



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:29 PM UTC

PDB ID : 6GH5 / pdb_00006gh5
EMDB ID : EMD-0001
Title : Cryo-EM structure of bacterial RNA polymerase-sigma54 holoenzyme transcription open complex
Authors : Glyde, R.; Ye, F.Z.; Zhang, X.D.
Deposited on : 2018-05-04
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

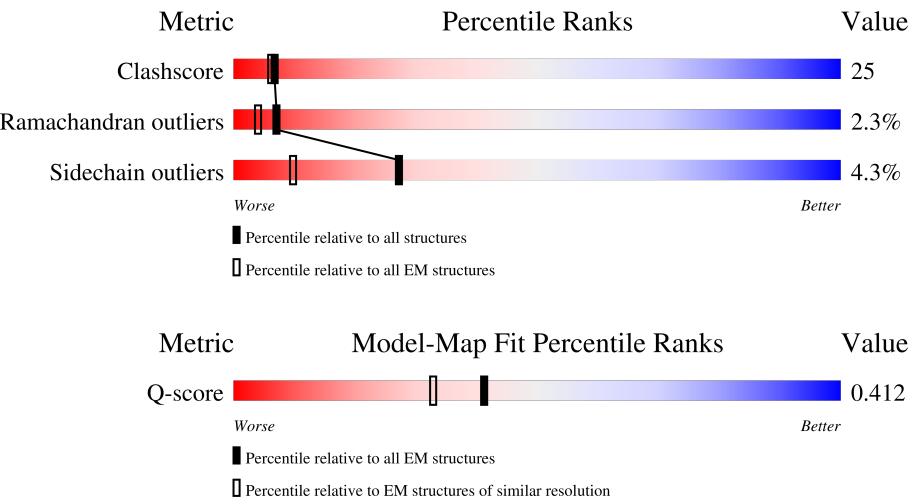
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	49% 29% 14% • 6%
1	B	329	38% 28% 5% 29%
2	C	1342	46% 34% 17% •
3	D	1407	41% 33% 18% • •

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Mol	Chain	Length	Quality of chain
4	E	91	43%26%12%18%
5	M	497	53%13%32%
6	F	63	6%16%43%14%27%
7	G	63	5%30%41%27%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 28316 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	309	Total	C	N	O	S	0	0
			2302	1441	400	454	7		
1	B	235	Total	C	N	O	S	0	0
			1733	1085	301	341	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0
			10034	6289	1746	1961	38		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1345	Total	C	N	O	S	0	0
			9790	6144	1746	1858	42		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	75	Total	C	N	O	S	0	0
			565	347	110	107	1		

- Molecule 5 is a protein called RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	338	Total	C	N	O	S	0	0
			2002	1243	356	400	3		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	initiating methionine	UNP A0A0J4U551
M	-18	GLY	-	expression tag	UNP A0A0J4U551
M	-17	SER	-	expression tag	UNP A0A0J4U551
M	-16	SER	-	expression tag	UNP A0A0J4U551
M	-15	HIS	-	expression tag	UNP A0A0J4U551
M	-14	HIS	-	expression tag	UNP A0A0J4U551
M	-13	HIS	-	expression tag	UNP A0A0J4U551
M	-12	HIS	-	expression tag	UNP A0A0J4U551
M	-11	HIS	-	expression tag	UNP A0A0J4U551
M	-10	HIS	-	expression tag	UNP A0A0J4U551
M	-9	SER	-	expression tag	UNP A0A0J4U551
M	-8	SER	-	expression tag	UNP A0A0J4U551
M	-7	GLY	-	expression tag	UNP A0A0J4U551
M	-6	LEU	-	expression tag	UNP A0A0J4U551
M	-5	VAL	-	expression tag	UNP A0A0J4U551
M	-4	PRO	-	expression tag	UNP A0A0J4U551
M	-3	ARG	-	expression tag	UNP A0A0J4U551
M	-2	GLY	-	expression tag	UNP A0A0J4U551
M	-1	SER	-	expression tag	UNP A0A0J4U551
M	0	HIS	-	expression tag	UNP A0A0J4U551
M	336	ALA	ARG	engineered mutation	UNP A0A0J4U551

- Molecule 6 is a DNA chain called nifH promoter template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	46	Total	C	N	O	P	0	0
			944	445	182	271	46		

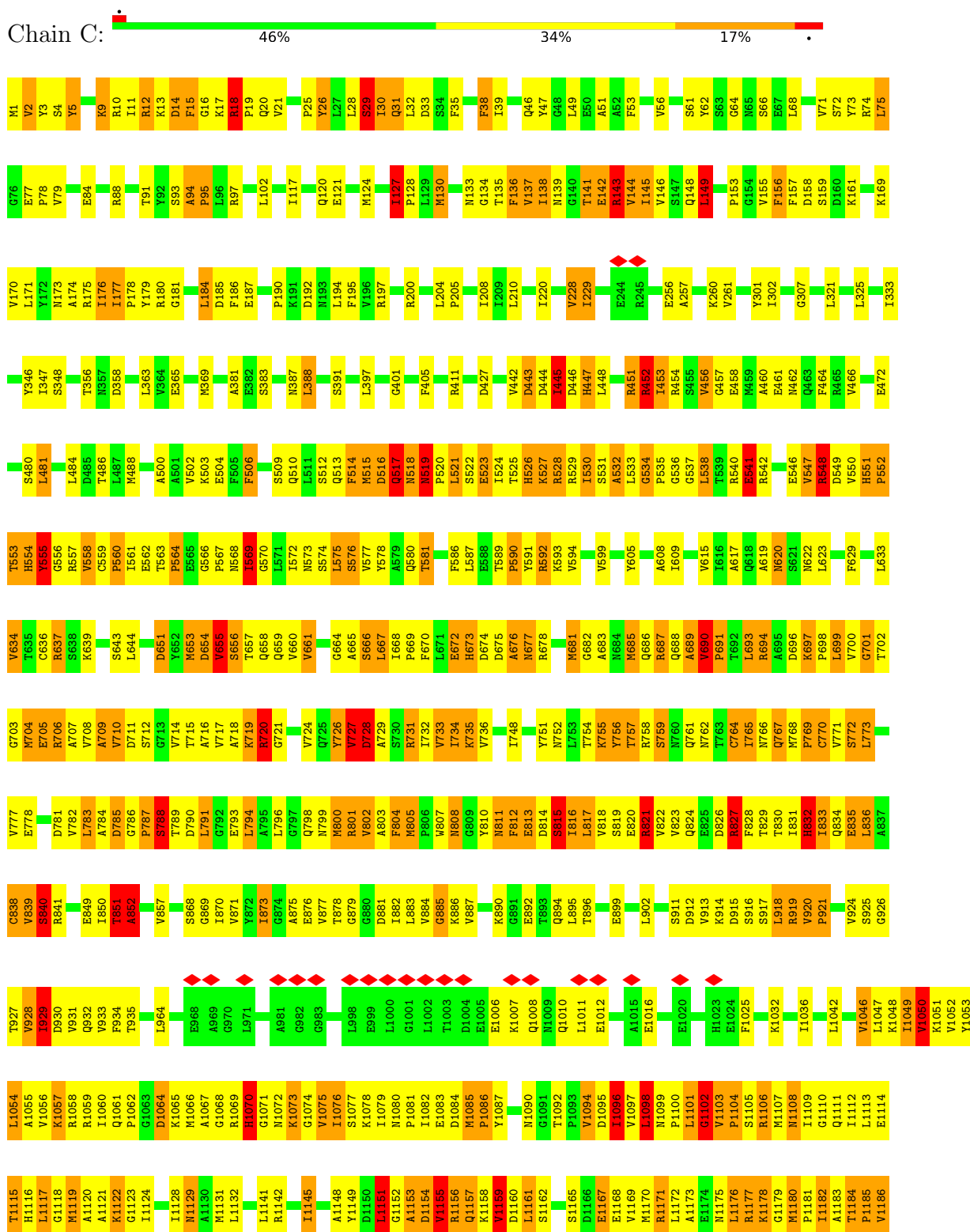
- Molecule 7 is a DNA chain called nifH promoter non-template DNA.

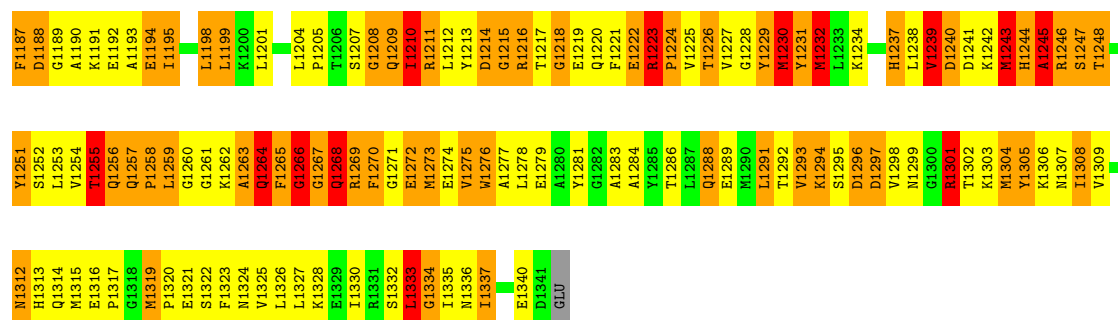
Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	46	Total	C	N	O	P	0	0
			946	448	173	279	46		

GLY
MET
ARG
LEU
GLU
ASN
TRP
PRO
PRO
ALA
SER
ILE
ALA
ASP
GLU

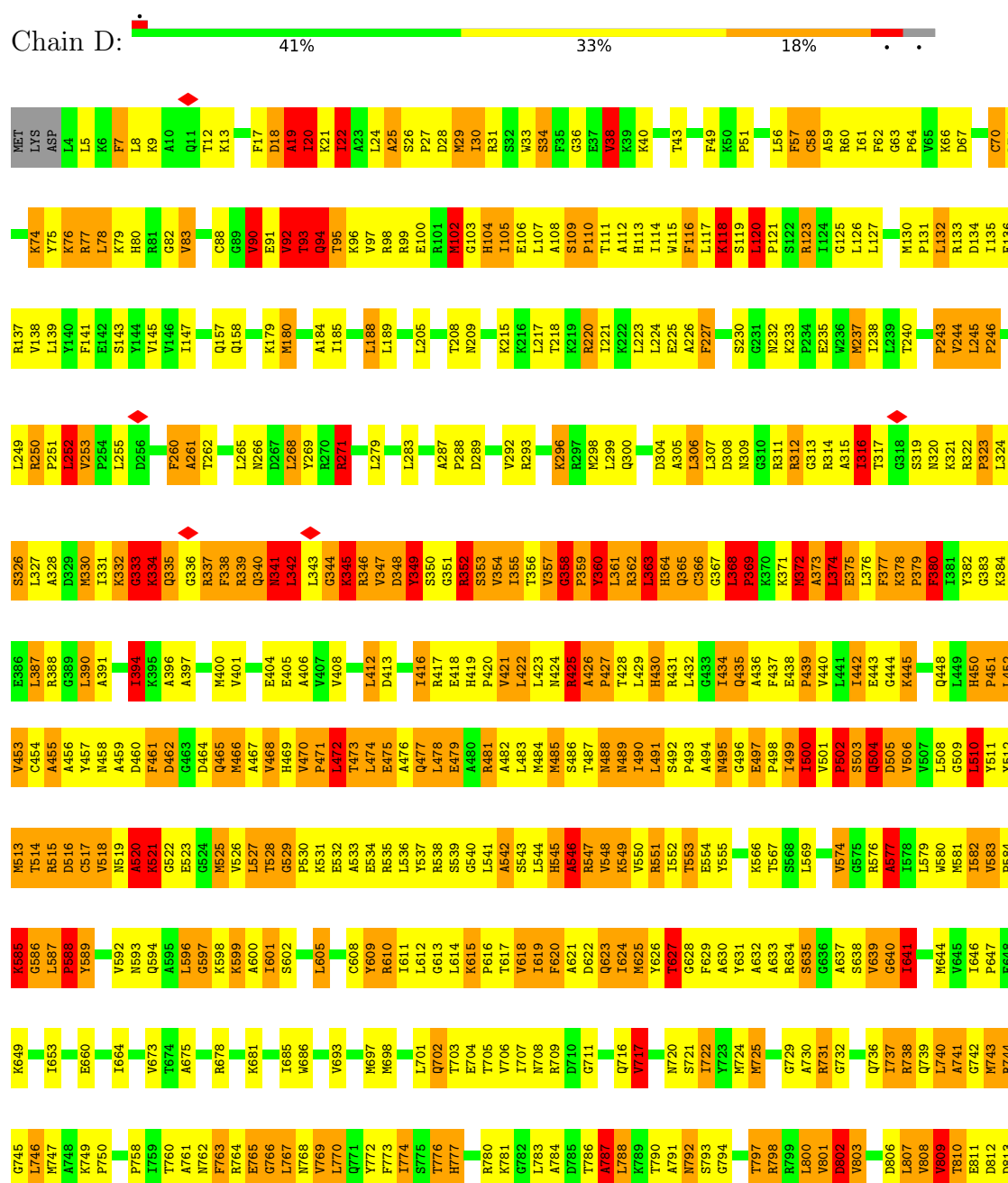
• Molecule 2: DNA-directed RNA polymerase subunit beta

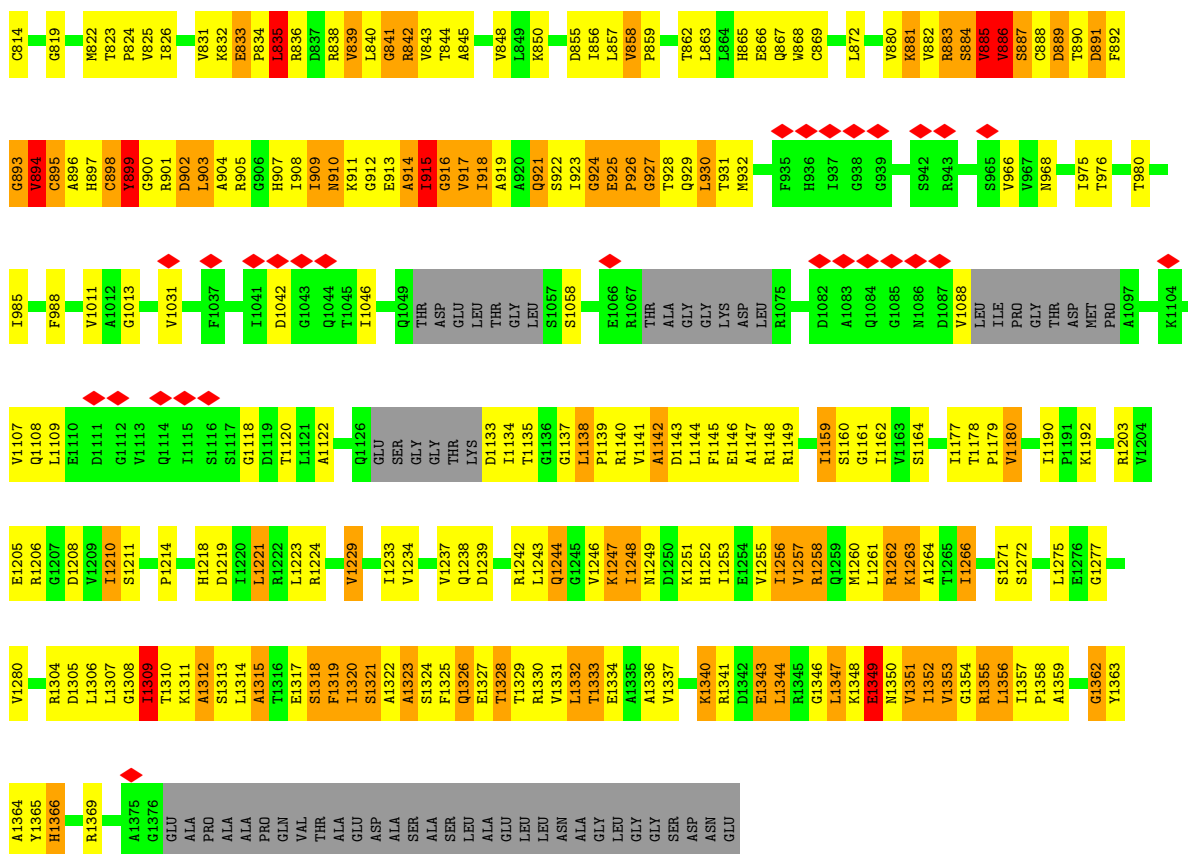
Chain C:



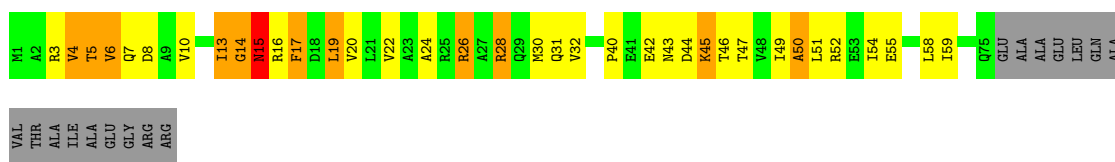


• Molecule 3: DNA-directed RNA polymerase subunit beta'

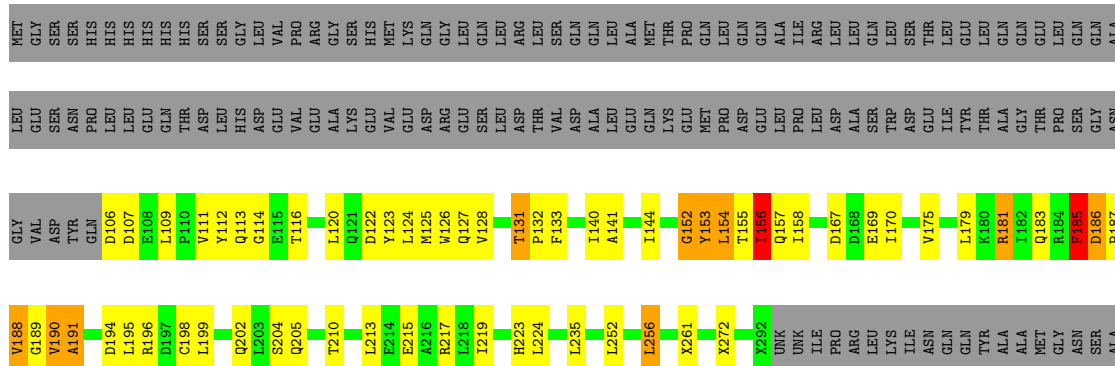


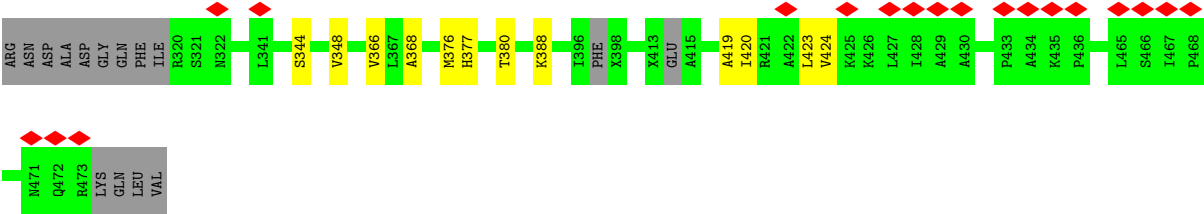


• Molecule 4: DNA-directed RNA polymerase subunit omega

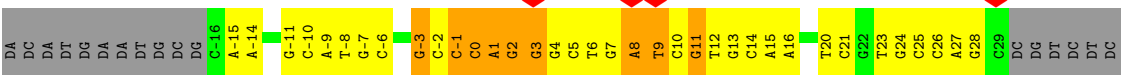
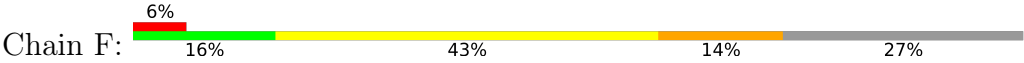


• Molecule 5: RNA polymerase sigma-54 factor, RNA polymerase sigma-54 factor, RNA polymerase sigma-54 factor, RNA polymerase sigma-54 factor, RNA polymerase sigma-54 factor

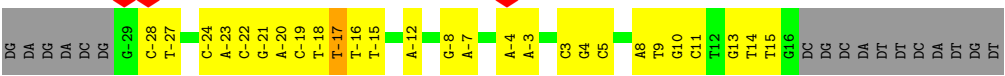




• Molecule 6: nifH promoter template DNA



• Molecule 7: nifH promoter non-template DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79678	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.227	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.018	Depositor
Map size ($\text{\AA}$)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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	2.02	85/2331 (3.6%)	1.82	59/3177 (1.9%)
1	B	1.58	19/1752 (1.1%)	1.50	21/2385 (0.9%)
2	C	2.45	641/10187 (6.3%)	2.16	558/13822 (4.0%)
3	D	2.41	562/9923 (5.7%)	2.17	546/13482 (4.0%)
4	E	1.69	11/567 (1.9%)	1.85	18/767 (2.3%)
5	M	1.27	14/1764 (0.8%)	1.35	22/2445 (0.9%)
6	F	0.51	1/1060 (0.1%)	1.31	19/1633 (1.2%)
7	G	0.39	0/1060	0.75	1/1635 (0.1%)
All	All	2.19	1333/28644 (4.7%)	1.98	1244/39346 (3.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	C	0	28
3	D	0	28
4	E	0	1
5	M	0	1
All	All	0	64

All (1333) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	526	HIS	C-O	-17.73	1.03	1.24
2	C	555	TYR	C-O	17.35	1.44	1.24
2	C	1225	VAL	C-O	17.28	1.41	1.24
3	D	333	GLY	N-CA	17.13	1.70	1.45
3	D	99	ARG	CZ-NH1	16.91	1.56	1.32
2	C	1216	ARG	CZ-NH1	16.80	1.56	1.32
3	D	339	ARG	C-O	16.67	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	813	GLU	C-O	15.89	1.39	1.24
3	D	597	GLY	C-O	15.49	1.39	1.23
2	C	827	ARG	N-CA	15.46	1.65	1.46
2	C	1243	MET	CA-C	15.43	1.73	1.52
3	D	462	ASP	CB-CG	15.31	1.90	1.52
3	D	360	TYR	N-CA	15.30	1.66	1.46
3	D	113	HIS	CA-C	-15.17	1.39	1.53
3	D	362	ARG	N-CA	-15.10	1.27	1.46
2	C	149	LEU	C-O	14.92	1.40	1.24
3	D	1323	ALA	C-O	14.88	1.41	1.24
3	D	357	VAL	CA-C	14.81	1.68	1.53
2	C	794	LEU	C-O	14.60	1.42	1.24
3	D	623	GLN	C-O	14.56	1.41	1.24
2	C	519	ASN	CG-OD1	14.41	1.50	1.23
2	C	1238	LEU	N-CA	14.33	1.63	1.45
2	C	668	ILE	CA-C	13.86	1.63	1.53
2	C	1247	SER	N-CA	13.83	1.61	1.46
2	C	143	ARG	C-O	-13.77	1.06	1.24
3	D	369	PRO	N-CA	13.60	1.64	1.47
3	D	359	PRO	CA-CB	13.58	1.73	1.53
3	D	352	ARG	N-CA	13.45	1.62	1.46
3	D	360	TYR	CA-C	13.34	1.70	1.52
3	D	365	GLN	CD-NE2	13.31	1.61	1.33
2	C	1298	VAL	C-O	13.27	1.36	1.24
3	D	429	LEU	C-O	13.15	1.41	1.23
5	M	190	VAL	C-O	13.11	1.37	1.24
2	C	519	ASN	N-CA	13.10	1.64	1.46
3	D	472	LEU	CA-CB	-13.08	1.36	1.53
3	D	337	ARG	N-CA	12.83	1.60	1.46
3	D	99	ARG	CZ-NH2	12.77	1.50	1.33
2	C	1246	ARG	CA-C	-12.72	1.37	1.52
2	C	577	VAL	C-O	12.69	1.38	1.24
3	D	373	ALA	N-CA	12.60	1.62	1.46
3	D	492	SER	C-O	-12.58	1.08	1.24
2	C	1299	ASN	CA-C	12.55	1.69	1.52
3	D	462	ASP	N-CA	12.39	1.60	1.46
2	C	590	PRO	CA-C	-12.34	1.40	1.52
2	C	931	VAL	C-O	12.30	1.36	1.24
2	C	699	LEU	C-O	-12.28	1.07	1.24
3	D	462	ASP	CA-C	12.27	1.68	1.52
3	D	425	ARG	C-O	-12.26	1.10	1.24
2	C	518	ASN	N-CA	12.22	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	683	ALA	C-O	12.20	1.38	1.24
1	A	181	GLU	N-CA	12.16	1.61	1.46
2	C	1078	LYS	C-O	12.15	1.38	1.23
3	D	451	PRO	C-O	12.13	1.40	1.24
2	C	177	ILE	N-CA	12.11	1.55	1.45
2	C	803	ALA	C-O	12.10	1.37	1.24
3	D	1365	TYR	C-O	-11.96	1.08	1.24
2	C	1099	ASN	CA-C	-11.94	1.38	1.52
3	D	894	VAL	C-O	-11.94	1.09	1.24
2	C	1246	ARG	N-CA	11.91	1.60	1.45
3	D	466	MET	SD-CE	-11.85	1.50	1.79
3	D	1363	TYR	C-O	11.83	1.37	1.24
3	D	345	LYS	CA-CB	11.82	1.71	1.53
2	C	1068	GLY	N-CA	11.81	1.56	1.45
3	D	492	SER	CA-C	-11.81	1.39	1.52
2	C	697	LYS	N-CA	11.75	1.61	1.45
2	C	1177	ARG	C-O	-11.74	1.10	1.24
3	D	769	VAL	N-CA	11.73	1.60	1.46
2	C	757	THR	C-O	-11.70	1.10	1.23
1	B	31	LEU	C-O	11.70	1.38	1.23
2	C	690	VAL	CA-C	-11.64	1.40	1.52
1	A	182	ARG	N-CA	11.64	1.59	1.45
2	C	804	PHE	N-CA	11.61	1.60	1.46
2	C	1111	GLN	C-O	11.51	1.37	1.24
3	D	908	ILE	CA-C	-11.48	1.40	1.52
3	D	456	ALA	N-CA	11.44	1.60	1.46
3	D	1340	LYS	C-O	-11.37	1.09	1.23
2	C	452	ARG	C-O	11.36	1.38	1.23
3	D	622	ASP	C-O	11.31	1.37	1.24
3	D	833	GLU	C-O	-11.30	1.14	1.25
2	C	879	GLY	C-O	-11.25	1.09	1.24
2	C	562	GLU	CA-CB	11.21	1.67	1.53
3	D	421	VAL	C-O	11.21	1.34	1.23
2	C	518	ASN	CG-OD1	11.18	1.44	1.23
2	C	764	CYS	N-CA	11.16	1.60	1.45
2	C	153	PRO	C-O	11.14	1.36	1.23
2	C	762	ASN	CA-C	11.10	1.67	1.53
2	C	524	ILE	N-CA	-11.05	1.34	1.46
3	D	808	VAL	C-O	-11.05	1.10	1.24
3	D	901	ARG	C-O	11.04	1.36	1.23
1	B	44	ARG	C-O	11.00	1.36	1.24
2	C	770	CYS	N-CA	10.99	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1256	ILE	N-CA	-10.90	1.33	1.46
3	D	545	HIS	C-O	-10.88	1.14	1.24
2	C	9	LYS	C-O	-10.87	1.11	1.24
3	D	308	ASP	N-CA	10.82	1.59	1.46
3	D	331	ILE	C-O	-10.80	1.11	1.24
2	C	515	MET	C-O	10.80	1.37	1.23
3	D	332	LYS	CA-CB	10.76	1.68	1.53
2	C	834	GLN	C-O	10.76	1.37	1.23
3	D	377	PHE	CA-C	10.76	1.68	1.52
2	C	678	ARG	CA-C	10.72	1.66	1.52
3	D	488	ASN	CA-C	-10.71	1.39	1.52
2	C	758	ARG	CA-C	10.70	1.66	1.52
2	C	677	ASN	C-O	10.69	1.38	1.24
2	C	659	GLN	CA-C	-10.67	1.39	1.52
2	C	133	ASN	N-CA	-10.58	1.32	1.46
2	C	818	VAL	CA-CB	10.54	1.69	1.54
2	C	1113	LEU	C-O	10.52	1.37	1.24
3	D	470	VAL	CA-CB	-10.48	1.43	1.53
3	D	1359	ALA	CA-C	-10.44	1.39	1.52
1	A	151	GLY	N-CA	10.41	1.60	1.45
2	C	1086	PRO	N-CA	10.40	1.59	1.47
3	D	1326	GLN	CA-C	-10.31	1.39	1.52
3	D	808	VAL	CA-CB	10.26	1.68	1.54
5	M	154	LEU	C-O	-10.22	1.11	1.24
3	D	632	ALA	CA-C	-10.20	1.39	1.52
2	C	834	GLN	CA-C	-10.20	1.39	1.52
3	D	889	ASP	CA-CB	10.19	1.69	1.53
2	C	1231	TYR	C-O	10.11	1.35	1.24
2	C	1271	GLY	C-O	10.08	1.33	1.23
2	C	693	LEU	CA-C	-10.07	1.39	1.52
3	D	914	ALA	CA-CB	-10.03	1.40	1.53
3	D	781	LYS	C-O	-10.00	1.12	1.24
3	D	582	ILE	CB-CG1	-10.00	1.33	1.53
3	D	476	ALA	CA-CB	-10.00	1.37	1.53
3	D	365	GLN	CA-CB	9.99	1.68	1.53
3	D	458	ASN	C-O	-9.99	1.10	1.23
2	C	514	PHE	C-O	9.98	1.36	1.23
2	C	1211	ARG	N-CA	9.98	1.58	1.46
2	C	521	LEU	N-CA	-9.95	1.34	1.46
3	D	770	LEU	C-O	9.92	1.35	1.24
2	C	1301	ARG	CZ-NH2	-9.91	1.20	1.33
1	A	129	VAL	C-O	-9.91	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	921	GLN	CD-OE1	9.89	1.42	1.23
1	A	178	SER	C-O	-9.88	1.11	1.24
2	C	667	LEU	C-O	9.87	1.37	1.24
2	C	1184	THR	N-CA	9.84	1.58	1.46
2	C	821	ARG	N-CA	-9.80	1.34	1.46
3	D	885	VAL	N-CA	9.77	1.58	1.46
1	A	41	ASN	C-O	9.74	1.35	1.24
2	C	551	HIS	CA-C	9.73	1.65	1.52
2	C	701	GLY	C-O	9.72	1.33	1.23
3	D	1323	ALA	CA-C	-9.72	1.40	1.52
3	D	506	VAL	C-O	9.71	1.35	1.24
3	D	468	VAL	C-O	9.70	1.33	1.24
3	D	784	ALA	C-O	-9.69	1.10	1.24
2	C	1277	ALA	CA-CB	-9.67	1.37	1.53
3	D	366	CYS	CA-C	-9.63	1.39	1.52
3	D	916	GLY	C-O	9.63	1.36	1.23
2	C	1334	GLY	C-O	9.60	1.36	1.23
3	D	501	VAL	N-CA	-9.60	1.34	1.46
1	A	96	ASP	C-O	-9.60	1.11	1.24
3	D	440	VAL	C-O	9.60	1.33	1.24
2	C	1247	SER	CA-C	-9.59	1.46	1.52
2	C	520	PRO	C-O	9.56	1.37	1.24
2	C	1248	THR	C-O	9.55	1.34	1.23
2	C	1096	ILE	N-CA	9.54	1.58	1.46
2	C	1111	GLN	N-CA	-9.54	1.35	1.46
2	C	700	VAL	CA-C	9.53	1.64	1.52
3	D	742	GLY	C-O	-9.53	1.12	1.24
3	D	460	ASP	CA-C	-9.52	1.41	1.53
2	C	1264	GLN	C-O	9.52	1.35	1.24
2	C	522	SER	N-CA	-9.51	1.34	1.46
2	C	1268	GLN	CA-CB	9.51	1.69	1.53
2	C	765	ILE	N-CA	9.51	1.58	1.46
2	C	811	ASN	CA-C	-9.51	1.41	1.52
2	C	138	ILE	C-O	9.50	1.34	1.24
3	D	365	GLN	CD-OE1	9.45	1.41	1.23
3	D	469	HIS	C-O	9.44	1.35	1.23
3	D	783	LEU	C-O	9.41	1.35	1.24
3	D	899	TYR	CA-CB	9.40	1.69	1.53
3	D	1248	ILE	C-O	9.39	1.33	1.24
2	C	1313	HIS	N-CA	9.32	1.58	1.46
3	D	483	LEU	CA-C	-9.30	1.40	1.52
1	A	51	MET	C-O	9.29	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	722	ILE	C-O	9.29	1.35	1.24
1	A	85	LEU	CA-C	-9.27	1.39	1.52
3	D	917	VAL	C-O	9.25	1.36	1.24
2	C	512	SER	C-O	9.24	1.34	1.24
2	C	765	ILE	CA-C	-9.23	1.40	1.52
2	C	1274	GLU	CA-C	-9.22	1.40	1.52
2	C	1277	ALA	C-O	9.22	1.35	1.24
2	C	1325	VAL	N-CA	-9.22	1.35	1.46
3	D	372	MET	C-O	-9.21	1.12	1.24
5	M	186	ASP	CA-C	-9.20	1.42	1.52
3	D	1352	ILE	C-O	-9.19	1.13	1.24
3	D	423	LEU	CA-C	-9.18	1.42	1.52
3	D	629	PHE	N-CA	-9.18	1.35	1.46
2	C	769	PRO	CA-CB	-9.17	1.41	1.53
2	C	1101	LEU	C-O	9.16	1.35	1.24
3	D	888	CYS	C-O	9.16	1.35	1.24
4	E	13	ILE	C-O	9.15	1.33	1.24
2	C	555	TYR	CE2-CZ	9.12	1.60	1.38
2	C	1322	SER	N-CA	-9.12	1.35	1.46
3	D	351	GLY	N-CA	9.10	1.55	1.44
2	C	777	VAL	C-O	9.09	1.33	1.24
3	D	921	GLN	CD-NE2	9.08	1.52	1.33
4	E	26	ARG	C-O	-9.07	1.12	1.24
2	C	557	ARG	N-CA	-9.07	1.34	1.46
2	C	800	MET	CA-CB	9.06	1.69	1.53
2	C	828	PHE	N-CA	9.06	1.57	1.46
2	C	1270	PHE	CA-CB	-9.06	1.37	1.53
3	D	351	GLY	C-O	9.06	1.33	1.23
2	C	548	ARG	CA-CB	9.05	1.67	1.53
3	D	539	SER	C-O	-9.05	1.14	1.24
2	C	525	THR	CA-C	-9.05	1.40	1.52
3	D	334	LYS	CA-CB	-9.04	1.38	1.53
3	D	360	TYR	CG-CD2	9.04	1.58	1.39
2	C	1232	MET	CA-C	-8.98	1.41	1.52
3	D	92	VAL	CA-C	8.98	1.64	1.52
3	D	582	ILE	CA-C	8.98	1.65	1.52
2	C	1239	VAL	N-CA	8.97	1.58	1.46
2	C	526	HIS	N-CA	8.96	1.57	1.46
2	C	803	ALA	CA-C	-8.92	1.41	1.52
3	D	514	THR	CA-CB	-8.92	1.41	1.53
3	D	104	HIS	CA-C	-8.92	1.41	1.52
3	D	445	LYS	N-CA	-8.91	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	705	GLU	C-O	8.88	1.35	1.24
2	C	1192	GLU	N-CA	8.88	1.57	1.46
2	C	808	ASN	CA-C	8.81	1.65	1.53
2	C	687	ARG	N-CA	-8.80	1.35	1.46
2	C	12	ARG	N-CA	8.79	1.57	1.45
3	D	1336	ALA	CA-C	-8.78	1.41	1.52
3	D	1277	GLY	N-CA	8.76	1.58	1.45
1	A	133	LEU	N-CA	-8.74	1.35	1.46
2	C	1323	PHE	N-CA	8.74	1.57	1.46
1	A	56	VAL	CA-CB	-8.73	1.45	1.54
3	D	443	GLU	C-O	8.73	1.34	1.24
2	C	29	SER	C-O	8.71	1.34	1.24
2	C	1181	PRO	C-O	-8.71	1.06	1.23
2	C	839	VAL	C-O	8.70	1.32	1.24
2	C	815	SER	CA-CB	-8.68	1.40	1.53
2	C	704	MET	CA-C	8.66	1.64	1.52
2	C	1096	ILE	CB-CG1	-8.63	1.36	1.53
2	C	1295	SER	CA-CB	8.62	1.68	1.53
1	B	38	THR	C-O	8.62	1.33	1.24
3	D	761	ALA	CA-C	8.61	1.62	1.52
2	C	673	HIS	CA-C	8.60	1.64	1.52
3	D	599	LYS	C-O	8.60	1.33	1.24
2	C	1246	ARG	NE-CZ	8.59	1.42	1.33
2	C	177	ILE	CA-CB	8.58	1.60	1.54
2	C	1107	MET	N-CA	8.57	1.58	1.46
2	C	655	VAL	C-O	8.57	1.34	1.24
2	C	819	SER	CA-C	-8.56	1.41	1.52
3	D	917	VAL	N-CA	-8.55	1.35	1.46
1	A	204	GLU	C-O	8.53	1.34	1.24
3	D	491	LEU	C-O	8.52	1.35	1.23
3	D	434	ILE	C-O	-8.51	1.15	1.24
1	A	151	GLY	C-O	-8.49	1.12	1.23
2	C	97	ARG	C-O	-8.48	1.13	1.24
3	D	64	PRO	CA-C	-8.47	1.43	1.53
3	D	809	VAL	C-O	-8.45	1.14	1.24
3	D	1321	SER	CB-OG	8.45	1.59	1.42
3	D	337	ARG	NE-CZ	-8.43	1.23	1.33
2	C	934	PHE	C-O	-8.43	1.13	1.23
5	M	152	GLY	C-O	-8.42	1.12	1.23
2	C	685	MET	C-O	-8.42	1.13	1.24
2	C	757	THR	CA-C	-8.40	1.42	1.52
3	D	914	ALA	C-N	-8.39	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1058	ARG	CA-C	8.38	1.62	1.52
1	B	197	ASP	C-O	8.37	1.34	1.24
2	C	1275	VAL	C-O	8.36	1.33	1.24
2	C	1047	LEU	C-O	-8.36	1.13	1.24
2	C	1239	VAL	CA-C	8.36	1.65	1.52
2	C	1273	MET	CA-CB	-8.36	1.39	1.53
3	D	424	ASN	CG-ND2	8.35	1.50	1.33
3	D	638	SER	C-O	-8.34	1.13	1.24
2	C	916	SER	C-O	-8.34	1.13	1.24
2	C	1240	ASP	N-CA	-8.34	1.35	1.46
3	D	1321	SER	C-O	8.34	1.35	1.23
3	D	374	LEU	N-CA	8.33	1.56	1.46
3	D	336	GLY	C-O	-8.31	1.13	1.23
2	C	1229	TYR	CA-CB	8.29	1.63	1.53
5	M	153	TYR	CA-CB	8.29	1.67	1.53
3	D	521	LYS	CA-CB	8.29	1.67	1.53
3	D	806	ASP	CB-CG	8.28	1.72	1.52
2	C	669	PRO	CA-C	-8.27	1.42	1.52
2	C	819	SER	N-CA	8.27	1.56	1.46
3	D	763	PHE	CG-CD2	8.27	1.56	1.38
1	A	225	ALA	C-O	-8.26	1.14	1.24
2	C	1227	VAL	N-CA	8.26	1.56	1.46
3	D	456	ALA	CA-C	-8.26	1.42	1.52
3	D	841	GLY	N-CA	8.25	1.58	1.45
3	D	902	ASP	C-O	8.25	1.34	1.24
2	C	706	ARG	C-O	8.24	1.33	1.24
3	D	372	MET	CA-C	-8.24	1.41	1.52
2	C	653	MET	C-O	8.22	1.33	1.23
3	D	452	LEU	C-O	8.22	1.34	1.24
2	C	811	ASN	CG-OD1	8.21	1.39	1.23
3	D	484	MET	N-CA	8.21	1.56	1.46
3	D	40	LYS	N-CA	8.20	1.56	1.45
2	C	521	LEU	CA-C	8.18	1.63	1.52
3	D	585	LYS	C-O	8.17	1.34	1.24
3	D	798	ARG	CD-NE	8.17	1.57	1.46
2	C	755	LYS	CA-CB	-8.16	1.41	1.53
3	D	112	ALA	CA-CB	8.16	1.65	1.53
3	D	1319	PHE	CG-CD1	8.16	1.55	1.38
1	A	70	THR	N-CA	8.16	1.55	1.45
3	D	406	ALA	C-O	-8.15	1.13	1.24
3	D	444	GLY	N-CA	8.14	1.54	1.45
3	D	92	VAL	C-O	-8.13	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1330	ARG	C-O	8.13	1.33	1.24
3	D	434	ILE	CA-CB	-8.11	1.44	1.54
2	C	1231	TYR	CA-CB	8.11	1.64	1.53
3	D	763	PHE	CG-CD1	8.10	1.55	1.38
2	C	818	VAL	C-O	-8.09	1.16	1.24
2	C	850	ILE	CA-C	8.07	1.62	1.52
3	D	900	GLY	C-O	-8.07	1.12	1.24
2	C	801	ARG	C-O	8.06	1.33	1.24
3	D	436	ALA	C-O	8.06	1.34	1.23
2	C	1069	ARG	CZ-NH1	8.06	1.44	1.32
1	A	211	ILE	CA-CB	8.06	1.64	1.54
2	C	727	VAL	CA-C	-8.06	1.43	1.52
2	C	552	PRO	CA-CB	-8.05	1.40	1.53
3	D	119	SER	N-CA	8.05	1.56	1.46
3	D	620	PHE	C-O	8.05	1.33	1.24
2	C	590	PRO	N-CA	8.04	1.54	1.46
3	D	519	ASN	C-O	-8.04	1.17	1.24
3	D	360	TYR	CA-CB	-8.03	1.40	1.53
3	D	422	LEU	CA-CB	8.02	1.69	1.53
1	A	205	MET	C-O	-8.02	1.14	1.23
3	D	841	GLY	C-O	8.02	1.33	1.24
2	C	1214	ASP	C-O	-8.01	1.14	1.23
3	D	501	VAL	C-N	8.01	1.43	1.33
2	C	458	GLU	C-O	8.00	1.33	1.24
3	D	419	HIS	CA-C	8.00	1.62	1.52
2	C	810	TYR	CA-C	-7.99	1.41	1.52
3	D	545	HIS	N-CA	-7.99	1.36	1.46
3	D	488	ASN	C-O	7.99	1.33	1.24
3	D	455	ALA	CA-C	-7.98	1.43	1.52
3	D	794	GLY	N-CA	-7.98	1.35	1.45
2	C	701	GLY	CA-C	-7.97	1.43	1.51
2	C	1172	LEU	CA-C	-7.97	1.42	1.52
2	C	550	VAL	CA-CB	7.97	1.63	1.53
2	C	724	VAL	C-O	-7.96	1.15	1.23
3	D	549	LYS	C-O	-7.95	1.14	1.24
5	M	186	ASP	N-CA	7.95	1.53	1.46
3	D	361	LEU	C-O	-7.94	1.14	1.24
3	D	787	ALA	C-O	7.91	1.33	1.24
4	E	28	ARG	CA-C	-7.90	1.42	1.52
2	C	1283	ALA	N-CA	-7.90	1.35	1.46
3	D	423	LEU	N-CA	7.88	1.55	1.45
2	C	672	GLU	CA-CB	-7.86	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	690	VAL	CA-CB	7.84	1.64	1.54
3	D	366	CYS	N-CA	7.84	1.56	1.46
3	D	912	GLY	CA-C	7.84	1.62	1.51
3	D	1256	ILE	CA-C	7.83	1.62	1.52
2	C	694	ARG	C-O	7.82	1.33	1.24
1	A	224	LEU	CA-C	-7.81	1.42	1.52
3	D	909	ILE	CA-CB	-7.81	1.45	1.54
2	C	1268	GLN	N-CA	7.80	1.56	1.46
2	C	1316	GLU	N-CA	7.80	1.57	1.46
2	C	687	ARG	CA-CB	7.79	1.66	1.53
2	C	1077	SER	N-CA	-7.78	1.36	1.46
3	D	325	LYS	CA-C	-7.77	1.43	1.52
2	C	1226	THR	C-O	7.76	1.33	1.24
3	D	1252	HIS	C-O	7.76	1.33	1.24
3	D	365	GLN	CG-CD	-7.76	1.32	1.52
2	C	689	ALA	CA-C	-7.75	1.42	1.53
4	E	40	PRO	C-O	-7.75	1.14	1.23
3	D	720	ASN	CA-C	-7.75	1.43	1.52
2	C	1295	SER	C-O	-7.72	1.14	1.24
3	D	105	ILE	CA-CB	7.72	1.66	1.54
2	C	731	ARG	CA-CB	7.72	1.66	1.53
2	C	1115	THR	CA-C	-7.72	1.43	1.52
3	D	419	HIS	CA-CB	-7.71	1.41	1.53
2	C	1123	GLY	C-O	7.71	1.33	1.23
3	D	422	LEU	N-CA	7.70	1.55	1.46
2	C	1333	LEU	C-O	-7.69	1.14	1.23
2	C	510	GLN	CA-C	7.69	1.62	1.52
2	C	726	TYR	CA-C	-7.68	1.42	1.52
3	D	922	SER	CA-C	7.68	1.62	1.52
3	D	430	HIS	CA-C	-7.68	1.42	1.53
2	C	591	TYR	CA-C	-7.68	1.43	1.52
2	C	1215	GLY	CA-C	-7.66	1.41	1.51
2	C	502	VAL	CA-CB	7.66	1.63	1.54
3	D	717	VAL	C-O	-7.66	1.16	1.24
3	D	514	THR	C-O	-7.64	1.14	1.23
3	D	465	GLN	C-O	7.63	1.33	1.23
3	D	483	LEU	N-CA	7.63	1.56	1.46
3	D	924	GLY	N-CA	-7.63	1.34	1.45
3	D	1357	ILE	C-O	-7.63	1.14	1.24
3	D	1315	ALA	CA-C	7.61	1.64	1.52
3	D	363	LEU	N-CA	-7.61	1.36	1.46
2	C	1278	LEU	C-O	7.61	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	681	MET	CA-CB	7.60	1.65	1.53
2	C	1210	ILE	CA-CB	7.60	1.66	1.55
2	C	1267	GLY	C-N	-7.60	1.23	1.33
3	D	766	GLY	N-CA	7.59	1.55	1.45
2	C	1222	GLU	N-CA	7.59	1.55	1.46
3	D	354	VAL	CA-C	7.59	1.62	1.52
3	D	823	THR	C-O	-7.59	1.14	1.24
3	D	619	ILE	C-O	7.55	1.33	1.24
2	C	1229	TYR	C-O	-7.55	1.15	1.24
1	A	229	GLU	N-CA	-7.55	1.36	1.46
2	C	668	ILE	CA-CB	-7.54	1.46	1.53
1	A	65	LEU	N-CA	-7.52	1.36	1.46
2	C	822	VAL	CA-C	7.52	1.62	1.52
2	C	1049	ILE	N-CA	7.52	1.55	1.46
2	C	1257	GLN	CA-C	-7.51	1.43	1.52
2	C	1222	GLU	CA-C	-7.50	1.43	1.52
2	C	1259	LEU	C-O	-7.50	1.13	1.23
3	D	910	ASN	N-CA	7.50	1.54	1.45
2	C	682	GLY	CA-C	7.50	1.60	1.52
2	C	677	ASN	CB-CG	-7.50	1.33	1.52
2	C	885	GLY	N-CA	7.49	1.52	1.44
2	C	674	ASP	N-CA	-7.48	1.37	1.45
3	D	488	ASN	CG-OD1	7.48	1.37	1.23
3	D	442	ILE	CA-C	-7.48	1.43	1.52
2	C	697	LYS	C-O	7.47	1.33	1.23
3	D	482	ALA	C-O	7.47	1.34	1.23
2	C	875	ALA	CA-C	-7.47	1.43	1.52
3	D	588	PRO	N-CA	-7.46	1.37	1.47
3	D	628	GLY	N-CA	7.46	1.56	1.45
3	D	1141	VAL	C-O	7.46	1.32	1.24
2	C	827	ARG	C-O	7.46	1.33	1.23
2	C	1071	GLY	CA-C	7.46	1.62	1.51
2	C	1284	ALA	C-O	7.46	1.34	1.24
2	C	791	LEU	C-O	7.45	1.32	1.23
2	C	1225	VAL	C-N	7.45	1.44	1.33
2	C	764	CYS	CA-CB	7.45	1.65	1.53
2	C	1069	ARG	C-O	7.45	1.33	1.24
2	C	137	VAL	C-O	7.45	1.32	1.24
1	A	177	TYR	N-CA	7.44	1.55	1.46
3	D	358	GLY	CA-C	7.44	1.62	1.51
2	C	1199	LEU	C-O	-7.43	1.14	1.24
1	A	50	SER	C-O	-7.43	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1108	ASN	CB-CG	7.43	1.70	1.52
3	D	633	ALA	CA-C	-7.40	1.43	1.52
3	D	437	PHE	CA-CB	7.40	1.67	1.53
2	C	1279	GLU	CA-C	-7.39	1.43	1.52
3	D	1356	LEU	N-CA	7.39	1.55	1.45
2	C	1114	GLU	C-O	7.38	1.32	1.24
3	D	519	ASN	CA-C	7.38	1.59	1.52
2	C	1321	GLU	CA-CB	7.38	1.65	1.53
2	C	1209	GLN	CA-C	7.37	1.61	1.52
2	C	518	ASN	CA-C	-7.37	1.43	1.52
2	C	568	ASN	C-O	-7.35	1.15	1.23
2	C	690	VAL	N-CA	7.35	1.55	1.46
3	D	907	HIS	C-O	-7.35	1.14	1.23
2	C	822	VAL	C-O	7.34	1.32	1.24
2	C	1244	HIS	CG-CD2	7.34	1.44	1.35
1	A	47	LEU	N-CA	-7.33	1.37	1.46
2	C	668	ILE	C-O	-7.33	1.15	1.24
2	C	1179	GLY	C-O	7.33	1.33	1.23
2	C	808	ASN	N-CA	-7.33	1.35	1.46
2	C	1158	LYS	N-CA	-7.33	1.36	1.46
2	C	1283	ALA	CA-C	-7.32	1.43	1.53
1	A	31	LEU	C-O	-7.32	1.14	1.23
2	C	451	ARG	C-O	-7.31	1.15	1.24
3	D	883	ARG	CA-C	-7.30	1.43	1.52
2	C	710	VAL	CA-CB	-7.30	1.43	1.54
2	C	1231	TYR	CG-CD2	-7.30	1.24	1.39
3	D	777	HIS	N-CA	7.30	1.55	1.46
2	C	10	ARG	CA-C	-7.30	1.44	1.52
2	C	1098	LEU	C-O	-7.30	1.14	1.23
3	D	335	GLN	CD-NE2	-7.30	1.18	1.33
2	C	522	SER	CA-C	7.29	1.63	1.52
3	D	899	TYR	CG-CD1	7.29	1.54	1.39
2	C	815	SER	N-CA	7.29	1.55	1.45
2	C	832	HIS	C-O	7.29	1.33	1.24
3	D	96	LYS	N-CA	-7.29	1.36	1.46
3	D	1258	ARG	CA-C	-7.29	1.43	1.52
3	D	553	THR	C-O	7.28	1.32	1.23
3	D	1359	ALA	C-O	-7.28	1.15	1.23
3	D	629	PHE	C-O	7.28	1.32	1.24
2	C	838	CYS	N-CA	7.27	1.54	1.46
3	D	510	LEU	CA-CB	7.26	1.64	1.53
5	M	127	GLN	CD-NE2	7.26	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	ASP	C-O	7.23	1.33	1.24
3	D	359	PRO	N-CA	7.23	1.56	1.47
2	C	689	ALA	N-CA	7.22	1.55	1.45
2	C	1215	GLY	N-CA	-7.22	1.34	1.45
5	M	127	GLN	CG-CD	-7.22	1.33	1.52
2	C	551	HIS	C-O	7.22	1.33	1.23
2	C	526	HIS	CA-CB	-7.22	1.41	1.53
3	D	349	TYR	C-O	7.21	1.33	1.24
2	C	516	ASP	C-O	-7.21	1.15	1.24
2	C	589	THR	CA-CB	7.21	1.64	1.54
2	C	1086	PRO	CA-C	-7.20	1.42	1.52
2	C	38	PHE	CG-CD2	7.19	1.53	1.38
1	B	198	LEU	CA-CB	-7.18	1.44	1.53
3	D	305	ALA	C-O	-7.18	1.14	1.24
3	D	601	ILE	CB-CG1	7.18	1.67	1.53
3	D	488	ASN	CG-ND2	7.18	1.48	1.33
2	C	558	VAL	C-O	-7.16	1.15	1.24
1	A	80	GLU	CA-C	7.16	1.62	1.52
3	D	632	ALA	N-CA	7.15	1.55	1.46
2	C	657	THR	C-O	7.15	1.33	1.24
2	C	1054	LEU	CA-C	7.13	1.61	1.52
2	C	1229	TYR	CA-C	7.12	1.62	1.52
3	D	1365	TYR	CA-C	7.12	1.62	1.52
2	C	157	PHE	N-CA	7.12	1.54	1.45
2	C	762	ASN	CA-CB	-7.12	1.42	1.53
3	D	332	LYS	N-CA	7.12	1.56	1.46
3	D	365	GLN	CA-C	-7.12	1.43	1.53
3	D	1331	VAL	C-O	7.12	1.32	1.24
3	D	494	ALA	N-CA	-7.11	1.37	1.46
3	D	839	VAL	C-O	-7.11	1.16	1.24
2	C	928	VAL	CA-C	-7.11	1.44	1.52
2	C	1095	ASP	CA-C	-7.11	1.43	1.52
2	C	527	LYS	CA-C	7.11	1.62	1.52
2	C	531	SER	N-CA	7.10	1.54	1.46
2	C	1244	HIS	CA-C	7.09	1.57	1.52
3	D	368	LEU	N-CA	7.09	1.58	1.45
2	C	12	ARG	CZ-NH2	-7.08	1.24	1.33
1	A	37	HIS	N-CA	-7.08	1.37	1.46
3	D	725	MET	CA-CB	-7.08	1.42	1.53
2	C	659	GLN	C-O	7.07	1.32	1.24
3	D	459	ALA	CA-C	7.06	1.60	1.52
3	D	94	GLN	N-CA	7.05	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1363	TYR	CA-C	-7.05	1.43	1.52
2	C	1070	HIS	CA-CB	-7.05	1.42	1.53
3	D	1364	ALA	N-CA	7.05	1.54	1.46
3	D	359	PRO	CG-CD	7.04	1.74	1.50
3	D	764	ARG	C-O	7.04	1.32	1.24
2	C	1172	LEU	C-O	7.04	1.32	1.24
3	D	342	LEU	CA-CB	7.04	1.65	1.53
2	C	1293	VAL	C-O	-7.02	1.15	1.24
3	D	363	LEU	C-O	7.01	1.32	1.24
2	C	587	LEU	N-CA	7.00	1.54	1.46
2	C	531	SER	C-O	7.00	1.32	1.24
2	C	30	ILE	CA-CB	-7.00	1.44	1.54
1	A	60	GLU	CA-C	-7.00	1.43	1.52
3	D	623	GLN	N-CA	-7.00	1.37	1.46
2	C	1257	GLN	C-O	7.00	1.31	1.24
3	D	376	LEU	C-O	7.00	1.32	1.24
2	C	1103	VAL	N-CA	-6.99	1.38	1.46
3	D	739	GLN	C-O	-6.99	1.15	1.24
2	C	666	SER	C-O	6.98	1.33	1.24
2	C	68	LEU	C-O	-6.97	1.15	1.23
3	D	491	LEU	CA-C	6.97	1.61	1.52
2	C	1212	LEU	CB-CG	-6.96	1.39	1.53
3	D	794	GLY	CA-C	-6.96	1.42	1.51
2	C	145	ILE	N-CA	6.96	1.55	1.46
2	C	765	ILE	C-O	6.96	1.31	1.24
3	D	536	LEU	CB-CG	6.94	1.67	1.53
2	C	1334	GLY	N-CA	6.94	1.55	1.45
3	D	94	GLN	CA-CB	6.94	1.65	1.53
2	C	145	ILE	C-O	-6.93	1.16	1.24
3	D	111	THR	C-O	-6.92	1.15	1.23
3	D	412	LEU	CA-CB	-6.92	1.42	1.53
3	D	891	ASP	N-CA	6.92	1.55	1.46
2	C	146	VAL	CA-C	-6.92	1.43	1.52
3	D	626	TYR	CG-CD2	6.92	1.53	1.39
2	C	453	ILE	CB-CG1	-6.91	1.39	1.53
2	C	761	GLN	CD-NE2	6.91	1.47	1.33
3	D	577	ALA	CA-C	-6.91	1.44	1.52
3	D	602	SER	N-CA	6.91	1.54	1.46
3	D	798	ARG	C-O	-6.90	1.16	1.24
2	C	759	SER	CB-OG	6.90	1.55	1.42
3	D	471	PRO	C-N	6.90	1.40	1.33
3	D	513	MET	C-O	6.90	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	518	VAL	C-O	6.90	1.33	1.24
3	D	271	ARG	C-O	6.89	1.32	1.24
2	C	818	VAL	CA-C	-6.89	1.44	1.52
2	C	1230	MET	CA-C	-6.89	1.44	1.52
3	D	490	ILE	N-CA	-6.89	1.36	1.46
2	C	1119	MET	CG-SD	6.89	1.98	1.80
3	D	706	VAL	C-O	6.88	1.31	1.24
2	C	1159	VAL	CA-C	-6.88	1.43	1.52
2	C	787	PRO	CA-CB	6.88	1.63	1.54
2	C	176	ILE	CA-C	6.88	1.60	1.52
3	D	783	LEU	CA-C	-6.88	1.44	1.52
3	D	534	GLU	CA-C	-6.87	1.43	1.52
3	D	834	PRO	CA-C	-6.87	1.44	1.52
3	D	351	GLY	CA-C	-6.87	1.43	1.51
2	C	808	ASN	C-O	6.87	1.33	1.23
2	C	810	TYR	CE2-CZ	6.86	1.54	1.38
2	C	576	SER	CA-CB	-6.86	1.42	1.53
2	C	1296	ASP	CG-OD1	-6.86	1.12	1.25
3	D	17	PHE	N-CA	-6.86	1.36	1.45
2	C	1148	ALA	CA-C	-6.85	1.44	1.52
3	D	543	SER	CA-CB	6.84	1.66	1.53
2	C	1283	ALA	C-O	6.84	1.31	1.23
3	D	807	LEU	CA-C	6.84	1.61	1.52
2	C	1218	GLY	N-CA	6.83	1.55	1.45
1	A	63	GLY	CA-C	6.82	1.61	1.51
2	C	1086	PRO	C-O	6.82	1.31	1.23
3	D	19	ALA	C-N	-6.82	1.24	1.33
2	C	1297	ASP	C-O	6.82	1.32	1.24
2	C	666	SER	CB-OG	6.81	1.55	1.42
3	D	515	ARG	CZ-NH1	-6.81	1.23	1.32
3	D	1180	VAL	C-O	-6.81	1.16	1.24
3	D	466	MET	N-CA	6.80	1.54	1.46
3	D	470	VAL	CA-C	-6.80	1.47	1.53
2	C	530	ILE	C-O	6.79	1.31	1.24
5	M	127	GLN	CD-OE1	6.79	1.36	1.23
2	C	458	GLU	N-CA	-6.78	1.38	1.46
2	C	1188	ASP	N-CA	6.78	1.54	1.46
2	C	782	VAL	C-O	-6.78	1.17	1.24
3	D	803	VAL	CA-C	-6.77	1.43	1.52
2	C	754	THR	CA-C	-6.77	1.44	1.52
3	D	20	ILE	CA-CB	6.76	1.63	1.54
2	C	656	SER	N-CA	6.75	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	812	PHE	C-O	6.75	1.32	1.23
3	D	90	VAL	C-O	-6.74	1.17	1.23
3	D	1214	PRO	CA-C	-6.74	1.44	1.52
1	A	66	HIS	C-O	6.74	1.32	1.24
3	D	512	TYR	C-O	-6.73	1.15	1.24
1	A	41	ASN	N-CA	-6.71	1.38	1.46
3	D	328	ALA	CA-C	-6.71	1.44	1.52
2	C	537	GLY	C-O	-6.71	1.13	1.23
3	D	640	GLY	N-CA	6.71	1.51	1.45
3	D	438	GLU	C-N	6.70	1.41	1.33
2	C	781	ASP	C-O	6.70	1.32	1.23
3	D	895	CYS	C-O	6.69	1.32	1.23
2	C	1288	GLN	CA-C	-6.69	1.43	1.52
2	C	1054	LEU	C-O	6.69	1.32	1.23
3	D	484	MET	CA-C	6.68	1.62	1.52
2	C	566	GLY	C-O	-6.68	1.15	1.24
3	D	479	GLU	CD-OE1	6.68	1.38	1.25
2	C	1111	GLN	CD-NE2	6.68	1.47	1.33
2	C	1298	VAL	CA-C	6.68	1.60	1.52
3	D	482	ALA	N-CA	-6.68	1.37	1.46
3	D	439	PRO	C-O	6.67	1.31	1.23
3	D	361	LEU	CA-C	-6.67	1.43	1.52
3	D	476	ALA	N-CA	-6.67	1.38	1.46
2	C	12	ARG	C-O	6.67	1.32	1.23
2	C	1288	GLN	CD-OE1	6.67	1.36	1.23
2	C	734	ILE	CA-C	-6.66	1.44	1.52
2	C	1157	GLN	C-O	6.66	1.32	1.24
2	C	145	ILE	CB-CG1	-6.66	1.40	1.53
3	D	364	HIS	C-O	6.66	1.32	1.24
2	C	733	VAL	N-CA	6.66	1.54	1.46
1	A	74	VAL	CA-CB	-6.65	1.46	1.54
2	C	1097	VAL	C-O	-6.65	1.17	1.24
2	C	1081	PRO	C-O	6.65	1.32	1.24
3	D	615	LYS	CA-C	6.64	1.60	1.52
1	A	38	THR	C-O	6.63	1.31	1.24
2	C	1094	VAL	CA-CB	-6.63	1.47	1.54
2	C	840	SER	N-CA	6.63	1.54	1.46
3	D	767	LEU	C-O	-6.63	1.15	1.24
3	D	338	PHE	N-CA	-6.62	1.38	1.46
2	C	572	ILE	C-O	6.62	1.31	1.24
3	D	1355	ARG	CZ-NH2	6.62	1.42	1.33
2	C	1082	ILE	C-O	6.62	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	577	ALA	N-CA	-6.62	1.38	1.46
2	C	32	LEU	N-CA	6.61	1.54	1.46
2	C	733	VAL	C-O	-6.60	1.16	1.24
3	D	268	LEU	N-CA	-6.60	1.38	1.46
2	C	555	TYR	CG-CD1	6.59	1.53	1.39
2	C	514	PHE	N-CA	6.59	1.54	1.46
2	C	145	ILE	CA-C	6.58	1.60	1.52
2	C	693	LEU	N-CA	6.58	1.54	1.46
2	C	691	PRO	C-O	6.58	1.30	1.23
3	D	405	GLU	N-CA	-6.58	1.37	1.45
3	D	633	ALA	C-O	-6.57	1.16	1.24
2	C	130	MET	C-O	6.57	1.32	1.24
2	C	1219	GLU	C-O	-6.57	1.16	1.23
3	D	335	GLN	CA-CB	-6.57	1.42	1.53
2	C	875	ALA	N-CA	6.56	1.54	1.46
3	D	1256	ILE	C-O	6.56	1.31	1.24
2	C	1182	ILE	CA-CB	-6.56	1.46	1.54
2	C	1279	GLU	C-O	6.56	1.31	1.24
2	C	510	GLN	N-CA	-6.55	1.38	1.46
3	D	499	ILE	N-CA	6.55	1.54	1.46
3	D	842	ARG	CG-CD	6.54	1.72	1.52
3	D	859	PRO	CA-C	-6.54	1.46	1.52
2	C	1226	THR	N-CA	6.52	1.54	1.46
3	D	621	ALA	C-O	6.52	1.31	1.24
2	C	1328	LYS	CA-C	-6.51	1.43	1.52
2	C	456	VAL	CA-CB	-6.51	1.45	1.54
3	D	621	ALA	CA-C	-6.51	1.44	1.52
3	D	924	GLY	CA-C	-6.50	1.42	1.51
1	B	204	GLU	CA-C	-6.50	1.44	1.52
3	D	781	LYS	N-CA	6.50	1.54	1.46
2	C	1046	VAL	CA-C	-6.50	1.44	1.52
1	A	153	VAL	N-CA	-6.49	1.41	1.46
2	C	787	PRO	CA-C	6.49	1.59	1.52
3	D	693	VAL	C-O	6.49	1.31	1.24
3	D	1248	ILE	CA-C	-6.49	1.44	1.52
2	C	1276	TRP	CD2-CE3	6.49	1.50	1.40
2	C	677	ASN	CG-OD1	6.48	1.35	1.23
3	D	859	PRO	C-O	-6.47	1.15	1.23
2	C	1303	LYS	C-O	6.47	1.32	1.24
3	D	886	VAL	CA-CB	6.47	1.63	1.54
3	D	352	ARG	C-O	-6.47	1.15	1.23
2	C	567	PRO	C-O	-6.46	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	19	ALA	CA-C	6.46	1.61	1.52
3	D	598	LYS	CA-CB	-6.46	1.43	1.53
1	A	173	VAL	CA-C	-6.46	1.45	1.52
2	C	10	ARG	CG-CD	6.45	1.71	1.52
3	D	918	ILE	CA-CB	-6.45	1.45	1.54
3	D	922	SER	C-O	-6.45	1.16	1.24
3	D	488	ASN	N-CA	6.44	1.54	1.46
3	D	794	GLY	C-O	6.44	1.31	1.24
1	B	18	GLN	CA-C	-6.44	1.44	1.52
3	D	250	ARG	C-O	-6.44	1.16	1.24
2	C	794	LEU	CA-C	-6.43	1.44	1.52
3	D	780	ARG	C-O	6.43	1.31	1.24
2	C	1120	ALA	C-O	6.43	1.32	1.24
2	C	674	ASP	CA-CB	6.43	1.63	1.53
2	C	593	LYS	CA-C	-6.42	1.44	1.52
2	C	932	GLN	C-O	6.42	1.31	1.23
1	A	168	ILE	C-O	6.42	1.31	1.24
2	C	810	TYR	CG-CD2	6.42	1.52	1.39
2	C	801	ARG	CA-C	6.41	1.60	1.52
2	C	1183	ALA	N-CA	6.41	1.54	1.46
3	D	1143	ASP	CA-C	6.41	1.61	1.52
1	B	180	VAL	CA-C	-6.40	1.44	1.52
3	D	469	HIS	CA-C	-6.40	1.44	1.52
3	D	369	PRO	C-O	6.40	1.30	1.23
1	A	61	ILE	C-O	6.40	1.30	1.23
1	A	153	VAL	C-O	-6.40	1.17	1.24
3	D	1333	THR	CA-C	6.39	1.61	1.52
3	D	617	THR	CB-CG2	-6.39	1.31	1.52
1	B	187	VAL	CA-CB	6.39	1.62	1.54
2	C	488	MET	C-O	-6.38	1.18	1.24
3	D	421	VAL	N-CA	6.38	1.56	1.45
2	C	444	ASP	C-O	-6.38	1.16	1.24
2	C	1102	GLY	N-CA	6.38	1.53	1.45
3	D	772	TYR	CA-C	-6.38	1.44	1.52
3	D	431	ARG	CA-CB	-6.37	1.42	1.53
2	C	49	LEU	C-O	6.37	1.32	1.24
2	C	1258	PRO	C-O	-6.37	1.16	1.23
3	D	502	PRO	CA-CB	-6.37	1.45	1.53
3	D	439	PRO	N-CA	-6.36	1.39	1.46
3	D	914	ALA	C-O	6.36	1.30	1.23
2	C	703	GLY	CA-C	-6.35	1.43	1.52
2	C	519	ASN	C-N	-6.35	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	610	ARG	N-CA	6.34	1.53	1.46
2	C	1224	PRO	CA-C	-6.34	1.45	1.53
3	D	630	ALA	CA-C	-6.33	1.44	1.52
3	D	104	HIS	C-O	-6.33	1.16	1.23
3	D	455	ALA	C-O	6.33	1.31	1.24
3	D	1353	VAL	C-O	-6.33	1.15	1.24
2	C	1052	VAL	CA-C	6.33	1.60	1.52
2	C	1176	LEU	C-O	6.33	1.32	1.24
2	C	1081	PRO	CA-C	6.32	1.61	1.52
3	D	461	PHE	C-O	6.32	1.32	1.23
3	D	1356	LEU	C-O	6.31	1.32	1.23
3	D	78	LEU	CA-C	6.31	1.61	1.52
2	C	1264	GLN	C-N	6.30	1.41	1.33
3	D	371	LYS	C-O	-6.30	1.16	1.24
3	D	747	MET	C-O	-6.29	1.16	1.23
2	C	10	ARG	C-O	6.29	1.31	1.23
3	D	408	VAL	N-CA	-6.29	1.39	1.46
3	D	413	ASP	C-O	6.28	1.31	1.24
1	A	76	GLU	N-CA	-6.28	1.37	1.45
2	C	575	LEU	CB-CG	-6.28	1.40	1.53
2	C	1055	ALA	C-O	-6.28	1.16	1.24
3	D	913	GLU	CA-C	-6.27	1.44	1.53
2	C	818	VAL	N-CA	6.27	1.53	1.46
3	D	471	PRO	C-O	6.27	1.30	1.23
2	C	506	PHE	C-O	-6.27	1.16	1.24
2	C	731	ARG	C-O	6.26	1.31	1.23
3	D	1317	GLU	C-O	6.26	1.31	1.24
3	D	1355	ARG	CZ-NH1	-6.25	1.24	1.32
1	A	154	PRO	C-O	6.24	1.31	1.23
2	C	1251	TYR	N-CA	6.24	1.54	1.45
3	D	1249	ASN	N-CA	6.23	1.53	1.45
1	A	45	ARG	CA-C	6.23	1.61	1.52
3	D	514	THR	CA-C	-6.23	1.45	1.53
2	C	734	ILE	N-CA	-6.22	1.39	1.46
2	C	4	SER	CA-C	-6.22	1.45	1.52
2	C	1312	ASN	C-O	6.22	1.31	1.24
3	D	899	TYR	C-O	6.22	1.31	1.24
2	C	677	ASN	C-N	-6.21	1.25	1.33
3	D	1347	LEU	C-O	6.21	1.31	1.24
2	C	1101	LEU	C-N	6.21	1.41	1.33
2	C	1289	GLU	C-O	-6.20	1.16	1.24
3	D	1323	ALA	N-CA	6.20	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	631	TYR	C-O	6.20	1.31	1.24
6	F	-3	DG	P-OP2	6.20	1.60	1.48
3	D	495	ASN	CG-OD1	-6.19	1.11	1.23
3	D	482	ALA	CA-C	-6.18	1.44	1.52
1	A	186	ASN	CA-C	-6.18	1.45	1.52
2	C	772	SER	C-O	6.18	1.31	1.24
3	D	345	LYS	CB-CG	6.18	1.71	1.52
3	D	489	ASN	CG-OD1	-6.18	1.11	1.23
2	C	673	HIS	C-O	6.16	1.31	1.24
2	C	686	GLN	CA-C	6.16	1.61	1.52
3	D	1262	ARG	CA-C	6.16	1.61	1.53
3	D	499	ILE	C-O	-6.16	1.16	1.24
2	C	533	LEU	CA-CB	-6.15	1.44	1.53
3	D	485	MET	C-O	6.15	1.31	1.23
3	D	457	TYR	CE2-CZ	6.15	1.53	1.38
3	D	596	LEU	CA-CB	-6.15	1.45	1.53
1	A	56	VAL	N-CA	6.15	1.54	1.46
5	M	123	TYR	CA-CB	-6.15	1.43	1.53
2	C	1326	LEU	C-O	6.15	1.31	1.24
2	C	1292	THR	N-CA	-6.14	1.38	1.46
3	D	40	LYS	CA-C	-6.14	1.46	1.52
2	C	569	ILE	CA-CB	6.14	1.62	1.54
2	C	700	VAL	C-O	6.14	1.30	1.24
2	C	1240	ASP	CA-C	6.14	1.61	1.52
3	D	731	ARG	CZ-NH1	6.14	1.41	1.32
2	C	95	PRO	C-O	-6.13	1.17	1.23
2	C	1083	GLU	CA-C	6.13	1.61	1.52
2	C	1097	VAL	N-CA	6.13	1.53	1.46
2	C	1216	ARG	CA-CB	-6.13	1.44	1.53
3	D	802	ASP	CB-CG	6.13	1.67	1.52
2	C	702	THR	C-O	-6.12	1.15	1.24
3	D	17	PHE	CA-C	6.12	1.60	1.52
3	D	534	GLU	CD-OE1	6.12	1.36	1.25
3	D	1321	SER	C-N	-6.12	1.25	1.33
2	C	840	SER	CA-C	-6.12	1.45	1.52
3	D	840	LEU	CA-C	-6.12	1.45	1.52
3	D	859	PRO	N-CA	-6.12	1.40	1.46
2	C	818	VAL	CB-CG2	-6.12	1.32	1.52
3	D	246	PRO	CA-CB	-6.11	1.48	1.53
2	C	1170	MET	C-O	6.11	1.31	1.24
3	D	359	PRO	C-N	6.11	1.42	1.33
2	C	1266	GLY	CA-C	-6.11	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	786	THR	CA-C	6.11	1.60	1.52
1	B	36	GLY	C-O	6.11	1.32	1.23
3	D	601	ILE	CA-C	-6.10	1.43	1.52
2	C	1255	THR	CA-CB	6.10	1.63	1.53
1	A	219	ARG	CA-C	-6.09	1.44	1.52
2	C	1335	ILE	CA-C	-6.09	1.45	1.52
3	D	342	LEU	C-O	-6.09	1.16	1.24
2	C	12	ARG	NE-CZ	-6.08	1.26	1.33
2	C	573	ASN	CA-C	-6.08	1.45	1.52
3	D	609	TYR	CA-C	-6.08	1.45	1.52
5	M	191	ALA	CA-CB	6.08	1.63	1.53
2	C	1241	ASP	CA-C	-6.07	1.44	1.52
3	D	807	LEU	CA-CB	-6.07	1.43	1.53
3	D	380	PHE	C-O	6.07	1.31	1.24
2	C	578	TYR	C-O	6.06	1.32	1.23
3	D	1362	GLY	C-N	-6.06	1.26	1.33
3	D	798	ARG	NE-CZ	6.05	1.39	1.33
1	A	88	LEU	C-O	6.05	1.31	1.24
2	C	687	ARG	CG-CD	6.05	1.70	1.52
3	D	339	ARG	N-CA	-6.05	1.38	1.45
1	A	56	VAL	CA-C	6.05	1.62	1.53
2	C	767	GLN	N-CA	6.05	1.53	1.46
2	C	1231	TYR	C-N	6.05	1.41	1.33
3	D	1311	LYS	N-CA	-6.05	1.38	1.46
2	C	443	ASP	C-O	-6.04	1.16	1.23
3	D	19	ALA	C-O	-6.04	1.16	1.24
2	C	128	PRO	CA-C	-6.04	1.44	1.52
2	C	549	ASP	CA-C	-6.04	1.45	1.52
2	C	881	ASP	N-CA	6.04	1.53	1.46
2	C	12	ARG	CA-C	6.03	1.60	1.52
2	C	1237	HIS	CA-CB	6.03	1.60	1.52
2	C	197	ARG	C-O	6.03	1.31	1.24
3	D	746	LEU	C-O	6.03	1.31	1.23
2	C	785	ASP	CA-C	6.03	1.59	1.52
3	D	1140	ARG	CA-C	6.02	1.60	1.52
3	D	378	LYS	CA-C	6.01	1.60	1.52
3	D	472	LEU	N-CA	6.01	1.55	1.45
3	D	1366	HIS	CA-C	-6.01	1.44	1.52
2	C	824	GLN	C-O	-6.01	1.17	1.24
2	C	827	ARG	C-N	-6.00	1.25	1.33
2	C	1087	TYR	CG-CD2	-6.00	1.26	1.39
1	A	43	LEU	N-CA	-6.00	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	ASP	CA-C	6.00	1.61	1.52
2	C	1067	ALA	C-O	6.00	1.30	1.24
3	D	1328	THR	CA-C	-5.99	1.44	1.52
2	C	1081	PRO	CA-CB	-5.98	1.45	1.53
3	D	20	ILE	C-O	-5.98	1.17	1.24
1	A	172	LEU	N-CA	-5.98	1.38	1.45
2	C	548	ARG	CZ-NH1	5.97	1.41	1.32
3	D	337	ARG	C-O	-5.97	1.15	1.24
3	D	1346	GLY	N-CA	5.97	1.49	1.44
3	D	345	LYS	CA-C	5.97	1.60	1.52
1	A	92	VAL	C-O	-5.97	1.16	1.23
2	C	12	ARG	CA-CB	5.96	1.63	1.53
2	C	143	ARG	C-N	-5.96	1.26	1.33
3	D	106	GLU	N-CA	5.95	1.53	1.46
3	D	473	THR	CB-OG1	-5.95	1.34	1.43
1	A	52	PRO	N-CA	-5.95	1.41	1.46
3	D	434	ILE	C-N	-5.95	1.25	1.33
2	C	721	GLY	C-O	-5.95	1.16	1.23
1	B	37	HIS	CA-CB	-5.94	1.44	1.53
2	C	1170	MET	N-CA	-5.94	1.38	1.46
2	C	94	ALA	CA-CB	-5.94	1.45	1.54
3	D	1251	LYS	C-O	5.94	1.31	1.24
2	C	807	TRP	CB-CG	-5.94	1.31	1.50
3	D	334	LYS	N-CA	5.93	1.53	1.46
3	D	923	ILE	N-CA	-5.93	1.39	1.46
3	D	341	ASN	CA-CB	5.92	1.63	1.53
1	A	218	ARG	C-O	5.92	1.30	1.24
2	C	586	PHE	C-O	5.92	1.31	1.23
2	C	768	MET	C-O	-5.92	1.16	1.24
2	C	1115	THR	CA-CB	5.92	1.62	1.53
3	D	763	PHE	CE2-CZ	5.92	1.56	1.38
5	M	152	GLY	N-CA	5.92	1.53	1.45
2	C	1227	VAL	C-O	-5.91	1.17	1.24
2	C	21	VAL	CA-CB	-5.91	1.46	1.54
2	C	1208	GLY	C-O	-5.90	1.16	1.23
3	D	252	LEU	C-O	-5.90	1.16	1.24
3	D	620	PHE	CA-CB	-5.90	1.43	1.53
2	C	1076	ILE	N-CA	-5.89	1.39	1.46
2	C	935	THR	N-CA	5.89	1.53	1.45
3	D	246	PRO	C-O	-5.89	1.20	1.25
3	D	90	VAL	CA-CB	-5.88	1.46	1.53
3	D	1328	THR	C-O	5.88	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	363	LEU	CA-C	5.88	1.60	1.52
2	C	1152	GLY	N-CA	5.86	1.52	1.45
3	D	429	LEU	N-CA	-5.86	1.38	1.46
1	A	35	PHE	C-O	5.86	1.31	1.24
2	C	673	HIS	N-CA	-5.86	1.38	1.46
2	C	1103	VAL	CA-C	5.86	1.59	1.52
2	C	156	PHE	N-CA	5.85	1.53	1.45
2	C	20	GLN	CA-C	-5.85	1.45	1.52
2	C	1281	TYR	CA-C	-5.85	1.44	1.52
3	D	496	GLY	N-CA	5.85	1.53	1.45
3	D	261	ALA	C-O	-5.85	1.17	1.23
3	D	478	LEU	N-CA	-5.84	1.38	1.46
2	C	524	ILE	CA-C	5.84	1.59	1.52
3	D	495	ASN	C-O	5.84	1.31	1.24
3	D	352	ARG	CG-CD	5.83	1.70	1.52
3	D	1308	GLY	C-O	5.83	1.31	1.23
2	C	1216	ARG	CZ-NH2	5.83	1.41	1.33
2	C	1232	MET	C-O	-5.83	1.16	1.23
2	C	547	VAL	N-CA	5.83	1.54	1.46
2	C	685	MET	CG-SD	5.83	1.95	1.80
2	C	15	PHE	C-O	-5.83	1.16	1.24
2	C	563	THR	CA-CB	5.83	1.62	1.54
2	C	694	ARG	N-CA	5.83	1.53	1.46
3	D	913	GLU	C-O	-5.83	1.16	1.23
1	A	184	ALA	CA-C	-5.82	1.45	1.52
1	B	191	ARG	N-CA	5.82	1.53	1.46
2	C	1186	VAL	CA-CB	-5.82	1.46	1.54
1	A	131	CYS	C-N	-5.82	1.26	1.33
4	E	26	ARG	CA-C	-5.82	1.45	1.52
3	D	362	ARG	NE-CZ	5.81	1.39	1.33
2	C	1182	ILE	N-CA	5.81	1.53	1.46
3	D	375	GLU	C-O	5.81	1.31	1.24
3	D	1355	ARG	CA-CB	5.81	1.63	1.53
3	D	493	PRO	CA-CB	-5.81	1.49	1.53
3	D	536	LEU	N-CA	5.81	1.53	1.46
3	D	608	CYS	CA-C	-5.81	1.45	1.52
3	D	1310	THR	CA-C	5.81	1.60	1.53
1	A	69	SER	CA-C	-5.80	1.45	1.53
3	D	516	ASP	C-O	-5.80	1.16	1.23
2	C	1123	GLY	N-CA	-5.79	1.38	1.45
3	D	776	THR	C-O	5.79	1.31	1.24
3	D	930	LEU	CB-CG	5.79	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	719	LYS	C-O	5.79	1.31	1.23
3	D	1326	GLN	N-CA	-5.79	1.38	1.46
3	D	534	GLU	CD-OE2	5.78	1.36	1.25
1	A	155	ALA	CA-C	5.78	1.60	1.52
2	C	729	ALA	C-O	5.78	1.30	1.24
3	D	550	VAL	C-O	-5.78	1.18	1.24
2	C	454	ARG	CZ-NH1	5.78	1.40	1.32
2	C	460	ALA	CA-CB	5.77	1.62	1.53
2	C	1210	ILE	N-CA	5.77	1.52	1.46
2	C	1160	ASP	N-CA	-5.77	1.38	1.45
3	D	25	ALA	N-CA	-5.77	1.39	1.46
2	C	1265	PHE	N-CA	5.76	1.54	1.46
2	C	697	LYS	CB-CG	5.76	1.69	1.52
2	C	93	SER	CA-CB	5.75	1.61	1.53
1	A	45	ARG	CZ-NH2	5.75	1.41	1.33
2	C	573	ASN	N-CA	5.75	1.53	1.45
3	D	613	GLY	N-CA	5.75	1.54	1.45
2	C	696	ASP	CG-OD2	5.75	1.36	1.25
2	C	1118	GLY	N-CA	5.75	1.52	1.45
2	C	793	GLU	CA-C	-5.74	1.45	1.52
2	C	878	THR	CA-C	-5.74	1.45	1.52
3	D	625	MET	C-O	5.74	1.30	1.24
3	D	1252	HIS	N-CA	-5.74	1.39	1.46
3	D	534	GLU	CG-CD	5.74	1.66	1.52
2	C	1122	LYS	C-N	-5.74	1.26	1.33
3	D	404	GLU	C-O	5.74	1.31	1.24
2	C	1261	GLY	N-CA	-5.73	1.39	1.45
3	D	585	LYS	CA-C	-5.73	1.45	1.52
3	D	761	ALA	CA-CB	5.73	1.63	1.53
2	C	538	LEU	N-CA	5.73	1.53	1.46
2	C	1117	LEU	CA-C	-5.73	1.45	1.52
2	C	25	PRO	CA-CB	-5.73	1.45	1.53
4	E	52	ARG	CA-C	-5.73	1.45	1.52
2	C	1110	GLY	CA-C	-5.72	1.45	1.51
3	D	1334	GLU	C-O	5.72	1.30	1.24
2	C	19	PRO	C-O	5.71	1.30	1.23
3	D	624	ILE	CA-C	5.71	1.60	1.52
2	C	524	ILE	CB-CG1	5.70	1.64	1.53
3	D	915	ILE	CB-CG1	5.70	1.64	1.53
3	D	517	CYS	CA-C	5.70	1.59	1.52
2	C	807	TRP	CA-C	5.69	1.59	1.53
3	D	544	LEU	CB-CG	-5.69	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	33	ASP	C-O	5.68	1.31	1.24
2	C	1256	GLN	CA-C	-5.68	1.46	1.53
2	C	790	ASP	CA-C	-5.68	1.46	1.52
3	D	566	LYS	C-O	5.68	1.30	1.24
3	D	332	LYS	C-O	-5.68	1.15	1.23
3	D	355	ILE	CA-CB	5.68	1.61	1.54
2	C	562	GLU	CA-C	-5.67	1.45	1.52
3	D	510	LEU	N-CA	-5.67	1.39	1.46
2	C	1322	SER	CA-C	5.67	1.60	1.52
2	C	1057	LYS	N-CA	5.67	1.53	1.46
2	C	1230	MET	CA-CB	-5.66	1.44	1.53
3	D	110	PRO	N-CA	5.66	1.53	1.47
1	A	142	MET	CA-C	-5.66	1.45	1.52
3	D	119	SER	CB-OG	5.66	1.53	1.42
3	D	307	LEU	C-O	-5.66	1.17	1.24
3	D	397	ALA	C-O	5.65	1.30	1.24
3	D	352	ARG	NE-CZ	5.65	1.39	1.33
2	C	1244	HIS	N-CA	-5.64	1.40	1.46
2	C	1321	GLU	N-CA	5.64	1.53	1.46
3	D	474	LEU	CA-C	-5.64	1.45	1.52
2	C	520	PRO	N-CD	-5.64	1.39	1.47
3	D	513	MET	CA-C	-5.63	1.45	1.52
2	C	664	GLY	C-O	-5.63	1.17	1.23
3	D	784	ALA	CA-C	5.63	1.60	1.52
2	C	827	ARG	CA-CB	-5.63	1.43	1.53
3	D	1350	ASN	C-O	5.63	1.31	1.24
3	D	896	ALA	C-O	-5.62	1.16	1.24
3	D	542	ALA	CA-C	-5.62	1.45	1.52
3	D	579	LEU	N-CA	-5.62	1.38	1.46
3	D	1229	VAL	C-O	5.62	1.30	1.24
2	C	615	VAL	CA-CB	-5.61	1.47	1.54
2	C	1223	ARG	CA-C	-5.61	1.45	1.52
3	D	227	PHE	CA-CB	-5.61	1.44	1.53
1	A	67	GLU	CA-C	-5.61	1.45	1.52
2	C	523	GLU	C-O	5.61	1.30	1.24
2	C	709	ALA	CA-CB	5.61	1.62	1.53
1	B	188	GLU	CA-C	-5.60	1.45	1.52
3	D	647	PRO	CA-CB	-5.60	1.46	1.53
1	A	150	ARG	N-CA	-5.59	1.40	1.46
2	C	735	LYS	CA-C	-5.59	1.46	1.52
2	C	1221	PHE	N-CA	5.59	1.52	1.46
3	D	1327	GLU	C-O	5.59	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	804	PHE	C-O	5.59	1.30	1.24
2	C	556	GLY	CA-C	-5.58	1.44	1.51
2	C	826	ASP	CA-C	-5.58	1.45	1.52
1	A	217	ILE	C-O	5.57	1.30	1.24
2	C	688	GLN	CA-CB	5.57	1.62	1.53
1	A	148	ARG	CA-CB	-5.57	1.44	1.53
2	C	1278	LEU	CA-CB	-5.57	1.44	1.53
2	C	1228	GLY	N-CA	5.56	1.53	1.45
1	B	203	ILE	C-O	5.56	1.30	1.24
2	C	759	SER	C-N	-5.56	1.26	1.34
1	A	174	ASP	C-O	5.56	1.30	1.24
2	C	702	THR	C-N	-5.56	1.26	1.33
2	C	1058	ARG	CZ-NH1	5.56	1.40	1.32
2	C	531	SER	CB-OG	5.56	1.53	1.42
3	D	773	PHE	CG-CD2	-5.55	1.27	1.38
2	C	658	GLN	N-CA	-5.55	1.38	1.46
3	D	360	TYR	C-N	-5.55	1.25	1.33
2	C	1214	ASP	CG-OD2	5.54	1.35	1.25
3	D	353	SER	CA-CB	5.54	1.61	1.53
2	C	1244	HIS	CA-CB	5.54	1.61	1.53
2	C	133	ASN	CG-OD1	5.54	1.34	1.23
3	D	503	SER	C-O	-5.54	1.16	1.23
2	C	871	VAL	CA-CB	-5.53	1.48	1.54
2	C	137	VAL	CA-C	5.52	1.58	1.52
2	C	178	PRO	CA-CB	-5.52	1.46	1.53
2	C	1288	GLN	CA-CB	-5.52	1.44	1.53
3	D	475	GLU	C-O	5.51	1.30	1.24
3	D	791	ALA	N-CA	-5.50	1.40	1.46
1	B	28	LEU	CA-CB	-5.50	1.45	1.53
3	D	585	LYS	N-CA	5.50	1.53	1.46
3	D	306	LEU	C-O	-5.50	1.17	1.24
2	C	1302	THR	CB-OG1	5.50	1.52	1.43
2	C	731	ARG	CA-C	-5.50	1.45	1.52
2	C	805	MET	C-N	-5.49	1.26	1.33
4	E	5	THR	C-O	-5.49	1.17	1.24
2	C	1272	GLU	C-N	5.49	1.41	1.34
2	C	1187	PHE	CG-CD1	5.49	1.50	1.38
1	A	47	LEU	CA-CB	5.49	1.62	1.53
2	C	47	TYR	N-CA	-5.49	1.39	1.46
2	C	703	GLY	C-O	5.48	1.31	1.24
2	C	840	SER	C-O	-5.48	1.17	1.24
2	C	527	LYS	C-O	-5.48	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1304	MET	CG-SD	5.48	1.94	1.80
2	C	548	ARG	CA-C	5.48	1.59	1.52
3	D	792	ASN	C-O	5.47	1.30	1.24
2	C	1056	VAL	CA-CB	-5.47	1.47	1.54
2	C	1219	GLU	CA-C	-5.47	1.46	1.52
2	C	1320	PRO	N-CA	5.47	1.53	1.47
3	D	30	ILE	CA-CB	-5.47	1.47	1.54
3	D	1142	ALA	CA-CB	-5.47	1.44	1.53
2	C	1226	THR	C-N	5.47	1.42	1.33
2	C	1320	PRO	CA-C	-5.47	1.45	1.52
3	D	366	CYS	CA-CB	5.47	1.62	1.53
2	C	1226	THR	CB-OG1	-5.46	1.35	1.43
3	D	807	LEU	C-N	-5.46	1.26	1.33
2	C	884	VAL	N-CA	5.45	1.53	1.46
1	B	179	PRO	CA-C	-5.45	1.46	1.53
3	D	766	GLY	C-O	5.45	1.31	1.23
3	D	439	PRO	N-CD	-5.44	1.40	1.47
2	C	137	VAL	CA-CB	-5.44	1.47	1.54
2	C	805	MET	N-CA	5.44	1.53	1.46
2	C	827	ARG	CB-CG	5.44	1.68	1.52
4	E	22	VAL	C-O	-5.44	1.18	1.24
2	C	816	ILE	CA-C	-5.43	1.45	1.52
4	E	50	ALA	CA-CB	-5.43	1.44	1.53
1	A	30	PRO	N-CA	5.43	1.54	1.47
3	D	57	PHE	C-O	5.43	1.30	1.24
3	D	550	VAL	CA-C	5.43	1.59	1.52
2	C	670	PHE	C-O	-5.43	1.17	1.24
3	D	1321	SER	CA-C	5.43	1.60	1.53
3	D	537	TYR	CG-CD1	5.43	1.50	1.39
3	D	269	TYR	N-CA	-5.43	1.39	1.46
2	C	620	ASN	C-O	5.42	1.30	1.23
3	D	251	PRO	CA-C	5.42	1.59	1.52
3	D	49	PHE	CA-C	5.42	1.60	1.53
2	C	839	VAL	N-CA	5.42	1.52	1.46
2	C	181	GLY	N-CA	5.42	1.51	1.44
2	C	1324	ASN	C-O	5.42	1.30	1.24
3	D	598	LYS	C-O	5.42	1.30	1.24
3	D	915	ILE	C-O	5.42	1.30	1.24
3	D	180	MET	C-O	-5.42	1.17	1.24
2	C	1223	ARG	N-CA	5.41	1.53	1.46
2	C	1246	ARG	CA-CB	-5.41	1.43	1.53
2	C	11	ILE	N-CA	5.41	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	691	PRO	CA-CB	-5.41	1.47	1.53
5	M	181	ARG	CA-C	5.40	1.59	1.52
2	C	1173	ALA	CA-CB	-5.40	1.44	1.53
2	C	452	ARG	CA-CB	5.39	1.66	1.53
2	C	5	TYR	C-O	-5.39	1.17	1.24
3	D	641	ILE	CB-CG1	5.39	1.64	1.53
2	C	731	ARG	N-CA	5.39	1.52	1.46
2	C	525	THR	C-O	5.38	1.30	1.24
2	C	1193	ALA	C-O	5.38	1.30	1.24
2	C	516	ASP	CA-CB	5.38	1.59	1.53
2	C	574	SER	N-CA	-5.38	1.39	1.46
2	C	1057	LYS	C-O	5.38	1.30	1.24
2	C	634	VAL	CA-C	-5.37	1.46	1.52
1	B	35	PHE	CA-C	-5.37	1.45	1.52
2	C	1187	PHE	CE2-CZ	5.37	1.54	1.38
3	D	111	THR	CA-C	-5.37	1.46	1.52
3	D	424	ASN	CA-C	-5.37	1.45	1.52
3	D	1355	ARG	C-O	5.36	1.30	1.23
5	M	122	ASP	C-O	5.36	1.30	1.24
3	D	456	ALA	C-O	5.36	1.30	1.24
2	C	1332	SER	CA-C	5.36	1.60	1.52
3	D	500	ILE	N-CA	5.36	1.53	1.46
3	D	1330	ARG	N-CA	-5.36	1.40	1.46
2	C	457	GLY	C-O	5.35	1.31	1.23
3	D	888	CYS	CA-C	-5.35	1.45	1.52
3	D	534	GLU	C-N	-5.35	1.26	1.33
3	D	244	VAL	CA-CB	-5.35	1.47	1.54
3	D	363	LEU	CA-CB	5.35	1.62	1.53
3	D	431	ARG	C-O	5.35	1.30	1.24
3	D	383	GLY	C-O	5.34	1.30	1.23
2	C	35	PHE	CG-CD2	5.34	1.50	1.38
2	C	849	GLU	C-O	-5.34	1.17	1.23
3	D	1260	MET	CA-C	5.34	1.60	1.52
3	D	232	ASN	C-O	-5.34	1.17	1.23
3	D	428	THR	N-CA	-5.34	1.39	1.46
2	C	835	GLU	N-CA	5.33	1.52	1.46
3	D	300	GLN	N-CA	5.33	1.52	1.46
1	A	180	VAL	N-CA	-5.33	1.39	1.46
2	C	929	ILE	CB-CG1	-5.33	1.42	1.53
2	C	1084	ASP	N-CA	-5.33	1.39	1.46
2	C	833	ILE	N-CA	-5.33	1.40	1.46
3	D	780	ARG	CA-C	-5.32	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1153	ALA	N-CA	5.32	1.52	1.46
2	C	789	THR	CB-CG2	-5.32	1.34	1.52
2	C	1078	LYS	CA-CB	5.32	1.62	1.53
3	D	919	ALA	C-O	5.32	1.30	1.24
2	C	674	ASP	C-O	5.32	1.30	1.23
3	D	724	MET	CA-C	-5.31	1.45	1.52
3	D	120	LEU	C-O	5.31	1.31	1.23
2	C	563	THR	C-O	5.31	1.30	1.24
3	D	580	TRP	CG-CD2	-5.31	1.34	1.43
2	C	1072	ASN	CG-ND2	5.31	1.44	1.33
3	D	793	SER	C-O	5.31	1.30	1.24
2	C	1102	GLY	CA-C	5.31	1.58	1.51
1	A	156	SER	N-CA	-5.30	1.39	1.46
2	C	926	GLY	C-O	-5.30	1.18	1.24
1	A	12	ARG	C-O	-5.30	1.17	1.23
3	D	253	VAL	CA-CB	5.29	1.61	1.54
2	C	137	VAL	N-CA	5.29	1.52	1.46
2	C	754	THR	N-CA	-5.29	1.39	1.46
1	A	207	THR	CA-C	-5.28	1.46	1.52
3	D	469	HIS	C-N	5.28	1.38	1.33
3	D	545	HIS	CA-CB	5.28	1.60	1.53
2	C	523	GLU	N-CA	5.28	1.52	1.46
3	D	819	GLY	C-O	5.28	1.29	1.23
2	C	931	VAL	C-N	5.28	1.40	1.33
2	C	1210	ILE	C-O	5.28	1.29	1.23
2	C	812	PHE	CG-CD2	5.27	1.50	1.38
2	C	820	GLU	CD-OE1	5.27	1.35	1.25
1	A	44	ARG	CZ-NH1	5.27	1.40	1.32
2	C	813	GLU	CA-C	5.27	1.58	1.53
2	C	574	SER	CB-OG	5.27	1.52	1.42
3	D	743	MET	CA-C	-5.27	1.46	1.53
3	D	787	ALA	CA-C	5.26	1.59	1.52
3	D	1329	THR	CA-CB	-5.26	1.45	1.53
2	C	771	VAL	C-O	5.25	1.31	1.24
2	C	810	TYR	C-O	-5.25	1.17	1.24
2	C	153	PRO	N-CD	-5.25	1.40	1.47
3	D	412	LEU	C-O	5.25	1.30	1.24
2	C	1167	GLU	C-O	-5.25	1.18	1.23
2	C	1194	GLU	CD-OE2	-5.25	1.15	1.25
3	D	546	ALA	N-CA	-5.25	1.39	1.46
3	D	431	ARG	CA-C	5.25	1.59	1.52
1	A	218	ARG	N-CA	-5.25	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	LYS	C-O	-5.24	1.17	1.23
1	A	47	LEU	C-O	5.24	1.30	1.24
3	D	730	ALA	N-CA	-5.24	1.39	1.46
3	D	1266	ILE	C-O	-5.24	1.18	1.24
2	C	783	LEU	CA-C	5.23	1.59	1.52
2	C	812	PHE	CA-C	-5.23	1.46	1.52
3	D	630	ALA	CA-CB	-5.23	1.44	1.53
2	C	136	PHE	CG-CD1	-5.22	1.27	1.38
2	C	752	ASN	N-CA	-5.22	1.39	1.46
2	C	756	TYR	CA-CB	-5.22	1.45	1.53
2	C	1305	TYR	N-CA	5.22	1.52	1.46
3	D	744	ARG	N-CA	5.22	1.52	1.46
2	C	1326	LEU	N-CA	-5.22	1.40	1.46
3	D	382	TYR	CB-CG	-5.22	1.40	1.51
3	D	1343	GLU	CA-CB	5.22	1.60	1.54
1	A	46	ILE	C-O	-5.22	1.17	1.24
1	A	89	ALA	N-CA	5.22	1.52	1.46
2	C	1048	LYS	N-CA	5.22	1.52	1.45
3	D	504	GLN	CA-CB	5.21	1.62	1.53
3	D	539	SER	CA-C	5.21	1.59	1.53
3	D	777	HIS	CA-C	-5.20	1.46	1.52
3	D	701	LEU	CA-C	-5.20	1.45	1.52
3	D	895	CYS	CB-SG	5.20	1.98	1.81
2	C	1317	PRO	CA-CB	-5.19	1.46	1.53
3	D	1310	THR	C-O	-5.19	1.17	1.23
1	A	61	ILE	CA-CB	-5.19	1.46	1.55
3	D	367	GLY	CA-C	-5.19	1.44	1.51
3	D	375	GLU	CA-C	-5.19	1.47	1.52
2	C	1056	VAL	N-CA	-5.19	1.40	1.46
3	D	1247	LYS	CA-CB	5.19	1.60	1.53
3	D	744	ARG	CZ-NH1	-5.18	1.25	1.32
2	C	142	GLU	CA-CB	-5.18	1.45	1.53
2	C	464	PHE	CA-CB	-5.18	1.44	1.53
2	C	816	ILE	CB-CG2	5.18	1.69	1.52
3	D	513	MET	SD-CE	5.18	1.92	1.79
2	C	1092	THR	CA-C	-5.17	1.46	1.52
3	D	535	ARG	CA-C	-5.17	1.46	1.52
3	D	1255	VAL	C-N	-5.17	1.27	1.33
3	D	98	ARG	CA-C	5.17	1.59	1.52
2	C	180	ARG	N-CA	5.16	1.52	1.46
3	D	296	LYS	C-O	5.16	1.30	1.24
3	D	479	GLU	CD-OE2	5.16	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	ILE	CA-CB	-5.16	1.48	1.54
3	D	542	ALA	C-O	-5.16	1.18	1.24
2	C	1224	PRO	N-CA	5.16	1.53	1.47
3	D	536	LEU	C-O	5.16	1.30	1.24
2	C	699	LEU	N-CA	5.15	1.52	1.46
2	C	852	ALA	N-CA	5.15	1.52	1.46
3	D	1221	LEU	CA-C	-5.15	1.46	1.52
4	E	13	ILE	CB-CG1	-5.15	1.43	1.53
3	D	589	TYR	CZ-OH	5.15	1.48	1.38
2	C	1068	GLY	C-O	5.15	1.30	1.23
2	C	1207	SER	C-O	-5.15	1.17	1.24
2	C	569	ILE	C-O	-5.14	1.18	1.24
2	C	447	HIS	CA-C	5.14	1.59	1.52
1	A	48	LEU	N-CA	5.14	1.52	1.46
3	D	1246	VAL	C-O	5.14	1.30	1.24
2	C	1075	VAL	CA-CB	-5.14	1.45	1.55
3	D	18	ASP	N-CA	-5.14	1.39	1.45
3	D	158	GLN	C-O	-5.14	1.17	1.23
2	C	576	SER	CB-OG	5.13	1.52	1.42
3	D	902	ASP	CA-C	5.13	1.59	1.52
2	C	731	ARG	CZ-NH1	-5.13	1.25	1.32
2	C	1321	GLU	CA-C	-5.13	1.45	1.52
3	D	19	ALA	CA-CB	5.13	1.62	1.53
3	D	486	SER	N-CA	5.13	1.52	1.46
2	C	711	ASP	CA-CB	5.13	1.61	1.53
2	C	1228	GLY	C-O	5.13	1.30	1.23
1	B	206	GLU	CA-C	-5.13	1.46	1.52
2	C	1231	TYR	N-CA	5.12	1.52	1.46
3	D	367	GLY	N-CA	5.12	1.52	1.45
3	D	917	VAL	CA-CB	-5.12	1.47	1.54
2	C	16	GLY	N-CA	5.12	1.52	1.45
3	D	881	LYS	C-O	-5.12	1.17	1.24
2	C	4	SER	C-O	-5.12	1.18	1.23
3	D	600	ALA	CA-C	5.12	1.59	1.52
2	C	26	TYR	C-O	-5.12	1.17	1.24
2	C	592	ARG	CA-CB	-5.12	1.45	1.53
2	C	711	ASP	CA-C	-5.11	1.45	1.52
3	D	892	PHE	CA-C	5.11	1.59	1.52
1	A	77	ASP	CA-C	-5.10	1.45	1.53
1	A	37	HIS	C-O	5.10	1.30	1.24
2	C	820	GLU	CD-OE2	5.10	1.35	1.25
2	C	1319	MET	C-O	5.10	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	450	HIS	CA-C	5.10	1.58	1.53
2	C	466	VAL	C-O	5.10	1.29	1.24
2	C	1226	THR	CB-CG2	5.09	1.69	1.52
1	B	50	SER	CA-C	-5.09	1.46	1.52
3	D	420	PRO	CA-CB	5.09	1.60	1.53
2	C	577	VAL	CA-C	-5.09	1.46	1.52
2	C	581	THR	CB-CG2	-5.09	1.35	1.52
2	C	870	ILE	CA-C	5.09	1.59	1.52
2	C	93	SER	CA-C	-5.08	1.46	1.53
3	D	626	TYR	N-CA	-5.08	1.40	1.46
3	D	309	ASN	N-CA	5.08	1.52	1.46
2	C	802	VAL	CA-CB	-5.08	1.47	1.55
2	C	1296	ASP	N-CA	5.08	1.52	1.45
2	C	14	ASP	C-O	-5.07	1.17	1.24
3	D	620	PHE	CG-CD1	5.07	1.49	1.38
2	C	35	PHE	CB-CG	-5.07	1.39	1.50
3	D	13	LYS	C-O	-5.07	1.18	1.23
2	C	1154	ASP	C-O	-5.07	1.17	1.24
2	C	128	PRO	N-CA	5.06	1.53	1.47
2	C	1232	MET	N-CA	-5.06	1.40	1.45
2	C	555	TYR	CA-C	-5.06	1.46	1.52
2	C	1096	ILE	CA-C	5.06	1.59	1.52
2	C	1171	ARG	CA-C	-5.06	1.46	1.52
3	D	92	VAL	C-N	-5.06	1.26	1.33
1	A	69	SER	N-CA	5.06	1.52	1.45
2	C	1199	LEU	CB-CG	-5.06	1.43	1.53
3	D	436	ALA	N-CA	5.05	1.52	1.45
3	D	1364	ALA	CA-C	5.05	1.59	1.52
3	D	116	PHE	CA-C	-5.05	1.46	1.52
2	C	1069	ARG	N-CA	5.05	1.52	1.46
2	C	1113	LEU	CB-CG	5.05	1.63	1.53
2	C	1213	TYR	C-O	5.05	1.30	1.24
3	D	341	ASN	CG-ND2	5.04	1.43	1.33
3	D	511	TYR	CG-CD2	5.04	1.50	1.39
2	C	587	LEU	CB-CG	5.04	1.63	1.53
1	A	213	PRO	N-CA	-5.04	1.41	1.47
2	C	1081	PRO	CG-CD	-5.04	1.33	1.50
1	A	219	ARG	C-O	5.04	1.30	1.24
3	D	701	LEU	C-O	-5.04	1.17	1.24
2	C	31	GLN	N-CA	5.03	1.52	1.46
2	C	1131	MET	C-O	-5.03	1.18	1.24
3	D	326	SER	CA-C	5.03	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	ARG	CA-C	-5.03	1.46	1.52
1	A	201	LEU	CA-C	-5.03	1.46	1.52
2	C	761	GLN	CA-C	5.03	1.60	1.52
1	A	182	ARG	CA-C	-5.03	1.46	1.52
3	D	862	THR	CA-C	-5.03	1.46	1.52
3	D	1349	GLU	CA-CB	5.02	1.61	1.53
2	C	541	GLU	N-CA	5.02	1.52	1.46
3	D	338	PHE	C-N	-5.02	1.26	1.33
3	D	745	GLY	C-O	-5.02	1.18	1.23
3	D	237	MET	N-CA	5.02	1.52	1.46
4	E	28	ARG	CZ-NH1	5.02	1.39	1.32
2	C	1294	LYS	CA-C	5.02	1.64	1.52
2	C	35	PHE	CA-CB	-5.01	1.45	1.53
3	D	95	THR	N-CA	5.01	1.54	1.47
2	C	461	GLU	C-O	5.01	1.30	1.24
2	C	728	ASP	CA-C	-5.01	1.46	1.52
2	C	1155	VAL	C-O	5.01	1.30	1.24
2	C	1264	GLN	CA-CB	5.01	1.61	1.53
3	D	401	VAL	CA-C	5.01	1.59	1.52
3	D	919	ALA	N-CA	-5.01	1.40	1.46
2	C	678	ARG	NE-CZ	5.01	1.38	1.33
3	D	300	GLN	CA-C	-5.00	1.46	1.52
2	C	554	HIS	CG-ND1	5.00	1.43	1.38
3	D	332	LYS	CG-CD	5.00	1.67	1.52

All (1244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	462	ASP	N-CA-C	-18.13	86.00	113.02
3	D	765	GLU	CA-C-N	-16.20	100.22	120.64
3	D	765	GLU	C-N-CA	-16.20	100.22	120.64
1	A	61	ILE	CB-CG1-CD1	-16.10	79.98	113.80
2	C	805	MET	CG-SD-CE	-16.07	65.55	100.90
5	M	186	ASP	N-CA-CB	15.87	129.15	110.42
6	F	9	DT	C2'-C3'-O3'	-15.43	88.35	111.50
3	D	358	GLY	CA-C-N	-14.10	102.21	119.84
3	D	358	GLY	C-N-CA	-14.10	102.21	119.84
2	C	786	GLY	CA-C-N	-14.10	105.30	120.66
2	C	786	GLY	C-N-CA	-14.10	105.30	120.66
3	D	434	ILE	CB-CG1-CD1	-14.04	84.31	113.80
3	D	492	SER	CA-C-O	-13.74	109.15	119.32
2	C	800	MET	CG-SD-CE	13.67	130.98	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	554	HIS	N-CA-CB	-13.33	91.25	110.57
2	C	519	ASN	CA-CB-CG	-13.07	99.53	112.60
2	C	149	LEU	CB-CG-CD1	-13.02	71.63	110.70
2	C	1117	LEU	CD1-CG-CD2	-12.93	82.35	110.80
3	D	422	LEU	CB-CG-CD2	-12.67	72.70	110.70
2	C	1216	ARG	NE-CZ-NH2	-12.62	107.84	119.20
3	D	1304	ARG	NE-CZ-NH1	-12.40	109.10	121.50
3	D	515	ARG	NE-CZ-NH2	12.38	130.34	119.20
2	C	527	LYS	N-CA-C	-12.30	97.97	113.23
2	C	521	LEU	CD1-CG-CD2	-12.10	84.17	110.80
3	D	353	SER	N-CA-CB	12.07	129.79	110.97
2	C	1180	MET	CB-CA-C	-12.03	92.06	109.38
2	C	1267	GLY	CA-C-N	-11.93	98.75	121.54
2	C	1267	GLY	C-N-CA	-11.93	98.75	121.54
3	D	1320	ILE	CB-CG1-CD1	-11.89	88.84	113.80
2	C	1270	PHE	CA-C-N	11.78	132.91	122.43
2	C	1270	PHE	C-N-CA	11.78	132.91	122.43
3	D	341	ASN	N-CA-CB	-11.77	90.60	110.49
2	C	727	VAL	CG1-CB-CG2	-11.74	84.97	110.80
3	D	366	CYS	CA-CB-SG	-11.74	87.40	114.40
2	C	1301	ARG	NE-CZ-NH2	-11.71	108.66	119.20
3	D	536	LEU	CD1-CG-CD2	-11.43	85.67	110.80
2	C	813	GLU	CA-C-N	-11.37	104.86	122.60
2	C	813	GLU	C-N-CA	-11.37	104.86	122.60
2	C	765	ILE	CG1-CB-CG2	-11.34	76.69	110.70
2	C	1081	PRO	CB-CA-C	-11.17	93.13	111.56
2	C	787	PRO	N-CA-C	-11.07	93.28	111.77
3	D	434	ILE	CG1-CB-CG2	-10.82	78.25	110.70
2	C	1153	ALA	CA-C-O	-10.80	109.27	121.15
2	C	1333	LEU	CD1-CG-CD2	-10.76	87.13	110.80
3	D	725	MET	CG-SD-CE	-10.72	77.31	100.90
3	D	347	VAL	N-CA-C	10.70	124.17	108.65
2	C	1246	ARG	NE-CZ-NH2	10.67	128.80	119.20
3	D	346	ARG	N-CA-C	-10.66	96.46	110.53
2	C	1216	ARG	NH1-CZ-NH2	10.64	133.13	119.30
3	D	345	LYS	CB-CA-C	10.62	127.67	109.51
3	D	99	ARG	NE-CZ-NH2	-10.62	109.64	119.20
1	A	102	LEU	CD1-CG-CD2	-10.60	87.48	110.80
3	D	113	HIS	CB-CA-C	-10.54	93.82	112.27
3	D	543	SER	N-CA-C	-10.52	100.45	113.28
2	C	577	VAL	CA-C-N	-10.47	105.26	122.54
2	C	577	VAL	C-N-CA	-10.47	105.26	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	535	ARG	CB-CG-CD	-10.46	87.24	111.30
2	C	1301	ARG	NE-CZ-NH1	10.45	131.95	121.50
2	C	1169	VAL	CB-CA-C	-10.43	98.80	111.94
2	C	146	VAL	CG1-CB-CG2	-10.42	87.88	110.80
2	C	1096	ILE	CG1-CB-CG2	-10.39	79.53	110.70
3	D	1323	ALA	O-C-N	10.35	134.69	122.17
2	C	12	ARG	NE-CZ-NH2	-10.29	109.94	119.20
2	C	1070	HIS	N-CA-C	10.21	124.36	112.93
3	D	337	ARG	N-CA-CB	-10.19	96.19	110.65
2	C	929	ILE	CA-CB-CG2	10.17	127.79	110.50
6	F	3	DG	C2'-C3'-O3'	-10.12	96.32	111.50
2	C	704	MET	N-CA-C	10.08	124.67	112.38
2	C	554	HIS	N-CA-C	-10.07	101.63	113.21
2	C	827	ARG	CB-CA-C	-10.06	91.61	109.62
3	D	1310	THR	N-CA-C	-9.98	97.67	112.04
1	A	81	ILE	CG1-CB-CG2	-9.94	80.89	110.70
3	D	373	ALA	O-C-N	-9.92	109.40	122.59
2	C	1217	THR	N-CA-C	-9.85	101.26	113.28
3	D	361	LEU	CA-CB-CG	9.79	150.58	116.30
2	C	1159	VAL	CB-CA-C	-9.78	96.27	111.71
3	D	536	LEU	CB-CG-CD2	9.76	139.99	110.70
6	F	0	DC	C2'-C3'-O3'	-9.74	96.89	111.50
3	D	914	ALA	CA-C-O	9.72	131.10	120.89
3	D	456	ALA	N-CA-C	-9.70	100.66	111.14
3	D	484	MET	N-CA-C	9.70	124.93	113.20
3	D	345	LYS	N-CA-C	-9.62	95.02	110.32
2	C	1246	ARG	CB-CA-C	-9.61	91.01	109.66
2	C	827	ARG	CG-CD-NE	9.54	132.99	112.00
3	D	915	ILE	CB-CG1-CD1	9.50	133.75	113.80
3	D	252	LEU	CB-CG-CD2	-9.50	82.20	110.70
6	F	-1	DC	P-O5'-C5'	9.46	134.19	120.00
2	C	1333	LEU	O-C-N	-9.43	110.50	122.20
5	M	256	LEU	N-CA-C	9.43	121.64	111.36
2	C	1238	LEU	CA-C-N	-9.43	104.99	120.64
2	C	1238	LEU	C-N-CA	-9.43	104.99	120.64
3	D	369	PRO	CB-CA-C	-9.41	100.07	111.46
3	D	506	VAL	N-CA-C	9.35	121.28	110.62
3	D	506	VAL	CA-CB-CG2	-9.34	94.52	110.40
3	D	617	THR	N-CA-C	9.31	122.62	111.82
2	C	1075	VAL	CA-CB-CG2	-9.30	94.58	110.40
2	C	932	GLN	CB-CG-CD	-9.29	96.81	112.60
6	F	8	DA	C2'-C3'-O3'	9.25	125.38	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	851	THR	N-CA-C	9.25	121.69	108.00
6	F	0	DC	N1-C1'-C2'	9.24	127.36	113.50
3	D	96	LYS	N-CA-C	-9.19	100.98	113.30
3	D	365	GLN	OE1-CD-NE2	9.15	131.75	122.60
2	C	530	ILE	CA-C-O	9.12	129.49	120.27
3	D	915	ILE	CG1-CB-CG2	-9.12	83.33	110.70
3	D	300	GLN	N-CA-CB	9.12	123.52	110.12
3	D	245	LEU	CD1-CG-CD2	-9.11	90.76	110.80
3	D	334	LYS	N-CA-C	9.09	130.16	110.80
2	C	135	THR	OG1-CB-CG2	-9.06	91.17	109.30
2	C	794	LEU	CB-CA-C	-9.06	95.86	110.81
2	C	1064	ASP	N-CA-C	9.03	121.12	111.28
6	F	0	DC	C4'-C3'-O3'	-9.03	96.46	110.00
2	C	1294	LYS	N-CA-CB	-9.02	97.48	110.57
3	D	798	ARG	NE-CZ-NH2	9.01	127.31	119.20
3	D	913	GLU	CA-C-O	-8.98	111.61	121.94
3	D	780	ARG	CG-CD-NE	-8.96	92.30	112.00
3	D	504	GLN	CB-CA-C	8.95	128.24	110.42
5	M	156	ILE	CB-CA-C	8.95	125.97	111.29
1	A	155	ALA	N-CA-C	8.95	122.16	111.33
2	C	1103	VAL	CA-CB-CG2	8.94	125.59	110.40
1	A	45	ARG	NE-CZ-NH1	-8.91	112.59	121.50
3	D	583	VAL	CB-CA-C	-8.90	101.28	110.89
2	C	833	ILE	N-CA-CB	-8.87	99.19	111.25
3	D	1262	ARG	N-CA-CB	-8.87	98.23	110.38
3	D	99	ARG	NH1-CZ-NH2	8.86	130.82	119.30
2	C	818	VAL	CG1-CB-CG2	-8.85	91.32	110.80
4	E	32	VAL	N-CA-C	-8.84	102.24	110.82
3	D	928	THR	N-CA-C	-8.82	101.66	111.28
3	D	1320	ILE	N-CA-C	8.82	119.62	110.62
2	C	851	THR	CB-CA-C	-8.82	104.00	116.34
3	D	885	VAL	CA-CB-CG1	8.82	125.39	110.40
6	F	11	DG	C4'-C3'-O3'	-8.80	96.80	110.00
3	D	377	PHE	N-CA-CB	-8.79	97.73	110.56
3	D	373	ALA	N-CA-C	-8.73	92.20	110.80
3	D	252	LEU	N-CA-C	8.71	123.48	113.02
2	C	1288	GLN	CB-CA-C	-8.71	93.95	110.67
3	D	513	MET	CG-SD-CE	-8.71	81.73	100.90
2	C	765	ILE	N-CA-CB	8.70	123.65	111.82
1	A	44	ARG	NE-CZ-NH1	-8.70	112.80	121.50
2	C	1232	MET	N-CA-C	8.68	123.87	110.42
1	B	205	MET	CG-SD-CE	-8.65	81.86	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	622	ASP	O-C-N	8.65	131.09	122.09
2	C	1050	VAL	CG1-CB-CG2	-8.63	91.80	110.80
2	C	1246	ARG	NH1-CZ-NH2	-8.63	108.09	119.30
2	C	1268	GLN	CB-CA-C	8.63	127.58	110.42
3	D	344	GLY	CA-C-N	-8.62	107.33	122.07
3	D	344	GLY	C-N-CA	-8.62	107.33	122.07
3	D	534	GLU	N-CA-CB	8.62	123.83	109.78
2	C	678	ARG	CB-CA-C	8.62	124.52	110.90
2	C	811	ASN	N-CA-C	-8.61	92.94	108.02
2	C	445	ILE	CB-CA-C	-8.60	100.35	112.22
2	C	819	SER	N-CA-CB	8.59	122.60	109.97
3	D	313	GLY	N-CA-C	8.56	124.36	111.18
2	C	555	TYR	N-CA-CB	8.55	122.39	109.91
2	C	12	ARG	CB-CG-CD	-8.55	91.64	111.30
5	M	185	PHE	CA-C-N	-8.52	109.22	119.78
5	M	185	PHE	C-N-CA	-8.52	109.22	119.78
2	C	700	VAL	CB-CA-C	-8.52	97.38	110.50
2	C	699	LEU	CD1-CG-CD2	8.51	129.53	110.80
2	C	700	VAL	CA-C-O	8.50	130.19	120.67
2	C	528	ARG	CB-CA-C	-8.48	96.98	111.23
2	C	681	MET	N-CA-CB	8.47	122.36	110.07
3	D	380	PHE	N-CA-CB	-8.45	97.70	110.12
3	D	90	VAL	CA-CB-CG1	-8.41	96.10	110.40
3	D	539	SER	CA-C-N	-8.40	109.76	122.28
3	D	539	SER	C-N-CA	-8.40	109.76	122.28
3	D	461	PHE	N-CA-CB	-8.38	98.40	111.23
3	D	808	VAL	N-CA-CB	-8.38	97.40	111.23
3	D	769	VAL	CB-CA-C	-8.38	101.06	112.04
3	D	515	ARG	NH1-CZ-NH2	-8.35	108.44	119.30
3	D	765	GLU	O-C-N	-8.35	113.42	123.19
5	M	186	ASP	N-CA-C	8.35	123.54	112.35
2	C	1077	SER	N-CA-C	-8.34	100.86	112.45
2	C	144	VAL	N-CA-C	8.32	120.61	109.37
3	D	345	LYS	CD-CE-NZ	8.32	138.52	111.90
2	C	677	ASN	CA-C-O	8.31	129.32	119.60
3	D	582	ILE	CG1-CB-CG2	-8.30	85.80	110.70
1	B	179	PRO	CB-CA-C	-8.28	100.20	112.04
3	D	90	VAL	N-CA-C	8.27	119.21	108.12
3	D	885	VAL	N-CA-CB	-8.25	97.61	111.23
2	C	1104	PRO	CB-CA-C	-8.24	99.95	113.06
2	C	1263	ALA	CA-C-O	-8.24	108.72	120.51
2	C	828	PHE	N-CA-C	8.24	128.35	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1182	ILE	N-CA-C	8.23	120.49	109.37
3	D	92	VAL	CA-CB-CG1	-8.21	96.44	110.40
3	D	807	LEU	O-C-N	-8.17	113.73	122.96
2	C	704	MET	CG-SD-CE	-8.16	82.94	100.90
2	C	758	ARG	N-CA-C	-8.15	99.27	110.35
3	D	1321	SER	N-CA-C	-8.15	100.02	110.53
2	C	515	MET	CA-C-O	-8.14	112.11	121.47
3	D	898	CYS	CA-C-N	-8.13	106.00	121.54
3	D	898	CYS	C-N-CA	-8.13	106.00	121.54
3	D	924	GLY	N-CA-C	8.13	124.00	114.16
3	D	896	ALA	N-CA-C	8.13	122.63	112.87
2	C	452	ARG	CA-C-O	-8.12	111.94	121.11
3	D	1246	VAL	CB-CA-C	-8.11	100.60	111.15
6	F	2	DG	C2'-C3'-O3'	-8.08	99.39	111.50
1	B	32	GLU	CA-C-O	-8.07	112.31	121.19
2	C	1182	ILE	CB-CA-C	-8.07	98.43	111.59
3	D	477	GLN	N-CA-C	8.06	121.08	111.33
3	D	502	PRO	CA-C-O	-8.05	112.61	121.23
3	D	102	MET	CG-SD-CE	-8.04	83.21	100.90
2	C	1107	MET	CA-C-O	8.02	131.57	122.27
3	D	885	VAL	N-CA-C	-8.01	92.67	109.34
2	C	575	LEU	CD1-CG-CD2	8.00	128.39	110.80
3	D	627	THR	CA-CB-CG2	-8.00	96.91	110.50
2	C	764	CYS	N-CA-CB	7.99	122.44	110.29
2	C	669	PRO	CB-CA-C	-7.99	100.81	111.12
3	D	474	LEU	CB-CG-CD2	-7.99	86.73	110.70
2	C	581	THR	CA-CB-OG1	7.99	121.58	109.60
3	D	471	PRO	CA-C-O	-7.96	111.75	121.31
2	C	704	MET	CB-CG-SD	7.96	136.58	112.70
2	C	1079	ILE	CA-C-O	-7.94	111.53	120.74
3	D	617	THR	OG1-CB-CG2	-7.93	93.44	109.30
3	D	519	ASN	CB-CA-C	-7.93	106.45	117.23
3	D	783	LEU	CB-CG-CD2	-7.92	86.95	110.70
3	D	268	LEU	CD1-CG-CD2	-7.91	93.41	110.80
2	C	146	VAL	CB-CA-C	-7.88	100.41	111.21
3	D	374	LEU	N-CA-CB	7.88	123.81	110.49
2	C	672	GLU	CB-CA-C	-7.88	98.51	110.88
2	C	857	VAL	CA-C-N	7.87	129.02	120.44
2	C	857	VAL	C-N-CA	7.87	129.02	120.44
3	D	722	ILE	CA-CB-CG2	7.87	123.88	110.50
3	D	1355	ARG	N-CA-CB	-7.85	99.28	111.05
2	C	144	VAL	CA-C-N	-7.84	113.05	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	144	VAL	C-N-CA	-7.84	113.05	122.93
3	D	456	ALA	O-C-N	7.83	130.54	122.09
2	C	1271	GLY	N-CA-C	-7.82	101.86	112.57
2	C	1231	TYR	CA-C-O	-7.82	112.09	120.46
2	C	177	ILE	CA-C-O	7.82	124.00	119.94
3	D	425	ARG	CA-C-O	-7.81	111.96	120.24
3	D	369	PRO	N-CD-CG	-7.80	91.50	103.20
3	D	908	ILE	CA-CB-CG1	7.80	123.66	110.40
6	F	2	DG	C4'-C3'-O3'	7.79	121.69	110.00
3	D	897	HIS	N-CA-C	-7.79	103.58	113.23
2	C	802	VAL	N-CA-C	-7.78	96.87	108.85
2	C	815	SER	N-CA-C	7.76	119.96	110.41
5	M	186	ASP	CB-CA-C	-7.75	100.40	113.04
2	C	802	VAL	CG1-CB-CG2	-7.74	93.78	110.80
3	D	351	GLY	CA-C-N	-7.74	106.78	121.63
3	D	351	GLY	C-N-CA	-7.74	106.78	121.63
2	C	515	MET	CG-SD-CE	7.73	117.91	100.90
2	C	527	LYS	O-C-N	-7.73	111.87	122.46
3	D	481	ARG	CB-CG-CD	-7.72	93.54	111.30
2	C	810	TYR	N-CA-CB	7.71	122.96	110.40
2	C	794	LEU	CA-C-N	-7.70	111.50	123.13
2	C	794	LEU	C-N-CA	-7.70	111.50	123.13
3	D	1363	TYR	O-C-N	7.68	129.98	122.07
3	D	586	GLY	N-CA-C	7.68	131.38	113.18
3	D	337	ARG	N-CA-C	-7.68	104.83	112.97
1	A	73	GLY	N-CA-C	7.68	131.38	113.18
2	C	137	VAL	CB-CA-C	-7.66	99.91	111.33
2	C	1245	ALA	N-CA-C	7.65	127.10	110.80
3	D	812	ASP	N-CA-C	7.64	119.39	111.14
3	D	77	ARG	N-CA-C	7.63	122.20	108.69
3	D	451	PRO	N-CA-CB	7.63	111.46	103.15
3	D	739	GLN	CA-C-O	7.63	128.76	119.38
3	D	893	GLY	CA-C-N	-7.62	108.25	121.97
3	D	893	GLY	C-N-CA	-7.62	108.25	121.97
6	F	-1	DC	O3'-P-O5'	7.61	115.41	104.00
2	C	12	ARG	NE-CZ-NH1	-7.60	113.90	121.50
6	F	8	DA	C4'-C3'-O3'	-7.58	98.63	110.00
2	C	1333	LEU	CB-CG-CD1	7.56	133.39	110.70
2	C	184	LEU	CD1-CG-CD2	-7.55	94.19	110.80
3	D	58	CYS	N-CA-C	7.54	120.48	110.53
2	C	1097	VAL	CB-CA-C	-7.54	99.48	110.63
3	D	337	ARG	CG-CD-NE	-7.51	95.47	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	489	ASN	N-CA-C	7.51	122.42	107.62
3	D	470	VAL	N-CA-C	7.51	115.64	107.60
2	C	13	LYS	N-CA-C	7.50	120.73	109.25
2	C	530	ILE	N-CA-C	-7.48	96.69	107.77
2	C	1081	PRO	CA-C-N	-7.48	109.80	120.42
2	C	1081	PRO	C-N-CA	-7.48	109.80	120.42
3	D	348	ASP	N-CA-C	7.48	121.46	109.79
2	C	1322	SER	CB-CA-C	7.48	123.57	110.85
3	D	1318	SER	N-CA-C	7.46	119.89	109.15
2	C	1106	ARG	NE-CZ-NH2	-7.45	112.49	119.20
3	D	1262	ARG	NE-CZ-NH2	7.45	125.90	119.20
3	D	365	GLN	CB-CA-C	-7.45	96.18	111.22
2	C	586	PHE	CA-C-O	-7.44	112.76	121.16
3	D	360	TYR	O-C-N	-7.44	112.70	122.59
3	D	903	LEU	N-CA-C	-7.42	94.99	110.80
3	D	807	LEU	N-CA-C	-7.42	99.50	110.48
3	D	1256	ILE	CA-CB-CG1	-7.42	97.79	110.40
2	C	1335	ILE	CA-C-O	-7.41	112.61	120.39
2	C	1096	ILE	CB-CA-C	7.41	123.43	111.29
3	D	1329	THR	N-CA-C	-7.40	103.15	111.14
3	D	387	LEU	CB-CG-CD2	-7.40	88.50	110.70
3	D	744	ARG	CB-CG-CD	-7.40	94.28	111.30
2	C	515	MET	O-C-N	7.39	131.31	122.96
2	C	1094	VAL	N-CA-C	7.38	120.26	109.63
2	C	1231	TYR	O-C-N	7.37	132.42	123.13
2	C	1298	VAL	CA-C-N	-7.37	110.28	120.38
2	C	1298	VAL	C-N-CA	-7.37	110.28	120.38
2	C	823	VAL	CA-CB-CG1	7.37	122.92	110.40
2	C	555	TYR	CA-C-N	-7.36	106.99	121.41
2	C	555	TYR	C-N-CA	-7.36	106.99	121.41
2	C	1244	HIS	CA-C-N	-7.36	107.49	121.54
2	C	1244	HIS	C-N-CA	-7.36	107.49	121.54
3	D	466	MET	CG-SD-CE	-7.34	84.75	100.90
2	C	1302	THR	CA-CB-CG2	-7.34	98.02	110.50
2	C	75	LEU	CD1-CG-CD2	-7.33	94.67	110.80
3	D	326	SER	N-CA-CB	-7.33	99.64	111.22
1	A	182	ARG	N-CA-C	7.31	121.58	109.95
5	M	127	GLN	OE1-CD-NE2	7.31	129.91	122.60
3	D	468	VAL	CB-CA-C	-7.31	99.24	110.50
2	C	577	VAL	O-C-N	7.30	129.49	121.90
1	A	51	MET	CA-C-N	-7.29	112.97	120.85
1	A	51	MET	C-N-CA	-7.29	112.97	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	LEU	CB-CG-CD2	7.29	132.57	110.70
2	C	1056	VAL	CA-C-N	-7.29	112.66	122.72
2	C	1056	VAL	C-N-CA	-7.29	112.66	122.72
3	D	22	ILE	CG1-CB-CG2	-7.29	88.85	110.70
3	D	625	MET	CA-C-O	7.28	128.26	120.55
3	D	1321	SER	CA-C-O	7.26	130.29	121.94
3	D	808	VAL	CB-CA-C	-7.26	99.39	111.29
3	D	361	LEU	N-CA-C	7.24	126.23	110.80
3	D	640	GLY	O-C-N	-7.24	117.77	123.27
3	D	1304	ARG	NH1-CZ-NH2	7.24	128.71	119.30
3	D	1356	LEU	N-CA-C	7.24	119.91	110.43
2	C	10	ARG	CB-CA-C	-7.23	99.68	110.24
3	D	338	PHE	N-CA-CB	-7.23	98.00	109.78
3	D	592	VAL	N-CA-C	7.23	122.02	112.98
3	D	806	ASP	N-CA-C	-7.22	104.34	113.01
3	D	892	PHE	CA-C-O	7.22	127.77	119.18
2	C	526	HIS	CB-CG-CD2	-7.21	121.83	131.20
3	D	582	ILE	CB-CG1-CD1	-7.21	98.66	113.80
2	C	1209	GLN	N-CA-CB	-7.20	99.76	110.85
2	C	704	MET	CA-C-O	7.19	128.19	119.49
2	C	1078	LYS	CB-CG-CD	7.19	127.83	111.30
1	A	76	GLU	N-CA-C	7.17	119.82	110.43
2	C	697	LYS	CB-CA-C	-7.17	97.71	109.46
2	C	454	ARG	NE-CZ-NH1	-7.17	114.33	121.50
4	E	4	VAL	N-CA-C	7.16	117.88	110.36
3	D	1214	PRO	CB-CA-C	-7.16	101.57	110.95
2	C	677	ASN	CA-C-N	-7.14	110.73	120.44
2	C	677	ASN	C-N-CA	-7.14	110.73	120.44
2	C	766	ASN	CB-CA-C	7.14	121.93	109.80
2	C	1176	LEU	CB-CG-CD2	-7.14	89.29	110.70
2	C	1328	LYS	N-CA-C	7.13	119.91	111.71
2	C	1107	MET	O-C-N	-7.12	114.31	122.86
3	D	641	ILE	CG1-CB-CG2	7.11	132.02	110.70
2	C	609	ILE	CB-CA-C	-7.10	102.42	112.22
2	C	1238	LEU	CA-C-O	-7.10	113.09	121.11
3	D	897	HIS	N-CA-CB	7.10	121.51	110.44
3	D	17	PHE	N-CA-CB	-7.09	100.16	111.43
3	D	807	LEU	CD1-CG-CD2	7.09	126.40	110.80
1	B	203	ILE	CA-CB-CG2	-7.08	98.46	110.50
2	C	929	ILE	N-CA-C	-7.08	104.08	111.58
3	D	529	GLY	C-N-CD	7.07	136.16	120.60
2	C	717	VAL	CG1-CB-CG2	-7.07	95.25	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	133	ASN	N-CA-CB	-7.05	100.05	110.49
2	C	10	ARG	CD-NE-CZ	-7.05	114.53	124.40
3	D	474	LEU	CB-CG-CD1	7.03	131.79	110.70
2	C	1323	PHE	CB-CA-C	-7.01	98.76	110.68
2	C	26	TYR	N-CA-C	7.01	121.28	112.87
3	D	334	LYS	CA-C-N	7.01	134.93	121.54
3	D	334	LYS	C-N-CA	7.01	134.93	121.54
3	D	1349	GLU	N-CA-C	-7.01	103.57	111.07
2	C	1074	GLY	CA-C-N	-7.01	114.77	122.27
2	C	1074	GLY	C-N-CA	-7.01	114.77	122.27
4	E	40	PRO	CA-C-O	-7.00	113.74	121.23
3	D	342	LEU	N-CA-CB	7.00	122.32	110.49
3	D	535	ARG	CA-C-O	-6.99	112.49	120.24
2	C	1237	HIS	CA-C-O	-6.98	113.66	120.92
3	D	250	ARG	CA-C-N	-6.97	113.52	120.21
3	D	250	ARG	C-N-CA	-6.97	113.52	120.21
2	C	1221	PHE	N-CA-CB	6.97	120.29	110.04
2	C	561	ILE	N-CA-C	-6.96	105.06	111.67
2	C	1159	VAL	O-C-N	6.96	129.54	122.79
2	C	801	ARG	CA-C-O	6.95	128.01	120.43
6	F	-3	DG	C2'-C3'-O3'	6.95	121.92	111.50
2	C	1086	PRO	CB-CA-C	-6.95	101.97	111.21
1	A	181	GLU	N-CA-CB	6.95	122.23	110.49
2	C	1101	LEU	N-CA-C	6.94	121.19	112.87
2	C	524	ILE	CA-CB-CG1	-6.93	98.62	110.40
1	A	182	ARG	O-C-N	6.91	131.87	123.16
2	C	688	GLN	CA-CB-CG	-6.91	100.28	114.10
3	D	423	LEU	CD1-CG-CD2	6.91	126.00	110.80
2	C	703	GLY	N-CA-C	6.90	124.40	114.67
3	D	488	ASN	CA-C-O	-6.90	113.16	120.55
2	C	517	GLN	N-CA-C	-6.90	103.98	112.88
3	D	574	VAL	CB-CA-C	-6.90	99.98	111.29
3	D	368	LEU	CB-CA-C	6.89	117.61	109.47
3	D	1244	GLN	N-CA-CB	6.89	120.69	110.49
2	C	1078	LYS	CA-C-N	-6.89	113.91	122.93
2	C	1078	LYS	C-N-CA	-6.89	113.91	122.93
2	C	929	ILE	N-CA-CB	-6.88	97.67	110.40
2	C	1177	ARG	CA-CB-CG	6.88	127.86	114.10
2	C	690	VAL	CA-CB-CG1	6.88	122.09	110.40
3	D	930	LEU	CB-CG-CD2	6.87	131.32	110.70
2	C	1094	VAL	CA-CB-CG1	-6.87	98.72	110.40
2	C	1237	HIS	N-CA-CB	-6.87	100.11	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	109	SER	CA-C-N	-6.87	112.57	119.99
3	D	109	SER	C-N-CA	-6.87	112.57	119.99
3	D	36	GLY	CA-C-O	-6.86	116.77	122.33
4	E	52	ARG	NH1-CZ-NH2	6.86	128.22	119.30
3	D	485	MET	CB-CA-C	-6.86	96.92	109.54
3	D	486	SER	N-CA-C	-6.86	104.88	113.18
2	C	1099	ASN	CA-C-O	-6.86	113.28	119.59
2	C	1296	ASP	CB-CA-C	-6.85	98.06	109.99
2	C	1145	ILE	N-CA-C	-6.85	104.09	110.53
2	C	1078	LYS	CA-C-O	-6.84	113.37	120.89
2	C	530	ILE	N-CA-CB	-6.83	102.53	111.82
2	C	1239	VAL	CB-CA-C	-6.83	96.26	111.77
2	C	522	SER	N-CA-C	6.83	122.64	111.37
2	C	808	ASN	CA-C-O	6.82	129.27	120.81
3	D	355	ILE	CA-CB-CG2	-6.82	98.90	110.50
3	D	453	VAL	CA-C-O	6.82	128.08	119.48
3	D	488	ASN	N-CA-CB	6.82	120.23	110.13
3	D	1344	LEU	N-CA-CB	-6.82	101.60	111.70
1	A	181	GLU	CA-C-N	-6.82	111.89	122.87
1	A	181	GLU	C-N-CA	-6.82	111.89	122.87
2	C	808	ASN	N-CA-CB	-6.82	101.94	112.30
3	D	1324	SER	N-CA-C	6.81	121.44	113.20
3	D	36	GLY	N-CA-C	-6.80	104.64	111.85
1	B	224	LEU	CD1-CG-CD2	6.79	125.75	110.80
3	D	1255	VAL	N-CA-C	6.79	117.49	110.36
3	D	1348	LYS	N-CA-CB	6.79	120.10	110.12
2	C	1231	TYR	N-CA-C	-6.78	95.99	107.99
2	C	677	ASN	OD1-CG-ND2	6.78	129.38	122.60
2	C	799	ASN	O-C-N	-6.77	115.31	123.10
3	D	344	GLY	O-C-N	-6.77	113.90	122.70
3	D	113	HIS	CA-C-O	-6.77	113.51	122.44
3	D	366	CYS	N-CA-CB	6.76	121.92	110.49
2	C	534	GLY	CA-C-N	6.76	128.29	119.84
2	C	534	GLY	C-N-CA	6.76	128.29	119.84
2	C	768	MET	CB-CA-C	6.75	120.15	110.02
4	E	52	ARG	NE-CZ-NH1	-6.75	114.75	121.50
2	C	1097	VAL	N-CA-C	6.75	117.56	108.11
2	C	1321	GLU	CA-C-N	-6.74	110.72	120.29
2	C	1321	GLU	C-N-CA	-6.74	110.72	120.29
1	B	187	VAL	N-CA-CB	6.74	121.96	111.99
2	C	731	ARG	N-CA-CB	6.73	123.17	111.39
2	C	1115	THR	N-CA-C	-6.73	103.88	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1145	PHE	N-CA-C	-6.73	104.55	112.89
2	C	1054	LEU	N-CA-CB	-6.71	99.61	111.08
3	D	470	VAL	CB-CA-C	-6.70	103.48	111.18
3	D	492	SER	O-C-N	6.69	127.51	121.35
2	C	693	LEU	N-CA-C	-6.68	103.24	111.40
2	C	1277	ALA	CA-C-N	-6.68	110.80	120.29
2	C	1277	ALA	C-N-CA	-6.68	110.80	120.29
3	D	309	ASN	N-CA-C	-6.68	105.13	113.28
2	C	1226	THR	CA-CB-CG2	-6.68	99.15	110.50
2	C	1051	LYS	CG-CD-CE	6.67	126.64	111.30
2	C	1246	ARG	CD-NE-CZ	-6.67	115.06	124.40
2	C	18	ARG	CG-CD-NE	6.65	126.64	112.00
2	C	145	ILE	CB-CG1-CD1	-6.65	99.83	113.80
2	C	550	VAL	CB-CA-C	-6.64	102.43	111.33
2	C	653	MET	CB-CA-C	-6.64	98.61	110.03
2	C	1198	LEU	CA-C-O	6.64	127.60	120.10
2	C	1317	PRO	CB-CA-C	-6.64	102.38	111.21
2	C	1069	ARG	CA-CB-CG	-6.63	100.84	114.10
3	D	808	VAL	CA-C-O	-6.62	112.50	120.78
3	D	470	VAL	CG1-CB-CG2	-6.62	96.23	110.80
3	D	1347	LEU	CA-C-N	-6.62	111.41	120.28
3	D	1347	LEU	C-N-CA	-6.62	111.41	120.28
2	C	1216	ARG	N-CA-C	-6.61	103.88	112.68
2	C	761	GLN	CB-CG-CD	-6.61	101.37	112.60
2	C	1195	ILE	N-CA-C	-6.61	103.80	111.00
3	D	1312	ALA	N-CA-C	-6.60	103.28	112.45
3	D	390	LEU	N-CA-C	6.60	120.92	112.34
2	C	800	MET	CA-CB-CG	6.60	127.29	114.10
2	C	1242	LYS	N-CA-C	6.59	121.45	112.68
2	C	929	ILE	CG1-CB-CG2	-6.59	90.93	110.70
3	D	427	PRO	CA-C-N	-6.59	114.01	122.77
3	D	427	PRO	C-N-CA	-6.59	114.01	122.77
2	C	157	PHE	CA-C-O	-6.59	113.40	121.11
2	C	1279	GLU	O-C-N	6.58	129.09	122.12
2	C	817	LEU	N-CA-C	6.58	119.96	109.24
2	C	698	PRO	N-CA-C	-6.56	100.89	111.19
2	C	681	MET	N-CA-C	-6.55	104.06	111.14
3	D	1253	ILE	CG1-CB-CG2	-6.55	91.06	110.70
2	C	177	ILE	CB-CA-C	-6.54	103.55	110.16
3	D	1309	ILE	CG1-CB-CG2	-6.54	91.08	110.70
3	D	513	MET	CB-CA-C	-6.54	100.62	110.88
3	D	598	LYS	CD-CE-NZ	6.54	132.82	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	670	PHE	N-CA-C	6.54	124.72	110.80
2	C	388	LEU	CB-CG-CD2	6.53	130.29	110.70
3	D	915	ILE	CB-CA-C	6.53	122.00	111.29
2	C	1283	ALA	CA-C-O	-6.53	113.79	120.84
3	D	641	ILE	CB-CG1-CD1	6.53	127.50	113.80
3	D	887	SER	CA-C-N	6.53	134.00	121.54
3	D	887	SER	C-N-CA	6.53	134.00	121.54
3	D	380	PHE	CA-C-O	6.52	127.46	120.55
3	D	452	LEU	CA-C-N	-6.51	112.14	121.52
3	D	452	LEU	C-N-CA	-6.51	112.14	121.52
3	D	423	LEU	CB-CA-C	-6.51	97.46	109.37
3	D	533	ALA	N-CA-C	-6.50	104.19	111.28
2	C	11	ILE	O-C-N	-6.50	116.35	123.18
2	C	782	VAL	CG1-CB-CG2	-6.50	96.50	110.80
2	C	702	THR	CA-C-N	-6.49	112.35	122.86
2	C	702	THR	C-N-CA	-6.49	112.35	122.86
2	C	1238	LEU	N-CA-C	6.48	120.09	109.72
3	D	442	ILE	O-C-N	6.48	130.61	123.09
3	D	889	ASP	N-CA-CB	6.47	119.65	109.82
3	D	473	THR	N-CA-C	6.46	121.22	109.32
3	D	505	ASP	CA-C-O	-6.46	112.54	119.97
3	D	798	ARG	CD-NE-CZ	6.46	133.45	124.40
2	C	816	ILE	CB-CA-C	-6.45	100.71	111.29
3	D	635	SER	CA-CB-OG	6.45	124.00	111.10
2	C	668	ILE	N-CA-C	6.45	113.42	107.56
3	D	807	LEU	CB-CG-CD1	-6.45	91.36	110.70
3	D	105	ILE	CB-CA-C	6.44	121.85	110.71
3	D	914	ALA	N-CA-C	6.43	121.01	111.04
2	C	12	ARG	NH1-CZ-NH2	6.43	127.66	119.30
2	C	705	GLU	O-C-N	6.42	129.74	122.22
3	D	767	LEU	CB-CG-CD2	6.42	129.95	110.70
4	E	4	VAL	N-CA-CB	-6.42	103.39	110.51
2	C	521	LEU	CB-CG-CD1	-6.41	91.46	110.70
3	D	253	VAL	O-C-N	6.41	128.41	121.10
3	D	355	ILE	CA-C-O	-6.41	113.47	120.71
2	C	1176	LEU	N-CA-C	6.41	120.71	113.02
3	D	588	PRO	CB-CG-CD	-6.40	85.61	106.10
2	C	446	ASP	N-CA-C	6.40	120.19	112.38
2	C	519	ASN	CB-CA-C	6.40	122.78	110.17
2	C	144	VAL	O-C-N	6.40	129.19	122.67
2	C	667	LEU	CA-C-N	-6.40	118.25	122.60
2	C	667	LEU	C-N-CA	-6.40	118.25	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ILE	N-CA-CB	-6.39	100.64	110.86
2	C	758	ARG	CA-C-O	6.39	128.32	121.55
2	C	1334	GLY	CA-C-N	-6.38	114.78	123.14
2	C	1334	GLY	C-N-CA	-6.38	114.78	123.14
3	D	610	ARG	NE-CZ-NH2	-6.38	113.46	119.20
3	D	375	GLU	N-CA-C	-6.38	103.57	112.12
2	C	97	ARG	CA-C-O	-6.38	113.81	120.70
2	C	555	TYR	CB-CA-C	6.38	120.78	110.96
3	D	337	ARG	NE-CZ-NH2	-6.38	113.46	119.20
3	D	19	ALA	O-C-N	-6.37	114.12	122.59
2	C	1072	ASN	CA-C-O	-6.37	114.90	120.88
2	C	886	LYS	CB-CA-C	6.36	121.80	110.16
3	D	368	LEU	CB-CG-CD1	-6.36	91.63	110.70
3	D	1148	ARG	NE-CZ-NH2	6.34	124.91	119.20
3	D	1323	ALA	CA-C-O	-6.34	113.77	120.55
2	C	1081	PRO	N-CA-CB	-6.34	96.60	103.25
2	C	72	SER	CB-CA-C	-6.33	108.25	115.79
1	A	72	GLU	CB-CA-C	-6.33	98.84	109.53
2	C	1100	PRO	CB-CA-C	-6.33	101.69	112.26
3	D	359	PRO	N-CA-CB	6.32	109.89	103.25
2	C	1076	ILE	CB-CG1-CD1	-6.32	100.52	113.80
2	C	788	SER	CB-CA-C	6.32	120.87	111.89
3	D	459	ALA	CA-C-O	6.32	127.18	120.36
4	E	40	PRO	CB-CA-C	-6.31	103.68	111.64
3	D	485	MET	CA-C-N	-6.31	109.27	121.58
3	D	485	MET	C-N-CA	-6.31	109.27	121.58
3	D	356	THR	CA-C-N	-6.31	111.93	120.95
3	D	356	THR	C-N-CA	-6.31	111.93	120.95
3	D	915	ILE	O-C-N	6.30	130.45	122.57
2	C	1223	ARG	CB-CG-CD	-6.30	96.81	111.30
2	C	764	CYS	CA-CB-SG	-6.28	99.95	114.40
2	C	1319	MET	CB-CG-SD	-6.28	93.87	112.70
3	D	637	ALA	CA-C-O	-6.28	113.30	120.58
2	C	1269	ARG	N-CA-CB	6.27	119.19	109.85
3	D	729	GLY	N-CA-C	-6.27	106.49	115.64
2	C	514	PHE	N-CA-C	-6.27	101.01	110.28
2	C	818	VAL	N-CA-CB	6.26	121.71	111.44
3	D	600	ALA	N-CA-C	-6.26	104.45	111.28
2	C	1298	VAL	CG1-CB-CG2	-6.25	97.04	110.80
3	D	488	ASN	O-C-N	6.25	129.73	122.17
2	C	452	ARG	CG-CD-NE	-6.24	98.26	112.00
2	C	12	ARG	CD-NE-CZ	-6.24	115.67	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	798	ARG	NH1-CZ-NH2	-6.23	111.20	119.30
3	D	363	LEU	CB-CG-CD1	6.22	129.37	110.70
3	D	629	PHE	CA-C-O	-6.22	114.24	120.90
2	C	144	VAL	CA-C-O	-6.22	113.92	121.13
3	D	1348	LYS	CB-CA-C	-6.22	100.47	110.79
2	C	518	ASN	O-C-N	-6.21	116.14	123.22
3	D	431	ARG	CG-CD-NE	-6.21	98.34	112.00
3	D	1262	ARG	NE-CZ-NH1	-6.21	115.29	121.50
3	D	1356	LEU	CD1-CG-CD2	-6.20	97.16	110.80
2	C	1308	ILE	N-CA-C	-6.20	104.25	111.00
3	D	438	GLU	N-CA-C	-6.20	100.63	109.62
3	D	744	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	B	43	LEU	CB-CG-CD1	-6.20	92.12	110.70
1	B	28	LEU	N-CA-CB	-6.19	100.85	110.57
3	D	340	GLN	CA-C-N	-6.19	109.71	121.54
3	D	340	GLN	C-N-CA	-6.19	109.71	121.54
3	D	536	LEU	CB-CG-CD1	6.19	129.26	110.70
2	C	1056	VAL	N-CA-CB	-6.17	101.32	111.44
3	D	1248	ILE	CG1-CB-CG2	-6.17	92.19	110.70
4	E	55	GLU	N-CA-C	-6.17	104.63	111.36
2	C	818	VAL	O-C-N	6.16	129.69	123.10
3	D	803	VAL	CA-CB-CG2	-6.16	99.93	110.40
3	D	443	GLU	N-CA-CB	6.16	119.49	109.95
3	D	1280	VAL	N-CA-C	-6.16	104.50	110.72
2	C	657	THR	N-CA-C	6.16	120.40	113.01
2	C	1273	MET	N-CA-CB	-6.15	100.74	110.22
2	C	1210	ILE	N-CA-C	-6.15	99.62	108.42
1	A	182	ARG	CA-C-O	-6.15	114.21	121.16
3	D	467	ALA	CB-CA-C	-6.14	99.09	109.83
3	D	764	ARG	NE-CZ-NH1	-6.13	115.37	121.50
3	D	702	GLN	N-CA-C	-6.13	100.91	110.17
2	C	817	LEU	N-CA-CB	-6.13	100.44	110.43
3	D	900	GLY	N-CA-C	6.13	122.89	114.92
2	C	1061	GLN	CA-C-N	-6.12	113.64	121.91
2	C	1061	GLN	C-N-CA	-6.12	113.64	121.91
3	D	401	VAL	N-CA-C	-6.12	104.33	111.00
2	C	716	ALA	CA-C-N	-6.11	115.22	123.10
2	C	716	ALA	C-N-CA	-6.11	115.22	123.10
3	D	894	VAL	CB-CA-C	6.11	121.31	111.29
2	C	529	ARG	N-CA-C	-6.11	99.40	108.99
2	C	921	PRO	CA-C-O	-6.10	114.38	121.34
3	D	583	VAL	CG1-CB-CG2	6.10	124.22	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	627	THR	CB-CA-C	6.10	122.39	110.67
2	C	1195	ILE	CG1-CB-CG2	-6.10	92.41	110.70
3	D	1363	TYR	CA-C-O	-6.10	114.42	120.82
3	D	1328	THR	N-CA-CB	6.10	119.37	110.47
1	A	51	MET	N-CA-CB	6.09	121.22	110.37
3	D	372	MET	CA-C-O	-6.09	112.97	119.97
3	D	797	THR	OG1-CB-CG2	-6.09	97.12	109.30
3	D	1280	VAL	N-CA-CB	6.09	119.72	110.58
2	C	502	VAL	CG1-CB-CG2	-6.09	97.41	110.80
2	C	787	PRO	CB-CA-C	6.08	118.99	110.17
2	C	690	VAL	N-CA-CB	6.08	119.72	111.21
3	D	1365	TYR	O-C-N	-6.07	114.50	122.39
3	D	112	ALA	CB-CA-C	-6.07	108.97	117.23
3	D	455	ALA	N-CA-C	-6.07	104.36	110.97
3	D	632	ALA	CB-CA-C	-6.07	100.53	110.85
3	D	442	ILE	CA-C-O	-6.07	114.41	120.90
3	D	361	LEU	CA-C-N	6.06	129.73	120.82
3	D	361	LEU	C-N-CA	6.06	129.73	120.82
3	D	927	GLY	N-CA-C	-6.05	107.49	114.69
3	D	1317	GLU	N-CA-C	6.05	118.37	111.11
3	D	78	LEU	CB-CA-C	6.04	122.44	110.42
3	D	434	ILE	CB-CA-C	6.03	119.14	110.33
2	C	578	TYR	O-C-N	6.03	129.88	122.34
2	C	661	VAL	N-CA-C	6.02	117.35	109.58
3	D	909	ILE	CB-CG1-CD1	-6.02	101.16	113.80
2	C	731	ARG	NE-CZ-NH1	-6.02	115.48	121.50
1	B	83	LEU	CD1-CG-CD2	6.01	124.03	110.80
2	C	520	PRO	CA-C-N	-6.01	111.75	120.29
2	C	520	PRO	C-N-CA	-6.01	111.75	120.29
3	D	466	MET	CB-CG-SD	-6.01	94.66	112.70
2	C	1115	THR	N-CA-CB	6.01	118.78	110.07
2	C	1192	GLU	CB-CA-C	-6.01	98.46	110.42
3	D	421	VAL	N-CA-CB	-6.01	105.22	112.07
3	D	599	LYS	O-C-N	6.01	128.34	122.09
2	C	814	ASP	N-CA-C	-6.01	105.13	112.88
2	C	523	GLU	CA-CB-CG	-6.00	102.09	114.10
5	M	183	GLN	N-CA-C	-6.00	105.22	112.54
2	C	752	ASN	CA-C-O	6.00	126.92	120.38
3	D	620	PHE	CB-CA-C	-6.00	100.65	110.85
2	C	676	ALA	CA-C-N	-6.00	110.48	121.52
2	C	676	ALA	C-N-CA	-6.00	110.48	121.52
2	C	705	GLU	N-CA-C	6.00	118.61	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	895	CYS	CB-CA-C	-5.99	98.89	109.62
2	C	770	CYS	N-CA-CB	5.99	118.76	110.07
1	A	88	LEU	CA-C-N	-5.99	113.96	122.94
1	A	88	LEU	C-N-CA	-5.99	113.96	122.94
3	D	1352	ILE	CB-CG1-CD1	-5.99	101.22	113.80
2	C	577	VAL	CA-CB-CG2	-5.99	100.22	110.40
2	C	79	VAL	N-CA-C	5.98	116.72	110.62
2	C	1102	GLY	CA-C-O	5.98	127.21	121.05
2	C	1291	LEU	N-CA-C	-5.98	104.33	111.69
3	D	834	PRO	CA-C-O	-5.98	114.42	122.08
1	B	179	PRO	CA-C-O	-5.98	116.89	121.31
3	D	115	TRP	CA-C-N	5.97	130.32	120.94
3	D	115	TRP	C-N-CA	5.97	130.32	120.94
3	D	470	VAL	CA-CB-CG1	-5.97	100.25	110.40
4	E	58	LEU	N-CA-C	5.96	118.74	111.82
3	D	802	ASP	N-CA-C	5.96	118.57	111.71
1	A	211	ILE	CB-CA-C	5.96	119.87	110.81
3	D	509	GLY	CA-C-N	-5.96	112.69	120.44
3	D	509	GLY	C-N-CA	-5.96	112.69	120.44
2	C	1070	HIS	N-CA-CB	5.96	118.78	110.56
3	D	917	VAL	CA-C-N	-5.95	111.07	120.47
3	D	917	VAL	C-N-CA	-5.95	111.07	120.47
2	C	707	ALA	N-CA-C	5.95	117.76	111.28
2	C	1210	ILE	CA-CB-CG2	5.95	120.61	110.50
2	C	453	ILE	N-CA-C	5.94	116.86	108.36
2	C	791	LEU	CB-CG-CD1	-5.94	92.87	110.70
5	M	185	PHE	CA-C-O	-5.94	112.01	120.51
2	C	124	MET	CB-CG-SD	-5.94	94.89	112.70
2	C	673	HIS	N-CA-CB	-5.94	100.46	110.49
3	D	897	HIS	CA-C-O	-5.93	112.33	119.27
2	C	832	HIS	CB-CA-C	-5.93	102.04	110.34
2	C	1075	VAL	CA-C-N	-5.93	114.95	122.37
2	C	1075	VAL	C-N-CA	-5.93	114.95	122.37
2	C	1266	GLY	CA-C-N	-5.93	109.78	121.41
2	C	1266	GLY	C-N-CA	-5.93	109.78	121.41
4	E	46	THR	OG1-CB-CG2	5.93	121.16	109.30
3	D	38	VAL	N-CA-CB	5.92	118.81	111.41
3	D	908	ILE	CB-CA-C	-5.92	103.32	111.49
2	C	520	PRO	CA-CB-CG	-5.92	93.26	104.50
2	C	1225	VAL	CA-C-O	-5.91	114.26	120.76
3	D	378	LYS	N-CA-C	5.91	122.88	109.81
1	A	94	GLY	CA-C-O	5.91	126.78	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	567	PRO	N-CA-C	-5.91	106.96	114.35
2	C	1281	TYR	CB-CA-C	-5.91	99.32	110.67
1	A	310	ARG	CA-C-N	5.91	126.65	120.03
1	A	310	ARG	C-N-CA	5.91	126.65	120.03
3	D	437	PHE	CE1-CZ-CE2	-5.91	109.37	120.00
2	C	801	ARG	N-CA-C	-5.90	99.62	109.24
2	C	1079	ILE	N-CA-C	5.90	116.30	107.51
3	D	17	PHE	CB-CA-C	5.90	121.98	110.30
5	M	141	ALA	N-CA-C	-5.90	104.77	111.14
2	C	1191	LYS	CA-C-O	-5.89	115.14	121.56
1	A	69	SER	CA-C-O	-5.89	115.04	121.87
2	C	654	ASP	N-CA-C	5.88	120.08	113.02
2	C	827	ARG	CA-C-N	-5.88	110.30	121.54
2	C	827	ARG	C-N-CA	-5.88	110.30	121.54
2	C	1071	GLY	CA-C-N	5.88	132.14	121.97
2	C	1071	GLY	C-N-CA	5.88	132.14	121.97
3	D	261	ALA	CA-C-O	-5.88	114.35	121.28
3	D	898	CYS	N-CA-C	-5.88	102.95	110.53
2	C	1321	GLU	N-CA-CB	5.87	118.87	110.06
3	D	115	TRP	N-CA-C	-5.87	104.79	111.07
1	A	130	ILE	CA-C-N	-5.86	110.34	121.54
1	A	130	ILE	C-N-CA	-5.86	110.34	121.54
2	C	678	ARG	NH1-CZ-NH2	-5.86	111.68	119.30
3	D	1309	ILE	CA-CB-CG1	5.86	120.37	110.40
3	D	1321	SER	O-C-N	-5.86	115.44	122.65
3	D	474	LEU	O-C-N	5.86	130.39	122.59
2	C	1172	LEU	N-CA-CB	5.86	118.73	110.12
3	D	506	VAL	CB-CA-C	-5.86	104.37	112.04
3	D	629	PHE	O-C-N	5.86	128.18	122.09
3	D	914	ALA	CA-C-N	-5.86	111.43	121.97
3	D	914	ALA	C-N-CA	-5.86	111.43	121.97
2	C	1309	VAL	N-CA-C	-5.85	103.77	111.09
2	C	1161	LEU	CD1-CG-CD2	-5.85	97.93	110.80
3	D	255	LEU	N-CA-C	5.85	119.43	110.36
3	D	332	LYS	CA-C-N	5.85	132.87	121.41
3	D	332	LYS	C-N-CA	5.85	132.87	121.41
3	D	587	LEU	CA-C-N	5.85	125.80	119.78
3	D	587	LEU	C-N-CA	5.85	125.80	119.78
2	C	1294	LYS	CB-CA-C	-5.84	100.37	110.72
2	C	762	ASN	CB-CA-C	-5.84	103.60	111.89
3	D	1352	ILE	O-C-N	-5.84	116.21	121.87
2	C	1225	VAL	CA-C-N	-5.84	112.83	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1225	VAL	C-N-CA	-5.84	112.83	121.24
3	D	738	ARG	N-CA-C	-5.83	105.00	111.71
2	C	453	ILE	N-CA-CB	5.83	117.98	110.99
2	C	1052	VAL	CG1-CB-CG2	-5.83	97.98	110.80
2	C	1159	VAL	CA-CB-CG2	5.82	120.30	110.40
3	D	1355	ARG	NE-CZ-NH2	5.82	124.44	119.20
3	D	806	ASP	N-CA-CB	-5.82	100.21	110.39
7	G	-17	DT	C5'-C4'-O4'	5.81	118.12	109.40
2	C	563	THR	O-C-N	5.81	126.36	121.83
3	D	618	VAL	CA-CB-CG2	5.81	120.28	110.40
2	C	1072	ASN	CA-C-N	-5.81	113.07	122.36
2	C	1072	ASN	C-N-CA	-5.81	113.07	122.36
2	C	816	ILE	N-CA-CB	5.80	120.81	111.23
3	D	246	PRO	CA-C-N	5.80	125.18	118.85
3	D	246	PRO	C-N-CA	5.80	125.18	118.85
2	C	1226	THR	CA-C-O	-5.80	113.85	120.58
3	D	438	GLU	CB-CA-C	5.80	116.45	109.31
1	A	182	ARG	N-CA-CB	5.80	120.13	110.85
3	D	1344	LEU	N-CA-C	5.79	119.39	111.39
2	C	1216	ARG	CD-NE-CZ	-5.79	116.29	124.40
3	D	76	LYS	CD-CE-NZ	5.79	130.43	111.90
3	D	539	SER	O-C-N	-5.79	110.30	121.42
1	A	146	VAL	CA-C-O	-5.78	114.34	120.53
3	D	476	ALA	CA-C-N	-5.78	112.46	120.38
3	D	476	ALA	C-N-CA	-5.78	112.46	120.38
2	C	836	LEU	CA-C-O	-5.77	113.91	120.32
3	D	908	ILE	CG1-CB-CG2	-5.77	93.38	110.70
2	C	537	GLY	N-CA-C	5.77	118.41	110.56
2	C	1265	PHE	CB-CA-C	-5.77	101.69	112.30
3	D	385	LEU	CB-CA-C	-5.76	101.23	110.79
3	D	640	GLY	N-CA-C	-5.76	102.00	110.87
2	C	1194	GLU	CA-C-O	5.76	126.47	119.38
2	C	1099	ASN	CA-C-N	5.76	126.15	119.47
2	C	1099	ASN	C-N-CA	5.76	126.15	119.47
3	D	738	ARG	CA-C-O	-5.76	113.59	120.10
3	D	95	THR	OG1-CB-CG2	-5.75	97.79	109.30
2	C	700	VAL	N-CA-C	-5.75	99.89	108.46
3	D	858	VAL	N-CA-CB	5.75	119.26	111.21
3	D	901	ARG	NE-CZ-NH2	-5.75	114.03	119.20
4	E	28	ARG	NE-CZ-NH2	-5.75	114.03	119.20
2	C	721	GLY	N-CA-C	5.75	121.39	112.60
6	F	2	DG	N9-C1'-C2'	-5.75	104.88	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1244	HIS	O-C-N	-5.74	115.16	121.76
3	D	92	VAL	CA-C-O	5.74	127.96	120.78
1	A	230	ALA	N-CA-C	-5.73	105.55	112.54
3	D	740	LEU	CD1-CG-CD2	5.73	123.41	110.80
3	D	793	SER	CA-C-N	-5.73	113.12	120.34
3	D	793	SER	C-N-CA	-5.73	113.12	120.34
2	C	1324	ASN	CA-C-N	-5.73	113.34	120.56
2	C	1324	ASN	C-N-CA	-5.73	113.34	120.56
3	D	464	ASP	N-CA-C	5.72	117.68	110.24
3	D	835	LEU	CD1-CG-CD2	-5.72	98.22	110.80
3	D	767	LEU	O-C-N	-5.71	114.99	122.59
3	D	809	VAL	N-CA-C	5.71	121.22	109.34
2	C	818	VAL	CA-C-O	-5.71	114.28	120.67
3	D	741	ALA	CA-C-N	-5.71	115.22	122.19
3	D	741	ALA	C-N-CA	-5.71	115.22	122.19
2	C	184	LEU	CB-CG-CD1	5.71	127.81	110.70
1	A	183	ILE	N-CA-C	5.70	117.04	107.18
2	C	454	ARG	NH1-CZ-NH2	5.70	126.71	119.30
2	C	1129	ASN	N-CA-C	-5.70	104.97	111.07
3	D	362	ARG	CD-NE-CZ	5.70	132.38	124.40
5	M	111	VAL	N-CA-C	-5.70	103.77	110.21
2	C	11	ILE	N-CA-CB	-5.69	103.51	111.25
3	D	635	SER	N-CA-C	-5.69	105.17	111.71
1	A	46	ILE	CA-CB-CG1	5.69	120.08	110.40
1	A	125	LYS	CD-CE-NZ	5.69	130.11	111.90
2	C	560	PRO	CA-C-N	-5.69	115.86	122.63
2	C	560	PRO	C-N-CA	-5.69	115.86	122.63
2	C	5	TYR	CA-C-O	-5.69	112.38	120.51
2	C	10	ARG	CA-C-N	-5.69	116.14	123.19
2	C	10	ARG	C-N-CA	-5.69	116.14	123.19
2	C	551	HIS	N-CA-C	-5.69	103.00	110.39
3	D	1328	THR	N-CA-C	-5.69	106.47	113.41
3	D	899	TYR	OH-CZ-CE2	-5.69	102.84	119.90
3	D	456	ALA	CA-C-O	-5.68	114.85	120.70
1	A	183	ILE	CA-CB-CG1	-5.68	100.74	110.40
3	D	40	LYS	N-CA-CB	5.68	121.42	111.19
1	A	175	ALA	CA-C-N	-5.68	112.10	122.38
1	A	175	ALA	C-N-CA	-5.68	112.10	122.38
2	C	688	GLN	N-CA-C	-5.68	105.93	112.92
3	D	380	PHE	CB-CG-CD1	-5.68	111.04	120.70
5	M	190	VAL	CA-C-N	-5.68	110.70	121.54
5	M	190	VAL	C-N-CA	-5.68	110.70	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	149	LEU	CA-C-O	5.67	126.25	120.24
3	D	768	ASN	N-CA-C	-5.67	101.63	110.42
2	C	1314	GLN	N-CA-CB	-5.67	101.83	111.69
3	D	731	ARG	CG-CD-NE	5.67	124.47	112.00
3	D	627	THR	N-CA-C	-5.67	105.25	111.82
2	C	1263	ALA	CB-CA-C	-5.66	99.15	110.42
3	D	34	SER	N-CA-C	5.66	118.45	109.96
2	C	729	ALA	N-CA-C	5.66	117.92	111.02
3	D	801	VAL	N-CA-CB	5.66	116.79	110.51
2	C	1301	ARG	CG-CD-NE	-5.66	99.56	112.00
2	C	1223	ARG	CA-C-N	-5.66	114.93	120.98
2	C	1223	ARG	C-N-CA	-5.66	114.93	120.98
2	C	1244	HIS	CB-CG-CD2	5.66	138.55	131.20
3	D	810	THR	N-CA-C	5.65	120.20	111.56
2	C	575	LEU	CB-CA-C	-5.65	100.34	109.72
3	D	1261	LEU	N-CA-CB	5.64	118.84	110.49
2	C	563	THR	CA-C-N	-5.63	114.13	119.76
2	C	563	THR	C-N-CA	-5.63	114.13	119.76
1	A	88	LEU	CD1-CG-CD2	5.63	123.19	110.80
2	C	559	CYS	CA-C-N	-5.63	112.80	119.84
2	C	559	CYS	C-N-CA	-5.63	112.80	119.84
3	D	624	ILE	N-CA-C	-5.63	104.88	110.62
3	D	1147	ALA	N-CA-C	-5.63	103.68	111.28
2	C	75	LEU	CA-C-N	-5.63	117.46	122.47
2	C	75	LEU	C-N-CA	-5.63	117.46	122.47
3	D	547	ARG	CA-C-O	5.62	128.36	121.84
3	D	300	GLN	CB-CA-C	-5.62	101.46	110.79
2	C	651	ASP	N-CA-C	5.62	120.12	113.16
5	M	125	MET	CB-CA-C	5.61	120.39	110.85
2	C	1295	SER	N-CA-CB	5.61	119.97	110.49
3	D	925	GLU	O-C-N	5.61	125.98	120.71
2	C	928	VAL	N-CA-CB	5.61	117.39	111.00
2	C	1255	THR	N-CA-CB	5.60	119.95	110.49
3	D	540	GLY	N-CA-C	-5.59	108.32	115.42
3	D	100	GLU	CB-CG-CD	5.59	122.11	112.60
1	A	101	THR	CA-C-O	-5.59	114.57	121.06
2	C	1301	ARG	NH1-CZ-NH2	-5.59	112.03	119.30
3	D	917	VAL	CG1-CB-CG2	5.59	123.10	110.80
2	C	884	VAL	CA-C-N	-5.59	115.79	122.16
2	C	884	VAL	C-N-CA	-5.59	115.79	122.16
2	C	687	ARG	NE-CZ-NH1	5.59	127.09	121.50
2	C	817	LEU	CD1-CG-CD2	-5.59	98.51	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	421	VAL	CA-CB-CG2	-5.59	100.90	110.40
3	D	495	ASN	N-CA-C	-5.58	105.19	112.23
1	A	64	VAL	CG1-CB-CG2	-5.58	98.52	110.80
2	C	801	ARG	CA-C-N	-5.58	113.30	122.67
2	C	801	ARG	C-N-CA	-5.58	113.30	122.67
3	D	1310	THR	N-CA-CB	5.58	118.83	110.19
2	C	1099	ASN	CB-CA-C	-5.57	103.98	110.17
3	D	253	VAL	N-CA-CB	5.57	119.01	111.21
4	E	20	VAL	CG1-CB-CG2	-5.57	98.55	110.80
5	M	190	VAL	CG1-CB-CG2	-5.57	98.55	110.80
3	D	440	VAL	CG1-CB-CG2	5.57	123.05	110.80
2	C	589	THR	CA-C-N	-5.57	114.59	120.66
2	C	589	THR	C-N-CA	-5.57	114.59	120.66
1	B	207	THR	CA-CB-CG2	-5.57	101.04	110.50
3	D	451	PRO	CB-CG-CD	5.57	123.91	106.10
2	C	445	ILE	N-CA-C	-5.56	105.10	110.72
2	C	1201	LEU	CD1-CG-CD2	-5.56	98.56	110.80
2	C	681	MET	CA-C-O	-5.56	114.97	120.70
3	D	1331	VAL	CG1-CB-CG2	-5.56	98.57	110.80
3	D	915	ILE	CA-CB-CG1	-5.56	100.95	110.40
2	C	452	ARG	CD-NE-CZ	-5.55	116.63	124.40
2	C	932	GLN	N-CA-C	5.55	119.79	111.96
2	C	734	ILE	CG1-CB-CG2	-5.55	94.06	110.70
1	B	228	LEU	CD1-CG-CD2	5.54	123.00	110.80
3	D	416	ILE	CA-CB-CG1	-5.54	100.98	110.40
1	A	79	LEU	CB-CG-CD2	5.54	127.31	110.70
1	A	10	LYS	CB-CA-C	5.53	116.11	109.31
2	C	177	ILE	CB-CG1-CD1	-5.53	102.19	113.80
3	D	349	TYR	CB-CA-C	-5.53	99.42	110.42
3	D	354	VAL	N-CA-CB	-5.52	100.68	110.95
3	D	631	TYR	CA-C-N	-5.52	112.45	120.29
3	D	631	TYR	C-N-CA	-5.52	112.45	120.29
1	B	56	VAL	CG1-CB-CG2	5.52	122.95	110.80
5	M	198	CYS	N-CA-CB	5.52	118.24	110.12
3	D	422	LEU	CB-CG-CD1	-5.52	94.14	110.70
1	A	140	ILE	CA-CB-CG1	-5.52	101.02	110.40
2	C	1246	ARG	CG-CD-NE	5.52	124.14	112.00
3	D	486	SER	CA-C-O	5.52	126.17	119.11
2	C	699	LEU	N-CA-CB	-5.51	101.42	110.40
2	C	1184	THR	CA-CB-CG2	-5.51	101.14	110.50
2	C	1246	ARG	N-CA-C	5.51	118.55	109.85
3	D	1327	GLU	CA-C-N	-5.51	112.23	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1327	GLU	C-N-CA	-5.51	112.23	122.09
2	C	688	GLN	N-CA-CB	5.50	118.60	110.56
1	B	182	ARG	CA-C-O	5.50	127.20	120.60
2	C	4	SER	CA-C-O	-5.50	113.49	120.20
2	C	452	ARG	NE-CZ-NH2	-5.50	114.25	119.20
3	D	1280	VAL	CG1-CB-CG2	5.50	122.91	110.80
1	A	44	ARG	CD-NE-CZ	-5.50	116.70	124.40
2	C	873	ILE	CA-C-N	-5.50	115.66	123.08
2	C	873	ILE	C-N-CA	-5.50	115.66	123.08
2	C	1229	TYR	CA-CB-CG	-5.50	104.00	113.90
2	C	1259	LEU	CB-CG-CD1	-5.50	94.21	110.70
3	D	598	LYS	N-CA-C	5.49	117.07	111.14
3	D	1354	GLY	CA-C-O	5.49	125.94	119.46
3	D	115	TRP	CH2-CZ2-CE2	-5.49	110.37	117.50
3	D	57	PHE	CB-CA-C	5.48	121.33	110.42
2	C	1324	ASN	CA-C-O	5.48	126.36	120.55
3	D	439	PRO	CA-N-CD	-5.48	104.33	112.00
2	C	525	THR	CA-C-N	-5.48	112.51	120.29
2	C	525	THR	C-N-CA	-5.48	112.51	120.29
3	D	442	ILE	CB-CA-C	-5.48	101.17	111.30
2	C	577	VAL	CG1-CB-CG2	-5.47	98.76	110.80
3	D	353	SER	CA-CB-OG	-5.47	100.15	111.10
1	A	182	ARG	CB-CA-C	-5.47	99.37	109.37
2	C	516	ASP	CA-C-N	-5.47	114.07	122.60
2	C	516	ASP	C-N-CA	-5.47	114.07	122.60
3	D	483	LEU	CD1-CG-CD2	-5.46	98.78	110.80
2	C	1265	PHE	CA-C-N	-5.46	114.36	120.53
2	C	1265	PHE	C-N-CA	-5.46	114.36	120.53
3	D	794	GLY	O-C-N	5.46	128.62	122.34
3	D	892	PHE	N-CA-CB	-5.46	101.89	110.46
4	E	19	LEU	CB-CG-CD1	-5.46	94.32	110.70
2	C	1083	GLU	N-CA-C	5.46	119.04	112.38
3	D	1313	SER	CA-CB-OG	-5.46	100.18	111.10
2	C	1227	VAL	CA-CB-CG1	-5.46	101.12	110.40
3	D	118	LYS	CD-CE-NZ	-5.46	94.44	111.90
2	C	515	MET	CA-CB-CG	-5.45	103.19	114.10
2	C	1301	ARG	N-CA-C	5.45	118.14	111.82
3	D	99	ARG	CG-CD-NE	-5.45	100.01	112.00
3	D	548	VAL	CG1-CB-CG2	-5.45	98.81	110.80
2	C	1097	VAL	CA-CB-CG2	-5.45	101.14	110.40
2	C	1243	MET	CG-SD-CE	-5.45	88.91	100.90
3	D	97	VAL	CG1-CB-CG2	5.45	122.78	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	721	GLY	CA-C-O	-5.45	114.85	122.36
3	D	525	MET	CG-SD-CE	-5.45	88.92	100.90
2	C	1337	ILE	CA-CB-CG2	5.44	119.75	110.50
3	D	316	ILE	N-CA-C	5.44	120.65	109.34
2	C	1124	ILE	CB-CG1-CD1	-5.44	102.39	113.80
2	C	1145	ILE	CA-CB-CG2	5.44	119.74	110.50
3	D	92	VAL	N-CA-C	5.44	120.65	109.34
2	C	771	VAL	O-C-N	5.43	128.13	122.54
3	D	7	PHE	CB-CA-C	5.43	119.10	110.19
2	C	144	VAL	CA-CB-CG2	-5.43	101.18	110.40
2	C	1072	ASN	CA-CB-CG	-5.42	107.18	112.60
2	C	1075	VAL	CA-CB-CG1	-5.42	101.18	110.40
3	D	1329	THR	OG1-CB-CG2	5.42	120.14	109.30
2	C	1327	LEU	CB-CA-C	-5.42	101.80	110.79
3	D	908	ILE	O-C-N	5.42	129.56	122.47
3	D	427	PRO	CB-CA-C	-5.41	102.63	111.56
3	D	504	GLN	CB-CG-CD	-5.41	103.40	112.60
2	C	553	THR	N-CA-C	-5.41	106.36	113.17
2	C	771	VAL	CB-CA-C	-5.41	105.40	111.45
3	D	598	LYS	CB-CG-CD	5.41	123.73	111.30
2	C	133	ASN	N-CA-C	-5.40	106.36	113.17
3	D	304	ASP	CB-CA-C	-5.40	100.30	110.67
2	C	1111	GLN	CA-C-N	-5.40	113.65	120.56
2	C	1111	GLN	C-N-CA	-5.40	113.65	120.56
3	D	639	VAL	CA-C-O	5.40	126.68	120.90
3	D	376	LEU	CB-CG-CD1	-5.40	94.50	110.70
2	C	564	PRO	N-CA-C	-5.39	102.72	111.19
2	C	127	ILE	CA-C-N	-5.39	114.17	119.99
2	C	127	ILE	C-N-CA	-5.39	114.17	119.99
2	C	1292	THR	OG1-CB-CG2	5.39	120.08	109.30
2	C	1175	ASN	CB-CA-C	5.39	120.01	110.85
3	D	352	ARG	NE-CZ-NH2	5.39	124.05	119.20
3	D	431	ARG	NE-CZ-NH2	-5.39	114.35	119.20
4	E	51	LEU	CD1-CG-CD2	-5.39	98.95	110.80
2	C	667	LEU	N-CA-CB	-5.39	102.04	110.44
3	D	451	PRO	CA-C-N	-5.39	112.52	120.38
3	D	451	PRO	C-N-CA	-5.39	112.52	120.38
3	D	451	PRO	CA-CB-CG	-5.39	94.27	104.50
3	D	354	VAL	CA-CB-CG2	-5.38	101.25	110.40
3	D	416	ILE	CG1-CB-CG2	5.38	126.85	110.70
1	A	181	GLU	CA-C-O	-5.38	112.82	120.51
2	C	822	VAL	CA-CB-CG2	-5.38	101.26	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	687	ARG	CB-CG-CD	5.38	123.67	111.30
2	C	857	VAL	O-C-N	5.38	129.01	123.20
2	C	1244	HIS	CB-CG-ND1	-5.38	114.64	122.70
3	D	605	LEU	CB-CA-C	-5.37	100.70	110.63
2	C	1256	GLN	CB-CA-C	-5.37	104.67	111.86
2	C	720	ARG	CA-C-N	-5.36	115.50	121.83
2	C	720	ARG	C-N-CA	-5.36	115.50	121.83
3	D	783	LEU	CA-C-N	-5.36	111.21	121.94
3	D	783	LEU	C-N-CA	-5.36	111.21	121.94
3	D	884	SER	CA-C-O	-5.36	115.68	121.36
2	C	1243	MET	CA-CB-CG	-5.35	103.39	114.10
3	D	1332	LEU	CB-CG-CD2	-5.35	94.64	110.70
2	C	531	SER	CA-C-O	5.35	126.38	120.71
3	D	721	SER	CA-C-O	-5.35	115.39	121.00
2	C	1108	ASN	OD1-CG-ND2	-5.34	117.26	122.60
3	D	1355	ARG	CD-NE-CZ	-5.34	116.92	124.40
3	D	1329	THR	O-C-N	5.34	127.86	122.09
2	C	1297	ASP	CA-C-N	-5.34	114.37	120.88
2	C	1297	ASP	C-N-CA	-5.34	114.37	120.88
2	C	682	GLY	N-CA-C	-5.34	105.94	112.77
3	D	1355	ARG	CB-CA-C	5.33	120.26	110.24
2	C	704	MET	O-C-N	-5.33	115.46	122.39
2	C	712	SER	CB-CA-C	-5.33	100.44	110.67
3	D	1327	GLU	N-CA-CB	-5.33	102.18	110.55
2	C	1222	GLU	N-CA-C	-5.33	101.78	110.20
3	D	1355	ARG	CB-CG-CD	-5.32	99.06	111.30
2	C	1057	LYS	CG-CD-CE	5.32	123.53	111.30
3	D	380	PHE	CB-CG-CD2	5.32	129.74	120.70
3	D	469	HIS	O-C-N	5.32	129.44	123.27
2	C	548	ARG	CB-CG-CD	5.32	123.53	111.30
3	D	362	ARG	N-CA-CB	-5.31	101.43	109.92
2	C	1222	GLU	CA-C-O	-5.31	115.00	121.05
3	D	899	TYR	CA-CB-CG	-5.30	104.36	113.90
2	C	1243	MET	N-CA-C	5.30	122.09	110.80
3	D	834	PRO	CB-CA-C	-5.30	104.01	110.95
3	D	908	ILE	CB-CG1-CD1	-5.30	102.68	113.80
3	D	926	PRO	N-CA-C	-5.30	103.24	111.13
2	C	1113	LEU	CD1-CG-CD2	-5.29	99.15	110.80
3	D	1256	ILE	CA-C-O	5.29	126.78	121.17
3	D	250	ARG	NE-CZ-NH1	-5.29	116.21	121.50
4	E	19	LEU	CB-CG-CD2	5.29	126.57	110.70
2	C	75	LEU	CB-CG-CD1	5.29	126.56	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1239	VAL	CA-CB-CG2	-5.28	101.42	110.40
3	D	220	ARG	CG-CD-NE	5.28	123.61	112.00
3	D	807	LEU	CA-C-O	5.28	127.54	121.47
2	C	524	ILE	N-CA-C	5.28	115.72	110.23
3	D	435	GLN	CB-CG-CD	-5.28	103.63	112.60
3	D	783	LEU	O-C-N	5.27	128.15	122.15
2	C	931	VAL	CA-CB-CG2	-5.26	101.45	110.40
2	C	1095	ASP	CA-C-N	-5.26	112.50	121.97
2	C	1095	ASP	C-N-CA	-5.26	112.50	121.97
3	D	528	THR	N-CA-C	5.26	117.65	108.76
3	D	245	LEU	N-CA-C	-5.26	103.03	110.29
4	E	19	LEU	CB-CA-C	-5.26	102.06	110.79
1	A	55	ALA	CA-C-N	-5.26	113.04	120.35
1	A	55	ALA	C-N-CA	-5.26	113.04	120.35
3	D	499	ILE	CA-C-N	-5.26	112.51	121.97
3	D	499	ILE	C-N-CA	-5.26	112.51	121.97
2	C	1050	VAL	CB-CA-C	-5.25	102.41	110.50
3	D	338	PHE	CA-C-O	5.25	126.81	120.92
3	D	352	ARG	NH1-CZ-NH2	-5.25	112.47	119.30
2	C	920	VAL	N-CA-C	5.25	114.74	108.96
2	C	1230	MET	O-C-N	-5.25	116.33	123.10
3	D	1237	VAL	CG1-CB-CG2	-5.25	99.25	110.80
2	C	143	ARG	NE-CZ-NH1	-5.25	116.25	121.50
2	C	784	ALA	N-CA-C	5.25	118.14	109.85
3	D	250	ARG	NH1-CZ-NH2	5.25	126.12	119.30
3	D	467	ALA	CA-C-N	-5.25	115.65	122.94
3	D	467	ALA	C-N-CA	-5.25	115.65	122.94
3	D	551	ARG	N-CA-C	-5.24	101.16	109.76
2	C	702	THR	OG1-CB-CG2	-5.24	98.81	109.30
2	C	1121	ALA	CA-C-O	-5.24	114.42	120.24
2	C	528	ARG	CG-CD-NE	-5.24	100.47	112.00
2	C	914	LYS	CG-CD-CE	5.24	123.34	111.30
3	D	430	HIS	CA-C-O	-5.23	115.27	121.60
2	C	758	ARG	NE-CZ-NH1	-5.23	116.27	121.50
2	C	920	VAL	CB-CA-C	-5.23	105.75	110.88
2	C	19	PRO	CA-C-N	-5.23	114.45	122.87
2	C	19	PRO	C-N-CA	-5.23	114.45	122.87
2	C	1267	GLY	N-CA-C	5.23	125.57	113.18
3	D	342	LEU	CD1-CG-CD2	-5.23	99.30	110.80
3	D	376	LEU	CD1-CG-CD2	5.23	122.30	110.80
4	E	17	PHE	CB-CA-C	-5.23	100.02	110.42
2	C	517	GLN	CA-C-N	-5.22	114.82	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	517	GLN	C-N-CA	-5.22	114.82	122.19
3	D	1144	LEU	N-CA-C	-5.22	106.06	112.90
2	C	1279	GLU	N-CA-C	-5.22	105.59	111.28
3	D	243	PRO	CB-CA-C	-5.22	103.16	110.63
3	D	803	VAL	CB-CA-C	-5.22	105.36	111.94
3	D	365	GLN	CA-CB-CG	-5.22	103.66	114.10
3	D	1264	ALA	N-CA-C	5.22	117.55	110.35
2	C	816	ILE	CG1-CB-CG2	-5.22	95.05	110.70
3	D	481	ARG	CD-NE-CZ	-5.22	117.10	124.40
2	C	1046	VAL	CB-CA-C	-5.21	101.47	110.65
3	D	332	LYS	CA-CB-CG	-5.21	103.67	114.10
3	D	361	LEU	CD1-CG-CD2	-5.21	99.33	110.80
2	C	1131	MET	CB-CA-C	5.21	119.14	110.90
2	C	1117	LEU	CB-CG-CD1	-5.21	95.08	110.70
3	D	888	CYS	CA-C-N	-5.21	113.55	120.79
3	D	888	CYS	C-N-CA	-5.21	113.55	120.79
1	B	230	ALA	CB-CA-C	-5.21	101.83	110.68
3	D	693	VAL	CG1-CB-CG2	-5.20	99.35	110.80
4	E	45	LYS	CA-CB-CG	5.20	124.50	114.10
2	C	1073	LYS	CA-CB-CG	-5.20	103.70	114.10
5	M	131	THR	CA-C-N	5.20	126.34	119.84
5	M	131	THR	C-N-CA	5.20	126.34	119.84
3	D	725	MET	N-CA-C	-5.20	105.53	111.14
1	A	44	ARG	NE-CZ-NH2	5.19	123.87	119.20
3	D	808	VAL	O-C-N	-5.19	116.08	122.57
2	C	637	ARG	NE-CZ-NH1	-5.19	116.31	121.50
2	C	520	PRO	N-CA-C	5.18	122.18	113.78
2	C	1304	MET	CB-CA-C	-5.18	102.98	110.96
2	C	170	VAL	N-CA-CB	-5.18	105.37	111.90
3	D	454	CYS	CA-CB-SG	-5.18	102.48	114.40
3	D	481	ARG	N-CA-CB	5.18	117.92	110.20
6	F	-1	DC	O5'-P-OP1	-5.18	93.46	109.00
2	C	1131	MET	CG-SD-CE	5.18	112.29	100.90
2	C	608	ALA	N-CA-C	5.17	117.66	111.71
2	C	1151	LEU	CA-CB-CG	5.17	134.41	116.30
3	D	220	ARG	NE-CZ-NH1	-5.17	116.33	121.50
3	D	332	LYS	CB-CA-C	5.17	121.82	112.30
3	D	901	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	A	171	LEU	CD1-CG-CD2	-5.17	99.42	110.80
2	C	1096	ILE	CA-CB-CG2	-5.17	101.71	110.50
2	C	1059	ARG	CA-CB-CG	-5.17	103.76	114.10
3	D	428	THR	CA-C-N	-5.17	112.88	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	428	THR	C-N-CA	-5.17	112.88	122.60
3	D	1355	ARG	CA-C-O	-5.17	115.58	121.68
1	B	56	VAL	N-CA-CB	-5.17	105.40	111.39
3	D	336	GLY	N-CA-C	-5.17	104.69	112.60
2	C	141	THR	N-CA-C	-5.16	101.22	109.23
2	C	176	ILE	CB-CA-C	5.16	118.26	110.98
3	D	397	ALA	O-C-N	5.16	127.39	122.07
3	D	436	ALA	CA-C-N	-5.16	113.41	121.87
3	D	436	ALA	C-N-CA	-5.16	113.41	121.87
6	F	0	DC	O5'-P-OP2	-5.16	92.52	108.00
3	D	1330	ARG	O-C-N	5.16	127.45	122.09
1	A	48	LEU	CB-CG-CD2	-5.15	95.24	110.70
3	D	1144	LEU	CB-CG-CD2	-5.15	95.24	110.70
3	D	298	MET	CB-CG-SD	-5.15	97.24	112.70
2	C	1101	LEU	CA-C-N	5.15	125.81	119.99
2	C	1101	LEU	C-N-CA	5.15	125.81	119.99
3	D	832	LYS	N-CA-C	5.15	116.70	111.14
3	D	621	ALA	O-C-N	5.14	127.37	122.07
2	C	1205	PRO	CA-C-N	5.14	127.42	120.38
2	C	1205	PRO	C-N-CA	5.14	127.42	120.38
3	D	472	LEU	CB-CA-C	-5.14	107.97	114.40
3	D	737	ILE	CA-CB-CG1	-5.14	101.66	110.40
3	D	800	LEU	N-CA-C	-5.14	105.75	111.36
2	C	829	THR	CA-CB-OG1	-5.14	101.89	109.60
3	D	111	THR	CA-C-O	-5.14	115.62	121.58
3	D	808	VAL	CA-CB-CG1	5.14	119.14	110.40
3	D	536	LEU	N-CA-CB	5.14	117.41	109.91
3	D	1363	TYR	CA-C-N	-5.13	113.03	121.19
3	D	1363	TYR	C-N-CA	-5.13	113.03	121.19
3	D	899	TYR	N-CA-CB	5.13	119.16	110.49
1	A	35	PHE	O-C-N	5.13	129.49	122.46
6	F	9	DT	C4'-C3'-O3'	5.13	117.69	110.00
2	C	451	ARG	NE-CZ-NH1	-5.13	116.37	121.50
3	D	63	GLY	CA-C-N	5.13	126.47	120.98
3	D	63	GLY	C-N-CA	5.13	126.47	120.98
3	D	366	CYS	O-C-N	5.13	129.41	122.59
3	D	538	ARG	N-CA-C	-5.13	106.71	113.17
3	D	777	HIS	CA-C-N	-5.13	113.88	120.34
3	D	777	HIS	C-N-CA	-5.13	113.88	120.34
3	D	1260	MET	N-CA-CB	-5.13	102.41	110.46
3	D	502	PRO	CA-C-N	-5.12	113.86	123.03
3	D	502	PRO	C-N-CA	-5.12	113.86	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	126	TRP	CA-C-O	5.12	125.89	120.10
1	B	35	PHE	O-C-N	5.12	129.48	122.46
3	D	619	ILE	O-C-N	5.12	128.60	121.84
3	D	774	ILE	CG1-CB-CG2	5.12	126.06	110.70
3	D	767	LEU	N-CA-C	5.12	121.71	110.80
1	A	86	LYS	O-C-N	5.12	127.54	122.12
1	B	44	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	C	1227	VAL	CA-C-O	-5.12	114.90	121.40
2	C	1264	GLN	O-C-N	5.12	129.39	122.59
2	C	758	ARG	N-CA-CB	-5.11	102.52	110.04
2	C	143	ARG	CA-C-N	5.11	127.43	120.63
2	C	143	ARG	C-N-CA	5.11	127.43	120.63
2	C	1231	TYR	N-CA-CB	5.11	118.96	110.47
2	C	520	PRO	N-CA-CB	5.11	108.72	103.15
2	C	538	LEU	CB-CG-CD2	-5.11	95.37	110.70
2	C	838	CYS	CA-CB-SG	-5.11	102.65	114.40
3	D	453	VAL	CG1-CB-CG2	5.11	122.04	110.80
2	C	452	ARG	O-C-N	5.11	129.83	123.19
2	C	552	PRO	CA-C-N	-5.11	114.12	122.54
2	C	552	PRO	C-N-CA	-5.11	114.12	122.54
2	C	827	ARG	CD-NE-CZ	5.11	131.55	124.40
1	B	201	LEU	CB-CG-CD1	-5.10	95.39	110.70
2	C	672	GLU	CG-CD-OE2	-5.10	106.66	118.40
2	C	590	PRO	CA-C-O	-5.10	115.86	122.13
3	D	8	LEU	CA-C-N	5.10	129.30	120.58
3	D	8	LEU	C-N-CA	5.10	129.30	120.58
3	D	862	THR	OG1-CB-CG2	-5.10	99.10	109.30
2	C	1090	ASN	CA-CB-CG	-5.10	107.50	112.60
2	C	562	GLU	N-CA-CB	5.09	118.09	109.94
3	D	394	ILE	CG1-CB-CG2	-5.09	95.42	110.70
3	D	123	ARG	CA-C-O	5.09	125.82	119.97
1	B	182	ARG	CA-CB-CG	5.09	124.27	114.10
3	D	29	MET	O-C-N	5.08	128.17	122.22
2	C	715	THR	O-C-N	5.08	128.70	122.96
2	C	1184	THR	CB-CA-C	-5.08	104.53	110.17
3	D	883	ARG	NE-CZ-NH1	-5.08	116.42	121.50
3	D	20	ILE	CB-CA-C	-5.08	102.96	111.29
6	F	1	DA	C4'-C3'-O3'	5.08	117.62	110.00
3	D	1234	VAL	CA-CB-CG1	5.08	119.03	110.40
2	C	824	GLN	CB-CA-C	-5.07	102.37	110.79
2	C	532	ALA	CB-CA-C	-5.07	99.98	109.72
1	A	223	ILE	CA-CB-CG2	-5.07	101.88	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	175	ARG	NE-CZ-NH1	-5.07	116.43	121.50
3	D	1319	PHE	N-CA-CB	5.07	118.66	110.40
2	C	1067	ALA	N-CA-CB	-5.07	101.75	110.87
2	C	1129	ASN	O-C-N	5.06	127.28	122.07
2	C	918	LEU	N-CA-C	5.06	118.49	112.72
2	C	1098	LEU	CB-CG-CD2	-5.06	95.53	110.70
3	D	504	GLN	CA-C-N	-5.06	112.62	120.31
3	D	504	GLN	C-N-CA	-5.06	112.62	120.31
3	D	824	PRO	O-C-N	-5.06	116.97	123.04
2	C	823	VAL	CA-CB-CG2	-5.05	101.81	110.40
3	D	497	GLU	N-CA-C	-5.05	103.59	110.36
2	C	1101	LEU	O-C-N	5.05	129.15	122.43
3	D	596	LEU	CD1-CG-CD2	5.05	121.91	110.80
3	D	1353	VAL	CA-CB-CG1	5.05	118.99	110.40
2	C	1176	LEU	CB-CG-CD1	-5.05	95.55	110.70
3	D	911	LYS	N-CA-CB	-5.05	102.55	109.97
2	C	1114	GLU	CG-CD-OE1	5.04	130.00	118.40
2	C	1326	LEU	CB-CG-CD1	-5.04	95.57	110.70
3	D	1257	VAL	O-C-N	5.04	126.76	121.87
2	C	451	ARG	NE-CZ-NH2	5.04	123.74	119.20
3	D	451	PRO	N-CD-CG	-5.04	95.64	103.20
2	C	720	ARG	NE-CZ-NH1	-5.04	116.46	121.50
2	C	712	SER	N-CA-C	-5.04	105.98	111.82
3	D	769	VAL	CA-CB-CG2	5.03	118.96	110.40
3	D	1340	LYS	CA-C-O	-5.03	115.68	121.47
3	D	520	ALA	CA-C-O	5.03	127.71	120.51
6	F	3	DG	C5'-C4'-C3'	5.03	122.45	114.90
1	A	231	PHE	N-CA-CB	5.03	118.07	110.28
2	C	1073	LYS	O-C-N	-5.03	116.62	122.96
3	D	345	LYS	O-C-N	-5.03	117.43	123.06
3	D	375	GLU	O-C-N	5.03	127.83	121.95
2	C	693	LEU	CA-C-N	-5.03	115.64	122.93
2	C	693	LEU	C-N-CA	-5.03	115.64	122.93
3	D	602	SER	N-CA-C	-5.03	105.69	111.07
3	D	619	ILE	CB-CA-C	5.03	118.97	112.24
1	A	29	GLU	CA-C-N	5.02	126.12	119.84
1	A	29	GLU	C-N-CA	5.02	126.12	119.84
1	B	198	LEU	CD1-CG-CD2	5.02	121.85	110.80
2	C	562	GLU	CA-C-O	-5.02	114.93	120.60
3	D	500	ILE	CA-CB-CG2	5.02	119.03	110.50
3	D	93	THR	CA-C-N	5.02	131.12	121.54
3	D	93	THR	C-N-CA	5.02	131.12	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1112	ILE	N-CA-C	5.01	115.24	110.53
3	D	400	MET	CB-CG-SD	-5.01	97.67	112.70
5	M	185	PHE	CB-CA-C	-5.01	100.46	110.42
1	A	64	VAL	O-C-N	5.00	128.59	123.18
3	D	102	MET	N-CA-C	5.00	121.46	110.80
3	D	508	LEU	CD1-CG-CD2	-5.00	99.79	110.80
2	C	691	PRO	CB-CA-C	-5.00	103.80	110.85
2	C	1246	ARG	N-CA-CB	5.00	119.30	111.20
3	D	366	CYS	CB-CA-C	-5.00	100.47	110.42
3	D	717	VAL	N-CA-CB	5.00	118.19	110.14
3	D	1275	LEU	N-CA-C	5.00	118.49	111.74
5	M	144	ILE	CA-CB-CG2	5.00	119.00	110.50

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	CYS	Mainchain
1	A	151	GLY	Mainchain,Peptide
1	A	47	LEU	Mainchain
1	A	63	GLY	Peptide
1	A	93	GLN	Peptide
2	C	1070	HIS	Mainchain
2	C	1085	MET	Mainchain
2	C	1098	LEU	Mainchain
2	C	1102	GLY	Peptide
2	C	1185	PRO	Peptide
2	C	12	ARG	Sidechain
2	C	1210	ILE	Mainchain
2	C	1230	MET	Mainchain
2	C	1266	GLY	Mainchain,Peptide
2	C	1270	PHE	Peptide
2	C	1301	ARG	Sidechain
2	C	1333	LEU	Mainchain
2	C	143	ARG	Peptide
2	C	452	ARG	Mainchain
2	C	519	ASN	Peptide
2	C	548	ARG	Mainchain
2	C	681	MET	Mainchain
2	C	687	ARG	Mainchain
2	C	709	ALA	Mainchain
2	C	788	SER	Mainchain

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Mol	Chain	Res	Type	Group
2	C	815	SER	Mainchain,Peptide
2	C	821	ARG	Mainchain
2	C	832	HIS	Sidechain
2	C	840	SER	Peptide
2	C	851	THR	Peptide
2	C	852	ALA	Peptide
3	D	1178	THR	Peptide
3	D	1349	GLU	Mainchain
3	D	19	ALA	Peptide
3	D	341	ASN	Mainchain
3	D	342	LEU	Mainchain
3	D	345	LYS	Mainchain
3	D	352	ARG	Mainchain
3	D	358	GLY	Peptide
3	D	361	LEU	Mainchain
3	D	365	GLN	Mainchain
3	D	369	PRO	Mainchain
3	D	372	MET	Mainchain
3	D	374	LEU	Mainchain
3	D	380	PHE	Sidechain
3	D	425	ARG	Peptide
3	D	435	GLN	Mainchain
3	D	455	ALA	Mainchain
3	D	5	LEU	Peptide
3	D	503	SER	Peptide
3	D	510	LEU	Mainchain
3	D	577	ALA	Mainchain
3	D	802	ASP	Mainchain
3	D	808	VAL	Mainchain
3	D	894	VAL	Mainchain
3	D	899	TYR	Sidechain
3	D	90	VAL	Mainchain
3	D	91	GLU	Peptide
3	D	92	VAL	Peptide
4	E	15	ASN	Mainchain
5	M	185	PHE	Peptide

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	2302	0	2266	95	0
1	B	1733	0	1720	82	0
2	C	10034	0	9668	455	0
3	D	9790	0	9539	604	0
4	E	565	0	563	27	0
5	M	2002	0	1412	64	0
6	F	944	0	513	100	0
7	G	946	0	518	42	0
All	All	28316	0	26199	1340	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1340) 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)
7:G:14:DT:H2''	7:G:15:DT:C7	1.31	1.55
2:C:1260:GLY:CA	3:D:346:ARG:HH12	1.20	1.52
2:C:1066:MET:CE	2:C:1232:MET:HE2	1.38	1.52
3:D:333:GLY:N	3:D:333:GLY:CA	1.70	1.51
3:D:316:ILE:CD1	3:D:317:THR:H	1.23	1.50
3:D:359:PRO:CD	3:D:359:PRO:CG	1.74	1.45
3:D:462:ASP:CB	3:D:462:ASP:CG	1.90	1.42
2:C:1260:GLY:HA2	3:D:346:ARG:NH1	1.34	1.40
3:D:316:ILE:HD12	3:D:317:THR:N	1.05	1.37
2:C:1066:MET:HE2	2:C:1232:MET:CE	1.54	1.37
3:D:261:ALA:HB1	6:F:6:DT:C7	1.65	1.26
3:D:316:ILE:CD1	3:D:317:THR:N	1.85	1.23
3:D:925:GLU:OE1	3:D:926:PRO:HD3	1.35	1.22
5:M:376:MET:CE	6:F:11:DG:H5''	1.69	1.21
3:D:889:ASP:CB	3:D:895:CYS:SG	2.30	1.19
7:G:14:DT:C2'	7:G:15:DT:C7	2.22	1.17
3:D:316:ILE:HD12	3:D:317:THR:CA	1.73	1.17
2:C:1262:LYS:O	2:C:1263:ALA:HB3	1.44	1.15
3:D:261:ALA:HB1	6:F:6:DT:H71	1.23	1.15
2:C:560:PRO:HB2	3:D:776:THR:HG21	1.27	1.15
3:D:426:ALA:HB1	3:D:427:PRO:HD2	1.23	1.15
2:C:933:VAL:HG22	2:C:1050:VAL:HG13	1.20	1.13
2:C:1066:MET:CE	2:C:1232:MET:CE	2.15	1.12
2:C:1260:GLY:C	3:D:346:ARG:HH12	1.55	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:4:DG:H1'	6:F:5:DC:H5'	1.28	1.12
7:G:14:DT:H2''	7:G:15:DT:H73	1.30	1.12
3:D:478:LEU:HD21	4:E:47:THR:HG23	1.27	1.12
6:F:4:DG:C1'	6:F:5:DC:H5'	1.79	1.12
2:C:1260:GLY:CA	3:D:346:ARG:NH1	1.99	1.11
2:C:1066:MET:HE1	2:C:1232:MET:HE2	1.24	1.10
6:F:-9:DA:H2''	6:F:-8:DT:H71	1.26	1.10
2:C:1275:VAL:HG11	3:D:343:LEU:HD22	1.15	1.09
2:C:1253:LEU:HG	5:M:114:GLY:HA3	1.12	1.09
3:D:426:ALA:HB1	3:D:427:PRO:CD	1.83	1.08
5:M:388:LYS:HE3	6:F:8:DA:OP2	1.53	1.08
2:C:1253:LEU:HB2	5:M:113:GLN:O	1.54	1.07
3:D:316:ILE:HD13	3:D:317:THR:O	1.54	1.07
2:C:1260:GLY:O	3:D:346:ARG:NH1	1.88	1.06
3:D:332:LYS:HB2	3:D:337:ARG:HA	1.36	1.05
3:D:528:THR:OG1	3:D:551:ARG:HD2	1.53	1.05
3:D:316:ILE:CD1	3:D:317:THR:O	2.05	1.05
2:C:1117:LEU:HD21	2:C:1182:ILE:HG21	1.34	1.04
3:D:426:ALA:CB	3:D:427:PRO:HD2	1.87	1.04
5:M:376:MET:HE1	6:F:11:DG:H5''	1.40	1.04
5:M:376:MET:HE2	6:F:11:DG:H5''	1.37	1.03
2:C:1260:GLY:C	3:D:346:ARG:NH1	2.14	1.03
2:C:1275:VAL:CG1	3:D:343:LEU:HD22	1.88	1.03
3:D:71:LEU:HD11	3:D:88:CYS:SG	2.00	1.02
3:D:925:GLU:OE1	3:D:926:PRO:CD	2.07	1.01
7:G:14:DT:H2''	7:G:15:DT:H71	1.08	1.01
6:F:-9:DA:C2'	6:F:-8:DT:H71	1.90	1.00
6:F:4:DG:H4'	6:F:5:DC:OP1	1.57	1.00
2:C:1209:GLN:HG2	2:C:1226:THR:HG22	1.41	1.00
1:A:312:LEU:HG	5:M:181:ARG:HG3	1.44	0.99
3:D:253:VAL:HG23	3:D:253:VAL:O	1.58	0.99
2:C:1262:LYS:O	2:C:1263:ALA:CB	2.11	0.99
7:G:8:DA:H2''	7:G:9:DT:H71	1.44	0.98
7:G:14:DT:C2'	7:G:15:DT:H73	1.90	0.97
3:D:57:PHE:HE2	3:D:252:LEU:HD12	1.27	0.97
3:D:114:ILE:HD11	3:D:311:ARG:HB3	1.43	0.97
2:C:1243:MET:HE1	3:D:445:LYS:HG2	1.47	0.96
3:D:261:ALA:HB1	6:F:6:DT:H72	1.45	0.96
2:C:1253:LEU:CG	5:M:114:GLY:HA3	1.95	0.95
7:G:14:DT:C2'	7:G:15:DT:H71	1.88	0.95
3:D:71:LEU:CD1	3:D:88:CYS:SG	2.56	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.50	0.94
6:F:7:DG:H2''	6:F:8:DA:O5'	1.66	0.94
3:D:530:PRO:HG2	3:D:577:ALA:HB1	1.49	0.94
3:D:57:PHE:CE2	3:D:252:LEU:HD12	2.02	0.93
2:C:685:MET:HE2	2:C:1073:LYS:HD3	1.48	0.93
6:F:12:DT:OP2	6:F:12:DT:H3'	1.68	0.93
7:G:14:DT:H2''	7:G:15:DT:C5	2.05	0.92
3:D:343:LEU:HD23	3:D:1351:VAL:HG11	1.50	0.92
2:C:1260:GLY:HA2	3:D:346:ARG:HH12	0.77	0.91
6:F:12:DT:H3'	6:F:12:DT:P	2.09	0.91
2:C:1275:VAL:HG11	3:D:343:LEU:CD2	2.00	0.90
2:C:1176:LEU:C	2:C:1176:LEU:HD12	1.94	0.90
2:C:685:MET:CE	2:C:1073:LYS:HD3	2.02	0.90
2:C:1066:MET:HE2	2:C:1232:MET:HE2	1.13	0.89
6:F:-9:DA:H2''	6:F:-8:DT:C7	2.02	0.89
2:C:540:ARG:HG2	2:C:541:GLU:H	1.37	0.88
2:C:56:VAL:HG11	2:C:472:GLU:HG3	1.54	0.88
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.54	0.88
7:G:8:DA:C2'	7:G:9:DT:H71	2.04	0.88
3:D:1262:ARG:O	3:D:1263:LYS:HB2	1.72	0.88
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.56	0.87
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.56	0.87
2:C:1222:GLU:O	2:C:1223:ARG:HB2	1.74	0.87
3:D:316:ILE:HD13	3:D:317:THR:H	1.39	0.87
2:C:1253:LEU:HD23	5:M:116:THR:HG22	1.54	0.87
3:D:311:ARG:O	3:D:312:ARG:CB	2.23	0.86
5:M:132:PRO:HD2	5:M:181:ARG:HH22	1.39	0.86
3:D:314:ARG:O	3:D:316:ILE:HG23	1.77	0.85
2:C:817:LEU:HD11	2:C:1080:ASN:HD21	1.38	0.85
3:D:528:THR:OG1	3:D:551:ARG:CD	2.24	0.85
3:D:20:ILE:CD1	3:D:1344:LEU:HD21	2.07	0.84
2:C:1132:LEU:HD21	2:C:1141:LEU:HD22	1.58	0.84
3:D:332:LYS:CB	3:D:337:ARG:HA	2.08	0.83
3:D:227:PHE:HZ	3:D:237:MET:HE1	1.41	0.83
2:C:1060:ILE:HD11	2:C:1064:ASP:CB	2.09	0.83
3:D:927:GLY:HA2	3:D:930:LEU:HG	1.61	0.83
2:C:727:VAL:HG12	2:C:728:ASP:H	1.44	0.83
1:A:279:GLY:HA3	1:A:321:TRP:HH2	1.44	0.83
7:G:13:DG:H2''	7:G:14:DT:C5	2.13	0.83
2:C:1267:GLY:HA3	3:D:347:VAL:O	1.79	0.82
3:D:56:LEU:O	3:D:57:PHE:HB2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:839:VAL:HG12	3:D:839:VAL:O	1.79	0.82
2:C:74:ARG:HG2	2:C:75:LEU:H	1.46	0.81
2:C:933:VAL:CG2	2:C:1050:VAL:HG13	2.06	0.81
2:C:1182:ILE:HD11	2:C:1198:LEU:HD21	1.63	0.81
3:D:117:LEU:O	3:D:118:LYS:HB2	1.77	0.81
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.61	0.81
6:F:9:DT:OP2	6:F:9:DT:H3'	1.80	0.81
3:D:927:GLY:HA2	3:D:930:LEU:CG	2.11	0.81
2:C:804:PHE:HE2	2:C:1115:THR:HG21	1.42	0.80
1:A:180:VAL:HA	1:A:207:THR:HG22	1.62	0.80
1:A:29:GLU:HB2	1:A:30:PRO:HD3	1.63	0.80
3:D:114:ILE:HD11	3:D:311:ARG:CB	2.10	0.80
3:D:127:LEU:HG	3:D:224:LEU:HD21	1.61	0.80
2:C:519:ASN:HD21	2:C:689:ALA:HB3	1.47	0.80
3:D:430:HIS:CE1	3:D:432:LEU:HB2	2.16	0.80
3:D:315:ALA:O	3:D:316:ILE:HG13	1.82	0.80
1:A:218:ARG:HD2	1:B:231:PHE:O	1.80	0.80
3:D:227:PHE:CZ	3:D:237:MET:HE1	2.17	0.80
3:D:34:SER:HB2	3:D:104:HIS:ND1	1.97	0.79
1:A:83:LEU:HD13	2:C:694:ARG:NH1	1.97	0.79
3:D:417:ARG:O	4:E:45:LYS:HE3	1.82	0.79
2:C:1253:LEU:HG	5:M:114:GLY:CA	2.05	0.79
3:D:848:VAL:HG22	3:D:858:VAL:HG22	1.63	0.79
5:M:156:ILE:HD12	5:M:157:GLN:H	1.48	0.79
6:F:20:DT:H2''	6:F:21:DC:C5	2.18	0.79
2:C:672:GLU:OE2	2:C:1187:PHE:HA	1.83	0.78
3:D:289:ASP:O	3:D:293:ARG:HB2	1.82	0.78
1:B:48:LEU:HD11	1:B:183:ILE:CG2	2.13	0.78
3:D:339:ARG:O	3:D:340:GLN:HB2	1.83	0.78
2:C:1042:LEU:HD13	2:C:1046:VAL:HG13	1.65	0.78
3:D:123:ARG:O	3:D:127:LEU:HB2	1.83	0.78
2:C:817:LEU:HD11	2:C:1080:ASN:ND2	1.98	0.78
3:D:139:LEU:HD23	3:D:185:ILE:CD1	2.12	0.78
3:D:1162:ILE:HG22	3:D:1164:SER:H	1.49	0.78
6:F:5:DC:H4'	6:F:6:DT:OP1	1.82	0.78
7:G:8:DA:H2''	7:G:9:DT:C7	2.13	0.78
1:B:83:LEU:CD1	3:D:526:VAL:HG12	2.13	0.77
3:D:902:ASP:O	3:D:903:LEU:HB2	1.85	0.77
2:C:179:TYR:H	2:C:397:LEU:HA	1.48	0.77
3:D:530:PRO:HB2	3:D:531:LYS:C	2.08	0.77
7:G:-7:DA:H4'	7:G:-7:DA:OP1	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1066:MET:HE2	2:C:1232:MET:HE3	1.62	0.77
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.66	0.77
3:D:262:THR:N	6:F:6:DT:H72	2.00	0.77
5:M:376:MET:HE2	6:F:11:DG:C5'	2.15	0.77
2:C:629:PHE:HD2	2:C:634:VAL:HG21	1.48	0.76
2:C:1243:MET:CE	3:D:445:LYS:HG2	2.14	0.76
3:D:803:VAL:HG21	3:D:1309:ILE:HG12	1.65	0.76
1:A:83:LEU:HD13	2:C:694:ARG:HH11	1.47	0.76
2:C:757:THR:HB	2:C:765:ILE:HD11	1.68	0.76
2:C:1307:ASN:HB3	2:C:1312:ASN:HB3	1.67	0.76
3:D:316:ILE:CD1	3:D:317:THR:C	2.59	0.76
6:F:-1:DC:H3'	6:F:-1:DC:P	2.25	0.76
2:C:445:ILE:H	2:C:445:ILE:HD12	1.49	0.76
2:C:661:VAL:CG2	2:C:665:ALA:HB3	2.17	0.75
3:D:261:ALA:CB	6:F:6:DT:H72	2.17	0.75
3:D:390:LEU:HD12	3:D:390:LEU:H	1.49	0.75
3:D:552:ILE:HD13	3:D:589:TYR:CE1	2.22	0.75
3:D:826:ILE:HG22	3:D:831:VAL:HB	1.68	0.75
3:D:287:ALA:HB1	3:D:288:PRO:HD2	1.69	0.75
2:C:1128:ILE:HD13	2:C:1176:LEU:HD11	1.69	0.75
3:D:335:GLN:HG3	3:D:335:GLN:O	1.84	0.75
3:D:338:PHE:HZ	3:D:798:ARG:HH11	1.34	0.74
1:A:312:LEU:CG	5:M:181:ARG:HG3	2.15	0.74
3:D:348:ASP:O	3:D:349:TYR:C	2.30	0.74
2:C:833:ILE:HA	2:C:1054:LEU:O	1.88	0.74
3:D:126:LEU:O	3:D:220:ARG:NH1	2.21	0.74
2:C:1007:LYS:O	2:C:1011:LEU:HB2	1.88	0.74
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.69	0.74
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.67	0.74
3:D:261:ALA:CB	6:F:6:DT:C7	2.58	0.74
3:D:347:VAL:HG12	3:D:348:ASP:N	2.03	0.74
3:D:925:GLU:HB3	3:D:926:PRO:CD	2.17	0.74
2:C:519:ASN:ND2	2:C:689:ALA:HB3	2.03	0.73
2:C:130:MET:HE3	2:C:134:GLY:HA2	1.71	0.73
2:C:1246:ARG:NH1	2:C:1265:PHE:O	2.20	0.73
3:D:697:MET:CE	3:D:737:ILE:HG22	2.19	0.73
3:D:798:ARG:NH1	3:D:1325:PHE:O	2.20	0.73
3:D:914:ALA:O	3:D:915:ILE:HB	1.87	0.73
2:C:705:GLU:HB3	2:C:794:LEU:H	1.52	0.73
3:D:848:VAL:HG22	3:D:858:VAL:CG2	2.17	0.73
2:C:500:ALA:O	2:C:504:GLU:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:117:LEU:O	3:D:118:LYS:CB	2.34	0.73
5:M:199:LEU:HD22	5:M:256:LEU:HD12	1.71	0.72
2:C:1272:GLU:HA	3:D:343:LEU:HB3	1.71	0.72
6:F:-1:DC:H3'	6:F:-1:DC:OP2	1.89	0.72
3:D:347:VAL:HG12	3:D:348:ASP:H	1.54	0.72
3:D:261:ALA:C	6:F:6:DT:H72	2.15	0.72
2:C:1260:GLY:HA2	3:D:346:ARG:CZ	2.18	0.72
3:D:499:ILE:O	3:D:500:ILE:HB	1.88	0.72
5:M:109:LEU:CB	6:F:2:DG:O6	2.38	0.72
3:D:26:SER:H	3:D:29:MET:HE3	1.55	0.71
3:D:250:ARG:NH2	3:D:266:ASN:OD1	2.23	0.71
3:D:1177:ILE:HG22	3:D:1179:PRO:HD3	1.71	0.71
3:D:478:LEU:HD21	4:E:47:THR:CG2	2.14	0.71
1:A:304:LYS:O	1:A:308:ALA:HB2	1.90	0.71
3:D:528:THR:OG1	3:D:551:ARG:CG	2.37	0.71
6:F:13:DG:H2'	6:F:14:DC:C6	2.24	0.71
3:D:531:LYS:HB3	3:D:581:MET:CE	2.20	0.71
2:C:102:LEU:HB3	2:C:117:ILE:O	1.91	0.71
2:C:1269:ARG:NH2	3:D:339:ARG:HA	2.06	0.71
7:G:-8:DG:N3	7:G:-8:DG:H5''	2.05	0.71
1:B:16:ILE:HD11	1:B:24:ALA:HB1	1.73	0.71
2:C:143:ARG:HG2	2:C:143:ARG:HH11	1.56	0.71
3:D:24:LEU:HD21	3:D:116:PHE:HE2	1.54	0.71
3:D:339:ARG:O	3:D:340:GLN:CB	2.38	0.71
3:D:516:ASP:O	3:D:716:GLN:NE2	2.23	0.71
5:M:156:ILE:HD12	5:M:157:GLN:N	2.06	0.71
3:D:71:LEU:HD12	3:D:71:LEU:O	1.90	0.71
2:C:902:LEU:CD1	5:M:195:LEU:HD13	2.21	0.70
3:D:426:ALA:CB	3:D:427:PRO:CD	2.53	0.70
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.73	0.70
3:D:531:LYS:HB3	3:D:581:MET:HE1	1.72	0.70
6:F:-3:DG:C2'	6:F:-2:DC:H5'	2.22	0.70
1:B:207:THR:HG22	1:B:208:ASN:N	2.05	0.70
3:D:92:VAL:HG12	3:D:93:THR:N	2.03	0.70
5:M:388:LYS:CE	6:F:8:DA:OP2	2.35	0.70
2:C:580:GLN:HG2	2:C:581:THR:H	1.56	0.69
3:D:848:VAL:CG2	3:D:858:VAL:HG22	2.20	0.69
3:D:130:MET:HE2	3:D:157:GLN:HB3	1.74	0.69
6:F:-9:DA:C2'	6:F:-8:DT:C7	2.65	0.69
1:A:228:LEU:HD11	1:B:224:LEU:HD13	1.72	0.69
1:B:59:VAL:HG22	1:B:144:ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:8:DA:C2'	7:G:9:DT:C7	2.70	0.69
1:A:41:ASN:ND2	2:C:1218:GLY:CA	2.56	0.69
2:C:1272:GLU:HA	3:D:343:LEU:CB	2.23	0.69
3:D:95:THR:HG23	3:D:95:THR:O	1.91	0.69
3:D:421:VAL:HG12	3:D:422:LEU:N	2.07	0.69
3:D:744:ARG:NH1	3:D:763:PHE:CZ	2.60	0.69
3:D:1307:LEU:N	3:D:1307:LEU:HD22	2.08	0.69
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.24	0.69
6:F:7:DG:H2'	6:F:8:DA:C8	2.28	0.68
1:B:179:PRO:O	1:B:207:THR:HG23	1.93	0.68
3:D:316:ILE:HD12	3:D:317:THR:C	2.19	0.68
3:D:530:PRO:HD2	3:D:531:LYS:O	1.93	0.68
6:F:6:DT:H2''	6:F:7:DG:C5'	2.24	0.68
3:D:478:LEU:CD2	4:E:47:THR:HG23	2.13	0.68
3:D:893:GLY:O	3:D:894:VAL:HB	1.91	0.68
3:D:114:ILE:CD1	3:D:311:ARG:CB	2.72	0.68
3:D:597:GLY:O	3:D:601:ILE:HG13	1.94	0.68
3:D:623:GLN:O	3:D:627:THR:HG22	1.94	0.68
2:C:1176:LEU:HD12	2:C:1176:LEU:O	1.93	0.68
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.76	0.67
3:D:227:PHE:CZ	3:D:237:MET:CE	2.76	0.67
1:A:279:GLY:HA3	1:A:321:TRP:CH2	2.29	0.67
6:F:4:DG:H3'	6:F:4:DG:OP2	1.93	0.67
2:C:448:LEU:HD13	2:C:554:HIS:HD2	1.58	0.67
2:C:633:LEU:HB3	2:C:644:LEU:HD23	1.76	0.67
3:D:925:GLU:CB	3:D:926:PRO:HD3	2.21	0.67
5:M:202:GLN:NE2	5:M:256:LEU:O	2.27	0.67
3:D:1221:LEU:HB2	3:D:1229:VAL:HG21	1.77	0.67
6:F:7:DG:C2'	6:F:8:DA:C8	2.78	0.67
1:A:110:VAL:HG21	1:A:140:ILE:HD11	1.76	0.67
1:B:48:LEU:HD11	1:B:183:ILE:HG22	1.75	0.67
2:C:540:ARG:HG2	2:C:541:GLU:N	2.08	0.67
6:F:9:DT:C2	6:F:10:DC:C5	2.83	0.67
3:D:324:LEU:O	3:D:325:LYS:HD3	1.95	0.67
2:C:629:PHE:CD2	2:C:634:VAL:HG21	2.30	0.66
3:D:474:LEU:HD11	4:E:31:GLN:HG2	1.77	0.66
5:M:190:VAL:O	5:M:191:ALA:HB3	1.93	0.66
2:C:159:SER:OG	2:C:442:VAL:HG21	1.95	0.66
1:B:28:LEU:HD12	1:B:28:LEU:N	2.10	0.66
3:D:252:LEU:CD2	3:D:260:PHE:HB3	2.25	0.66
6:F:-15:DA:H61	7:G:15:DT:H3	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:GLN:HB3	2:C:130:MET:HE1	1.76	0.66
3:D:1323:ALA:O	3:D:1328:THR:HG22	1.94	0.66
1:A:180:VAL:HG13	1:A:183:ILE:CD1	2.26	0.66
2:C:442:VAL:HG12	2:C:443:ASP:N	2.11	0.66
3:D:1325:PHE:CD2	3:D:1326:GLN:HG2	2.30	0.66
2:C:540:ARG:CG	2:C:541:GLU:H	2.06	0.66
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.77	0.66
2:C:1244:HIS:CE1	2:C:1265:PHE:HA	2.30	0.66
2:C:356:THR:HG22	2:C:358:ASP:H	1.59	0.65
7:G:3:DC:H2''	7:G:4:DG:H5''	1.78	0.65
2:C:1182:ILE:CD1	2:C:1198:LEU:HD21	2.26	0.65
1:A:29:GLU:CB	1:A:30:PRO:HD3	2.26	0.65
3:D:24:LEU:HD21	3:D:116:PHE:CE2	2.31	0.65
2:C:9:LYS:HG2	2:C:1171:ARG:HH22	1.61	0.65
2:C:540:ARG:C	2:C:542:ARG:H	2.05	0.65
2:C:677:ASN:N	2:C:677:ASN:OD1	2.28	0.65
2:C:155:VAL:HG22	2:C:176:ILE:HD13	1.78	0.65
3:D:355:ILE:HD11	3:D:466:MET:HB2	1.78	0.65
2:C:18:ARG:O	2:C:1156:ARG:NH1	2.30	0.65
2:C:890:LYS:H	2:C:912:ASP:HB2	1.63	0.64
6:F:6:DT:H2''	6:F:7:DG:O5'	1.97	0.64
2:C:145:ILE:CG2	2:C:456:VAL:HG12	2.27	0.64
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.79	0.64
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.79	0.64
3:D:340:GLN:HE21	5:M:107:ASP:CB	2.11	0.64
3:D:582:ILE:HD11	3:D:627:THR:HG21	1.80	0.64
4:E:14:GLY:O	4:E:15:ASN:C	2.36	0.64
2:C:895:LEU:HG	2:C:896:THR:H	1.63	0.64
3:D:227:PHE:HZ	3:D:237:MET:CE	2.11	0.64
3:D:338:PHE:HZ	3:D:798:ARG:HE	1.45	0.64
3:D:529:GLY:N	3:D:530:PRO:HA	2.13	0.64
3:D:1190:ILE:HG22	3:D:1192:LYS:H	1.62	0.64
3:D:1307:LEU:HB3	3:D:1312:ALA:HB2	1.79	0.64
3:D:1356:LEU:N	3:D:1356:LEU:HD12	2.12	0.64
3:D:71:LEU:HD12	3:D:71:LEU:C	2.22	0.64
3:D:678:ARG:HH21	3:D:678:ARG:HG2	1.63	0.63
3:D:21:LYS:HG2	3:D:22:ILE:N	2.13	0.63
2:C:704:MET:O	2:C:708:VAL:HG23	1.98	0.63
2:C:442:VAL:HG12	2:C:443:ASP:H	1.63	0.63
3:D:910:ASN:HD22	4:E:15:ASN:HA	1.64	0.63
3:D:135:ILE:HA	3:D:138:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:7:DG:H2''	6:F:8:DA:C5'	2.29	0.63
1:B:91:ARG:HB2	1:B:122:GLU:HB3	1.81	0.63
2:C:706:ARG:O	2:C:710:VAL:HG12	1.98	0.63
3:D:1356:LEU:HD12	3:D:1356:LEU:H	1.62	0.63
2:C:1275:VAL:HG21	3:D:343:LEU:HA	1.81	0.63
3:D:377:PHE:O	3:D:380:PHE:HB2	1.99	0.63
3:D:741:ALA:O	3:D:762:ASN:ND2	2.22	0.62
3:D:898:CYS:O	3:D:899:TYR:CB	2.46	0.62
3:D:1120:THR:HG22	3:D:1122:ALA:H	1.63	0.62
2:C:256:GLU:HA	2:C:261:VAL:HA	1.82	0.62
2:C:1154:ASP:O	2:C:1155:VAL:HG22	1.99	0.62
3:D:323:PRO:O	3:D:324:LEU:HB2	1.98	0.62
3:D:899:TYR:CE2	3:D:909:ILE:HD12	2.35	0.62
2:C:804:PHE:CE2	2:C:1115:THR:HG21	2.31	0.62
1:B:192:VAL:HG23	1:B:198:LEU:CD1	2.30	0.62
2:C:902:LEU:HD12	5:M:195:LEU:HD13	1.82	0.62
1:A:275:ILE:HG21	1:A:281:LEU:HB2	1.81	0.62
2:C:710:VAL:HG22	2:C:710:VAL:O	1.98	0.62
3:D:130:MET:CE	3:D:157:GLN:HB3	2.30	0.62
1:B:27:THR:C	1:B:28:LEU:HD12	2.24	0.62
1:B:83:LEU:HD12	3:D:526:VAL:HG12	1.82	0.62
2:C:764:CYS:SG	2:C:831:ILE:HB	2.39	0.62
2:C:1185:PRO:HB2	2:C:1188:ASP:OD1	2.00	0.62
2:C:1257:GLN:HB3	2:C:1258:PRO:HD2	1.82	0.62
2:C:302:ILE:HB	2:C:307:GLY:HA2	1.81	0.62
3:D:185:ILE:O	3:D:189:LEU:HB2	1.99	0.62
2:C:851:THR:CG2	2:C:885:GLY:H	2.13	0.61
3:D:338:PHE:HZ	3:D:798:ARG:NH1	1.97	0.61
3:D:139:LEU:HD23	3:D:185:ILE:HD11	1.82	0.61
3:D:678:ARG:HG2	3:D:678:ARG:NH2	2.14	0.61
3:D:843:VAL:CG1	3:D:844:THR:N	2.64	0.61
6:F:11:DG:H2'	6:F:12:DT:H71	1.81	0.61
3:D:843:VAL:HG12	3:D:844:THR:N	2.15	0.61
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.82	0.61
6:F:1:DA:N3	6:F:1:DA:H2'	2.16	0.61
1:A:222:THR:HA	1:B:232:VAL:HG12	1.81	0.61
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.83	0.61
3:D:1325:PHE:CE2	3:D:1326:GLN:HG2	2.36	0.61
3:D:133:ARG:O	3:D:137:ARG:HB2	2.01	0.61
2:C:1330:ILE:HG22	2:C:1337:ILE:HG22	1.83	0.61
3:D:279:LEU:O	3:D:279:LEU:HD23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:316:ILE:CD1	3:D:317:THR:CA	2.59	0.60
1:B:52:PRO:HG2	1:B:219:ARG:HH22	1.67	0.60
1:A:41:ASN:HD22	2:C:1218:GLY:CA	2.14	0.60
5:M:376:MET:CE	6:F:11:DG:C5'	2.62	0.60
7:G:-21:DG:C2	7:G:-20:DA:C2	2.90	0.60
3:D:59:ALA:O	3:D:60:ARG:CB	2.49	0.60
2:C:883:LEU:HD11	2:C:920:VAL:CG2	2.31	0.60
3:D:316:ILE:CG1	3:D:317:THR:N	2.49	0.60
3:D:488:ASN:HB3	4:E:16:ARG:HH22	1.67	0.60
5:M:366:VAL:HG12	5:M:368:ALA:H	1.67	0.60
3:D:341:ASN:OD1	3:D:342:LEU:N	2.35	0.60
1:B:16:ILE:HD13	1:B:26:VAL:HG12	1.83	0.60
2:C:75:LEU:HD21	2:C:127:ILE:HD11	1.84	0.60
3:D:61:ILE:O	3:D:62:PHE:HB2	2.01	0.60
3:D:373:ALA:C	3:D:375:GLU:H	2.09	0.60
3:D:1321:SER:C	3:D:1323:ALA:H	2.10	0.60
6:F:12:DT:H3	7:G:-12:DA:H2	1.45	0.60
3:D:147:ILE:HG22	3:D:188:LEU:HD12	1.83	0.60
2:C:691:PRO:HB3	2:C:788:SER:HB3	1.83	0.59
3:D:364:HIS:HB3	3:D:487:THR:HG21	1.82	0.59
3:D:384:LYS:HD2	3:D:387:LEU:HD12	1.84	0.59
3:D:527:LEU:HD12	3:D:527:LEU:O	2.01	0.59
3:D:925:GLU:CB	3:D:926:PRO:CD	2.78	0.59
1:A:218:ARG:HG2	1:B:234:LEU:HD23	1.84	0.59
2:C:1254:VAL:O	2:C:1255:THR:OG1	2.19	0.59
2:C:26:TYR:HB3	2:C:29:SER:HB3	1.82	0.59
2:C:1167:GLU:O	2:C:1168:GLU:HB2	2.01	0.59
3:D:205:LEU:HD12	3:D:217:LEU:CB	2.33	0.59
3:D:341:ASN:O	3:D:342:LEU:C	2.41	0.59
3:D:584:PRO:O	3:D:585:LYS:HB2	2.01	0.59
2:C:136:PHE:HE2	2:C:145:ILE:HD12	1.67	0.59
2:C:883:LEU:HD11	2:C:920:VAL:HG22	1.84	0.59
1:B:48:LEU:CD1	1:B:183:ILE:CG2	2.80	0.59
1:B:219:ARG:O	1:B:223:ILE:HD12	2.03	0.59
2:C:143:ARG:HG2	2:C:143:ARG:NH1	2.17	0.59
2:C:518:ASN:N	2:C:518:ASN:OD1	2.36	0.59
3:D:842:ARG:HD2	3:D:882:VAL:HG11	1.85	0.59
1:A:214:GLU:O	1:A:218:ARG:HB2	2.02	0.59
2:C:169:LYS:HE3	2:C:190:PRO:HA	1.85	0.59
3:D:20:ILE:HD11	3:D:1344:LEU:HD21	1.83	0.59
2:C:796:LEU:N	2:C:1231:TYR:OH	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1153:ALA:O	2:C:1155:VAL:HG13	2.03	0.58
5:M:213:LEU:O	5:M:217:ARG:CB	2.51	0.58
6:F:0:DC:H4'	6:F:0:DC:OP2	2.03	0.58
2:C:675:ASP:OD1	2:C:676:ALA:N	2.36	0.58
3:D:279:LEU:HD11	3:D:296:LYS:HD3	1.84	0.58
6:F:0:DC:OP2	6:F:0:DC:C4'	2.50	0.58
7:G:-17:DT:C6	7:G:-16:DT:H72	2.38	0.58
2:C:447:HIS:CE1	2:C:553:THR:HG21	2.39	0.58
2:C:830:THR:HG22	2:C:1234:LYS:NZ	2.19	0.58
3:D:909:ILE:HG23	3:D:909:ILE:O	2.03	0.58
1:B:48:LEU:CD1	1:B:183:ILE:HG21	2.33	0.58
2:C:448:LEU:CD1	2:C:554:HIS:HD2	2.16	0.58
3:D:615:LYS:O	3:D:618:VAL:HG12	2.03	0.58
3:D:765:GLU:O	3:D:766:GLY:C	2.42	0.58
3:D:885:VAL:C	3:D:887:SER:H	2.12	0.58
6:F:-9:DA:H2''	6:F:-8:DT:C5	2.38	0.58
1:A:41:ASN:HD22	2:C:1218:GLY:HA3	1.69	0.58
3:D:905:ARG:HG3	3:D:905:ARG:HH11	1.69	0.58
7:G:-21:DG:H2''	7:G:-20:DA:C8	2.38	0.58
2:C:5:TYR:HE2	2:C:778:GLU:HG3	1.68	0.58
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.27	0.58
3:D:528:THR:OG1	3:D:551:ARG:HG2	2.03	0.58
3:D:582:ILE:CD1	3:D:627:THR:HG21	2.34	0.58
6:F:-9:DA:H2'	6:F:-8:DT:H71	1.82	0.58
3:D:70:CYS:SG	3:D:92:VAL:HG22	2.44	0.58
2:C:551:HIS:O	2:C:554:HIS:HB2	2.03	0.58
3:D:108:ALA:CB	3:D:279:LEU:HD22	2.34	0.57
3:D:530:PRO:CG	3:D:577:ALA:HB1	2.30	0.57
7:G:8:DA:H2''	7:G:9:DT:C5	2.38	0.57
2:C:619:ALA:HA	2:C:654:ASP:HB2	1.86	0.57
6:F:5:DC:O3'	6:F:6:DT:H3'	2.04	0.57
2:C:885:GLY:HA2	2:C:917:SER:HB2	1.86	0.57
2:C:918:LEU:O	2:C:919:ARG:C	2.46	0.57
2:C:685:MET:HE2	2:C:1073:LYS:CD	2.30	0.57
3:D:19:ALA:HA	3:D:1343:GLU:H	1.69	0.57
3:D:20:ILE:HD12	3:D:1344:LEU:HD21	1.87	0.57
3:D:261:ALA:CA	6:F:6:DT:H72	2.34	0.57
2:C:918:LEU:O	2:C:918:LEU:HG	2.02	0.57
4:E:6:VAL:HG13	4:E:10:VAL:CG2	2.35	0.57
6:F:9:DT:H4'	6:F:10:DC:H5'	1.85	0.57
3:D:138:VAL:HG12	3:D:143:SER:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:583:VAL:HA	3:D:620:PHE:CE1	2.39	0.57
4:E:6:VAL:HG13	4:E:10:VAL:HG23	1.87	0.57
2:C:448:LEU:CD1	2:C:554:HIS:CD2	2.88	0.57
2:C:1269:ARG:HH22	3:D:339:ARG:HA	1.69	0.57
3:D:355:ILE:N	3:D:355:ILE:HD13	2.20	0.57
3:D:360:TYR:H	3:D:360:TYR:HD1	1.51	0.57
3:D:510:LEU:HD23	3:D:513:MET:CE	2.35	0.57
2:C:770:CYS:HB3	2:C:791:LEU:CD2	2.35	0.57
1:A:39:LEU:O	1:A:43:LEU:HB2	2.05	0.56
1:A:42:ALA:HB1	1:A:224:LEU:HD11	1.86	0.56
2:C:1145:ILE:HG23	2:C:1149:TYR:HE2	1.68	0.56
2:C:1267:GLY:O	3:D:347:VAL:O	2.22	0.56
1:A:92:VAL:HG21	1:A:98:VAL:HG21	1.88	0.56
2:C:532:ALA:HB1	2:C:538:LEU:HD13	1.86	0.56
2:C:1155:VAL:O	2:C:1157:GLN:N	2.38	0.56
1:A:80:GLU:O	1:A:84:ASN:ND2	2.39	0.56
1:A:180:VAL:HG13	1:A:183:ILE:HD11	1.86	0.56
1:B:9:LEU:HD13	1:B:32:GLU:OE2	2.04	0.56
3:D:546:ALA:O	3:D:547:ARG:C	2.48	0.56
3:D:551:ARG:C	3:D:552:ILE:HG13	2.29	0.56
6:F:-7:DG:H2''	6:F:-6:DC:C6	2.40	0.56
2:C:130:MET:CE	2:C:134:GLY:HA2	2.35	0.56
2:C:1248:THR:HG23	2:C:1251:TYR:OH	2.05	0.56
3:D:56:LEU:O	3:D:57:PHE:CB	2.50	0.56
3:D:205:LEU:HD11	3:D:218:THR:HG23	1.86	0.56
6:F:-11:DG:H2''	6:F:-10:DC:C5	2.40	0.56
7:G:13:DG:H2''	7:G:14:DT:C6	2.40	0.56
1:A:53:GLY:O	1:A:148:ARG:HA	2.05	0.56
3:D:675:ALA:HA	3:D:678:ARG:HB3	1.87	0.56
3:D:925:GLU:CD	3:D:926:PRO:HD3	2.27	0.56
3:D:927:GLY:HA2	3:D:930:LEU:CD1	2.35	0.56
2:C:1268:GLN:HB3	3:D:350:SER:HB3	1.86	0.56
2:C:64:GLY:C	2:C:66:SER:H	2.14	0.56
2:C:383:SER:O	2:C:387:ASN:HB2	2.04	0.56
2:C:530:ILE:HD11	2:C:575:LEU:HD23	1.88	0.56
2:C:887:VAL:HB	2:C:913:VAL:HB	1.88	0.56
2:C:28:LEU:O	2:C:30:ILE:N	2.39	0.56
2:C:655:VAL:HG12	2:C:656:SER:N	2.20	0.56
2:C:1333:LEU:HD12	3:D:327:LEU:HD13	1.88	0.56
1:A:130:ILE:O	1:A:131:CYS:C	2.46	0.55
1:B:104:LYS:HD3	1:B:110:VAL:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.89	0.55
3:D:885:VAL:O	3:D:886:VAL:HG12	2.06	0.55
5:M:175:VAL:O	5:M:179:LEU:HB2	2.06	0.55
3:D:491:LEU:HD12	3:D:904:ALA:O	2.06	0.55
5:M:210:THR:HB	5:M:213:LEU:HD12	1.87	0.55
1:B:84:ASN:O	1:B:128:HIS:NE2	2.25	0.55
2:C:155:VAL:HG23	2:C:405:PHE:HD1	1.70	0.55
2:C:540:ARG:O	2:C:542:ARG:N	2.33	0.55
3:D:333:GLY:N	3:D:333:GLY:C	2.57	0.55
3:D:610:ARG:NH1	3:D:866:GLU:OE2	2.38	0.55
3:D:800:LEU:HD22	3:D:1256:ILE:HD13	1.87	0.55
1:B:52:PRO:HG2	1:B:219:ARG:NH2	2.22	0.55
3:D:707:ILE:HG22	3:D:708:ASN:H	1.69	0.55
7:G:-8:DG:H3'	7:G:-7:DA:H5''	1.87	0.55
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.40	0.55
2:C:693:LEU:HD21	2:C:831:ILE:HD11	1.89	0.55
3:D:474:LEU:HD12	4:E:28:ARG:HE	1.72	0.55
5:M:158:ILE:H	5:M:158:ILE:HD12	1.71	0.55
3:D:289:ASP:O	3:D:293:ARG:CB	2.54	0.55
3:D:432:LEU:HD13	3:D:499:ILE:HD13	1.89	0.55
3:D:646:ILE:HG12	3:D:762:ASN:HD21	1.72	0.55
3:D:716:GLN:HG2	3:D:717:VAL:N	2.20	0.55
6:F:-11:DG:H2''	6:F:-10:DC:C6	2.42	0.55
6:F:-3:DG:H2'	6:F:-2:DC:H5'	1.88	0.55
1:A:60:GLU:OE2	1:A:143:ARG:NH2	2.39	0.55
1:A:252:ILE:HG22	1:A:252:ILE:O	2.05	0.55
3:D:347:VAL:CG1	3:D:348:ASP:H	2.18	0.55
3:D:366:CYS:O	3:D:439:PRO:HA	2.07	0.55
6:F:7:DG:H2'	6:F:8:DA:N7	2.21	0.55
2:C:667:LEU:HD23	2:C:704:MET:HB3	1.87	0.55
3:D:185:ILE:O	3:D:189:LEU:CB	2.55	0.55
3:D:835:LEU:CD2	3:D:839:VAL:HG21	2.37	0.55
3:D:884:SER:C	3:D:885:VAL:O	2.48	0.55
3:D:1159:ILE:HG22	3:D:1160:SER:H	1.70	0.55
3:D:139:LEU:CD2	3:D:185:ILE:CD1	2.82	0.55
3:D:374:LEU:O	3:D:374:LEU:HG	2.06	0.55
6:F:6:DT:H2''	6:F:7:DG:H5''	1.88	0.55
3:D:585:LYS:O	3:D:587:LEU:N	2.40	0.54
3:D:845:ALA:HB3	3:D:881:LYS:HG3	1.89	0.54
4:E:3:ARG:HH22	4:E:8:ASP:HB2	1.72	0.54
1:A:100:LEU:HD13	1:A:115:ILE:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:CG1	1:A:183:ILE:HD12	2.37	0.54
2:C:710:VAL:O	2:C:710:VAL:CG2	2.55	0.54
3:D:245:LEU:HD22	3:D:250:ARG:HG3	1.88	0.54
3:D:810:THR:HG23	3:D:811:GLU:OE1	2.07	0.54
6:F:7:DG:H2''	6:F:8:DA:C8	2.42	0.54
6:F:15:DA:H2''	6:F:16:DA:C8	2.43	0.54
2:C:1:MET:O	2:C:2:VAL:HG22	2.07	0.54
2:C:205:PRO:HG2	2:C:208:ILE:HG12	1.89	0.54
3:D:842:ARG:HD2	3:D:882:VAL:CG1	2.38	0.54
1:B:28:LEU:N	1:B:28:LEU:CD1	2.69	0.54
2:C:1151:LEU:HD11	2:C:1198:LEU:HA	1.88	0.54
3:D:92:VAL:O	3:D:94:GLN:N	2.37	0.54
1:A:18:GLN:NE2	1:A:20:SER:O	2.34	0.54
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.38	0.54
3:D:372:MET:HE1	3:D:468:VAL:HG21	1.89	0.54
3:D:432:LEU:HD13	3:D:499:ILE:CD1	2.37	0.54
3:D:1358:PRO:HA	3:D:1366:HIS:CD2	2.43	0.54
6:F:-15:DA:N1	7:G:15:DT:O2	2.40	0.54
1:B:16:ILE:HD12	1:B:17:GLU:N	2.22	0.54
2:C:839:VAL:HG22	2:C:841:ARG:HG3	1.90	0.54
1:B:44:ARG:HG2	1:B:44:ARG:HH21	1.72	0.54
2:C:346:TYR:C	2:C:348:SER:H	2.16	0.54
3:D:905:ARG:HG3	3:D:905:ARG:NH1	2.23	0.54
1:B:16:ILE:HD12	1:B:17:GLU:H	1.72	0.54
2:C:530:ILE:HD11	2:C:575:LEU:CD2	2.38	0.54
2:C:1252:SER:O	2:C:1256:GLN:HA	2.07	0.54
3:D:355:ILE:HG22	3:D:461:PHE:HE1	1.73	0.54
1:A:100:LEU:HD12	1:A:100:LEU:C	2.33	0.54
1:A:106:GLY:HA2	1:A:136:GLU:HG3	1.90	0.54
2:C:924:VAL:CG1	2:C:925:SER:N	2.71	0.54
2:C:1101:LEU:HG	3:D:725:MET:CE	2.38	0.54
3:D:51:PRO:HB2	3:D:58:CYS:HA	1.90	0.54
3:D:287:ALA:HB1	3:D:288:PRO:CD	2.37	0.54
5:M:194:ASP:O	5:M:195:LEU:HB3	2.08	0.54
3:D:472:LEU:N	3:D:472:LEU:CD1	2.71	0.53
3:D:541:LEU:HD12	3:D:542:ALA:H	1.72	0.53
6:F:12:DT:H2''	6:F:13:DG:H5''	1.90	0.53
2:C:1066:MET:CE	2:C:1232:MET:HE3	2.23	0.53
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.43	0.53
3:D:841:GLY:O	3:D:842:ARG:HB2	2.07	0.53
3:D:915:ILE:HD13	3:D:918:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:685:MET:HE1	2:C:1073:LYS:HD3	1.90	0.53
3:D:530:PRO:HB2	3:D:532:GLU:CB	2.38	0.53
3:D:697:MET:SD	3:D:738:ARG:HA	2.48	0.53
1:B:14:VAL:HG12	1:B:28:LEU:HG	1.91	0.53
3:D:360:TYR:CD1	3:D:360:TYR:N	2.74	0.53
3:D:551:ARG:HA	3:D:569:LEU:HA	1.89	0.53
3:D:750:PRO:HD3	3:D:777:HIS:HB3	1.90	0.53
3:D:788:LEU:CD1	3:D:792:ASN:ND2	2.72	0.53
3:D:898:CYS:O	3:D:899:TYR:HB3	2.08	0.53
6:F:-3:DG:H4'	6:F:-2:DC:OP1	2.08	0.53
6:F:3:DG:H2'	6:F:4:DG:C8	2.43	0.53
6:F:4:DG:O4'	6:F:5:DC:H5'	2.07	0.53
3:D:347:VAL:CG1	3:D:348:ASP:N	2.72	0.53
3:D:1210:ILE:HG22	3:D:1211:SER:H	1.73	0.53
3:D:117:LEU:O	3:D:117:LEU:HD23	2.09	0.53
3:D:179:LYS:HB2	3:D:184:ALA:HB2	1.91	0.53
2:C:1273:MET:HA	2:C:1276:TRP:CE3	2.44	0.53
3:D:528:THR:CB	3:D:551:ARG:HG2	2.39	0.53
3:D:554:GLU:O	3:D:555:TYR:HB2	2.09	0.53
3:D:639:VAL:HG22	3:D:640:GLY:N	2.22	0.53
3:D:746:LEU:HD23	3:D:758:PRO:HB3	1.90	0.53
3:D:902:ASP:O	3:D:903:LEU:CB	2.56	0.53
5:M:132:PRO:HD2	5:M:181:ARG:NH2	2.17	0.53
3:D:510:LEU:HD23	3:D:513:MET:HE2	1.91	0.53
6:F:3:DG:H3'	6:F:4:DG:H3'	1.91	0.53
7:G:8:DA:H2''	7:G:9:DT:C6	2.44	0.53
2:C:138:ILE:CD1	2:C:506:PHE:HB3	2.36	0.53
2:C:811:ASN:O	2:C:811:ASN:OD1	2.27	0.53
2:C:924:VAL:HG12	2:C:925:SER:N	2.24	0.53
2:C:1222:GLU:O	2:C:1223:ARG:CB	2.51	0.53
2:C:1336:ASN:HB3	3:D:33:TRP:CZ2	2.44	0.52
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.74	0.52
1:A:179:PRO:HG3	1:A:211:ILE:HD12	1.89	0.52
2:C:30:ILE:HG23	2:C:31:GLN:N	2.23	0.52
2:C:448:LEU:HD13	2:C:554:HIS:CD2	2.42	0.52
3:D:809:VAL:HA	3:D:893:GLY:O	2.09	0.52
6:F:-9:DA:H2''	6:F:-8:DT:C6	2.44	0.52
2:C:1263:ALA:O	2:C:1264:GLN:HB2	2.10	0.52
4:E:13:ILE:HD12	4:E:13:ILE:N	2.25	0.52
1:A:26:VAL:HG11	1:A:217:ILE:HD12	1.90	0.52
1:A:81:ILE:HG12	1:A:131:CYS:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:136:PHE:CE2	2:C:145:ILE:HD12	2.44	0.52
2:C:917:SER:OG	2:C:919:ARG:NH2	2.42	0.52
3:D:123:ARG:O	3:D:127:LEU:CB	2.53	0.52
3:D:865:HIS:CE1	3:D:867:GLN:HB3	2.45	0.52
1:A:228:LEU:HD23	1:A:231:PHE:CD2	2.45	0.52
2:C:31:GLN:HB3	2:C:130:MET:CE	2.39	0.52
2:C:143:ARG:NH1	2:C:143:ARG:CG	2.70	0.52
2:C:1263:ALA:O	2:C:1264:GLN:CB	2.57	0.52
3:D:316:ILE:HG22	3:D:323:PRO:HA	1.90	0.52
1:A:100:LEU:HD13	1:A:115:ILE:CG2	2.40	0.52
2:C:159:SER:C	2:C:161:LYS:H	2.17	0.52
2:C:661:VAL:HG22	2:C:665:ALA:HB3	1.91	0.52
2:C:1222:GLU:OE1	3:D:635:SER:HA	2.09	0.52
3:D:732:GLY:HA2	3:D:736:GLN:OE1	2.10	0.52
3:D:843:VAL:CG1	3:D:844:THR:H	2.23	0.52
3:D:1341:ARG:NH2	3:D:1343:GLU:OE2	2.43	0.52
5:M:120:LEU:HD11	5:M:261:UNK:CB	2.39	0.52
1:A:218:ARG:CD	1:B:231:PHE:O	2.54	0.52
3:D:549:LYS:HB3	3:D:569:LEU:HD21	1.91	0.52
1:A:51:MET:HG3	1:A:180:VAL:CG2	2.40	0.52
1:A:158:ARG:NH2	1:A:173:VAL:O	2.42	0.52
2:C:155:VAL:CG2	2:C:405:PHE:HD1	2.23	0.52
3:D:141:PHE:HA	3:D:180:MET:HE2	1.91	0.52
3:D:317:THR:HG23	3:D:319:SER:H	1.73	0.52
3:D:338:PHE:HZ	3:D:798:ARG:NE	2.08	0.52
1:A:312:LEU:HD23	5:M:181:ARG:HE	1.74	0.52
2:C:770:CYS:HB3	2:C:791:LEU:HD23	1.91	0.52
3:D:576:ARG:HD3	3:D:593:ASN:HA	1.92	0.52
3:D:1356:LEU:H	3:D:1356:LEU:CD1	2.23	0.52
6:F:4:DG:C2'	6:F:5:DC:H5'	2.40	0.52
2:C:120:GLN:HG2	2:C:121:GLU:H	1.75	0.52
2:C:548:ARG:HD3	2:C:569:ILE:HG23	1.92	0.52
2:C:1176:LEU:C	2:C:1176:LEU:CD1	2.74	0.52
3:D:138:VAL:HB	3:D:145:VAL:CG2	2.40	0.52
3:D:788:LEU:HD12	3:D:792:ASN:ND2	2.25	0.52
6:F:-15:DA:H2'	6:F:-14:DA:C8	2.45	0.52
2:C:831:ILE:HG22	2:C:832:HIS:N	2.26	0.51
2:C:1294:LYS:HG3	3:D:348:ASP:HB2	1.92	0.51
3:D:338:PHE:CZ	3:D:798:ARG:NE	2.78	0.51
3:D:205:LEU:HD12	3:D:217:LEU:HB2	1.91	0.51
3:D:253:VAL:O	3:D:253:VAL:CG2	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:478:LEU:HD12	4:E:24:ALA:HB2	1.93	0.51
3:D:857:LEU:HD11	3:D:872:LEU:HD21	1.91	0.51
5:M:224:LEU:HD13	5:M:235:LEU:HD22	1.92	0.51
1:A:57:THR:HG23	1:A:158:ARG:NH1	2.26	0.51
2:C:1268:GLN:CB	3:D:350:SER:HB3	2.40	0.51
3:D:109:SER:CB	3:D:296:LYS:HD2	2.40	0.51
3:D:116:PHE:O	3:D:117:LEU:HB3	2.08	0.51
7:G:8:DA:H2'	7:G:9:DT:H71	1.88	0.51
1:A:41:ASN:ND2	2:C:1218:GLY:HA3	2.22	0.51
1:A:180:VAL:HG13	1:A:183:ILE:HD12	1.92	0.51
2:C:727:VAL:HG12	2:C:728:ASP:N	2.17	0.51
2:C:1119:MET:HG3	2:C:1204:LEU:HD13	1.92	0.51
3:D:226:ALA:O	3:D:230:SER:CB	2.59	0.51
3:D:835:LEU:HD21	3:D:839:VAL:HG21	1.92	0.51
1:A:68:TYR:CD2	2:C:929:ILE:HD11	2.46	0.51
1:A:231:PHE:CE2	1:B:39:LEU:HD23	2.46	0.51
2:C:192:ASP:HB3	2:C:346:TYR:CE1	2.46	0.51
3:D:92:VAL:HG12	3:D:93:THR:H	1.75	0.51
3:D:92:VAL:C	3:D:94:GLN:H	2.18	0.51
3:D:902:ASP:C	3:D:903:LEU:O	2.44	0.51
3:D:1263:LYS:HB2	3:D:1307:LEU:HD21	1.93	0.51
2:C:546:GLU:HG2	2:C:547:VAL:N	2.24	0.51
2:C:816:ILE:HB	2:C:1075:VAL:O	2.11	0.51
2:C:1288:GLN:O	2:C:1288:GLN:CG	2.59	0.51
3:D:233:LYS:HB3	3:D:235:GLU:OE1	2.11	0.51
3:D:744:ARG:HH12	3:D:763:PHE:HZ	1.57	0.51
5:M:419:ALA:O	5:M:423:LEU:HB2	2.11	0.51
1:A:41:ASN:ND2	2:C:1218:GLY:HA2	2.24	0.51
1:A:85:LEU:HD21	1:A:130:ILE:HD13	1.93	0.51
2:C:9:LYS:HG2	2:C:1171:ARG:NH2	2.25	0.51
2:C:143:ARG:HH11	2:C:143:ARG:CG	2.18	0.51
2:C:1065:LYS:O	2:C:1065:LYS:HG3	2.11	0.51
3:D:34:SER:CB	3:D:104:HIS:ND1	2.71	0.51
3:D:1161:GLY:HA3	3:D:1203:ARG:HA	1.93	0.51
3:D:1355:ARG:HD3	3:D:1369:ARG:HH22	1.75	0.51
6:F:6:DT:H1'	6:F:7:DG:O4'	2.10	0.51
6:F:20:DT:H2''	6:F:21:DC:H5	1.73	0.51
1:B:47:LEU:HD23	1:B:51:MET:CE	2.41	0.51
3:D:43:THR:HG22	3:D:56:LEU:HB2	1.92	0.51
3:D:510:LEU:HD11	3:D:624:ILE:HG23	1.93	0.51
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:16:ARG:O	4:E:17:PHE:C	2.48	0.51
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.76	0.50
2:C:701:GLY:O	2:C:1184:THR:N	2.39	0.50
3:D:681:LYS:O	3:D:685:ILE:HD12	2.11	0.50
4:E:5:THR:HG22	4:E:7:GLN:H	1.75	0.50
4:E:16:ARG:O	4:E:19:LEU:N	2.44	0.50
6:F:4:DG:H3'	6:F:4:DG:P	2.50	0.50
3:D:75:TYR:HB3	3:D:80:HIS:CD2	2.45	0.50
3:D:205:LEU:HD12	3:D:217:LEU:HB3	1.92	0.50
3:D:357:VAL:HG22	3:D:358:GLY:N	2.27	0.50
3:D:523:GLU:HA	3:D:546:ALA:HB1	1.93	0.50
3:D:587:LEU:HB3	3:D:588:PRO:HD2	1.93	0.50
3:D:646:ILE:HG12	3:D:762:ASN:ND2	2.26	0.50
3:D:822:MET:CE	3:D:838:ARG:HB3	2.42	0.50
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.93	0.50
3:D:857:LEU:HD12	3:D:858:VAL:HG13	1.94	0.50
5:M:420:ILE:O	5:M:424:VAL:CB	2.59	0.50
1:A:71:LYS:HB3	1:A:74:VAL:CG2	2.41	0.50
2:C:365:GLU:O	2:C:369:MET:HB2	2.11	0.50
3:D:262:THR:H	6:F:6:DT:H72	1.76	0.50
3:D:762:ASN:OD1	3:D:765:GLU:HG2	2.12	0.50
3:D:1233:ILE:CD1	3:D:1257:VAL:HG22	2.42	0.50
6:F:12:DT:N3	7:G:-12:DA:C2	2.74	0.50
1:A:211:ILE:CG2	1:A:216:ALA:HB2	2.41	0.50
2:C:894:GLN:HG2	2:C:895:LEU:N	2.27	0.50
2:C:1257:GLN:HG2	2:C:1296:ASP:OD1	2.11	0.50
3:D:108:ALA:HB3	3:D:279:LEU:HD22	1.94	0.50
3:D:886:VAL:HG23	3:D:1258:ARG:HA	1.92	0.50
3:D:1159:ILE:CG1	3:D:1206:ARG:HB2	2.42	0.50
5:M:380:THR:HB	6:F:11:DG:OP2	2.11	0.50
1:A:110:VAL:HG21	1:A:140:ILE:CD1	2.41	0.50
2:C:523:GLU:O	2:C:527:LYS:HG3	2.12	0.50
2:C:633:LEU:CB	2:C:644:LEU:HD23	2.41	0.50
2:C:928:VAL:HG23	2:C:928:VAL:O	2.11	0.50
2:C:1085:MET:HE2	2:C:1094:VAL:O	2.12	0.50
2:C:1132:LEU:HD21	2:C:1141:LEU:CD2	2.36	0.50
2:C:1272:GLU:HA	3:D:343:LEU:HB2	1.94	0.50
3:D:425:ARG:HG2	3:D:426:ALA:HB3	1.94	0.50
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.94	0.50
3:D:825:VAL:CG2	3:D:833:GLU:H	2.25	0.50
3:D:1307:LEU:N	3:D:1307:LEU:CD2	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HG22	1:B:232:VAL:HA	1.94	0.50
1:B:51:MET:H	1:B:150:ARG:HG3	1.77	0.50
2:C:580:GLN:HG2	2:C:581:THR:N	2.23	0.50
2:C:654:ASP:O	2:C:655:VAL:HB	2.12	0.50
3:D:649:LYS:O	3:D:653:ILE:HD12	2.11	0.50
6:F:3:DG:H2''	6:F:4:DG:H5'	1.93	0.50
6:F:24:DG:H2''	6:F:25:DC:C6	2.47	0.50
7:G:13:DG:H2''	7:G:14:DT:C7	2.41	0.50
2:C:756:TYR:HB3	2:C:833:ILE:HD11	1.94	0.50
2:C:841:ARG:NH1	5:M:272:UNK:CB	2.74	0.50
2:C:1254:VAL:O	2:C:1255:THR:CB	2.59	0.50
3:D:388:ARG:HB2	3:D:390:LEU:HD12	1.94	0.50
3:D:890:THR:HG23	3:D:891:ASP:N	2.26	0.50
2:C:851:THR:HG21	2:C:869:GLY:HA3	1.94	0.50
2:C:1065:LYS:HG2	2:C:1237:HIS:HB2	1.94	0.50
3:D:660:GLU:O	3:D:664:ILE:HD12	2.12	0.50
2:C:171:LEU:HD12	2:C:171:LEU:N	2.27	0.49
2:C:500:ALA:O	2:C:504:GLU:CB	2.59	0.49
3:D:38:VAL:O	3:D:105:ILE:HD13	2.11	0.49
3:D:350:SER:HA	3:D:468:VAL:O	2.12	0.49
3:D:530:PRO:N	3:D:531:LYS:HA	2.27	0.49
2:C:660:VAL:HG23	2:C:661:VAL:N	2.27	0.49
2:C:1336:ASN:HB3	3:D:33:TRP:HZ2	1.76	0.49
3:D:390:LEU:HD12	3:D:390:LEU:N	2.24	0.49
3:D:490:ILE:HA	3:D:500:ILE:HD13	1.93	0.49
3:D:1142:ALA:O	3:D:1146:GLU:HG2	2.12	0.49
6:F:-7:DG:H2''	6:F:-6:DC:H6	1.77	0.49
6:F:23:DT:H2''	6:F:24:DG:C8	2.47	0.49
1:A:282:VAL:HG23	1:A:307:LEU:HD21	1.94	0.49
2:C:732:ILE:O	2:C:751:TYR:HB2	2.12	0.49
2:C:1211:ARG:HD2	2:C:1220:GLN:NE2	2.27	0.49
3:D:1314:LEU:HD21	3:D:1326:GLN:HB2	1.95	0.49
2:C:321:LEU:HG	2:C:325:LEU:HD23	1.94	0.49
2:C:1122:LYS:HD2	2:C:1229:TYR:CZ	2.48	0.49
2:C:1267:GLY:O	2:C:1268:GLN:CB	2.52	0.49
3:D:340:GLN:OE1	3:D:340:GLN:HA	2.12	0.49
3:D:546:ALA:CB	3:D:548:VAL:HG23	2.41	0.49
6:F:12:DT:N3	7:G:-12:DA:H2	2.09	0.49
2:C:15:PHE:CG	2:C:1190:ALA:HB2	2.47	0.49
2:C:851:THR:CB	2:C:869:GLY:HA3	2.41	0.49
2:C:1101:LEU:CD2	3:D:504:GLN:OE1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:353:SER:O	3:D:465:GLN:HG3	2.12	0.49
3:D:528:THR:O	3:D:528:THR:HG23	2.13	0.49
7:G:14:DT:H2'	7:G:15:DT:H73	1.83	0.49
1:A:312:LEU:CD2	5:M:181:ARG:HG3	2.42	0.49
2:C:515:MET:HG2	2:C:516:ASP:N	2.27	0.49
3:D:139:LEU:CD2	3:D:185:ILE:HD13	2.42	0.49
3:D:889:ASP:CB	3:D:898:CYS:SG	3.01	0.49
1:A:181:GLU:HB2	1:A:206:GLU:O	2.11	0.49
1:B:215:GLU:O	1:B:219:ARG:HG3	2.12	0.49
2:C:1:MET:C	2:C:3:TYR:H	2.20	0.49
2:C:851:THR:OG1	2:C:868:SER:O	2.31	0.49
3:D:30:ILE:HD13	3:D:243:PRO:HD3	1.94	0.49
3:D:226:ALA:O	3:D:230:SER:HB2	2.12	0.49
3:D:880:VAL:HG12	3:D:882:VAL:HG23	1.94	0.49
3:D:1058:SER:HA	3:D:1108:GLN:HA	1.94	0.49
2:C:619:ALA:HB3	3:D:769:VAL:HG21	1.95	0.49
2:C:964:LEU:HD11	2:C:1025:PHE:CB	2.42	0.49
2:C:1304:MET:HE1	2:C:1315:MET:HA	1.94	0.49
5:M:106:ASP:CG	5:M:107:ASP:H	2.20	0.49
1:A:103:ASN:HA	1:A:140:ILE:O	2.12	0.49
1:B:80:GLU:O	1:B:84:ASN:ND2	2.46	0.49
2:C:690:VAL:HG23	2:C:691:PRO:HD2	1.95	0.49
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.94	0.49
2:C:902:LEU:CD1	5:M:195:LEU:CD1	2.90	0.49
2:C:930:ASP:HB3	2:C:1053:TYR:HD2	1.77	0.49
3:D:481:ARG:HA	3:D:485:MET:HG2	1.95	0.49
4:E:26:ARG:HH12	4:E:30:MET:HG3	1.77	0.49
1:B:207:THR:CG2	1:B:208:ASN:N	2.74	0.48
3:D:157:GLN:HE21	3:D:188:LEU:HD21	1.78	0.48
3:D:530:PRO:CB	3:D:531:LYS:C	2.84	0.48
2:C:767:GLN:HA	2:C:785:ASP:O	2.13	0.48
7:G:13:DG:H2''	7:G:14:DT:H72	1.94	0.48
2:C:540:ARG:C	2:C:542:ARG:N	2.71	0.48
2:C:661:VAL:HG13	2:C:666:SER:OG	2.13	0.48
2:C:838:CYS:HB2	2:C:918:LEU:HD22	1.95	0.48
3:D:71:LEU:CD1	3:D:71:LEU:C	2.86	0.48
3:D:116:PHE:HE1	3:D:1333:THR:HG22	1.77	0.48
3:D:362:ARG:O	3:D:363:LEU:C	2.55	0.48
3:D:839:VAL:O	3:D:839:VAL:CG1	2.50	0.48
3:D:914:ALA:C	3:D:916:GLY:H	2.21	0.48
3:D:1239:ASP:OD1	3:D:1242:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:O	1:B:15:ASP:OD1	2.31	0.48
2:C:77:GLU:HG3	2:C:78:PRO:HD2	1.95	0.48
3:D:442:ILE:HG13	3:D:442:ILE:O	2.13	0.48
3:D:1149:ARG:HE	3:D:1218:HIS:CD2	2.31	0.48
3:D:914:ALA:O	3:D:915:ILE:CB	2.42	0.48
5:M:152:GLY:O	5:M:154:LEU:N	2.45	0.48
1:B:10:LYS:HD2	1:B:10:LYS:N	2.28	0.48
2:C:785:ASP:OD2	2:C:791:LEU:N	2.43	0.48
3:D:208:THR:HG22	3:D:209:ASN:H	1.79	0.48
1:A:158:ARG:NH2	1:A:173:VAL:H	2.11	0.48
1:B:13:LEU:HD22	1:B:29:GLU:HB3	1.96	0.48
3:D:227:PHE:CE1	3:D:237:MET:CE	2.97	0.48
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.94	0.48
3:D:814:CYS:CB	3:D:895:CYS:SG	3.02	0.48
2:C:1304:MET:HE1	3:D:473:THR:CG2	2.44	0.48
3:D:126:LEU:HD11	3:D:223:LEU:HD22	1.95	0.48
3:D:802:ASP:HB2	3:D:1325:PHE:CE1	2.49	0.48
2:C:447:HIS:ND1	2:C:553:THR:HG21	2.29	0.48
2:C:1145:ILE:HG23	2:C:1149:TYR:CE2	2.48	0.48
3:D:495:ASN:ND2	3:D:497:GLU:HB2	2.29	0.48
6:F:9:DT:H3'	6:F:9:DT:P	2.53	0.48
1:A:18:GLN:NE2	1:A:23:HIS:O	2.46	0.48
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.14	0.48
2:C:800:MET:HE1	2:C:827:ARG:HD3	1.95	0.48
3:D:127:LEU:HG	3:D:224:LEU:CD2	2.40	0.48
3:D:1321:SER:O	3:D:1323:ALA:N	2.47	0.48
5:M:156:ILE:CD1	5:M:157:GLN:H	2.24	0.48
6:F:7:DG:C2'	6:F:8:DA:O5'	2.49	0.48
6:F:11:DG:C4	6:F:12:DT:H73	2.49	0.48
6:F:27:DA:H2''	6:F:28:DG:C8	2.49	0.48
1:B:5:VAL:C	1:B:7:GLU:H	2.23	0.47
2:C:1104:PRO:HG2	2:C:1105:SER:H	1.79	0.47
2:C:1117:LEU:HD21	2:C:1182:ILE:CG2	2.22	0.47
2:C:1188:ASP:OD1	2:C:1188:ASP:N	2.47	0.47
3:D:521:LYS:O	3:D:541:LEU:HD12	2.14	0.47
3:D:788:LEU:CD1	3:D:792:ASN:HD21	2.27	0.47
1:A:231:PHE:HE2	1:B:39:LEU:HD23	1.79	0.47
1:B:193:GLU:HG2	1:B:194:GLN:N	2.28	0.47
2:C:145:ILE:HG21	2:C:145:ILE:HD13	1.51	0.47
3:D:66:LYS:HB2	3:D:66:LYS:HE2	1.61	0.47
3:D:583:VAL:HG13	3:D:584:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:985:ILE:HG23	3:D:988:PHE:O	2.14	0.47
1:A:98:VAL:HG11	1:A:121:VAL:HG22	1.95	0.47
2:C:228:VAL:HG13	2:C:229:ILE:H	1.80	0.47
2:C:515:MET:CG	2:C:516:ASP:N	2.77	0.47
2:C:1102:GLY:HA2	2:C:1106:ARG:NH2	2.29	0.47
3:D:221:ILE:O	3:D:225:GLU:HB2	2.15	0.47
2:C:839:VAL:CG2	2:C:1046:VAL:HG23	2.43	0.47
2:C:1253:LEU:HD23	5:M:116:THR:CG2	2.37	0.47
3:D:857:LEU:HD11	3:D:872:LEU:CD2	2.45	0.47
5:M:188:VAL:HG12	5:M:189:GLY:N	2.29	0.47
6:F:1:DA:OP2	6:F:1:DA:O3'	2.33	0.47
2:C:142:GLU:HG3	2:C:515:MET:HE2	1.97	0.47
2:C:148:GLN:HG2	2:C:149:LEU:N	2.29	0.47
2:C:673:HIS:HB3	2:C:1109:ILE:HB	1.95	0.47
2:C:1293:VAL:O	2:C:1301:ARG:HB3	2.14	0.47
3:D:103:GLY:C	3:D:244:VAL:HG22	2.39	0.47
3:D:373:ALA:O	3:D:375:GLU:N	2.48	0.47
3:D:553:THR:HG22	3:D:567:THR:HB	1.95	0.47
3:D:1177:ILE:C	3:D:1179:PRO:HD3	2.39	0.47
4:E:50:ALA:O	4:E:54:ILE:HG12	2.15	0.47
6:F:9:DT:C4'	6:F:10:DC:H5'	2.45	0.47
1:B:11:PRO:HG2	1:B:28:LEU:HD23	1.97	0.47
3:D:1319:PHE:HB3	3:D:1340:LYS:HD2	1.97	0.47
1:A:59:VAL:HG21	1:A:85:LEU:HD13	1.96	0.47
1:B:179:PRO:HG3	1:B:211:ILE:HD13	1.97	0.47
2:C:228:VAL:HG13	2:C:229:ILE:N	2.30	0.47
3:D:450:HIS:O	3:D:453:VAL:HG22	2.14	0.47
3:D:770:LEU:O	3:D:774:ILE:HG13	2.15	0.47
1:B:46:ILE:HG21	1:B:46:ILE:HD13	1.61	0.47
2:C:851:THR:HG1	2:C:869:GLY:HA3	1.80	0.47
3:D:442:ILE:O	3:D:442:ILE:CG1	2.63	0.47
3:D:527:LEU:HD12	3:D:527:LEU:H	1.79	0.47
5:M:186:ASP:N	5:M:187:PRO:HD2	2.29	0.47
1:B:9:LEU:C	1:B:10:LYS:HD2	2.39	0.47
1:B:219:ARG:O	1:B:222:THR:OG1	2.26	0.47
2:C:257:ALA:N	2:C:260:LYS:O	2.43	0.47
2:C:1006:GLU:O	2:C:1010:GLN:CB	2.63	0.47
3:D:292:VAL:O	3:D:296:LYS:HG2	2.15	0.47
3:D:587:LEU:CB	3:D:588:PRO:HD2	2.44	0.47
3:D:627:THR:HG22	3:D:627:THR:H	1.47	0.47
5:M:133:PHE:HE1	5:M:181:ARG:HD3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:CB	1:A:30:PRO:CD	2.92	0.47
1:B:155:ALA:N	1:B:174:ASP:OD1	2.48	0.47
2:C:800:MET:CE	2:C:827:ARG:HD3	2.45	0.47
3:D:929:GLN:O	3:D:929:GLN:HG3	2.15	0.47
2:C:452:ARG:HH21	2:C:452:ARG:HD3	1.43	0.46
3:D:114:ILE:HG12	3:D:311:ARG:HG3	1.96	0.46
3:D:342:LEU:C	3:D:344:GLY:N	2.72	0.46
3:D:426:ALA:HB3	3:D:427:PRO:HD2	1.87	0.46
3:D:863:LEU:HD12	3:D:863:LEU:HA	1.76	0.46
3:D:1248:ILE:HD13	3:D:1248:ILE:HG21	1.54	0.46
1:A:37:HIS:HB2	1:B:45:ARG:HH21	1.80	0.46
1:A:71:LYS:HB3	1:A:74:VAL:HG22	1.96	0.46
2:C:727:VAL:HG21	2:C:772:SER:O	2.15	0.46
2:C:1106:ARG:HH21	2:C:1106:ARG:HD2	1.33	0.46
3:D:391:ALA:HB1	3:D:396:ALA:HB3	1.97	0.46
3:D:475:GLU:OE1	3:D:475:GLU:N	2.40	0.46
1:A:59:VAL:O	1:A:171:LEU:HB2	2.16	0.46
1:B:55:ALA:HB2	1:B:176:CYS:O	2.15	0.46
2:C:136:PHE:CE2	2:C:506:PHE:HE1	2.32	0.46
2:C:186:PHE:HA	2:C:195:PHE:O	2.15	0.46
2:C:1064:ASP:CB	2:C:1076:ILE:HD12	2.46	0.46
2:C:1244:HIS:O	2:C:1245:ALA:HB3	2.14	0.46
2:C:1291:LEU:O	3:D:345:LYS:HD3	2.14	0.46
3:D:787:ALA:O	3:D:790:THR:OG1	2.25	0.46
2:C:622:ASN:O	2:C:623:LEU:HB2	2.15	0.46
2:C:915:ASP:OD1	2:C:915:ASP:O	2.34	0.46
2:C:1065:LYS:NZ	2:C:1073:LYS:HD2	2.31	0.46
3:D:582:ILE:HG21	3:D:582:ILE:HD13	1.32	0.46
3:D:1042:ASP:HA	3:D:1046:ILE:HB	1.97	0.46
3:D:1305:ASP:OD1	3:D:1306:LEU:N	2.47	0.46
1:A:37:HIS:HB2	1:B:45:ARG:NH2	2.30	0.46
1:A:192:VAL:C	1:A:194:GLN:H	2.24	0.46
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.71	0.46
1:B:74:VAL:O	1:B:75:GLN:HB3	2.15	0.46
2:C:26:TYR:CG	2:C:26:TYR:O	2.68	0.46
2:C:46:GLN:HA	2:C:51:ALA:HB2	1.98	0.46
2:C:91:THR:HA	2:C:139:ASN:H	1.81	0.46
2:C:187:GLU:O	2:C:194:LEU:HA	2.16	0.46
3:D:925:GLU:OE1	3:D:926:PRO:CG	2.62	0.46
1:B:205:MET:HE1	1:B:213:PRO:O	2.15	0.46
2:C:30:ILE:HD12	2:C:575:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:451:ARG:HH11	2:C:451:ARG:HD3	1.52	0.46
2:C:655:VAL:HG12	2:C:656:SER:H	1.79	0.46
2:C:1269:ARG:HH22	3:D:340:GLN:H	1.64	0.46
2:C:1304:MET:CE	2:C:1315:MET:HA	2.46	0.46
3:D:107:LEU:HB2	3:D:240:THR:O	2.15	0.46
2:C:38:PHE:CD2	2:C:39:ILE:CD1	2.99	0.46
2:C:1297:ASP:O	2:C:1301:ARG:HG2	2.15	0.46
3:D:95:THR:O	3:D:95:THR:CG2	2.64	0.46
3:D:893:GLY:O	3:D:894:VAL:C	2.53	0.46
3:D:1223:LEU:HD12	3:D:1224:ARG:N	2.31	0.46
4:E:15:ASN:O	4:E:16:ARG:C	2.57	0.46
6:F:0:DC:P	6:F:0:DC:O4'	2.73	0.46
1:B:99:ILE:HG13	1:B:145:LYS:HG3	1.97	0.46
3:D:502:PRO:HD3	3:D:605:LEU:HD11	1.98	0.46
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.97	0.46
3:D:1233:ILE:HD13	3:D:1257:VAL:HG22	1.98	0.46
1:B:25:LYS:HA	1:B:203:ILE:O	2.15	0.46
1:B:31:LEU:HB2	1:B:199:ASP:HB2	1.97	0.46
2:C:1129:ASN:OD1	2:C:1177:ARG:HD2	2.16	0.46
3:D:352:ARG:HA	3:D:466:MET:O	2.16	0.46
2:C:204:LEU:HD11	2:C:369:MET:HG2	1.98	0.45
2:C:401:GLY:O	2:C:405:PHE:HB2	2.17	0.45
2:C:620:ASN:HD21	3:D:769:VAL:H	1.63	0.45
2:C:877:VAL:HG11	2:C:920:VAL:HG21	1.98	0.45
2:C:1334:GLY:C	3:D:25:ALA:HB3	2.41	0.45
3:D:74:LYS:HB3	3:D:74:LYS:HE3	1.77	0.45
3:D:412:LEU:HG	3:D:416:ILE:HD12	1.97	0.45
3:D:975:ILE:HG21	3:D:980:THR:HG21	1.98	0.45
7:G:-19:DC:H2''	7:G:-18:DT:C6	2.51	0.45
7:G:8:DA:H2'	7:G:9:DT:C7	2.44	0.45
2:C:798:GLN:OE1	2:C:827:ARG:NH1	2.48	0.45
2:C:816:ILE:O	2:C:1076:ILE:HA	2.16	0.45
2:C:885:GLY:HA2	2:C:917:SER:CB	2.46	0.45
2:C:895:LEU:O	2:C:896:THR:OG1	2.26	0.45
3:D:352:ARG:HG3	3:D:352:ARG:NH2	2.30	0.45
3:D:541:LEU:CD1	3:D:542:ALA:H	2.29	0.45
3:D:743:MET:HE3	3:D:760:THR:HG22	1.99	0.45
3:D:1162:ILE:HD13	3:D:1179:PRO:HB3	1.99	0.45
5:M:223:HIS:O	5:M:224:LEU:HG	2.16	0.45
1:A:124:VAL:HG21	1:A:209:GLY:HA3	1.99	0.45
1:B:83:LEU:HD13	3:D:526:VAL:HG12	1.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1094:VAL:H	2:C:1094:VAL:HG13	1.46	0.45
2:C:1101:LEU:HD22	3:D:504:GLN:OE1	2.17	0.45
3:D:515:ARG:HD2	3:D:515:ARG:HA	1.91	0.45
2:C:714:VAL:HG21	2:C:787:PRO:HD2	1.98	0.45
3:D:339:ARG:C	3:D:340:GLN:HG2	2.41	0.45
7:G:-23:DA:H2''	7:G:-22:DC:C6	2.51	0.45
3:D:252:LEU:HD23	3:D:260:PHE:HB3	1.95	0.45
3:D:337:ARG:HH21	3:D:337:ARG:HD2	1.46	0.45
3:D:495:ASN:HB3	3:D:1247:LYS:O	2.16	0.45
3:D:541:LEU:HG	3:D:542:ALA:H	1.82	0.45
6:F:0:DC:H2''	6:F:1:DA:H5'	1.98	0.45
1:A:45:ARG:NH2	1:B:34:GLY:O	2.47	0.45
2:C:448:LEU:HD11	2:C:554:HIS:CD2	2.52	0.45
2:C:513:GLN:HE21	2:C:526:HIS:HE1	1.64	0.45
2:C:1007:LYS:HA	2:C:1011:LEU:HD13	1.98	0.45
2:C:1268:GLN:HE22	3:D:352:ARG:HD2	1.81	0.45
3:D:530:PRO:HB2	3:D:532:GLU:N	2.31	0.45
3:D:541:LEU:CG	3:D:542:ALA:H	2.29	0.45
3:D:858:VAL:HG12	3:D:868:TRP:CZ3	2.52	0.45
3:D:921:GLN:O	3:D:925:GLU:HB2	2.16	0.45
5:M:376:MET:HE2	6:F:11:DG:OP1	2.17	0.45
2:C:137:VAL:HA	2:C:141:THR:O	2.16	0.45
3:D:354:VAL:C	3:D:355:ILE:HD13	2.41	0.45
3:D:709:ARG:C	3:D:711:GLY:H	2.25	0.45
3:D:966:VAL:HG21	3:D:976:THR:HG23	1.98	0.45
3:D:1011:VAL:HG22	3:D:1013:GLY:H	1.82	0.45
6:F:9:DT:H4'	6:F:10:DC:C5'	2.45	0.45
2:C:1116:HIS:CD2	2:C:1208:GLY:HA3	2.51	0.45
3:D:138:VAL:HG21	3:D:145:VAL:HG22	1.99	0.45
3:D:421:VAL:HG12	3:D:422:LEU:H	1.82	0.45
3:D:1332:LEU:HA	3:D:1332:LEU:HD23	1.80	0.45
5:M:215:GLU:O	5:M:219:ILE:HD12	2.16	0.45
7:G:10:DG:H2''	7:G:11:DC:C6	2.52	0.45
1:A:51:MET:HE3	1:A:52:PRO:HD2	1.99	0.45
1:A:273:GLU:HB3	1:A:275:ILE:HG12	1.99	0.45
2:C:94:ALA:HA	2:C:95:PRO:HD3	1.81	0.45
2:C:179:TYR:OH	2:C:462:ASN:OD1	2.30	0.45
2:C:503:LYS:HE2	2:C:503:LYS:HB3	1.69	0.45
2:C:653:MET:HG3	2:C:654:ASP:N	2.32	0.45
2:C:839:VAL:CG2	2:C:840:SER:N	2.77	0.45
1:A:155:ALA:N	1:A:174:ASP:OD1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:76:LYS:HE3	3:D:76:LYS:HB3	1.70	0.45
6:F:1:DA:OP2	6:F:1:DA:H3'	2.17	0.45
2:C:177:ILE:HD12	2:C:177:ILE:HG23	1.69	0.44
2:C:1340:GLU:O	3:D:18:ASP:O	2.35	0.44
3:D:250:ARG:HG2	3:D:265:LEU:HD23	1.99	0.44
3:D:372:MET:HE1	3:D:468:VAL:CG2	2.47	0.44
3:D:506:VAL:H	3:D:506:VAL:HG23	1.37	0.44
3:D:614:LEU:HD23	4:E:5:THR:HG23	1.98	0.44
3:D:1356:LEU:N	3:D:1356:LEU:CD1	2.80	0.44
1:A:56:VAL:H	1:A:56:VAL:HG23	1.63	0.44
1:B:168:ILE:HD12	1:B:169:GLY:N	2.32	0.44
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.47	0.44
5:M:213:LEU:HD13	5:M:252:LEU:HD22	1.99	0.44
2:C:156:PHE:O	2:C:174:ALA:HA	2.17	0.44
2:C:210:LEU:HD22	2:C:220:ILE:HG12	1.98	0.44
2:C:528:ARG:NH1	2:C:576:SER:O	2.51	0.44
2:C:637:ARG:HH11	2:C:637:ARG:HD2	1.59	0.44
2:C:1267:GLY:CA	3:D:347:VAL:O	2.59	0.44
3:D:373:ALA:C	3:D:375:GLU:N	2.76	0.44
1:A:158:ARG:HH22	1:A:173:VAL:H	1.65	0.44
2:C:1247:SER:OG	2:C:1248:THR:N	2.48	0.44
2:C:1259:LEU:O	2:C:1266:GLY:HA2	2.18	0.44
3:D:322:ARG:C	3:D:324:LEU:H	2.25	0.44
3:D:472:LEU:N	3:D:472:LEU:HD12	2.33	0.44
3:D:740:LEU:C	3:D:762:ASN:HB2	2.43	0.44
1:B:33:ARG:HH11	1:B:33:ARG:CG	2.29	0.44
2:C:30:ILE:CG2	2:C:31:GLN:N	2.79	0.44
2:C:177:ILE:HA	2:C:177:ILE:HD13	1.71	0.44
2:C:791:LEU:HD23	2:C:791:LEU:HA	1.86	0.44
2:C:1101:LEU:N	2:C:1101:LEU:HD12	2.32	0.44
3:D:110:PRO:HB3	3:D:240:THR:HG22	1.99	0.44
3:D:252:LEU:HD21	3:D:260:PHE:HB3	1.95	0.44
3:D:529:GLY:N	3:D:530:PRO:CA	2.81	0.44
3:D:531:LYS:HB3	3:D:581:MET:HE2	1.99	0.44
6:F:4:DG:C4'	6:F:5:DC:C5'	2.95	0.44
6:F:10:DC:P	6:F:10:DC:H3'	2.57	0.44
1:A:81:ILE:CG1	1:A:131:CYS:HB3	2.48	0.44
2:C:899:GLU:OE2	2:C:899:GLU:HA	2.18	0.44
2:C:1161:LEU:O	2:C:1162:SER:OG	2.28	0.44
3:D:388:ARG:HB2	3:D:390:LEU:CD1	2.47	0.44
3:D:813:ASP:OD1	3:D:814:CYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:10:VAL:O	4:E:13:ILE:O	2.35	0.44
1:B:109:PRO:HA	1:B:132:HIS:HA	2.00	0.44
2:C:155:VAL:CG2	2:C:405:PHE:CD1	3.01	0.44
2:C:592:ARG:HD2	2:C:653:MET:HG2	2.00	0.44
3:D:394:ILE:H	3:D:394:ILE:HD12	1.82	0.44
3:D:848:VAL:O	3:D:856:ILE:HG22	2.18	0.44
3:D:925:GLU:CD	3:D:925:GLU:C	2.86	0.44
3:D:1219:ASP:O	3:D:1223:LEU:HG	2.18	0.44
2:C:765:ILE:C	2:C:765:ILE:HD12	2.42	0.44
2:C:1288:GLN:O	2:C:1288:GLN:HG2	2.16	0.44
3:D:133:ARG:O	3:D:137:ARG:CB	2.66	0.44
3:D:342:LEU:C	3:D:344:GLY:H	2.26	0.44
7:G:13:DG:C2'	7:G:14:DT:H72	2.48	0.44
1:B:47:LEU:HD23	1:B:51:MET:HE1	1.99	0.44
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.80	0.44
3:D:387:LEU:HA	3:D:387:LEU:HD23	1.89	0.44
3:D:704:GLU:O	3:D:705:THR:C	2.61	0.44
3:D:1159:ILE:HG12	3:D:1206:ARG:HB2	2.00	0.44
2:C:144:VAL:HG11	2:C:527:LYS:HA	2.00	0.43
2:C:1286:THR:OG1	3:D:479:GLU:OE1	2.28	0.43
3:D:338:PHE:HZ	3:D:798:ARG:CZ	2.30	0.43
3:D:1307:LEU:HD22	3:D:1307:LEU:H	1.79	0.43
6:F:8:DA:H2''	6:F:9:DT:H3'	1.99	0.43
1:A:71:LYS:O	1:A:74:VAL:HG22	2.18	0.43
1:B:104:LYS:NZ	1:B:109:PRO:O	2.51	0.43
2:C:532:ALA:HB1	2:C:538:LEU:CD1	2.49	0.43
2:C:1066:MET:HE2	2:C:1066:MET:HB3	1.82	0.43
2:C:1244:HIS:HB2	2:C:1262:LYS:HD2	2.00	0.43
3:D:102:MET:HG2	3:D:246:PRO:HG3	2.00	0.43
3:D:238:ILE:O	3:D:238:ILE:CG1	2.66	0.43
3:D:625:MET:HE2	3:D:625:MET:HB3	1.86	0.43
3:D:850:LYS:HD2	3:D:855:ASP:HB3	2.00	0.43
3:D:1031:VAL:HG21	3:D:1088:VAL:HG11	2.00	0.43
1:A:234:LEU:HD12	1:A:234:LEU:N	2.33	0.43
2:C:61:SER:OG	2:C:62:TYR:N	2.48	0.43
2:C:200:ARG:HA	2:C:200:ARG:HD3	1.87	0.43
2:C:718:ALA:HB2	2:C:783:LEU:HG	2.00	0.43
2:C:801:ARG:HB2	2:C:1229:TYR:CE2	2.52	0.43
1:B:102:LEU:HD11	1:B:142:MET:HE3	2.01	0.43
2:C:617:ALA:HA	2:C:636:CYS:SG	2.59	0.43
3:D:322:ARG:O	3:D:324:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:610:ARG:HA	3:D:610:ARG:HD3	1.80	0.43
3:D:1159:ILE:HG22	3:D:1160:SER:N	2.33	0.43
3:D:1352:ILE:HD13	3:D:1352:ILE:HG21	1.72	0.43
1:B:43:LEU:HA	1:B:43:LEU:HD12	1.85	0.43
2:C:73:TYR:HD2	2:C:74:ARG:O	2.01	0.43
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.33	0.43
2:C:1142:ARG:HH22	2:C:1165:SER:HA	1.82	0.43
2:C:1239:VAL:HG23	2:C:1240:ASP:N	2.33	0.43
3:D:520:ALA:HB3	3:D:545:HIS:CB	2.48	0.43
3:D:807:LEU:HD12	3:D:807:LEU:HA	1.55	0.43
3:D:1323:ALA:O	3:D:1328:THR:CG2	2.64	0.43
5:M:204:SER:OG	5:M:205:GLN:OE1	2.37	0.43
7:G:-28:DC:H2'	7:G:-27:DT:H72	2.01	0.43
1:A:219:ARG:O	1:A:223:ILE:HG13	2.18	0.43
2:C:84:GLU:OE2	2:C:88:ARG:NE	2.50	0.43
2:C:1178:LYS:HB2	2:C:1178:LYS:HE3	1.93	0.43
5:M:124:LEU:O	5:M:128:VAL:HG23	2.18	0.43
2:C:127:ILE:H	2:C:127:ILE:HG12	1.77	0.43
2:C:301:TYR:CE2	2:C:333:ILE:HG23	2.54	0.43
2:C:540:ARG:CG	2:C:541:GLU:N	2.71	0.43
2:C:708:VAL:HG23	2:C:708:VAL:H	1.58	0.43
3:D:60:ARG:H	3:D:90:VAL:HG22	1.83	0.43
3:D:132:LEU:O	3:D:136:GLU:CB	2.66	0.43
5:M:131:THR:HB	5:M:181:ARG:NH2	2.33	0.43
2:C:1032:LYS:O	2:C:1036:ILE:HG12	2.19	0.43
2:C:1195:ILE:HD13	2:C:1195:ILE:HG21	1.69	0.43
3:D:527:LEU:CD1	3:D:527:LEU:C	2.92	0.43
3:D:707:ILE:HG22	3:D:708:ASN:N	2.33	0.43
7:G:-24:DC:H2''	7:G:-23:DA:C8	2.53	0.43
3:D:20:ILE:HD12	3:D:20:ILE:H	1.83	0.43
3:D:82:GLY:O	3:D:83:VAL:HB	2.19	0.43
3:D:279:LEU:HD13	3:D:299:LEU:HD13	1.99	0.43
3:D:545:HIS:O	3:D:546:ALA:HB3	2.17	0.43
3:D:968:ASN:HA	3:D:1118:GLY:HA3	2.01	0.43
3:D:1133:ASP:C	3:D:1135:THR:H	2.26	0.43
6:F:-1:DC:H6	6:F:-1:DC:H2'	1.63	0.43
1:B:19:VAL:HB	1:B:23:HIS:CD2	2.53	0.43
2:C:755:LYS:HD3	2:C:755:LYS:HA	1.84	0.43
3:D:584:PRO:HD3	3:D:620:PHE:CD1	2.54	0.43
3:D:788:LEU:HD12	3:D:792:ASN:HD21	1.84	0.43
3:D:800:LEU:HD22	3:D:1256:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLU:HB2	1:A:35:PHE:CD2	2.54	0.42
1:A:42:ALA:O	1:A:46:ILE:HG12	2.19	0.42
2:C:933:VAL:O	2:C:933:VAL:HG12	2.18	0.42
3:D:19:ALA:CB	3:D:1343:GLU:H	2.32	0.42
3:D:450:HIS:HE1	3:D:625:MET:HE1	1.84	0.42
3:D:541:LEU:HG	3:D:542:ALA:N	2.33	0.42
6:F:12:DT:H1'	6:F:13:DG:C8	2.54	0.42
1:A:218:ARG:HH21	1:B:231:PHE:HA	1.83	0.42
2:C:517:GLN:HB3	2:C:759:SER:HB2	1.99	0.42
2:C:815:SER:HB2	2:C:816:ILE:H	1.66	0.42
2:C:902:LEU:HD11	5:M:195:LEU:CD1	2.50	0.42
2:C:1012:GLU:O	2:C:1016:GLU:CB	2.66	0.42
3:D:576:ARG:NH1	3:D:593:ASN:OD1	2.50	0.42
3:D:842:ARG:O	3:D:843:VAL:HG23	2.20	0.42
3:D:929:GLN:O	3:D:930:LEU:HG	2.19	0.42
3:D:1177:ILE:HD11	3:D:1190:ILE:HD11	2.01	0.42
3:D:1233:ILE:HD13	3:D:1233:ILE:HG21	1.61	0.42
4:E:42:GLU:O	4:E:43:ASN:HB3	2.18	0.42
1:A:279:GLY:HA2	1:A:282:VAL:HG12	2.00	0.42
2:C:877:VAL:CG1	2:C:920:VAL:HG21	2.49	0.42
2:C:1259:LEU:HD23	2:C:1259:LEU:HA	1.56	0.42
3:D:215:LYS:O	3:D:218:THR:OG1	2.31	0.42
3:D:321:LYS:O	3:D:322:ARG:HB2	2.19	0.42
3:D:339:ARG:HA	3:D:339:ARG:HD3	1.90	0.42
6:F:1:DA:H3'	6:F:1:DA:P	2.58	0.42
1:A:118:ASP:OD1	1:A:119:GLY:N	2.51	0.42
2:C:830:THR:HG22	2:C:1234:LYS:HZ1	1.83	0.42
3:D:9:LYS:O	3:D:12:THR:HG22	2.19	0.42
3:D:271:ARG:HE	3:D:271:ARG:HB2	1.63	0.42
5:M:344:SER:O	5:M:348:VAL:CB	2.66	0.42
2:C:31:GLN:C	2:C:130:MET:HE1	2.44	0.42
2:C:718:ALA:HB2	2:C:783:LEU:HD21	2.00	0.42
2:C:835:GLU:HG3	2:C:1053:TYR:CE1	2.55	0.42
3:D:355:ILE:HD12	3:D:355:ILE:HG23	1.59	0.42
3:D:452:LEU:HD23	3:D:452:LEU:HA	1.86	0.42
3:D:932:MET:O	3:D:1137:GLY:HA3	2.19	0.42
2:C:1226:THR:HG21	3:D:639:VAL:O	2.20	0.42
3:D:62:PHE:HE1	3:D:102:MET:O	2.03	0.42
3:D:180:MET:CE	3:D:293:ARG:HD2	2.50	0.42
3:D:279:LEU:O	3:D:283:LEU:HB2	2.20	0.42
3:D:883:ARG:O	3:D:883:ARG:CG	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1107:VAL:HG12	3:D:1109:LEU:H	1.84	0.42
3:D:1318:SER:OG	3:D:1321:SER:OG	2.36	0.42
2:C:148:GLN:HE22	2:C:536:GLY:H	1.68	0.42
2:C:192:ASP:HB3	2:C:346:TYR:HE1	1.83	0.42
2:C:590:PRO:HB3	2:C:605:TYR:CE1	2.55	0.42
2:C:1253:LEU:CB	5:M:113:GLN:O	2.46	0.42
3:D:123:ARG:HD2	3:D:1337:VAL:HG21	2.01	0.42
3:D:368:LEU:HD12	3:D:369:PRO:CD	2.47	0.42
3:D:477:GLN:O	3:D:481:ARG:HG2	2.20	0.42
3:D:843:VAL:CG1	3:D:883:ARG:HD3	2.50	0.42
1:B:89:ALA:HB3	1:B:124:VAL:CG2	2.50	0.42
1:B:92:VAL:O	1:B:148:ARG:NH1	2.52	0.42
2:C:480:SER:O	2:C:481:LEU:CB	2.68	0.42
2:C:484:LEU:HD21	2:C:486:THR:HG23	2.02	0.42
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.54	0.42
2:C:833:ILE:HD13	2:C:833:ILE:HG21	1.67	0.42
2:C:1239:VAL:H	2:C:1239:VAL:HG22	1.51	0.42
3:D:77:ARG:C	3:D:79:LYS:H	2.28	0.42
3:D:702:GLN:O	3:D:703:THR:C	2.63	0.42
1:B:124:VAL:HG23	1:B:125:LYS:N	2.34	0.42
2:C:726:TYR:HB3	2:C:733:VAL:HG22	2.01	0.42
2:C:757:THR:HB	2:C:765:ILE:CD1	2.45	0.42
2:C:812:PHE:CE2	2:C:813:GLU:HG2	2.55	0.42
2:C:1214:ASP:OD1	2:C:1215:GLY:N	2.50	0.42
3:D:116:PHE:CE1	3:D:1333:THR:HG22	2.55	0.42
3:D:432:LEU:HD23	3:D:432:LEU:HA	1.93	0.42
3:D:530:PRO:HD2	3:D:531:LYS:C	2.44	0.42
3:D:698:MET:O	3:D:702:GLN:HG3	2.20	0.42
6:F:2:DG:H2''	6:F:3:DG:H1'	2.02	0.42
3:D:374:LEU:O	3:D:378:LYS:HG3	2.20	0.42
3:D:546:ALA:HB3	3:D:548:VAL:HG23	2.02	0.42
3:D:634:ARG:HE	3:D:634:ARG:HB3	1.70	0.42
3:D:1205:GLU:N	3:D:1208:ASP:OD2	2.52	0.42
4:E:49:ILE:HD12	4:E:49:ILE:HG23	1.81	0.42
7:G:-16:DT:C6	7:G:-15:DT:H72	2.54	0.42
1:A:136:GLU:O	1:A:137:ASN:CB	2.67	0.41
2:C:53:PHE:HE2	2:C:73:TYR:HB3	1.85	0.41
2:C:667:LEU:CD2	2:C:704:MET:HB3	2.50	0.41
2:C:933:VAL:HG22	2:C:1050:VAL:CG1	2.15	0.41
2:C:1167:GLU:O	2:C:1168:GLU:CB	2.61	0.41
2:C:1269:ARG:HA	3:D:346:ARG:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:378:LYS:CB	3:D:379:PRO:HD3	2.50	0.41
3:D:489:ASN:OD1	3:D:489:ASN:O	2.38	0.41
3:D:518:VAL:HB	3:D:707:ILE:HB	2.02	0.41
3:D:1320:ILE:HG21	3:D:1320:ILE:HD13	1.43	0.41
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.90	0.41
1:A:89:ALA:O	1:A:124:VAL:HG12	2.20	0.41
2:C:851:THR:OG1	2:C:869:GLY:HA3	2.20	0.41
2:C:1268:GLN:NE2	3:D:352:ARG:HD2	2.36	0.41
3:D:686:TRP:HB3	3:D:758:PRO:HG3	2.02	0.41
1:A:131:CYS:O	1:A:132:HIS:CG	2.74	0.41
1:B:86:LYS:HE2	1:B:174:ASP:HB2	2.02	0.41
1:B:190:ALA:O	1:B:198:LEU:HB2	2.21	0.41
2:C:14:ASP:O	2:C:1155:VAL:HB	2.19	0.41
2:C:594:VAL:HB	2:C:651:ASP:C	2.44	0.41
2:C:830:THR:HG22	2:C:1234:LYS:HZ3	1.84	0.41
2:C:831:ILE:HD13	2:C:1057:LYS:HG2	2.02	0.41
2:C:894:GLN:HG2	2:C:895:LEU:H	1.84	0.41
2:C:1333:LEU:HD11	3:D:327:LEU:HB3	2.02	0.41
3:D:134:ASP:O	3:D:138:VAL:HG13	2.20	0.41
7:G:4:DG:C4	7:G:5:DC:C5	3.08	0.41
2:C:519:ASN:HD21	2:C:689:ALA:CB	2.25	0.41
2:C:553:THR:C	2:C:555:TYR:H	2.29	0.41
2:C:1159:VAL:HG13	2:C:1159:VAL:O	2.21	0.41
2:C:1222:GLU:O	3:D:635:SER:O	2.37	0.41
2:C:1243:MET:HB3	2:C:1243:MET:HE3	1.80	0.41
3:D:1271:SER:O	3:D:1272:SER:OG	2.26	0.41
3:D:1314:LEU:HA	3:D:1322:ALA:HB1	2.01	0.41
5:M:377:HIS:O	5:M:380:THR:OG1	2.37	0.41
6:F:10:DC:H3'	6:F:10:DC:OP2	2.20	0.41
2:C:911:SER:OG	2:C:912:ASP:N	2.53	0.41
3:D:31:ARG:HA	3:D:34:SER:OG	2.21	0.41
3:D:120:LEU:HA	3:D:121:PRO:HA	1.83	0.41
3:D:332:LYS:HD3	3:D:332:LYS:HA	1.55	0.41
3:D:731:ARG:HD2	3:D:731:ARG:HA	1.51	0.41
3:D:1243:LEU:HA	3:D:1243:LEU:HD12	1.85	0.41
2:C:534:GLY:HA3	2:C:535:PRO:HD2	1.78	0.41
2:C:551:HIS:H	2:C:554:HIS:CE1	2.39	0.41
2:C:1062:PRO:HA	2:C:1076:ILE:HB	2.02	0.41
2:C:1101:LEU:HA	3:D:725:MET:HE1	2.03	0.41
2:C:1195:ILE:O	2:C:1199:LEU:HB2	2.21	0.41
3:D:19:ALA:HB2	3:D:1343:GLU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:125:GLY:HA2	3:D:135:ILE:HD12	2.03	0.41
3:D:807:LEU:HD23	3:D:915:ILE:HB	2.03	0.41
3:D:931:THR:H	3:D:1244:GLN:HE21	1.68	0.41
3:D:1263:LYS:HE2	3:D:1315:ALA:HB1	2.03	0.41
5:M:131:THR:HA	5:M:132:PRO:HD3	1.84	0.41
1:B:57:THR:HG21	1:B:147:GLN:CD	2.46	0.41
2:C:387:ASN:HA	2:C:391:SER:OG	2.20	0.41
2:C:1075:VAL:H	2:C:1075:VAL:HG22	1.54	0.41
3:D:357:VAL:C	3:D:359:PRO:HD3	2.45	0.41
3:D:599:LYS:HA	3:D:599:LYS:HD2	1.77	0.41
3:D:641:ILE:H	3:D:641:ILE:HG12	1.27	0.41
5:M:175:VAL:O	5:M:179:LEU:CB	2.68	0.41
5:M:186:ASP:N	5:M:187:PRO:CD	2.83	0.41
2:C:731:ARG:HH11	2:C:731:ARG:HD3	1.47	0.41
2:C:1230:MET:CG	2:C:1231:TYR:N	2.83	0.41
3:D:61:ILE:HG21	3:D:61:ILE:HD13	1.73	0.41
3:D:279:LEU:HD23	3:D:279:LEU:C	2.45	0.41
3:D:418:GLU:OE1	4:E:44:ASP:HB2	2.21	0.41
3:D:430:HIS:HD2	3:D:925:GLU:HG3	1.85	0.41
1:A:47:LEU:HD13	1:A:183:ILE:HD13	2.03	0.41
1:B:178:SER:HA	1:B:179:PRO:HD2	1.93	0.41
1:B:210:THR:OG1	1:B:211:ILE:HD12	2.20	0.41
2:C:136:PHE:CD2	2:C:506:PHE:HE1	2.38	0.41
2:C:174:ALA:O	2:C:185:ASP:HA	2.20	0.41
2:C:346:TYR:C	2:C:348:SER:N	2.79	0.41
2:C:756:TYR:CD1	2:C:756:TYR:N	2.88	0.41
2:C:1101:LEU:HD12	2:C:1101:LEU:H	1.86	0.41
2:C:1101:LEU:O	3:D:731:ARG:HG3	2.21	0.41
2:C:1330:ILE:CG2	2:C:1337:ILE:CG2	2.99	0.41
3:D:253:VAL:HA	5:M:112:TYR:CB	2.51	0.41
3:D:326:SER:O	3:D:330:MET:N	2.52	0.41
3:D:770:LEU:HA	3:D:770:LEU:HD12	1.85	0.41
3:D:797:THR:O	3:D:801:VAL:HG23	2.21	0.41
3:D:917:VAL:H	3:D:917:VAL:HG23	1.36	0.41
5:M:194:ASP:C	5:M:196:ARG:H	2.29	0.41
2:C:660:VAL:CG2	2:C:661:VAL:N	2.83	0.41
2:C:705:GLU:CD	2:C:705:GLU:H	2.29	0.41
2:C:805:MET:O	2:C:805:MET:HG3	2.19	0.41
2:C:882:ILE:CG1	2:C:919:ARG:HG2	2.51	0.41
6:F:25:DC:H2''	6:F:26:DC:C6	2.56	0.41
1:B:27:THR:HG22	1:B:202:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:LEU:HD21	2:C:527:LYS:HD2	2.03	0.40
2:C:802:VAL:HG13	2:C:1098:LEU:HD13	2.03	0.40
2:C:813:GLU:HB2	3:D:461:PHE:HD2	1.85	0.40
2:C:836:LEU:HD23	2:C:836:LEU:HA	1.83	0.40
2:C:1168:GLU:OE1	2:C:1171:ARG:NH1	2.47	0.40
3:D:490:ILE:HD11	3:D:609:TYR:CD1	2.56	0.40
3:D:522:GLY:O	3:D:525:MET:HE2	2.20	0.40
3:D:527:LEU:HD12	3:D:527:LEU:C	2.45	0.40
6:F:-3:DG:C4'	6:F:-2:DC:OP1	2.69	0.40
2:C:515:MET:HG3	2:C:526:HIS:HD2	1.87	0.40
2:C:1085:MET:HA	2:C:1086:PRO:HD3	1.92	0.40
3:D:366:CYS:SG	3:D:448:GLN:O	2.78	0.40
3:D:514:THR:O	3:D:515:ARG:HG2	2.21	0.40
3:D:788:LEU:HD11	3:D:792:ASN:ND2	2.37	0.40
3:D:1238:GLN:HB3	3:D:1242:ARG:NH2	2.36	0.40
4:E:4:VAL:H	4:E:4:VAL:HG23	1.42	0.40
6:F:-9:DA:C2	7:G:10:DG:C2	3.09	0.40
1:A:102:LEU:HD12	1:A:102:LEU:C	2.46	0.40
2:C:38:PHE:CD2	2:C:39:ILE:HD11	2.56	0.40
2:C:141:THR:HG21	2:C:514:PHE:CD1	2.56	0.40
2:C:453:ILE:HG21	2:C:453:ILE:HD13	1.40	0.40
2:C:765:ILE:HD12	2:C:765:ILE:O	2.21	0.40
2:C:1008:GLN:O	2:C:1012:GLU:CB	2.69	0.40
2:C:1046:VAL:HG13	2:C:1046:VAL:O	2.19	0.40
3:D:61:ILE:O	3:D:62:PHE:CB	2.67	0.40
3:D:245:LEU:HD23	3:D:246:PRO:O	2.22	0.40
3:D:514:THR:HG21	3:D:596:LEU:HD22	2.02	0.40
3:D:619:ILE:HD13	3:D:619:ILE:HG21	1.87	0.40
1:A:179:PRO:O	1:A:180:VAL:C	2.64	0.40
1:B:34:GLY:N	1:B:199:ASP:OD2	2.49	0.40
2:C:720:ARG:O	2:C:736:VAL:HG23	2.22	0.40
2:C:920:VAL:HG12	2:C:921:PRO:O	2.22	0.40
2:C:1291:LEU:HD23	2:C:1291:LEU:HA	1.65	0.40
2:C:1308:ILE:HD13	2:C:1308:ILE:HA	1.82	0.40
3:D:421:VAL:CG1	3:D:422:LEU:N	2.78	0.40
3:D:1244:GLN:N	3:D:1244:GLN:OE1	2.54	0.40
7:G:-4:DA:H2''	7:G:-3:DA:H8	1.87	0.40
2:C:17:LYS:HZ2	2:C:1194:GLU:CD	2.28	0.40
2:C:1076:ILE:HG21	2:C:1076:ILE:HD13	1.86	0.40
2:C:1096:ILE:HD13	2:C:1096:ILE:HG21	1.28	0.40
3:D:499:ILE:O	3:D:500:ILE:CB	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	2.04	0.40
3:D:1362:GLY:O	3:D:1366:HIS:HD2	2.05	0.40
4:E:59:ILE:HG23	4:E:59:ILE:HD12	1.83	0.40
5:M:155:THR:O	5:M:156:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	305/329 (93%)	269 (88%)	32 (10%)	4 (1%)	9	33
1	B	233/329 (71%)	209 (90%)	22 (9%)	2 (1%)	14	42
2	C	1339/1342 (100%)	1183 (88%)	128 (10%)	28 (2%)	5	24
3	D	1335/1407 (95%)	1127 (84%)	169 (13%)	39 (3%)	3	19
4	E	73/91 (80%)	68 (93%)	3 (4%)	2 (3%)	4	20
5	M	283/497 (57%)	236 (83%)	40 (14%)	7 (2%)	4	21
All	All	3568/3995 (89%)	3092 (87%)	394 (11%)	82 (2%)	7	23

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ILE
2	C	29	SER
2	C	347	ILE
2	C	541	GLU
2	C	1155	VAL
3	D	118	LYS
3	D	312	ARG
3	D	334	LYS

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Mol	Chain	Res	Type
3	D	426	ALA
3	D	500	ILE
3	D	521	LYS
3	D	586	GLY
3	D	886	VAL
3	D	1134	ILE
4	E	15	ASN
5	M	153	TYR
2	C	2	VAL
2	C	228	VAL
2	C	570	GLY
2	C	728	ASP
2	C	773	LEU
2	C	919	ARG
2	C	1156	ARG
2	C	1189	GLY
2	C	1264	GLN
2	C	1268	GLN
3	D	94	GLN
3	D	349	TYR
3	D	574	VAL
3	D	915	ILE
3	D	1159	ILE
3	D	1309	ILE
5	M	169	GLU
1	A	98	VAL
1	A	177	TYR
1	B	168	ILE
2	C	481	LEU
2	C	509	SER
2	C	852	ALA
2	C	1255	THR
3	D	360	TYR
3	D	363	LEU
3	D	585	LYS
3	D	594	GLN
3	D	767	LEU
3	D	787	ALA
3	D	1210	ILE
4	E	14	GLY
5	M	156	ILE
5	M	167	ASP

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Mol	Chain	Res	Type
5	M	188	VAL
1	A	131	CYS
2	C	519	ASN
2	C	655	VAL
2	C	720	ARG
3	D	20	ILE
3	D	316	ILE
3	D	320	ASN
3	D	520	ALA
3	D	899	TYR
2	C	643	SER
2	C	1223	ARG
3	D	67	ASP
3	D	260	PHE
3	D	323	PRO
3	D	333	GLY
3	D	546	ALA
3	D	1180	VAL
5	M	185	PHE
2	C	892	GLU
2	C	1245	ALA
3	D	92	VAL
3	D	83	VAL
3	D	809	VAL
3	D	885	VAL
2	C	229	ILE
3	D	673	VAL
5	M	170	ILE
1	B	159	ILE
2	C	558	VAL
2	C	1186	VAL
3	D	894	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 PDB entries followed by that with respect to all EM entries.

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	244/286 (85%)	235 (96%)	9 (4%)	30	55
1	B	183/286 (64%)	176 (96%)	7 (4%)	29	54
2	C	1029/1157 (89%)	987 (96%)	42 (4%)	27	52
3	D	961/1168 (82%)	911 (95%)	50 (5%)	21	48
4	E	56/75 (75%)	55 (98%)	1 (2%)	51	67
5	M	113/393 (29%)	111 (98%)	2 (2%)	51	67
All	All	2586/3365 (77%)	2475 (96%)	111 (4%)	27	51

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	72	GLU
1	A	79	LEU
1	A	96	ASP
1	A	98	VAL
1	A	140	ILE
1	A	168	ILE
1	A	213	PRO
1	A	224	LEU
1	B	6	THR
1	B	16	ILE
1	B	33	ARG
1	B	45	ARG
1	B	201	LEU
1	B	223	ILE
1	B	224	LEU
2	C	18	ARG
2	C	71	VAL
2	C	127	ILE
2	C	149	LEU
2	C	184	LEU
2	C	388	LEU
2	C	445	ILE
2	C	517	GLN
2	C	521	LEU
2	C	552	PRO
2	C	555	TYR
2	C	564	PRO
2	C	569	ILE
2	C	639	LYS

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Mol	Chain	Res	Type
2	C	690	VAL
2	C	697	LYS
2	C	699	LEU
2	C	719	LYS
2	C	727	VAL
2	C	734	ILE
2	C	773	LEU
2	C	821	ARG
2	C	827	ARG
2	C	873	ILE
2	C	929	ILE
2	C	1049	ILE
2	C	1050	VAL
2	C	1070	HIS
2	C	1096	ILE
2	C	1108	ASN
2	C	1151	LEU
2	C	1159	VAL
2	C	1178	LYS
2	C	1180	MET
2	C	1210	ILE
2	C	1224	PRO
2	C	1232	MET
2	C	1239	VAL
2	C	1243	MET
2	C	1268	GLN
2	C	1306	LYS
2	C	1319	MET
3	D	7	PHE
3	D	22	ILE
3	D	27	PRO
3	D	28	ASP
3	D	38	VAL
3	D	70	CYS
3	D	74	LYS
3	D	78	LEU
3	D	93	THR
3	D	102	MET
3	D	120	LEU
3	D	132	LEU
3	D	188	LEU
3	D	249	LEU

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Mol	Chain	Res	Type
3	D	252	LEU
3	D	271	ARG
3	D	316	ILE
3	D	330	MET
3	D	334	LYS
3	D	352	ARG
3	D	368	LEU
3	D	379	PRO
3	D	394	ILE
3	D	434	ILE
3	D	470	VAL
3	D	471	PRO
3	D	472	LEU
3	D	502	PRO
3	D	504	GLN
3	D	505	ASP
3	D	527	LEU
3	D	588	PRO
3	D	616	PRO
3	D	627	THR
3	D	641	ILE
3	D	644	MET
3	D	717	VAL
3	D	722	ILE
3	D	788	LEU
3	D	835	LEU
3	D	885	VAL
3	D	886	VAL
3	D	1138	LEU
3	D	1263	LYS
3	D	1266	ILE
3	D	1309	ILE
3	D	1347	LEU
3	D	1349	GLU
3	D	1351	VAL
3	D	1353	VAL
4	E	6	VAL
5	M	140	ILE
5	M	156	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	103	ASN
1	A	132	HIS
1	A	268	ASN
1	A	294	ASN
1	B	37	HIS
2	C	165	HIS
2	C	513	GLN
2	C	519	ASN
2	C	526	HIS
2	C	554	HIS
2	C	573	ASN
2	C	604	HIS
2	C	686	GLN
2	C	688	GLN
2	C	725	GLN
2	C	760	ASN
2	C	761	GLN
2	C	1072	ASN
2	C	1080	ASN
2	C	1135	GLN
2	C	1136	GLN
2	C	1175	ASN
2	C	1244	HIS
2	C	1268	GLN
2	C	1313	HIS
3	D	157	GLN
3	D	186	GLN
3	D	335	GLN
3	D	364	HIS
3	D	365	GLN
3	D	419	HIS
3	D	477	GLN
3	D	667	GLN
3	D	669	GLN
3	D	792	ASN
3	D	875	ASN
3	D	907	HIS
3	D	1366	HIS
5	M	157	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

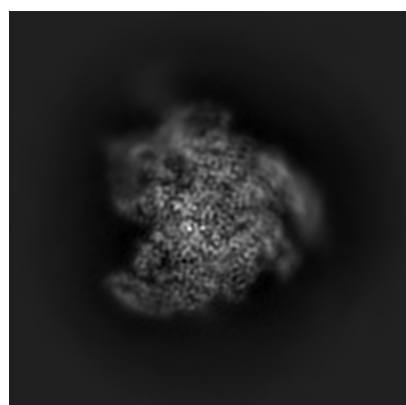
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0001. These allow visual inspection of the internal detail of the map and identification of artifacts.

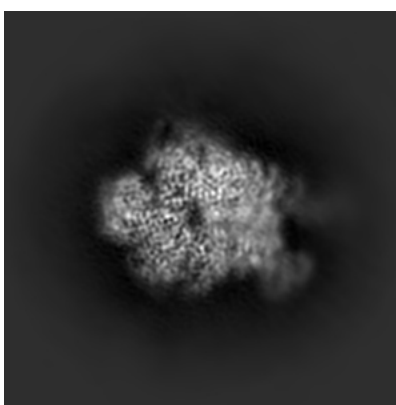
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

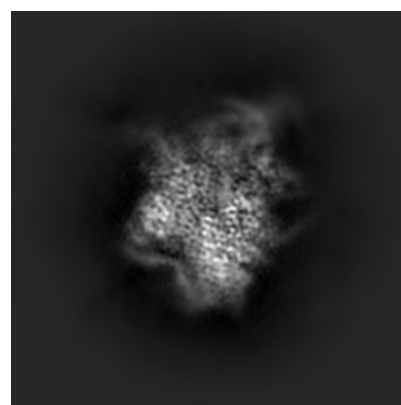
6.1.1 Primary map



X



Y

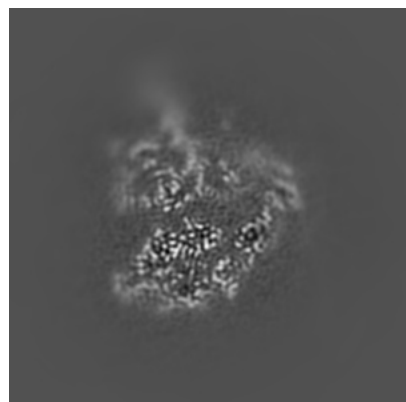


Z

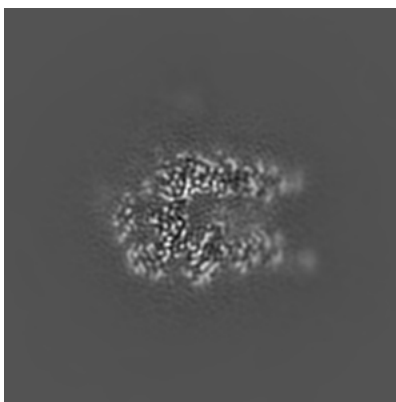
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

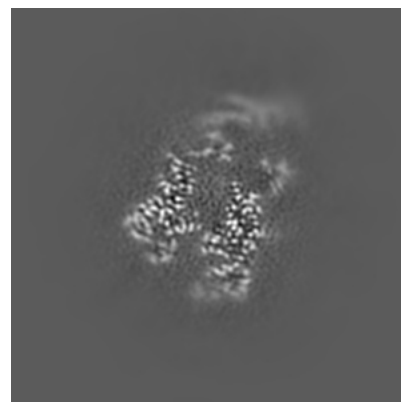
6.2.1 Primary map



X Index: 128



Y Index: 128

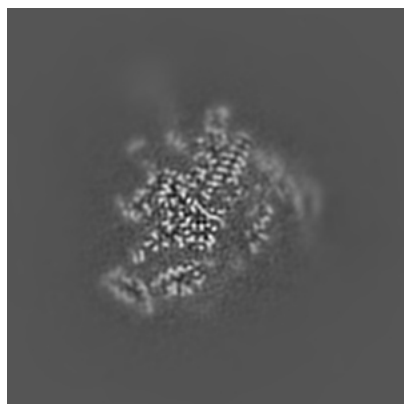


Z Index: 128

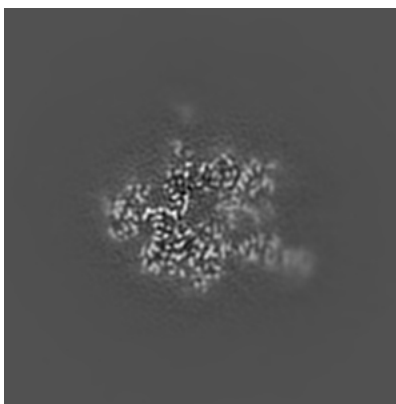
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

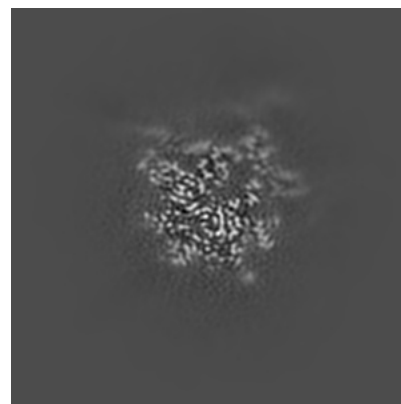
6.3.1 Primary map



X Index: 140



Y Index: 122

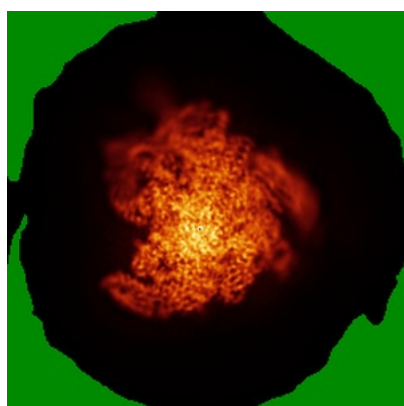


Z Index: 108

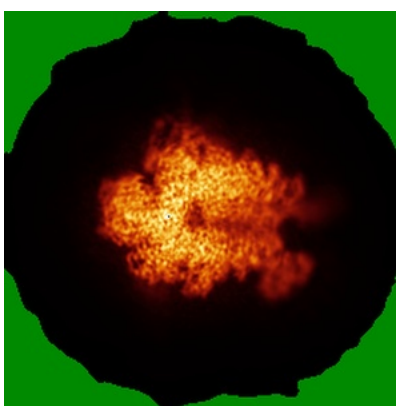
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

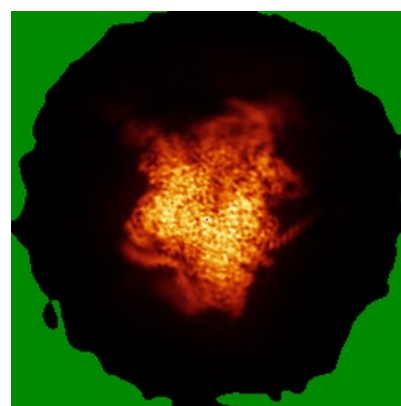
6.4.1 Primary map



X



Y

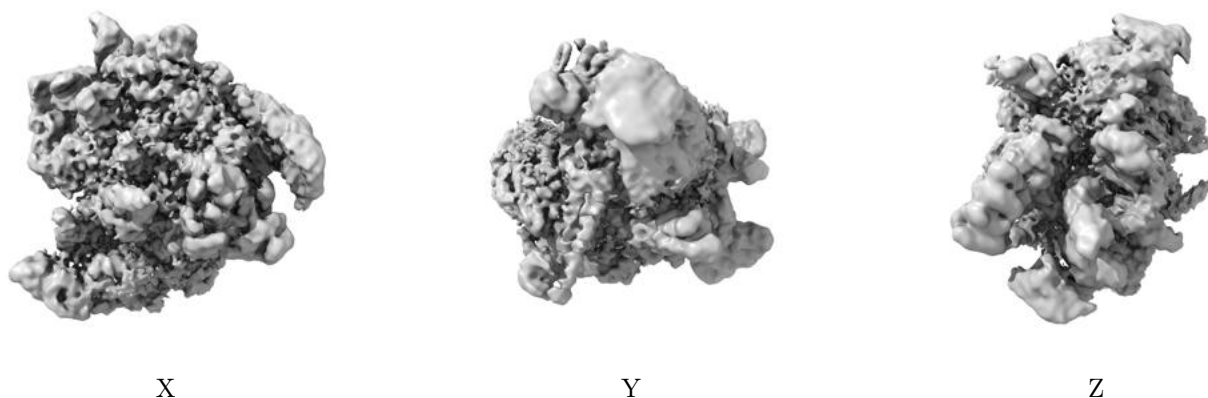


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

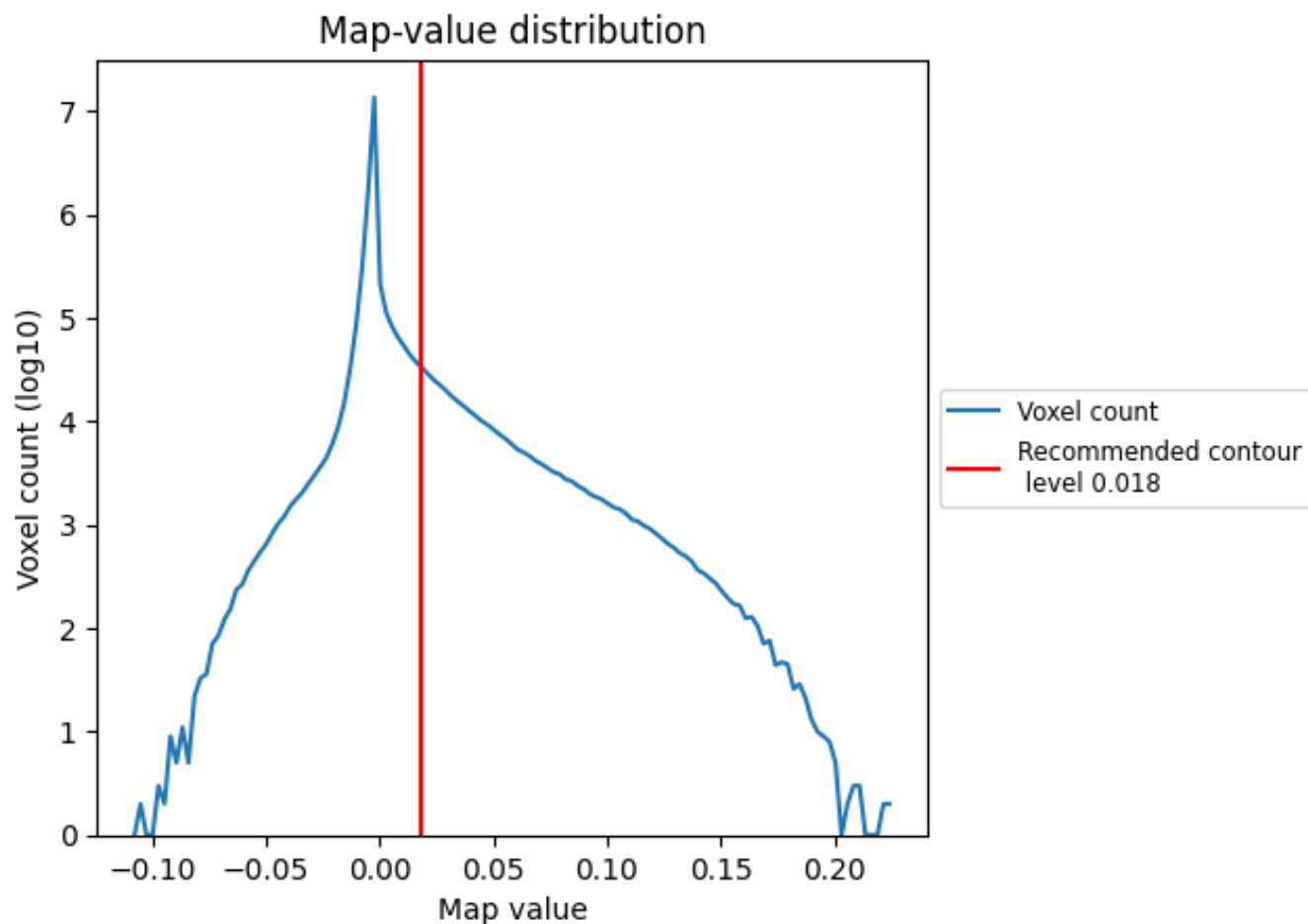
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

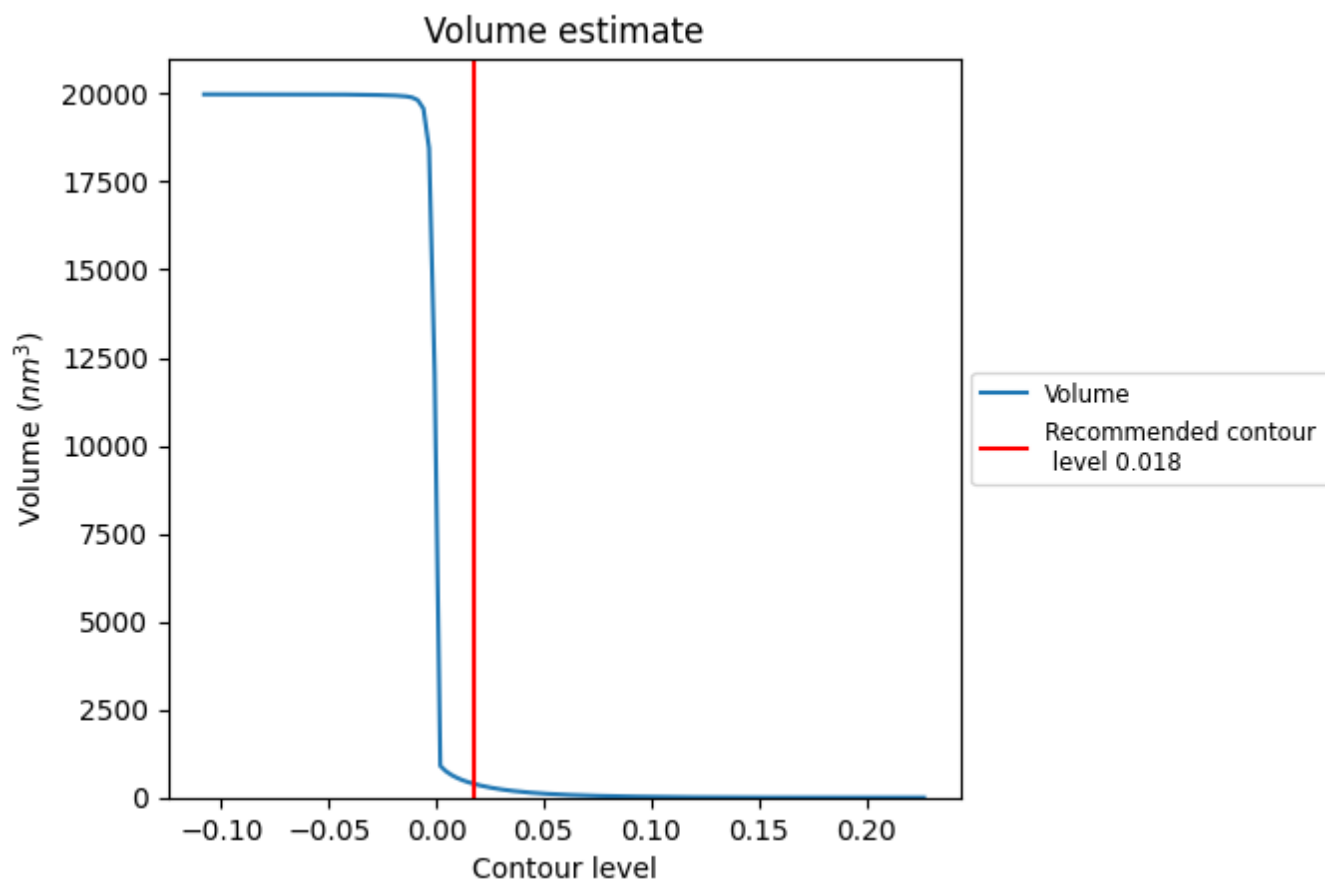
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

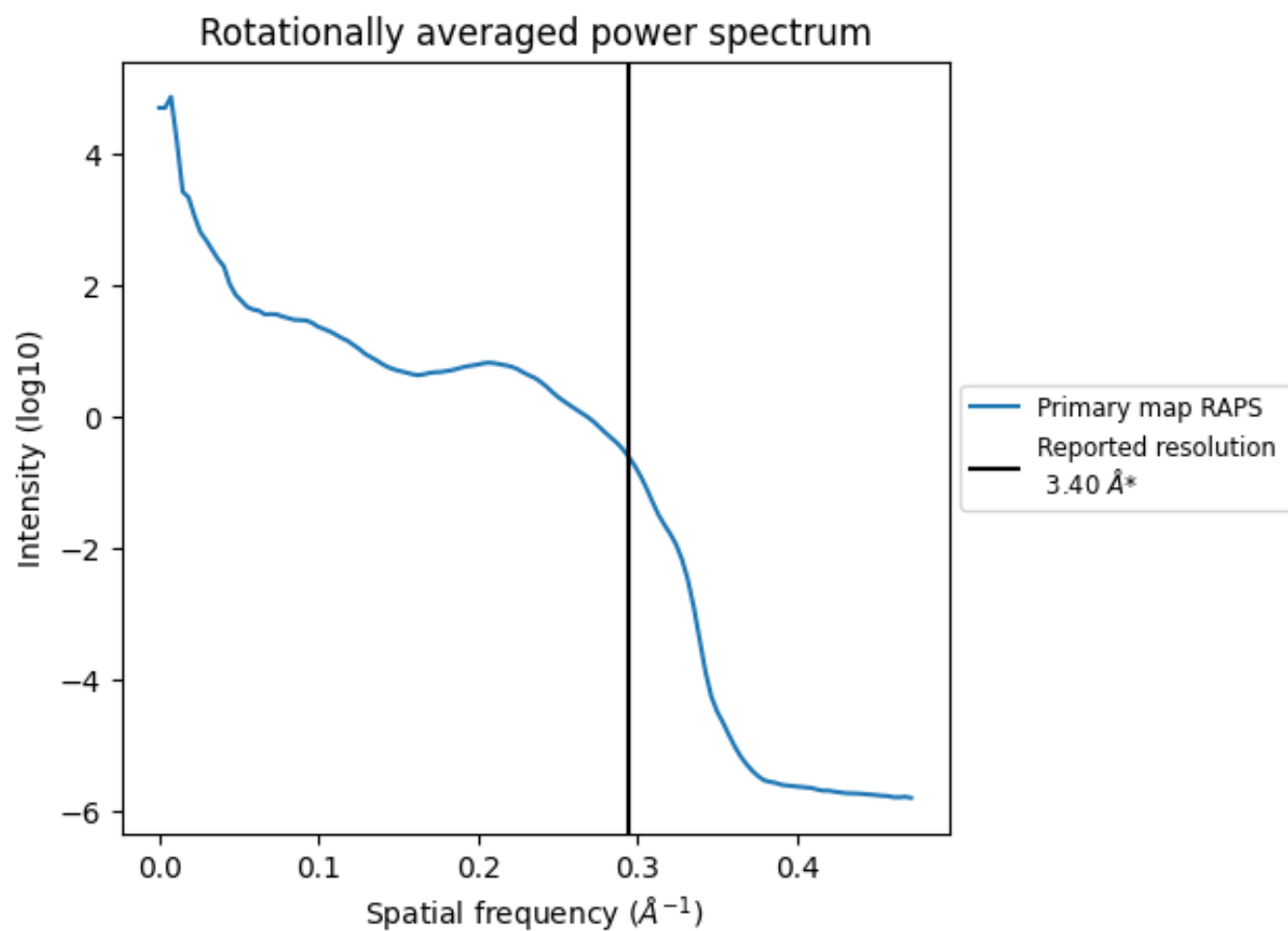
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 383 nm^3 ; this corresponds to an approximate mass of 346 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

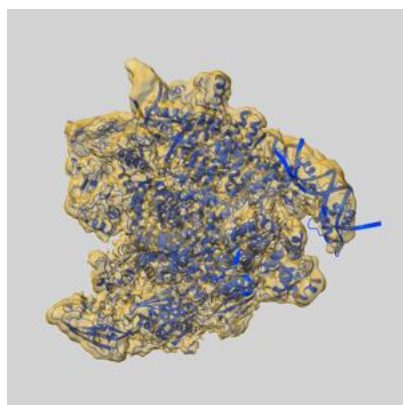
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

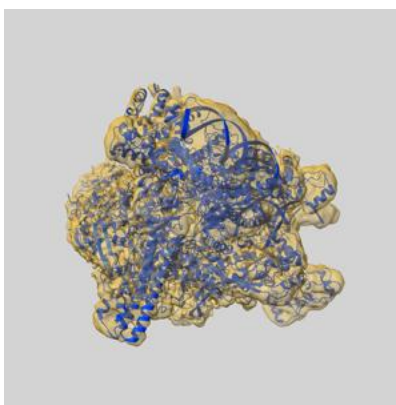
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0001 and PDB model 6GH5. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

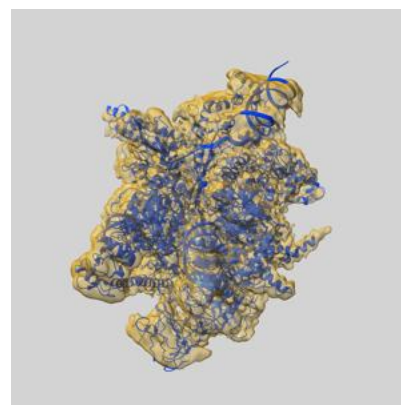
9.1 Map-model overlay [i](#)



X



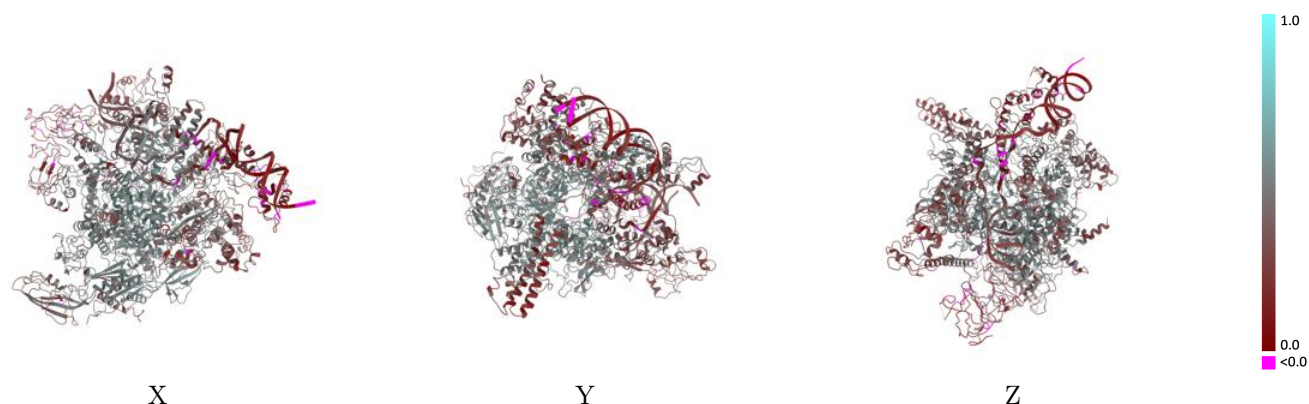
Y



Z

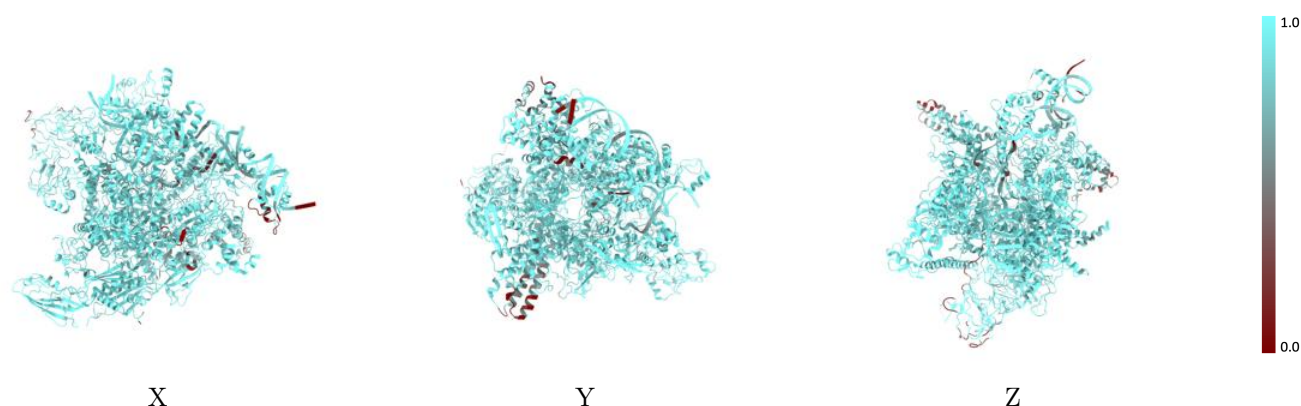
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



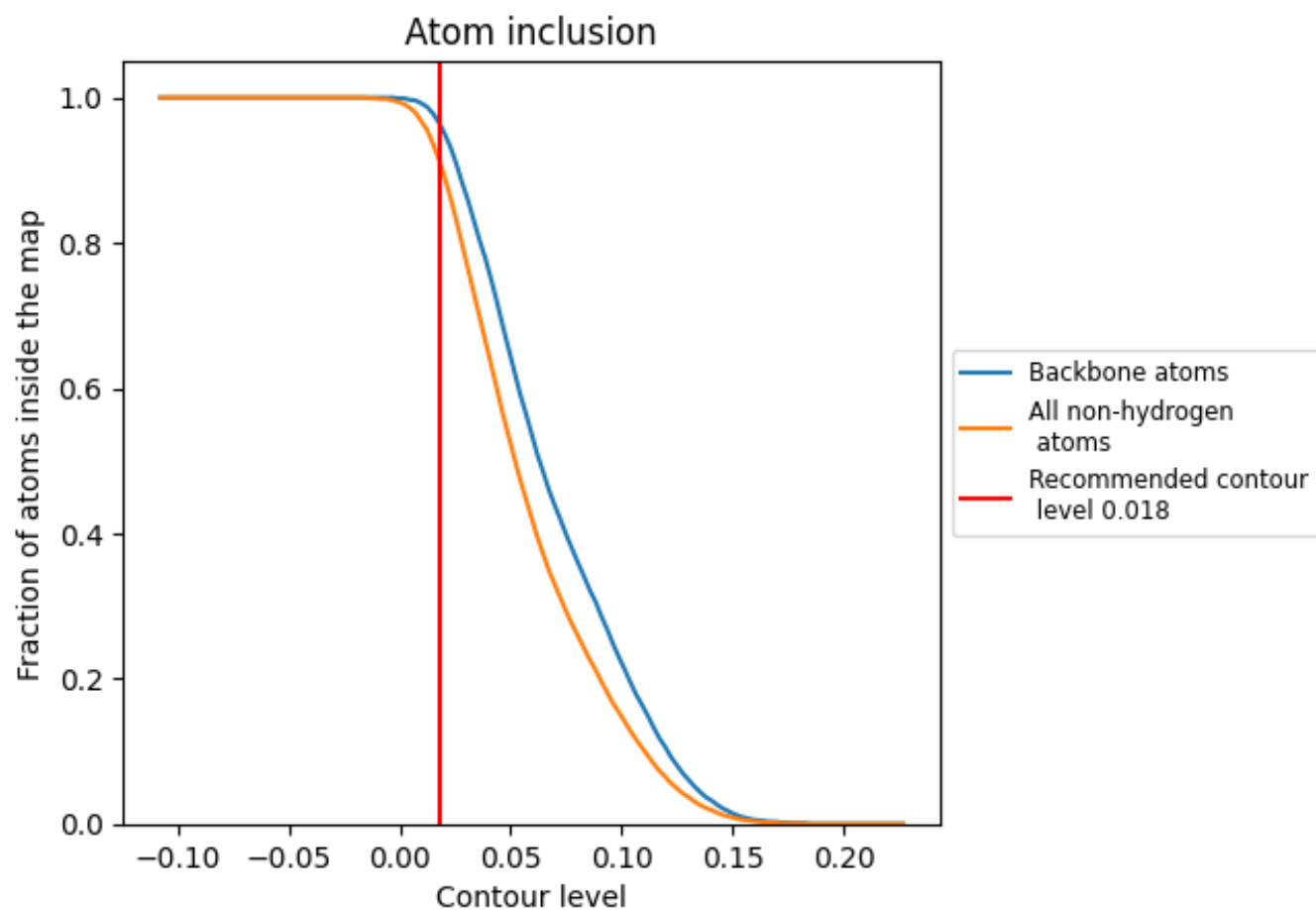
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9120	0.4120
A	0.8810	0.4420
B	0.9370	0.4200
C	0.9280	0.4460
D	0.9210	0.4290
E	0.9400	0.4620
F	0.7720	0.1950
G	0.8450	0.2120
M	0.9010	0.3010

1.0

0.0

<0.0