Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:08 am GMT

PDB ID	:	6GH5
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:

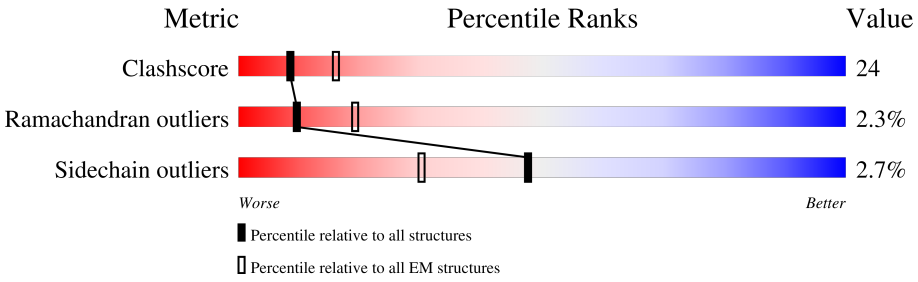
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	56% 30% 8% • 6%
1	B	329	41% 25% 5% • 29%
2	C	1342	54% 30% 13% •
3	D	1407	48% 31% 13% • •
4	E	91	47% 24% 10% • 18%
5	M	497	55% 10% • 32%
6	F	63	6% 14% 46% 13% 27%
7	G	63	5% 29% 44% 27%

2 Entry composition

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.

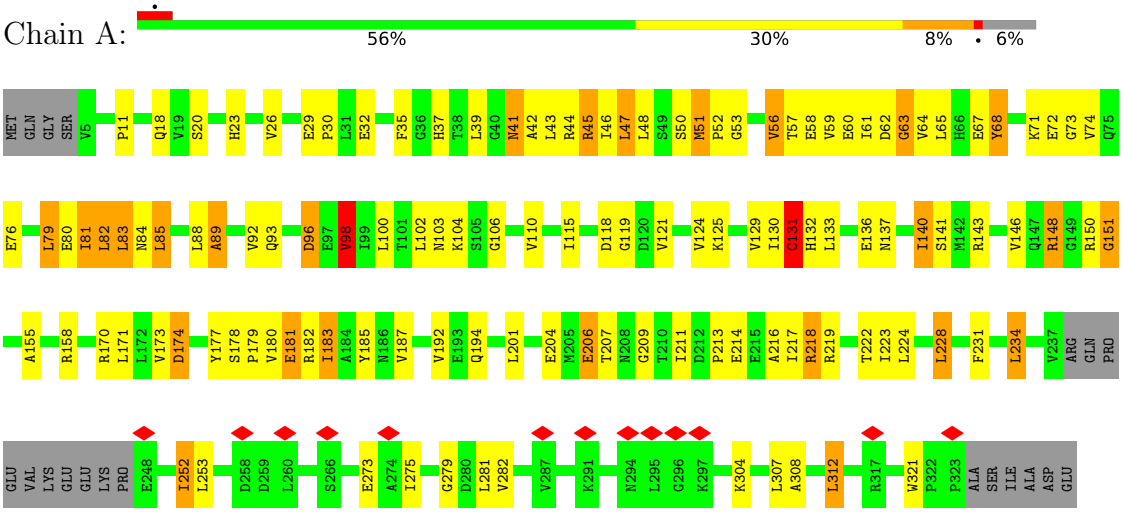
Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	46	Total	C	N	O	P	0	0
			946	448	173	279	46		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

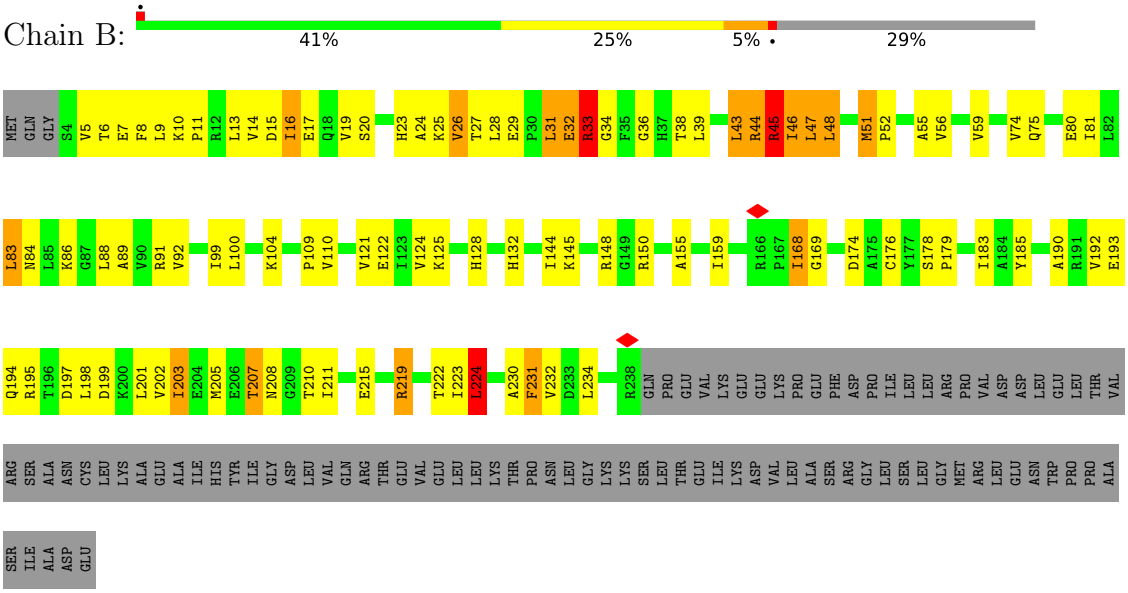
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



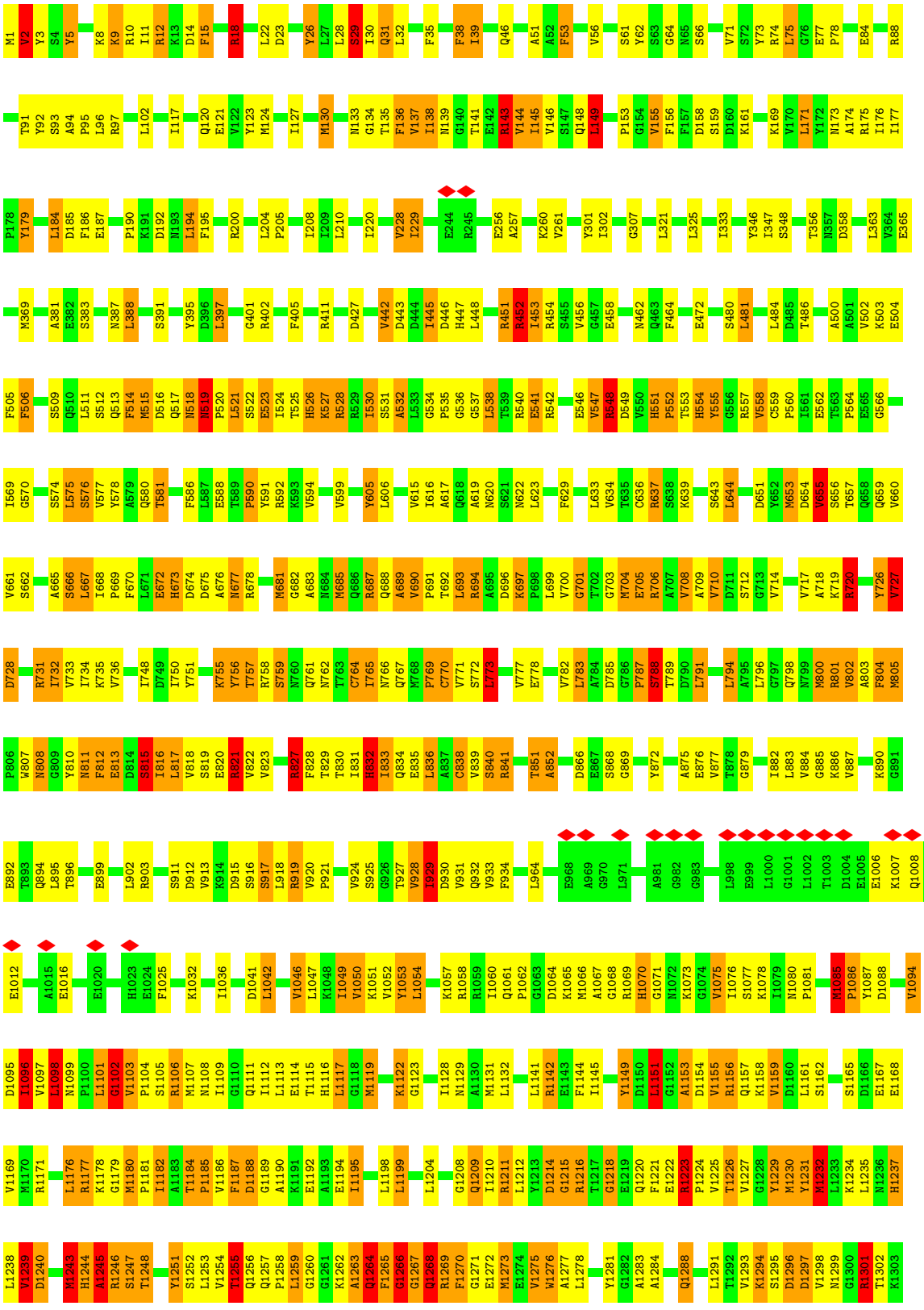
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



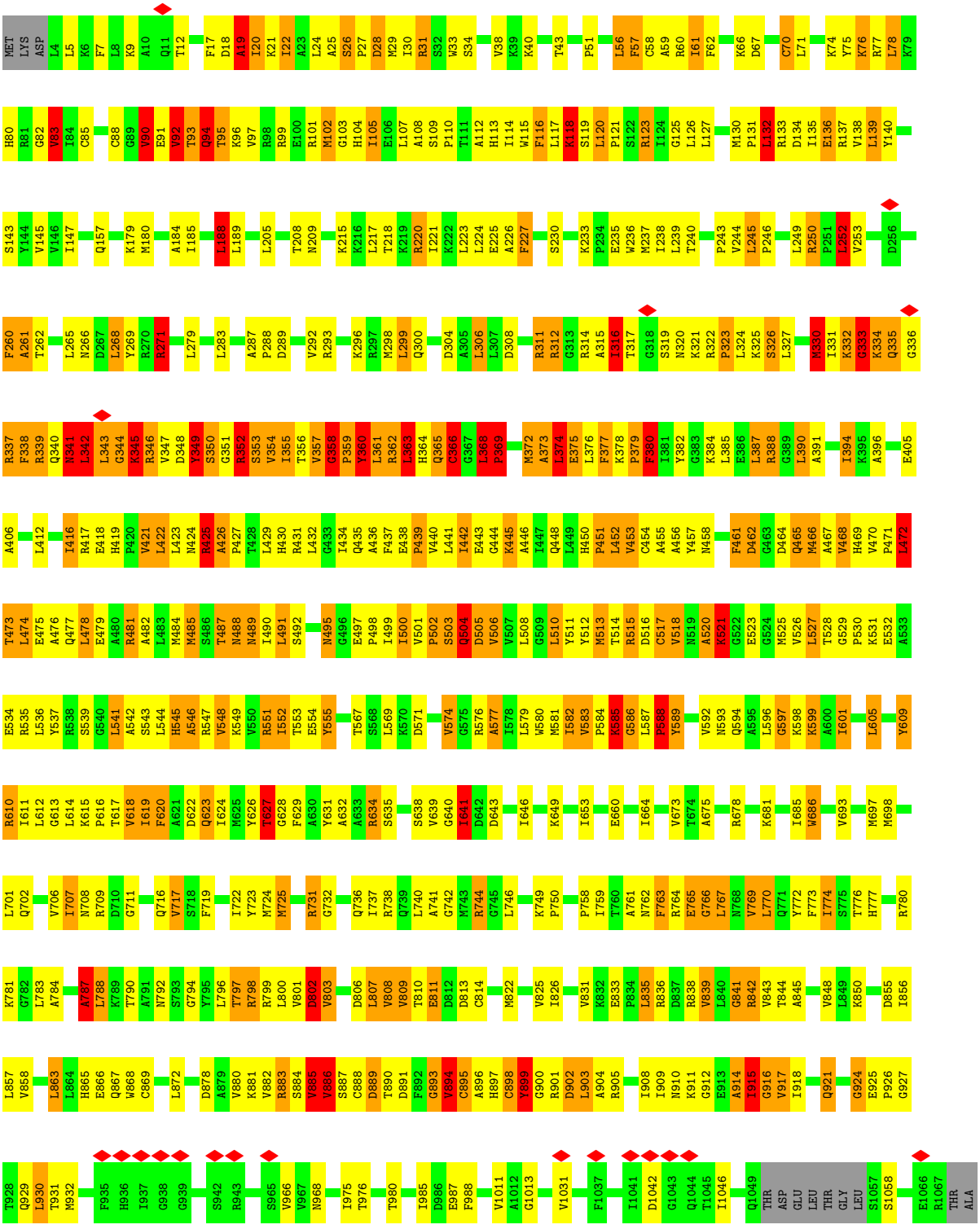
• Molecule 2: DNA-directed RNA polymerase subunit beta

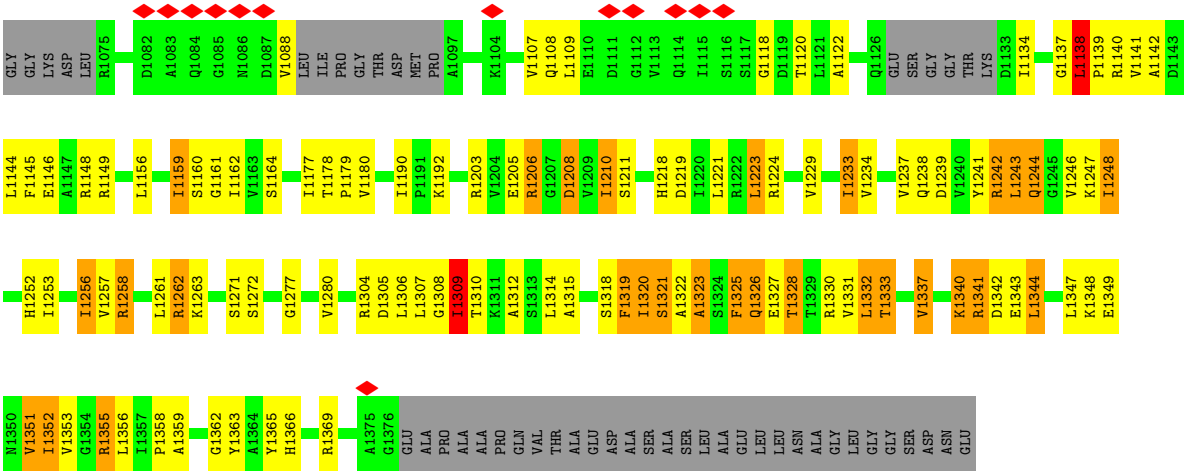
Chain C:



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

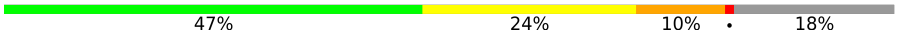
Chain D:

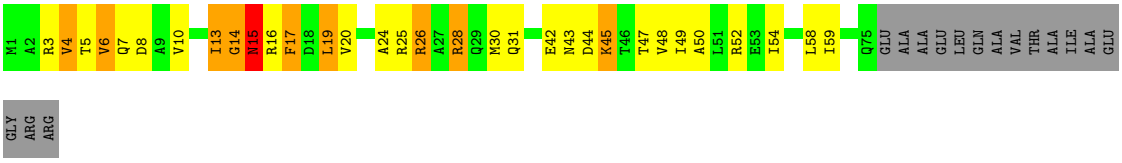




• Molecule 4: DNA-directed RNA polymerase subunit omega

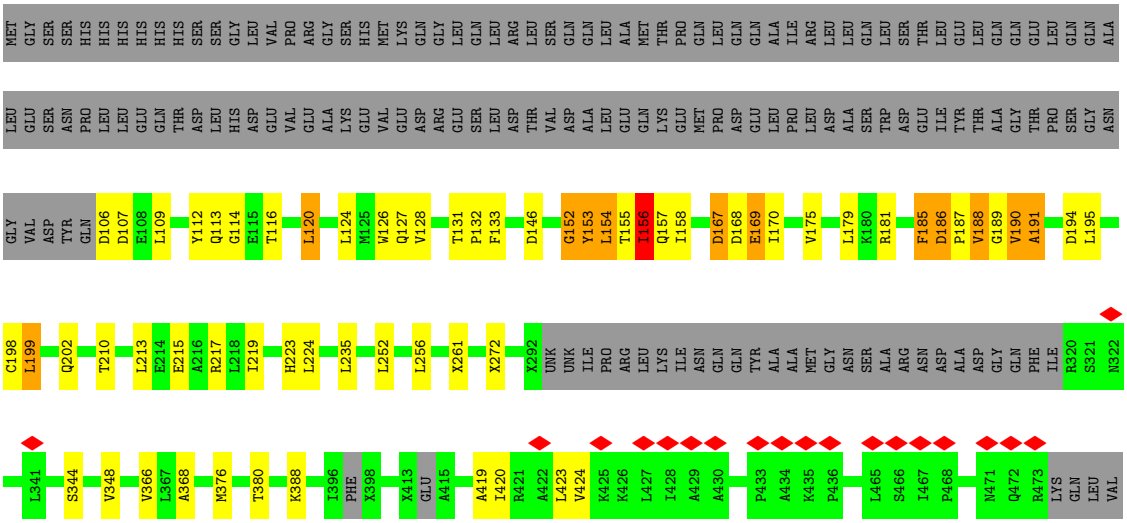
Chain E:





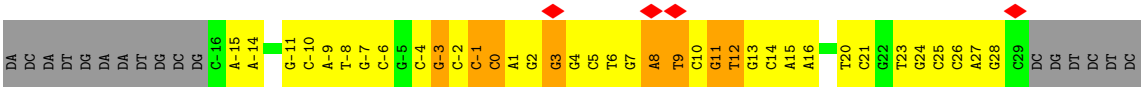
• Molecule 5: RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor

Chain M:

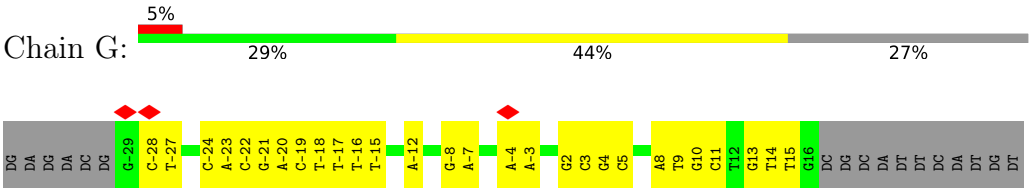


• Molecule 6: nifH promoter template DNA

Chain F:



• Molecule 7: nifH promoter non-template DNA



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	1.46	24/2331 (1.0%)	1.65	48/3177 (1.5%)
1	B	1.15	8/1752 (0.5%)	1.41	29/2385 (1.2%)
2	C	1.84	276/10187 (2.7%)	1.96	384/13822 (2.8%)
3	D	1.84	272/9923 (2.7%)	1.98	394/13482 (2.9%)
4	E	1.21	3/567 (0.5%)	1.72	15/767 (2.0%)
5	M	0.93	11/1764 (0.6%)	1.02	8/2445 (0.3%)
6	F	0.70	1/1060 (0.1%)	1.31	17/1633 (1.0%)
7	G	0.54	0/1060	0.84	1/1635 (0.1%)
All	All	1.66	595/28644 (2.1%)	1.81	896/39346 (2.3%)

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 (595) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	462	ASP	CB-CG	18.37	1.90	1.51
3	D	99	ARG	CZ-NH1	17.98	1.56	1.33
2	C	1216	ARG	CZ-NH1	17.86	1.56	1.33
2	C	555	TYR	CE2-CZ	16.61	1.60	1.38
3	D	333	GLY	N-CA	16.11	1.70	1.46
3	D	360	TYR	CG-CD2	14.76	1.58	1.39
3	D	99	ARG	CZ-NH2	13.07	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1321	SER	CB-OG	12.92	1.59	1.42
2	C	810	TYR	CE2-CZ	12.44	1.54	1.38
2	C	519	ASN	CG-OD1	12.27	1.50	1.24
3	D	899	TYR	CG-CD1	11.94	1.54	1.39
3	D	763	PHE	CG-CD2	11.64	1.56	1.38
2	C	1231	TYR	CG-CD2	-11.64	1.24	1.39
3	D	1319	PHE	CG-CD1	11.50	1.55	1.38
3	D	763	PHE	CG-CD1	11.41	1.55	1.38
3	D	365	GLN	CD-NE2	11.34	1.61	1.32
3	D	626	TYR	CG-CD2	11.33	1.53	1.39
3	D	479	GLU	CD-OE1	11.27	1.38	1.25
3	D	457	TYR	CE2-CZ	11.12	1.53	1.38
3	D	339	ARG	C-O	11.05	1.44	1.23
2	C	555	TYR	C-O	10.89	1.44	1.23
2	C	555	TYR	CG-CD1	10.80	1.53	1.39
2	C	526	HIS	C-O	-10.71	1.03	1.23
2	C	759	SER	CB-OG	10.54	1.55	1.42
2	C	810	TYR	CG-CD2	10.53	1.52	1.39
2	C	666	SER	CB-OG	10.40	1.55	1.42
3	D	534	GLU	CD-OE1	10.30	1.36	1.25
2	C	807	TRP	CB-CG	-10.22	1.31	1.50
2	C	38	PHE	CG-CD2	10.14	1.53	1.38
2	C	1295	SER	CA-CB	10.06	1.68	1.52
3	D	763	PHE	CE2-CZ	10.03	1.56	1.37
3	D	806	ASP	CB-CG	9.99	1.72	1.51
3	D	369	PRO	N-CA	9.84	1.64	1.47
3	D	360	TYR	N-CA	9.79	1.66	1.46
2	C	794	LEU	C-O	9.79	1.42	1.23
2	C	818	VAL	CB-CG2	-9.75	1.32	1.52
3	D	359	PRO	CA-CB	9.75	1.73	1.53
3	D	534	GLU	CD-OE2	9.71	1.36	1.25
3	D	1323	ALA	C-O	9.68	1.41	1.23
3	D	534	GLU	CG-CD	9.64	1.66	1.51
3	D	429	LEU	C-O	9.63	1.41	1.23
1	A	151	GLY	N-CA	9.61	1.60	1.46
2	C	1301	ARG	CZ-NH2	-9.61	1.20	1.33
3	D	362	ARG	N-CA	-9.61	1.27	1.46
3	D	597	GLY	C-O	9.59	1.39	1.23
2	C	1087	TYR	CG-CD2	-9.54	1.26	1.39
2	C	1225	VAL	C-O	9.53	1.41	1.23
3	D	895	CYS	CB-SG	9.50	1.98	1.82
2	C	827	ARG	N-CA	9.49	1.65	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	518	ASN	CG-OD1	9.47	1.44	1.24
3	D	623	GLN	C-O	9.37	1.41	1.23
2	C	1194	GLU	CD-OE2	-9.34	1.15	1.25
2	C	1187	PHE	CE2-CZ	9.16	1.54	1.37
2	C	149	LEU	C-O	9.13	1.40	1.23
2	C	519	ASN	N-CA	9.13	1.64	1.46
3	D	537	TYR	CG-CD1	8.92	1.50	1.39
2	C	820	GLU	CD-OE1	8.83	1.35	1.25
2	C	143	ARG	C-O	-8.80	1.06	1.23
2	C	815	SER	CA-CB	-8.69	1.40	1.52
3	D	457	TYR	CE1-CZ	8.69	1.49	1.38
3	D	451	PRO	C-O	8.67	1.40	1.23
3	D	772	TYR	CE1-CZ	-8.67	1.27	1.38
2	C	879	GLY	C-O	-8.67	1.09	1.23
3	D	543	SER	CA-CB	8.65	1.66	1.52
3	D	479	GLU	CD-OE2	8.64	1.35	1.25
3	D	119	SER	CB-OG	8.63	1.53	1.42
2	C	1238	LEU	N-CA	8.57	1.63	1.46
2	C	813	GLU	C-O	8.55	1.39	1.23
2	C	820	GLU	CD-OE2	8.53	1.35	1.25
2	C	1108	ASN	CB-CG	8.51	1.70	1.51
3	D	841	GLY	N-CA	8.51	1.58	1.46
2	C	531	SER	CB-OG	8.47	1.53	1.42
2	C	1069	ARG	CZ-NH1	8.45	1.44	1.33
2	C	1181	PRO	C-O	-8.43	1.06	1.23
3	D	921	GLN	CD-OE1	8.36	1.42	1.24
3	D	511	TYR	CG-CD2	8.30	1.50	1.39
3	D	916	GLY	C-O	8.30	1.36	1.23
2	C	764	CYS	CB-SG	-8.29	1.68	1.82
2	C	1334	GLY	C-O	8.27	1.36	1.23
2	C	1078	LYS	C-O	8.18	1.38	1.23
2	C	699	LEU	C-O	-8.18	1.07	1.23
3	D	360	TYR	CG-CD1	8.15	1.49	1.39
2	C	591	TYR	CE1-CZ	-8.14	1.27	1.38
3	D	719	PHE	CE1-CZ	8.13	1.52	1.37
3	D	352	ARG	N-CA	8.09	1.62	1.46
3	D	345	LYS	CA-CB	8.09	1.71	1.53
2	C	452	ARG	C-O	8.08	1.38	1.23
3	D	763	PHE	CE1-CZ	8.06	1.52	1.37
3	D	373	ALA	N-CA	8.05	1.62	1.46
3	D	842	ARG	CG-CD	8.05	1.72	1.51
2	C	574	SER	CB-OG	8.03	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1277	GLY	N-CA	8.02	1.58	1.46
2	C	26	TYR	CG-CD1	8.00	1.49	1.39
3	D	365	GLN	CG-CD	-8.00	1.32	1.51
3	D	899	TYR	CE1-CZ	7.99	1.49	1.38
3	D	365	GLN	CD-OE1	7.98	1.41	1.24
3	D	269	TYR	CG-CD1	7.96	1.49	1.39
2	C	10	ARG	CG-CD	7.94	1.71	1.51
3	D	492	SER	C-O	-7.91	1.08	1.23
2	C	1243	MET	CA-C	7.88	1.73	1.52
2	C	577	VAL	C-O	7.88	1.38	1.23
2	C	576	SER	CB-OG	7.82	1.52	1.42
3	D	921	GLN	CD-NE2	7.79	1.52	1.32
2	C	677	ASN	C-O	7.77	1.38	1.23
1	B	31	LEU	C-O	7.77	1.38	1.23
2	C	683	ALA	C-O	7.76	1.38	1.23
1	A	181	GLU	N-CA	7.76	1.61	1.46
2	C	1187	PHE	CG-CD1	7.75	1.50	1.38
2	C	518	ASN	N-CA	7.75	1.61	1.46
2	C	697	LYS	N-CA	7.73	1.61	1.46
3	D	382	TYR	CE1-CZ	7.73	1.48	1.38
2	C	677	ASN	CB-CG	-7.71	1.33	1.51
3	D	773	PHE	CG-CD2	-7.71	1.27	1.38
3	D	1365	TYR	C-O	-7.69	1.08	1.23
2	C	605	TYR	CG-CD1	-7.69	1.29	1.39
3	D	382	TYR	CB-CG	-7.66	1.40	1.51
2	C	803	ALA	C-O	7.59	1.37	1.23
2	C	1270	PHE	CA-CB	-7.58	1.37	1.53
3	D	472	LEU	CA-CB	-7.57	1.36	1.53
3	D	515	ARG	CZ-NH1	-7.56	1.23	1.33
3	D	1363	TYR	C-O	7.56	1.37	1.23
1	A	68	TYR	CE1-CZ	7.55	1.48	1.38
2	C	35	PHE	CG-CD2	7.54	1.50	1.38
3	D	811	GLU	CD-OE1	7.54	1.33	1.25
2	C	515	MET	C-O	7.50	1.37	1.23
3	D	26	SER	CB-OG	7.46	1.51	1.42
2	C	687	ARG	CG-CD	7.46	1.70	1.51
2	C	812	PHE	CG-CD2	7.45	1.50	1.38
3	D	802	ASP	CB-CG	7.44	1.67	1.51
2	C	1215	GLY	N-CA	-7.43	1.34	1.46
5	M	127	GLN	CG-CD	-7.41	1.33	1.51
3	D	924	GLY	N-CA	-7.39	1.34	1.46
3	D	269	TYR	CE1-CZ	-7.38	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1111	GLN	C-O	7.36	1.37	1.23
3	D	582	ILE	CB-CG1	-7.36	1.33	1.54
2	C	1086	PRO	N-CA	7.35	1.59	1.47
2	C	1247	SER	N-CA	7.33	1.61	1.46
3	D	1340	LYS	C-O	-7.31	1.09	1.23
2	C	1113	LEU	C-O	7.31	1.37	1.23
3	D	349	TYR	CE1-CZ	-7.29	1.29	1.38
3	D	359	PRO	CG-CD	7.29	1.74	1.50
2	C	578	TYR	CE1-CZ	7.28	1.48	1.38
2	C	35	PHE	CB-CG	-7.27	1.39	1.51
2	C	1246	ARG	NE-CZ	7.27	1.42	1.33
3	D	462	ASP	N-CA	7.26	1.60	1.46
2	C	667	LEU	C-O	7.25	1.37	1.23
2	C	136	PHE	CG-CD1	-7.25	1.27	1.38
5	M	190	VAL	C-O	7.24	1.37	1.23
3	D	360	TYR	CD2-CE2	7.23	1.50	1.39
3	D	622	ASP	C-O	7.23	1.37	1.23
2	C	834	GLN	C-O	7.21	1.37	1.23
3	D	352	ARG	CG-CD	7.20	1.70	1.51
2	C	818	VAL	CA-CB	7.18	1.69	1.54
2	C	1298	VAL	C-O	7.17	1.36	1.23
3	D	1319	PHE	CE1-CZ	7.17	1.50	1.37
3	D	424	ASN	CG-ND2	7.17	1.50	1.32
3	D	620	PHE	CG-CD1	7.17	1.49	1.38
3	D	334	LYS	CA-CB	-7.17	1.38	1.53
2	C	576	SER	CA-CB	-7.16	1.42	1.52
2	C	133	ASN	N-CA	-7.16	1.32	1.46
2	C	804	PHE	N-CA	7.15	1.60	1.46
3	D	337	ARG	NE-CZ	-7.14	1.23	1.33
3	D	901	ARG	C-O	7.13	1.36	1.23
3	D	437	PHE	CD2-CE2	7.13	1.53	1.39
3	D	337	ARG	N-CA	7.12	1.60	1.46
2	C	577	VAL	CB-CG1	-7.11	1.38	1.52
3	D	889	ASP	CA-CB	7.11	1.69	1.53
3	D	894	VAL	C-O	-7.10	1.09	1.23
2	C	1268	GLN	CA-CB	7.09	1.69	1.53
3	D	360	TYR	CB-CG	7.08	1.62	1.51
2	C	764	CYS	N-CA	7.07	1.60	1.46
3	D	609	TYR	CG-CD2	-7.06	1.29	1.39
2	C	1114	GLU	CB-CG	7.06	1.65	1.52
1	B	44	ARG	C-O	7.05	1.36	1.23
2	C	1246	ARG	N-CA	7.05	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	742	GLY	C-O	-7.03	1.12	1.23
2	C	800	MET	CA-CB	7.01	1.69	1.53
2	C	705	GLU	CG-CD	7.00	1.62	1.51
3	D	899	TYR	CA-CB	7.00	1.69	1.53
6	F	-3	DG	P-OP2	6.99	1.60	1.49
1	A	151	GLY	C-O	-6.99	1.12	1.23
3	D	769	VAL	N-CA	6.98	1.60	1.46
3	D	1355	ARG	CZ-NH1	-6.96	1.24	1.33
3	D	476	ALA	CA-CB	-6.95	1.37	1.52
5	M	152	GLY	C-O	-6.94	1.12	1.23
3	D	794	GLY	N-CA	-6.94	1.35	1.46
3	D	917	VAL	CB-CG1	6.93	1.67	1.52
2	C	520	PRO	C-O	6.93	1.37	1.23
2	C	1277	ALA	CA-CB	-6.93	1.37	1.52
3	D	1355	ARG	CZ-NH2	6.93	1.42	1.33
3	D	900	GLY	C-O	-6.92	1.12	1.23
2	C	811	ASN	CG-OD1	6.91	1.39	1.24
3	D	1280	VAL	CB-CG1	6.89	1.67	1.52
3	D	425	ARG	C-O	-6.89	1.10	1.23
3	D	456	ALA	N-CA	6.87	1.60	1.46
2	C	1276	TRP	CD2-CE3	6.85	1.50	1.40
2	C	934	PHE	CG-CD1	6.85	1.49	1.38
3	D	85	CYS	CB-SG	-6.84	1.70	1.82
3	D	115	TRP	CD2-CE2	6.83	1.49	1.41
3	D	479	GLU	CG-CD	6.83	1.62	1.51
2	C	1177	ARG	C-O	-6.83	1.10	1.23
3	D	345	LYS	CB-CG	6.83	1.71	1.52
3	D	686	TRP	CE3-CZ3	6.83	1.50	1.38
3	D	360	TYR	CA-C	6.81	1.70	1.52
2	C	931	VAL	C-O	6.78	1.36	1.23
2	C	1052	VAL	CB-CG2	-6.78	1.38	1.52
2	C	12	ARG	CZ-NH2	-6.78	1.24	1.33
3	D	628	GLY	N-CA	6.76	1.56	1.46
2	C	1068	GLY	N-CA	6.75	1.56	1.46
2	C	552	PRO	CA-CB	-6.74	1.40	1.53
2	C	1215	GLY	CA-C	-6.74	1.41	1.51
3	D	338	PHE	CE1-CZ	6.73	1.50	1.37
1	A	51	MET	C-O	6.72	1.36	1.23
2	C	505	PHE	CG-CD1	6.72	1.48	1.38
3	D	917	VAL	C-O	6.71	1.36	1.23
2	C	770	CYS	CB-SG	-6.71	1.70	1.82
2	C	1071	GLY	CA-C	6.70	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	308	ASP	N-CA	6.70	1.59	1.46
3	D	1319	PHE	CG-CD2	6.70	1.48	1.38
2	C	823	VAL	CB-CG1	6.69	1.67	1.52
2	C	1270	PHE	CG-CD1	6.69	1.48	1.38
3	D	512	TYR	CE2-CZ	6.69	1.47	1.38
3	D	358	GLY	CA-C	6.69	1.62	1.51
2	C	514	PHE	C-O	6.68	1.36	1.23
1	A	182	ARG	N-CA	6.67	1.59	1.46
3	D	349	TYR	CG-CD1	-6.65	1.30	1.39
2	C	1264	GLN	C-O	6.64	1.35	1.23
3	D	458	ASN	C-O	-6.64	1.10	1.23
3	D	422	LEU	CA-CB	6.63	1.69	1.53
2	C	153	PRO	C-O	6.62	1.36	1.23
3	D	770	LEU	C-O	6.62	1.35	1.23
3	D	798	ARG	CD-NE	6.61	1.57	1.46
2	C	770	CYS	N-CA	6.61	1.59	1.46
2	C	1231	TYR	C-O	6.59	1.35	1.23
3	D	360	TYR	CE1-CZ	6.56	1.47	1.38
1	A	67	GLU	CD-OE2	6.55	1.32	1.25
2	C	757	THR	C-O	-6.55	1.10	1.23
2	C	1101	LEU	C-O	6.54	1.35	1.23
3	D	808	VAL	C-O	-6.54	1.10	1.23
3	D	269	TYR	CE2-CZ	6.54	1.47	1.38
3	D	912	GLY	CA-C	6.53	1.62	1.51
3	D	899	TYR	CE2-CZ	6.53	1.47	1.38
3	D	784	ALA	C-O	-6.53	1.10	1.23
2	C	1273	MET	CA-CB	-6.51	1.39	1.53
3	D	808	VAL	CA-CB	6.51	1.68	1.54
1	A	41	ASN	C-O	6.50	1.35	1.23
3	D	332	LYS	CA-CB	6.50	1.68	1.53
3	D	589	TYR	CZ-OH	6.48	1.48	1.37
3	D	506	VAL	C-O	6.47	1.35	1.23
2	C	1119	MET	CG-SD	6.47	1.98	1.81
2	C	1218	GLY	N-CA	6.46	1.55	1.46
2	C	1299	ASN	CA-C	6.44	1.69	1.52
3	D	365	GLN	CA-CB	6.44	1.68	1.53
3	D	350	SER	CB-OG	6.43	1.50	1.42
3	D	841	GLY	C-O	6.42	1.33	1.23
2	C	395	TYR	CG-CD1	6.42	1.47	1.39
3	D	351	GLY	N-CA	6.42	1.55	1.46
3	D	631	TYR	CE1-CZ	6.41	1.46	1.38
2	C	590	PRO	CA-C	-6.41	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	437	PHE	CE2-CZ	6.41	1.49	1.37
3	D	888	CYS	C-O	6.41	1.35	1.23
3	D	112	ALA	CA-CB	6.40	1.65	1.52
2	C	726	TYR	CE2-CZ	-6.40	1.30	1.38
1	A	185	TYR	CE2-CZ	-6.40	1.30	1.38
3	D	336	GLY	C-O	-6.40	1.13	1.23
3	D	331	ILE	C-O	-6.39	1.11	1.23
3	D	360	TYR	CA-CB	-6.38	1.40	1.53
2	C	1096	ILE	CB-CG1	-6.38	1.36	1.54
3	D	731	ARG	CZ-NH1	6.38	1.41	1.33
2	C	1270	PHE	CE1-CZ	6.38	1.49	1.37
1	A	131	CYS	CB-SG	-6.37	1.71	1.82
3	D	1319	PHE	CE2-CZ	6.36	1.49	1.37
2	C	697	LYS	CB-CG	6.36	1.69	1.52
3	D	115	TRP	CB-CG	-6.36	1.38	1.50
5	M	198	CYS	CB-SG	6.36	1.93	1.82
2	C	1179	GLY	C-O	6.35	1.33	1.23
3	D	382	TYR	CG-CD1	6.35	1.47	1.39
2	C	701	GLY	C-O	6.34	1.33	1.23
3	D	351	GLY	C-O	6.34	1.33	1.23
3	D	617	THR	CB-CG2	-6.33	1.31	1.52
2	C	555	TYR	CG-CD2	6.32	1.47	1.39
3	D	469	HIS	C-O	6.31	1.35	1.23
3	D	766	GLY	N-CA	6.31	1.55	1.46
1	A	178	SER	C-O	-6.30	1.11	1.23
3	D	783	LEU	C-O	6.29	1.35	1.23
1	A	129	VAL	C-O	-6.29	1.11	1.23
2	C	9	LYS	C-O	-6.29	1.11	1.23
3	D	488	ASN	CG-OD1	6.28	1.37	1.24
2	C	35	PHE	CE1-CZ	6.27	1.49	1.37
3	D	1256	ILE	N-CA	-6.26	1.33	1.46
5	M	127	GLN	CD-NE2	6.26	1.48	1.32
2	C	1114	GLU	CD-OE1	6.26	1.32	1.25
2	C	1239	VAL	N-CA	6.26	1.58	1.46
2	C	1334	GLY	N-CA	6.26	1.55	1.46
3	D	57	PHE	CG-CD2	-6.25	1.29	1.38
3	D	899	TYR	CB-CG	6.23	1.61	1.51
2	C	705	GLU	C-O	6.23	1.35	1.23
2	C	548	ARG	CZ-NH1	6.20	1.41	1.33
3	D	457	TYR	CG-CD1	6.20	1.47	1.39
1	B	8	PHE	CB-CG	-6.20	1.40	1.51
3	D	488	ASN	CG-ND2	6.19	1.48	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1321	SER	C-O	6.19	1.35	1.23
2	C	1277	ALA	C-O	6.18	1.35	1.23
3	D	1325	PHE	CG-CD1	-6.16	1.29	1.38
2	C	537	GLY	C-O	-6.15	1.13	1.23
3	D	722	ILE	C-O	6.15	1.35	1.23
5	M	153	TYR	CA-CB	6.15	1.67	1.53
3	D	521	LYS	CA-CB	6.15	1.67	1.53
5	M	154	LEU	C-O	-6.14	1.11	1.23
2	C	1216	ARG	CZ-NH2	6.14	1.41	1.33
3	D	491	LEU	C-O	6.13	1.35	1.23
2	C	1107	MET	N-CA	6.12	1.58	1.46
2	C	672	GLU	CB-CG	-6.12	1.40	1.52
2	C	521	LEU	N-CA	-6.11	1.34	1.46
2	C	1184	THR	N-CA	6.11	1.58	1.46
3	D	431	ARG	CG-CD	6.11	1.67	1.51
1	A	96	ASP	C-O	-6.11	1.11	1.23
2	C	29	SER	C-O	6.11	1.34	1.23
3	D	885	VAL	N-CA	6.11	1.58	1.46
2	C	548	ARG	CA-CB	6.10	1.67	1.53
2	C	524	ILE	N-CA	-6.10	1.34	1.46
3	D	902	ASP	C-O	6.09	1.34	1.23
2	C	765	ILE	N-CA	6.09	1.58	1.46
1	A	45	ARG	CZ-NH2	6.06	1.41	1.33
3	D	421	VAL	C-O	6.05	1.34	1.23
3	D	445	LYS	N-CA	-6.05	1.34	1.46
2	C	512	SER	CB-OG	-6.05	1.34	1.42
2	C	512	SER	C-O	6.05	1.34	1.23
3	D	377	PHE	CA-C	6.04	1.68	1.52
1	A	63	GLY	CA-C	6.03	1.61	1.51
3	D	437	PHE	CA-CB	6.02	1.67	1.53
2	C	562	GLU	CA-CB	6.01	1.67	1.53
2	C	756	TYR	CE1-CZ	-6.01	1.30	1.38
2	C	827	ARG	CB-CG	6.00	1.68	1.52
3	D	438	GLU	CD-OE2	6.00	1.32	1.25
2	C	1246	ARG	CA-C	-5.99	1.37	1.52
2	C	454	ARG	CZ-NH1	5.99	1.40	1.33
2	C	514	PHE	CB-CG	-5.99	1.41	1.51
2	C	1248	THR	C-O	5.98	1.34	1.23
2	C	1187	PHE	CD2-CE2	5.97	1.51	1.39
3	D	335	GLN	CD-NE2	-5.97	1.18	1.32
2	C	761	GLN	CD-NE2	5.96	1.47	1.32
2	C	1096	ILE	N-CA	5.96	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1271	GLY	C-O	5.96	1.33	1.23
3	D	613	GLY	N-CA	5.96	1.54	1.46
3	D	357	VAL	CA-C	5.96	1.68	1.52
2	C	1211	ARG	N-CA	5.96	1.58	1.46
3	D	227	PHE	CG-CD2	5.94	1.47	1.38
2	C	179	TYR	CE1-CZ	5.93	1.46	1.38
2	C	1313	HIS	N-CA	5.93	1.58	1.46
3	D	686	TRP	CB-CG	-5.93	1.39	1.50
2	C	557	ARG	N-CA	-5.93	1.34	1.46
3	D	1327	GLU	CG-CD	5.92	1.60	1.51
2	C	769	PRO	CA-CB	-5.92	1.41	1.53
2	C	917	SER	CB-OG	5.92	1.50	1.42
2	C	1281	TYR	CZ-OH	-5.90	1.27	1.37
2	C	672	GLU	CG-CD	-5.89	1.43	1.51
3	D	368	LEU	N-CA	5.89	1.58	1.46
2	C	755	LYS	CA-CB	-5.88	1.41	1.53
3	D	443	GLU	C-O	5.88	1.34	1.23
2	C	1123	GLY	C-O	5.88	1.33	1.23
2	C	522	SER	N-CA	-5.88	1.34	1.46
3	D	462	ASP	CA-C	5.86	1.68	1.52
3	D	227	PHE	CB-CG	-5.84	1.41	1.51
1	A	204	GLU	C-O	5.84	1.34	1.23
3	D	744	ARG	CZ-NH1	-5.82	1.25	1.33
3	D	380	PHE	CG-CD1	-5.81	1.30	1.38
3	D	512	TYR	CG-CD1	5.81	1.46	1.39
2	C	672	GLU	CA-CB	-5.81	1.41	1.53
5	M	126	TRP	CG-CD1	5.81	1.44	1.36
3	D	375	GLU	CG-CD	5.80	1.60	1.51
3	D	436	ALA	CA-CB	5.80	1.64	1.52
3	D	501	VAL	N-CA	-5.80	1.34	1.46
2	C	1149	TYR	CG-CD1	5.79	1.46	1.39
2	C	549	ASP	CB-CG	5.78	1.63	1.51
3	D	419	HIS	CA-CB	-5.77	1.41	1.53
2	C	1111	GLN	CD-NE2	5.77	1.47	1.32
2	C	828	PHE	N-CA	5.76	1.57	1.46
2	C	731	ARG	CZ-NH1	-5.76	1.25	1.33
1	B	197	ASP	C-O	5.76	1.34	1.23
2	C	1058	ARG	CZ-NH1	5.75	1.40	1.33
2	C	559	CYS	CB-SG	5.75	1.92	1.82
3	D	781	LYS	C-O	-5.75	1.12	1.23
3	D	452	LEU	C-O	5.75	1.34	1.23
3	D	585	LYS	C-O	5.75	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	924	GLY	CA-C	-5.75	1.42	1.51
2	C	655	VAL	C-O	5.74	1.34	1.23
2	C	731	ARG	CA-CB	5.74	1.66	1.53
3	D	482	ALA	C-O	5.74	1.34	1.23
2	C	1099	ASN	CA-C	-5.74	1.38	1.52
1	A	187	VAL	CB-CG1	-5.74	1.40	1.52
2	C	138	ILE	C-O	5.73	1.34	1.23
2	C	821	ARG	N-CA	-5.73	1.34	1.46
3	D	372	MET	C-O	-5.73	1.12	1.23
2	C	520	PRO	N-CD	-5.71	1.39	1.47
3	D	511	TYR	CE1-CZ	5.70	1.46	1.38
2	C	1231	TYR	CE1-CZ	-5.70	1.31	1.38
3	D	515	ARG	CG-CD	5.69	1.66	1.51
2	C	93	SER	CA-CB	5.69	1.61	1.52
2	C	452	ARG	CA-CB	5.68	1.66	1.53
3	D	236	TRP	CD2-CE2	-5.68	1.34	1.41
5	M	127	GLN	CD-OE1	5.68	1.36	1.24
2	C	1296	ASP	CG-OD1	-5.67	1.12	1.25
2	C	1111	GLN	N-CA	-5.66	1.35	1.46
3	D	1145	PHE	CG-CD2	5.66	1.47	1.38
2	C	932	GLN	CG-CD	5.65	1.64	1.51
2	C	1192	GLU	N-CA	5.65	1.57	1.46
2	C	762	ASN	CA-C	5.63	1.67	1.52
3	D	794	GLY	CA-C	-5.62	1.42	1.51
2	C	53	PHE	CG-CD1	5.62	1.47	1.38
2	C	838	CYS	CB-SG	-5.62	1.72	1.81
3	D	436	ALA	C-O	5.62	1.34	1.23
2	C	1284	ALA	C-O	5.61	1.34	1.23
2	C	1322	SER	N-CA	-5.60	1.35	1.46
1	B	38	THR	C-O	5.60	1.33	1.23
2	C	1251	TYR	CE2-CZ	-5.59	1.31	1.38
3	D	599	LYS	C-O	5.58	1.33	1.23
2	C	1288	GLN	CD-OE1	5.58	1.36	1.24
3	D	787	ALA	C-O	5.57	1.33	1.23
2	C	687	ARG	N-CA	-5.57	1.35	1.46
1	B	185	TYR	CG-CD1	5.57	1.46	1.39
3	D	580	TRP	CG-CD2	-5.57	1.34	1.43
2	C	701	GLY	CA-C	-5.56	1.43	1.51
2	C	928	VAL	CB-CG2	-5.56	1.41	1.52
2	C	31	GLN	CG-CD	5.56	1.63	1.51
3	D	588	PRO	N-CA	-5.56	1.37	1.47
3	D	1241	TYR	CE1-CZ	-5.55	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	13	ILE	C-O	5.55	1.33	1.23
3	D	917	VAL	N-CA	-5.54	1.35	1.46
1	A	133	LEU	N-CA	-5.54	1.35	1.46
3	D	803	VAL	CB-CG1	-5.53	1.41	1.52
3	D	495	ASN	CG-OD1	-5.53	1.11	1.24
3	D	914	ALA	CA-CB	-5.53	1.40	1.52
3	D	382	TYR	CG-CD2	5.52	1.46	1.39
2	C	526	HIS	CA-CB	-5.52	1.41	1.53
2	C	526	HIS	N-CA	5.52	1.57	1.46
3	D	489	ASN	CG-OD1	-5.52	1.11	1.24
2	C	1281	TYR	CE1-CZ	5.51	1.45	1.38
3	D	439	PRO	N-CD	-5.51	1.40	1.47
2	C	1323	PHE	CB-CG	-5.51	1.42	1.51
2	C	682	GLY	CA-C	5.51	1.60	1.51
3	D	629	PHE	N-CA	-5.50	1.35	1.46
3	D	338	PHE	CE2-CZ	5.49	1.47	1.37
3	D	353	SER	CA-CB	5.49	1.61	1.52
3	D	470	VAL	CA-CB	-5.49	1.43	1.54
2	C	801	ARG	C-O	5.48	1.33	1.23
3	D	359	PRO	N-CA	5.48	1.56	1.47
2	C	672	GLU	CD-OE2	-5.47	1.19	1.25
2	C	687	ARG	CA-CB	5.46	1.66	1.53
2	C	685	MET	CG-SD	5.45	1.95	1.81
4	E	26	ARG	C-O	-5.45	1.12	1.23
2	C	808	ASN	C-O	5.44	1.33	1.23
3	D	811	GLU	CG-CD	5.44	1.60	1.51
1	A	44	ARG	CZ-NH1	5.44	1.40	1.33
2	C	566	GLY	C-O	-5.44	1.15	1.23
3	D	382	TYR	CE2-CZ	5.44	1.45	1.38
3	D	620	PHE	C-O	5.44	1.33	1.23
3	D	537	TYR	CE2-CZ	5.43	1.45	1.38
3	D	574	VAL	CB-CG1	-5.43	1.41	1.52
3	D	468	VAL	C-O	5.43	1.33	1.23
1	A	141	SER	CB-OG	-5.42	1.35	1.42
2	C	677	ASN	CG-OD1	5.42	1.35	1.24
2	C	816	ILE	CB-CG2	5.42	1.69	1.52
3	D	444	GLY	N-CA	5.42	1.54	1.46
3	D	629	PHE	CG-CD2	5.41	1.46	1.38
2	C	458	GLU	C-O	5.41	1.33	1.23
3	D	457	TYR	CB-CG	-5.41	1.43	1.51
3	D	574	VAL	CB-CG2	-5.41	1.41	1.52
2	C	1069	ARG	C-O	5.40	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1229	TYR	CG-CD2	5.40	1.46	1.39
2	C	551	HIS	C-O	5.40	1.33	1.23
2	C	708	VAL	CB-CG1	5.40	1.64	1.52
2	C	92	TYR	CG-CD1	-5.40	1.32	1.39
3	D	440	VAL	C-O	5.39	1.33	1.23
2	C	1316	GLU	N-CA	5.39	1.57	1.46
2	C	694	ARG	C-O	5.39	1.33	1.23
2	C	97	ARG	C-O	-5.38	1.13	1.23
2	C	706	ARG	C-O	5.38	1.33	1.23
3	D	1326	GLN	CA-C	-5.38	1.39	1.52
2	C	1323	PHE	N-CA	5.38	1.57	1.46
5	M	191	ALA	CA-CB	5.38	1.63	1.52
2	C	12	ARG	N-CA	5.38	1.57	1.46
3	D	421	VAL	CB-CG1	-5.37	1.41	1.52
3	D	488	ASN	C-O	5.37	1.33	1.23
3	D	725	MET	CA-CB	-5.36	1.42	1.53
2	C	659	GLN	CA-C	-5.35	1.39	1.52
2	C	653	MET	C-O	5.35	1.33	1.23
2	C	697	LYS	C-O	5.35	1.33	1.23
2	C	685	MET	C-O	-5.34	1.13	1.23
3	D	488	ASN	CA-C	-5.34	1.39	1.52
2	C	808	ASN	N-CA	-5.34	1.35	1.46
3	D	1248	ILE	C-O	5.34	1.33	1.23
3	D	537	TYR	CE1-CZ	5.34	1.45	1.38
3	D	723	TYR	CE1-CZ	5.33	1.45	1.38
2	C	153	PRO	N-CD	-5.33	1.40	1.47
2	C	1240	ASP	N-CA	-5.33	1.35	1.46
2	C	756	TYR	CE2-CZ	5.32	1.45	1.38
1	B	36	GLY	C-O	5.32	1.32	1.23
3	D	351	GLY	CA-C	-5.32	1.43	1.51
3	D	113	HIS	CA-C	-5.32	1.39	1.52
3	D	505	ASP	CB-CG	5.31	1.62	1.51
3	D	484	MET	N-CA	5.31	1.56	1.46
3	D	1330	ARG	C-O	5.30	1.33	1.23
3	D	374	LEU	N-CA	5.29	1.56	1.46
3	D	761	ALA	CA-CB	5.29	1.63	1.52
2	C	1325	VAL	N-CA	-5.28	1.35	1.46
3	D	492	SER	CA-C	-5.28	1.39	1.52
3	D	335	GLN	CA-CB	-5.27	1.42	1.53
5	M	152	GLY	N-CA	5.27	1.53	1.46
2	C	789	THR	CB-CG2	-5.26	1.34	1.52
3	D	619	ILE	C-O	5.26	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	758	ARG	CA-C	5.25	1.66	1.52
3	D	518	VAL	C-O	5.25	1.33	1.23
3	D	1352	ILE	C-O	-5.23	1.13	1.23
3	D	421	VAL	N-CA	5.23	1.56	1.46
2	C	1275	VAL	C-O	5.22	1.33	1.23
2	C	1053	TYR	CE1-CZ	5.22	1.45	1.38
2	C	1305	TYR	CE2-CZ	5.22	1.45	1.38
2	C	1047	LEU	C-O	-5.21	1.13	1.23
2	C	657	THR	C-O	5.21	1.33	1.23
3	D	465	GLN	C-O	5.20	1.33	1.23
3	D	638	SER	C-O	-5.20	1.13	1.23
2	C	1283	ALA	N-CA	-5.20	1.35	1.46
2	C	916	SER	C-O	-5.20	1.13	1.23
2	C	1122	LYS	CB-CG	5.19	1.66	1.52
2	C	681	MET	CA-CB	5.18	1.65	1.53
2	C	703	GLY	C-O	5.18	1.31	1.23
2	C	1305	TYR	CE1-CZ	-5.18	1.31	1.38
2	C	777	VAL	C-O	5.18	1.33	1.23
2	C	710	VAL	CA-CB	-5.17	1.43	1.54
4	E	28	ARG	CZ-NH1	5.17	1.39	1.33
3	D	517	CYS	CB-SG	5.17	1.91	1.82
2	C	1278	LEU	C-O	5.16	1.33	1.23
2	C	1081	PRO	CG-CD	-5.16	1.33	1.50
1	B	231	PHE	CG-CD1	5.16	1.46	1.38
2	C	1226	THR	CB-CG2	5.15	1.69	1.52
2	C	453	ILE	CB-CG1	-5.15	1.39	1.54
2	C	678	ARG	CA-C	5.15	1.66	1.52
2	C	788	SER	CA-CB	5.15	1.60	1.52
3	D	116	PHE	CG-CD2	-5.15	1.31	1.38
3	D	512	TYR	CG-CD2	5.15	1.45	1.39
2	C	12	ARG	NE-CZ	-5.15	1.26	1.33
3	D	802	ASP	C-O	5.14	1.33	1.23
2	C	1123	GLY	N-CA	-5.14	1.38	1.46
3	D	914	ALA	C-N	-5.14	1.22	1.34
2	C	827	ARG	C-O	5.13	1.33	1.23
2	C	1226	THR	C-O	5.12	1.33	1.23
2	C	1114	GLU	CG-CD	5.12	1.59	1.51
3	D	798	ARG	NE-CZ	5.12	1.39	1.33
3	D	632	ALA	CA-C	-5.12	1.39	1.52
2	C	1304	MET	CG-SD	5.11	1.94	1.81
3	D	94	GLN	CA-CB	5.11	1.65	1.53
3	D	349	TYR	C-O	5.11	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	119	SER	N-CA	5.11	1.56	1.46
3	D	431	ARG	CA-CB	-5.11	1.42	1.53
3	D	503	SER	CB-OG	5.10	1.48	1.42
1	A	185	TYR	CG-CD2	-5.10	1.32	1.39
3	D	536	LEU	CB-CG	5.10	1.67	1.52
2	C	666	SER	C-O	5.09	1.33	1.23
3	D	1252	HIS	C-O	5.09	1.33	1.23
1	A	85	LEU	CA-C	-5.09	1.39	1.52
3	D	1308	GLY	C-O	5.09	1.31	1.23
3	D	1359	ALA	CA-C	-5.09	1.39	1.52
2	C	832	HIS	C-O	5.09	1.33	1.23
2	C	1102	GLY	N-CA	5.09	1.53	1.46
1	A	68	TYR	CD1-CE1	5.08	1.47	1.39
2	C	764	CYS	CA-CB	5.08	1.65	1.53
3	D	406	ALA	C-O	-5.07	1.13	1.23
3	D	40	LYS	N-CA	5.07	1.56	1.46
2	C	1259	LEU	C-O	-5.07	1.13	1.23
2	C	1070	HIS	CA-CB	-5.07	1.42	1.53
2	C	669	PRO	CA-C	-5.06	1.42	1.52
2	C	1270	PHE	CB-CG	-5.06	1.42	1.51
3	D	332	LYS	CD-CE	5.06	1.64	1.51
3	D	545	HIS	N-CA	-5.06	1.36	1.46
2	C	1077	SER	N-CA	-5.05	1.36	1.46
3	D	766	GLY	C-O	5.05	1.31	1.23
3	D	342	LEU	CA-CB	5.05	1.65	1.53
3	D	638	SER	CA-CB	5.05	1.60	1.52
3	D	1337	VAL	CB-CG2	5.05	1.63	1.52
2	C	1321	GLU	CA-CB	5.04	1.65	1.53
2	C	562	GLU	CD-OE2	5.04	1.31	1.25
3	D	366	CYS	CA-C	-5.03	1.39	1.52
2	C	581	THR	CB-CG2	-5.03	1.35	1.52
3	D	96	LYS	N-CA	-5.03	1.36	1.46
2	C	693	LEU	CA-C	-5.03	1.39	1.52
1	A	50	SER	CA-CB	5.02	1.60	1.52
2	C	834	GLN	CA-C	-5.02	1.39	1.52
2	C	1058	ARG	CG-CD	5.02	1.64	1.51
2	C	1231	TYR	CZ-OH	5.01	1.46	1.37
2	C	934	PHE	C-O	-5.01	1.13	1.23
3	D	543	SER	CB-OG	5.01	1.48	1.42
2	C	703	GLY	CA-C	-5.00	1.43	1.51
2	C	1158	LYS	N-CA	-5.00	1.36	1.46
2	C	1144	PHE	CG-CD2	5.00	1.46	1.38

All (896) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1216	ARG	NE-CZ-NH2	-24.92	107.84	120.30
2	C	1301	ARG	NE-CZ-NH1	23.30	131.95	120.30
2	C	1301	ARG	NE-CZ-NH2	-23.28	108.66	120.30
2	C	149	LEU	CB-CG-CD1	-23.16	71.63	111.00
3	D	422	LEU	CB-CG-CD2	-22.53	72.70	111.00
3	D	1304	ARG	NE-CZ-NH1	-22.39	109.10	120.30
2	C	805	MET	CG-SD-CE	-21.66	65.55	100.20
3	D	99	ARG	NE-CZ-NH2	-21.31	109.64	120.30
2	C	12	ARG	NE-CZ-NH2	-20.73	109.94	120.30
3	D	515	ARG	NE-CZ-NH2	20.08	130.34	120.30
2	C	800	MET	CG-SD-CE	19.24	130.98	100.20
3	D	536	LEU	CB-CG-CD2	17.05	139.99	111.00
2	C	1246	ARG	NE-CZ-NH2	17.01	128.80	120.30
3	D	252	LEU	CB-CG-CD2	-16.94	82.20	111.00
2	C	727	VAL	CG1-CB-CG2	-16.20	84.97	110.90
2	C	765	ILE	CG1-CB-CG2	-15.78	76.69	111.40
2	C	1106	ARG	NE-CZ-NH2	-15.62	112.49	120.30
1	A	45	ARG	NE-CZ-NH1	-15.42	112.59	120.30
3	D	361	LEU	CA-CB-CG	15.34	150.58	115.30
3	D	434	ILE	CG1-CB-CG2	-15.07	78.25	111.40
1	A	44	ARG	NE-CZ-NH1	-15.00	112.80	120.30
3	D	366	CYS	CA-CB-SG	-14.78	87.40	114.00
6	F	0	DC	O5'-P-OP2	-14.64	92.52	105.70
2	C	1096	ILE	CG1-CB-CG2	-14.48	79.53	111.40
2	C	146	VAL	CG1-CB-CG2	-14.38	87.88	110.90
3	D	725	MET	CG-SD-CE	-14.31	77.31	100.20
3	D	474	LEU	CB-CG-CD2	-14.28	86.73	111.00
3	D	783	LEU	CB-CG-CD2	-14.14	86.95	111.00
3	D	798	ARG	NE-CZ-NH2	14.01	127.31	120.30
3	D	380	PHE	CB-CG-CD1	-13.94	111.04	120.80
1	A	81	ILE	CG1-CB-CG2	-13.87	80.89	111.40
3	D	610	ARG	NE-CZ-NH2	-13.68	113.46	120.30
3	D	337	ARG	NE-CZ-NH2	-13.68	113.46	120.30
6	F	-1	DC	O5'-P-OP1	-13.60	93.46	105.70
2	C	687	ARG	NE-CZ-NH1	13.57	127.09	120.30
3	D	387	LEU	CB-CG-CD2	-13.24	88.50	111.00
2	C	1333	LEU	CB-CG-CD1	13.17	133.39	111.00
3	D	353	SER	N-CA-CB	12.86	129.79	110.50
2	C	12	ARG	NE-CZ-NH1	-12.79	113.90	120.30
3	D	380	PHE	CB-CG-CD2	12.78	129.74	120.80
2	C	1176	LEU	CB-CG-CD2	-12.77	89.29	111.00
3	D	915	ILE	CG1-CB-CG2	-12.76	83.33	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	901	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	A	234	LEU	CB-CG-CD2	12.69	132.57	111.00
3	D	464	ASP	CB-CG-OD1	12.56	129.60	118.30
3	D	901	ARG	NE-CZ-NH2	-12.55	114.03	120.30
4	E	28	ARG	NE-CZ-NH2	-12.55	114.03	120.30
2	C	1216	ARG	NH1-CZ-NH2	12.48	133.13	119.40
3	D	899	TYR	CB-CG-CD2	-12.26	113.64	121.00
2	C	818	VAL	CG1-CB-CG2	-12.23	91.32	110.90
3	D	474	LEU	CB-CG-CD1	12.23	131.79	111.00
2	C	810	TYR	CB-CG-CD1	-12.21	113.67	121.00
2	C	827	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	A	61	ILE	CB-CG1-CD1	-12.11	79.98	113.90
2	C	452	ARG	NE-CZ-NH2	-12.10	114.25	120.30
2	C	1296	ASP	CB-CG-OD1	-12.00	107.50	118.30
3	D	930	LEU	CB-CG-CD2	11.96	131.32	111.00
2	C	1050	VAL	CG1-CB-CG2	-11.94	91.80	110.90
2	C	454	ARG	NE-CZ-NH1	-11.93	114.33	120.30
3	D	431	ARG	NE-CZ-NH2	-11.90	114.35	120.30
2	C	1296	ASP	CB-CG-OD2	11.88	129.00	118.30
2	C	678	ARG	NE-CZ-NH1	11.87	126.23	120.30
3	D	345	LYS	CD-CE-NZ	11.66	138.52	111.70
3	D	582	ILE	CG1-CB-CG2	-11.64	85.80	111.40
3	D	807	LEU	CB-CG-CD1	-11.55	91.36	111.00
3	D	513	MET	CG-SD-CE	-11.54	81.73	100.20
2	C	521	LEU	CB-CG-CD1	-11.49	91.46	111.00
1	B	205	MET	CG-SD-CE	-11.46	81.86	100.20
3	D	368	LEU	CB-CG-CD1	-11.39	91.63	111.00
2	C	388	LEU	CB-CG-CD2	11.35	130.29	111.00
2	C	1106	ARG	NE-CZ-NH1	11.34	125.97	120.30
3	D	1262	ARG	NE-CZ-NH2	11.21	125.90	120.30
3	D	123	ARG	NE-CZ-NH1	11.17	125.89	120.30
3	D	767	LEU	CB-CG-CD2	11.14	129.95	111.00
1	B	43	LEU	CB-CG-CD1	-11.11	92.12	111.00
3	D	341	ASN	N-CA-CB	-11.11	90.60	110.60
4	E	52	ARG	NE-CZ-NH1	-11.10	114.75	120.30
3	D	627	THR	CA-CB-CG2	-11.07	96.91	112.40
2	C	515	MET	CG-SD-CE	11.07	117.91	100.20
3	D	620	PHE	CB-CG-CD1	10.93	128.45	120.80
3	D	506	VAL	CA-CB-CG2	-10.92	94.52	110.90
2	C	1075	VAL	CA-CB-CG2	-10.88	94.58	110.90
3	D	363	LEU	CB-CG-CD1	10.80	129.37	111.00
2	C	704	MET	CG-SD-CE	-10.79	82.94	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	554	HIS	N-CA-CB	-10.75	91.25	110.60
3	D	101	ARG	NE-CZ-NH2	-10.75	114.92	120.30
3	D	536	LEU	CB-CG-CD1	10.74	129.26	111.00
2	C	802	VAL	CG1-CB-CG2	-10.70	93.78	110.90
3	D	362	ARG	NE-CZ-NH1	10.68	125.64	120.30
3	D	338	PHE	CB-CG-CD1	-10.68	113.33	120.80
2	C	791	LEU	CB-CG-CD1	-10.66	92.87	111.00
3	D	620	PHE	CB-CG-CD2	-10.64	113.36	120.80
3	D	102	MET	CG-SD-CE	-10.62	83.21	100.20
3	D	269	TYR	CB-CG-CD2	-10.61	114.63	121.00
3	D	434	ILE	CB-CG1-CD1	-10.57	84.31	113.90
3	D	765	GLU	C-N-CA	-10.51	100.22	122.30
1	A	148	ARG	NE-CZ-NH2	-10.43	115.09	120.30
2	C	1240	ASP	CB-CG-OD1	-10.39	108.95	118.30
3	D	99	ARG	NH1-CZ-NH2	10.38	130.82	119.40
3	D	349	TYR	CB-CG-CD2	10.37	127.22	121.00
5	M	186	ASP	N-CA-CB	10.30	129.15	110.60
2	C	1246	ARG	NH1-CZ-NH2	-10.29	108.09	119.40
2	C	1302	THR	CA-CB-CG2	-10.27	98.02	112.40
3	D	22	ILE	CG1-CB-CG2	-10.25	88.85	111.40
2	C	10	ARG	NE-CZ-NH1	10.21	125.41	120.30
2	C	827	ARG	CG-CD-NE	10.09	132.99	111.80
6	F	-1	DC	O5'-P-OP2	10.06	122.78	110.70
3	D	1262	ARG	NE-CZ-NH1	-10.01	115.29	120.30
3	D	899	TYR	CB-CG-CD1	10.01	127.00	121.00
2	C	10	ARG	NE-CZ-NH2	-9.97	115.32	120.30
3	D	515	ARG	NH1-CZ-NH2	-9.96	108.44	119.40
3	D	802	ASP	CB-CG-OD1	9.93	127.24	118.30
3	D	422	LEU	CB-CG-CD1	-9.92	94.14	111.00
2	C	184	LEU	CB-CG-CD1	9.89	127.81	111.00
2	C	1259	LEU	CB-CG-CD1	-9.88	94.21	111.00
3	D	90	VAL	CA-CB-CG1	-9.87	96.10	110.90
3	D	764	ARG	NE-CZ-NH1	-9.87	115.37	120.30
3	D	505	ASP	CB-CG-OD1	9.86	127.17	118.30
4	E	19	LEU	CB-CG-CD1	-9.81	94.32	111.00
2	C	1103	VAL	CA-CB-CG2	9.79	125.59	110.90
2	C	717	VAL	CG1-CB-CG2	-9.78	95.25	110.90
3	D	799	ARG	NE-CZ-NH2	-9.78	115.41	120.30
2	C	548	ARG	NE-CZ-NH1	9.78	125.19	120.30
2	C	1221	PHE	CB-CG-CD1	-9.74	113.98	120.80
3	D	376	LEU	CB-CG-CD1	-9.70	94.50	111.00
2	C	1246	ARG	CB-CA-C	-9.70	91.01	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	466	MET	CG-SD-CE	-9.66	84.75	100.20
3	D	885	VAL	CA-CB-CG1	9.66	125.39	110.90
3	D	92	VAL	CA-CB-CG1	-9.64	96.44	110.90
2	C	731	ARG	NE-CZ-NH1	-9.64	115.48	120.30
3	D	1332	LEU	CB-CG-CD2	-9.62	94.64	111.00
2	C	1142	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	79	LEU	CB-CG-CD2	9.59	127.31	111.00
2	C	1194	GLU	OE1-CD-OE2	-9.58	111.81	123.30
1	B	231	PHE	CB-CG-CD2	-9.57	114.10	120.80
2	C	1226	THR	CA-CB-CG2	-9.46	99.15	112.40
3	D	481	ARG	NE-CZ-NH2	-9.42	115.59	120.30
2	C	827	ARG	CB-CA-C	-9.39	91.61	110.40
2	C	1117	LEU	CD1-CG-CD2	-9.38	82.35	110.50
3	D	641	ILE	CG1-CB-CG2	9.37	132.02	111.40
3	D	535	ARG	CB-CG-CD	-9.37	87.24	111.60
2	C	1117	LEU	CB-CG-CD1	-9.37	95.08	111.00
1	A	174	ASP	CB-CG-OD2	9.34	126.71	118.30
2	C	929	ILE	CG1-CB-CG2	-9.30	90.93	111.40
3	D	780	ARG	CG-CD-NE	-9.29	92.30	111.80
3	D	899	TYR	CD1-CE1-CZ	-9.28	111.44	119.80
1	A	48	LEU	CB-CG-CD2	-9.27	95.24	111.00
2	C	1270	PHE	CB-CG-CD2	-9.27	114.31	120.80
3	D	1144	LEU	CB-CG-CD2	-9.27	95.24	111.00
3	D	462	ASP	N-CA-C	-9.26	86.00	111.00
3	D	1253	ILE	CG1-CB-CG2	-9.24	91.06	111.40
3	D	1309	ILE	CG1-CB-CG2	-9.24	91.08	111.40
3	D	763	PHE	CB-CG-CD2	-9.22	114.34	120.80
3	D	1148	ARG	NE-CZ-NH2	9.22	124.91	120.30
2	C	538	LEU	CB-CG-CD2	-9.19	95.37	111.00
3	D	598	LYS	CD-CE-NZ	9.19	132.82	111.70
1	B	201	LEU	CB-CG-CD1	-9.18	95.39	111.00
2	C	1267	GLY	C-N-CA	-9.18	98.75	121.70
2	C	1180	MET	CB-CA-C	-9.17	92.06	110.40
3	D	470	VAL	CG1-CB-CG2	-9.17	96.23	110.90
4	E	19	LEU	CB-CG-CD2	9.16	126.57	111.00
2	C	75	LEU	CB-CG-CD1	9.15	126.56	111.00
3	D	269	TYR	CB-CG-CD1	9.11	126.47	121.00
2	C	1098	LEU	CB-CG-CD2	-9.10	95.53	111.00
2	C	1176	LEU	CB-CG-CD1	-9.09	95.55	111.00
2	C	1326	LEU	CB-CG-CD1	-9.08	95.57	111.00
2	C	782	VAL	CG1-CB-CG2	-9.00	96.50	110.90
3	D	744	ARG	NE-CZ-NH2	8.96	124.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1320	ILE	CB-CG1-CD1	-8.95	88.84	113.90
3	D	504	GLN	CB-CA-C	8.92	128.24	110.40
3	D	441	LEU	CB-CG-CD1	-8.91	95.85	111.00
2	C	395	TYR	CB-CG-CD2	-8.90	115.66	121.00
2	C	528	ARG	NE-CZ-NH1	8.89	124.75	120.30
3	D	390	LEU	CB-CG-CD2	-8.89	95.89	111.00
3	D	605	LEU	CB-CG-CD2	-8.87	95.92	111.00
2	C	693	LEU	CB-CG-CD2	-8.87	95.92	111.00
1	B	47	LEU	CB-CG-CD2	-8.80	96.05	111.00
2	C	521	LEU	CD1-CG-CD2	-8.78	84.17	110.50
2	C	810	TYR	CG-CD2-CE2	-8.76	114.29	121.30
3	D	1330	ARG	NE-CZ-NH1	8.74	124.67	120.30
3	D	1248	ILE	CG1-CB-CG2	-8.73	92.19	111.40
2	C	1305	TYR	CB-CG-CD1	-8.72	115.77	121.00
5	M	146	ASP	CB-CG-OD1	-8.68	110.49	118.30
2	C	1298	VAL	CG1-CB-CG2	-8.66	97.04	110.90
2	C	1195	ILE	CG1-CB-CG2	-8.63	92.41	111.40
3	D	345	LYS	CB-CA-C	8.63	127.67	110.40
3	D	349	TYR	CB-CG-CD1	-8.62	115.83	121.00
2	C	511	LEU	CB-CG-CD2	-8.60	96.38	111.00
2	C	1268	GLN	CB-CA-C	8.59	127.58	110.40
3	D	308	ASP	CB-CG-OD1	-8.58	110.58	118.30
2	C	22	LEU	CB-CG-CD2	-8.58	96.42	111.00
1	A	88	LEU	CB-CG-CD1	-8.55	96.46	111.00
2	C	505	PHE	CB-CG-CD2	-8.50	114.85	120.80
3	D	462	ASP	CB-CG-OD2	8.50	125.95	118.30
3	D	1304	ARG	NH1-CZ-NH2	8.46	128.71	119.40
2	C	929	ILE	CA-CB-CG2	8.44	127.79	110.90
2	C	502	VAL	CG1-CB-CG2	-8.43	97.41	110.90
2	C	578	TYR	CB-CG-CD2	-8.40	115.96	121.00
3	D	583	VAL	CG1-CB-CG2	8.33	124.22	110.90
3	D	373	ALA	O-C-N	-8.31	109.40	122.70
2	C	1151	LEU	CA-CB-CG	8.31	134.41	115.30
6	F	-1	DC	P-O5'-C5'	8.30	134.19	120.90
3	D	113	HIS	CB-CA-C	-8.29	93.82	110.40
3	D	536	LEU	CD1-CG-CD2	-8.28	85.67	110.50
3	D	1243	LEU	CB-CG-CD1	-8.27	96.93	111.00
3	D	1355	ARG	NE-CZ-NH2	8.27	124.44	120.30
2	C	800	MET	CA-CB-CG	8.23	127.29	113.30
2	C	1288	GLN	CB-CA-C	-8.23	93.95	110.40
3	D	719	PHE	CB-CG-CD2	-8.23	115.04	120.80
1	A	170	ARG	NE-CZ-NH2	-8.19	116.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	908	ILE	CG1-CB-CG2	-8.19	93.38	111.40
2	C	135	THR	OG1-CB-CG2	-8.19	91.17	110.00
3	D	250	ARG	NE-CZ-NH1	-8.19	116.21	120.30
2	C	1231	TYR	CG-CD1-CE1	8.18	127.84	121.30
2	C	22	LEU	CB-CG-CD1	-8.17	97.11	111.00
3	D	626	TYR	CB-CG-CD1	-8.16	116.10	121.00
2	C	1305	TYR	CD1-CE1-CZ	-8.16	112.46	119.80
3	D	622	ASP	CB-CG-OD2	8.15	125.64	118.30
3	D	76	LYS	CD-CE-NZ	8.14	130.43	111.70
1	B	45	ARG	NE-CZ-NH1	8.14	124.37	120.30
2	C	1094	VAL	CA-CB-CG1	-8.12	98.72	110.90
1	B	207	THR	CA-CB-CG2	-8.12	101.04	112.40
2	C	143	ARG	NE-CZ-NH1	-8.10	116.25	120.30
2	C	1265	PHE	CB-CG-CD2	-8.09	115.14	120.80
2	C	1052	VAL	CG1-CB-CG2	-8.08	97.98	110.90
2	C	819	SER	N-CA-CB	8.07	122.60	110.50
2	C	758	ARG	NE-CZ-NH1	-8.07	116.27	120.30
2	C	704	MET	CB-CG-SD	8.06	136.58	112.40
3	D	132	LEU	CB-CG-CD2	8.06	124.69	111.00
2	C	1184	THR	CA-CB-CG2	-8.04	101.14	112.40
4	E	52	ARG	NH1-CZ-NH2	8.02	128.22	119.40
2	C	866	ASP	CB-CG-OD2	-8.02	111.08	118.30
2	C	823	VAL	CA-CB-CG1	8.02	122.92	110.90
3	D	337	ARG	N-CA-CB	-8.01	96.19	110.60
1	A	125	LYS	CD-CE-NZ	8.00	130.11	111.70
2	C	96	LEU	CB-CG-CD1	-7.98	97.43	111.00
2	C	38	PHE	CB-CG-CD1	-7.98	115.22	120.80
3	D	537	TYR	CB-CG-CD2	-7.98	116.21	121.00
2	C	637	ARG	NE-CZ-NH1	-7.97	116.31	120.30
2	C	1159	VAL	CB-CA-C	-7.97	96.27	111.40
2	C	1239	VAL	CB-CA-C	-7.97	96.26	111.40
1	B	219	ARG	NE-CZ-NH2	-7.95	116.33	120.30
3	D	220	ARG	NE-CZ-NH1	-7.95	116.33	120.30
5	M	120	LEU	CB-CG-CD1	-7.95	97.48	111.00
2	C	734	ILE	CG1-CB-CG2	-7.88	94.06	111.40
2	C	395	TYR	CB-CG-CD1	7.88	125.73	121.00
2	C	451	ARG	NE-CZ-NH1	-7.86	116.37	120.30
2	C	18	ARG	NE-CZ-NH1	7.85	124.22	120.30
2	C	23	ASP	CB-CG-OD1	7.83	125.35	118.30
3	D	343	LEU	CB-CG-CD2	7.83	124.32	111.00
2	C	764	CYS	CA-CB-SG	-7.80	99.95	114.00
3	D	369	PRO	N-CD-CG	-7.80	91.50	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1333	LEU	CD1-CG-CD2	-7.79	87.13	110.50
3	D	337	ARG	CG-CD-NE	-7.78	95.47	111.80
6	F	0	DC	N1-C1'-C2'	7.77	127.36	112.60
3	D	511	TYR	CZ-CE2-CD2	-7.76	112.82	119.80
3	D	883	ARG	NE-CZ-NH1	-7.76	116.42	120.30
1	A	64	VAL	CG1-CB-CG2	-7.74	98.52	110.90
2	C	175	ARG	NE-CZ-NH1	-7.74	116.43	120.30
4	E	20	VAL	CG1-CB-CG2	-7.72	98.55	110.90
5	M	190	VAL	CG1-CB-CG2	-7.72	98.55	110.90
2	C	827	ARG	NE-CZ-NH2	-7.71	116.44	120.30
3	D	1331	VAL	CG1-CB-CG2	-7.71	98.57	110.90
2	C	1187	PHE	CG-CD2-CE2	-7.69	112.34	120.80
2	C	12	ARG	CB-CG-CD	-7.68	91.64	111.60
1	A	102	LEU	CD1-CG-CD2	-7.67	87.48	110.50
2	C	720	ARG	NE-CZ-NH1	-7.67	116.46	120.30
2	C	1221	PHE	CB-CG-CD2	7.67	126.17	120.80
1	B	219	ARG	NE-CZ-NH1	7.67	124.14	120.30
3	D	1138	LEU	CB-CG-CD1	7.66	124.02	111.00
3	D	917	VAL	CG1-CB-CG2	7.63	123.10	110.90
3	D	440	VAL	CG1-CB-CG2	7.59	123.05	110.90
2	C	577	VAL	CG1-CB-CG2	-7.59	98.76	110.90
3	D	539	SER	O-C-N	-7.59	110.30	123.20
3	D	239	LEU	CB-CG-CD2	-7.57	98.13	111.00
2	C	1131	MET	CG-SD-CE	7.56	112.29	100.20
3	D	548	VAL	CG1-CB-CG2	-7.56	98.81	110.90
2	C	794	LEU	CB-CA-C	-7.55	95.86	110.20
2	C	1081	PRO	CB-CA-C	-7.55	93.13	112.00
1	B	224	LEU	CB-CG-CD1	-7.54	98.19	111.00
1	B	56	VAL	CG1-CB-CG2	7.53	122.95	110.90
3	D	835	LEU	CB-CG-CD2	7.53	123.80	111.00
2	C	12	ARG	NH1-CZ-NH2	7.51	127.66	119.40
3	D	118	LYS	CD-CE-NZ	-7.50	94.44	111.70
3	D	1280	VAL	CG1-CB-CG2	7.50	122.91	110.90
3	D	352	ARG	NE-CZ-NH2	7.50	124.05	120.30
3	D	1323	ALA	O-C-N	7.49	134.69	122.70
2	C	1095	ASP	CB-CG-OD2	-7.49	111.56	118.30
3	D	306	LEU	CB-CG-CD2	-7.49	98.27	111.00
2	C	1333	LEU	O-C-N	-7.47	110.50	123.20
2	C	690	VAL	CA-CB-CG1	7.46	122.09	110.90
3	D	508	LEU	CB-CG-CD2	-7.46	98.32	111.00
3	D	798	ARG	NH1-CZ-NH2	-7.45	111.20	119.40
2	C	816	ILE	CG1-CB-CG2	-7.43	95.05	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	97	VAL	CG1-CB-CG2	7.43	122.78	110.90
4	E	28	ARG	NE-CZ-NH1	7.40	124.00	120.30
2	C	700	VAL	CB-CA-C	-7.38	97.38	111.40
3	D	338	PHE	CZ-CE2-CD2	-7.36	111.27	120.10
3	D	534	GLU	N-CA-CB	7.35	123.83	110.60
6	F	9	DT	C2'-C3'-O3'	-7.35	88.35	112.60
2	C	817	LEU	CB-CG-CD2	-7.34	98.52	111.00
3	D	467	ALA	CB-CA-C	-7.34	99.09	110.10
3	D	1242	ARG	NE-CZ-NH1	7.33	123.96	120.30
3	D	586	GLY	N-CA-C	7.31	131.38	113.10
3	D	803	VAL	CA-CB-CG2	-7.31	99.93	110.90
1	A	73	GLY	N-CA-C	7.31	131.38	113.10
2	C	1263	ALA	CB-CA-C	-7.30	99.15	110.10
2	C	555	TYR	C-N-CA	-7.29	106.99	122.30
2	C	1294	LYS	N-CA-CB	-7.29	97.48	110.60
3	D	1237	VAL	CG1-CB-CG2	-7.28	99.25	110.90
3	D	116	PHE	CB-CG-CD2	7.28	125.90	120.80
3	D	394	ILE	CG1-CB-CG2	-7.26	95.42	111.40
2	C	97	ARG	NE-CZ-NH2	-7.26	116.67	120.30
2	C	506	PHE	CB-CG-CD1	-7.25	115.73	120.80
3	D	390	LEU	CB-CG-CD1	-7.24	98.69	111.00
2	C	1269	ARG	NE-CZ-NH1	-7.24	116.68	120.30
3	D	326	SER	N-CA-CB	-7.24	99.64	110.50
3	D	1342	ASP	CB-CG-OD1	7.24	124.81	118.30
2	C	787	PRO	N-CA-C	-7.24	93.28	112.10
3	D	579	LEU	CB-CG-CD2	7.22	123.27	111.00
3	D	693	VAL	CG1-CB-CG2	-7.22	99.35	110.90
3	D	28	ASP	CB-CG-OD1	7.21	124.79	118.30
2	C	821	ARG	NE-CZ-NH2	-7.20	116.70	120.30
3	D	617	THR	OG1-CB-CG2	-7.20	93.44	110.00
3	D	1206	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	C	801	ARG	NE-CZ-NH2	-7.19	116.70	120.30
2	C	829	THR	CA-CB-CG2	-7.19	102.34	112.40
5	M	156	ILE	CB-CA-C	7.19	125.97	111.60
3	D	300	GLN	N-CA-CB	7.18	123.52	110.60
3	D	380	PHE	N-CA-CB	-7.17	97.70	110.60
3	D	511	TYR	CB-CG-CD1	-7.16	116.71	121.00
3	D	377	PHE	N-CA-CB	-7.15	97.73	110.60
1	A	44	ARG	NE-CZ-NH2	7.15	123.87	120.30
3	D	701	LEU	CB-CG-CD2	-7.14	98.87	111.00
2	C	577	VAL	CA-CB-CG2	-7.12	100.22	110.90
3	D	365	GLN	CB-CA-C	-7.11	96.18	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	376	LEU	CB-CG-CD2	7.10	123.07	111.00
3	D	334	LYS	N-CA-C	7.10	130.16	111.00
3	D	470	VAL	CA-CB-CG1	-7.10	100.25	110.90
3	D	915	ILE	CB-CG1-CD1	7.09	133.75	113.90
2	C	1322	SER	CB-CA-C	7.09	123.57	110.10
2	C	1199	LEU	CB-CG-CD2	-7.08	98.97	111.00
2	C	18	ARG	CG-CD-NE	7.07	126.64	111.80
2	C	678	ARG	CB-CA-C	7.06	124.52	110.40
2	C	1243	MET	CG-SD-CE	-7.05	88.91	100.20
3	D	525	MET	CG-SD-CE	-7.05	88.92	100.20
3	D	511	TYR	CG-CD1-CE1	-7.04	115.67	121.30
3	D	798	ARG	CD-NE-CZ	7.04	133.45	123.60
2	C	528	ARG	NE-CZ-NH2	-7.03	116.78	120.30
3	D	115	TRP	CH2-CZ2-CE2	-7.03	110.37	117.40
4	E	52	ARG	NE-CZ-NH2	-7.03	116.79	120.30
2	C	678	ARG	NH1-CZ-NH2	-7.02	111.68	119.40
3	D	416	ILE	CG1-CB-CG2	7.02	126.85	111.40
3	D	1344	LEU	CB-CG-CD2	7.02	122.93	111.00
1	B	44	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	B	46	ILE	CG1-CB-CG2	-7.00	95.99	111.40
3	D	338	PHE	N-CA-CB	-7.00	98.00	110.60
2	C	731	ARG	N-CA-CB	6.98	123.17	110.60
1	A	228	LEU	CB-CG-CD2	-6.98	99.13	111.00
1	A	65	LEU	CB-CG-CD2	-6.97	99.16	111.00
3	D	373	ALA	N-CA-C	-6.96	92.20	111.00
3	D	453	VAL	CG1-CB-CG2	6.96	122.04	110.90
2	C	692	THR	CA-CB-CG2	-6.96	102.66	112.40
3	D	1256	ILE	CA-CB-CG1	-6.95	97.79	111.00
1	A	96	ASP	CB-CG-OD1	6.95	124.55	118.30
3	D	481	ARG	CB-CG-CD	-6.95	93.54	111.60
3	D	740	LEU	CB-CG-CD1	-6.93	99.22	111.00
2	C	35	PHE	CB-CG-CD2	-6.91	115.97	120.80
3	D	388	ARG	NE-CZ-NH1	6.90	123.75	120.30
3	D	56	LEU	CB-CG-CD2	-6.89	99.29	111.00
2	C	667	LEU	CB-CG-CD2	6.89	122.71	111.00
2	C	464	PHE	CB-CG-CD2	-6.88	115.98	120.80
2	C	451	ARG	NE-CZ-NH2	6.88	123.74	120.30
3	D	1262	ARG	N-CA-CB	-6.87	98.23	110.60
2	C	810	TYR	N-CA-CB	6.87	122.96	110.60
2	C	35	PHE	CG-CD1-CE1	-6.86	113.25	120.80
3	D	77	ARG	NE-CZ-NH1	-6.86	116.87	120.30
3	D	1355	ARG	NE-CZ-NH1	-6.84	116.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1305	TYR	CB-CG-CD2	6.83	125.10	121.00
3	D	780	ARG	NE-CZ-NH1	-6.82	116.89	120.30
3	D	451	PRO	N-CA-CB	6.80	111.46	103.30
3	D	885	VAL	N-CA-C	-6.79	92.67	111.00
3	D	271	ARG	NE-CZ-NH2	-6.78	116.91	120.30
3	D	461	PHE	N-CA-CB	-6.78	98.40	110.60
2	C	527	LYS	O-C-N	-6.77	111.87	122.70
3	D	769	VAL	CG1-CB-CG2	-6.76	100.08	110.90
2	C	453	ILE	CG1-CB-CG2	-6.76	96.53	111.40
3	D	1261	LEU	CB-CG-CD1	6.75	122.48	111.00
2	C	532	ALA	CB-CA-C	-6.75	99.98	110.10
3	D	485	MET	CB-CA-C	-6.74	96.92	110.40
3	D	707	ILE	CG1-CB-CG2	-6.74	96.57	111.40
2	C	813	GLU	C-N-CA	-6.73	104.86	121.70
1	A	48	LEU	CB-CG-CD1	6.73	122.44	111.00
2	C	528	ARG	CB-CA-C	-6.71	96.98	110.40
3	D	574	VAL	CG1-CB-CG2	-6.71	100.16	110.90
3	D	374	LEU	N-CA-CB	6.70	123.81	110.40
3	D	423	LEU	CB-CA-C	-6.70	97.46	110.20
2	C	1238	LEU	CB-CG-CD2	-6.70	99.61	111.00
2	C	1301	ARG	NH1-CZ-NH2	-6.70	112.03	119.40
2	C	811	ASN	N-CA-C	-6.69	92.94	111.00
2	C	1214	ASP	CB-CG-OD2	-6.69	112.28	118.30
3	D	1233	ILE	CG1-CB-CG2	-6.68	96.69	111.40
2	C	1238	LEU	C-N-CA	-6.68	104.99	121.70
2	C	821	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	C	171	LEU	CB-CG-CD1	-6.67	99.65	111.00
3	D	421	VAL	CA-CB-CG2	-6.67	100.90	110.90
3	D	774	ILE	CG1-CB-CG2	6.67	126.06	111.40
3	D	744	ARG	CB-CG-CD	-6.66	94.28	111.60
2	C	657	THR	CA-CB-CG2	-6.66	103.07	112.40
3	D	908	ILE	CA-CB-CG1	6.66	123.66	111.00
3	D	1319	PHE	CB-CG-CD1	-6.66	116.14	120.80
3	D	472	LEU	CA-CB-CG	6.65	130.60	115.30
3	D	374	LEU	CB-CG-CD2	6.65	122.30	111.00
2	C	454	ARG	NH1-CZ-NH2	6.64	126.71	119.40
3	D	356	THR	CA-CB-CG2	-6.64	103.10	112.40
3	D	78	LEU	CB-CG-CD1	6.64	122.29	111.00
2	C	1169	VAL	CB-CA-C	-6.63	98.80	111.40
2	C	750	ILE	CG1-CB-CG2	-6.63	96.82	111.40
2	C	931	VAL	CG1-CB-CG2	-6.60	100.34	110.90
2	C	1227	VAL	CG1-CB-CG2	-6.59	100.35	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1182	ILE	CB-CA-C	-6.58	98.43	111.60
3	D	245	LEU	CD1-CG-CD2	-6.58	90.76	110.50
2	C	764	CYS	N-CA-CB	6.58	122.44	110.60
2	C	577	VAL	C-N-CA	-6.58	105.26	121.70
2	C	1177	ARG	CA-CB-CG	6.57	127.86	113.40
2	C	388	LEU	CB-CG-CD1	-6.56	99.85	111.00
1	A	82	LEU	CA-CB-CG	-6.55	100.23	115.30
2	C	555	TYR	N-CA-CB	6.55	122.39	110.60
2	C	773	LEU	CB-CG-CD1	-6.54	99.88	111.00
2	C	681	MET	N-CA-CB	6.53	122.36	110.60
3	D	188	LEU	CB-CG-CD1	6.53	122.10	111.00
3	D	539	SER	CA-C-N	6.53	129.26	116.20
3	D	863	LEU	CB-CG-CD1	-6.52	99.91	111.00
3	D	701	LEU	CA-CB-CG	6.52	130.30	115.30
2	C	1227	VAL	CA-CB-CG1	-6.52	101.12	110.90
2	C	524	ILE	CA-CB-CG1	-6.52	98.62	111.00
2	C	26	TYR	CB-CG-CD1	6.51	124.91	121.00
2	C	1097	VAL	CA-CB-CG2	-6.51	101.14	110.90
4	E	58	LEU	CB-CG-CD2	6.50	122.06	111.00
3	D	722	ILE	CA-CB-CG2	6.49	123.88	110.90
2	C	144	VAL	CA-CB-CG2	-6.48	101.18	110.90
2	C	10	ARG	CD-NE-CZ	-6.48	114.53	123.60
2	C	1075	VAL	CA-CB-CG1	-6.48	101.18	110.90
2	C	1058	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	181	GLU	N-CA-CB	6.46	122.23	110.60
2	C	1188	ASP	CB-CG-OD2	6.46	124.11	118.30
2	C	452	ARG	CG-CD-NE	-6.45	98.26	111.80
2	C	606	LEU	CB-CG-CD2	-6.45	100.04	111.00
3	D	78	LEU	CB-CA-C	6.44	122.44	110.20
3	D	354	VAL	CA-CB-CG2	-6.43	101.25	110.90
2	C	822	VAL	CA-CB-CG2	-6.43	101.26	110.90
2	C	828	PHE	N-CA-C	6.43	128.35	111.00
3	D	626	TYR	CZ-CE2-CD2	-6.43	114.02	119.80
3	D	808	VAL	N-CA-CB	-6.41	97.40	111.50
1	B	195	ARG	NE-CZ-NH1	6.41	123.50	120.30
3	D	431	ARG	CG-CD-NE	-6.41	98.34	111.80
3	D	454	CYS	CA-CB-SG	-6.40	102.48	114.00
3	D	468	VAL	CB-CA-C	-6.40	99.24	111.40
1	B	81	ILE	CG1-CB-CG2	-6.40	97.33	111.40
3	D	899	TYR	OH-CZ-CE2	-6.39	102.84	120.10
3	D	380	PHE	CZ-CE2-CD2	-6.38	112.44	120.10
3	D	632	ALA	CB-CA-C	-6.38	100.53	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	32	LEU	CB-CG-CD2	-6.37	100.17	111.00
3	D	139	LEU	CB-CG-CD2	-6.36	100.19	111.00
2	C	1182	ILE	CG1-CB-CG2	6.36	125.39	111.40
3	D	405	GLU	OE1-CD-OE2	6.36	130.93	123.30
1	A	83	LEU	CB-CG-CD2	6.36	121.81	111.00
2	C	697	LYS	CB-CA-C	-6.35	97.71	110.40
2	C	1231	TYR	CB-CG-CD1	6.35	124.81	121.00
2	C	699	LEU	CD1-CG-CD2	6.34	129.53	110.50
2	C	39	ILE	CG1-CB-CG2	6.34	125.35	111.40
2	C	11	ILE	CG1-CB-CG2	-6.32	97.49	111.40
3	D	806	ASP	CB-CG-OD1	6.32	123.99	118.30
3	D	808	VAL	CB-CA-C	-6.32	99.39	111.40
2	C	1151	LEU	CB-CG-CD1	-6.32	100.26	111.00
2	C	1239	VAL	CA-CB-CG2	-6.32	101.42	110.90
6	F	8	DA	P-O3'-C3'	6.31	127.28	119.70
2	C	1295	SER	N-CA-CB	6.31	119.97	110.50
3	D	885	VAL	N-CA-CB	-6.31	97.61	111.50
2	C	838	CYS	CA-CB-SG	-6.31	102.65	114.00
2	C	519	ASN	CA-CB-CG	-6.30	99.53	113.40
3	D	609	TYR	CB-CG-CD1	6.30	124.78	121.00
3	D	352	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
2	C	872	TYR	CB-CG-CD1	-6.30	117.22	121.00
3	D	1341	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	C	931	VAL	CA-CB-CG2	-6.30	101.45	110.90
3	D	366	CYS	N-CA-CB	6.29	121.92	110.60
3	D	1355	ARG	N-CA-CB	-6.29	99.28	110.60
1	A	148	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	C	1051	LYS	CD-CE-NZ	6.28	126.15	111.70
2	C	1212	LEU	CB-CG-CD1	-6.28	100.32	111.00
3	D	898	CYS	C-N-CA	-6.28	106.00	121.70
2	C	1097	VAL	CB-CA-C	-6.28	99.48	111.40
7	G	2	DG	O4'-C4'-C3'	-6.27	101.99	104.50
3	D	239	LEU	CB-CG-CD1	6.27	121.66	111.00
3	D	362	ARG	CD-NE-CZ	6.27	132.38	123.60
2	C	1159	VAL	CA-CB-CG2	6.27	120.30	110.90
2	C	1231	TYR	CZ-CE2-CD2	6.26	125.44	119.80
3	D	360	TYR	O-C-N	-6.25	112.70	122.70
3	D	618	VAL	CA-CB-CG2	6.25	120.28	110.90
3	D	299	LEU	CB-CG-CD2	-6.25	100.38	111.00
3	D	724	MET	CG-SD-CE	-6.25	90.20	100.20
2	C	1078	LYS	CB-CG-CD	6.24	127.83	111.60
2	C	820	GLU	OE1-CD-OE2	6.24	130.78	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	48	LEU	CB-CG-CD2	-6.22	100.42	111.00
1	B	203	ILE	CA-CB-CG2	-6.22	98.46	110.90
1	B	51	MET	CG-SD-CE	-6.21	90.26	100.20
2	C	1305	TYR	CG-CD2-CE2	-6.21	116.33	121.30
2	C	616	ILE	CG1-CB-CG2	-6.19	97.78	111.40
1	A	312	LEU	CA-CB-CG	6.19	129.53	115.30
2	C	519	ASN	CB-CA-C	6.19	122.78	110.40
1	A	218	ARG	NE-CZ-NH2	6.18	123.39	120.30
2	C	1319	MET	CB-CG-SD	-6.18	93.87	112.40
3	D	360	TYR	CD1-CE1-CZ	6.17	125.36	119.80
1	A	68	TYR	CB-CG-CD1	6.17	124.70	121.00
2	C	1296	ASP	CB-CA-C	-6.17	98.06	110.40
2	C	706	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	A	206	GLU	OE1-CD-OE2	-6.16	115.91	123.30
2	C	1305	TYR	CG-CD1-CE1	6.15	126.22	121.30
2	C	605	TYR	CB-CG-CD2	6.13	124.68	121.00
3	D	1333	THR	CA-CB-CG2	-6.13	103.82	112.40
2	C	1149	TYR	CD1-CE1-CZ	-6.12	114.29	119.80
3	D	643	ASP	CB-CG-OD1	6.12	123.81	118.30
3	D	250	ARG	NH1-CZ-NH2	6.11	126.12	119.40
3	D	473	THR	CA-CB-CG2	-6.11	103.85	112.40
2	C	15	PHE	CB-CG-CD1	6.10	125.07	120.80
1	A	82	LEU	CB-CG-CD2	6.10	121.37	111.00
2	C	1246	ARG	CD-NE-CZ	-6.10	115.06	123.60
5	M	199	LEU	CB-CG-CD2	-6.09	100.64	111.00
2	C	674	ASP	CB-CG-OD2	6.09	123.78	118.30
3	D	462	ASP	OD1-CG-OD2	-6.08	111.74	123.30
2	C	388	LEU	CA-CB-CG	6.08	129.28	115.30
2	C	689	ALA	CB-CA-C	-6.08	100.98	110.10
2	C	1231	TYR	O-C-N	6.07	132.42	122.70
2	C	1169	VAL	CG1-CB-CG2	6.07	120.61	110.90
1	A	56	VAL	CG1-CB-CG2	6.07	120.61	110.90
3	D	618	VAL	CG1-CB-CG2	-6.07	101.19	110.90
3	D	835	LEU	CB-CG-CD1	-6.07	100.69	111.00
2	C	823	VAL	CA-CB-CG2	-6.06	101.81	110.90
3	D	897	HIS	N-CA-CB	6.06	121.51	110.60
2	C	615	VAL	CG1-CB-CG2	-6.06	101.21	110.90
3	D	634	ARG	NE-CZ-NH1	-6.05	117.28	120.30
2	C	137	VAL	CB-CA-C	-6.05	99.91	111.40
2	C	402	ARG	NE-CZ-NH1	-6.04	117.28	120.30
6	F	-4	DC	O5'-P-OP2	-6.04	100.26	105.70
3	D	1328	THR	CA-CB-CG2	-6.04	103.95	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	731	ARG	CG-CD-NE	6.03	124.47	111.80
1	A	253	LEU	CB-CG-CD2	6.03	121.25	111.00
3	D	464	ASP	CB-CG-OD2	-6.03	112.88	118.30
3	D	332	LYS	CD-CE-NZ	6.03	125.56	111.70
2	C	1209	GLN	N-CA-CB	-6.02	99.76	110.60
3	D	342	LEU	CB-CG-CD1	-6.02	100.77	111.00
3	D	40	LYS	N-CA-CB	6.01	121.42	110.60
3	D	574	VAL	CB-CA-C	-6.01	99.98	111.40
2	C	732	ILE	CG1-CB-CG2	-6.01	98.19	111.40
3	D	342	LEU	CB-CG-CD2	-6.00	100.80	111.00
6	F	-1	DC	O3'-P-O5'	6.00	115.41	104.00
3	D	338	PHE	CB-CG-CD2	6.00	125.00	120.80
3	D	355	ILE	CA-CB-CG2	-6.00	98.90	110.90
3	D	245	LEU	CB-CG-CD2	-6.00	100.80	111.00
2	C	581	THR	CA-CB-OG1	5.99	121.58	109.00
3	D	719	PHE	CB-CG-CD1	5.99	124.99	120.80
2	C	1088	ASP	CB-CG-OD2	5.98	123.68	118.30
2	C	875	ALA	CB-CA-C	-5.98	101.13	110.10
3	D	539	SER	C-N-CA	-5.97	109.76	122.30
2	C	1192	GLU	CB-CA-C	-5.97	98.46	110.40
3	D	351	GLY	C-N-CA	-5.97	106.78	121.70
2	C	575	LEU	CD1-CG-CD2	5.96	128.39	110.50
3	D	61	ILE	CG1-CB-CG2	-5.96	98.28	111.40
2	C	688	GLN	CA-CB-CG	-5.96	100.28	113.40
2	C	1245	ALA	N-CA-C	5.96	127.10	111.00
2	C	1067	ALA	N-CA-CB	-5.96	101.75	110.10
2	C	1266	GLY	C-N-CA	-5.96	109.78	122.30
2	C	1323	PHE	CB-CG-CD2	-5.96	116.63	120.80
3	D	342	LEU	N-CA-CB	5.96	122.32	110.40
3	D	452	LEU	CA-CB-CG	-5.96	101.59	115.30
3	D	1141	VAL	CA-CB-CG1	-5.96	101.96	110.90
2	C	1049	ILE	CG1-CB-CG2	-5.95	98.31	111.40
2	C	672	GLU	CB-CA-C	-5.95	98.51	110.40
2	C	515	MET	CA-CB-CG	-5.94	103.19	113.30
2	C	397	LEU	CB-CG-CD2	-5.93	100.92	111.00
3	D	903	LEU	N-CA-C	-5.93	94.99	111.00
3	D	361	LEU	CB-CG-CD2	-5.93	100.92	111.00
3	D	345	LYS	N-CA-C	-5.92	95.02	111.00
2	C	1096	ILE	CB-CA-C	5.92	123.43	111.60
3	D	466	MET	CB-CG-SD	-5.91	94.66	112.40
3	D	457	TYR	CD1-CE1-CZ	-5.91	114.48	119.80
3	D	437	PHE	CE1-CZ-CE2	-5.91	109.37	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	179	TYR	CB-CG-CD2	-5.91	117.46	121.00
2	C	866	ASP	CB-CG-OD1	5.91	123.61	118.30
2	C	194	LEU	CB-CG-CD2	5.90	121.04	111.00
1	A	51	MET	N-CA-CB	5.90	121.22	110.60
3	D	1141	VAL	CG1-CB-CG2	-5.90	101.46	110.90
5	M	146	ASP	CB-CG-OD2	5.90	123.61	118.30
2	C	653	MET	CB-CA-C	-5.89	98.61	110.40
3	D	773	PHE	CB-CG-CD1	5.89	124.92	120.80
2	C	578	TYR	CG-CD2-CE2	5.89	126.01	121.30
3	D	355	ILE	CG1-CB-CG2	-5.88	98.47	111.40
2	C	1246	ARG	CG-CD-NE	5.88	124.14	111.80
3	D	487	THR	CA-CB-CG2	-5.87	104.18	112.40
2	C	133	ASN	N-CA-CB	-5.86	100.05	110.60
2	C	651	ASP	CB-CG-OD1	-5.86	113.03	118.30
2	C	1114	GLU	CG-CD-OE1	5.85	130.00	118.30
1	A	76	GLU	OE1-CD-OE2	5.84	130.31	123.30
3	D	552	ILE	CG1-CB-CG2	-5.84	98.55	111.40
3	D	421	VAL	CG1-CB-CG2	-5.84	101.55	110.90
2	C	547	VAL	CA-CB-CG2	-5.84	102.14	110.90
2	C	124	MET	CB-CG-SD	-5.84	94.89	112.40
1	A	98	VAL	CA-CB-CG1	-5.83	102.15	110.90
1	A	234	LEU	CB-CG-CD1	-5.83	101.08	111.00
1	A	62	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	88	LEU	CB-CG-CD1	-5.83	101.09	111.00
2	C	687	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	C	1301	ARG	CG-CD-NE	-5.83	99.56	111.80
2	C	1149	TYR	CB-CG-CD2	-5.83	117.50	121.00
3	D	453	VAL	CA-CB-CG2	-5.83	102.16	110.90
2	C	1243	MET	CA-CB-CG	-5.83	103.39	113.30
2	C	1237	HIS	N-CA-CB	-5.83	100.11	110.60
2	C	1323	PHE	CB-CA-C	-5.82	98.76	110.40
2	C	672	GLU	CG-CD-OE2	-5.82	106.66	118.30
2	C	823	VAL	CG1-CB-CG2	5.80	120.18	110.90
3	D	17	PHE	N-CA-CB	-5.80	100.16	110.60
3	D	626	TYR	CB-CG-CD2	5.80	124.48	121.00
2	C	841	ARG	NE-CZ-NH2	-5.80	117.40	120.30
3	D	17	PHE	CB-CA-C	5.79	121.98	110.40
2	C	696	ASP	CB-CG-OD1	-5.79	113.09	118.30
2	C	146	VAL	CB-CA-C	-5.78	100.41	111.40
1	A	72	GLU	CB-CA-C	-5.78	98.84	110.40
2	C	1078	LYS	CD-CE-NZ	5.78	124.99	111.70
3	D	136	GLU	OE1-CD-OE2	-5.77	116.37	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	806	ASP	N-CA-CB	-5.77	100.21	110.60
3	D	886	VAL	CG1-CB-CG2	-5.77	101.67	110.90
2	C	766	ASN	CB-CA-C	5.77	121.93	110.40
6	F	-3	DG	OP1-P-OP2	5.76	128.25	119.60
3	D	123	ARG	NE-CZ-NH2	-5.76	117.42	120.30
3	D	763	PHE	CD1-CG-CD2	5.76	125.78	118.30
3	D	765	GLU	O-C-N	-5.75	113.42	123.20
3	D	895	CYS	CB-CA-C	-5.75	98.89	110.40
2	C	822	VAL	CA-CB-CG1	-5.75	102.27	110.90
3	D	344	GLY	C-N-CA	-5.75	107.33	121.70
2	C	1235	LEU	CB-CG-CD2	5.75	120.77	111.00
3	D	468	VAL	CG1-CB-CG2	-5.75	101.71	110.90
2	C	9	LYS	CD-CE-NZ	-5.74	98.50	111.70
1	A	182	ARG	O-C-N	5.73	131.87	122.70
2	C	708	VAL	CA-CB-CG2	-5.72	102.32	110.90
2	C	929	ILE	N-CA-CB	-5.71	97.67	110.80
2	C	1069	ARG	CA-CB-CG	-5.71	100.84	113.40
3	D	332	LYS	CB-CA-C	5.71	121.82	110.40
3	D	446	ALA	CB-CA-C	-5.71	101.54	110.10
3	D	916	GLY	CA-C-N	-5.70	104.66	117.20
1	B	44	ARG	NE-CZ-NH1	-5.70	117.45	120.30
2	C	886	LYS	CB-CA-C	5.70	121.80	110.40
3	D	878	ASP	CB-CG-OD2	5.70	123.43	118.30
3	D	268	LEU	CD1-CG-CD2	-5.70	93.41	110.50
2	C	932	GLN	CB-CG-CD	-5.69	96.81	111.60
2	C	1223	ARG	CB-CG-CD	-5.69	96.81	111.60
2	C	1244	HIS	C-N-CA	-5.68	107.49	121.70
3	D	544	LEU	CA-CB-CG	5.68	128.37	115.30
3	D	1246	VAL	CB-CA-C	-5.68	100.60	111.40
2	C	827	ARG	CD-NE-CZ	5.68	131.55	123.60
2	C	130	MET	CG-SD-CE	5.67	109.27	100.20
2	C	788	SER	CB-CA-C	5.67	120.87	110.10
2	C	12	ARG	CD-NE-CZ	-5.66	115.67	123.60
1	B	26	VAL	CG1-CB-CG2	-5.66	101.84	110.90
3	D	541	LEU	CB-CG-CD1	5.66	120.62	111.00
2	C	520	PRO	CA-CB-CG	-5.65	93.26	104.00
3	D	361	LEU	N-CA-C	5.64	126.23	111.00
3	D	140	TYR	CB-CG-CD2	-5.64	117.62	121.00
3	D	1325	PHE	CB-CG-CD2	5.64	124.75	120.80
3	D	132	LEU	CA-CB-CG	5.64	128.26	115.30
2	C	673	HIS	N-CA-CB	-5.63	100.46	110.60
2	C	445	ILE	CB-CA-C	-5.63	100.35	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	220	ARG	CG-CD-NE	5.62	123.61	111.80
2	C	38	PHE	CB-CG-CD2	5.62	124.73	120.80
3	D	99	ARG	CG-CD-NE	-5.62	100.01	111.80
1	B	45	ARG	NE-CZ-NH2	-5.61	117.49	120.30
2	C	578	TYR	CB-CG-CD1	5.61	124.36	121.00
3	D	807	LEU	O-C-N	-5.61	113.73	122.70
3	D	1244	GLN	N-CA-CB	5.61	120.69	110.60
3	D	797	THR	OG1-CB-CG2	-5.60	97.12	110.00
3	D	306	LEU	CB-CG-CD1	-5.60	101.48	111.00
3	D	85	CYS	CA-CB-SG	5.60	124.08	114.00
2	C	765	ILE	N-CA-CB	5.59	123.65	110.80
3	D	1337	VAL	CG1-CB-CG2	5.58	119.83	110.90
3	D	1325	PHE	CG-CD1-CE1	5.57	126.93	120.80
3	D	802	ASP	OD1-CG-OD2	-5.56	112.73	123.30
2	C	1231	TYR	N-CA-C	-5.56	95.99	111.00
2	C	555	TYR	CG-CD2-CE2	-5.55	116.86	121.30
3	D	759	ILE	CG1-CB-CG2	-5.55	99.19	111.40
3	D	352	ARG	NE-CZ-NH1	5.55	123.07	120.30
2	C	836	LEU	CB-CG-CD2	-5.54	101.57	111.00
2	C	155	VAL	CG1-CB-CG2	-5.54	102.03	110.90
2	C	1281	TYR	CB-CA-C	-5.54	99.32	110.40
3	D	784	ALA	CB-CA-C	5.53	118.39	110.10
3	D	764	ARG	NH1-CZ-NH2	5.52	125.48	119.40
1	A	182	ARG	CB-CA-C	-5.52	99.37	110.40
2	C	442	VAL	CA-CB-CG1	-5.51	102.63	110.90
1	B	230	ALA	CB-CA-C	-5.51	101.83	110.10
2	C	685	MET	CA-CB-CG	5.51	122.67	113.30
1	A	89	ALA	N-CA-CB	5.51	117.81	110.10
2	C	1177	ARG	NE-CZ-NH1	-5.50	117.55	120.30
3	D	344	GLY	O-C-N	-5.50	113.90	122.70
2	C	15	PHE	CZ-CE2-CD2	5.50	126.70	120.10
3	D	349	TYR	CB-CA-C	-5.49	99.42	110.40
2	C	731	ARG	NE-CZ-NH2	5.49	123.05	120.30
3	D	359	PRO	N-CA-CB	5.49	109.89	103.30
3	D	808	VAL	CA-CB-CG1	5.49	119.14	110.90
2	C	506	PHE	CB-CG-CD2	5.48	124.64	120.80
2	C	558	VAL	CA-CB-CG1	-5.48	102.68	110.90
3	D	501	VAL	CA-CB-CG1	-5.48	102.68	110.90
2	C	1273	MET	N-CA-CB	-5.48	100.74	110.60
2	C	1067	ALA	CB-CA-C	-5.47	101.89	110.10
3	D	57	PHE	CB-CA-C	5.47	121.33	110.40
3	D	911	LYS	CD-CE-NZ	5.46	124.27	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1107	MET	CA-C-O	5.46	131.57	120.10
2	C	1081	PRO	N-CA-CB	-5.46	96.60	102.60
3	D	478	LEU	CB-CG-CD2	-5.46	101.72	111.00
3	D	839	VAL	CB-CA-C	-5.46	101.03	111.40
3	D	1310	THR	CA-CB-CG2	-5.46	104.76	112.40
2	C	816	ILE	CB-CA-C	-5.44	100.71	111.60
3	D	582	ILE	CB-CG1-CD1	-5.44	98.66	113.90
3	D	769	VAL	CB-CA-C	-5.44	101.06	111.40
2	C	771	VAL	CG1-CB-CG2	-5.44	102.20	110.90
2	C	184	LEU	CD1-CG-CD2	-5.43	94.19	110.50
2	C	1314	GLN	CB-CA-C	-5.43	99.53	110.40
2	C	727	VAL	CA-CB-CG1	-5.43	102.75	110.90
2	C	149	LEU	CA-C-N	-5.43	105.26	117.20
3	D	250	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	C	1259	LEU	CA-CB-CG	-5.42	102.82	115.30
3	D	1208	ASP	CB-CG-OD1	5.42	123.18	118.30
6	F	3	DG	C1'-O4'-C4'	-5.42	104.68	110.10
2	C	1263	ALA	CA-C-O	-5.42	108.72	120.10
3	D	1234	VAL	CA-CB-CG1	5.42	119.03	110.90
1	B	203	ILE	CG1-CB-CG2	5.41	123.31	111.40
3	D	571	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	183	ILE	CA-CB-CG1	-5.40	100.74	111.00
6	F	0	DC	C1'-O4'-C4'	-5.40	104.70	110.10
2	C	123	TYR	CB-CG-CD2	-5.40	117.76	121.00
2	C	1054	LEU	N-CA-CB	-5.40	99.61	110.40
2	C	528	ARG	CG-CD-NE	-5.39	100.47	111.80
3	D	1353	VAL	CA-CB-CG1	5.39	118.99	110.90
2	C	1187	PHE	CB-CG-CD1	-5.39	117.03	120.80
3	D	346	ARG	N-CA-C	-5.39	96.46	111.00
2	C	644	LEU	CB-CG-CD2	-5.38	101.85	111.00
2	C	928	VAL	CG1-CB-CG2	-5.38	102.28	110.90
2	C	783	LEU	CB-CG-CD1	-5.38	101.85	111.00
2	C	515	MET	O-C-N	5.38	131.31	122.70
2	C	1221	PHE	N-CA-CB	5.38	120.29	110.60
2	C	525	THR	CA-CB-CG2	-5.38	104.87	112.40
3	D	717	VAL	CG1-CB-CG2	5.38	119.51	110.90
3	D	893	GLY	C-N-CA	-5.38	108.25	121.70
2	C	1058	ARG	NE-CZ-NH2	-5.38	117.61	120.30
3	D	484	MET	CA-CB-CG	-5.38	104.16	113.30
3	D	769	VAL	CA-CB-CG2	5.37	118.96	110.90
3	D	357	VAL	CA-CB-CG1	-5.37	102.85	110.90
3	D	19	ALA	O-C-N	-5.36	114.12	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	538	LEU	CB-CG-CD1	5.36	120.12	111.00
3	D	706	VAL	CG1-CB-CG2	-5.36	102.32	110.90
2	C	10	ARG	CB-CA-C	-5.36	99.68	110.40
3	D	31	ARG	NE-CZ-NH2	-5.36	117.62	120.30
3	D	588	PRO	CB-CG-CD	-5.36	85.61	106.50
2	C	884	VAL	CG1-CB-CG2	-5.35	102.34	110.90
2	C	1041	ASP	CB-CG-OD2	-5.35	113.48	118.30
3	D	894	VAL	CG1-CB-CG2	-5.35	102.34	110.90
3	D	488	ASN	N-CA-CB	5.35	120.23	110.60
3	D	105	ILE	CG1-CB-CG2	-5.34	99.64	111.40
3	D	610	ARG	NH1-CZ-NH2	5.34	125.27	119.40
3	D	583	VAL	CB-CA-C	-5.33	101.28	111.40
2	C	1085	MET	CG-SD-CE	-5.32	91.69	100.20
2	C	1315	MET	CG-SD-CE	-5.32	91.69	100.20
3	D	261	ALA	N-CA-CB	-5.31	102.66	110.10
3	D	796	LEU	CB-CG-CD2	5.31	120.03	111.00
2	C	1188	ASP	CB-CG-OD1	-5.31	113.52	118.30
3	D	95	THR	OG1-CB-CG2	-5.31	97.79	110.00
3	D	511	TYR	CD1-CG-CD2	5.30	123.73	117.90
2	C	586	PHE	CB-CG-CD2	-5.30	117.09	120.80
3	D	807	LEU	CD1-CG-CD2	5.30	126.40	110.50
3	D	1344	LEU	CB-CG-CD1	-5.30	101.99	111.00
2	C	530	ILE	N-CA-C	-5.30	96.69	111.00
6	F	0	DC	C4'-C3'-O3'	-5.30	96.46	109.70
1	A	182	ARG	N-CA-CB	5.29	120.13	110.60
3	D	334	LYS	C-N-CA	5.29	134.93	121.70
1	B	83	LEU	CB-CG-CD2	-5.29	102.01	111.00
2	C	668	ILE	CG1-CB-CG2	5.29	123.04	111.40
3	D	915	ILE	CA-CB-CG1	-5.29	100.95	111.00
3	D	17	PHE	CD1-CE1-CZ	-5.28	113.76	120.10
2	C	75	LEU	CD1-CG-CD2	-5.28	94.67	110.50
3	D	1348	LYS	N-CA-CB	5.28	120.10	110.60
6	F	9	DT	P-O3'-C3'	5.28	126.03	119.70
2	C	588	GLU	CB-CA-C	-5.27	99.85	110.40
3	D	416	ILE	CA-CB-CG1	-5.27	100.98	111.00
3	D	1258	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	C	697	LYS	CD-CE-NZ	-5.26	99.61	111.70
2	C	1042	LEU	CA-CB-CG	5.26	127.39	115.30
3	D	337	ARG	NH1-CZ-NH2	5.26	125.18	119.40
1	A	140	ILE	CA-CB-CG1	-5.25	101.02	111.00
2	C	1107	MET	O-C-N	-5.24	114.31	122.70
3	D	622	ASP	O-C-N	5.24	131.09	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	511	LEU	CB-CG-CD1	5.24	119.90	111.00
3	D	914	ALA	CA-C-O	5.24	131.10	120.10
3	D	1138	LEU	CB-CG-CD2	-5.24	102.09	111.00
2	C	506	PHE	CD1-CE1-CZ	5.24	126.38	120.10
2	C	802	VAL	N-CA-C	-5.24	96.87	111.00
5	M	198	CYS	CA-CB-SG	-5.24	104.58	114.00
2	C	35	PHE	CD1-CG-CD2	5.23	125.10	118.30
4	E	48	VAL	CG1-CB-CG2	-5.23	102.54	110.90
2	C	1046	VAL	CB-CA-C	-5.22	101.47	111.40
2	C	26	TYR	CB-CG-CD2	-5.22	117.87	121.00
2	C	1216	ARG	CD-NE-CZ	-5.22	116.29	123.60
2	C	1088	ASP	CB-CG-OD1	-5.22	113.61	118.30
3	D	442	ILE	CB-CA-C	-5.22	101.17	111.60
1	A	185	TYR	OH-CZ-CE2	-5.21	106.02	120.10
3	D	83	VAL	CG1-CB-CG2	-5.21	102.56	110.90
3	D	492	SER	CA-C-O	-5.21	109.15	120.10
3	D	894	VAL	CB-CA-C	5.21	121.31	111.40
4	E	4	VAL	CG1-CB-CG2	5.21	119.23	110.90
3	D	535	ARG	CG-CD-NE	5.20	122.72	111.80
3	D	915	ILE	CB-CA-C	5.20	122.00	111.60
6	F	12	DT	O5'-P-OP2	5.20	116.94	110.70
2	C	555	TYR	CB-CA-C	5.19	120.78	110.40
4	E	17	PHE	CB-CA-C	-5.19	100.02	110.40
2	C	575	LEU	CB-CA-C	-5.19	100.34	110.20
2	C	578	TYR	CG-CD1-CE1	-5.18	117.16	121.30
1	B	32	GLU	OE1-CD-OE2	-5.17	117.09	123.30
3	D	1156	LEU	CA-CB-CG	5.17	127.19	115.30
3	D	592	VAL	CA-CB-CG1	-5.17	103.15	110.90
2	C	1232	MET	CA-CB-CG	-5.17	104.52	113.30
3	D	423	LEU	CD1-CG-CD2	5.17	126.00	110.50
1	A	45	ARG	NH1-CZ-NH2	5.16	125.08	119.40
2	C	1153	ALA	CA-C-O	-5.16	109.27	120.10
3	D	484	MET	N-CA-C	5.16	124.93	111.00
3	D	808	VAL	CG1-CB-CG2	-5.16	102.64	110.90
6	F	11	DG	C4'-C3'-O3'	-5.16	96.80	109.70
1	B	83	LEU	CB-CG-CD1	-5.16	102.23	111.00
6	F	-3	DG	O4'-C1'-N9	5.15	111.61	108.00
2	C	446	ASP	CB-CG-OD2	-5.15	113.67	118.30
2	C	523	GLU	CA-CB-CG	-5.14	102.09	113.40
4	E	25	ARG	NE-CZ-NH1	-5.14	117.73	120.30
3	D	1365	TYR	O-C-N	-5.13	114.50	122.70
2	C	903	ARG	NE-CZ-NH1	5.13	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	105	ILE	CB-CA-C	5.13	121.85	111.60
3	D	439	PRO	CA-N-CD	-5.12	104.33	111.50
3	D	451	PRO	CA-CB-CG	-5.12	94.27	104.00
2	C	446	ASP	CB-CG-OD1	5.12	122.91	118.30
3	D	551	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	C	2	VAL	CG1-CB-CG2	5.12	119.09	110.90
3	D	188	LEU	CB-CG-CD2	-5.12	102.30	111.00
3	D	811	GLU	CG-CD-OE1	5.12	128.53	118.30
2	C	1114	GLU	OE1-CD-OE2	-5.11	117.17	123.30
3	D	731	ARG	NE-CZ-NH1	5.11	122.85	120.30
3	D	437	PHE	CZ-CE2-CD2	5.10	126.22	120.10
3	D	1223	LEU	CA-CB-CG	5.10	127.03	115.30
3	D	362	ARG	N-CA-CB	-5.10	101.43	110.60
2	C	872	TYR	CB-CG-CD2	5.09	124.06	121.00
3	D	360	TYR	CG-CD1-CE1	-5.09	117.23	121.30
2	C	71	VAL	CG1-CB-CG2	5.09	119.04	110.90
2	C	712	SER	CB-CA-C	-5.08	100.44	110.10
1	B	224	LEU	CD1-CG-CD2	5.08	125.75	110.50
2	C	670	PHE	N-CA-C	5.08	124.72	111.00
2	C	1255	THR	N-CA-CB	5.08	119.95	110.30
3	D	1140	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	C	5	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	B	33	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	C	1232	MET	CG-SD-CE	5.08	108.32	100.20
1	A	146	VAL	CA-CB-CG2	-5.07	103.29	110.90
3	D	555	TYR	CB-CG-CD2	-5.07	117.96	121.00
3	D	1342	ASP	OD1-CG-OD2	-5.07	113.66	123.30
3	D	770	LEU	CB-CG-CD1	-5.07	102.39	111.00
2	C	704	MET	N-CA-C	5.06	124.67	111.00
4	E	17	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	A	150	ARG	C-N-CA	-5.06	111.68	122.30
3	D	601	ILE	CG1-CB-CG2	5.05	122.52	111.40
2	C	1177	ARG	CG-CD-NE	-5.05	101.19	111.80
2	C	1270	PHE	C-N-CA	5.05	132.91	122.30
3	D	298	MET	CB-CG-SD	-5.05	97.24	112.40
3	D	304	ASP	CB-CA-C	-5.05	100.30	110.40
2	C	833	ILE	N-CA-CB	-5.05	99.19	110.80
4	E	45	LYS	CA-CB-CG	5.05	124.50	113.40
3	D	330	MET	CB-CG-SD	5.05	127.54	112.40
2	C	1297	ASP	CB-CG-OD1	5.04	122.84	118.30
3	D	451	PRO	N-CD-CG	-5.04	95.64	103.20
2	C	1112	ILE	CG1-CB-CG2	-5.04	100.32	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	332	LYS	C-N-CA	5.03	132.87	122.30
3	D	889	ASP	N-CA-CB	5.03	119.65	110.60
2	C	145	ILE	CB-CG1-CD1	-5.02	99.83	113.90
2	C	1061	GLN	C-N-CD	5.02	138.94	128.40
2	C	1187	PHE	CG-CD1-CE1	5.01	126.31	120.80
2	C	1294	LYS	CB-CA-C	-5.01	100.37	110.40
3	D	772	TYR	CG-CD1-CE1	5.01	125.31	121.30
3	D	896	ALA	CB-CA-C	-5.01	102.58	110.10
1	A	201	LEU	CB-CG-CD2	-5.01	102.48	111.00
2	C	548	ARG	CG-CD-NE	5.01	122.32	111.80
3	D	363	LEU	CA-CB-CG	-5.01	103.78	115.30
2	C	605	TYR	CB-CG-CD1	-5.00	118.00	121.00
2	C	1325	VAL	CG1-CB-CG2	-5.00	102.90	110.90
3	D	605	LEU	CB-CA-C	-5.00	100.70	110.20

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

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Mol	Chain	Res	Type	Group
2	C	709	ALA	Mainchain
2	C	788	SER	Mainchain
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2302	0	2266	94	0
1	B	1733	0	1720	80	0
2	C	10034	0	9668	444	0
3	D	9790	0	9539	583	0
4	E	565	0	563	27	0
5	M	2002	0	1412	62	0
6	F	944	0	513	99	0
7	G	946	0	518	42	0
All	All	28316	0	26199	1305	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 24.

All (1305) 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:1066:MET:CE	2:C:1232:MET:HE2	1.31	1.53
2:C:1260:GLY:CA	3:D:346:ARG:HH12	1.20	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
2:C:1066:MET:HE2	2:C:1232:MET:CE	1.51	1.40
2:C:1260:GLY:HA2	3:D:346:ARG:NH1	1.34	1.40
3:D:462:ASP:CB	3:D:462:ASP:CG	1.90	1.39
3:D:316:ILE:HD12	3:D:317:THR:N	1.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:1260:GLY:C	3:D:346:ARG:HH12	1.55	1.07
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
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
2:C:1066:MET:HE1	2:C:1232:MET:HE2	1.39	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
2:C:1260:GLY:C	3:D:346:ARG:NH1	2.14	0.98
5:M:376:MET:HE1	6:F:11:DG:C5'	1.93	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
5:M:376:MET:HE1	6:F:11:DG:H5"	0.97	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:1066:MET:HE2	2:C:1232:MET:HE2	0.97	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
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
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:1243:MET:HE1	3:D:445:LYS:HG2	1.51	0.90
2:C:685:MET:CE	2:C:1073:LYS:HD3	2.02	0.90
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
2:C:1176:LEU:C	2:C:1176:LEU:HD12	1.94	0.86
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:685:MET:HE1	2:C:1073:LYS:HD3	1.64	0.77
7:G:-7:DA:H4'	7:G:-7:DA:OP1	1.84	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
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
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
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: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
3:D:92:VAL:HG12	3:D:93:THR:N	2.03	0.73
3:D:117:LEU:O	3:D:118:LYS:CB	2.34	0.73
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:530:PRO:HB2	3:D:531:LYS:C	2.08	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
2:C:1066:MET:HE2	2:C:1232:MET:HE1	1.69	0.72
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:316:ILE:CD1	3:D:317:THR:C	2.59	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
2:C:685:MET:HE2	2:C:1073:LYS:HD3	1.73	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:348:ASP:O	3:D:349:TYR:C	2.30	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:531:LYS:HB3	3:D:581:MET:HE1	1.73	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
7:G:8:DA:C2'	7:G:9:DT:C7	2.70	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:M:168:ASP:O	5:M:169:GLU:CB	2.41	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
5:M:190:VAL:O	5:M:191:ALA:HB3	1.93	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
2:C:1176:LEU:HD12	2:C:1176:LEU:O	1.93	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
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:261:ALA:C	6:F:6:DT:H72	2.15	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
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)
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: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
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: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
3:D:316:ILE:HD12	3:D:317:THR:C	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:M:376:MET:CE	6:F:11:DG:C5'	2.62	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
3:D:130:MET:CE	3:D:157:GLN:HB3	2.30	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
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:843:VAL:HG12	3:D:844:THR:N	2.15	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: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
3:D:584:PRO:O	3:D:585:LYS: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
4:E:14:GLY:O	4:E:15:ASN:C	2.36	0.60
3:D:316:ILE:CD1	3:D:317:THR:CA	2.59	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:540:ARG:C	2:C:542:ARG:H	2.05	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
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: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
2:C:136:PHE:HE2	2:C:145:ILE:HD12	1.67	0.59
3:D:227:PHE:CZ	3:D:237:MET:HE1	2.38	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
3:D:71:LEU:HD12	3:D:71:LEU:C	2.22	0.59
2:C:796:LEU:N	2:C:1231:TYR:OH	2.36	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:130:MET:HE2	3:D:157:GLN:HB3	1.85	0.58
3:D:227:PHE:HZ	3:D:237:MET:HE2	1.66	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
2:C:1085:MET:HE2	2:C:1094:VAL:O	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:1304:MET:HE1	2:C:1315:MET:HA	1.86	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
1:B:27:THR:C	1:B:28:LEU:HD12	2.24	0.57
3:D:138:VAL:HG12	3:D:143:SER:HB2	1.86	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:716:GLN:HG2	3:D:717:VAL:N	2.20	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
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: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: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:B:104:LYS:HD3	1:B:110:VAL:HG22	1.87	0.55
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
1:A:252:ILE:HG22	1:A:252:ILE:O	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:373:ALA:C	3:D:375:GLU:H	2.09	0.55
3:D:474:LEU:HD12	4:E:28:ARG:HE	1.72	0.55
3:D:1321:SER:C	3:D:1323:ALA:H	2.10	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
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
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: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:341:ASN:O	3:D:342:LEU:C	2.41	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:841:GLY:O	3:D:842:ARG:HB2	2.07	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
3:D:885:VAL:C	3:D:887:SER:H	2.12	0.53
6:F:12:DT:H2"	6:F:13:DG:H5"	1.90	0.53
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.43	0.53
3:D:902:ASP:C	3:D:903:LEU:O	2.44	0.53
3:D:915:ILE:HD13	3:D:918:ILE:HD12	1.89	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
2:C:130:MET:HE2	2:C:134:GLY:HA2	1.89	0.53
2:C:1254:VAL:O	2:C:1255:THR:OG1	2.19	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:765:GLU:O	3:D:766:GLY:C	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:1066:MET:HE3	2:C:1232:MET:CE	2.29	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
2:C:918:LEU:O	2:C:919:ARG:C	2.46	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:546:GLU:HG2	2:C:547:VAL:N	2.24	0.52
2:C:548:ARG:HD3	2:C:569:ILE:HG23	1.92	0.52
3:D:138:VAL:HB	3:D:145:VAL:CG2	2.40	0.52
3:D:180:MET:HE1	3:D:293:ARG:HD2	1.92	0.52
3:D:546:ALA:O	3:D:547:ARG:C	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:551:ARG:C	3:D:552:ILE:HG13	2.29	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:130:ILE:O	1:A:131:CYS:C	2.46	0.51
1:A:231:PHE:CE2	1:B:39:LEU:HD23	2.46	0.51
2:C:64:GLY:C	2:C:66:SER:H	2.14	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:1263:LYS:HB2	3:D:1307:LEU:HD21	1.93	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
3:D:890:THR:HG23	3:D:891:ASP:N	2.26	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:333:GLY:N	3:D:333:GLY:C	2.57	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:1176:LEU:C	2:C:1176:LEU:CD1	2.74	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:51:MET:HE3	1:A:52:PRO:HD2	1.93	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
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:346:TYR:C	2:C:348:SER:H	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:M:376:MET:HE2	6:F:11:DG:H5"	1.84	0.49
1:A:100:LEU:HD12	1:A:100:LEU:C	2.33	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: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
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
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: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:116:PHE:HE1	3:D:1333:THR:HG22	1.77	0.48
3:D:839:VAL:O	3:D:839:VAL:CG1	2.50	0.48
3:D:1239:ASP:OD1	3:D:1242:ARG:NH1	2.46	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:47:LEU:HD23	1:B:51:MET:HE2	1.94	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
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
5:M:167:ASP:O	5:M:168:ASP:CB	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:C:159:SER:C	2:C:161:LYS:H	2.17	0.47
3:D:1319:PHE:HB3	3:D:1340:LYS:HD2	1.97	0.47
4:E:16:ARG:O	4:E:17:PHE:C	2.48	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
2:C:662:SER:O	2:C:666:SER:OG	2.15	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
3:D:884:SER:C	3:D:885:VAL:O	2.48	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: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
3:D:929:GLN:O	3:D:929:GLN:HG3	2.15	0.47
5:M:133:PHE:HE1	5:M:181:ARG:HD3	1.80	0.47
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
2:C:452:ARG:HH21	2:C:452:ARG:HD3	1.43	0.46
2:C:800:MET:HE1	2:C:827:ARG:HD3	1.97	0.46
3:D:114:ILE:HG12	3:D:311:ARG:HG3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:30:ILE:HD12	2:C:575:LEU:HD11	1.97	0.46
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:1223:LEU:HD12	3:D:1224:ARG:N	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1247:SER:OG	2:C:1248:THR:N	2.48	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:31:GLN:HB3	2:C:130:MET:HE3	1.98	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: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
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:531:LYS:HB3	3:D:581:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:137:VAL:HA	2:C:141:THR:O	2.16	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:830:THR:HG22	2:C:1234:LYS:HZ1	1.81	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: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
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: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:1321:SER:C	3:D:1323:ALA:N	2.69	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:1:MET:C	2:C:3:TYR:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1267:GLY:CA	3:D:347:VAL:O	2.59	0.44
1:A:158:ARG:HH22	1:A:173:VAL:H	1.65	0.44
2:C:1259:LEU:O	2:C:1266:GLY:HA2	2.18	0.44
3:D:472:LEU:N	3:D:472:LEU:HD12	2.33	0.44
5:M:106:ASP:CG	5:M:107:ASP:H	2.20	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
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:530:PRO:CB	3:D:531:LYS:C	2.84	0.44
3:D:813:ASP:OD1	3:D:814:CYS:N	2.51	0.44
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:26:SER:H	3:D:29:MET:HE3	1.82	0.44
3:D:362:ARG:O	3:D:363:LEU:C	2.55	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:1219:ASP:O	3:D:1223:LEU:HG	2.18	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
7:G:13:DG:C2'	7:G:14:DT:H72	2.48	0.44
2:C:540:ARG:C	2:C:542:ARG:N	2.71	0.44
3:D:71:LEU:CD1	3:D:71:LEU:C	2.86	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:914:ALA:C	3:D:916:GLY:H	2.21	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
3:D:338:PHE:HZ	3:D:798:ARG:CZ	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1195:ILE:HD13	2:C:1195:ILE:HG21	1.69	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
1:B:5:VAL:C	1:B:7:GLU:H	2.23	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
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
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
1:B:19:VAL:O	1:B:20:SER:OG	2.35	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:103:GLY:C	3:D:244:VAL:HG22	2.39	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:1177:ILE:C	3:D:1179:PRO:HD3	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
3:D:893:GLY:O	3:D:894:VAL:CB	2.52	0.42
3:D:925:GLU:CD	3:D:926:PRO:HD3	2.27	0.42
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
1:B:9:LEU:C	1:B:10:LYS:HD2	2.39	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
4:E:15:ASN:O	4:E:16:ARG:C	2.57	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:342:LEU:C	3:D:344:GLY:N	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:1304:MET:HE1	3:D:473:THR:CG2	2.50	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
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:31:GLN:C	2:C:130:MET:HE1	2.41	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:A:192:VAL:C	1:A:194:GLN:H	2.24	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: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: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
3:D:1271:SER:O	3:D:1272:SER:OG	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1314:LEU:HA	3:D:1322:ALA:HB1	2.01	0.41
6:F:10:DC:H3'	6:F:10:DC:OP2	2.20	0.41
2:C:31:GLN:HB3	2:C:130:MET:HE1	2.03	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: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
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:893:GLY:O	3:D:894:VAL:C	2.53	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
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: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: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
3:D:889:ASP:CB	3:D:895:CYS:HG	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1334:GLY:C	3:D:25:ALA:HB3	2.41	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
2:C:660:VAL:CG2	2:C:661:VAL:N	2.83	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
3:D:227:PHE:CZ	3:D:237:MET:HE2	2.46	0.41
3:D:339:ARG:C	3:D:340:GLN:HG2	2.41	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
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
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:354:VAL:C	3:D:355:ILE:HD13	2.41	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:709:ARG:C	3:D:711:GLY:H	2.25	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
1:A:103:ASN:O	1:A:104:LYS:HB2	2.22	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
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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	12 39
1	B	233/329 (71%)	209 (90%)	22 (9%)	2 (1%)	17 49
2	C	1339/1342 (100%)	1183 (88%)	128 (10%)	28 (2%)	7 30
3	D	1335/1407 (95%)	1127 (84%)	169 (13%)	39 (3%)	4 24
4	E	73/91 (80%)	68 (93%)	3 (4%)	2 (3%)	5 26
5	M	283/497 (57%)	236 (83%)	40 (14%)	7 (2%)	5 26
All	All	3568/3995 (89%)	3092 (87%)	394 (11%)	82 (2%)	9 28

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
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

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Mol	Chain	Res	Type
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
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 (i)

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%)	241 (99%)	3 (1%)	71 85
1	B	183/286 (64%)	178 (97%)	5 (3%)	44 70
2	C	1029/1157 (89%)	1003 (98%)	26 (2%)	47 72
3	D	961/1168 (82%)	925 (96%)	36 (4%)	34 62
4	E	56/75 (75%)	55 (98%)	1 (2%)	59 79
5	M	113/393 (29%)	113 (100%)	0	100 100
All	All	2586/3365 (77%)	2515 (97%)	71 (3%)	48 70

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	96	ASP
1	A	213	PRO
1	B	6	THR
1	B	16	ILE
1	B	33	ARG
1	B	45	ARG
1	B	224	LEU
2	C	8	LYS
2	C	18	ARG
2	C	149	LEU
2	C	184	LEU
2	C	388	LEU
2	C	521	LEU
2	C	552	PRO
2	C	555	TYR
2	C	564	PRO
2	C	639	LYS
2	C	697	LYS
2	C	719	LYS
2	C	727	VAL
2	C	773	LEU

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Mol	Chain	Res	Type
2	C	821	ARG
2	C	827	ARG
2	C	929	ILE
2	C	1049	ILE
2	C	1096	ILE
2	C	1151	LEU
2	C	1180	MET
2	C	1224	PRO
2	C	1232	MET
2	C	1239	VAL
2	C	1243	MET
2	C	1319	MET
3	D	7	PHE
3	D	27	PRO
3	D	28	ASP
3	D	70	CYS
3	D	78	LEU
3	D	93	THR
3	D	120	LEU
3	D	132	LEU
3	D	188	LEU
3	D	249	LEU
3	D	252	LEU
3	D	271	ARG
3	D	311	ARG
3	D	316	ILE
3	D	330	MET
3	D	352	ARG
3	D	366	CYS
3	D	368	LEU
3	D	379	PRO
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	788	LEU

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Mol	Chain	Res	Type
3	D	886	VAL
3	D	987	GLU
3	D	1138	LEU
3	D	1309	ILE
3	D	1347	LEU
3	D	1351	VAL
4	E	6	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	103	ASN
1	A	132	HIS
1	A	294	ASN
1	B	23	HIS
2	C	65	ASN
2	C	165	HIS
2	C	513	GLN
2	C	519	ASN
2	C	526	HIS
2	C	554	HIS
2	C	604	HIS
2	C	688	GLN
2	C	799	ASN
2	C	1080	ASN
2	C	1136	GLN
2	C	1175	ASN
2	C	1244	HIS
2	C	1268	GLN
3	D	157	GLN
3	D	450	HIS
3	D	560	ASN
3	D	792	ASN
3	D	897	HIS
3	D	907	HIS
3	D	1238	GLN
3	D	1366	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

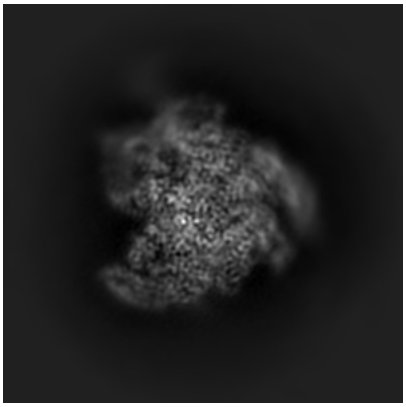
6 Map visualisation

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.

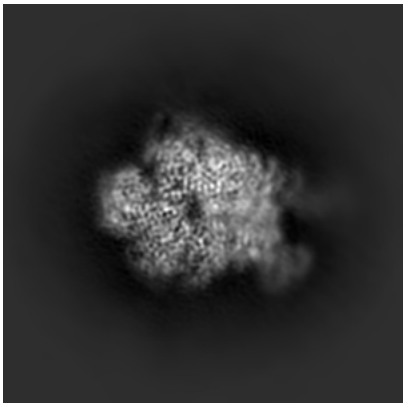
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

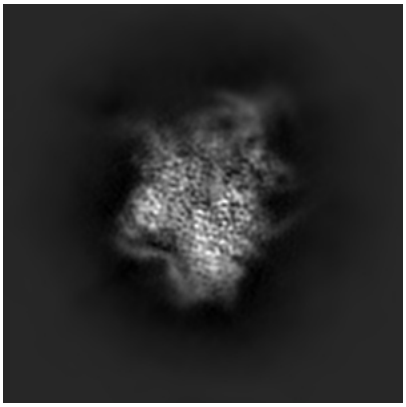
6.1.1 Primary map



X



Y

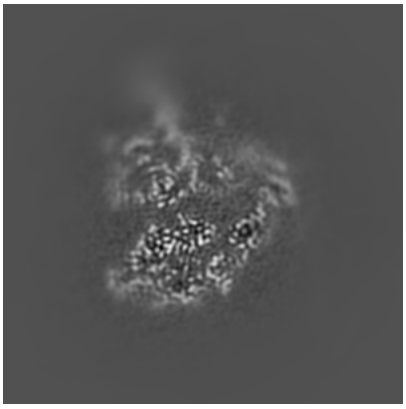


Z

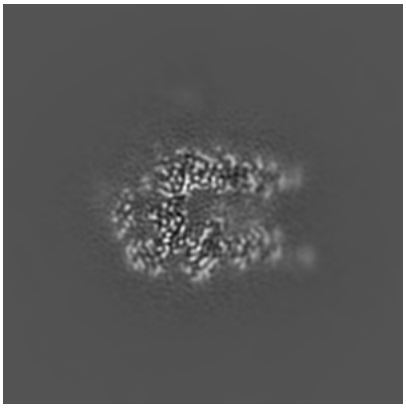
The images above show the map projected in three orthogonal directions.

6.2 Central slices

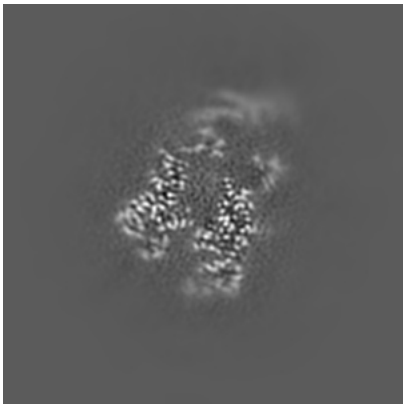
6.2.1 Primary map



X Index: 128



Y Index: 128

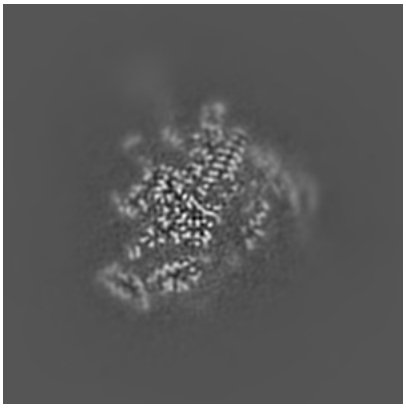


Z Index: 128

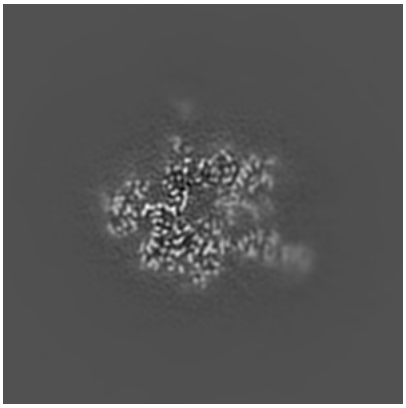
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

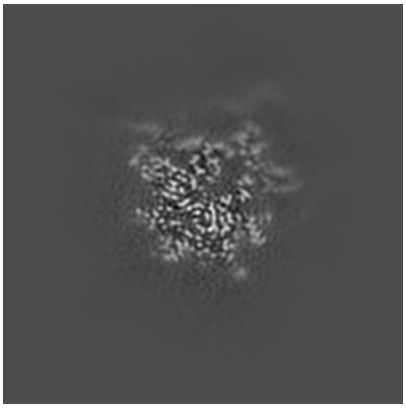
6.3.1 Primary map



X Index: 140



Y Index: 122

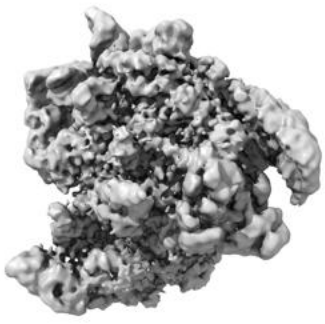


Z Index: 108

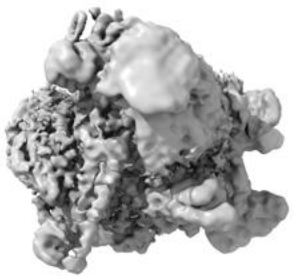
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

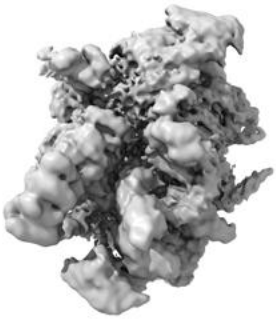
6.4.1 Primary map



X



Y



Z

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.

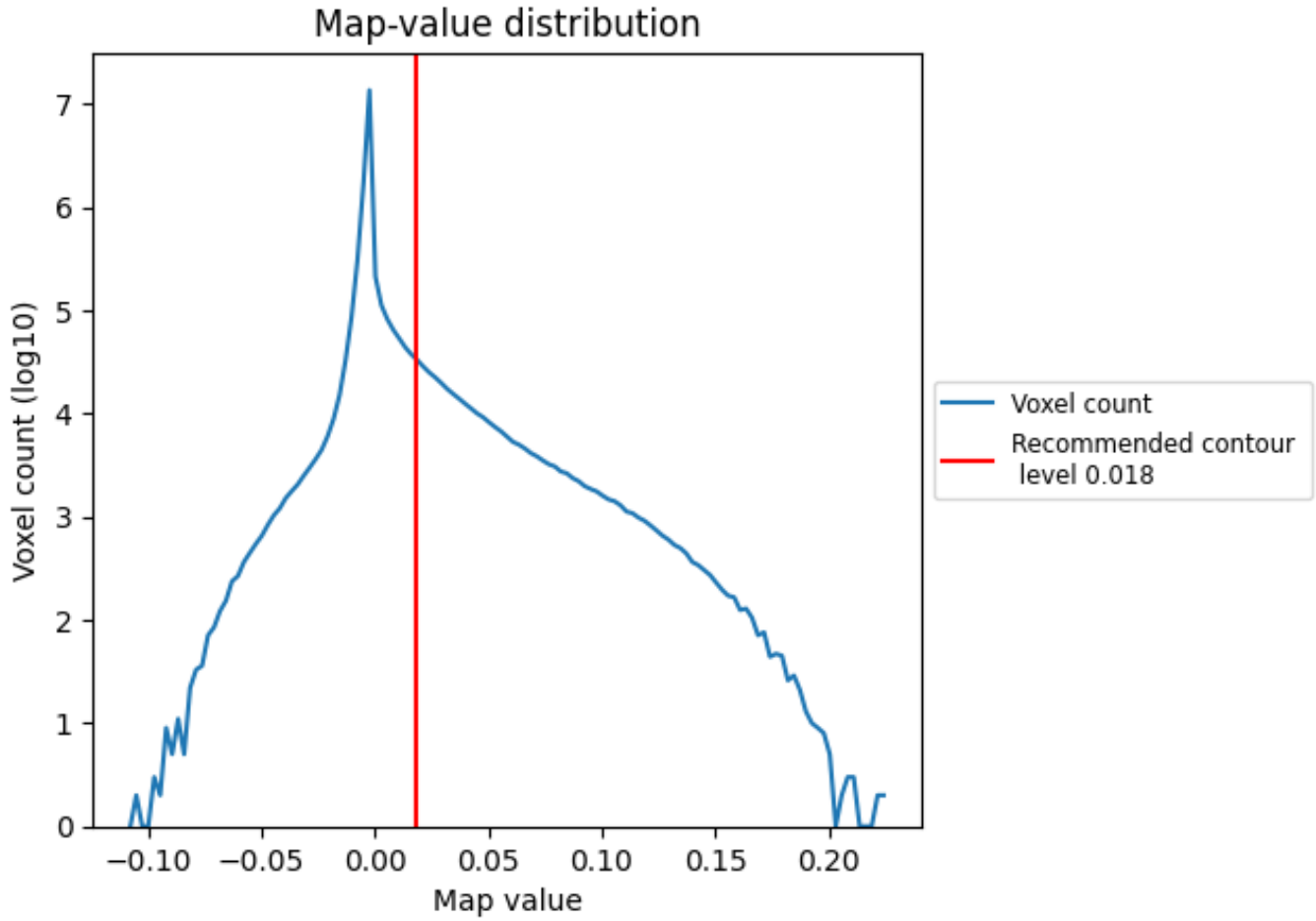
6.5 Mask visualisation (i)

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

7 Map analysis

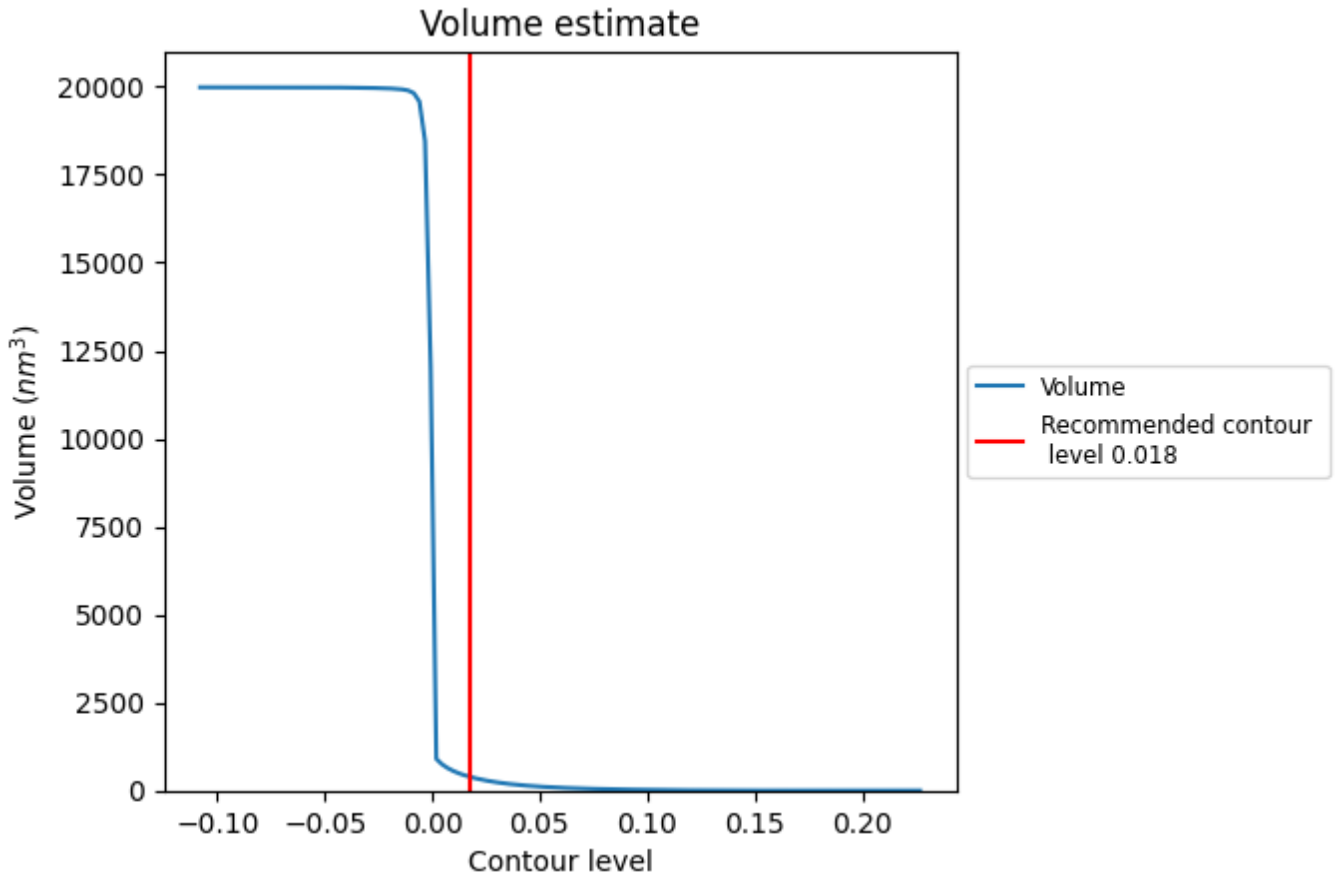
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

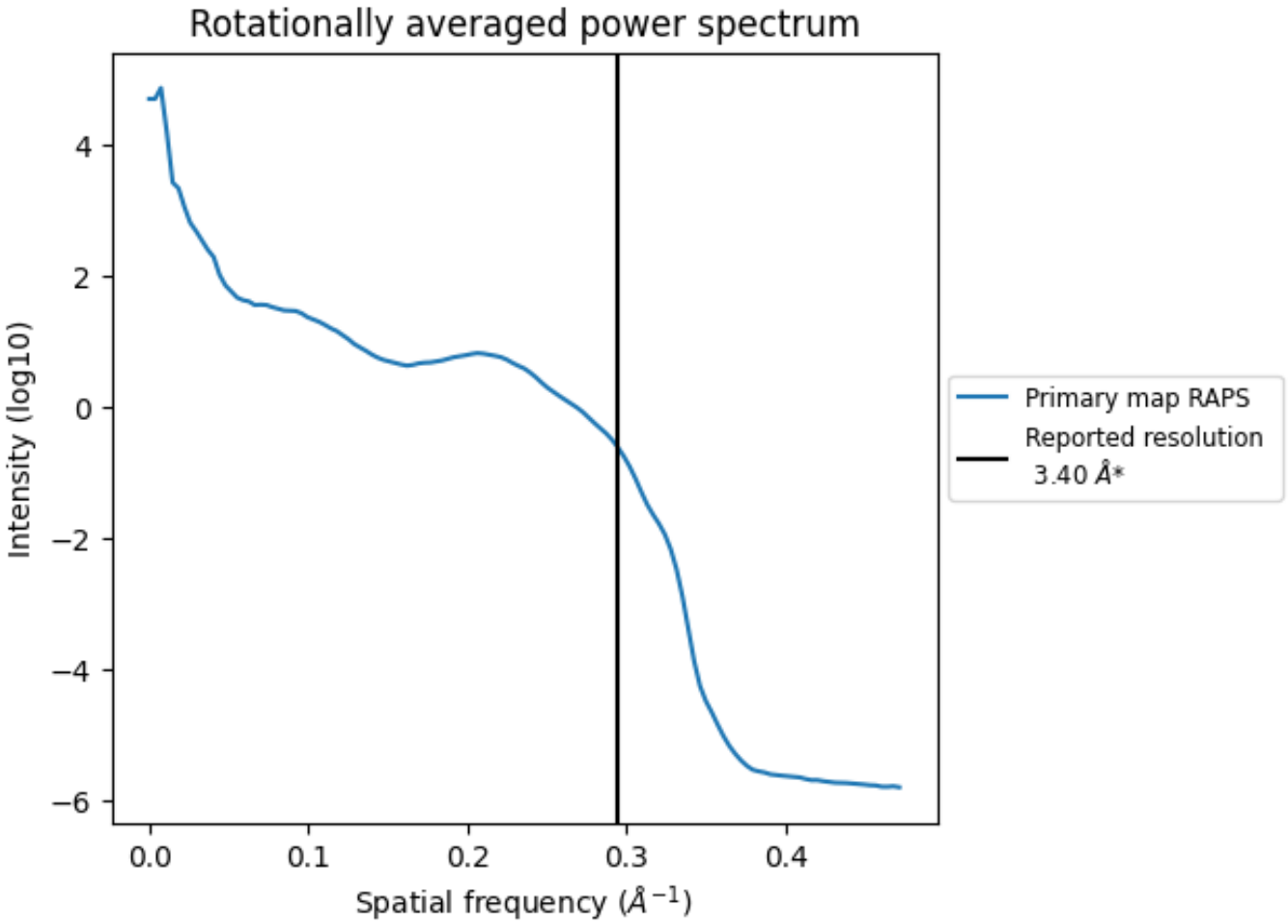
7.2 Volume estimate



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 (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

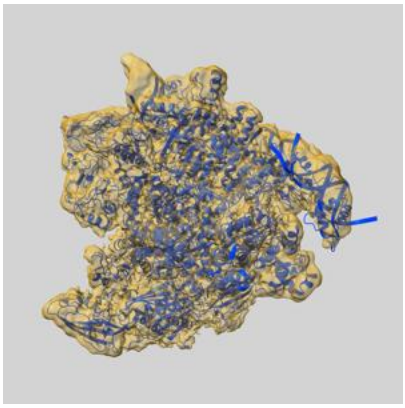
8 Fourier-Shell correlation

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

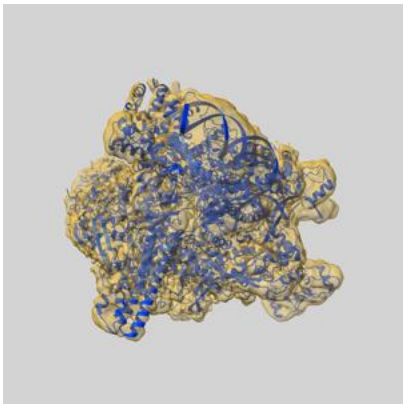
9 Map-model fit

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 5.

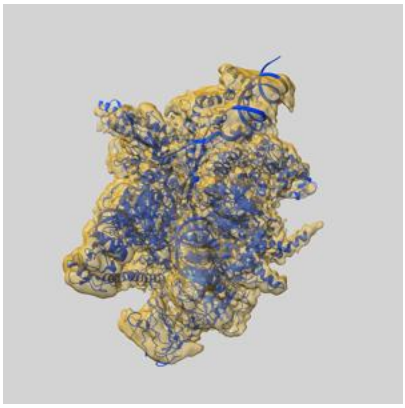
9.1 Map-model overlay



X



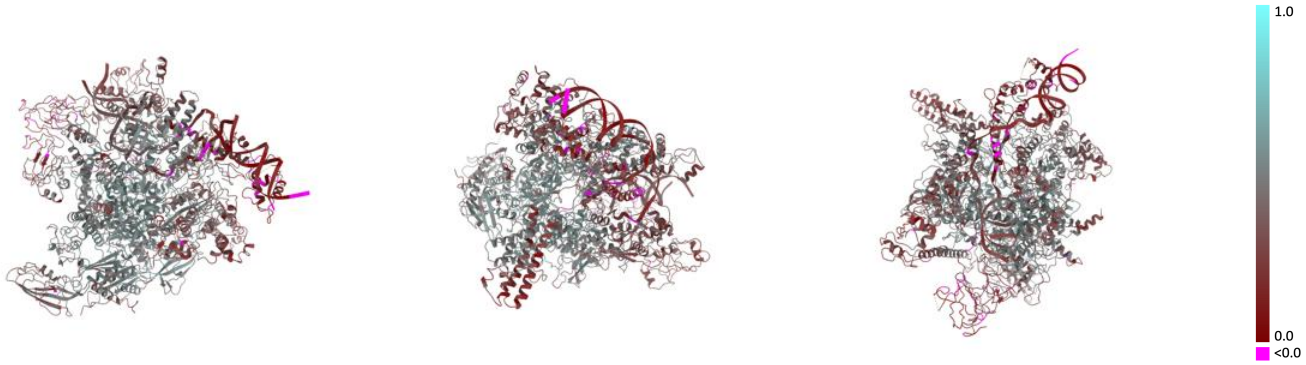
Y



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.

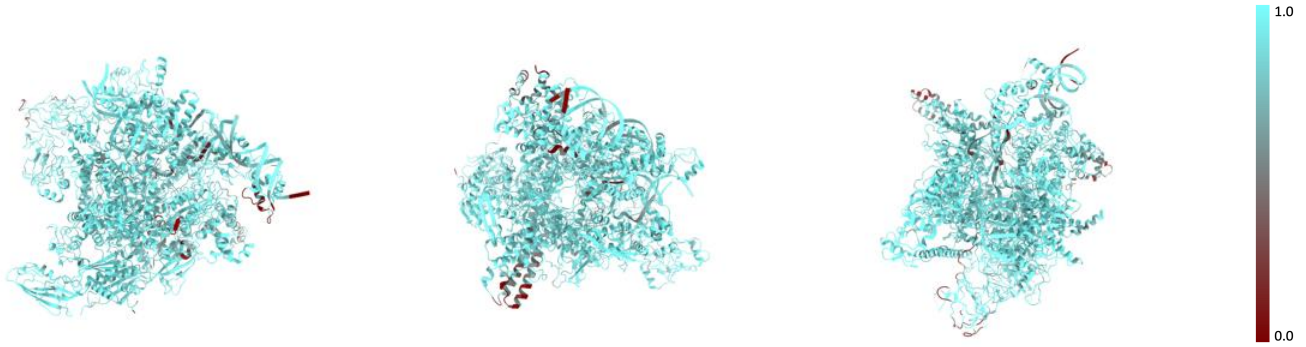
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

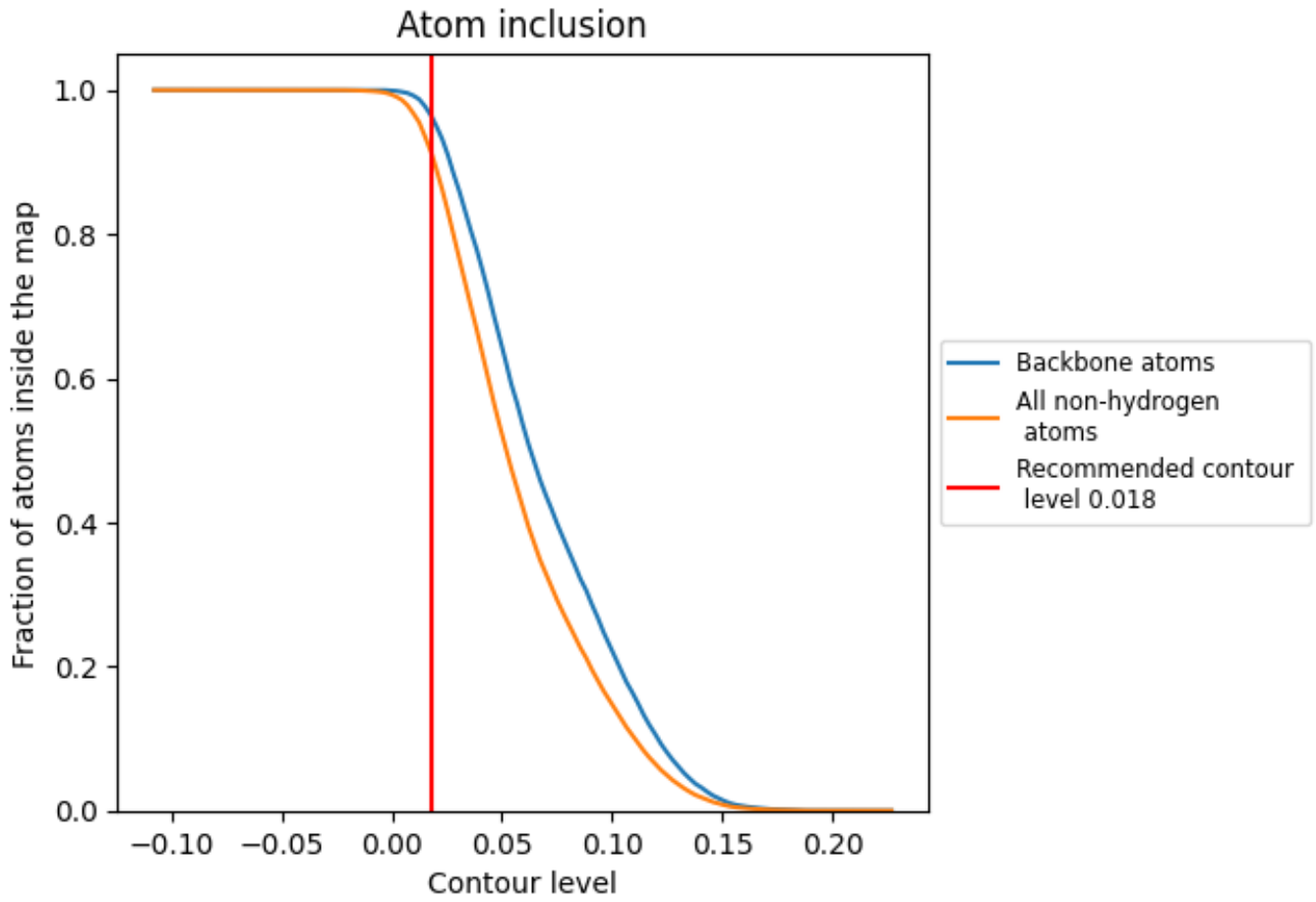
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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	0.9124	0.4120
A	0.8806	0.4420
B	0.9367	0.4200
C	0.9279	0.4460
D	0.9209	0.4290
E	0.9399	0.4620
F	0.7722	0.1950
G	0.8446	0.2120
M	0.9009	0.3010