48
1:G:307:ASN:O	1:G:311:LYS:HG3	2.13	0.48
1:H:58:ALA:HB1	1:H:80:HIS:HD2	1.79	0.48
1:H:218:LYS:HB3	1:H:218:LYS:HE2	1.55	0.48
1:A:209:MET:CG	1:A:214:LEU:CD2	2.91	0.48
1:B:209:MET:HE3	1:B:209:MET:HB2	1.68	0.48
1:C:15:MET:O	1:C:47:GLU:HG3	2.14	0.48
1:C:15:MET:HE3	1:D:295:ARG:CB	2.44	0.48
1:D:54:ASN:ND2	1:D:56:SER:HB2	2.27	0.48
1:D:299:ARG:C	1:D:300:GLU:HG3	2.37	0.48
1:E:209:MET:HE3	1:G:304:ILE:HB	1.96	0.48
1:F:15:MET:HB2	1:F:19:GLY:N	2.28	0.48
1:F:295:ARG:NH1	1:F:295:ARG:O	2.46	0.48
1:G:47:GLU:HB3	1:G:79:TRP:CH2	2.49	0.48
1:G:145:TYR:HE1	1:G:329:PHE:HE2	1.57	0.48
1:H:46:ASP:C	1:H:47:GLU:HG3	2.38	0.48
1:H:144:THR:HG21	1:H:286:TYR:CD2	2.48	0.48
1:H:276:LEU:CD2	1:H:279:LEU:CB	2.92	0.48
1:A:221:GLU:O	1:A:222:ALA:C	2.57	0.48
1:B:138:ASN:HB2	4:B:352:NAD:HO2N	1.72	0.48
1:E:223:GLN:OE1	1:E:223:GLN:HA	2.10	0.48
1:F:146:ALA:CB	1:F:329:PHE:CZ	2.97	0.48
1:H:213:LYS:C	1:H:216:GLU:HB3	2.39	0.48
1:A:122:GLU:O	1:A:126:ALA:CB	2.61	0.47
1:B:124:VAL:HG22	1:B:129:PHE:HB3	1.96	0.47
1:B:169:ARG:HG2	1:C:67:HIS:CG	2.49	0.47
1:B:182:PRO:C	1:B:184:ASN:N	2.72	0.47
1:B:265:ASN:HA	1:B:295:ARG:H	1.79	0.47
1:C:16:LYS:NZ	1:D:264:HIS:CB	2.74	0.47
1:C:226:LEU:O	1:C:229:ILE:HB	2.13	0.47
1:E:65:PHE:HB3	1:E:78:ILE:HD13	1.96	0.47
1:E:193:HIS:HB2	5:E:377:HOH:O	2.13	0.47
1:G:44:ILE:HG22	1:G:263:LEU:HD12	1.97	0.47
1:G:106:ARG:HG2	1:G:138:ASN:CG	2.39	0.47
1:H:191:GLY:HA2	1:H:287:ILE:HD11	1.96	0.47
1:A:41:ASN:HB2	1:D:41:ASN:HB3	1.96	0.47
1:A:125:MET:SD	1:A:153:LEU:HD11	2.54	0.47
1:A:295:ARG:HB3	1:B:15:MET:CE	2.42	0.47
1:B:118:ARG:NH2	1:B:330:THR:HG21	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:ARG:O	1:C:260:ARG:HB2	2.14	0.47
1:D:36:VAL:HG21	1:D:50:LEU:CD2	2.44	0.47
1:D:130:GLN:O	1:D:157:ARG:NH1	2.39	0.47
1:D:198:LEU:HA	1:D:199:PRO:HD3	1.79	0.47
1:D:260:ARG:HH11	1:D:260:ARG:HD3	1.44	0.47
1:H:136:ALA:O	4:H:352:NAD:H2N	2.14	0.47
1:H:243:LYS:HB2	1:H:243:LYS:HZ2	1.77	0.47
1:A:48:ILE:O	1:A:78:ILE:HA	2.15	0.47
1:A:83:TYR:O	1:A:86:CYS:HB2	2.14	0.47
1:A:198:LEU:HD22	1:A:313:ARG:HB2	1.95	0.47
1:B:272:VAL:O	1:B:288:GLY:HA2	2.14	0.47
1:C:324:VAL:O	1:C:328:ALA:N	2.46	0.47
1:E:208:VAL:CG2	1:G:304:ILE:HG21	2.45	0.47
1:F:87:ARG:HD2	1:F:128:GLY:HA3	1.95	0.47
1:G:159:ILE:HD11	1:G:297:GLY:HA2	1.96	0.47
1:G:325:LEU:HD22	1:G:329:PHE:CE2	2.49	0.47
1:H:175:GLY:CA	1:H:185:VAL:HG21	2.45	0.47
1:A:41:ASN:CB	1:D:41:ASN:HB3	2.44	0.47
1:B:16:LYS:NZ	1:B:46:ASP:OD1	2.39	0.47
1:B:39:LEU:CD2	1:B:44:ILE:HD12	2.42	0.47
1:B:182:PRO:C	1:B:184:ASN:H	2.23	0.47
1:C:24:VAL:HG11	1:C:51:ILE:HD11	1.97	0.47
1:D:189:ILE:HA	1:D:198:LEU:O	2.14	0.47
1:D:324:VAL:O	1:D:328:ALA:HB3	2.14	0.47
1:G:112:LYS:CA	1:G:112:LYS:CE	2.89	0.47
1:H:166:ASP:HB3	1:H:189:ILE:HG21	1.96	0.47
5:A:419:HOH:O	1:B:295:ARG:CD	2.58	0.47
1:B:15:MET:CB	1:B:19:GLY:CA	2.90	0.47
1:C:177:TYR:CE1	1:C:225:ASP:OD2	2.68	0.47
1:D:177:TYR:HD2	1:D:178:PHE:CZ	2.32	0.47
1:E:322:LYS:O	1:E:325:LEU:HB2	2.14	0.47
1:F:205:TYR:CE2	1:H:205:TYR:CE2	3.02	0.47
1:G:52:ASP:HB3	1:G:58:ALA:HB2	1.96	0.47
1:G:202:SER:OG	1:G:310:GLU:OE1	2.32	0.47
5:G:557:HOH:O	1:H:295:ARG:HG3	2.15	0.47
1:H:125:MET:HA	1:H:125:MET:HE3	1.95	0.47
1:B:299:ARG:C	1:B:300:GLU:HG3	2.38	0.47
1:B:305:GLU:OE1	1:D:213:LYS:HE2	2.15	0.47
1:E:55:GLU:O	1:E:59:ILE:HG13	2.15	0.47
1:E:203:GLN:NE2	1:G:209:MET:CE	2.74	0.47
1:F:87:ARG:CZ	1:F:87:ARG:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:ARG:CG	1:H:15:MET:HG3	2.43	0.47
1:H:65:PHE:O	1:H:67:HIS:N	2.48	0.47
1:H:150:PHE:CZ	1:H:330:THR:HB	2.49	0.47
1:H:279:LEU:HD22	5:H:407:HOH:O	2.14	0.47
1:A:170:PHE:HE2	1:A:187:ALA:HB1	1.79	0.47
1:B:31:VAL:HG13	1:B:251:ILE:CG2	2.45	0.47
1:B:38:ALA:O	1:B:42:GLN:HG3	2.15	0.47
1:B:203:GLN:HG3	1:D:208:VAL:O	2.15	0.47
1:C:35:TYR:CE1	1:C:255:LEU:HB3	2.50	0.47
1:C:231:VAL:O	1:C:235:ASP:HB2	2.14	0.47
1:D:170:PHE:CG	1:D:189:ILE:HD11	2.49	0.47
1:D:260:ARG:O	1:D:261:ALA:C	2.57	0.47
1:E:164:ILE:CD1	1:E:258:VAL:HG23	2.45	0.47
1:F:200:VAL:HG11	1:F:304:ILE:CD1	2.45	0.47
1:F:308:ASP:O	1:F:312:ASN:HB2	2.15	0.47
1:G:86:CYS:O	1:G:89:ALA:N	2.41	0.47
1:G:93:VAL:HG13	1:G:134:LEU:HG	1.96	0.47
1:G:93:VAL:HG13	1:G:134:LEU:O	2.14	0.47
1:G:279:LEU:CD2	1:G:301:VAL:HB	2.45	0.47
1:H:132:LEU:HD22	5:H:376:HOH:O	2.15	0.47
1:A:291:ALA:HB1	1:A:298:ILE:CG2	2.44	0.47
1:B:41:ASN:O	1:B:73:PRO:HG3	2.14	0.47
1:B:94:ILE:HG21	1:B:117:PHE:CE2	2.50	0.47
1:B:304:ILE:CB	1:D:209:MET:HE3	2.42	0.47
1:D:92:VAL:HG12	1:D:133:PHE:CD1	2.50	0.47
1:D:185:VAL:HG22	1:D:206:ILE:HD12	1.97	0.47
1:G:83:TYR:C	1:G:85:ASP:N	2.71	0.47
1:A:327:ARG:NH2	1:A:328:ALA:HB2	2.30	0.47
1:B:16:LYS:HE3	1:B:75:PRO:O	2.15	0.47
1:B:24:VAL:HB	1:B:92:VAL:HG22	1.95	0.47
1:B:102:PRO:C	1:B:104:GLU:H	2.23	0.47
1:C:220:GLU:O	1:C:221:GLU:O	2.31	0.47
1:D:118:ARG:CG	1:D:118:ARG:NH1	2.77	0.47
1:D:145:TYR:CD1	1:D:329:PHE:HE2	2.32	0.47
1:E:15:MET:CB	1:E:19:GLY:CA	2.77	0.47
1:E:218:LYS:HB3	1:E:218:LYS:HE2	1.55	0.47
1:F:212:ARG:NH1	1:F:226:LEU:HD13	2.27	0.47
1:F:247:THR:HG21	3:F:351:OXM:O3	2.15	0.47
1:F:251:ILE:HG13	1:F:255:LEU:HD22	1.97	0.47
5:F:422:HOH:O	1:G:75:PRO:HA	2.15	0.47
1:G:280:TYR:CZ	1:G:303:GLU:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:VAL:CB	1:H:222:ALA:CB	2.69	0.47
1:B:243:LYS:HD3	1:C:59:ILE:CG2	2.45	0.47
1:C:148:TRP:CZ3	1:C:275:TYR:CE2	3.03	0.47
1:D:118:ARG:HH11	1:D:118:ARG:HG2	1.80	0.47
1:F:74:LYS:HB2	5:F:361:HOH:O	2.15	0.47
1:F:215:VAL:HA	1:F:218:LYS:HE3	1.97	0.47
1:G:229:ILE:O	1:G:233:VAL:HG23	2.14	0.47
1:A:107:LEU:CD2	1:A:324:VAL:HG21	2.46	0.46
1:A:109:LEU:O	1:A:113:ASN:ND2	2.48	0.46
1:A:243:LYS:HD2	1:D:63:MET:HE3	1.97	0.46
1:B:110:VAL:HG12	1:B:114:ILE:CD1	2.45	0.46
1:C:15:MET:HA	1:D:265:ASN:CB	2.45	0.46
1:D:47:GLU:CD	5:D:363:HOH:O	2.57	0.46
1:E:173:LEU:O	5:E:383:HOH:O	2.20	0.46
1:F:58:ALA:HB1	1:F:80:HIS:HD2	1.80	0.46
1:F:221:GLU:O	1:F:222:ALA:C	2.56	0.46
1:F:237:ALA:O	1:F:241:ILE:HD12	2.15	0.46
1:G:240:ILE:HB	1:G:247:THR:HG22	1.98	0.46
1:A:174:LEU:HD23	1:A:229:ILE:HD13	1.97	0.46
1:C:15:MET:N	1:C:20:GLY:CA	2.78	0.46
1:E:109:LEU:CD2	5:E:374:HOH:O	2.62	0.46
1:E:173:LEU:HD12	1:E:233:VAL:HG23	1.97	0.46
1:E:213:LYS:O	1:E:213:LYS:HG2	2.15	0.46
1:G:137:THR:HG22	1:G:143:LEU:HD13	1.96	0.46
1:G:222:ALA:O	1:G:223:GLN:C	2.58	0.46
1:A:67:HIS:HE1	1:D:240:ILE:HD11	1.81	0.46
1:D:16:LYS:CE	1:D:75:PRO:O	2.63	0.46
1:D:26:ILE:HD13	1:D:83:TYR:HE1	1.81	0.46
1:D:30:PHE:HB3	1:D:248:TYR:CG	2.50	0.46
1:D:228:ARG:NH1	1:D:228:ARG:HA	2.29	0.46
1:E:120:ILE:O	1:E:121:VAL:C	2.58	0.46
1:E:189:ILE:CG2	1:E:197:GLU:HB2	2.46	0.46
1:F:18:ASN:N	1:F:47:GLU:OE2	2.47	0.46
1:G:24:VAL:HG21	1:G:89:ALA:HB2	1.97	0.46
1:H:111:ASP:O	1:H:112:LYS:C	2.58	0.46
1:H:276:LEU:HD22	1:H:279:LEU:CB	2.45	0.46
1:A:206:ILE:HG12	1:A:211:ILE:HG12	1.96	0.46
1:B:174:LEU:HD23	1:B:229:ILE:HD13	1.96	0.46
1:D:136:ALA:O	4:D:352:NAD:H2N	2.16	0.46
1:F:15:MET:O	1:F:47:GLU:OE2	2.33	0.46
1:H:26:ILE:HD11	1:H:92:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TYR:HE2	1:A:124:VAL:HG12	1.81	0.46
1:C:219:GLY:O	1:C:221:GLU:N	2.48	0.46
1:C:250:GLY:CA	5:C:355:HOH:O	2.62	0.46
1:D:287:ILE:HG13	1:D:321:LEU:CD1	2.44	0.46
1:F:21:ALA:HB1	1:F:263:LEU:HD22	1.96	0.46
1:F:229:ILE:O	1:F:233:VAL:HG23	2.15	0.46
1:H:219:GLY:C	1:H:221:GLU:H	2.24	0.46
1:A:56:SER:HA	1:A:59:ILE:HD12	1.97	0.46
1:A:265:ASN:HA	1:A:295:ARG:H	1.80	0.46
1:B:275:TYR:CZ	1:B:284:ASP:HA	2.50	0.46
1:C:16:LYS:HE2	1:D:264:HIS:O	2.14	0.46
1:C:134:LEU:HA	1:C:159:ILE:O	2.16	0.46
1:C:138:ASN:HB3	1:C:139:PRO:HA	1.96	0.46
1:C:166:ASP:OD2	1:C:193:HIS:ND1	2.37	0.46
1:C:294:ASN:C	1:C:294:ASN:ND2	2.71	0.46
1:D:140:VAL:HG21	1:D:162:GLY:H	1.80	0.46
1:D:181:ALA:HB3	1:D:184:ASN:OD1	2.16	0.46
1:E:155:HIS:CD2	1:E:275:TYR:HB3	2.50	0.46
1:E:251:ILE:HD13	5:E:381:HOH:O	2.15	0.46
1:G:16:LYS:HZ2	1:H:264:HIS:C	2.22	0.46
1:G:107:LEU:N	1:G:107:LEU:HD23	2.29	0.46
1:G:262:ILE:O	1:G:265:ASN:N	2.45	0.46
1:H:267:ASN:ND2	1:H:294:ASN:CB	2.75	0.46
1:A:36:VAL:HG13	1:A:48:ILE:HG21	1.97	0.46
1:A:50:LEU:C	1:A:51:ILE:HG13	2.41	0.46
1:A:224:LYS:HE3	1:A:224:LYS:HB3	1.82	0.46
1:B:216:GLU:HA	5:B:400:HOH:O	2.16	0.46
1:B:244:LYS:NZ	1:C:61:ASP:OD1	2.45	0.46
1:C:110:VAL:HG13	1:C:142:ILE:HG21	1.97	0.46
1:C:114:ILE:HD11	1:C:142:ILE:CG2	2.46	0.46
1:C:177:TYR:HE1	1:C:225:ASP:OD2	1.98	0.46
1:D:60:GLY:HA2	1:D:63:MET:HG3	1.97	0.46
1:E:163:THR:HA	1:E:166:ASP:OD1	2.16	0.46
1:F:138:ASN:HA	1:F:140:VAL:N	2.31	0.46
1:H:173:LEU:O	1:H:174:LEU:C	2.59	0.46
1:H:178:PHE:HZ	1:H:211:ILE:HG23	1.81	0.46
1:B:258:VAL:O	1:B:259:THR:C	2.58	0.46
1:C:52:ASP:OD2	1:C:54:ASN:HB3	2.15	0.46
1:D:137:THR:HG23	4:D:352:NAD:O3D	2.16	0.46
1:D:164:ILE:HD13	1:D:258:VAL:HG23	1.96	0.46
1:F:208:VAL:CG2	1:H:203:GLN:HG3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:HIS:CD2	1:G:207:GLY:O	2.69	0.46
1:H:325:LEU:O	1:H:326:ALA:C	2.58	0.46
1:B:59:ILE:N	1:B:59:ILE:CD1	2.79	0.46
1:D:247:THR:C	1:D:248:TYR:CD1	2.94	0.46
1:E:15:MET:SD	1:E:17:ASN:O	2.73	0.46
1:F:35:TYR:CE2	1:F:93:VAL:HG21	2.50	0.46
1:F:114:ILE:HG23	1:F:330:THR:HA	1.95	0.46
1:H:15:MET:HB2	1:H:19:GLY:CA	2.46	0.46
1:A:120:ILE:O	1:A:124:VAL:CG1	2.60	0.46
1:C:120:ILE:O	1:C:124:VAL:CG1	2.64	0.46
1:D:129:PHE:CG	1:D:130:GLN:N	2.83	0.46
1:D:270:LEU:HD12	1:D:293:ILE:HG13	1.97	0.46
1:E:64:ASP:OD2	1:H:244:LYS:CE	2.64	0.46
1:F:157:ARG:HH11	1:F:157:ARG:HD3	1.33	0.46
1:H:249:TYR:O	1:H:253:MET:HG2	2.16	0.46
1:A:175:GLY:HA2	1:A:185:VAL:HG21	1.97	0.45
1:B:35:TYR:CZ	1:B:93:VAL:HG21	2.51	0.45
1:B:159:ILE:HD12	1:B:262:ILE:HD11	1.98	0.45
1:B:209:MET:HA	1:B:210:PRO:HD3	1.67	0.45
1:C:266:GLU:CG	1:D:75:PRO:HG3	2.47	0.45
1:D:138:ASN:CB	4:D:352:NAD:O2D	2.53	0.45
1:E:295:ARG:CD	1:F:15:MET:HG3	2.39	0.45
1:F:110:VAL:HG21	1:F:324:VAL:CG1	2.46	0.45
1:G:44:ILE:HD13	1:G:260:ARG:HG2	1.98	0.45
1:G:251:ILE:HG13	1:G:255:LEU:HD22	1.97	0.45
1:A:123:SER:O	1:A:126:ALA:HB3	2.16	0.45
1:C:148:TRP:CE2	1:C:155:HIS:HB3	2.51	0.45
1:D:18:ASN:N	1:D:47:GLU:OE2	2.49	0.45
1:F:87:ARG:CG	1:F:128:GLY:C	2.81	0.45
1:F:177:TYR:CE1	1:F:225:ASP:HB3	2.52	0.45
1:F:208:VAL:HG23	1:F:208:VAL:O	2.15	0.45
1:F:275:TYR:CZ	1:F:284:ASP:HA	2.51	0.45
1:G:74:LYS:HE3	1:G:74:LYS:HB3	1.53	0.45
1:A:327:ARG:HH21	1:A:328:ALA:HB2	1.81	0.45
1:C:99:ASN:HA	5:C:373:HOH:O	2.16	0.45
1:C:120:ILE:O	1:C:124:VAL:HG13	2.17	0.45
1:C:164:ILE:HD12	1:C:258:VAL:HG23	1.97	0.45
1:D:265:ASN:HD22	1:D:295:ARG:CB	2.24	0.45
1:H:149:LYS:HA	1:H:149:LYS:CE	2.45	0.45
1:H:230:PHE:O	1:H:233:VAL:HB	2.17	0.45
1:A:37:PHE:HD1	1:A:37:PHE:HA	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:HA	1:A:149:LYS:HE3	1.98	0.45
1:A:175:GLY:CA	1:A:185:VAL:HG21	2.46	0.45
1:B:299:ARG:CZ	1:B:300:GLU:OE2	2.64	0.45
1:C:180:VAL:HG21	1:C:206:ILE:CG2	2.43	0.45
1:C:276:LEU:HD11	1:C:287:ILE:CG2	2.47	0.45
1:E:57:LYS:NZ	1:E:61:ASP:OD2	2.39	0.45
1:E:239:GLN:O	1:E:243:LYS:HD2	2.16	0.45
1:E:244:LYS:HD2	1:H:60:GLY:CA	2.45	0.45
1:F:52:ASP:OD1	4:F:352:NAD:O2B	2.21	0.45
1:F:165:LEU:HA	5:F:424:HOH:O	2.15	0.45
1:A:15:MET:HG3	1:B:295:ARG:HD3	1.98	0.45
1:A:279:LEU:HB2	5:A:399:HOH:O	2.16	0.45
1:D:113:ASN:CB	1:D:143:LEU:HD11	2.47	0.45
1:F:16:LYS:HE3	1:F:46:ASP:HA	1.99	0.45
1:F:101:LYS:O	1:F:104:GLU:HB2	2.16	0.45
1:F:201:TRP:C	1:F:203:GLN:N	2.75	0.45
1:G:16:LYS:HZ1	1:H:264:HIS:CA	2.28	0.45
1:G:153:LEU:HB3	1:G:154:PRO:CD	2.46	0.45
1:G:180:VAL:HG23	1:G:181:ALA:O	2.17	0.45
1:H:112:LYS:HA	1:H:112:LYS:CE	2.47	0.45
1:H:145:TYR:O	1:H:148:TRP:HB3	2.17	0.45
1:A:151:SER:OG	1:A:153:LEU:HD12	2.16	0.45
1:C:101:LYS:HB2	1:C:104:GLU:OE1	2.17	0.45
1:C:299:ARG:O	1:C:300:GLU:HG3	2.16	0.45
1:G:36:VAL:HG21	1:G:50:LEU:CD2	2.46	0.45
1:H:313:ARG:HH11	1:H:313:ARG:HD2	1.43	0.45
1:H:313:ARG:HA	1:H:316:HIS:HB3	1.98	0.45
1:A:125:MET:CE	1:A:153:LEU:HD11	2.46	0.45
1:A:196:THR:OG1	1:A:317:SER:CB	2.65	0.45
1:A:244:LYS:O	1:A:244:LYS:HG2	2.17	0.45
1:C:213:LYS:HA	1:C:216:GLU:HB3	1.99	0.45
1:D:220:GLU:HA	1:D:223:GLN:CB	2.36	0.45
1:E:142:ILE:N	1:E:142:ILE:CD1	2.78	0.45
1:A:110:VAL:HB	1:A:111:ASP:H	1.68	0.45
1:B:57:LYS:NZ	1:B:61:ASP:OD2	2.49	0.45
1:C:189:ILE:CD1	1:C:230:PHE:HE1	2.19	0.45
1:C:264:HIS:O	1:C:265:ASN:C	2.59	0.45
1:D:125:MET:O	1:D:126:ALA:C	2.59	0.45
1:D:138:ASN:HA	1:D:140:VAL:N	2.32	0.45
1:E:290:PRO:HG3	1:E:304:ILE:HG21	1.99	0.45
1:F:22:ARG:HE	1:F:22:ARG:HB2	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:TRP:HB2	1:F:158:VAL:CG2	2.46	0.45
1:F:257:ARG:HH12	1:F:266:GLU:CD	2.24	0.45
1:H:274:ALA:HB1	1:H:301:VAL:CG2	2.46	0.45
1:H:278:GLY:CA	1:H:282:GLU:O	2.65	0.45
1:A:15:MET:CB	1:A:19:GLY:CA	2.62	0.45
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.71	0.45
1:B:35:TYR:O	1:B:38:ALA:HB3	2.17	0.45
1:B:54:ASN:O	1:B:55:GLU:C	2.60	0.45
1:C:110:VAL:O	1:C:114:ILE:HG12	2.17	0.45
1:C:264:HIS:O	1:D:16:LYS:HD3	2.16	0.45
1:E:208:VAL:HG22	1:G:188:TYR:CE2	2.52	0.45
1:F:159:ILE:HD12	1:F:262:ILE:HD11	1.99	0.45
1:F:201:TRP:C	1:F:203:GLN:H	2.25	0.45
1:H:189:ILE:CD1	1:H:230:PHE:CE1	2.99	0.45
1:A:16:LYS:HE3	1:A:46:ASP:CB	2.47	0.45
1:A:107:LEU:HA	1:A:139:PRO:CG	2.46	0.45
1:A:242:GLU:O	1:A:242:GLU:HG3	2.17	0.45
1:A:265:ASN:HA	1:A:265:ASN:HD22	1.61	0.45
1:B:49:VAL:HG22	1:B:79:TRP:CZ2	2.52	0.45
1:B:243:LYS:HD2	1:C:59:ILE:HG22	1.98	0.45
1:C:172:PHE:CD1	1:C:172:PHE:C	2.92	0.45
1:C:257:ARG:O	1:C:257:ARG:NH1	2.49	0.45
1:E:16:LYS:HZ1	1:E:46:ASP:CG	2.20	0.45
1:E:264:HIS:CA	1:F:16:LYS:NZ	2.80	0.45
1:G:74:LYS:HD2	1:G:75:PRO:CD	2.34	0.45
1:G:291:ALA:HB1	1:G:298:ILE:CG2	2.44	0.45
1:H:15:MET:C	1:H:17:ASN:H	2.05	0.45
1:H:65:PHE:O	1:H:66:ASN:C	2.60	0.45
1:A:15:MET:CB	1:A:19:GLY:N	2.75	0.44
1:B:30:PHE:N	4:B:352:NAD:O2N	2.49	0.44
1:C:15:MET:N	1:C:20:GLY:N	2.65	0.44
1:D:129:PHE:CE1	1:D:131:GLY:N	2.71	0.44
1:D:187:ALA:HB2	1:D:204:ALA:HB1	1.98	0.44
1:E:134:LEU:HD13	1:E:258:VAL:HG11	1.99	0.44
1:E:200:VAL:HG12	1:E:200:VAL:O	2.17	0.44
1:E:280:TYR:OH	1:E:304:ILE:HG12	2.16	0.44
1:G:83:TYR:O	1:G:84:ASP:C	2.60	0.44
1:H:27:GLY:O	1:H:32:GLY:HA3	2.16	0.44
1:H:173:LEU:O	1:H:176:GLU:N	2.49	0.44
1:H:280:TYR:HB3	1:H:314:PHE:CE2	2.52	0.44
1:A:16:LYS:HD3	1:A:16:LYS:HA	1.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:N	1:A:132:LEU:CD2	2.80	0.44
1:C:30:PHE:HB3	1:C:248:TYR:CG	2.52	0.44
1:D:153:LEU:HB3	1:D:154:PRO:CD	2.47	0.44
1:D:170:PHE:CG	1:D:189:ILE:CD1	3.00	0.44
1:D:221:GLU:OE1	5:D:425:HOH:O	2.20	0.44
1:F:16:LYS:HE2	1:F:75:PRO:O	2.18	0.44
1:F:171:ARG:O	1:F:175:GLY:N	2.49	0.44
1:G:210:PRO:O	1:G:211:ILE:C	2.60	0.44
1:G:220:GLU:N	1:G:223:GLN:HB2	2.32	0.44
1:H:133:PHE:CD1	1:H:153:LEU:HD11	2.53	0.44
1:A:80:HIS:NE2	5:A:359:HOH:O	2.19	0.44
1:A:90:ASP:HA	5:A:367:HOH:O	2.18	0.44
1:B:100:GLN:HA	1:B:109:LEU:HD21	1.99	0.44
1:B:165:LEU:HD22	1:B:251:ILE:CA	2.47	0.44
1:D:116:ILE:CG2	1:D:120:ILE:HD11	2.47	0.44
1:D:269:ILE:HG21	1:D:302:ILE:HD12	2.00	0.44
1:G:107:LEU:HD21	1:G:192:GLU:OE2	2.18	0.44
1:H:112:LYS:CA	1:H:112:LYS:CE	2.95	0.44
1:H:294:ASN:ND2	1:H:294:ASN:C	2.74	0.44
1:A:54:ASN:ND2	1:A:54:ASN:O	2.49	0.44
1:A:160:GLY:HA3	1:A:273:SER:CB	2.48	0.44
1:C:16:LYS:HZ3	1:D:264:HIS:CA	2.31	0.44
1:F:51:ILE:HD11	1:F:82:ASP:C	2.42	0.44
1:G:86:CYS:CB	1:G:124:VAL:HG23	2.47	0.44
1:H:165:LEU:HD12	1:H:165:LEU:O	2.17	0.44
1:C:15:MET:HB3	1:C:17:ASN:C	2.43	0.44
1:D:100:GLN:NE2	1:D:241:ILE:HD11	2.33	0.44
1:E:92:VAL:HG23	1:E:129:PHE:CE1	2.53	0.44
1:F:148:TRP:CB	1:F:158:VAL:HG21	2.47	0.44
1:F:169:ARG:HD3	1:F:236:ALA:CB	2.47	0.44
1:F:266:GLU:O	1:F:267:ASN:HB2	2.17	0.44
1:G:66:ASN:ND2	5:G:442:HOH:O	2.50	0.44
1:H:159:ILE:HG12	1:H:298:ILE:HD12	1.99	0.44
1:A:171:ARG:HD2	1:A:185:VAL:O	2.17	0.44
1:C:209:MET:HG3	1:C:214:LEU:HD21	1.99	0.44
1:E:67:HIS:CG	1:H:169:ARG:HG2	2.51	0.44
1:E:70:VAL:HG21	1:H:171:ARG:HB2	1.99	0.44
1:E:240:ILE:HG23	1:E:244:LYS:HD3	1.99	0.44
1:E:276:LEU:HD23	1:E:276:LEU:HA	1.80	0.44
1:F:148:TRP:HA	1:F:158:VAL:HG21	1.99	0.44
1:G:280:TYR:CE1	1:G:289:VAL:CG2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:298:ILE:HG22	1:H:300:GLU:N	2.32	0.44
1:A:52:ASP:OD2	4:A:352:NAD:H1B	2.17	0.44
1:A:206:ILE:CG1	1:A:211:ILE:CD1	2.96	0.44
1:A:215:VAL:HB	1:A:222:ALA:CB	2.47	0.44
1:C:173:LEU:HA	1:C:173:LEU:HD23	1.67	0.44
1:D:274:ALA:HB3	1:D:289:VAL:HG12	2.00	0.44
1:D:274:ALA:HB1	1:D:301:VAL:HG22	2.00	0.44
1:D:280:TYR:CE1	1:D:289:VAL:HG21	2.53	0.44
1:E:167:THR:O	1:E:171:ARG:HG3	2.17	0.44
1:G:74:LYS:NZ	1:G:75:PRO:O	2.47	0.44
1:H:155:HIS:CD2	1:H:275:TYR:HB3	2.53	0.44
1:H:189:ILE:HD13	1:H:230:PHE:CE1	2.50	0.44
1:H:248:TYR:HA	1:H:251:ILE:CG2	2.48	0.44
1:H:306:LEU:C	1:H:307:ASN:O	2.58	0.44
1:B:64:ASP:HB2	1:C:244:LYS:HE2	2.00	0.44
1:B:100:GLN:HE21	3:B:351:OXM:HN1	1.64	0.44
1:B:282:GLU:HG3	1:B:318:ALA:HB1	2.00	0.44
1:C:15:MET:CG	1:C:19:GLY:CA	2.94	0.44
1:C:101:LYS:HB3	1:C:101:LYS:HZ3	1.79	0.44
1:D:227:GLU:O	1:D:231:VAL:HG23	2.18	0.44
1:E:113:ASN:HB3	1:E:143:LEU:HD11	2.00	0.44
1:E:205:TYR:CZ	1:G:205:TYR:CE2	3.06	0.44
1:E:209:MET:HA	1:E:210:PRO:HD3	1.86	0.44
1:E:220:GLU:HA	1:E:223:GLN:CB	2.35	0.44
1:E:228:ARG:O	1:E:229:ILE:C	2.59	0.44
1:E:261:ALA:HA	1:E:266:GLU:HB2	2.00	0.44
1:G:18:ASN:N	1:G:47:GLU:OE2	2.51	0.44
1:G:186:HIS:HB2	1:G:205:TYR:HB2	2.00	0.44
1:G:218:LYS:HG3	1:G:222:ALA:CB	2.39	0.44
1:A:56:SER:CA	1:A:59:ILE:HD12	2.48	0.44
1:A:100:GLN:CB	1:A:109:LEU:HD11	2.47	0.44
1:B:19:GLY:N	5:B:357:HOH:O	2.51	0.44
1:C:267:ASN:HD22	1:C:292:VAL:HG12	1.83	0.44
1:D:34:SER:O	1:D:35:TYR:C	2.59	0.44
1:D:275:TYR:HB2	1:D:286:TYR:CE1	2.53	0.44
1:E:21:ALA:HB1	1:E:263:LEU:HD13	2.00	0.44
1:F:94:ILE:HG21	1:F:117:PHE:CE2	2.52	0.44
1:G:70:VAL:HG22	5:G:440:HOH:O	2.17	0.44
1:G:125:MET:HA	1:G:125:MET:HE3	1.99	0.44
1:G:299:ARG:CZ	1:G:300:GLU:OE2	2.66	0.44
1:H:124:VAL:C	1:H:126:ALA:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:SER:O	1:A:162:GLY:C	2.61	0.43
1:A:265:ASN:OD1	1:B:17:ASN:HB2	2.17	0.43
1:A:272:VAL:O	1:A:288:GLY:HA2	2.18	0.43
1:B:25:VAL:HG21	1:B:36:VAL:CG2	2.48	0.43
1:C:221:GLU:HB3	1:C:224:LYS:N	2.26	0.43
1:C:309:ASP:O	1:C:313:ARG:HG2	2.16	0.43
1:D:15:MET:N	1:D:20:GLY:HA3	2.32	0.43
1:D:329:PHE:HD1	1:D:330:THR:H	1.65	0.43
1:E:89:ALA:O	1:E:129:PHE:HE1	2.01	0.43
1:E:166:ASP:OD2	1:E:197:GLU:OE1	2.36	0.43
1:E:209:MET:HG2	1:G:304:ILE:HG22	2.00	0.43
1:E:304:ILE:HG13	1:E:306:LEU:HD23	1.98	0.43
1:F:110:VAL:O	1:F:114:ILE:HB	2.18	0.43
1:F:172:PHE:CE2	1:F:173:LEU:HD23	2.53	0.43
1:F:279:LEU:HD12	1:F:279:LEU:HA	1.77	0.43
1:G:145:TYR:HD1	1:G:329:PHE:CZ	2.36	0.43
1:G:273:SER:HA	1:G:287:ILE:O	2.18	0.43
1:H:201:TRP:HZ3	1:H:211:ILE:HD13	1.83	0.43
1:H:325:LEU:HD23	1:H:325:LEU:HA	1.76	0.43
1:A:220:GLU:CA	1:A:223:GLN:HB2	2.46	0.43
1:B:92:VAL:HG12	1:B:133:PHE:CE1	2.53	0.43
1:B:101:LYS:CB	1:B:102:PRO:CD	2.92	0.43
1:C:101:LYS:CB	1:C:101:LYS:HZ2	2.31	0.43
1:D:221:GLU:O	1:D:225:ASP:HB2	2.18	0.43
1:E:75:PRO:CA	5:H:356:HOH:O	2.60	0.43
1:E:173:LEU:CB	1:E:229:ILE:HG23	2.48	0.43
1:F:313:ARG:NH1	1:F:313:ARG:CG	2.68	0.43
1:H:23:VAL:O	1:H:48:ILE:HA	2.19	0.43
1:H:96:ALA:O	1:H:137:THR:CG2	2.66	0.43
1:B:117:PHE:O	1:B:121:VAL:HB	2.18	0.43
1:C:15:MET:CE	1:D:265:ASN:ND2	2.81	0.43
1:C:299:ARG:HG2	1:C:300:GLU:HG3	1.99	0.43
1:D:18:ASN:N	1:D:18:ASN:OD1	2.50	0.43
1:D:170:PHE:CD2	1:D:189:ILE:HD11	2.52	0.43
1:E:106:ARG:NH1	1:E:194:GLY:HA2	2.34	0.43
1:E:264:HIS:O	1:F:16:LYS:HD3	2.18	0.43
1:F:244:LYS:HE3	1:G:64:ASP:OD2	2.17	0.43
1:G:16:LYS:NZ	1:H:264:HIS:C	2.76	0.43
1:G:215:VAL:CG2	1:G:222:ALA:CB	2.96	0.43
1:A:246:ALA:O	1:A:248:TYR:CD1	2.71	0.43
1:A:265:ASN:CB	1:B:15:MET:HA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ILE:O	1:B:245:GLY:N	2.52	0.43
1:B:280:TYR:CZ	1:B:303:GLU:HA	2.54	0.43
1:E:129:PHE:CZ	1:E:131:GLY:C	2.97	0.43
1:H:72:ALA:C	1:H:74:LYS:N	2.75	0.43
1:H:121:VAL:O	1:H:124:VAL:HG13	2.18	0.43
1:A:253:MET:HE1	1:D:72:ALA:HA	2.00	0.43
1:B:309:ASP:O	1:B:313:ARG:HG3	2.17	0.43
1:C:112:LYS:HB2	5:C:377:HOH:O	2.18	0.43
1:C:117:PHE:HE2	1:C:135:VAL:HG13	1.83	0.43
1:C:328:ALA:HB1	5:C:408:HOH:O	2.18	0.43
1:D:132:LEU:N	1:D:132:LEU:HD22	2.34	0.43
1:F:31:VAL:HG23	4:F:352:NAD:PN	2.58	0.43
1:H:148:TRP:CD1	1:H:153:LEU:O	2.72	0.43
1:A:137:THR:HB	1:A:143:LEU:CD1	2.48	0.43
1:A:218:LYS:HB3	1:A:218:LYS:HE2	1.85	0.43
1:B:124:VAL:HG23	1:B:129:PHE:HB2	2.00	0.43
1:B:203:GLN:NE2	1:B:305:GLU:O	2.52	0.43
1:D:113:ASN:HB2	1:D:143:LEU:HD11	2.01	0.43
1:D:237:ALA:HB2	3:D:351:OXM:C2	2.48	0.43
1:E:70:VAL:HG11	1:H:171:ARG:CZ	2.48	0.43
1:G:145:TYR:HA	1:G:286:TYR:CE1	2.53	0.43
1:H:314:PHE:O	1:H:317:SER:N	2.52	0.43
1:A:16:LYS:HZ3	1:B:264:HIS:HB3	1.83	0.43
1:A:289:VAL:HA	1:A:290:PRO:HD2	1.91	0.43
1:B:118:ARG:HE	1:B:330:THR:HG1	1.63	0.43
1:D:228:ARG:NH1	1:D:228:ARG:C	2.76	0.43
1:D:253:MET:HE3	1:D:253:MET:HB3	1.74	0.43
1:D:265:ASN:CG	1:D:295:ARG:HB2	2.43	0.43
1:D:275:TYR:HB2	1:D:286:TYR:CD1	2.54	0.43
1:E:52:ASP:OD1	4:E:352:NAD:H1B	2.18	0.43
1:E:292:VAL:N	1:E:300:GLU:O	2.50	0.43
1:E:294:ASN:ND2	1:E:295:ARG:N	2.65	0.43
1:F:86:CYS:O	1:F:87:ARG:C	2.59	0.43
1:F:91:LEU:HD11	1:F:134:LEU:HB3	2.01	0.43
1:G:23:VAL:O	1:G:48:ILE:HA	2.19	0.43
1:H:279:LEU:HD12	1:H:279:LEU:HA	1.86	0.43
1:A:209:MET:O	1:A:210:PRO:C	2.62	0.43
1:B:168:ALA:HA	1:C:70:VAL:HG21	2.01	0.43
1:B:177:TYR:CZ	1:B:225:ASP:HB3	2.54	0.43
1:D:279:LEU:HD22	5:D:407:HOH:O	2.18	0.43
1:D:318:ALA:O	1:D:322:LYS:CG	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:LEU:O	1:E:284:ASP:N	2.51	0.43
1:F:67:HIS:CG	1:G:169:ARG:HG2	2.54	0.43
1:F:177:TYR:HD2	1:F:178:PHE:CE2	2.37	0.43
1:G:128:GLY:O	1:G:130:GLN:HG2	2.18	0.43
1:G:174:LEU:HB3	1:G:185:VAL:HG11	2.01	0.43
1:H:28:ALA:N	1:H:52:ASP:OD2	2.49	0.43
1:H:280:TYR:CZ	1:H:303:GLU:HA	2.53	0.43
1:A:55:GLU:O	1:A:59:ILE:CD1	2.66	0.43
1:A:83:TYR:CD2	1:A:124:VAL:HG12	2.54	0.43
1:A:133:PHE:HE1	1:A:153:LEU:CD1	2.32	0.43
1:A:209:MET:HG2	1:A:214:LEU:HD21	2.01	0.43
1:A:304:ILE:HA	1:C:209:MET:CE	2.48	0.43
1:B:119:SER:O	1:B:120:ILE:C	2.61	0.43
1:B:209:MET:HE1	1:D:203:GLN:NE2	2.34	0.43
1:C:15:MET:HE2	1:D:265:ASN:ND2	2.34	0.43
1:C:290:PRO:HG3	1:C:304:ILE:HG21	2.01	0.43
1:D:91:LEU:HD11	1:D:134:LEU:HB2	2.01	0.43
1:E:212:ARG:O	1:E:213:LYS:CB	2.67	0.43
1:E:240:ILE:CG1	1:H:63:MET:CE	2.91	0.43
1:G:15:MET:N	1:G:20:GLY:HA3	2.34	0.43
1:H:327:ARG:NH2	1:H:328:ALA:HB2	2.33	0.43
1:A:209:MET:SD	1:A:213:LYS:CE	3.07	0.43
1:B:248:TYR:HA	1:B:251:ILE:CG2	2.49	0.43
1:B:248:TYR:HA	1:B:251:ILE:HG22	2.00	0.43
1:B:253:MET:HE3	1:B:253:MET:HB3	1.90	0.43
1:B:265:ASN:HB2	1:B:295:ARG:HG2	2.00	0.43
1:C:275:TYR:CZ	1:C:284:ASP:HA	2.53	0.43
1:D:274:ALA:HB1	1:D:301:VAL:CG2	2.49	0.43
1:E:35:TYR:HA	1:E:252:ALA:HB1	2.00	0.43
1:E:212:ARG:O	1:E:213:LYS:HB2	2.19	0.43
1:E:218:LYS:O	1:E:219:GLY:O	2.36	0.43
1:F:29:GLY:HA2	5:F:408:HOH:O	2.19	0.43
1:F:189:ILE:CD1	1:F:199:PRO:HA	2.48	0.43
1:H:15:MET:SD	1:H:17:ASN:O	2.77	0.43
1:B:213:LYS:HG2	1:B:214:LEU:HG	2.00	0.42
1:B:251:ILE:O	1:B:255:LEU:HD22	2.19	0.42
1:D:39:LEU:HD22	1:D:44:ILE:CB	2.49	0.42
1:F:60:GLY:C	1:G:244:LYS:HE2	2.44	0.42
1:G:307:ASN:O	1:G:308:ASP:C	2.62	0.42
1:G:309:ASP:OD2	1:G:313:ARG:HD2	2.18	0.42
1:H:69:LYS:C	1:H:71:PHE:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:TYR:CE1	1:A:329:PHE:HE2	2.35	0.42
1:B:60:GLY:HA3	1:C:244:LYS:HD2	2.00	0.42
1:B:75:PRO:HA	5:B:364:HOH:O	2.19	0.42
1:B:83:TYR:O	1:B:84:ASP:C	2.60	0.42
1:B:211:ILE:O	1:B:215:VAL:HG13	2.19	0.42
1:C:170:PHE:CE2	1:C:187:ALA:HB1	2.55	0.42
1:D:60:GLY:O	1:D:61:ASP:C	2.61	0.42
1:D:242:GLU:OE1	1:D:243:LYS:NZ	2.47	0.42
1:F:182:PRO:HG3	5:F:390:HOH:O	2.18	0.42
1:F:202:SER:HB3	1:F:310:GLU:OE2	2.19	0.42
1:H:148:TRP:CA	1:H:158:VAL:HG21	2.49	0.42
1:A:180:VAL:CG1	1:C:269:ILE:HD11	2.46	0.42
1:B:87:ARG:CZ	1:B:87:ARG:CB	2.97	0.42
1:C:116:ILE:CG2	1:C:120:ILE:CD1	2.96	0.42
1:C:311:LYS:HA	5:C:402:HOH:O	2.19	0.42
1:D:294:ASN:HD21	1:D:296:ASN:HB2	1.84	0.42
1:E:92:VAL:CG2	1:E:129:PHE:CZ	3.01	0.42
1:G:121:VAL:HA	1:G:124:VAL:HG12	2.01	0.42
1:H:235:ASP:O	1:H:236:ALA:C	2.62	0.42
1:A:16:LYS:NZ	1:B:264:HIS:HB3	2.34	0.42
1:B:210:PRO:O	1:B:213:LYS:HB3	2.20	0.42
1:F:106:ARG:O	1:F:109:LEU:HD12	2.19	0.42
1:F:198:LEU:HA	1:F:199:PRO:HD3	1.84	0.42
1:F:294:ASN:HD22	1:F:294:ASN:C	2.27	0.42
1:H:318:ALA:O	1:H:322:LYS:HG3	2.18	0.42
1:A:29:GLY:HA3	4:A:352:NAD:O5B	2.19	0.42
1:A:212:ARG:HH11	1:A:226:LEU:CD1	2.30	0.42
1:A:243:LYS:CD	1:D:59:ILE:HG22	2.49	0.42
1:A:271:THR:HG22	1:A:290:PRO:HD3	2.01	0.42
1:A:295:ARG:HG2	1:A:295:ARG:HH11	1.85	0.42
1:C:156:GLU:O	1:C:297:GLY:HA3	2.19	0.42
1:C:200:VAL:HG13	1:C:306:LEU:HD22	2.01	0.42
1:E:313:ARG:O	1:E:314:PHE:C	2.62	0.42
1:G:165:LEU:HD12	1:G:165:LEU:O	2.20	0.42
1:G:219:GLY:O	1:G:220:GLU:C	2.62	0.42
1:H:279:LEU:O	1:H:303:GLU:HG3	2.20	0.42
1:A:62:ALA:O	1:A:66:ASN:ND2	2.52	0.42
1:A:148:TRP:CD1	1:A:153:LEU:O	2.73	0.42
1:B:314:PHE:C	1:B:314:PHE:CD1	2.97	0.42
1:C:189:ILE:CD1	1:C:233:VAL:HG11	2.50	0.42
1:C:292:VAL:CG2	1:C:302:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:VAL:HA	1:D:134:LEU:O	2.19	0.42
1:D:164:ILE:HD13	1:D:258:VAL:CG2	2.49	0.42
1:E:24:VAL:HG11	1:E:86:CYS:SG	2.60	0.42
1:G:265:ASN:CG	1:H:15:MET:HA	2.40	0.42
1:H:65:PHE:C	1:H:67:HIS:N	2.77	0.42
1:H:118:ARG:HD2	1:H:330:THR:HG1	1.80	0.42
1:H:118:ARG:HA	1:H:150:PHE:CD2	2.54	0.42
1:H:124:VAL:O	1:H:127:SER:N	2.44	0.42
1:H:279:LEU:O	1:H:303:GLU:OE2	2.38	0.42
1:A:169:ARG:NH1	5:A:386:HOH:O	2.53	0.42
1:A:192:GLU:H	1:A:317:SER:HG	1.67	0.42
1:A:223:GLN:HG2	5:A:397:HOH:O	2.19	0.42
1:C:148:TRP:CD1	1:C:155:HIS:HA	2.55	0.42
1:C:275:TYR:HB2	1:C:286:TYR:CZ	2.55	0.42
1:D:154:PRO:C	1:D:156:GLU:N	2.76	0.42
1:E:40:MET:CE	1:E:72:ALA:HB2	2.38	0.42
1:E:106:ARG:O	1:E:109:LEU:HD12	2.20	0.42
1:F:140:VAL:O	1:F:144:THR:OG1	2.22	0.42
1:F:159:ILE:CD1	1:F:262:ILE:HD11	2.50	0.42
1:H:204:ALA:HB3	1:H:211:ILE:HD12	2.01	0.42
1:A:279:LEU:HA	1:A:279:LEU:HD12	1.29	0.42
1:A:281:GLY:C	1:A:282:GLU:HG2	2.45	0.42
1:C:40:MET:HE2	1:C:69:LYS:HB3	2.00	0.42
1:C:279:LEU:HD12	1:C:279:LEU:HA	1.62	0.42
1:C:324:VAL:HG13	1:C:327:ARG:HH11	1.83	0.42
1:E:63:MET:HE1	1:H:243:LYS:HD2	2.02	0.42
1:E:145:TYR:O	1:E:148:TRP:HB3	2.20	0.42
1:F:139:PRO:CD	1:F:143:LEU:HD12	2.49	0.42
1:G:40:MET:HE3	1:G:72:ALA:HB2	2.02	0.42
1:G:262:ILE:C	1:G:264:HIS:N	2.76	0.42
1:H:124:VAL:HG22	1:H:125:MET:N	2.34	0.42
1:H:265:ASN:HB2	1:H:295:ARG:HB2	2.01	0.42
1:C:107:LEU:C	1:C:109:LEU:N	2.78	0.42
1:C:280:TYR:CB	1:C:314:PHE:CE2	3.03	0.42
1:D:56:SER:CA	1:D:59:ILE:HD12	2.50	0.42
1:E:287:ILE:HD12	1:E:318:ALA:HA	2.02	0.42
1:E:295:ARG:HG3	1:F:15:MET:HG3	2.00	0.42
1:F:200:VAL:HG11	1:F:304:ILE:HD12	2.02	0.42
1:F:217:SER:O	1:F:218:LYS:CB	2.68	0.42
1:G:240:ILE:O	1:G:241:ILE:C	2.61	0.42
1:H:148:TRP:CZ3	1:H:275:TYR:CE2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ASN:O	1:A:117:PHE:HD1	2.03	0.42
1:A:172:PHE:HB2	5:A:422:HOH:O	2.20	0.42
1:A:248:TYR:HA	1:A:251:ILE:HG22	2.02	0.42
1:B:35:TYR:OH	1:B:93:VAL:HG21	2.20	0.42
1:C:24:VAL:HG23	1:C:89:ALA:HB2	2.01	0.42
1:D:56:SER:N	1:D:59:ILE:HD12	2.35	0.42
1:D:107:LEU:N	1:D:107:LEU:HD23	2.35	0.42
1:D:215:VAL:HA	1:D:218:LYS:HG2	2.01	0.42
1:E:16:LYS:HB3	1:E:77:ASP:HB2	2.02	0.42
1:E:74:LYS:HE3	1:E:74:LYS:HB3	1.88	0.42
1:E:153:LEU:HB3	1:E:154:PRO:CD	2.50	0.42
1:E:170:PHE:CE2	1:E:187:ALA:CB	2.99	0.42
1:E:325:LEU:HD23	1:E:325:LEU:HA	1.81	0.42
1:F:36:VAL:HG13	1:F:48:ILE:HG21	2.02	0.42
1:A:99:ASN:HA	4:A:352:NAD:H3D	2.01	0.41
1:A:181:ALA:HA	1:A:182:PRO:HD3	1.96	0.41
1:B:148:TRP:NE1	5:B:384:HOH:O	2.52	0.41
1:B:287:ILE:HD13	1:B:287:ILE:HG21	1.85	0.41
1:C:36:VAL:HG21	1:C:50:LEU:CD2	2.48	0.41
1:C:323:SER:O	1:C:327:ARG:N	2.53	0.41
1:D:206:ILE:HD11	1:D:211:ILE:HD11	2.02	0.41
1:D:293:ILE:HD13	1:D:298:ILE:HD13	2.02	0.41
1:E:74:LYS:HD2	1:E:75:PRO:CD	2.46	0.41
1:E:89:ALA:O	1:E:129:PHE:CE1	2.73	0.41
1:E:142:ILE:CD1	1:E:321:LEU:HD22	2.50	0.41
1:E:164:ILE:HD12	1:E:258:VAL:CG2	2.48	0.41
1:E:205:TYR:O	1:E:206:ILE:CD1	2.67	0.41
1:E:257:ARG:O	1:E:258:VAL:C	2.63	0.41
1:F:56:SER:O	1:F:57:LYS:C	2.62	0.41
1:F:112:LYS:HB2	5:F:375:HOH:O	2.20	0.41
1:F:117:PHE:O	1:F:121:VAL:HG23	2.20	0.41
1:F:117:PHE:CZ	1:F:137:THR:HB	2.55	0.41
1:F:290:PRO:HB2	1:F:302:ILE:HB	2.02	0.41
1:G:325:LEU:HD23	1:G:325:LEU:HA	1.63	0.41
1:H:26:ILE:HD11	1:H:92:VAL:CG1	2.50	0.41
1:H:113:ASN:C	1:H:115:ALA:N	2.72	0.41
1:H:274:ALA:HB1	1:H:301:VAL:HG21	2.02	0.41
1:A:72:ALA:HB1	1:A:73:PRO:HD2	2.01	0.41
1:B:228:ARG:O	1:B:229:ILE:C	2.62	0.41
1:C:114:ILE:HD11	1:C:142:ILE:HG23	2.03	0.41
1:D:118:ARG:O	1:D:122:GLU:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:PRO:HG2	1:E:142:ILE:HB	2.02	0.41
1:E:157:ARG:HH11	1:E:157:ARG:HD3	1.63	0.41
1:F:318:ALA:O	1:F:319:ALA:C	2.63	0.41
1:G:209:MET:O	1:G:214:LEU:HD11	2.20	0.41
1:H:209:MET:HE2	1:H:209:MET:HB2	1.65	0.41
4:H:352:NAD:H6N	5:H:377:HOH:O	2.19	0.41
1:A:164:ILE:O	1:A:164:ILE:HG12	2.20	0.41
1:B:25:VAL:HG21	1:B:36:VAL:HG23	2.02	0.41
1:B:59:ILE:CB	1:C:243:LYS:HD3	2.50	0.41
1:B:182:PRO:HB2	1:C:70:VAL:CG1	2.51	0.41
1:C:87:ARG:HB2	1:C:87:ARG:CZ	2.50	0.41
1:C:280:TYR:HB3	1:C:314:PHE:CE2	2.54	0.41
1:D:98:ALA:O	1:D:109:LEU:HD13	2.20	0.41
1:D:162:GLY:O	1:D:193:HIS:HB2	2.20	0.41
1:D:196:THR:HB	1:D:317:SER:CB	2.50	0.41
1:F:138:ASN:HB2	4:F:352:NAD:O2D	2.20	0.41
1:B:240:ILE:CG2	1:B:244:LYS:HD2	2.50	0.41
1:C:137:THR:HG22	1:C:138:ASN:N	2.34	0.41
1:C:156:GLU:HA	5:C:382:HOH:O	2.19	0.41
1:D:134:LEU:C	1:D:134:LEU:HD12	2.46	0.41
1:E:57:LYS:HG2	5:E:408:HOH:O	2.20	0.41
1:E:162:GLY:HA2	5:E:377:HOH:O	2.19	0.41
1:F:198:LEU:HB2	1:F:313:ARG:CD	2.49	0.41
1:G:31:VAL:HG21	4:G:352:NAD:C6N	2.51	0.41
1:H:223:GLN:HG2	5:H:405:HOH:O	2.20	0.41
1:A:116:ILE:HG23	1:A:120:ILE:HD11	2.01	0.41
1:A:317:SER:O	1:A:320:THR:HB	2.20	0.41
1:B:84:ASP:C	1:B:86:CYS:H	2.28	0.41
1:B:203:GLN:O	1:B:205:TYR:CE2	2.74	0.41
1:C:24:VAL:HG22	1:C:49:VAL:HB	2.02	0.41
1:C:255:LEU:O	1:C:256:ALA:C	2.62	0.41
1:E:117:PHE:O	1:E:118:ARG:C	2.62	0.41
1:E:251:ILE:O	1:E:255:LEU:HB2	2.21	0.41
1:F:201:TRP:HZ3	1:F:211:ILE:HD13	1.86	0.41
1:G:145:TYR:HE1	1:G:329:PHE:CE2	2.34	0.41
1:H:16:LYS:CB	1:H:77:ASP:OD1	2.68	0.41
1:H:317:SER:O	1:H:320:THR:HB	2.20	0.41
1:A:181:ALA:O	1:A:182:PRO:C	2.63	0.41
1:C:262:ILE:HG22	1:C:263:LEU:N	2.35	0.41
1:D:69:LYS:C	1:D:71:PHE:N	2.78	0.41
1:D:93:VAL:HG13	1:D:134:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:LEU:CD2	1:E:132:LEU:H	2.32	0.41
1:F:172:PHE:CE2	1:F:173:LEU:CD2	3.04	0.41
1:G:15:MET:HG2	1:H:265:ASN:HB2	2.01	0.41
1:A:129:PHE:HE2	1:A:133:PHE:CE1	2.38	0.41
1:B:172:PHE:CE1	1:C:69:LYS:NZ	2.85	0.41
1:B:173:LEU:HD12	1:B:233:VAL:HG23	2.03	0.41
1:C:40:MET:HE1	1:C:65:PHE:O	2.20	0.41
1:C:165:LEU:O	1:C:169:ARG:HG3	2.21	0.41
1:D:55:GLU:O	1:D:59:ILE:CG1	2.69	0.41
1:E:193:HIS:CE1	3:E:351:OXM:O2	2.73	0.41
1:F:230:PHE:O	1:F:233:VAL:HB	2.21	0.41
1:G:144:THR:OG1	1:G:160:GLY:HA3	2.21	0.41
1:G:174:LEU:CB	1:G:185:VAL:HG11	2.50	0.41
1:H:148:TRP:CH2	1:H:275:TYR:CE2	3.09	0.41
1:H:308:ASP:OD1	1:H:311:LYS:HD2	2.21	0.41
1:H:313:ARG:HE	1:H:313:ARG:HB3	1.51	0.41
1:A:15:MET:CE	1:B:296:ASN:OD1	2.68	0.41
1:A:279:LEU:O	1:A:303:GLU:OE2	2.39	0.41
1:B:203:GLN:CD	1:D:209:MET:HE1	2.44	0.41
1:B:277:ASP:HA	1:B:283:ARG:HB3	2.01	0.41
1:C:38:ALA:O	1:C:39:LEU:C	2.64	0.41
1:C:165:LEU:HD21	1:C:169:ARG:NH2	2.35	0.41
1:D:215:VAL:C	1:D:217:SER:N	2.77	0.41
1:E:118:ARG:HG2	1:E:150:PHE:CE2	2.56	0.41
1:E:262:ILE:HD13	1:E:262:ILE:HG21	1.87	0.41
1:G:171:ARG:HD2	1:G:185:VAL:O	2.20	0.41
1:H:181:ALA:HB3	1:H:184:ASN:OD1	2.19	0.41
1:A:63:MET:CE	1:D:243:LYS:CD	2.98	0.41
1:A:76:VAL:HB	5:A:357:HOH:O	2.21	0.41
1:A:212:ARG:HH12	1:A:226:LEU:HB2	1.81	0.41
1:A:248:TYR:HA	1:A:251:ILE:CG2	2.51	0.41
1:B:54:ASN:HD21	1:B:57:LYS:H	1.67	0.41
1:B:138:ASN:HA	1:B:140:VAL:N	2.36	0.41
1:C:81:GLY:HA3	1:C:85:ASP:OD2	2.21	0.41
1:D:15:MET:HG3	1:D:19:GLY:CA	2.51	0.41
1:E:262:ILE:O	1:E:263:LEU:C	2.62	0.41
1:F:257:ARG:NH1	1:F:266:GLU:OE2	2.47	0.41
1:G:16:LYS:HZ1	1:H:264:HIS:HA	1.86	0.41
1:G:35:TYR:CD1	1:G:255:LEU:HB3	2.56	0.41
1:G:83:TYR:O	1:G:86:CYS:N	2.41	0.41
1:G:92:VAL:HG12	1:G:133:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:PHE:HA	1:G:182:PRO:HB3	2.02	0.41
1:G:220:GLU:OE1	1:G:224:LYS:HD3	2.21	0.41
1:G:316:HIS:O	1:G:319:ALA:HB3	2.20	0.41
1:H:54:ASN:HD21	1:H:56:SER:HB2	1.86	0.41
1:H:74:LYS:CG	1:H:75:PRO:HD2	2.51	0.41
1:H:124:VAL:HG23	1:H:129:PHE:CD2	2.56	0.41
1:H:221:GLU:C	1:H:223:GLN:N	2.71	0.41
1:H:241:ILE:HG23	1:H:245:GLY:O	2.21	0.41
1:B:172:PHE:HA	1:B:182:PRO:HB3	2.03	0.41
1:C:40:MET:HG3	1:C:76:VAL:HG11	2.03	0.41
1:C:279:LEU:CD2	1:C:301:VAL:HB	2.46	0.41
1:D:16:LYS:HE2	1:D:75:PRO:O	2.21	0.41
1:D:220:GLU:O	1:D:221:GLU:CD	2.64	0.41
1:F:323:SER:O	1:F:324:VAL:C	2.60	0.41
1:G:209:MET:HE3	1:G:209:MET:HB2	1.87	0.41
1:G:230:PHE:O	1:G:230:PHE:CG	2.74	0.41
1:G:328:ALA:HB1	5:G:490:HOH:O	2.21	0.41
1:B:320:THR:O	1:B:321:LEU:C	2.64	0.40
1:C:213:LYS:HA	1:C:216:GLU:HB2	2.02	0.40
1:D:16:LYS:O	1:D:47:GLU:HG2	2.21	0.40
1:E:29:GLY:HA3	4:E:352:NAD:PA	2.60	0.40
1:F:77:ASP:HB3	1:F:79:TRP:CZ3	2.53	0.40
1:G:38:ALA:O	1:G:42:GLN:HG3	2.21	0.40
1:H:69:LYS:C	1:H:71:PHE:H	2.29	0.40
1:A:100:GLN:CA	1:A:109:LEU:HD21	2.52	0.40
1:A:107:LEU:HD22	1:A:324:VAL:HG21	2.02	0.40
1:C:116:ILE:HG23	1:C:120:ILE:CD1	2.52	0.40
1:D:58:ALA:HB1	1:D:80:HIS:CD2	2.56	0.40
1:D:207:GLY:C	1:D:208:VAL:CG1	2.94	0.40
1:E:160:GLY:HA3	1:E:273:SER:HB2	2.03	0.40
1:E:265:ASN:CB	1:F:16:LYS:H	2.29	0.40
1:E:280:TYR:HE1	1:E:302:ILE:O	2.02	0.40
1:F:31:VAL:HG23	4:F:352:NAD:O5D	2.21	0.40
1:F:109:LEU:HD23	5:F:376:HOH:O	2.20	0.40
1:F:110:VAL:HG13	1:F:142:ILE:HG21	2.03	0.40
1:F:253:MET:HE3	1:F:253:MET:HB3	1.78	0.40
1:G:264:HIS:HB3	1:H:16:LYS:CE	2.51	0.40
1:G:309:ASP:OD1	1:G:313:ARG:NH1	2.54	0.40
1:H:36:VAL:HG11	1:H:65:PHE:CE2	2.56	0.40
1:H:219:GLY:C	1:H:221:GLU:N	2.79	0.40
1:B:18:ASN:N	1:B:47:GLU:OE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLU:C	1:B:59:ILE:CD1	2.91	0.40
1:B:279:LEU:HD12	1:B:279:LEU:HA	1.64	0.40
1:F:154:PRO:HA	5:F:381:HOH:O	2.21	0.40
1:G:16:LYS:HA	1:G:47:GLU:HG2	2.02	0.40
1:A:142:ILE:HG13	1:A:324:VAL:HG11	2.03	0.40
1:B:15:MET:O	1:B:47:GLU:OE2	2.40	0.40
1:B:169:ARG:O	1:B:173:LEU:HG	2.21	0.40
1:B:276:LEU:HD23	1:B:276:LEU:HA	1.57	0.40
1:C:251:ILE:HD12	1:C:251:ILE:HA	1.74	0.40
1:D:26:ILE:HD13	1:D:83:TYR:CE1	2.56	0.40
1:D:145:TYR:HD2	1:D:286:TYR:HD1	1.69	0.40
1:E:203:GLN:HG3	1:G:208:VAL:HB	2.04	0.40
1:F:41:ASN:O	1:F:73:PRO:HG3	2.20	0.40
1:G:230:PHE:O	1:G:230:PHE:CD1	2.75	0.40
1:H:15:MET:SD	1:H:18:ASN:C	3.04	0.40
1:H:16:LYS:HB2	1:H:77:ASP:OD1	2.21	0.40
1:H:198:LEU:HA	1:H:199:PRO:HD3	1.93	0.40
1:H:280:TYR:OH	1:H:303:GLU:HA	2.22	0.40
1:A:100:GLN:HG3	1:A:105:THR:O	2.21	0.40
1:A:237:ALA:HA	1:A:247:THR:HG21	2.04	0.40
1:A:247:THR:OG1	3:A:351:OXM:N1	2.54	0.40
1:B:263:LEU:HD23	1:B:263:LEU:HA	1.90	0.40
1:D:280:TYR:HB3	1:D:314:PHE:CE2	2.57	0.40
1:E:94:ILE:CG2	1:E:117:PHE:CE2	3.03	0.40
1:F:114:ILE:HG21	1:F:330:THR:CA	2.50	0.40
1:F:142:ILE:O	1:F:145:TYR:HB3	2.21	0.40
1:G:156:GLU:O	1:G:297:GLY:HA3	2.21	0.40
1:H:119:SER:O	1:H:120:ILE:C	2.63	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ASN:OD1	5:B:384:HOH:O[2_645]	2.13	0.07
1:C:312:ASN:ND2	5:B:384:HOH:O[2_645]	2.14	0.06

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	314/316 (99%)	255 (81%)	48 (15%)	11 (4%)	3	4
1	B	314/316 (99%)	266 (85%)	40 (13%)	8 (2%)	4	7
1	C	314/316 (99%)	273 (87%)	30 (10%)	11 (4%)	3	4
1	D	314/316 (99%)	273 (87%)	35 (11%)	6 (2%)	6	11
1	E	314/316 (99%)	271 (86%)	34 (11%)	9 (3%)	3	5
1	F	314/316 (99%)	268 (85%)	38 (12%)	8 (2%)	4	7
1	G	314/316 (99%)	269 (86%)	35 (11%)	10 (3%)	3	4
1	H	314/316 (99%)	258 (82%)	48 (15%)	8 (2%)	4	7
All	All	2512/2528 (99%)	2133 (85%)	308 (12%)	71 (3%)	4	6

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	LYS
1	B	110	VAL
1	C	213	LYS
1	C	220	GLU
1	C	221	GLU
1	E	213	LYS
1	E	220	GLU
1	F	140	VAL
1	F	213	LYS
1	F	218	LYS
1	G	213	LYS
1	G	219	GLY
1	G	220	GLU
1	G	262	ILE
1	G	263	LEU
1	H	213	LYS
1	A	110	VAL

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Mol	Chain	Res	Type
1	A	295	ARG
1	B	162	GLY
1	B	213	LYS
1	B	219	GLY
1	D	87	ARG
1	D	213	LYS
1	D	248	TYR
1	E	110	VAL
1	E	219	GLY
1	F	248	TYR
1	F	263	LEU
1	G	110	VAL
1	H	66	ASN
1	H	265	ASN
1	A	140	VAL
1	A	218	LYS
1	A	219	GLY
1	A	248	TYR
1	B	248	TYR
1	C	55	GLU
1	C	140	VAL
1	C	183	GLN
1	D	19	GLY
1	E	248	TYR
1	H	219	GLY
1	H	325	LEU
1	A	19	GLY
1	B	295	ARG
1	C	19	GLY
1	C	248	TYR
1	E	19	GLY
1	E	87	ARG
1	G	197	GLU
1	G	265	ASN
1	H	223	GLN
1	A	112	LYS
1	B	328	ALA
1	C	149	LYS
1	D	221	GLU
1	E	121	VAL
1	F	219	GLY
1	H	112	LYS

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Mol	Chain	Res	Type
1	A	217	SER
1	B	19	GLY
1	C	262	ILE
1	D	219	GLY
1	G	19	GLY
1	H	120	ILE
1	F	139	PRO
1	F	262	ILE
1	A	162	GLY
1	E	262	ILE
1	G	233	VAL
1	C	110	VAL

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	254/254 (100%)	201 (79%)	53 (21%)	1	2
1	B	254/254 (100%)	208 (82%)	46 (18%)	2	3
1	C	254/254 (100%)	213 (84%)	41 (16%)	2	4
1	D	254/254 (100%)	203 (80%)	51 (20%)	1	2
1	E	254/254 (100%)	207 (82%)	47 (18%)	1	3
1	F	254/254 (100%)	214 (84%)	40 (16%)	2	5
1	G	254/254 (100%)	206 (81%)	48 (19%)	1	3
1	H	254/254 (100%)	207 (82%)	47 (18%)	1	3
All	All	2032/2032 (100%)	1659 (82%)	373 (18%)	1	3

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	17	ASN
1	A	31	VAL

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Mol	Chain	Res	Type
1	A	40	MET
1	A	54	ASN
1	A	56	SER
1	A	59	ILE
1	A	63	MET
1	A	70	VAL
1	A	77	ASP
1	A	95	CYS
1	A	100	GLN
1	A	104	GLU
1	A	105	THR
1	A	106	ARG
1	A	107	LEU
1	A	110	VAL
1	A	111	ASP
1	A	114	ILE
1	A	118	ARG
1	A	119	SER
1	A	122	GLU
1	A	124	VAL
1	A	132	LEU
1	A	134	LEU
1	A	142	ILE
1	A	149	LYS
1	A	153	LEU
1	A	171	ARG
1	A	179	SER
1	A	180	VAL
1	A	198	LEU
1	A	202	SER
1	A	203	GLN
1	A	206	ILE
1	A	211	ILE
1	A	213	LYS
1	A	218	LYS
1	A	227	GLU
1	A	228	ARG
1	A	244	LYS
1	A	255	LEU
1	A	260	ARG
1	A	263	LEU
1	A	265	ASN

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Mol	Chain	Res	Type
1	A	273	SER
1	A	287	ILE
1	A	293	ILE
1	A	294	ASN
1	A	300	GLU
1	A	312	ASN
1	A	329	PHE
1	A	330	THR
1	B	17	ASN
1	B	48	ILE
1	B	54	ASN
1	B	55	GLU
1	B	59	ILE
1	B	63	MET
1	B	77	ASP
1	B	87	ARG
1	B	92	VAL
1	B	100	GLN
1	B	105	THR
1	B	110	VAL
1	B	118	ARG
1	B	119	SER
1	B	122	GLU
1	B	124	VAL
1	B	132	LEU
1	B	149	LYS
1	B	179	SER
1	B	203	GLN
1	B	209	MET
1	B	213	LYS
1	B	215	VAL
1	B	217	SER
1	B	223	GLN
1	B	227	GLU
1	B	228	ARG
1	B	243	LYS
1	B	244	LYS
1	B	247	THR
1	B	255	LEU
1	B	260	ARG
1	B	279	LEU
1	B	282	GLU

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Mol	Chain	Res	Type
1	B	283	ARG
1	B	289	VAL
1	B	292	VAL
1	B	293	ILE
1	B	294	ASN
1	B	295	ARG
1	B	298	ILE
1	B	300	GLU
1	B	312	ASN
1	B	313	ARG
1	B	327	ARG
1	B	330	THR
1	C	16	LYS
1	C	18	ASN
1	C	51	ILE
1	C	54	ASN
1	C	69	LYS
1	C	70	VAL
1	C	76	VAL
1	C	77	ASP
1	C	78	ILE
1	C	100	GLN
1	C	105	THR
1	C	107	LEU
1	C	112	LYS
1	C	114	ILE
1	C	118	ARG
1	C	119	SER
1	C	124	VAL
1	C	127	SER
1	C	149	LYS
1	C	156	GLU
1	C	164	ILE
1	C	171	ARG
1	C	198	LEU
1	C	203	GLN
1	C	211	ILE
1	C	213	LYS
1	C	216	GLU
1	C	223	GLN
1	C	224	LYS
1	C	227	GLU

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Mol	Chain	Res	Type
1	C	228	ARG
1	C	229	ILE
1	C	243	LYS
1	C	244	LYS
1	C	247	THR
1	C	255	LEU
1	C	294	ASN
1	C	295	ARG
1	C	300	GLU
1	C	313	ARG
1	C	329	PHE
1	D	17	ASN
1	D	18	ASN
1	D	22	ARG
1	D	23	VAL
1	D	48	ILE
1	D	50	LEU
1	D	69	LYS
1	D	70	VAL
1	D	77	ASP
1	D	87	ARG
1	D	91	LEU
1	D	92	VAL
1	D	100	GLN
1	D	101	LYS
1	D	107	LEU
1	D	110	VAL
1	D	114	ILE
1	D	118	ARG
1	D	124	VAL
1	D	132	LEU
1	D	134	LEU
1	D	142	ILE
1	D	165	LEU
1	D	189	ILE
1	D	196	THR
1	D	198	LEU
1	D	203	GLN
1	D	213	LYS
1	D	215	VAL
1	D	216	GLU
1	D	218	LYS

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Mol	Chain	Res	Type
1	D	227	GLU
1	D	228	ARG
1	D	241	ILE
1	D	243	LYS
1	D	244	LYS
1	D	260	ARG
1	D	269	ILE
1	D	273	SER
1	D	275	TYR
1	D	279	LEU
1	D	287	ILE
1	D	294	ASN
1	D	295	ARG
1	D	300	GLU
1	D	313	ARG
1	D	320	THR
1	D	323	SER
1	D	327	ARG
1	D	329	PHE
1	D	330	THR
1	E	17	ASN
1	E	26	ILE
1	E	54	ASN
1	E	56	SER
1	E	74	LYS
1	E	77	ASP
1	E	85	ASP
1	E	100	GLN
1	E	101	LYS
1	E	105	THR
1	E	110	VAL
1	E	111	ASP
1	E	114	ILE
1	E	118	ARG
1	E	122	GLU
1	E	123	SER
1	E	124	VAL
1	E	125	MET
1	E	127	SER
1	E	132	LEU
1	E	142	ILE
1	E	156	GLU

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Mol	Chain	Res	Type
1	E	164	ILE
1	E	174	LEU
1	E	179	SER
1	E	189	ILE
1	E	203	GLN
1	E	216	GLU
1	E	218	LYS
1	E	224	LYS
1	E	227	GLU
1	E	228	ARG
1	E	242	GLU
1	E	243	LYS
1	E	247	THR
1	E	273	SER
1	E	283	ARG
1	E	289	VAL
1	E	294	ASN
1	E	295	ARG
1	E	300	GLU
1	E	306	LEU
1	E	312	ASN
1	E	313	ARG
1	E	323	SER
1	E	329	PHE
1	E	330	THR
1	F	17	ASN
1	F	54	ASN
1	F	70	VAL
1	F	77	ASP
1	F	111	ASP
1	F	112	LYS
1	F	114	ILE
1	F	118	ARG
1	F	122	GLU
1	F	124	VAL
1	F	130	GLN
1	F	132	LEU
1	F	149	LYS
1	F	157	ARG
1	F	164	ILE
1	F	171	ARG
1	F	198	LEU

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Mol	Chain	Res	Type
1	F	200	VAL
1	F	203	GLN
1	F	215	VAL
1	F	216	GLU
1	F	217	SER
1	F	223	GLN
1	F	227	GLU
1	F	228	ARG
1	F	241	ILE
1	F	243	LYS
1	F	244	LYS
1	F	255	LEU
1	F	260	ARG
1	F	273	SER
1	F	283	ARG
1	F	289	VAL
1	F	294	ASN
1	F	295	ARG
1	F	300	GLU
1	F	305	GLU
1	F	312	ASN
1	F	321	LEU
1	F	327	ARG
1	G	16	LYS
1	G	17	ASN
1	G	22	ARG
1	G	39	LEU
1	G	54	ASN
1	G	55	GLU
1	G	70	VAL
1	G	74	LYS
1	G	77	ASP
1	G	92	VAL
1	G	94	ILE
1	G	100	GLN
1	G	101	LYS
1	G	107	LEU
1	G	109	LEU
1	G	111	ASP
1	G	112	LYS
1	G	116	ILE
1	G	119	SER

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Mol	Chain	Res	Type
1	G	130	GLN
1	G	132	LEU
1	G	134	LEU
1	G	149	LYS
1	G	159	ILE
1	G	164	ILE
1	G	190	ILE
1	G	203	GLN
1	G	209	MET
1	G	213	LYS
1	G	215	VAL
1	G	227	GLU
1	G	228	ARG
1	G	240	ILE
1	G	244	LYS
1	G	247	THR
1	G	255	LEU
1	G	269	ILE
1	G	287	ILE
1	G	294	ASN
1	G	295	ARG
1	G	298	ILE
1	G	300	GLU
1	G	302	ILE
1	G	305	GLU
1	G	312	ASN
1	G	313	ARG
1	G	327	ARG
1	G	329	PHE
1	H	16	LYS
1	H	17	ASN
1	H	70	VAL
1	H	74	LYS
1	H	77	ASP
1	H	100	GLN
1	H	112	LYS
1	H	114	ILE
1	H	116	ILE
1	H	118	ARG
1	H	119	SER
1	H	123	SER
1	H	124	VAL

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Mol	Chain	Res	Type
1	H	127	SER
1	H	130	GLN
1	H	132	LEU
1	H	144	THR
1	H	149	LYS
1	H	159	ILE
1	H	164	ILE
1	H	189	ILE
1	H	198	LEU
1	H	203	GLN
1	H	214	LEU
1	H	216	GLU
1	H	218	LYS
1	H	224	LYS
1	H	227	GLU
1	H	228	ARG
1	H	241	ILE
1	H	243	LYS
1	H	244	LYS
1	H	247	THR
1	H	251	ILE
1	H	255	LEU
1	H	260	ARG
1	H	283	ARG
1	H	293	ILE
1	H	294	ASN
1	H	295	ARG
1	H	302	ILE
1	H	312	ASN
1	H	313	ARG
1	H	323	SER
1	H	327	ARG
1	H	329	PHE
1	H	330	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	66	ASN
1	A	99	ASN
1	A	138	ASN

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Mol	Chain	Res	Type
1	A	203	GLN
1	A	223	GLN
1	A	267	ASN
1	A	294	ASN
1	A	316	HIS
1	B	54	ASN
1	B	130	GLN
1	B	203	GLN
1	B	265	ASN
1	B	267	ASN
1	B	294	ASN
1	B	316	HIS
1	C	17	ASN
1	C	54	ASN
1	C	138	ASN
1	C	155	HIS
1	C	264	HIS
1	C	267	ASN
1	C	294	ASN
1	D	17	ASN
1	D	54	ASN
1	D	66	ASN
1	D	100	GLN
1	D	138	ASN
1	D	267	ASN
1	D	294	ASN
1	D	316	HIS
1	E	54	ASN
1	E	138	ASN
1	E	155	HIS
1	E	267	ASN
1	E	294	ASN
1	F	54	ASN
1	F	67	HIS
1	F	138	ASN
1	F	223	GLN
1	F	265	ASN
1	F	267	ASN
1	F	294	ASN
1	G	54	ASN
1	G	66	ASN
1	G	138	ASN

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Mol	Chain	Res	Type
1	G	203	GLN
1	G	264	HIS
1	G	267	ASN
1	G	294	ASN
1	G	296	ASN
1	G	312	ASN
1	G	315	HIS
1	H	54	ASN
1	H	138	ASN
1	H	267	ASN
1	H	294	ASN
1	H	316	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	FBP	A	353[A]	-	18,20,20	0.79	0	21,32,32	0.91	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXM	G	351	-	5,5,5	6.33	2 (40%)	2,6,6	1.52	1 (50%)
3	OXM	B	351	-	5,5,5	6.14	2 (40%)	2,6,6	1.68	1 (50%)
4	NAD	H	352	-	46,48,48	1.35	6 (13%)	64,73,73	2.67	18 (28%)
3	OXM	A	351	-	5,5,5	6.18	2 (40%)	2,6,6	1.46	0
2	FBP	F	353[F]	-	18,20,20	0.78	0	21,32,32	0.95	1 (4%)
2	FBP	A	353[C]	-	18,20,20	0.79	0	21,32,32	0.96	1 (4%)
4	NAD	D	352	-	46,48,48	1.00	3 (6%)	64,73,73	2.22	11 (17%)
4	NAD	E	352	-	46,48,48	1.22	5 (10%)	64,73,73	2.51	10 (15%)
3	OXM	D	351	-	5,5,5	6.47	2 (40%)	2,6,6	1.74	1 (50%)
2	FBP	E	353[E]	-	18,20,20	0.79	0	21,32,32	0.95	1 (4%)
2	FBP	F	353[H]	-	18,20,20	0.79	0	21,32,32	0.95	1 (4%)
4	NAD	F	352	-	46,48,48	1.32	7 (15%)	64,73,73	2.42	12 (18%)
4	NAD	A	352	-	46,48,48	1.21	5 (10%)	64,73,73	2.35	15 (23%)
4	NAD	C	352	-	46,48,48	1.18	4 (8%)	64,73,73	2.65	10 (15%)
3	OXM	H	351	-	5,5,5	6.60	2 (40%)	2,6,6	3.26	2 (100%)
2	FBP	E	353[G]	-	18,20,20	0.80	0	21,32,32	0.95	1 (4%)
3	OXM	F	351	-	5,5,5	6.26	2 (40%)	2,6,6	1.39	0
4	NAD	B	352	-	46,48,48	1.22	4 (8%)	64,73,73	2.28	14 (21%)
2	FBP	B	353[B]	-	18,20,20	0.79	0	21,32,32	0.96	1 (4%)
4	NAD	G	352	-	46,48,48	1.16	5 (10%)	64,73,73	2.27	11 (17%)
3	OXM	E	351	-	5,5,5	6.43	2 (40%)	2,6,6	3.31	2 (100%)
2	FBP	B	353[D]	-	18,20,20	0.79	0	21,32,32	0.95	1 (4%)
3	OXM	C	351	-	5,5,5	6.02	2 (40%)	2,6,6	0.95	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	A	353[A]	-	-	4/13/32/32	0/1/1/1
3	OXM	G	351	-	-	0/4/4/4	-
3	OXM	B	351	-	-	3/4/4/4	-
4	NAD	H	352	-	-	12/30/62/62	0/5/5/5
3	OXM	A	351	-	-	4/4/4/4	-
2	FBP	F	353[F]	-	-	1/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	A	353[C]	-	-	1/13/32/32	0/1/1/1
4	NAD	D	352	-	-	8/30/62/62	0/5/5/5
4	NAD	E	352	-	-	8/30/62/62	0/5/5/5
3	OXM	D	351	-	-	2/4/4/4	-
2	FBP	E	353[E]	-	-	1/13/32/32	0/1/1/1
2	FBP	F	353[H]	-	-	1/13/32/32	0/1/1/1
4	NAD	F	352	-	-	9/30/62/62	0/5/5/5
4	NAD	A	352	-	-	12/30/62/62	0/5/5/5
4	NAD	C	352	-	-	9/30/62/62	0/5/5/5
3	OXM	H	351	-	-	0/4/4/4	-
2	FBP	E	353[G]	-	-	1/13/32/32	0/1/1/1
3	OXM	F	351	-	-	2/4/4/4	-
4	NAD	B	352	-	-	6/30/62/62	0/5/5/5
2	FBP	B	353[B]	-	-	1/13/32/32	0/1/1/1
4	NAD	G	352	-	-	8/30/62/62	0/5/5/5
3	OXM	E	351	-	-	1/4/4/4	-
2	FBP	B	353[D]	-	-	1/13/32/32	0/1/1/1
3	OXM	C	351	-	-	2/4/4/4	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	351	OXM	C1-C2	-14.52	1.38	1.55
3	D	351	OXM	C1-C2	-14.26	1.38	1.55
3	E	351	OXM	C1-C2	-14.14	1.38	1.55
3	G	351	OXM	C1-C2	-13.86	1.38	1.55
3	F	351	OXM	C1-C2	-13.65	1.39	1.55
3	A	351	OXM	C1-C2	-13.56	1.39	1.55
3	B	351	OXM	C1-C2	-13.49	1.39	1.55
3	C	351	OXM	C1-C2	-13.23	1.39	1.55
4	F	352	NAD	C3N-C7N	4.50	1.57	1.50
4	H	352	NAD	O7N-C7N	4.34	1.32	1.24
4	C	352	NAD	C3N-C7N	4.24	1.56	1.50
4	B	352	NAD	C3N-C7N	3.99	1.56	1.50
4	E	352	NAD	C3N-C7N	3.97	1.56	1.50
4	A	352	NAD	C3N-C7N	3.92	1.56	1.50
4	H	352	NAD	C3N-C7N	3.90	1.56	1.50
4	D	352	NAD	C3N-C7N	3.90	1.56	1.50
4	E	352	NAD	PA-O3	3.52	1.63	1.59
4	G	352	NAD	C3N-C7N	3.51	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	352	NAD	O7N-C7N	-3.22	1.18	1.24
4	B	352	NAD	C6N-N1N	3.06	1.42	1.35
3	F	351	OXM	O3-C2	-3.00	1.22	1.30
4	G	352	NAD	PA-O3	2.96	1.62	1.59
4	A	352	NAD	C6N-N1N	2.85	1.41	1.35
4	H	352	NAD	C6N-N1N	2.81	1.41	1.35
4	B	352	NAD	C2A-N1A	2.79	1.38	1.33
4	H	352	NAD	PA-O3	2.70	1.62	1.59
3	G	351	OXM	O3-C2	-2.66	1.23	1.30
4	C	352	NAD	C6N-N1N	2.66	1.41	1.35
4	E	352	NAD	C6N-N1N	2.65	1.41	1.35
4	B	352	NAD	PA-O3	2.61	1.62	1.59
3	A	351	OXM	O3-C2	-2.57	1.23	1.30
4	A	352	NAD	O4D-C1D	2.54	1.44	1.40
4	C	352	NAD	C2A-N3A	-2.53	1.29	1.33
4	D	352	NAD	C6N-N1N	2.48	1.41	1.35
4	F	352	NAD	C6N-N1N	2.45	1.40	1.35
3	B	351	OXM	O3-C2	-2.43	1.23	1.30
4	G	352	NAD	PN-O3	2.43	1.62	1.59
3	H	351	OXM	O3-C2	-2.41	1.24	1.30
4	G	352	NAD	C6N-N1N	2.37	1.40	1.35
3	E	351	OXM	O3-C2	-2.34	1.24	1.30
3	D	351	OXM	O3-C2	-2.32	1.24	1.30
4	A	352	NAD	C2A-N1A	2.31	1.38	1.33
4	F	352	NAD	C4N-C3N	2.28	1.42	1.39
4	F	352	NAD	C2N-N1N	2.28	1.37	1.35
3	C	351	OXM	O3-C2	-2.22	1.24	1.30
4	D	352	NAD	C2A-N1A	2.21	1.37	1.33
4	E	352	NAD	C2A-N1A	2.18	1.37	1.33
4	C	352	NAD	O7N-C7N	2.18	1.28	1.24
4	F	352	NAD	C2A-N3A	-2.17	1.30	1.33
4	A	352	NAD	PA-O3	2.16	1.61	1.59
4	G	352	NAD	C2N-N1N	2.15	1.37	1.35
4	H	352	NAD	PN-O3	2.11	1.61	1.59
4	H	352	NAD	C2A-N1A	2.10	1.37	1.33
4	E	352	NAD	PN-O3	2.07	1.61	1.59
4	F	352	NAD	C2A-N1A	2.04	1.37	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	352	NAD	C6N-N1N-C1D	10.56	140.44	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	352	NAD	C2N-N1N-C1D	-9.84	97.41	119.13
4	A	352	NAD	C5N-C4N-C3N	-8.84	111.67	120.36
4	H	352	NAD	C5N-C4N-C3N	-8.81	111.71	120.36
4	C	352	NAD	C6N-N1N-C1D	8.78	136.95	119.73
4	C	352	NAD	C2N-N1N-C1D	-8.59	100.16	119.13
4	F	352	NAD	C5N-C4N-C3N	-8.39	112.11	120.36
4	D	352	NAD	C5N-C4N-C3N	-7.96	112.54	120.36
4	F	352	NAD	C6N-N1N-C1D	7.87	135.18	119.73
4	B	352	NAD	C2N-N1N-C1D	-7.57	102.43	119.13
4	E	352	NAD	C5N-C4N-C3N	-7.44	113.05	120.36
4	H	352	NAD	O7N-C7N-N7N	7.41	133.32	122.62
4	G	352	NAD	C4D-O4D-C1D	-7.36	103.19	109.92
4	F	352	NAD	C2N-N1N-C1D	-7.30	103.01	119.13
4	B	352	NAD	C6N-N1N-C1D	7.23	133.91	119.73
4	A	352	NAD	C6N-N1N-C1D	7.13	133.72	119.73
4	G	352	NAD	C5N-C4N-C3N	-7.09	113.40	120.36
4	C	352	NAD	O7N-C7N-C3N	-7.07	110.96	119.60
4	H	352	NAD	C6N-N1N-C1D	6.94	133.35	119.73
4	D	352	NAD	C6N-C5N-C4N	6.69	129.09	119.45
4	C	352	NAD	C6N-C5N-C4N	6.63	129.01	119.45
4	G	352	NAD	C2N-N1N-C1D	-6.62	104.53	119.13
4	B	352	NAD	C5N-C4N-C3N	-6.59	113.88	120.36
4	H	352	NAD	C2N-N1N-C1D	-6.59	104.59	119.13
4	H	352	NAD	C6N-C5N-C4N	6.53	128.85	119.45
4	C	352	NAD	C5N-C4N-C3N	-6.49	113.98	120.36
4	G	352	NAD	C6N-N1N-C1D	6.40	132.29	119.73
4	F	352	NAD	C6N-C5N-C4N	6.38	128.64	119.45
4	A	352	NAD	C2N-N1N-C1D	-6.33	105.17	119.13
4	A	352	NAD	C6N-C5N-C4N	6.32	128.56	119.45
4	C	352	NAD	O7N-C7N-N7N	6.27	131.67	122.62
4	D	352	NAD	C2N-N1N-C1D	-6.18	105.49	119.13
4	C	352	NAD	C5N-C6N-N1N	-5.95	112.27	120.38
4	H	352	NAD	C3N-C7N-N7N	-5.79	110.61	117.74
4	G	352	NAD	C6N-C5N-C4N	5.76	127.74	119.45
4	D	352	NAD	C6N-N1N-C1D	5.71	130.94	119.73
4	E	352	NAD	C6N-C5N-C4N	5.64	127.58	119.45
4	D	352	NAD	C5N-C6N-N1N	-5.62	112.71	120.38
4	B	352	NAD	C6N-C5N-C4N	5.58	127.48	119.45
4	A	352	NAD	C4D-O4D-C1D	-5.34	105.04	109.92
4	D	352	NAD	C4D-O4D-C1D	-5.22	105.15	109.92
4	B	352	NAD	C5N-C6N-N1N	-5.17	113.33	120.38
4	G	352	NAD	C5N-C6N-N1N	-4.99	113.58	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	352	NAD	C2N-C3N-C4N	4.86	123.91	118.26
4	H	352	NAD	C4D-O4D-C1D	-4.83	105.50	109.92
4	H	352	NAD	C5N-C6N-N1N	-4.83	113.80	120.38
4	F	352	NAD	C4D-O4D-C1D	-4.65	105.67	109.92
4	F	352	NAD	C5N-C6N-N1N	-4.54	114.19	120.38
4	A	352	NAD	C2N-C3N-C4N	4.47	123.46	118.26
4	E	352	NAD	C5N-C6N-N1N	-4.13	114.75	120.38
4	C	352	NAD	C4D-O4D-C1D	-4.12	106.16	109.92
4	A	352	NAD	C5N-C6N-N1N	-4.11	114.78	120.38
3	H	351	OXM	O3-C2-O2	-4.06	114.24	123.90
4	F	352	NAD	C2N-C3N-C4N	3.96	122.86	118.26
4	E	352	NAD	O4B-C1B-N9A	-3.95	100.50	108.09
4	D	352	NAD	C2N-C3N-C4N	3.89	122.79	118.26
4	A	352	NAD	C3N-C7N-N7N	-3.77	113.09	117.74
4	F	352	NAD	C4N-C3N-C7N	-3.75	110.83	121.06
3	E	351	OXM	O3-C2-O2	-3.73	115.01	123.90
4	D	352	NAD	C3N-C7N-N7N	-3.71	113.17	117.74
4	E	352	NAD	C2N-C3N-C4N	3.71	122.57	118.26
4	G	352	NAD	C2N-C3N-C4N	3.61	122.46	118.26
4	G	352	NAD	O2A-PA-O3	3.56	116.89	107.27
4	C	352	NAD	O2A-PA-O3	3.54	116.85	107.27
4	B	352	NAD	C4D-O4D-C1D	-3.27	106.93	109.92
4	A	352	NAD	PN-O5D-C5D	3.23	139.88	121.35
4	B	352	NAD	C2N-C3N-C4N	3.23	122.01	118.26
4	F	352	NAD	O7N-C7N-N7N	3.23	127.28	122.62
4	B	352	NAD	N6A-C6A-N1A	3.22	125.55	118.38
4	E	352	NAD	C4N-C3N-C7N	-3.12	112.57	121.06
4	H	352	NAD	C3B-C2B-C1B	-3.06	95.68	101.46
4	B	352	NAD	C4N-C3N-C7N	-3.03	112.81	121.06
4	H	352	NAD	O7N-C7N-C3N	-2.98	115.95	119.60
4	F	352	NAD	O7N-C7N-C3N	-2.84	116.13	119.60
3	E	351	OXM	O1-C1-N1	-2.83	116.56	122.89
4	D	352	NAD	O2A-PA-O3	2.75	114.69	107.27
4	B	352	NAD	C4B-O4B-C1B	-2.74	103.41	109.47
4	H	352	NAD	O4B-C1B-C2B	-2.72	100.79	106.62
4	H	352	NAD	O3-PA-O1A	2.55	118.36	110.70
4	D	352	NAD	C4N-C3N-C7N	-2.54	114.14	121.06
4	B	352	NAD	O4B-C1B-C2B	-2.53	101.19	106.62
4	H	352	NAD	O2B-C2B-C1B	2.53	118.82	110.10
4	B	352	NAD	O7N-C7N-C3N	-2.51	116.53	119.60
3	D	351	OXM	O3-C2-O2	-2.42	118.14	123.90
4	G	352	NAD	O5D-C5D-C4D	-2.42	100.76	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	352	NAD	C3B-C2B-C1B	-2.40	96.92	101.46
4	F	352	NAD	C2N-C3N-C7N	2.37	126.30	119.46
4	G	352	NAD	O2B-C2B-C1B	2.36	118.22	110.10
4	D	352	NAD	O7N-C7N-C3N	2.36	122.48	119.60
4	H	352	NAD	C4N-C3N-C7N	-2.35	114.66	121.06
4	A	352	NAD	C4N-C3N-C7N	-2.32	114.73	121.06
4	H	352	NAD	O2A-PA-O3	2.31	113.52	107.27
3	B	351	OXM	O3-C2-O2	-2.30	118.44	123.90
4	A	352	NAD	O7N-C7N-N7N	2.25	125.87	122.62
4	E	352	NAD	C2B-C1B-N9A	2.21	118.80	113.30
4	H	352	NAD	C4B-O4B-C1B	-2.21	104.59	109.47
3	H	351	OXM	O1-C1-N1	-2.20	117.95	122.89
4	H	352	NAD	O3-PN-O1N	-2.17	104.17	110.70
4	A	352	NAD	O3D-C3D-C4D	-2.13	104.95	111.08
4	A	352	NAD	O3D-C3D-C2D	2.07	118.47	111.82
4	A	352	NAD	C2B-C1B-N9A	2.07	118.46	113.30
4	E	352	NAD	O7N-C7N-C3N	-2.07	117.06	119.60
4	B	352	NAD	C6N-N1N-C2N	2.07	123.64	121.88
4	A	352	NAD	C1B-N9A-C8A	2.07	131.68	127.09
2	A	353[C]	FBP	O2P-P1-O1P	2.06	118.86	110.83
2	E	353[G]	FBP	O2P-P1-O1P	2.06	118.85	110.83
2	E	353[E]	FBP	O2P-P1-O1P	2.05	118.84	110.83
2	A	353[A]	FBP	O2P-P1-O1P	2.05	118.84	110.83
2	B	353[B]	FBP	O2P-P1-O1P	2.05	118.83	110.83
2	F	353[F]	FBP	O2P-P1-O1P	2.05	118.82	110.83
2	B	353[D]	FBP	O2P-P1-O1P	2.05	118.82	110.83
2	F	353[H]	FBP	O2P-P1-O1P	2.05	118.82	110.83
4	F	352	NAD	C4B-O4B-C1B	-2.04	104.95	109.47
4	G	352	NAD	O5D-PN-O1N	2.03	116.97	108.94
4	C	352	NAD	C4N-C3N-C7N	-2.03	115.54	121.06
3	G	351	OXM	O3-C2-O2	-2.02	119.09	123.90

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	353[A]	FBP	C6-O6-P2-O5P
2	A	353[A]	FBP	C6-O6-P2-O6P
3	A	351	OXM	N1-C1-C2-O2
3	A	351	OXM	N1-C1-C2-O3
3	A	351	OXM	O1-C1-C2-O3
3	B	351	OXM	N1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	351	OXM	N1-C1-C2-O3
3	B	351	OXM	O1-C1-C2-O3
3	C	351	OXM	N1-C1-C2-O2
3	C	351	OXM	N1-C1-C2-O3
3	D	351	OXM	O1-C1-C2-O3
3	E	351	OXM	O1-C1-C2-O3
3	F	351	OXM	N1-C1-C2-O3
4	A	352	NAD	C5D-O5D-PN-O3
4	A	352	NAD	C5D-O5D-PN-O1N
4	A	352	NAD	C5D-O5D-PN-O2N
4	A	352	NAD	O4D-C1D-N1N-C6N
4	A	352	NAD	C2D-C1D-N1N-C2N
4	B	352	NAD	C5D-O5D-PN-O3
4	B	352	NAD	C5D-O5D-PN-O1N
4	B	352	NAD	C5D-O5D-PN-O2N
4	B	352	NAD	O4D-C4D-C5D-O5D
4	C	352	NAD	C5D-O5D-PN-O1N
4	C	352	NAD	C5D-O5D-PN-O2N
4	C	352	NAD	O4D-C4D-C5D-O5D
4	C	352	NAD	O4D-C1D-N1N-C6N
4	D	352	NAD	C5D-O5D-PN-O2N
4	D	352	NAD	O4D-C4D-C5D-O5D
4	E	352	NAD	C5D-O5D-PN-O1N
4	E	352	NAD	C5D-O5D-PN-O2N
4	E	352	NAD	O4D-C1D-N1N-C6N
4	F	352	NAD	C5D-O5D-PN-O2N
4	F	352	NAD	O4D-C4D-C5D-O5D
4	F	352	NAD	O4D-C1D-N1N-C2N
4	F	352	NAD	O4D-C1D-N1N-C6N
4	F	352	NAD	C2D-C1D-N1N-C2N
4	F	352	NAD	C2D-C1D-N1N-C6N
4	G	352	NAD	C5D-O5D-PN-O1N
4	G	352	NAD	C5D-O5D-PN-O2N
4	G	352	NAD	O4D-C4D-C5D-O5D
4	G	352	NAD	C3D-C4D-C5D-O5D
4	H	352	NAD	C5D-O5D-PN-O2N
4	H	352	NAD	O4D-C1D-N1N-C2N
4	H	352	NAD	O4D-C1D-N1N-C6N
4	H	352	NAD	C2D-C1D-N1N-C2N
4	H	352	NAD	C2D-C1D-N1N-C6N
4	A	352	NAD	O4D-C4D-C5D-O5D
4	D	352	NAD	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
4	H	352	NAD	O4D-C4D-C5D-O5D
4	B	352	NAD	C3D-C4D-C5D-O5D
4	E	352	NAD	O4D-C4D-C5D-O5D
4	C	352	NAD	C3D-C4D-C5D-O5D
4	F	352	NAD	C3D-C4D-C5D-O5D
4	G	352	NAD	O4B-C4B-C5B-O5B
4	H	352	NAD	O4B-C4B-C5B-O5B
4	H	352	NAD	C3B-C4B-C5B-O5B
4	H	352	NAD	C3D-C4D-C5D-O5D
4	A	352	NAD	C3D-C4D-C5D-O5D
4	G	352	NAD	C3B-C4B-C5B-O5B
2	A	353[A]	FBP	C6-O6-P2-O4P
4	E	352	NAD	C3D-C4D-C5D-O5D
4	D	352	NAD	O4B-C4B-C5B-O5B
4	C	352	NAD	C5D-O5D-PN-O3
4	D	352	NAD	C5D-O5D-PN-O3
4	D	352	NAD	C5D-O5D-PN-O1N
4	E	352	NAD	C5D-O5D-PN-O3
4	F	352	NAD	C5D-O5D-PN-O3
4	F	352	NAD	C5D-O5D-PN-O1N
4	G	352	NAD	C5B-O5B-PA-O3
4	G	352	NAD	C5D-O5D-PN-O3
4	H	352	NAD	C5B-O5B-PA-O1A
4	H	352	NAD	C5D-O5D-PN-O3
4	H	352	NAD	C5D-O5D-PN-O1N
4	A	352	NAD	C2D-C1D-N1N-C6N
4	C	352	NAD	C2D-C1D-N1N-C2N
4	E	352	NAD	C2D-C1D-N1N-C2N
3	A	351	OXM	O1-C1-C2-O2
3	D	351	OXM	N1-C1-C2-O2
3	F	351	OXM	N1-C1-C2-O2
4	A	352	NAD	O4D-C1D-N1N-C2N
4	B	352	NAD	O4D-C1D-N1N-C2N
4	C	352	NAD	O4D-C1D-N1N-C2N
4	E	352	NAD	O4D-C1D-N1N-C2N
4	D	352	NAD	PA-O3-PN-O2N
4	C	352	NAD	C2B-C1B-N9A-C8A
2	A	353[A]	FBP	C1-O1-P1-O2P
2	A	353[C]	FBP	C1-O1-P1-O2P
2	B	353[B]	FBP	C1-O1-P1-O2P
2	B	353[D]	FBP	C1-O1-P1-O2P
2	E	353[E]	FBP	C1-O1-P1-O2P

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Mol	Chain	Res	Type	Atoms
2	E	353[G]	FBP	C1-O1-P1-O2P
2	F	353[F]	FBP	C1-O1-P1-O2P
2	F	353[H]	FBP	C1-O1-P1-O2P
4	A	352	NAD	PA-O3-PN-O2N
4	A	352	NAD	O4B-C4B-C5B-O5B
4	D	352	NAD	C3B-C4B-C5B-O5B
4	A	352	NAD	PA-O3-PN-O1N

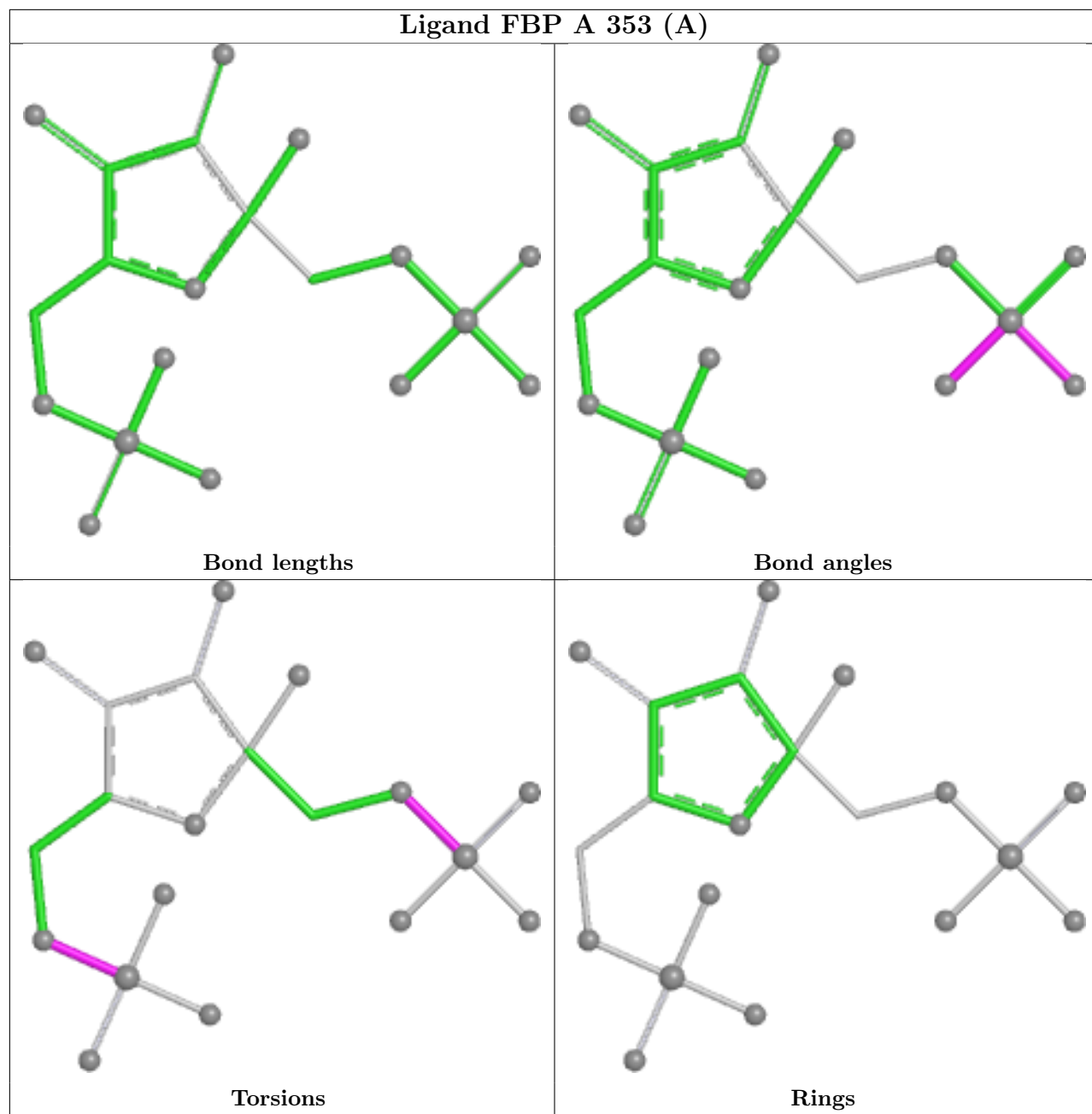
There are no ring outliers.

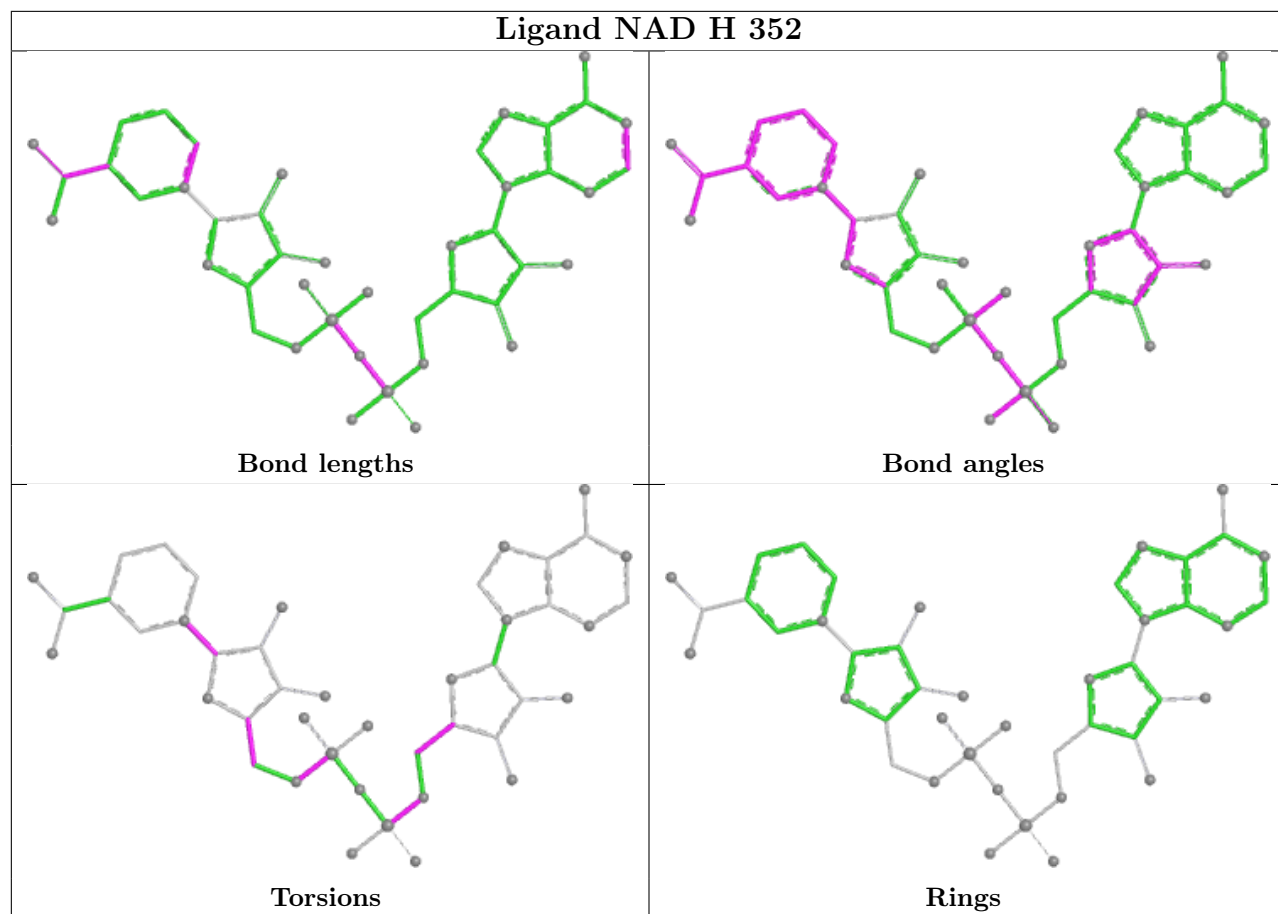
15 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	351	OXM	1	0
3	B	351	OXM	2	0
4	H	352	NAD	4	0
3	A	351	OXM	2	0
4	D	352	NAD	6	0
4	E	352	NAD	9	0
3	D	351	OXM	1	0
4	F	352	NAD	6	0
4	A	352	NAD	7	0
4	C	352	NAD	3	0
3	F	351	OXM	1	0
4	B	352	NAD	9	0
4	G	352	NAD	9	0
3	E	351	OXM	2	0
3	C	351	OXM	2	0

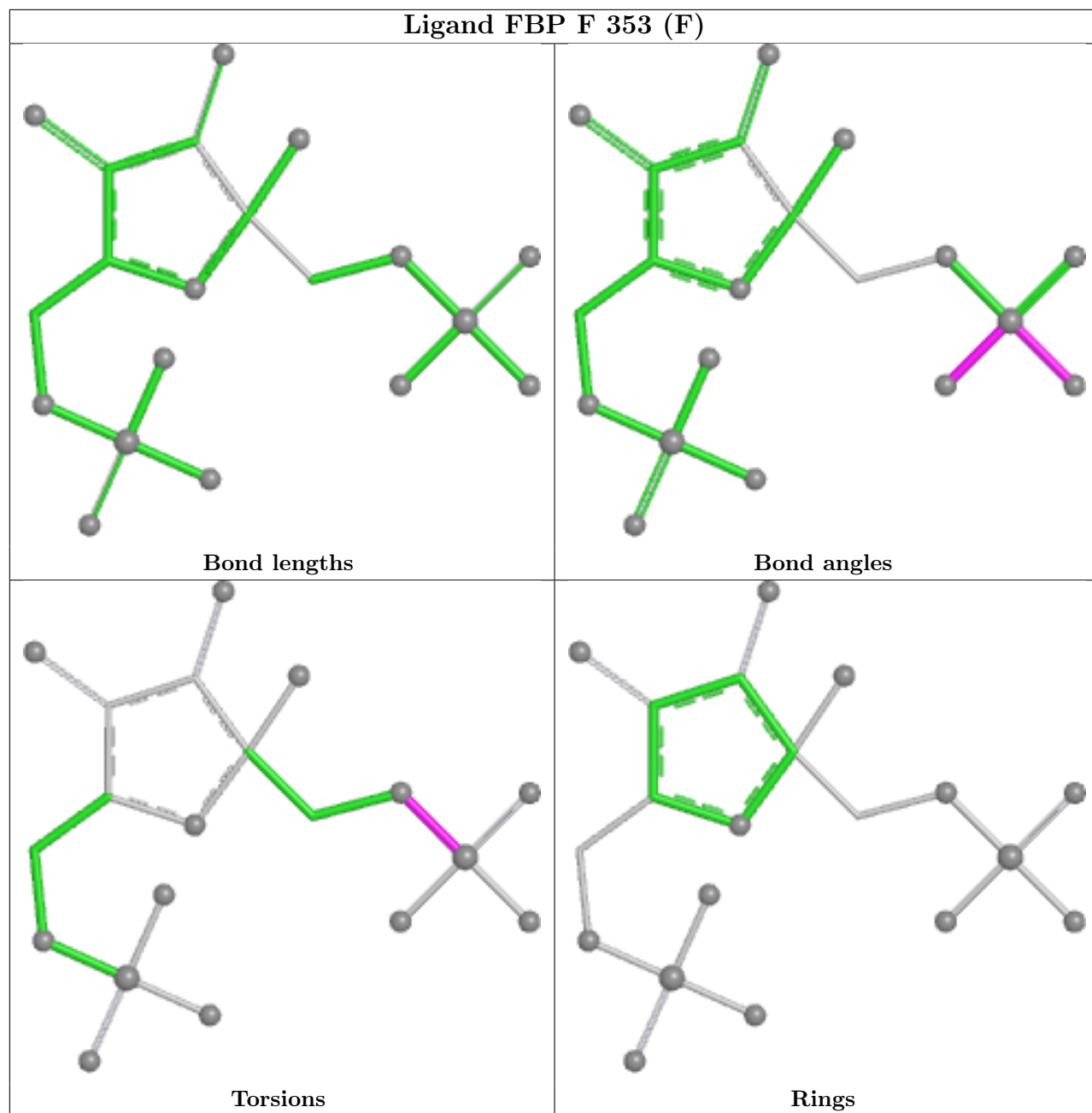
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FBP A 353 (A)

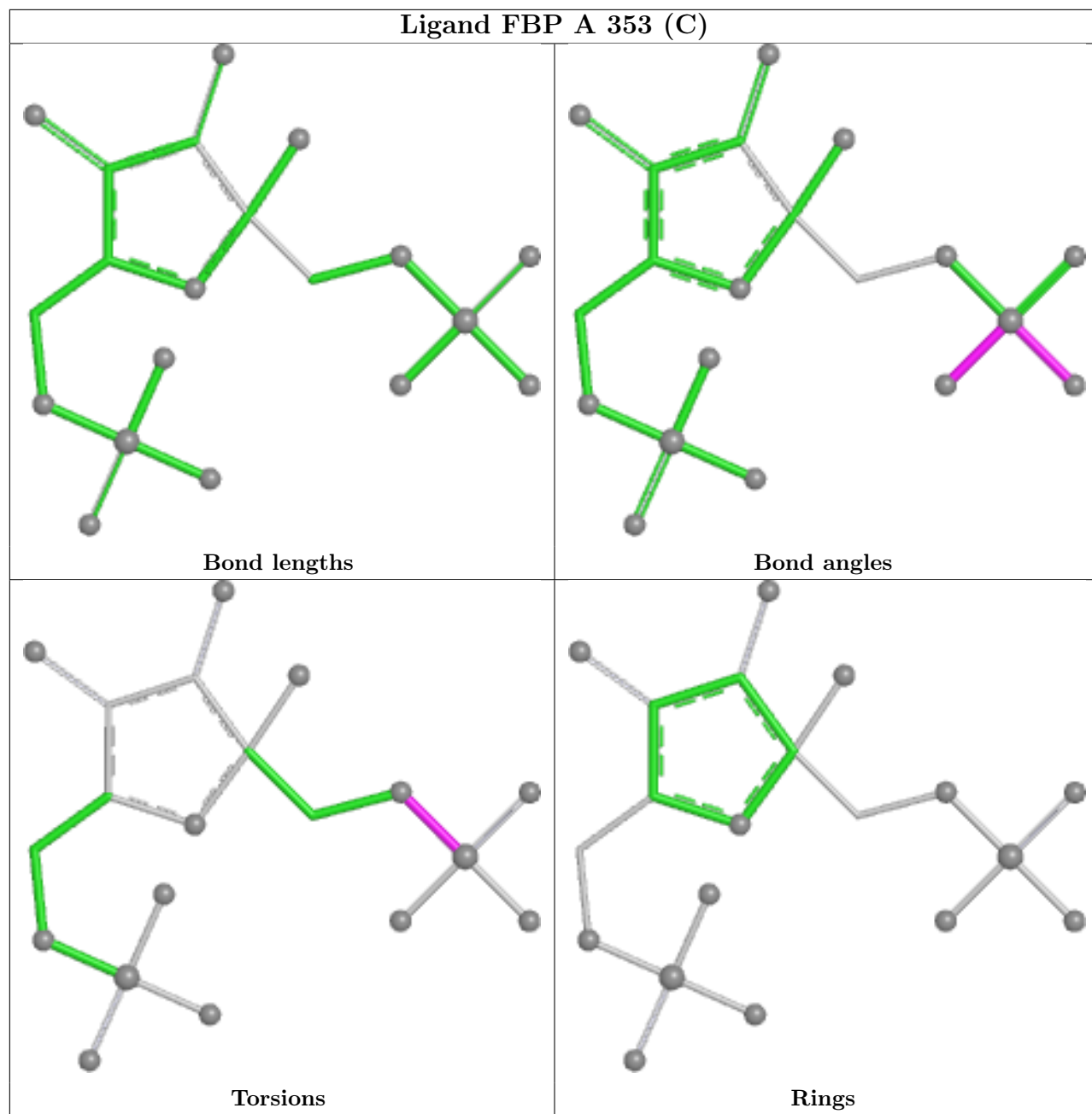


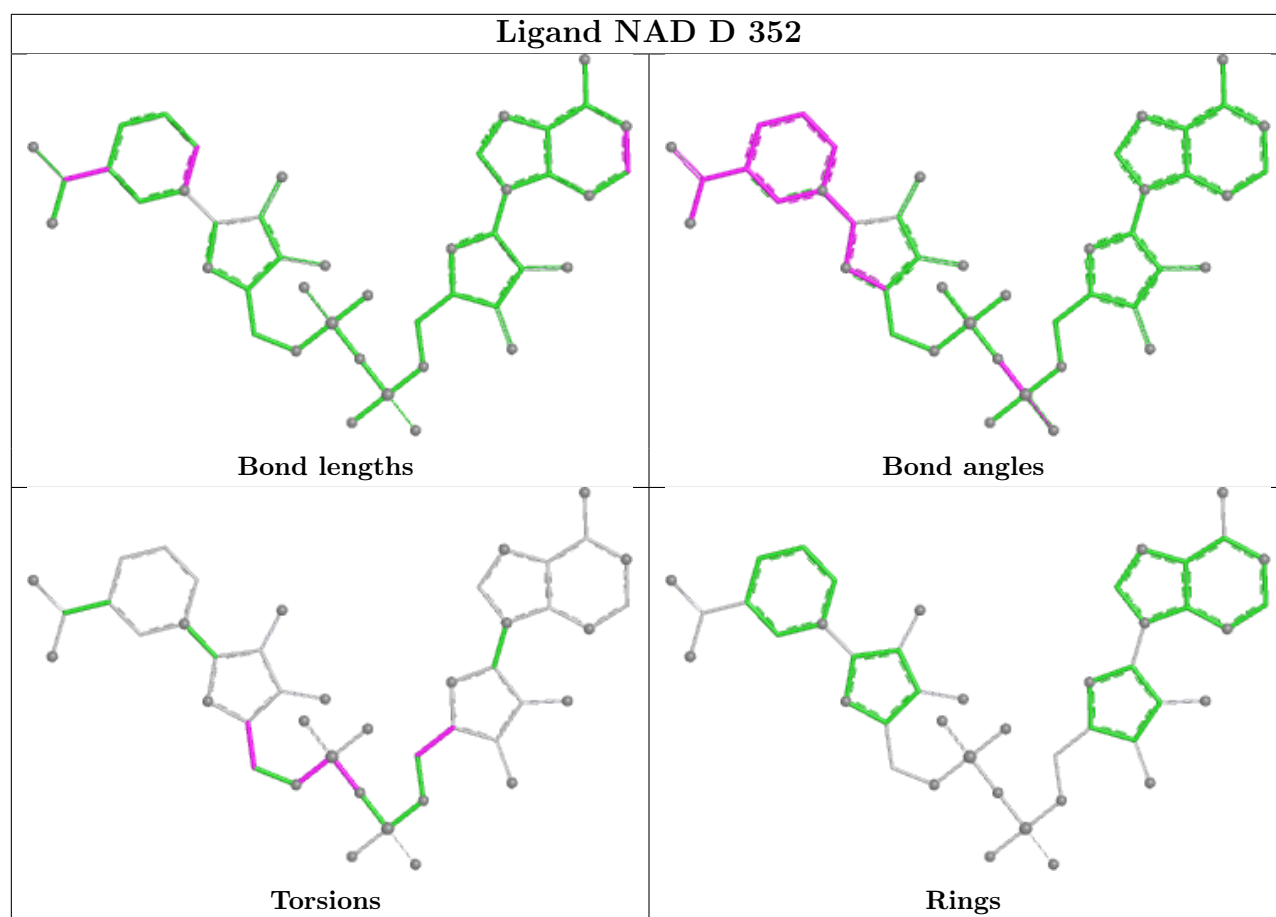


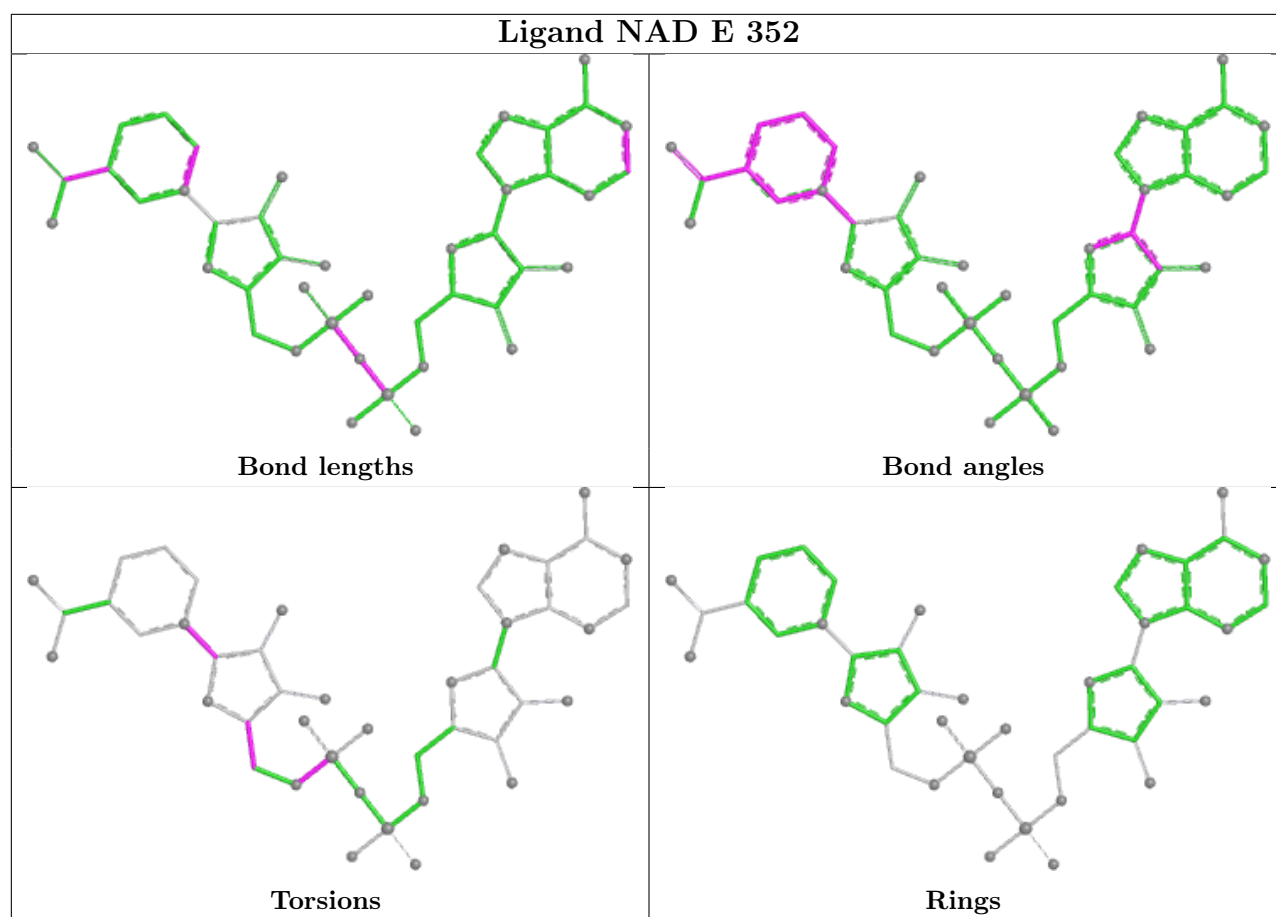
Ligand FBP F 353 (F)



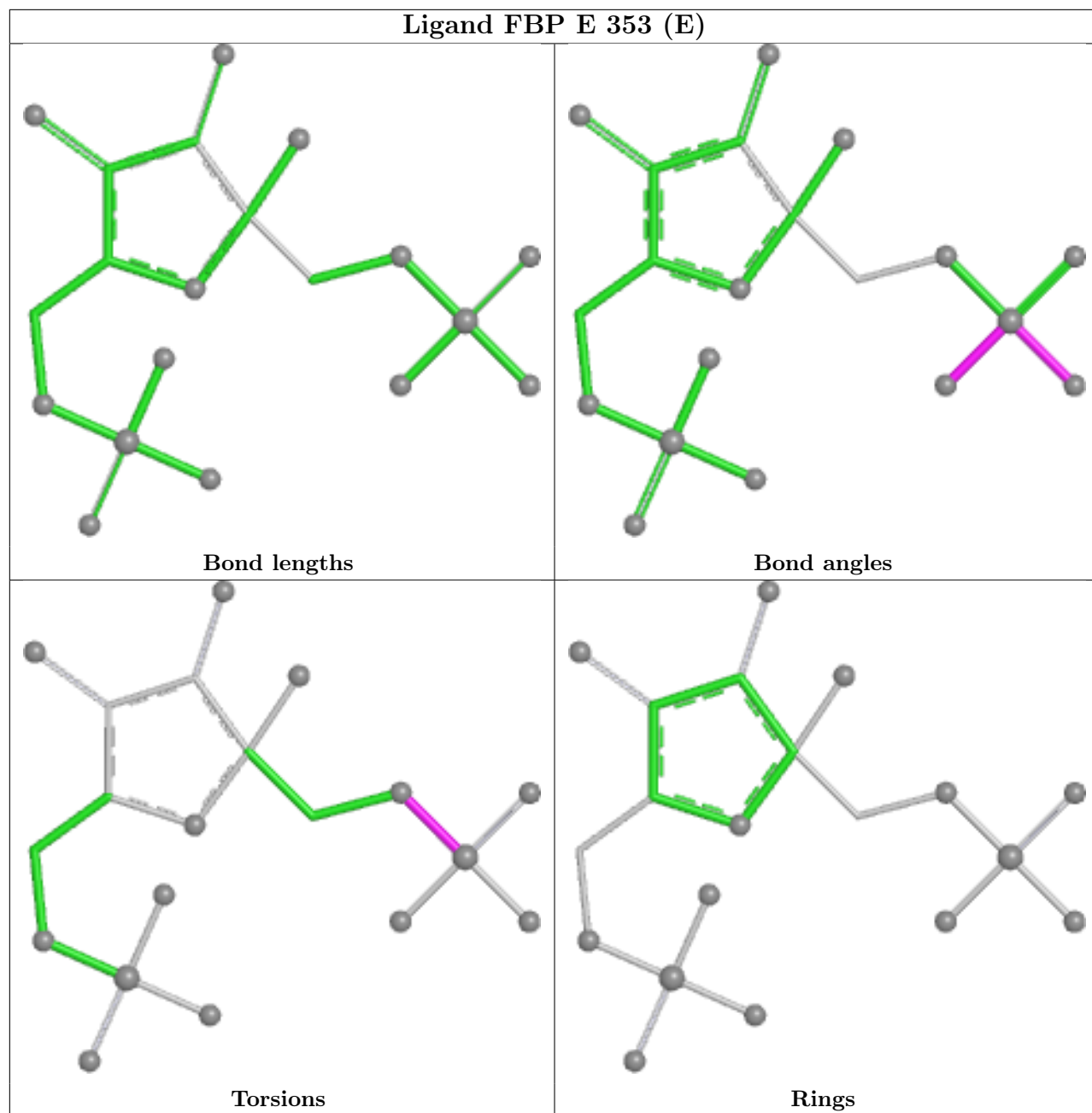
Ligand FBP A 353 (C)



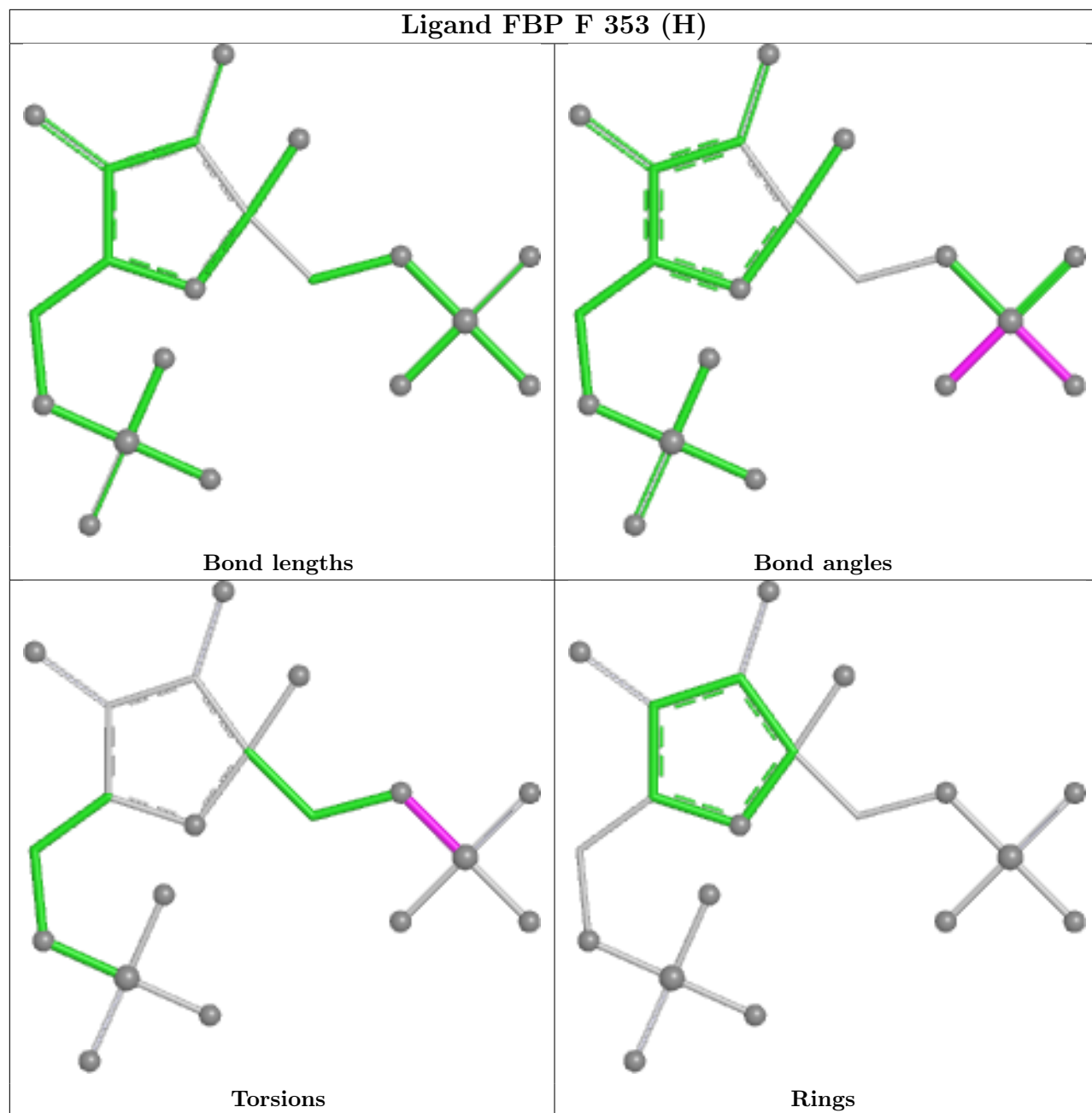


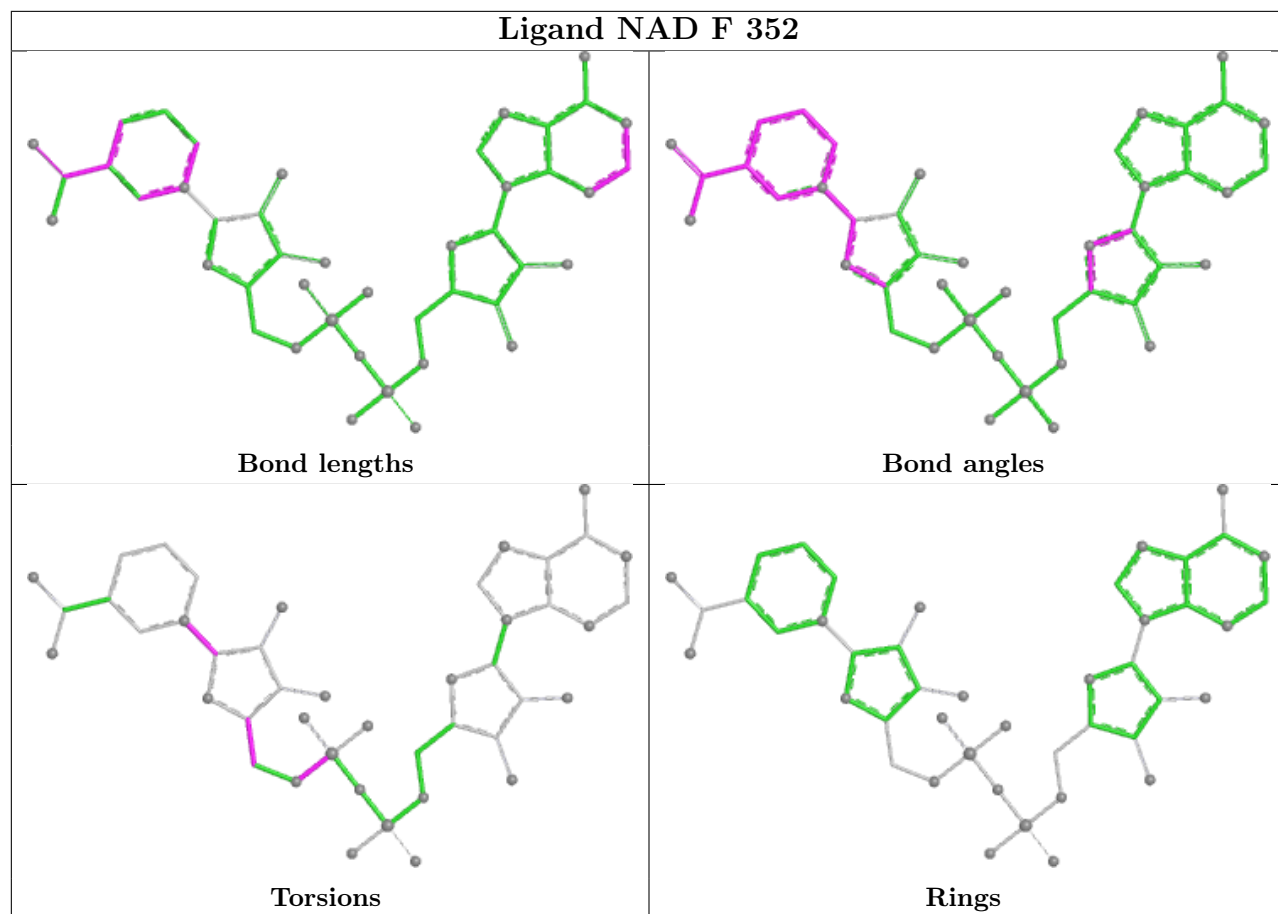


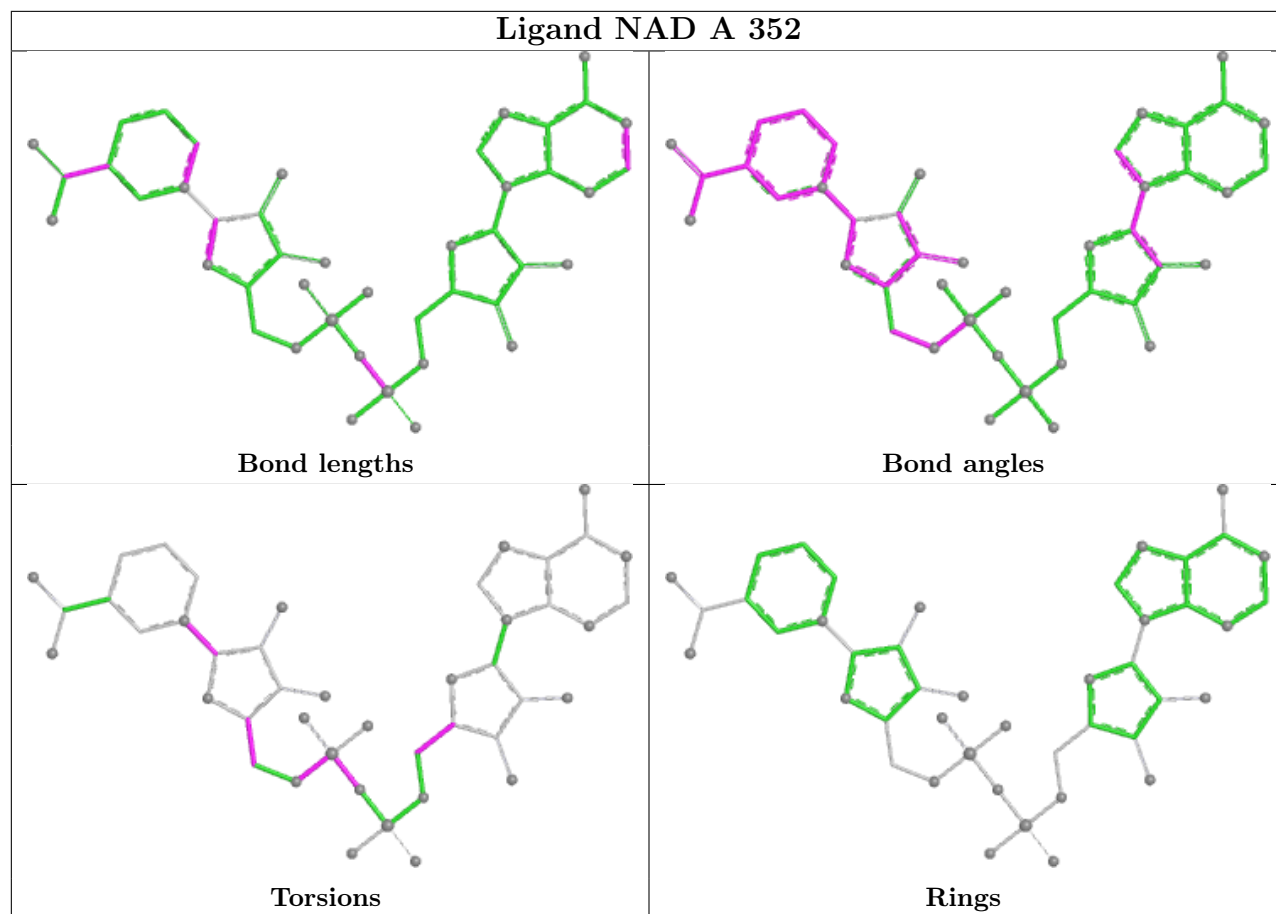
Ligand FBP E 353 (E)

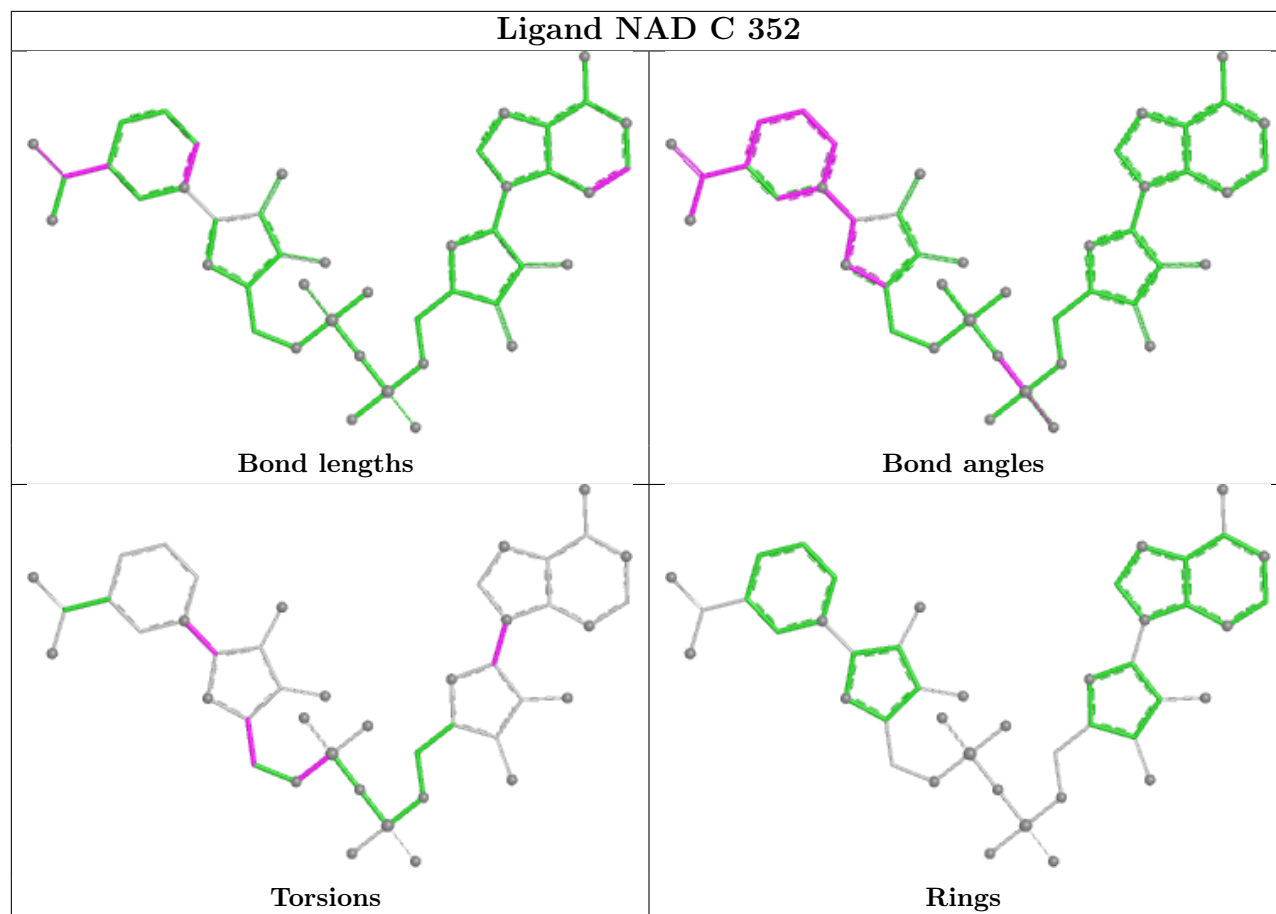


Ligand FBP F 353 (H)

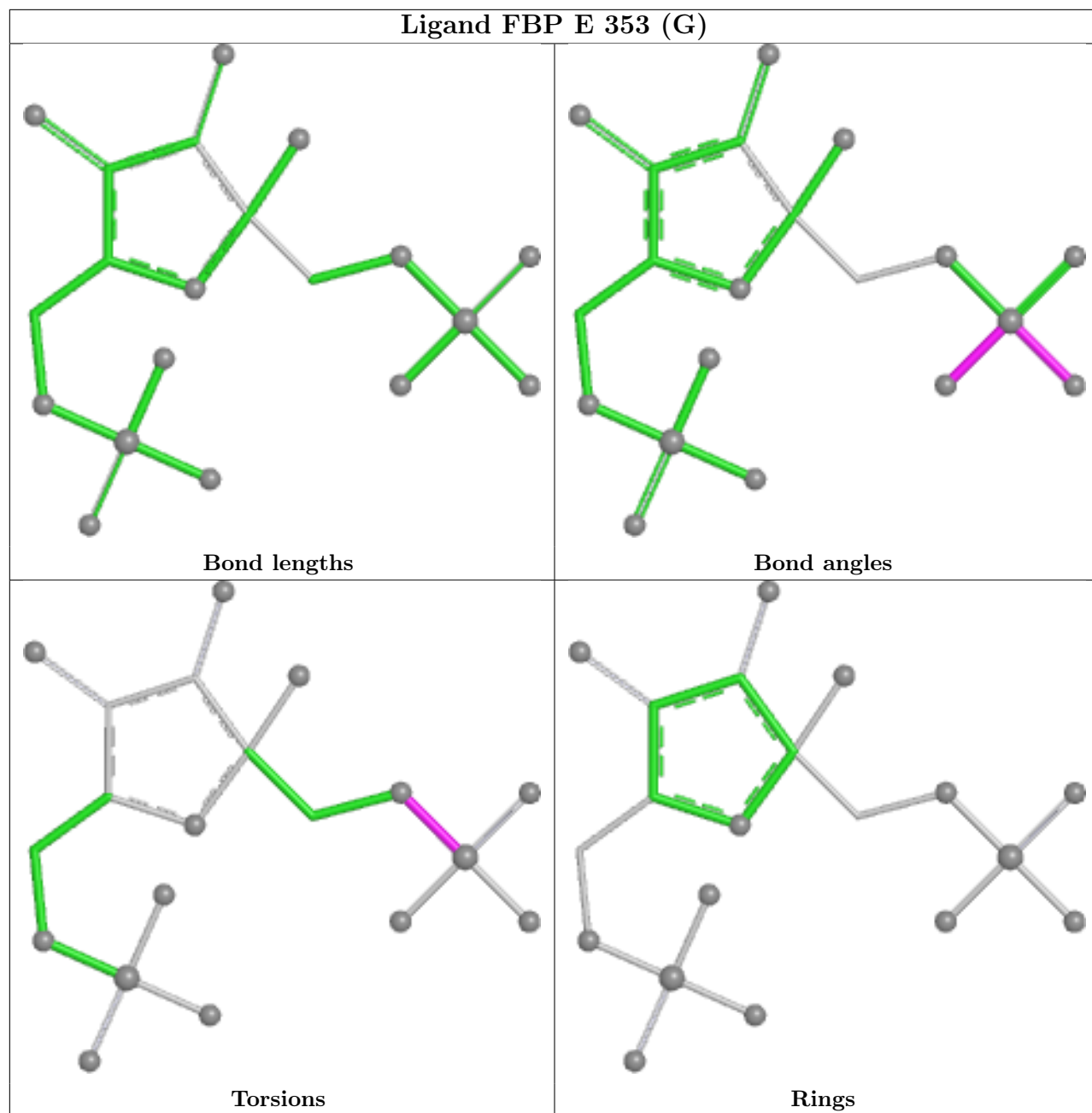


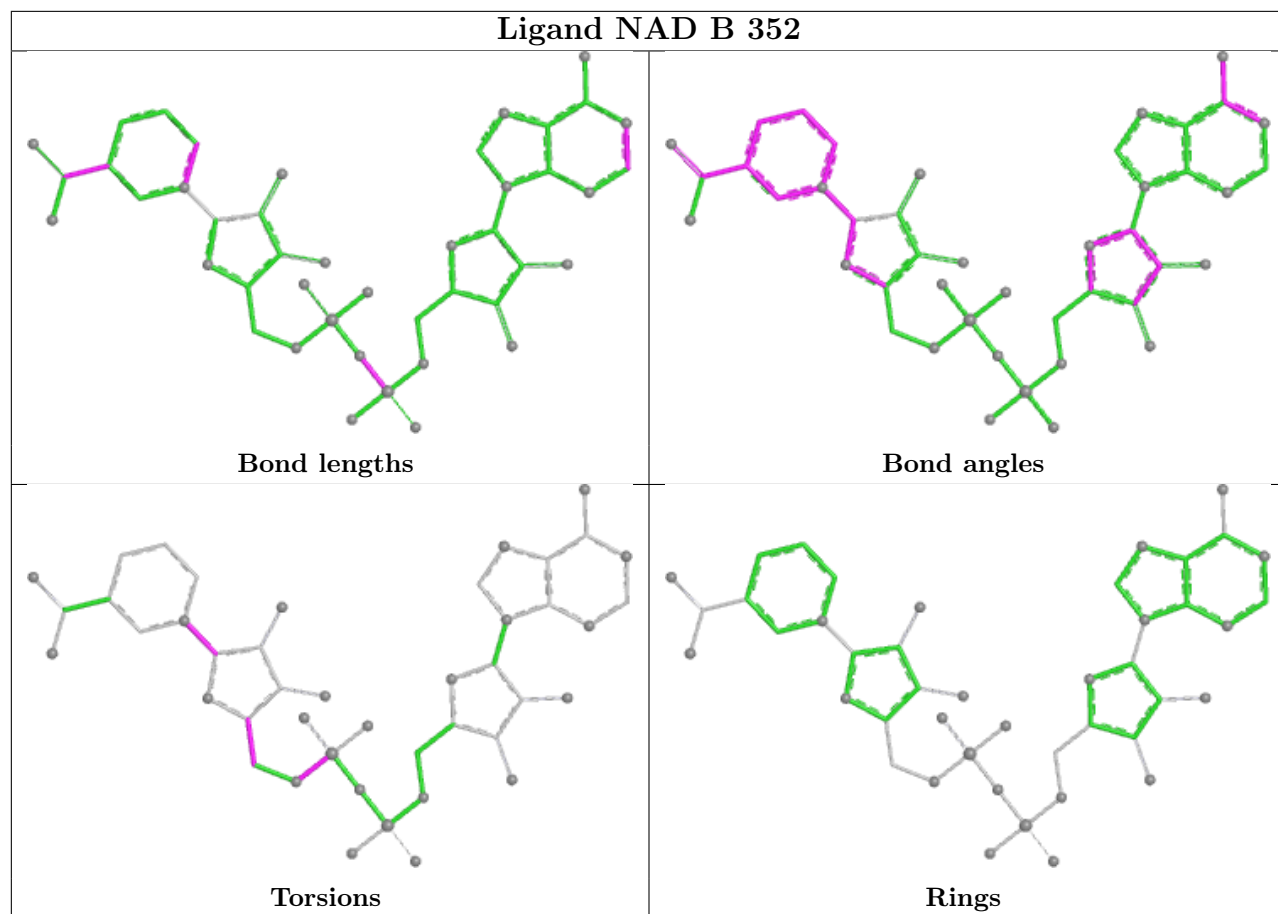




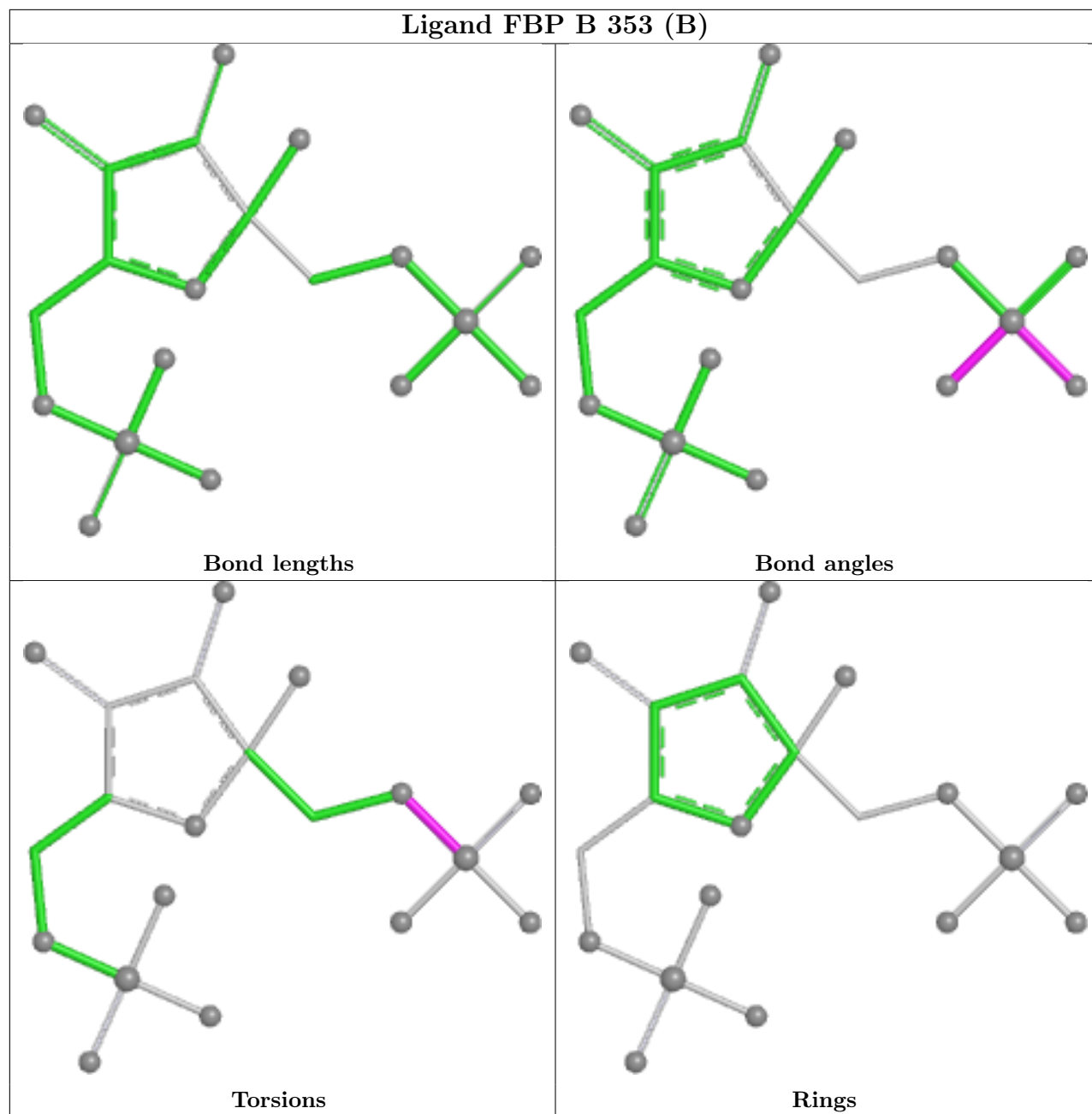


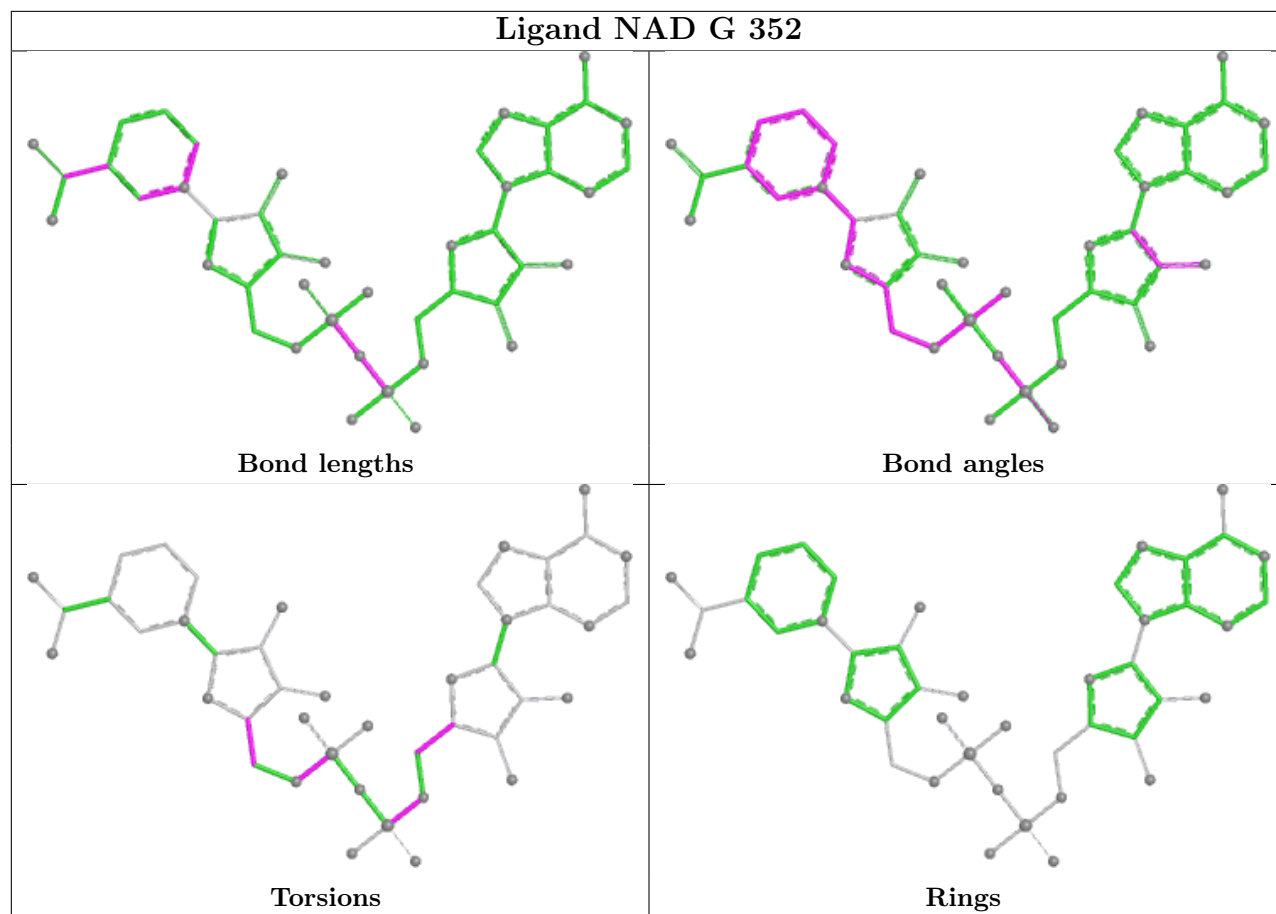
Ligand FBP E 353 (G)

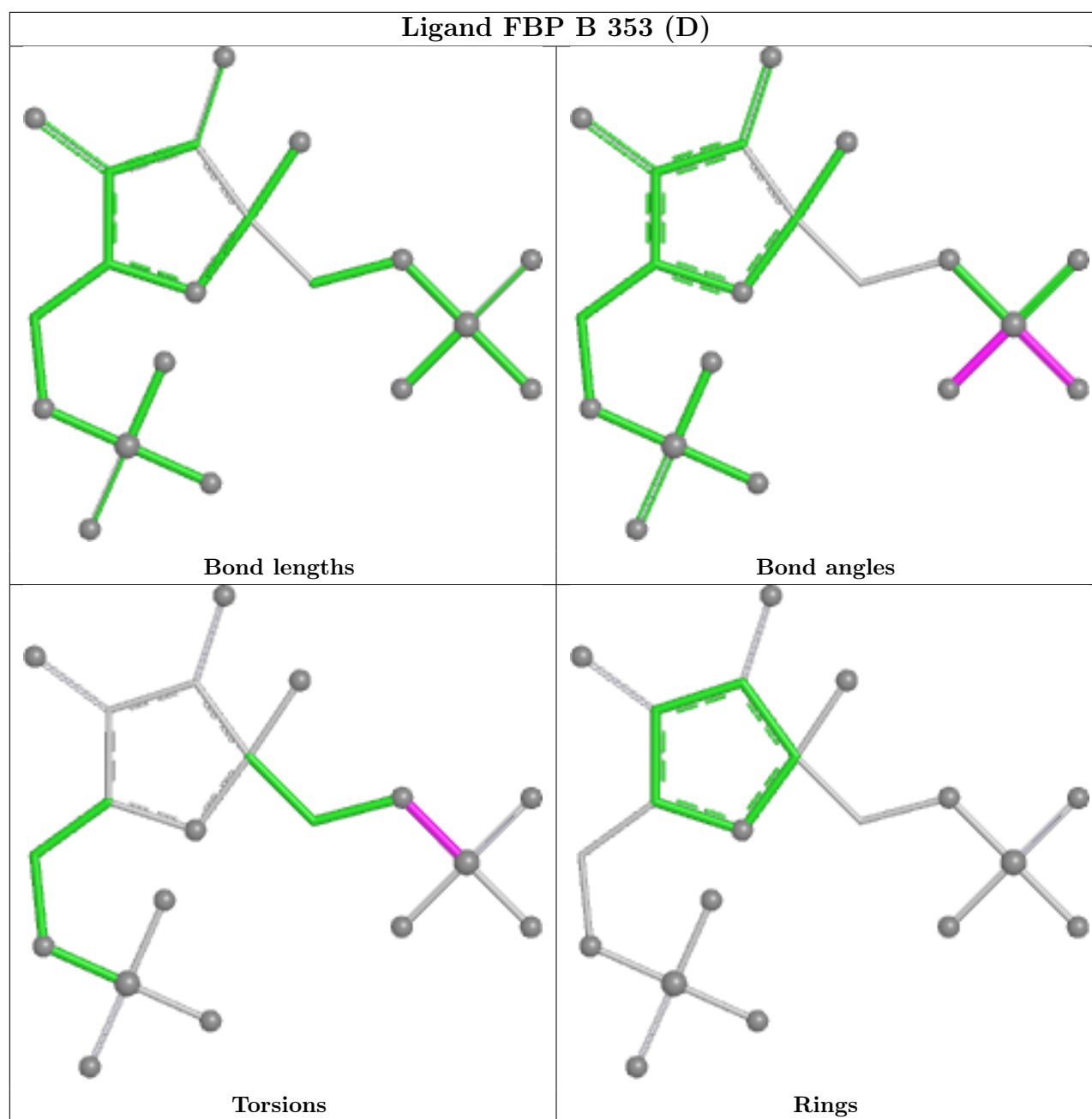




Ligand FBP B 353 (B)







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	316/316 (100%)	-0.61	1 (0%) 90 87	9, 25, 44, 56	0
1	B	316/316 (100%)	-0.72	1 (0%) 90 87	10, 23, 39, 56	0
1	C	316/316 (100%)	-0.70	1 (0%) 90 87	8, 23, 39, 51	0
1	D	316/316 (100%)	-0.68	0 100 100	9, 24, 42, 50	0
1	E	316/316 (100%)	-0.62	1 (0%) 90 87	10, 26, 41, 51	0
1	F	316/316 (100%)	-0.71	1 (0%) 90 87	8, 23, 40, 54	0
1	G	316/316 (100%)	-0.72	0 100 100	12, 24, 40, 53	0
1	H	316/316 (100%)	-0.66	3 (0%) 81 78	13, 25, 43, 52	0
All	All	2528/2528 (100%)	-0.68	8 (0%) 90 87	8, 24, 41, 56	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	MET	4.5
1	F	17	ASN	3.2
1	H	16	LYS	2.8
1	B	17	ASN	2.7
1	A	17	ASN	2.4
1	H	15	MET	2.3
1	H	18	ASN	2.3
1	E	15	MET	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

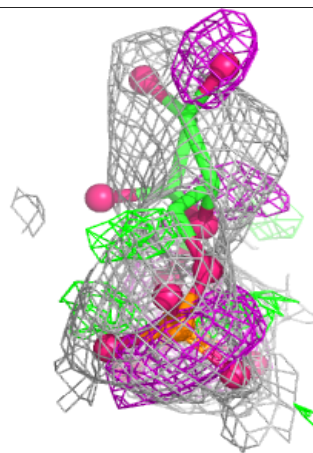
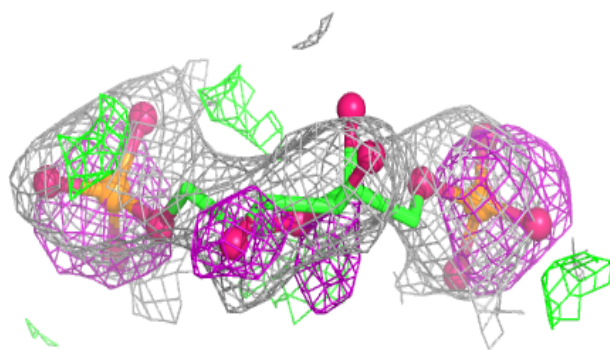
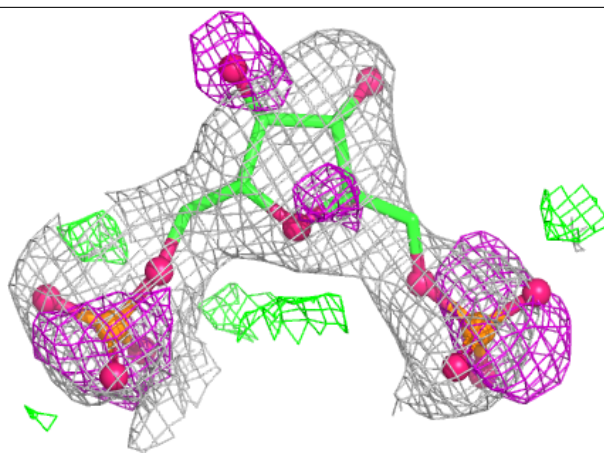
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FBP	E	353[E]	20/20	0.82	0.12	23,40,50,52	20
2	FBP	E	353[G]	20/20	0.82	0.12	22,39,52,52	20
2	FBP	B	353[B]	20/20	0.85	0.11	25,41,49,53	20
2	FBP	B	353[D]	20/20	0.85	0.11	24,39,49,52	20
2	FBP	F	353[F]	20/20	0.87	0.09	22,40,50,54	20
2	FBP	F	353[H]	20/20	0.87	0.09	24,39,48,50	20
2	FBP	A	353[A]	20/20	0.91	0.09	24,38,54,57	20
2	FBP	A	353[C]	20/20	0.91	0.09	25,39,52,59	20
3	OXM	B	351	6/6	0.95	0.07	22,32,41,53	0
3	OXM	D	351	6/6	0.95	0.07	28,32,38,45	0
3	OXM	C	351	6/6	0.96	0.06	9,23,27,50	0
4	NAD	H	352	44/44	0.96	0.07	14,31,55,65	0
3	OXM	F	351	6/6	0.97	0.05	18,25,34,35	0
3	OXM	G	351	6/6	0.97	0.04	15,20,27,34	0
4	NAD	A	352	44/44	0.97	0.06	8,31,48,58	0
4	NAD	B	352	44/44	0.97	0.07	6,26,43,65	0
4	NAD	E	352	44/44	0.97	0.06	7,29,38,52	0
4	NAD	F	352	44/44	0.97	0.06	13,27,44,52	0
3	OXM	A	351	6/6	0.97	0.05	20,41,43,68	0
4	NAD	D	352	44/44	0.98	0.05	8,27,44,51	0
3	OXM	E	351	6/6	0.98	0.04	19,32,42,48	0
3	OXM	H	351	6/6	0.98	0.04	21,24,32,38	0
4	NAD	G	352	44/44	0.98	0.05	0,25,36,60	0
4	NAD	C	352	44/44	0.98	0.05	5,23,41,48	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.

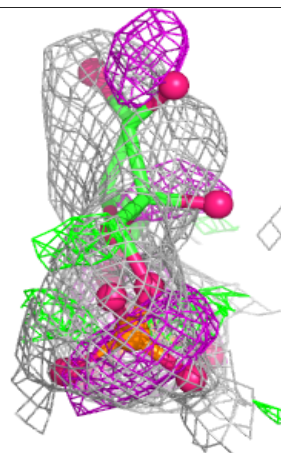
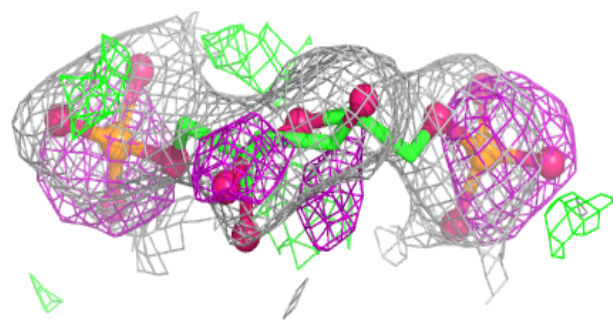
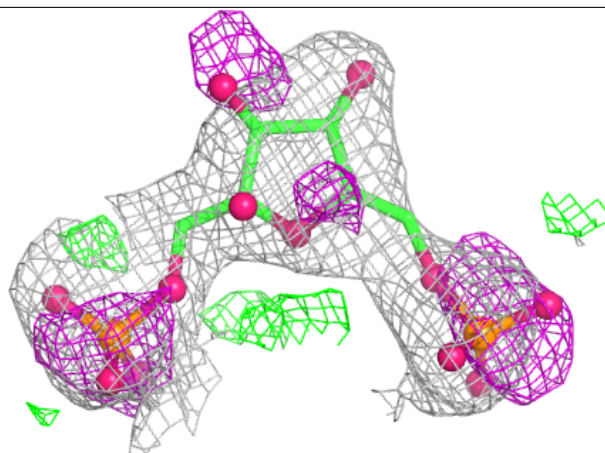
Electron density around FBP E 353 (E):

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



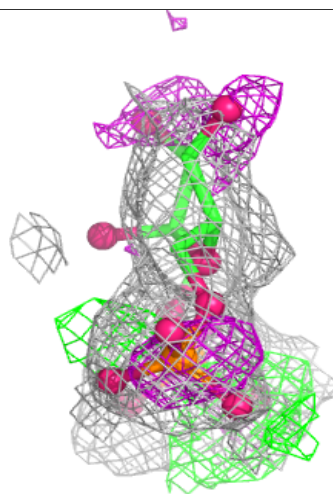
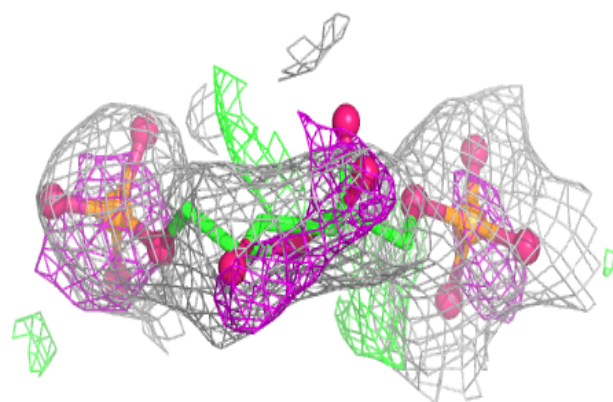
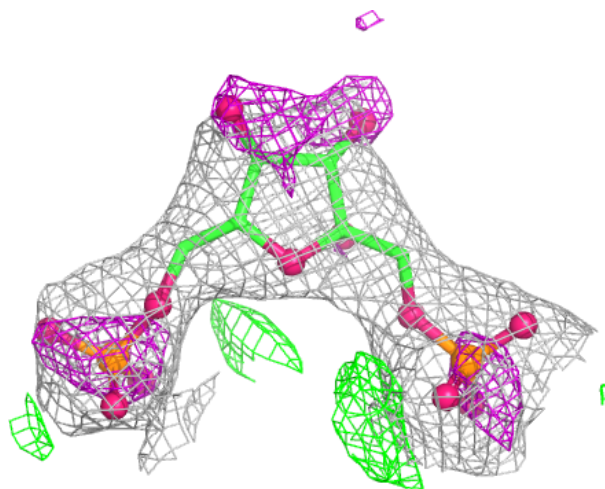
Electron density around FBP E 353 (G):

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



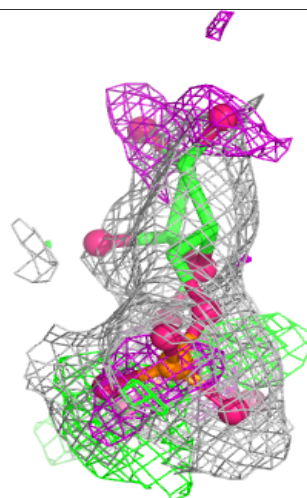
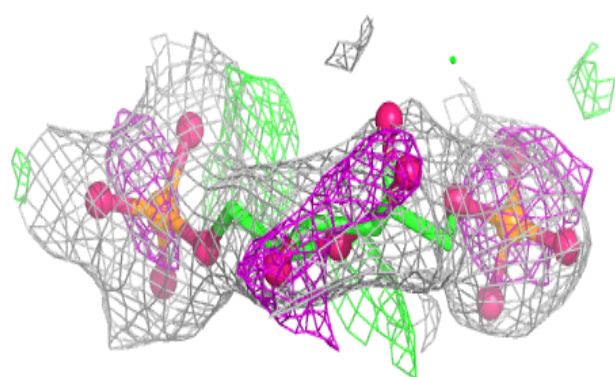
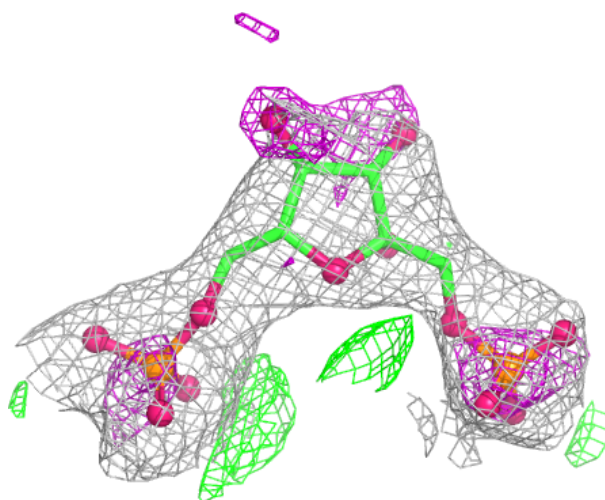
Electron density around FBP B 353 (B):

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



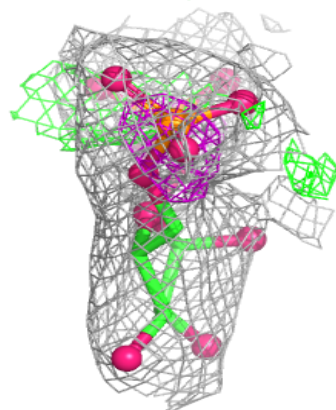
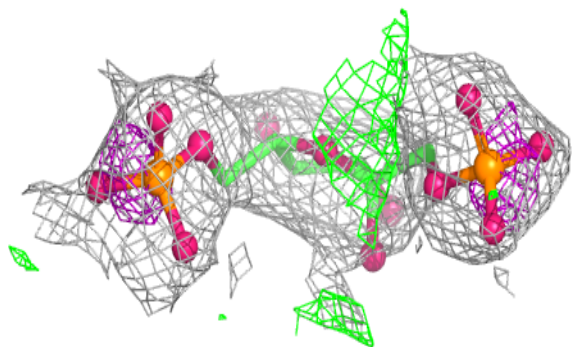
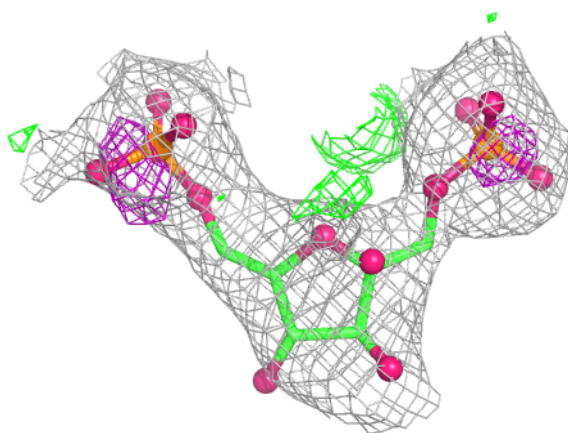
Electron density around FBP B 353 (D):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



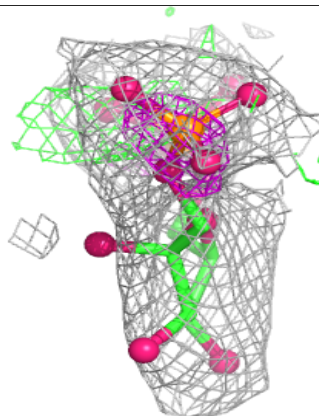
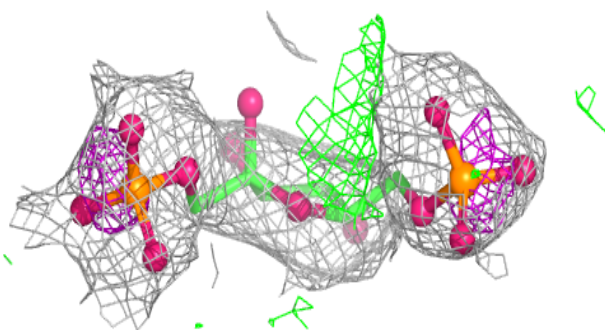
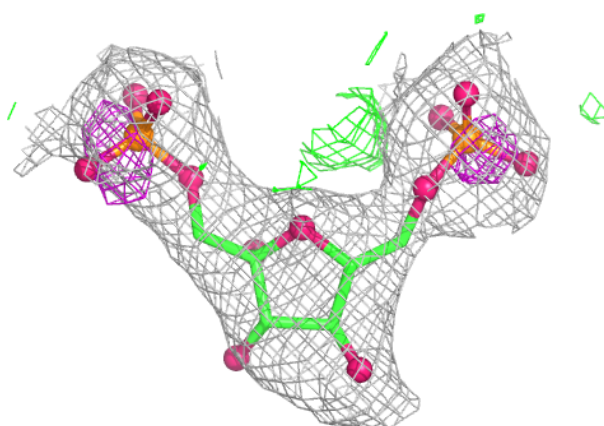
Electron density around FBP F 353 (F):

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

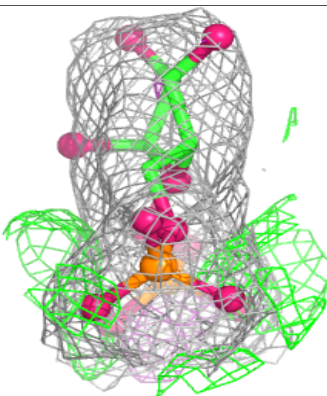
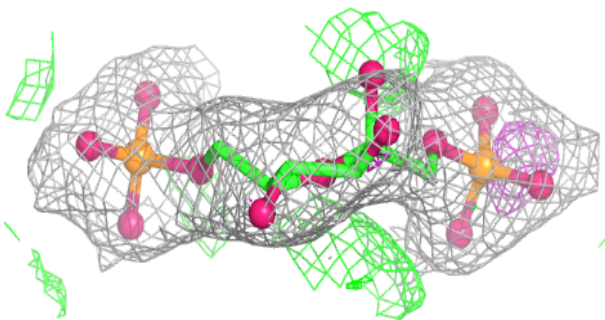
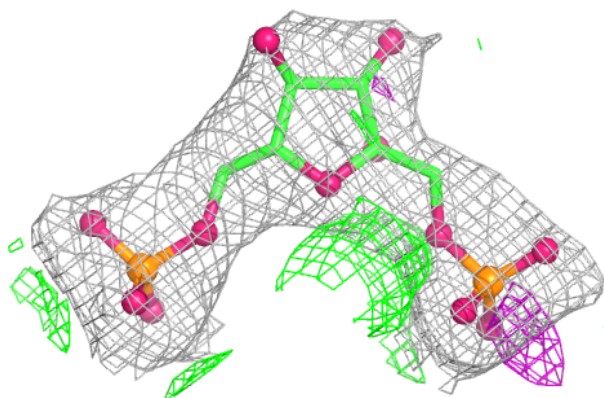


Electron density around FBP F 353 (H):

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and green (positive)

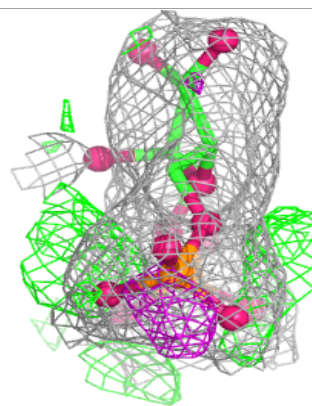
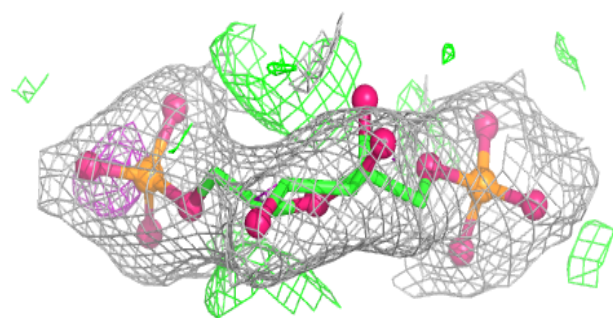
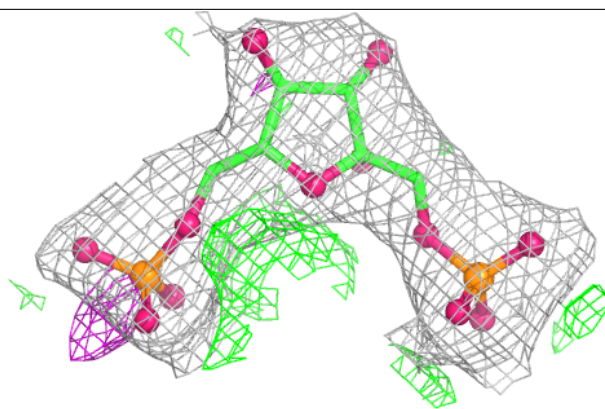
**Electron density around FBP A 353 (A):**

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and green (positive)

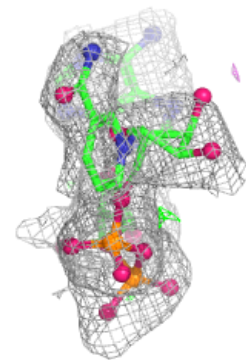
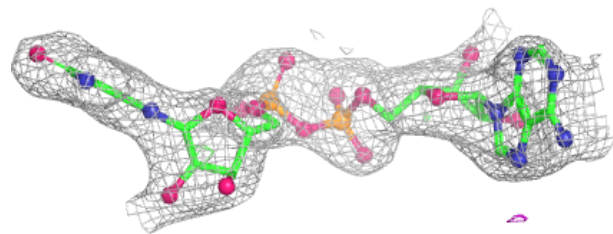
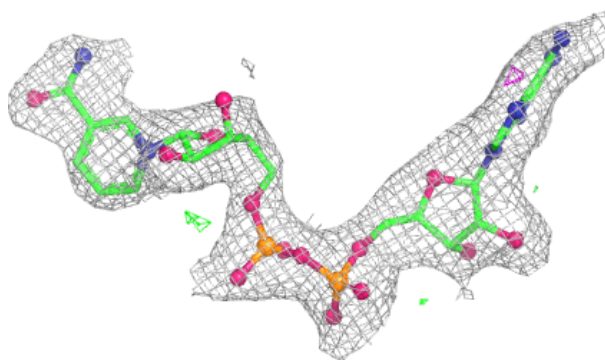


Electron density around FBP A 353 (C):

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

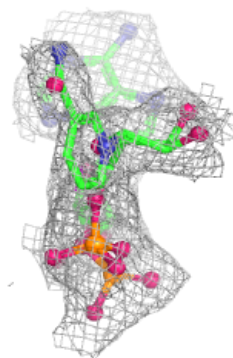
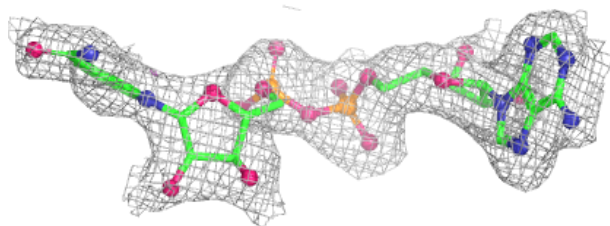
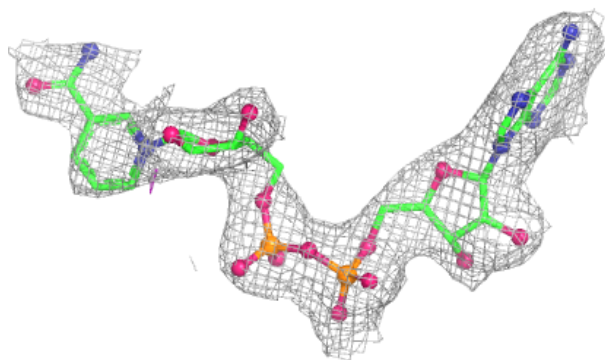
**Electron density around NAD H 352:**

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

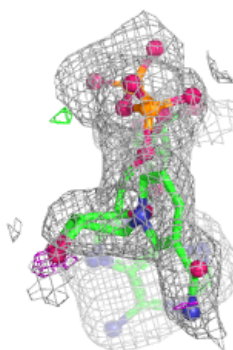
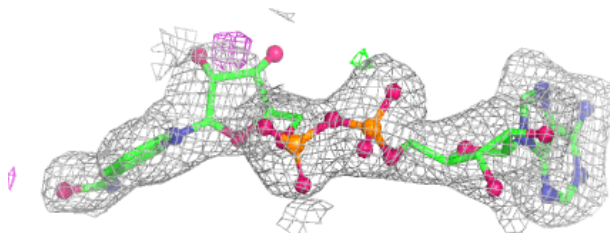
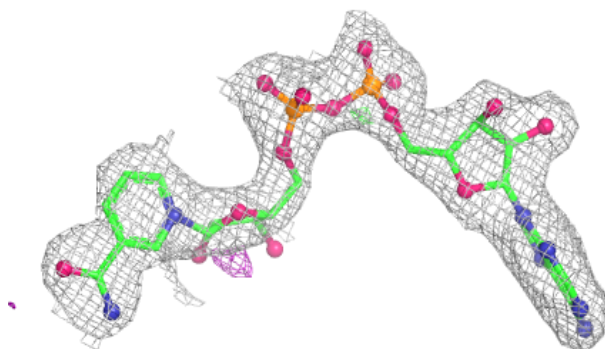


Electron density around NAD A 352:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

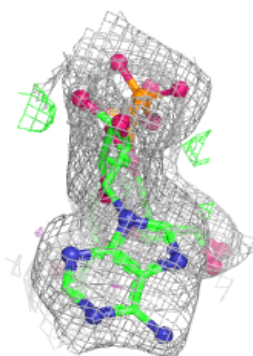
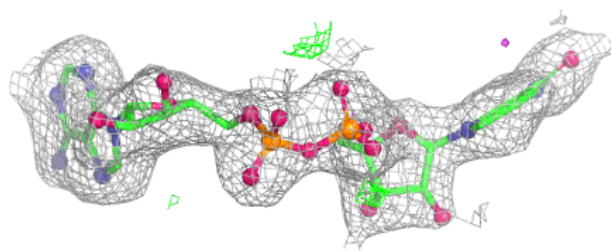
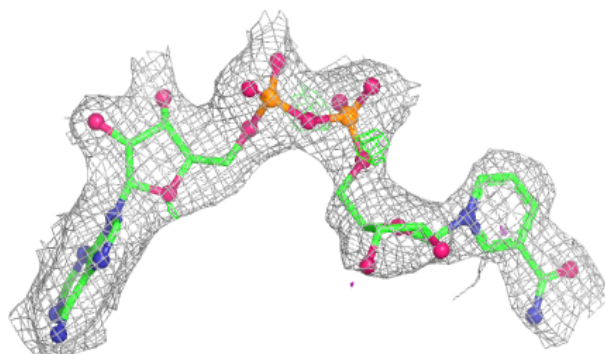
**Electron density around NAD B 352:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

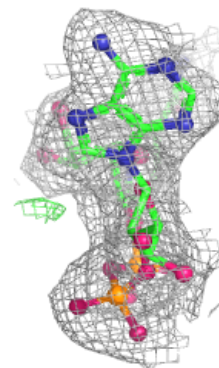
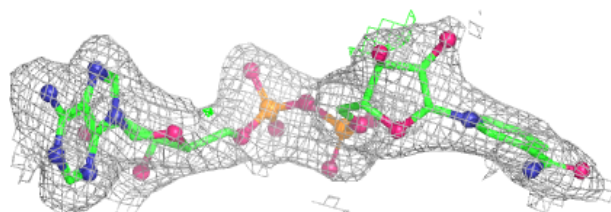
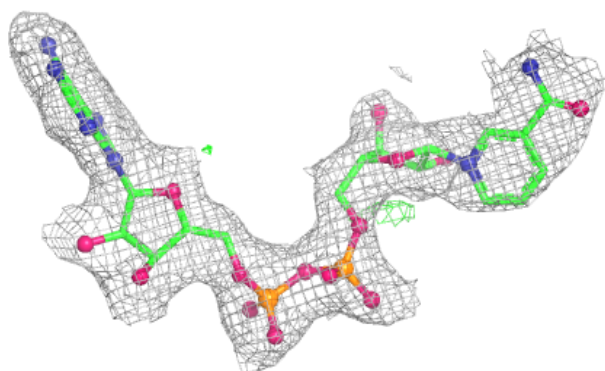


Electron density around NAD E 352:

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and green (positive)

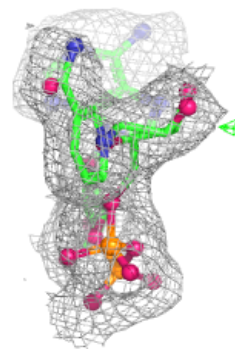
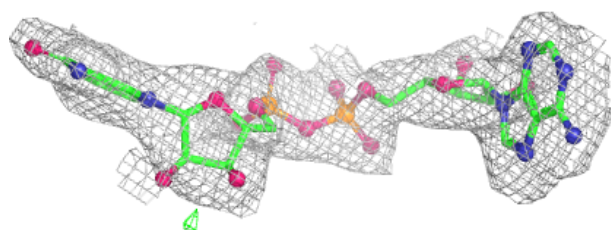
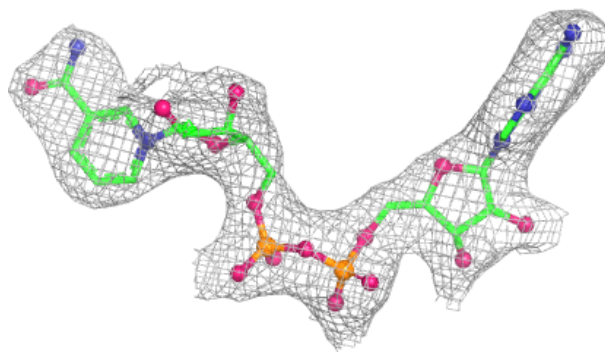
**Electron density around NAD F 352:**

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and green (positive)

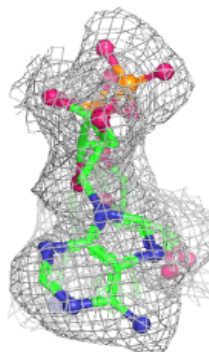
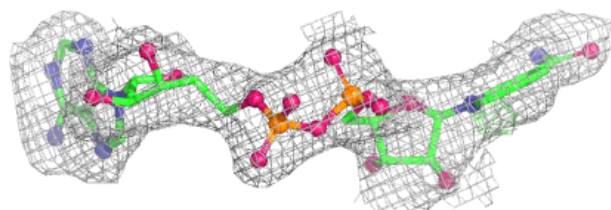
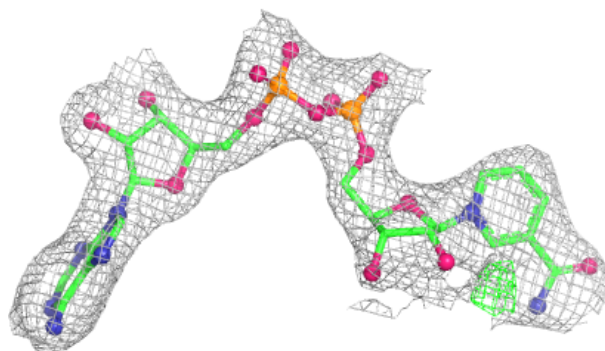


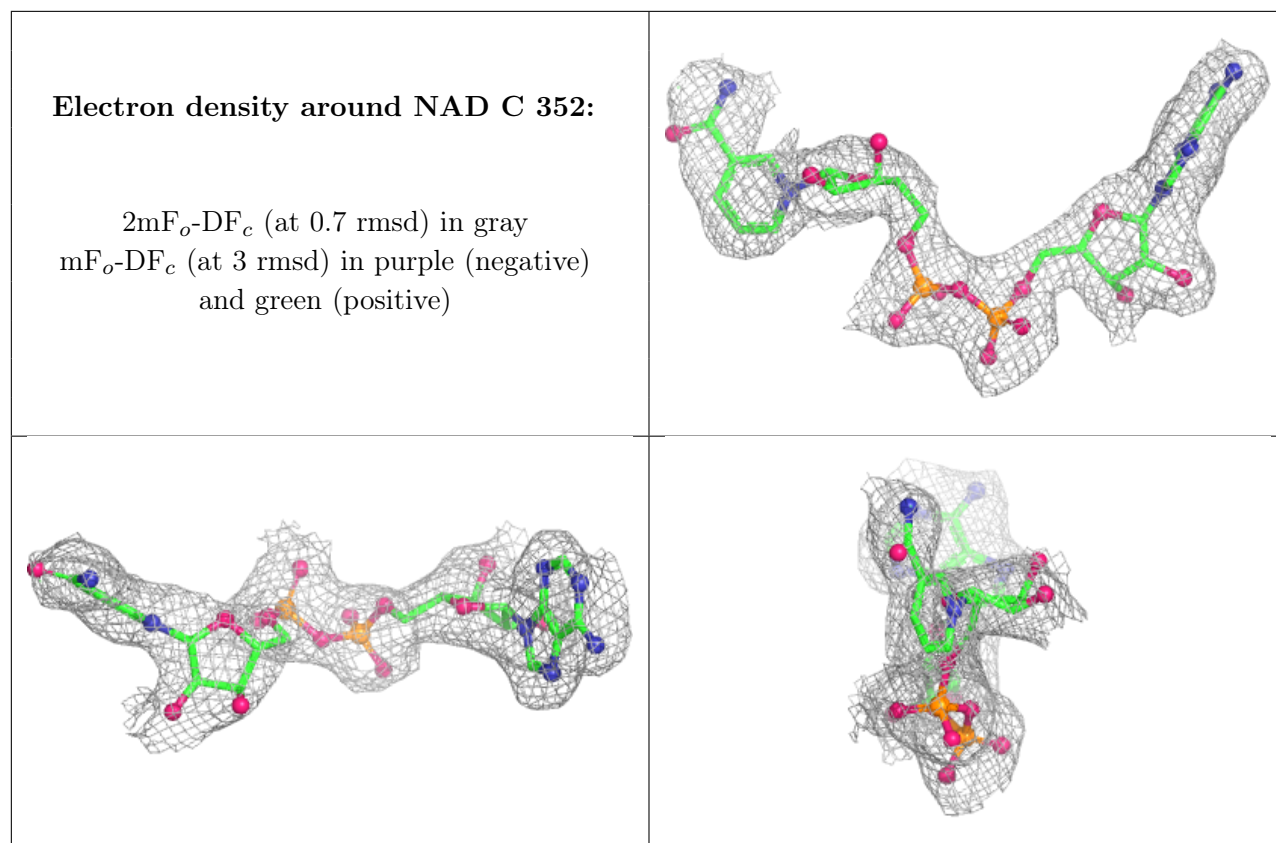
Electron density around NAD D 352:

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

**Electron density around NAD G 352:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.