



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:39 PM UTC

PDB ID : 7R4R / pdb_00007r4r
EMDB ID : EMD-14315
Title : The SARS-CoV-2 spike in complex with the 1.10 neutralizing nanobody
Authors : Casasnovas, J.M.; Melero, R.; Arranz, R.; Fernandez, L.A.
Deposited on : 2022-02-09
Resolution : 3.90 Å (reported)
Based on initial models : 1ZV5, 6ZXN

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

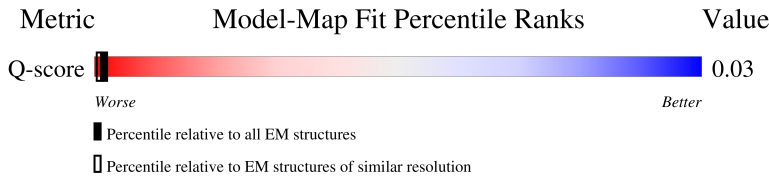
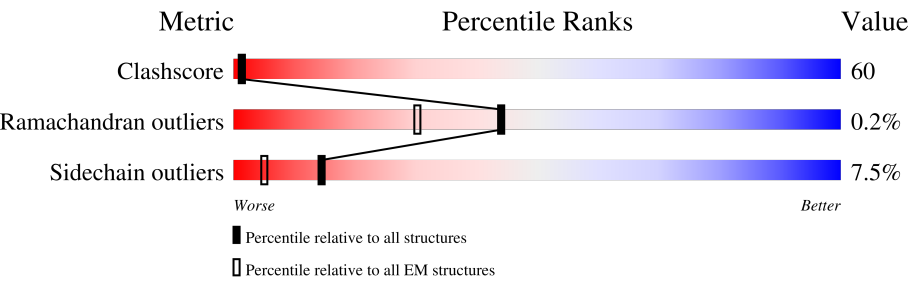
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



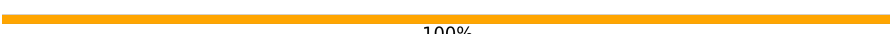
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1264	9% 28% 43% 9% 16%
1	B	1264	11% 27% 44% 9% 17%
1	C	1264	10% 27% 44% 10% 16%
2	D	124	66% 44% 47% 6%

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Mol	Chain	Length	Quality of chain
3	E	2	 50%50%
3	F	2	 50%100%
3	G	2	 50%100%
3	H	2	 100%
3	I	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	1	-	-	X	-
4	NAG	A	1312	-	-	X	-
4	NAG	B	1302	-	-	X	-
4	NAG	B	1304	-	-	X	-
4	NAG	C	1303	X	-	-	-
4	NAG	C	1306	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51042 atoms, of which 24708 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1060	Total	C	H	N	O	S	1	0
			16360	5292	8068	1382	1580	38		
1	B	1054	Total	C	H	N	O	S	3	0
			16287	5268	8034	1376	1571	38		
1	C	1060	Total	C	H	N	O	S	1	0
			16361	5292	8069	1382	1580	38		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	TYR	-	expression tag	UNP P0DTC2
A	1215	ILE	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	GLU	-	expression tag	UNP P0DTC2
A	1218	ALA	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	ASP	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLN	-	expression tag	UNP P0DTC2
A	1224	ALA	-	expression tag	UNP P0DTC2
A	1225	TYR	-	expression tag	UNP P0DTC2
A	1226	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ARG	-	expression tag	UNP P0DTC2
A	1228	LYS	-	expression tag	UNP P0DTC2
A	1229	ASP	-	expression tag	UNP P0DTC2
A	1230	GLY	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	TRP	-	expression tag	UNP P0DTC2
A	1233	VAL	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	SER	-	expression tag	UNP P0DTC2
A	1237	THR	-	expression tag	UNP P0DTC2
A	1238	PHE	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	ASN	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	TYR	-	expression tag	UNP P0DTC2
A	1246	PHE	-	expression tag	UNP P0DTC2
A	1247	GLN	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	ASP	-	expression tag	UNP P0DTC2
A	1250	TYR	-	expression tag	UNP P0DTC2
A	1251	LYS	-	expression tag	UNP P0DTC2
A	1252	ASP	-	expression tag	UNP P0DTC2
A	1253	ASP	-	expression tag	UNP P0DTC2
A	1254	ASP	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	LYS	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	HIS	-	expression tag	UNP P0DTC2
A	1264	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	TYR	-	expression tag	UNP P0DTC2
B	1215	ILE	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	GLU	-	expression tag	UNP P0DTC2
B	1218	ALA	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	ASP	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLN	-	expression tag	UNP P0DTC2
B	1224	ALA	-	expression tag	UNP P0DTC2
B	1225	TYR	-	expression tag	UNP P0DTC2
B	1226	VAL	-	expression tag	UNP P0DTC2
B	1227	ARG	-	expression tag	UNP P0DTC2
B	1228	LYS	-	expression tag	UNP P0DTC2
B	1229	ASP	-	expression tag	UNP P0DTC2
B	1230	GLY	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	TRP	-	expression tag	UNP P0DTC2
B	1233	VAL	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	SER	-	expression tag	UNP P0DTC2
B	1237	THR	-	expression tag	UNP P0DTC2
B	1238	PHE	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	THR	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	ASN	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	TYR	-	expression tag	UNP P0DTC2
B	1246	PHE	-	expression tag	UNP P0DTC2
B	1247	GLN	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1249	ASP	-	expression tag	UNP P0DTC2
B	1250	TYR	-	expression tag	UNP P0DTC2
B	1251	LYS	-	expression tag	UNP P0DTC2
B	1252	ASP	-	expression tag	UNP P0DTC2
B	1253	ASP	-	expression tag	UNP P0DTC2
B	1254	ASP	-	expression tag	UNP P0DTC2
B	1255	ASP	-	expression tag	UNP P0DTC2
B	1256	LYS	-	expression tag	UNP P0DTC2
B	1257	GLY	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	HIS	-	expression tag	UNP P0DTC2
B	1264	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	TYR	-	expression tag	UNP P0DTC2
C	1215	ILE	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	GLU	-	expression tag	UNP P0DTC2
C	1218	ALA	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	ASP	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLN	-	expression tag	UNP P0DTC2
C	1224	ALA	-	expression tag	UNP P0DTC2
C	1225	TYR	-	expression tag	UNP P0DTC2
C	1226	VAL	-	expression tag	UNP P0DTC2
C	1227	ARG	-	expression tag	UNP P0DTC2
C	1228	LYS	-	expression tag	UNP P0DTC2

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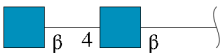
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1229	ASP	-	expression tag	UNP P0DTC2
C	1230	GLY	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	TRP	-	expression tag	UNP P0DTC2
C	1233	VAL	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	SER	-	expression tag	UNP P0DTC2
C	1237	THR	-	expression tag	UNP P0DTC2
C	1238	PHE	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	THR	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	ASN	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	TYR	-	expression tag	UNP P0DTC2
C	1246	PHE	-	expression tag	UNP P0DTC2
C	1247	GLN	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	ASP	-	expression tag	UNP P0DTC2
C	1250	TYR	-	expression tag	UNP P0DTC2
C	1251	LYS	-	expression tag	UNP P0DTC2
C	1252	ASP	-	expression tag	UNP P0DTC2
C	1253	ASP	-	expression tag	UNP P0DTC2
C	1254	ASP	-	expression tag	UNP P0DTC2
C	1255	ASP	-	expression tag	UNP P0DTC2
C	1256	LYS	-	expression tag	UNP P0DTC2
C	1257	GLY	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	HIS	-	expression tag	UNP P0DTC2
C	1264	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Camel-derived nanobody 1.10.

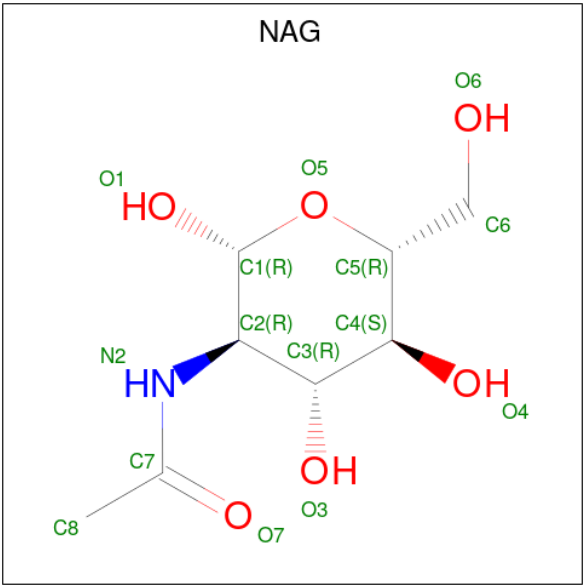
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	119	Total	C	N	O	S	0	0
			895	554	154	182	5		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	F	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	G	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	H	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	I	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	

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Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			26	8	12	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			26	8	12	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			26	8	12	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	

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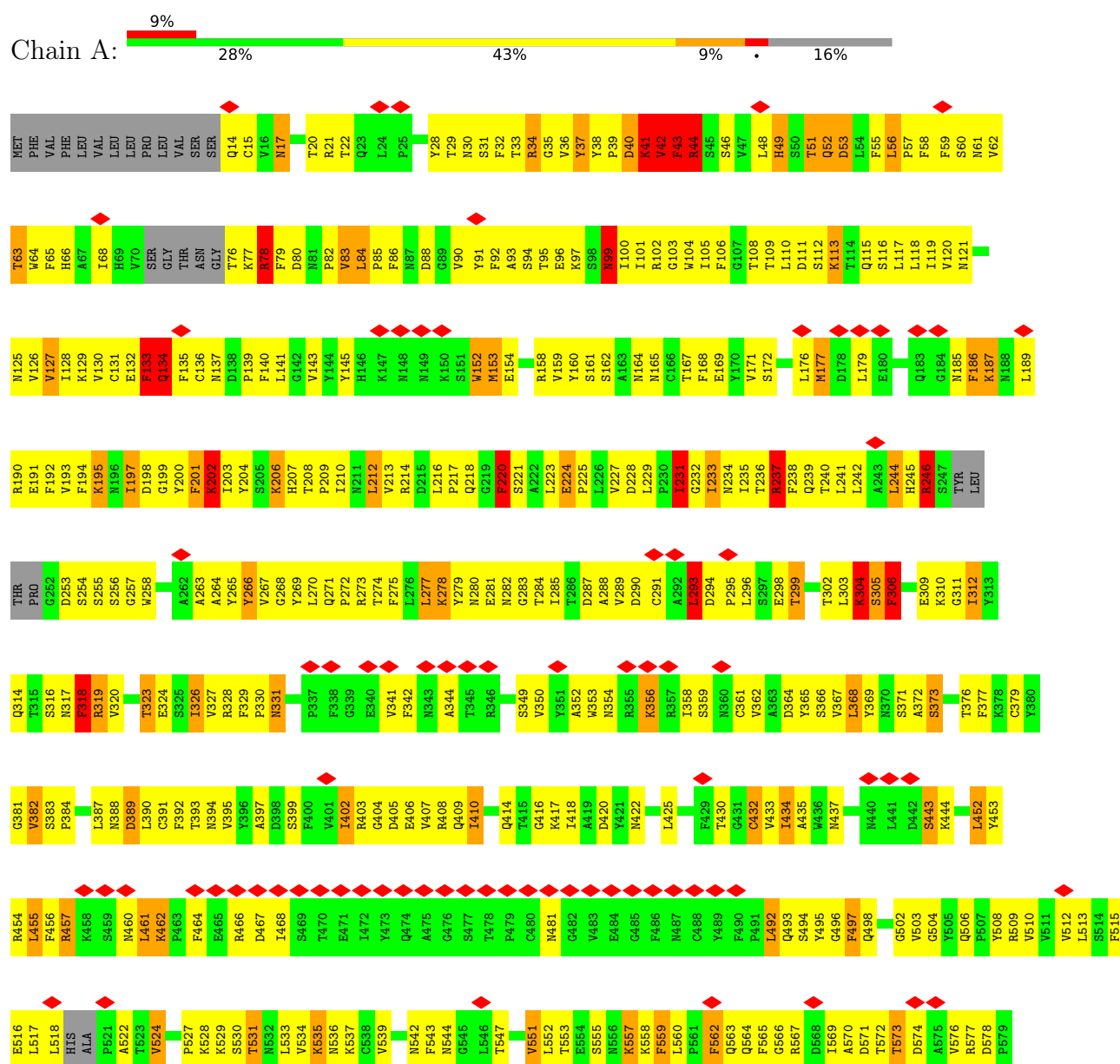
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Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	H	N	O	0
			26	8	12	1	5	
4	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	N	O		0
			14	8	1	5		

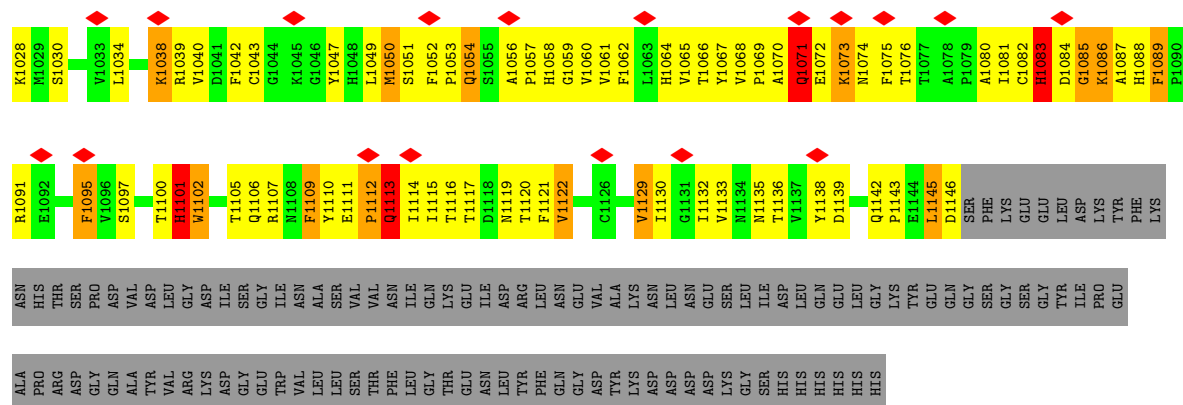
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

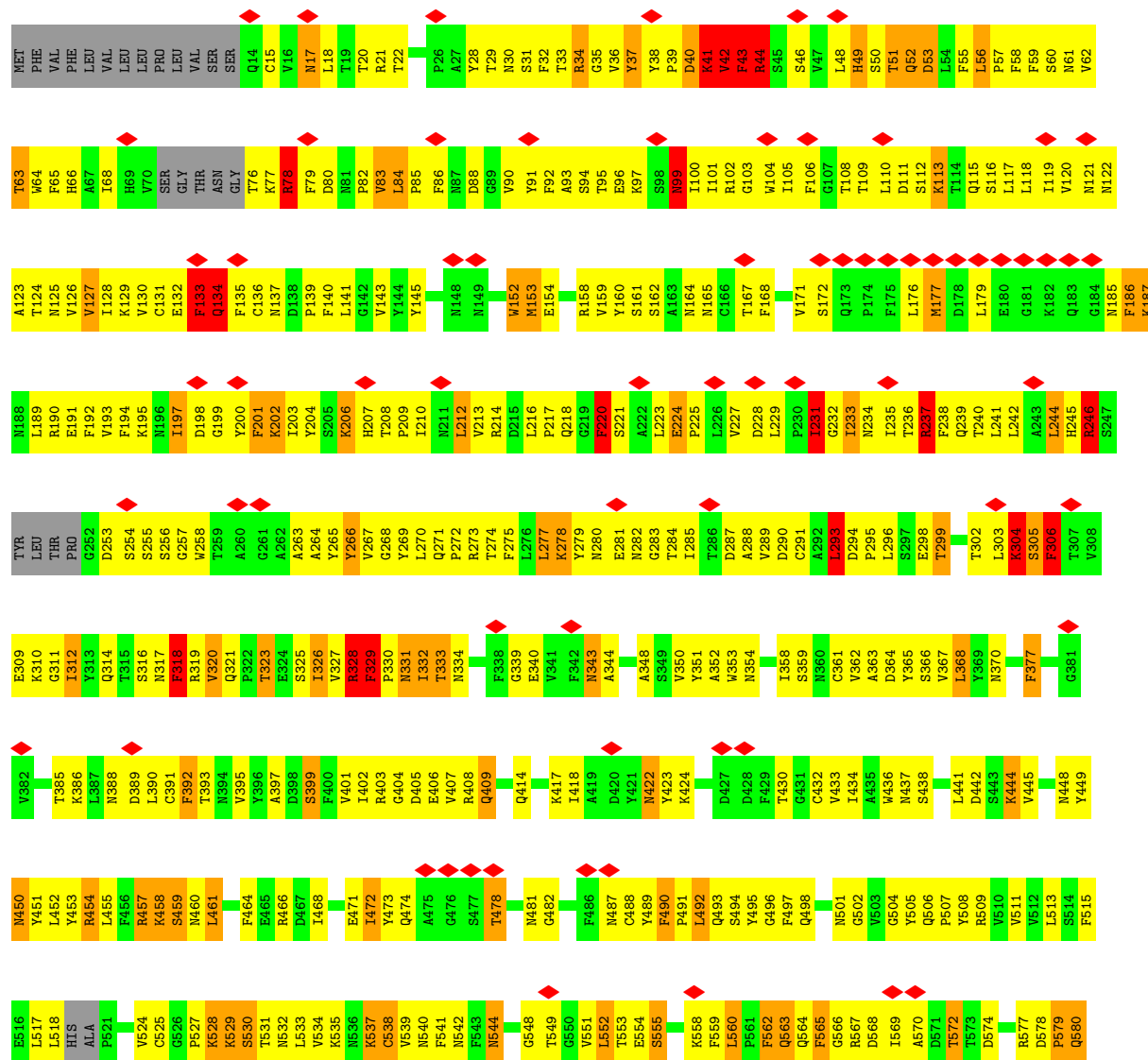
• Molecule 1: Spike glycoprotein

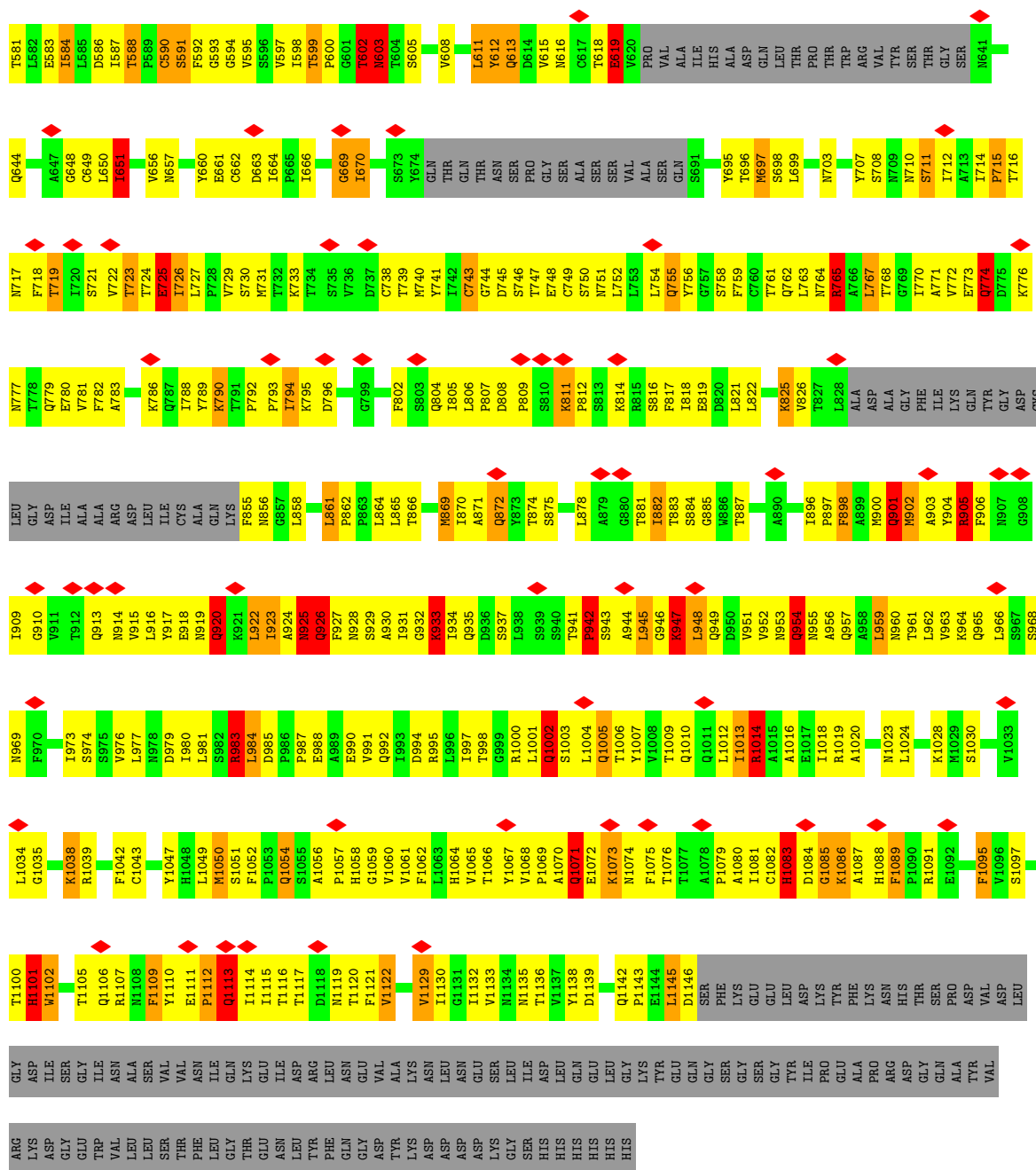




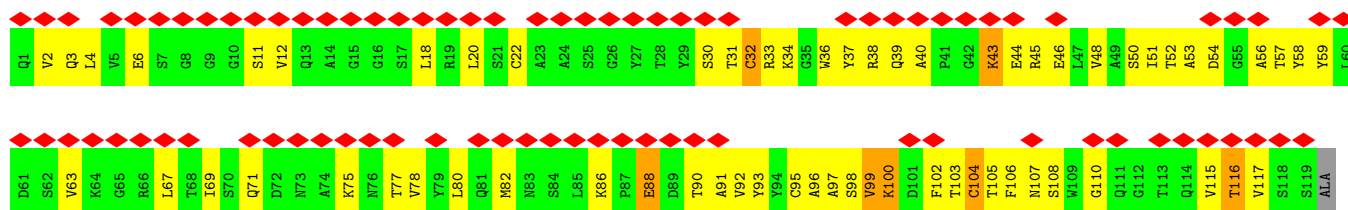
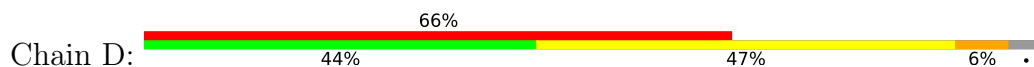


• Molecule 1: Spike glycoprotein





• Molecule 2: Camel-derived nanobody 1.10





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.871	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	418.2, 418.2, 418.2	wwPDB
Map dimensions	492, 492, 492	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.59	151/8490 (1.8%)	2.34	371/11550 (3.2%)
1	B	1.60	148/8452 (1.8%)	2.36	377/11495 (3.3%)
1	C	1.60	152/8490 (1.8%)	2.35	372/11550 (3.2%)
2	D	0.12	0/910	0.41	0/1233
All	All	1.57	451/26342 (1.7%)	2.31	1120/35828 (3.1%)

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	5	53
1	B	5	54
1	C	5	54
All	All	15	161

All (451) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1083	HIS	CE1-NE2	-29.78	1.02	1.32
1	C	1083	HIS	CE1-NE2	-29.77	1.02	1.32
1	B	1083	HIS	CE1-NE2	-29.77	1.02	1.32
1	C	983	ARG	NE-CZ	-28.42	1.01	1.33
1	B	983	ARG	NE-CZ	-28.41	1.01	1.33
1	A	983	ARG	NE-CZ	-28.40	1.01	1.33
1	A	1113	GLN	CD-OE1	-27.50	0.71	1.23
1	C	1113	GLN	CD-OE1	-27.47	0.71	1.23
1	B	1113	GLN	CD-OE1	-27.44	0.71	1.23
1	A	954	GLN	CD-NE2	-27.42	0.75	1.33
1	C	954	GLN	CD-NE2	-27.40	0.75	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	954	GLN	CD-NE2	-27.39	0.75	1.33
1	A	41	LYS	CB-CG	25.24	2.28	1.52
1	B	41	LYS	CB-CG	25.23	2.28	1.52
1	C	41	LYS	CB-CG	25.21	2.28	1.52
1	A	600	PRO	N-CD	22.79	1.79	1.47
1	C	600	PRO	N-CD	22.79	1.79	1.47
1	B	600	PRO	N-CD	22.78	1.79	1.47
1	C	774	GLN	CG-CD	-22.05	0.96	1.52
1	A	774	GLN	CG-CD	-22.03	0.96	1.52
1	B	774	GLN	CG-CD	-22.03	0.96	1.52
1	C	304	LYS	CG-CD	-20.81	0.90	1.52
1	A	304	LYS	CG-CD	-20.80	0.90	1.52
1	B	304	LYS	CG-CD	-20.79	0.90	1.52
1	B	318	PHE	CG-CD1	-19.32	0.98	1.38
1	C	318	PHE	CG-CD1	-19.30	0.98	1.38
1	A	318	PHE	CG-CD1	-19.28	0.98	1.38
1	C	41	LYS	CA-C	19.20	1.76	1.52
1	B	41	LYS	CA-C	19.18	1.76	1.52
1	A	41	LYS	CA-C	19.18	1.76	1.52
1	B	1002	GLN	CG-CD	-18.95	1.04	1.52
1	A	1002	GLN	CG-CD	-18.95	1.04	1.52
1	C	1002	GLN	CG-CD	-18.94	1.04	1.52
1	B	1071	GLN	CD-NE2	18.11	1.71	1.33
1	A	1071	GLN	CD-NE2	18.09	1.71	1.33
1	C	1071	GLN	CD-NE2	18.07	1.71	1.33
1	B	177	MET	SD-CE	-17.47	1.35	1.79
1	C	177	MET	SD-CE	-17.46	1.35	1.79
1	A	177	MET	SD-CE	-17.45	1.35	1.79
1	C	1071	GLN	CG-CD	-17.42	1.08	1.52
1	B	1071	GLN	CG-CD	-17.41	1.08	1.52
1	A	1071	GLN	CG-CD	-17.41	1.08	1.52
1	A	600	PRO	CG-CD	-16.47	0.94	1.50
1	B	600	PRO	CG-CD	-16.46	0.94	1.50
1	C	600	PRO	CG-CD	-16.44	0.94	1.50
1	B	231	ILE	CB-CG2	16.41	2.06	1.52
1	C	231	ILE	CB-CG2	16.38	2.06	1.52
1	A	231	ILE	CB-CG2	16.37	2.06	1.52
1	C	1014	ARG	CG-CD	-16.01	1.04	1.52
1	B	1014	ARG	CG-CD	-16.00	1.04	1.52
1	A	1014	ARG	CG-CD	-15.97	1.04	1.52
1	C	153	MET	SD-CE	-15.59	1.40	1.79
1	B	153	MET	SD-CE	-15.57	1.40	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	MET	SD-CE	-15.56	1.40	1.79
1	B	41	LYS	CG-CD	15.06	1.97	1.52
1	C	41	LYS	CG-CD	15.04	1.97	1.52
1	A	41	LYS	CG-CD	15.02	1.97	1.52
1	C	983	ARG	CA-C	-14.16	1.34	1.52
1	A	983	ARG	CA-C	-14.08	1.34	1.52
1	B	983	ARG	CA-C	-14.07	1.34	1.52
1	C	42	VAL	CB-CG2	-14.07	1.06	1.52
1	B	42	VAL	CB-CG2	-14.04	1.06	1.52
1	A	42	VAL	CB-CG2	-14.03	1.06	1.52
1	A	948	LEU	CA-CB	-13.89	1.31	1.53
1	C	948	LEU	CA-CB	-13.86	1.31	1.53
1	B	948	LEU	CA-CB	-13.83	1.31	1.53
1	A	983	ARG	CD-NE	13.54	1.65	1.46
1	B	983	ARG	CD-NE	13.53	1.65	1.46
1	C	983	ARG	CD-NE	13.52	1.65	1.46
1	A	304	LYS	CA-C	-13.36	1.31	1.52
1	B	304	LYS	CA-C	-13.36	1.31	1.52
1	C	304	LYS	CA-C	-13.36	1.31	1.52
1	C	723	THR	CB-CG2	13.31	1.96	1.52
1	A	723	THR	CB-CG2	13.30	1.96	1.52
1	B	723	THR	CB-CG2	13.30	1.96	1.52
1	A	1083	HIS	CG-CD2	-12.72	1.21	1.35
1	C	1083	HIS	CG-CD2	-12.71	1.21	1.35
1	B	1083	HIS	CG-CD2	-12.70	1.21	1.35
1	C	811	LYS	CB-CG	-12.66	1.14	1.52
1	A	811	LYS	CB-CG	-12.62	1.14	1.52
1	B	811	LYS	CB-CG	-12.62	1.14	1.52
1	A	134	GLN	CG-CD	-12.54	1.20	1.52
1	C	134	GLN	CG-CD	-12.53	1.20	1.52
1	B	134	GLN	CG-CD	-12.52	1.20	1.52
1	C	1002	GLN	CD-OE1	-12.51	0.99	1.23
1	B	1002	GLN	CD-OE1	-12.50	0.99	1.23
1	A	1002	GLN	CD-OE1	-12.49	0.99	1.23
1	C	983	ARG	CZ-NH1	12.42	1.50	1.32
1	A	983	ARG	CZ-NH1	12.40	1.50	1.32
1	B	983	ARG	CZ-NH1	12.38	1.50	1.32
1	A	237	ARG	NE-CZ	-12.03	1.19	1.33
1	B	651	ILE	CB-CG2	12.02	1.92	1.52
1	C	651	ILE	CB-CG2	12.01	1.92	1.52
1	A	651	ILE	CB-CG2	11.98	1.92	1.52
1	C	237	ARG	NE-CZ	-11.98	1.19	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	ARG	NE-CZ	-11.94	1.20	1.33
1	C	723	THR	CB-OG1	-11.87	1.24	1.43
1	B	723	THR	CB-OG1	-11.85	1.24	1.43
1	A	723	THR	CB-OG1	-11.82	1.24	1.43
1	C	755	GLN	CD-OE1	11.41	1.45	1.23
1	A	755	GLN	CD-OE1	11.38	1.45	1.23
1	B	755	GLN	CD-OE1	11.38	1.45	1.23
1	B	78	ARG	NE-CZ	-11.10	1.20	1.33
1	A	78	ARG	NE-CZ	-11.10	1.20	1.33
1	C	78	ARG	NE-CZ	-11.07	1.20	1.33
1	B	99	ASN	CG-OD1	-10.91	1.02	1.23
1	A	99	ASN	CG-OD1	-10.90	1.02	1.23
1	C	99	ASN	CG-OD1	-10.86	1.02	1.23
1	A	1129	VAL	CB-CG1	-10.80	1.16	1.52
1	B	1129	VAL	CB-CG1	-10.80	1.17	1.52
1	C	1129	VAL	CB-CG1	-10.79	1.17	1.52
1	A	670	ILE	CB-CG2	10.65	1.87	1.52
1	B	670	ILE	CB-CG2	10.64	1.87	1.52
1	C	670	ILE	CB-CG2	10.62	1.87	1.52
1	A	1002	GLN	CD-NE2	-10.61	1.10	1.33
1	C	1002	GLN	CD-NE2	-10.58	1.11	1.33
1	B	1002	GLN	CD-NE2	-10.57	1.11	1.33
1	A	983	ARG	CB-CG	-10.53	1.20	1.52
1	B	983	ARG	CB-CG	-10.52	1.20	1.52
1	C	983	ARG	CB-CG	-10.51	1.21	1.52
1	A	651	ILE	CG1-CD1	10.47	1.92	1.51
1	B	651	ILE	CG1-CD1	10.45	1.92	1.51
1	C	651	ILE	CG1-CD1	10.43	1.92	1.51
1	C	1014	ARG	CD-NE	-10.40	1.31	1.46
1	A	947	LYS	CD-CE	-10.39	1.21	1.52
1	B	947	LYS	CD-CE	-10.39	1.21	1.52
1	B	1014	ARG	CD-NE	-10.39	1.31	1.46
1	C	947	LYS	CD-CE	-10.39	1.21	1.52
1	A	1014	ARG	CD-NE	-10.37	1.31	1.46
1	B	872	GLN	CG-CD	-10.35	1.26	1.52
1	C	872	GLN	CG-CD	-10.34	1.26	1.52
1	A	872	GLN	CG-CD	-10.34	1.26	1.52
1	B	1050	MET	CB-CG	-10.32	1.21	1.52
1	C	1050	MET	CB-CG	-10.31	1.21	1.52
1	A	303	LEU	C-N	10.27	1.48	1.33
1	A	1050	MET	CB-CG	-10.27	1.21	1.52
1	B	303	LEU	C-N	10.26	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	303	LEU	C-N	10.22	1.48	1.33
1	A	611	LEU	CG-CD2	9.91	1.85	1.52
1	C	983	ARG	CZ-NH2	9.91	1.46	1.33
1	C	611	LEU	CG-CD2	9.91	1.85	1.52
1	B	599	THR	CA-C	9.91	1.61	1.52
1	B	611	LEU	CG-CD2	9.90	1.85	1.52
1	C	599	THR	CA-C	9.90	1.61	1.52
1	A	1071	GLN	CD-OE1	9.87	1.42	1.23
1	B	983	ARG	CZ-NH2	9.85	1.46	1.33
1	B	41	LYS	C-O	9.84	1.38	1.24
1	C	41	LYS	C-O	9.84	1.38	1.24
1	A	983	ARG	CZ-NH2	9.83	1.46	1.33
1	A	599	THR	CA-C	9.82	1.61	1.52
1	B	1071	GLN	CD-OE1	9.82	1.42	1.23
1	A	41	LYS	C-O	9.82	1.38	1.24
1	C	1071	GLN	CD-OE1	9.82	1.42	1.23
1	B	187	LYS	CE-NZ	-9.80	1.20	1.49
1	C	905	ARG	CD-NE	-9.77	1.32	1.46
1	A	187	LYS	CE-NZ	-9.77	1.20	1.49
1	C	187	LYS	CE-NZ	-9.77	1.20	1.49
1	B	905	ARG	CD-NE	-9.73	1.32	1.46
1	A	905	ARG	CD-NE	-9.69	1.32	1.46
1	A	187	LYS	CA-CB	-9.67	1.40	1.53
1	B	187	LYS	CA-CB	-9.63	1.40	1.53
1	C	187	LYS	CA-CB	-9.63	1.40	1.53
1	B	651	ILE	CB-CG1	-9.59	1.34	1.53
1	A	651	ILE	CB-CG1	-9.56	1.34	1.53
1	C	651	ILE	CB-CG1	-9.55	1.34	1.53
1	A	78	ARG	CD-NE	-9.54	1.32	1.46
1	C	187	LYS	CA-C	9.53	1.66	1.52
1	C	78	ARG	CD-NE	-9.53	1.32	1.46
1	B	78	ARG	CD-NE	-9.53	1.32	1.46
1	B	187	LYS	CA-C	9.51	1.66	1.52
1	A	187	LYS	CA-C	9.49	1.66	1.52
1	C	1002	GLN	CB-CG	-9.28	1.24	1.52
1	A	1002	GLN	CB-CG	-9.27	1.24	1.52
1	B	1002	GLN	CB-CG	-9.27	1.24	1.52
1	B	187	LYS	C-O	9.16	1.32	1.24
1	A	187	LYS	C-O	9.12	1.32	1.24
1	C	187	LYS	C-O	9.07	1.31	1.24
1	C	237	ARG	CD-NE	-8.95	1.33	1.46
1	B	237	ARG	CD-NE	-8.95	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	901	GLN	CD-OE1	-8.94	1.06	1.23
1	A	237	ARG	CD-NE	-8.94	1.33	1.46
1	C	901	GLN	CD-OE1	-8.92	1.06	1.23
1	B	901	GLN	CD-OE1	-8.89	1.06	1.23
1	C	954	GLN	CD-OE1	-8.84	1.06	1.23
1	B	954	GLN	CD-OE1	-8.82	1.06	1.23
1	A	954	GLN	CD-OE1	-8.78	1.06	1.23
1	C	923	ILE	CB-CG1	-8.76	1.35	1.53
1	A	923	ILE	CB-CG1	-8.74	1.35	1.53
1	B	923	ILE	CB-CG1	-8.72	1.36	1.53
1	C	983	ARG	N-CA	8.55	1.57	1.45
1	B	983	ARG	N-CA	8.53	1.57	1.45
1	A	983	ARG	N-CA	8.53	1.57	1.45
1	A	954	GLN	CB-CG	-8.53	1.26	1.52
1	C	954	GLN	CB-CG	-8.53	1.26	1.52
1	B	954	GLN	CB-CG	-8.50	1.26	1.52
1	A	318	PHE	CG-CD2	8.50	1.56	1.38
1	B	318	PHE	CG-CD2	8.49	1.56	1.38
1	C	318	PHE	CG-CD2	8.49	1.56	1.38
1	B	922	LEU	CB-CG	-8.44	1.36	1.53
1	B	755	GLN	CD-NE2	8.43	1.50	1.33
1	A	922	LEU	CB-CG	-8.42	1.36	1.53
1	A	755	GLN	CD-NE2	8.41	1.50	1.33
1	C	755	GLN	CD-NE2	8.40	1.50	1.33
1	C	922	LEU	CB-CG	-8.40	1.36	1.53
1	B	231	ILE	CA-CB	-8.39	1.46	1.55
1	A	774	GLN	CD-OE1	-8.35	1.07	1.23
1	B	293	LEU	C-N	8.35	1.45	1.33
1	B	774	GLN	CD-OE1	-8.35	1.07	1.23
1	C	293	LEU	C-N	8.32	1.45	1.33
1	C	774	GLN	CD-OE1	-8.32	1.07	1.23
1	B	206	LYS	CB-CG	-8.31	1.27	1.52
1	A	293	LEU	C-N	8.30	1.45	1.33
1	B	40	ASP	C-N	8.30	1.46	1.33
1	A	206	LYS	CB-CG	-8.29	1.27	1.52
1	C	206	LYS	CB-CG	-8.29	1.27	1.52
1	B	63	THR	CB-OG1	-8.28	1.30	1.43
1	A	63	THR	CB-OG1	-8.27	1.30	1.43
1	C	63	THR	CB-OG1	-8.26	1.30	1.43
1	A	40	ASP	C-N	8.24	1.46	1.33
1	C	40	ASP	C-N	8.23	1.46	1.33
1	C	712	ILE	CB-CG1	-8.19	1.37	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	712	ILE	CB-CG1	-8.18	1.37	1.53
1	A	712	ILE	CB-CG1	-8.12	1.37	1.53
1	B	44	ARG	NE-CZ	-8.12	1.24	1.33
1	C	44	ARG	NE-CZ	-8.12	1.24	1.33
1	A	44	ARG	NE-CZ	-8.08	1.24	1.33
1	A	1113	GLN	CG-CD	8.02	1.72	1.52
1	B	905	ARG	CB-CG	-8.01	1.28	1.52
1	C	1113	GLN	CG-CD	8.01	1.72	1.52
1	A	153	MET	CG-SD	-8.01	1.60	1.80
1	B	1113	GLN	CG-CD	8.00	1.72	1.52
1	C	905	ARG	CB-CG	-8.00	1.28	1.52
1	B	153	MET	CG-SD	-7.99	1.60	1.80
1	A	905	ARG	CB-CG	-7.98	1.28	1.52
1	C	52	GLN	CG-CD	-7.98	1.32	1.52
1	C	153	MET	CG-SD	-7.97	1.60	1.80
1	A	52	GLN	CG-CD	-7.97	1.32	1.52
1	B	52	GLN	CG-CD	-7.96	1.32	1.52
1	C	1113	GLN	CB-CG	-7.88	1.28	1.52
1	B	1113	GLN	CB-CG	-7.87	1.28	1.52
1	B	946	GLY	C-N	-7.86	1.23	1.34
1	A	1113	GLN	CB-CG	-7.86	1.28	1.52
1	C	946	GLY	C-N	-7.83	1.23	1.34
1	A	922	LEU	CG-CD2	-7.80	1.26	1.52
1	B	922	LEU	CG-CD2	-7.79	1.26	1.52
1	A	925	ASN	CB-CG	-7.78	1.32	1.52
1	C	922	LEU	CG-CD2	-7.78	1.26	1.52
1	C	133	PHE	CB-CG	-7.78	1.32	1.50
1	A	946	GLY	C-N	-7.76	1.23	1.34
1	B	133	PHE	CB-CG	-7.75	1.32	1.50
1	A	133	PHE	CB-CG	-7.75	1.32	1.50
1	C	925	ASN	CB-CG	-7.75	1.32	1.52
1	B	925	ASN	CB-CG	-7.75	1.32	1.52
1	B	44	ARG	CB-CG	-7.73	1.29	1.52
1	C	44	ARG	CB-CG	-7.73	1.29	1.52
1	A	44	ARG	CB-CG	-7.71	1.29	1.52
1	B	237	ARG	CZ-NH1	-7.71	1.22	1.32
1	A	237	ARG	CZ-NH1	-7.69	1.22	1.32
1	C	237	ARG	CZ-NH1	-7.68	1.22	1.32
1	C	922	LEU	C-N	-7.63	1.24	1.34
1	A	922	LEU	C-N	-7.62	1.24	1.34
1	B	922	LEU	C-N	-7.61	1.24	1.34
1	C	206	LYS	CD-CE	-7.61	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	LYS	CD-CE	-7.60	1.29	1.52
1	C	246	ARG	CZ-NH1	7.59	1.43	1.32
1	A	206	LYS	CD-CE	-7.56	1.29	1.52
1	A	246	ARG	CZ-NH1	7.55	1.43	1.32
1	B	246	ARG	CZ-NH1	7.48	1.43	1.32
1	B	237	ARG	CB-CG	-7.46	1.30	1.52
1	A	237	ARG	CB-CG	-7.43	1.30	1.52
1	C	237	ARG	CB-CG	-7.42	1.30	1.52
1	A	774	GLN	CB-CG	-7.34	1.30	1.52
1	C	774	GLN	CB-CG	-7.33	1.30	1.52
1	B	774	GLN	CB-CG	-7.31	1.30	1.52
1	B	611	LEU	CG-CD1	-7.31	1.28	1.52
1	C	611	LEU	CG-CD1	-7.30	1.28	1.52
1	A	611	LEU	CG-CD1	-7.28	1.28	1.52
1	B	281	GLU	CG-CD	-7.27	1.33	1.52
1	A	281	GLU	CG-CD	-7.25	1.33	1.52
1	C	281	GLU	CG-CD	-7.25	1.33	1.52
1	B	1014	ARG	CB-CG	-7.21	1.30	1.52
1	A	1014	ARG	CB-CG	-7.20	1.30	1.52
1	C	1014	ARG	CB-CG	-7.19	1.30	1.52
1	A	42	VAL	CB-CG1	7.16	1.76	1.52
1	B	42	VAL	CB-CG1	7.15	1.76	1.52
1	C	42	VAL	CB-CG1	7.15	1.76	1.52
1	C	926	GLN	CD-OE1	-7.12	1.10	1.23
1	C	328	ARG	C-N	7.11	1.41	1.33
1	B	926	GLN	CD-OE1	-7.11	1.10	1.23
1	A	926	GLN	CD-OE1	-7.08	1.10	1.23
1	B	41	LYS	CA-CB	7.07	1.65	1.53
1	C	811	LYS	CD-CE	-7.05	1.31	1.52
1	A	811	LYS	CD-CE	-7.04	1.31	1.52
1	A	41	LYS	CA-CB	7.04	1.65	1.53
1	B	811	LYS	CD-CE	-7.04	1.31	1.52
1	C	1073	LYS	CE-NZ	7.04	1.70	1.49
1	B	1073	LYS	CE-NZ	7.04	1.70	1.49
1	C	41	LYS	CA-CB	7.02	1.65	1.53
1	A	1073	LYS	CE-NZ	7.02	1.70	1.49
1	C	948	LEU	CG-CD1	6.98	1.75	1.52
1	A	948	LEU	CG-CD1	6.96	1.75	1.52
1	B	933	LYS	CD-CE	6.96	1.73	1.52
1	C	63	THR	CB-CG2	6.96	1.75	1.52
1	C	933	LYS	CD-CE	6.96	1.73	1.52
1	B	63	THR	CB-CG2	6.96	1.75	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	933	LYS	CD-CE	6.96	1.73	1.52
1	B	948	LEU	CG-CD1	6.96	1.75	1.52
1	A	63	THR	CB-CG2	6.95	1.75	1.52
1	A	1086	LYS	CD-CE	6.95	1.73	1.52
1	A	1005	GLN	CD-NE2	-6.94	1.18	1.33
1	B	947	LYS	CG-CD	-6.93	1.31	1.52
1	C	947	LYS	CG-CD	-6.93	1.31	1.52
1	A	947	LYS	CG-CD	-6.93	1.31	1.52
1	B	1086	LYS	CD-CE	6.93	1.73	1.52
1	C	1086	LYS	CD-CE	6.92	1.73	1.52
1	C	231	ILE	CG1-CD1	-6.92	1.24	1.51
1	A	231	ILE	CG1-CD1	-6.92	1.24	1.51
1	B	231	ILE	CG1-CD1	-6.91	1.24	1.51
1	A	187	LYS	CD-CE	6.91	1.73	1.52
1	C	1005	GLN	CD-NE2	-6.91	1.18	1.33
1	B	187	LYS	CD-CE	6.91	1.73	1.52
1	C	1054	GLN	CD-NE2	6.90	1.47	1.33
1	C	187	LYS	CD-CE	6.90	1.73	1.52
1	B	1005	GLN	CD-NE2	-6.89	1.18	1.33
1	C	78	ARG	CZ-NH1	-6.89	1.23	1.32
1	A	1054	GLN	CD-NE2	6.86	1.47	1.33
1	B	1054	GLN	CD-NE2	6.85	1.47	1.33
1	A	78	ARG	CZ-NH1	-6.84	1.23	1.32
1	B	78	ARG	CZ-NH1	-6.82	1.23	1.32
1	B	774	GLN	CD-NE2	-6.76	1.19	1.33
1	C	774	GLN	CD-NE2	-6.75	1.19	1.33
1	A	774	GLN	CD-NE2	-6.74	1.19	1.33
1	B	948	LEU	CB-CG	-6.59	1.40	1.53
1	A	948	LEU	CB-CG	-6.54	1.40	1.53
1	B	767	LEU	CB-CG	-6.53	1.40	1.53
1	C	948	LEU	CB-CG	-6.51	1.40	1.53
1	A	318	PHE	CE2-CZ	-6.49	1.19	1.38
1	B	318	PHE	CE2-CZ	-6.49	1.19	1.38
1	A	767	LEU	CB-CG	-6.48	1.40	1.53
1	C	767	LEU	CB-CG	-6.48	1.40	1.53
1	C	318	PHE	CE2-CZ	-6.47	1.19	1.38
1	B	212	LEU	CG-CD2	-6.42	1.31	1.52
1	A	933	LYS	CE-NZ	6.41	1.68	1.49
1	B	933	LYS	CE-NZ	6.41	1.68	1.49
1	C	933	LYS	CE-NZ	6.41	1.68	1.49
1	A	212	LEU	CG-CD2	-6.41	1.31	1.52
1	C	212	LEU	CG-CD2	-6.39	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	LYS	CB-CG	-6.39	1.33	1.52
1	C	187	LYS	CB-CG	-6.37	1.33	1.52
1	B	187	LYS	CB-CG	-6.36	1.33	1.52
1	A	113	LYS	CD-CE	-6.36	1.33	1.52
1	B	113	LYS	CD-CE	-6.36	1.33	1.52
1	C	113	LYS	CD-CE	-6.35	1.33	1.52
1	C	78	ARG	CA-CB	6.29	1.64	1.53
1	B	78	ARG	CA-CB	6.27	1.64	1.53
1	A	78	ARG	CA-CB	6.25	1.64	1.53
1	B	278	LYS	CB-CG	-6.15	1.34	1.52
1	C	278	LYS	CB-CG	-6.15	1.34	1.52
1	A	278	LYS	CB-CG	-6.14	1.34	1.52
1	C	231	ILE	CA-CB	-6.14	1.46	1.54
1	A	231	ILE	CA-CB	-6.09	1.46	1.54
1	B	1129	VAL	CB-CG2	5.96	1.72	1.52
1	A	1129	VAL	CB-CG2	5.96	1.72	1.52
1	C	231	ILE	C-N	5.96	1.42	1.33
1	A	1145	LEU	CG-CD2	5.95	1.72	1.52
1	C	1129	VAL	CB-CG2	5.95	1.72	1.52
1	C	1145	LEU	CG-CD2	5.95	1.72	1.52
1	B	1145	LEU	CG-CD2	5.94	1.72	1.52
1	A	231	ILE	C-N	5.92	1.42	1.33
1	B	231	ILE	C-N	5.91	1.42	1.33
1	C	608	VAL	CB-CG2	5.87	1.72	1.52
1	B	608	VAL	CB-CG2	5.87	1.72	1.52
1	A	599	THR	C-O	-5.87	1.16	1.24
1	A	608	VAL	CB-CG2	5.86	1.71	1.52
1	A	231	ILE	N-CA	-5.86	1.39	1.46
1	B	599	THR	C-O	-5.85	1.16	1.24
1	C	599	THR	C-O	-5.84	1.16	1.24
1	B	171	VAL	CB-CG2	-5.82	1.33	1.52
1	A	171	VAL	CB-CG2	-5.82	1.33	1.52
1	C	171	VAL	CB-CG2	-5.81	1.33	1.52
1	C	231	ILE	N-CA	-5.80	1.39	1.46
1	A	318	PHE	CE1-CZ	-5.80	1.21	1.38
1	C	318	PHE	CE1-CZ	-5.79	1.21	1.38
1	B	318	PHE	CE1-CZ	-5.78	1.21	1.38
1	A	948	LEU	CG-CD2	5.77	1.71	1.52
1	B	948	LEU	CG-CD2	5.76	1.71	1.52
1	C	948	LEU	CG-CD2	5.75	1.71	1.52
1	C	767	LEU	CG-CD1	-5.74	1.33	1.52
1	B	767	LEU	CG-CD1	-5.73	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	ARG	CG-CD	-5.71	1.35	1.52
1	A	78	ARG	CG-CD	-5.71	1.35	1.52
1	A	767	LEU	CG-CD1	-5.71	1.33	1.52
1	B	78	ARG	CG-CD	-5.70	1.35	1.52
1	A	727	LEU	CG-CD2	-5.68	1.33	1.52
1	C	727	LEU	CG-CD2	-5.68	1.33	1.52
1	B	727	LEU	CG-CD2	-5.66	1.33	1.52
1	A	52	GLN	CB-CG	-5.52	1.35	1.52
1	B	52	GLN	CB-CG	-5.51	1.35	1.52
1	B	920	GLN	CD-NE2	5.50	1.44	1.33
1	B	133	PHE	CE2-CZ	-5.50	1.22	1.38
1	C	52	GLN	CB-CG	-5.49	1.35	1.52
1	C	920	GLN	CD-NE2	5.48	1.44	1.33
1	A	133	PHE	CE2-CZ	-5.48	1.22	1.38
1	C	133	PHE	CE2-CZ	-5.47	1.22	1.38
1	A	920	GLN	CD-NE2	5.44	1.44	1.33
1	C	40	ASP	C-O	5.42	1.30	1.24
1	C	995	ARG	CB-CG	-5.42	1.36	1.52
1	A	995	ARG	CB-CG	-5.42	1.36	1.52
1	B	995	ARG	CB-CG	-5.41	1.36	1.52
1	B	40	ASP	C-O	5.40	1.30	1.24
1	B	44	ARG	CD-NE	-5.40	1.38	1.46
1	C	329	PHE	C-N	5.39	1.46	1.33
1	C	1113	GLN	N-CA	5.38	1.53	1.46
1	C	44	ARG	CD-NE	-5.37	1.38	1.46
1	A	669	GLY	C-N	-5.37	1.26	1.33
1	B	246	ARG	CG-CD	-5.36	1.36	1.52
1	A	44	ARG	CD-NE	-5.36	1.38	1.46
1	A	1113	GLN	N-CA	5.36	1.53	1.46
1	B	1113	GLN	N-CA	5.36	1.53	1.46
1	A	246	ARG	CG-CD	-5.34	1.36	1.52
1	A	40	ASP	C-O	5.34	1.30	1.24
1	A	1083	HIS	ND1-CE1	5.34	1.37	1.32
1	C	246	ARG	CG-CD	-5.34	1.36	1.52
1	B	1083	HIS	ND1-CE1	5.33	1.37	1.32
1	C	669	GLY	C-N	-5.32	1.26	1.33
1	B	669	GLY	C-N	-5.31	1.26	1.33
1	C	1083	HIS	ND1-CE1	5.27	1.37	1.32
1	C	726	ILE	CG1-CD1	5.27	1.72	1.51
1	B	726	ILE	CG1-CD1	5.24	1.72	1.51
1	B	901	GLN	CD-NE2	-5.23	1.22	1.33
1	A	726	ILE	CG1-CD1	5.23	1.72	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1113	GLN	CA-C	-5.22	1.45	1.52
1	A	901	GLN	CD-NE2	-5.22	1.22	1.33
1	C	1113	GLN	CA-C	-5.18	1.45	1.52
1	A	1113	GLN	CA-C	-5.18	1.45	1.52
1	C	901	GLN	CD-NE2	-5.18	1.22	1.33
1	A	206	LYS	CG-CD	-5.17	1.36	1.52
1	C	206	LYS	CG-CD	-5.16	1.36	1.52
1	B	712	ILE	CG1-CD1	-5.15	1.31	1.51
1	A	712	ILE	CG1-CD1	-5.14	1.31	1.51
1	B	1129	VAL	CA-C	-5.14	1.45	1.53
1	C	712	ILE	CG1-CD1	-5.14	1.31	1.51
1	C	983	ARG	CG-CD	5.14	1.67	1.52
1	B	983	ARG	CG-CD	5.14	1.67	1.52
1	A	1129	VAL	CA-C	-5.13	1.45	1.53
1	A	983	ARG	CG-CD	5.13	1.67	1.52
1	B	206	LYS	CG-CD	-5.12	1.37	1.52
1	C	1129	VAL	CA-C	-5.11	1.45	1.53
1	C	922	LEU	CA-CB	-5.05	1.45	1.53
1	A	304	LYS	CB-CG	-5.01	1.37	1.52
1	A	44	ARG	CA-CB	-5.00	1.46	1.52

All (1120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	983	ARG	NE-CZ-NH1	-64.03	57.47	121.50
1	C	983	ARG	NE-CZ-NH1	-63.99	57.51	121.50
1	B	983	ARG	NE-CZ-NH1	-63.93	57.57	121.50
1	B	983	ARG	CD-NE-CZ	-53.50	49.50	124.40
1	C	983	ARG	CD-NE-CZ	-53.50	49.51	124.40
1	A	983	ARG	CD-NE-CZ	-53.45	49.57	124.40
1	A	774	GLN	CG-CD-NE2	-33.31	66.44	116.40
1	B	774	GLN	CG-CD-NE2	-33.30	66.45	116.40
1	C	774	GLN	CG-CD-NE2	-33.27	66.49	116.40
1	B	42	VAL	CA-CB-CG2	33.08	166.63	110.40
1	C	42	VAL	CA-CB-CG2	33.03	166.56	110.40
1	A	42	VAL	CA-CB-CG2	33.03	166.55	110.40
1	A	983	ARG	NH1-CZ-NH2	-32.89	76.55	119.30
1	C	983	ARG	NH1-CZ-NH2	-32.88	76.55	119.30
1	B	983	ARG	NH1-CZ-NH2	-32.85	76.59	119.30
1	A	723	THR	OG1-CB-CG2	-31.67	45.96	109.30
1	B	723	THR	OG1-CB-CG2	-31.66	45.99	109.30
1	C	723	THR	OG1-CB-CG2	-31.64	46.01	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	LYS	N-CA-CB	30.74	162.30	111.27
1	B	41	LYS	N-CA-CB	30.74	162.30	111.27
1	A	41	LYS	N-CA-CB	30.74	162.29	111.27
1	C	983	ARG	CB-CG-CD	29.86	179.98	111.30
1	B	983	ARG	CB-CG-CD	29.86	179.97	111.30
1	A	983	ARG	CB-CG-CD	29.86	179.97	111.30
1	A	63	THR	CA-CB-OG1	29.32	153.58	109.60
1	B	63	THR	CA-CB-OG1	29.29	153.54	109.60
1	C	63	THR	CA-CB-OG1	29.29	153.54	109.60
1	C	63	THR	OG1-CB-CG2	-27.03	55.24	109.30
1	A	63	THR	OG1-CB-CG2	-27.03	55.24	109.30
1	B	63	THR	OG1-CB-CG2	-27.03	55.25	109.30
1	A	1113	GLN	CG-CD-OE1	-26.66	67.49	120.80
1	C	1113	GLN	CG-CD-OE1	-26.65	67.49	120.80
1	B	1113	GLN	CG-CD-OE1	-26.64	67.53	120.80
1	A	187	LYS	CB-CG-CD	24.91	168.59	111.30
1	C	187	LYS	CB-CG-CD	24.89	168.55	111.30
1	B	187	LYS	CB-CG-CD	24.87	168.50	111.30
1	C	947	LYS	CA-CB-CG	24.66	163.42	114.10
1	A	947	LYS	CA-CB-CG	24.65	163.39	114.10
1	B	947	LYS	CA-CB-CG	24.64	163.38	114.10
1	A	600	PRO	N-CD-CG	-24.21	66.88	103.20
1	B	600	PRO	N-CD-CG	-24.21	66.88	103.20
1	C	600	PRO	N-CD-CG	-24.19	66.92	103.20
1	C	901	GLN	OE1-CD-NE2	-22.75	99.85	122.60
1	A	901	GLN	OE1-CD-NE2	-22.69	99.91	122.60
1	B	901	GLN	OE1-CD-NE2	-22.67	99.93	122.60
1	A	651	ILE	CA-CB-CG1	22.38	148.44	110.40
1	C	651	ILE	CA-CB-CG1	22.37	148.43	110.40
1	B	651	ILE	CA-CB-CG1	22.36	148.42	110.40
1	A	187	LYS	CG-CD-CE	-21.13	62.69	111.30
1	B	187	LYS	CG-CD-CE	-21.13	62.70	111.30
1	C	187	LYS	CG-CD-CE	-21.12	62.73	111.30
1	C	318	PHE	CA-CB-CG	20.75	134.55	113.80
1	B	318	PHE	CA-CB-CG	20.75	134.55	113.80
1	A	318	PHE	CA-CB-CG	20.73	134.53	113.80
1	B	947	LYS	N-CA-CB	-20.70	78.19	110.28
1	A	947	LYS	N-CA-CB	-20.70	78.20	110.28
1	C	947	LYS	N-CA-CB	-20.69	78.21	110.28
1	A	304	LYS	CB-CG-CD	19.98	157.26	111.30
1	B	304	LYS	CB-CG-CD	19.97	157.23	111.30
1	C	304	LYS	CB-CG-CD	19.95	157.18	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	PHE	CD1-CG-CD2	-19.87	88.80	118.60
1	C	318	PHE	CD1-CG-CD2	-19.87	88.80	118.60
1	A	318	PHE	CD1-CG-CD2	-19.86	88.81	118.60
1	A	901	GLN	CG-CD-NE2	-19.62	86.97	116.40
1	C	901	GLN	CG-CD-NE2	-19.60	87.00	116.40
1	B	901	GLN	CG-CD-NE2	-19.59	87.02	116.40
1	A	52	GLN	CA-CB-CG	19.31	152.71	114.10
1	B	52	GLN	CA-CB-CG	19.29	152.69	114.10
1	C	52	GLN	CA-CB-CG	19.28	152.67	114.10
1	B	651	ILE	CB-CG1-CD1	-19.15	73.59	113.80
1	B	171	VAL	CA-CB-CG1	19.14	142.94	110.40
1	A	171	VAL	CA-CB-CG1	19.14	142.93	110.40
1	A	651	ILE	CB-CG1-CD1	-19.14	73.61	113.80
1	C	651	ILE	CB-CG1-CD1	-19.13	73.63	113.80
1	C	171	VAL	CA-CB-CG1	19.12	142.91	110.40
1	B	1071	GLN	CG-CD-NE2	-19.04	87.84	116.40
1	A	1071	GLN	CG-CD-NE2	-18.99	87.91	116.40
1	C	1071	GLN	CG-CD-NE2	-18.99	87.91	116.40
1	B	948	LEU	N-CA-CB	-18.97	81.99	110.26
1	C	948	LEU	N-CA-CB	-18.96	82.01	110.26
1	A	948	LEU	N-CA-CB	-18.93	82.05	110.26
1	B	774	GLN	OE1-CD-NE2	-18.89	103.72	122.60
1	A	774	GLN	OE1-CD-NE2	-18.83	103.77	122.60
1	C	774	GLN	OE1-CD-NE2	-18.83	103.77	122.60
1	A	231	ILE	CA-CB-CG1	18.44	141.75	110.40
1	C	231	ILE	CA-CB-CG1	18.42	141.72	110.40
1	B	231	ILE	CA-CB-CG1	18.37	141.64	110.40
1	A	42	VAL	CG1-CB-CG2	-17.87	71.48	110.80
1	C	1083	HIS	CE1-NE2-CD2	-17.86	91.14	109.00
1	C	42	VAL	CG1-CB-CG2	-17.85	71.52	110.80
1	B	42	VAL	CG1-CB-CG2	-17.84	71.55	110.80
1	A	1083	HIS	CE1-NE2-CD2	-17.82	91.18	109.00
1	B	1083	HIS	CE1-NE2-CD2	-17.80	91.19	109.00
1	B	78	ARG	NE-CZ-NH1	-17.68	103.82	121.50
1	C	78	ARG	NE-CZ-NH1	-17.64	103.86	121.50
1	A	78	ARG	NE-CZ-NH1	-17.64	103.86	121.50
1	A	153	MET	CG-SD-CE	17.50	139.39	100.90
1	B	153	MET	CG-SD-CE	17.48	139.36	100.90
1	C	153	MET	CG-SD-CE	17.48	139.36	100.90
1	B	231	ILE	CA-CB-CG2	-17.13	81.38	110.50
1	C	231	ILE	CA-CB-CG2	-17.11	81.42	110.50
1	A	231	ILE	CA-CB-CG2	-17.09	81.44	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	LYS	CB-CA-C	-17.07	81.77	110.44
1	A	41	LYS	CB-CA-C	-17.06	81.78	110.44
1	C	41	LYS	CB-CA-C	-17.05	81.79	110.44
1	C	133	PHE	CB-CG-CD2	-16.86	92.04	120.70
1	B	133	PHE	CB-CG-CD2	-16.85	92.05	120.70
1	A	133	PHE	CB-CG-CD2	-16.84	92.07	120.70
1	B	231	ILE	CG1-CB-CG2	-16.81	60.26	110.70
1	C	231	ILE	CG1-CB-CG2	-16.80	60.30	110.70
1	A	231	ILE	CG1-CB-CG2	-16.79	60.32	110.70
1	A	811	LYS	CG-CD-CE	16.53	149.31	111.30
1	B	811	LYS	CG-CD-CE	16.52	149.29	111.30
1	C	811	LYS	CG-CD-CE	16.50	149.25	111.30
1	A	954	GLN	OE1-CD-NE2	-16.37	106.23	122.60
1	C	774	GLN	CB-CG-CD	16.32	140.35	112.60
1	A	774	GLN	CB-CG-CD	16.32	140.34	112.60
1	B	774	GLN	CB-CG-CD	16.31	140.33	112.60
1	C	954	GLN	OE1-CD-NE2	-16.31	106.29	122.60
1	B	954	GLN	OE1-CD-NE2	-16.31	106.29	122.60
1	C	983	ARG	NE-CZ-NH2	-16.29	104.54	119.20
1	A	983	ARG	NE-CZ-NH2	-16.26	104.57	119.20
1	B	983	ARG	NE-CZ-NH2	-16.21	104.61	119.20
1	B	948	LEU	CA-CB-CG	15.91	171.98	116.30
1	A	948	LEU	CA-CB-CG	15.89	171.92	116.30
1	C	948	LEU	CA-CB-CG	15.88	171.89	116.30
1	A	40	ASP	CA-C-N	-15.78	96.99	122.08
1	A	40	ASP	C-N-CA	-15.78	96.99	122.08
1	B	40	ASP	CA-C-N	-15.78	97.00	122.08
1	B	40	ASP	C-N-CA	-15.78	97.00	122.08
1	C	40	ASP	CA-C-N	-15.76	97.02	122.08
1	C	40	ASP	C-N-CA	-15.76	97.02	122.08
1	A	611	LEU	CD1-CG-CD2	-15.53	76.63	110.80
1	B	611	LEU	CD1-CG-CD2	-15.52	76.66	110.80
1	C	611	LEU	CD1-CG-CD2	-15.51	76.67	110.80
1	B	1014	ARG	CG-CD-NE	15.41	145.91	112.00
1	C	1014	ARG	CG-CD-NE	15.41	145.90	112.00
1	A	1014	ARG	CG-CD-NE	15.41	145.90	112.00
1	B	1002	GLN	CA-CB-CG	15.23	144.56	114.10
1	A	1002	GLN	CA-CB-CG	15.22	144.54	114.10
1	B	1002	GLN	OE1-CD-NE2	-15.21	107.39	122.60
1	C	1002	GLN	OE1-CD-NE2	-15.20	107.40	122.60
1	C	1002	GLN	CA-CB-CG	15.20	144.50	114.10
1	A	1002	GLN	OE1-CD-NE2	-15.16	107.44	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	723	THR	CA-CB-OG1	14.87	131.90	109.60
1	B	723	THR	CA-CB-OG1	14.84	131.87	109.60
1	A	723	THR	CA-CB-OG1	14.81	131.81	109.60
1	B	983	ARG	CA-CB-CG	14.65	143.39	114.10
1	A	983	ARG	CA-CB-CG	14.64	143.38	114.10
1	C	983	ARG	CA-CB-CG	14.64	143.38	114.10
1	C	233	ILE	CG1-CB-CG2	-14.55	67.05	110.70
1	B	233	ILE	CG1-CB-CG2	-14.55	67.06	110.70
1	A	233	ILE	CG1-CB-CG2	-14.54	67.08	110.70
1	A	926	GLN	CA-CB-CG	14.51	143.11	114.10
1	C	99	ASN	OD1-CG-ND2	-14.47	108.13	122.60
1	C	926	GLN	CA-CB-CG	14.47	143.04	114.10
1	B	926	GLN	CA-CB-CG	14.46	143.03	114.10
1	A	99	ASN	OD1-CG-ND2	-14.44	108.16	122.60
1	B	99	ASN	OD1-CG-ND2	-14.34	108.26	122.60
1	C	600	PRO	CA-N-CD	-14.26	92.03	112.00
1	B	237	ARG	CD-NE-CZ	14.25	144.35	124.40
1	C	237	ARG	CD-NE-CZ	14.25	144.35	124.40
1	A	600	PRO	CA-N-CD	-14.25	92.05	112.00
1	A	237	ARG	CD-NE-CZ	14.24	144.34	124.40
1	B	600	PRO	CA-N-CD	-14.24	92.06	112.00
1	C	1002	GLN	CG-CD-NE2	-14.13	95.20	116.40
1	B	1002	GLN	CG-CD-NE2	-14.13	95.21	116.40
1	B	925	ASN	CB-CG-ND2	-14.08	95.28	116.40
1	A	1002	GLN	CG-CD-NE2	-14.08	95.28	116.40
1	C	925	ASN	CB-CG-ND2	-14.07	95.29	116.40
1	A	925	ASN	CB-CG-ND2	-14.06	95.31	116.40
1	B	1083	HIS	ND1-CG-CD2	-13.95	92.15	106.10
1	A	1083	HIS	ND1-CG-CD2	-13.95	92.16	106.10
1	C	1083	HIS	ND1-CG-CD2	-13.92	92.18	106.10
1	B	133	PHE	CB-CG-CD1	13.86	144.25	120.70
1	A	133	PHE	CB-CG-CD1	13.85	144.25	120.70
1	C	133	PHE	CB-CG-CD1	13.81	144.18	120.70
1	B	946	GLY	CA-C-N	13.77	141.24	120.31
1	B	946	GLY	C-N-CA	13.77	141.24	120.31
1	C	946	GLY	CA-C-N	13.76	141.22	120.31
1	C	946	GLY	C-N-CA	13.76	141.22	120.31
1	A	946	GLY	CA-C-N	13.75	141.21	120.31
1	A	946	GLY	C-N-CA	13.75	141.21	120.31
1	A	52	GLN	CG-CD-NE2	-13.59	96.01	116.40
1	B	608	VAL	CG1-CB-CG2	-13.57	80.94	110.80
1	A	608	VAL	CG1-CB-CG2	-13.56	80.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	608	VAL	CG1-CB-CG2	-13.56	80.97	110.80
1	C	52	GLN	CG-CD-NE2	-13.54	96.09	116.40
1	B	52	GLN	CG-CD-NE2	-13.54	96.09	116.40
1	C	901	GLN	CG-CD-OE1	13.51	147.82	120.80
1	B	901	GLN	CG-CD-OE1	13.51	147.82	120.80
1	A	901	GLN	CG-CD-OE1	13.49	147.79	120.80
1	B	651	ILE	CG1-CB-CG2	-13.48	70.25	110.70
1	C	651	ILE	CG1-CB-CG2	-13.48	70.25	110.70
1	A	651	ILE	CG1-CB-CG2	-13.48	70.27	110.70
1	B	1129	VAL	CG1-CB-CG2	-13.46	81.18	110.80
1	A	1129	VAL	CG1-CB-CG2	-13.46	81.19	110.80
1	C	1129	VAL	CG1-CB-CG2	-13.45	81.22	110.80
1	A	305	SER	CA-CB-OG	13.42	137.94	111.10
1	C	305	SER	CA-CB-OG	13.41	137.92	111.10
1	B	305	SER	CA-CB-OG	13.41	137.91	111.10
1	B	1083	HIS	ND1-CE1-NE2	-13.37	95.03	108.40
1	A	99	ASN	CB-CG-ND2	-13.34	96.40	116.40
1	A	1083	HIS	ND1-CE1-NE2	-13.33	95.07	108.40
1	B	99	ASN	CB-CG-ND2	-13.32	96.42	116.40
1	C	99	ASN	CB-CG-ND2	-13.32	96.42	116.40
1	A	41	LYS	CG-CD-CE	-13.32	80.67	111.30
1	A	318	PHE	CB-CG-CD1	13.31	143.33	120.70
1	B	41	LYS	CG-CD-CE	-13.31	80.69	111.30
1	C	41	LYS	CG-CD-CE	-13.31	80.69	111.30
1	C	1083	HIS	ND1-CE1-NE2	-13.31	95.09	108.40
1	B	318	PHE	CB-CG-CD1	13.27	143.26	120.70
1	A	861	LEU	CB-CG-CD1	13.25	150.44	110.70
1	C	318	PHE	CB-CG-CD1	13.24	143.21	120.70
1	B	861	LEU	CB-CG-CD1	13.23	150.40	110.70
1	C	861	LEU	CB-CG-CD1	13.22	150.37	110.70
1	B	318	PHE	N-CA-CB	13.02	128.35	110.38
1	A	318	PHE	N-CA-CB	13.01	128.34	110.38
1	C	318	PHE	N-CA-CB	13.01	128.34	110.38
1	B	186	PHE	CA-C-N	-12.80	101.95	121.53
1	B	186	PHE	C-N-CA	-12.80	101.95	121.53
1	A	186	PHE	CA-C-N	-12.78	101.97	121.53
1	A	186	PHE	C-N-CA	-12.78	101.97	121.53
1	C	186	PHE	CA-C-N	-12.77	101.99	121.53
1	C	186	PHE	C-N-CA	-12.77	101.99	121.53
1	A	959	LEU	CA-CB-CG	12.76	160.96	116.30
1	B	959	LEU	CA-CB-CG	12.75	160.92	116.30
1	C	959	LEU	CA-CB-CG	12.74	160.89	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ILE	CB-CG1-CD1	12.68	140.43	113.80
1	C	231	ILE	CB-CG1-CD1	12.65	140.38	113.80
1	B	231	ILE	CB-CG1-CD1	12.65	140.37	113.80
1	A	237	ARG	NH1-CZ-NH2	-12.65	102.86	119.30
1	C	237	ARG	NH1-CZ-NH2	-12.65	102.85	119.30
1	B	237	ARG	NH1-CZ-NH2	-12.60	102.92	119.30
1	C	1113	GLN	OE1-CD-NE2	-12.58	110.02	122.60
1	B	195	LYS	CB-CG-CD	12.56	140.19	111.30
1	A	195	LYS	CB-CG-CD	12.55	140.17	111.30
1	B	237	ARG	CB-CG-CD	12.55	140.17	111.30
1	A	237	ARG	CB-CG-CD	12.54	140.15	111.30
1	B	1113	GLN	OE1-CD-NE2	-12.53	110.07	122.60
1	C	237	ARG	CB-CG-CD	12.53	140.12	111.30
1	C	195	LYS	CB-CG-CD	12.51	140.08	111.30
1	B	1071	GLN	OE1-CD-NE2	12.48	135.08	122.60
1	C	1071	GLN	OE1-CD-NE2	12.48	135.08	122.60
1	A	1071	GLN	OE1-CD-NE2	12.48	135.08	122.60
1	B	726	ILE	N-CA-C	-12.45	90.74	108.17
1	A	1113	GLN	OE1-CD-NE2	-12.44	110.16	122.60
1	C	726	ILE	N-CA-C	-12.43	90.77	108.17
1	A	726	ILE	N-CA-C	-12.42	90.78	108.17
1	B	246	ARG	NE-CZ-NH2	-12.33	108.11	119.20
1	C	246	ARG	NE-CZ-NH2	-12.28	108.15	119.20
1	A	246	ARG	NE-CZ-NH2	-12.27	108.16	119.20
1	B	197	ILE	CA-CB-CG1	12.21	131.15	110.40
1	C	197	ILE	CA-CB-CG1	12.20	131.15	110.40
1	A	197	ILE	CA-CB-CG1	12.20	131.14	110.40
1	A	212	LEU	CB-CG-CD1	12.15	147.16	110.70
1	C	1129	VAL	CA-CB-CG1	12.15	131.06	110.40
1	A	1129	VAL	CA-CB-CG1	12.15	131.05	110.40
1	C	212	LEU	CB-CG-CD1	12.15	147.14	110.70
1	B	1129	VAL	CA-CB-CG1	12.14	131.05	110.40
1	B	212	LEU	CB-CG-CD1	12.14	147.13	110.70
1	C	861	LEU	CD1-CG-CD2	-12.13	84.10	110.80
1	B	861	LEU	CD1-CG-CD2	-12.13	84.12	110.80
1	A	861	LEU	CD1-CG-CD2	-12.13	84.12	110.80
1	B	187	LYS	N-CA-C	-12.13	96.10	110.41
1	A	187	LYS	N-CA-C	-12.10	96.13	110.41
1	C	187	LYS	N-CA-C	-12.09	96.14	110.41
1	C	948	LEU	CB-CG-CD2	-11.99	74.74	110.70
1	B	948	LEU	CB-CG-CD2	-11.98	74.76	110.70
1	A	948	LEU	CB-CG-CD2	-11.98	74.76	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	922	LEU	CB-CG-CD2	11.94	146.51	110.70
1	B	922	LEU	CB-CG-CD2	11.93	146.49	110.70
1	C	922	LEU	CB-CG-CD2	11.91	146.42	110.70
1	C	774	GLN	CG-CD-OE1	11.84	144.47	120.80
1	A	774	GLN	CG-CD-OE1	11.82	144.45	120.80
1	B	774	GLN	CG-CD-OE1	11.82	144.44	120.80
1	B	861	LEU	CB-CG-CD2	-11.75	75.45	110.70
1	C	861	LEU	CB-CG-CD2	-11.75	75.45	110.70
1	A	861	LEU	CB-CG-CD2	-11.74	75.49	110.70
1	A	872	GLN	CB-CG-CD	11.71	132.50	112.60
1	C	206	LYS	CB-CG-CD	11.70	138.20	111.30
1	C	872	GLN	CB-CG-CD	11.68	132.46	112.60
1	B	206	LYS	CB-CG-CD	11.68	138.16	111.30
1	B	872	GLN	CB-CG-CD	11.67	132.44	112.60
1	A	206	LYS	CB-CG-CD	11.66	138.13	111.30
1	B	790	LYS	CD-CE-NZ	11.66	149.21	111.90
1	A	790	LYS	CD-CE-NZ	11.65	149.17	111.90
1	C	790	LYS	CD-CE-NZ	11.64	149.15	111.90
1	A	78	ARG	CB-CG-CD	-11.62	84.57	111.30
1	C	78	ARG	CB-CG-CD	-11.62	84.57	111.30
1	B	78	ARG	CB-CG-CD	-11.62	84.58	111.30
1	B	925	ASN	CA-CB-CG	11.62	124.22	112.60
1	A	925	ASN	CA-CB-CG	11.61	124.20	112.60
1	A	922	LEU	CA-CB-CG	11.57	156.81	116.30
1	C	925	ASN	CA-CB-CG	11.57	124.17	112.60
1	B	922	LEU	CA-CB-CG	11.56	156.78	116.30
1	C	922	LEU	CA-CB-CG	11.56	156.76	116.30
1	B	767	LEU	CB-CG-CD1	11.49	145.16	110.70
1	B	177	MET	CG-SD-CE	11.47	126.14	100.90
1	A	767	LEU	CB-CG-CD1	11.47	145.10	110.70
1	C	767	LEU	CB-CG-CD1	11.46	145.09	110.70
1	C	177	MET	CG-SD-CE	11.44	126.07	100.90
1	A	177	MET	CG-SD-CE	11.44	126.06	100.90
1	C	712	ILE	CB-CG1-CD1	11.26	137.46	113.80
1	C	726	ILE	CG1-CB-CG2	-11.24	76.98	110.70
1	A	712	ILE	CB-CG1-CD1	11.24	137.40	113.80
1	B	712	ILE	CB-CG1-CD1	11.23	137.39	113.80
1	A	41	LYS	N-CA-C	-11.23	96.29	113.02
1	B	41	LYS	N-CA-C	-11.23	96.29	113.02
1	C	197	ILE	CG1-CB-CG2	-11.22	77.03	110.70
1	A	197	ILE	CG1-CB-CG2	-11.22	77.04	110.70
1	A	726	ILE	CG1-CB-CG2	-11.22	77.04	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	LYS	N-CA-C	-11.22	96.30	113.02
1	B	197	ILE	CG1-CB-CG2	-11.22	77.05	110.70
1	B	726	ILE	CG1-CB-CG2	-11.21	77.05	110.70
1	C	1050	MET	CB-CG-SD	11.19	146.28	112.70
1	A	1050	MET	CB-CG-SD	11.18	146.25	112.70
1	B	1050	MET	CB-CG-SD	11.18	146.23	112.70
1	A	923	ILE	CB-CA-C	11.14	126.64	112.04
1	B	923	ILE	CB-CA-C	11.14	126.63	112.04
1	C	923	ILE	CB-CA-C	11.13	126.62	112.04
1	C	133	PHE	CD1-CG-CD2	-11.06	102.02	118.60
1	A	133	PHE	CD1-CG-CD2	-11.04	102.04	118.60
1	B	133	PHE	CD1-CG-CD2	-11.04	102.04	118.60
1	B	811	LYS	CD-CE-NZ	10.99	147.07	111.90
1	A	811	LYS	CD-CE-NZ	10.98	147.05	111.90
1	B	1113	GLN	CB-CG-CD	10.98	131.26	112.60
1	C	811	LYS	CD-CE-NZ	10.98	147.03	111.90
1	B	926	GLN	CB-CG-CD	10.97	131.24	112.60
1	C	926	GLN	CB-CG-CD	10.96	131.24	112.60
1	A	926	GLN	CB-CG-CD	10.96	131.22	112.60
1	A	1113	GLN	CB-CG-CD	10.95	131.22	112.60
1	C	1113	GLN	CB-CG-CD	10.95	131.21	112.60
1	C	1083	HIS	CB-CG-ND1	10.92	139.08	122.70
1	B	1083	HIS	CB-CG-ND1	10.89	139.04	122.70
1	A	1083	HIS	CB-CG-ND1	10.89	139.04	122.70
1	B	187	LYS	CA-CB-CG	10.87	135.84	114.10
1	A	187	LYS	CA-CB-CG	10.87	135.83	114.10
1	C	278	LYS	CB-CG-CD	10.86	136.28	111.30
1	C	187	LYS	CA-CB-CG	10.85	135.81	114.10
1	B	278	LYS	CB-CG-CD	10.85	136.26	111.30
1	A	278	LYS	CB-CG-CD	10.83	136.21	111.30
1	B	1114	ILE	CG1-CB-CG2	-10.83	78.21	110.70
1	C	1114	ILE	CG1-CB-CG2	-10.83	78.22	110.70
1	A	1114	ILE	CG1-CB-CG2	-10.82	78.23	110.70
1	B	765	ARG	CD-NE-CZ	-10.74	109.36	124.40
1	C	765	ARG	CD-NE-CZ	-10.73	109.37	124.40
1	A	765	ARG	CD-NE-CZ	-10.73	109.38	124.40
1	C	948	LEU	CB-CA-C	10.69	130.31	110.11
1	A	948	LEU	CB-CA-C	10.67	130.28	110.11
1	B	948	LEU	CB-CA-C	10.66	130.26	110.11
1	A	304	LYS	N-CA-C	10.59	125.78	112.86
1	A	600	PRO	CA-CB-CG	-10.58	84.40	104.50
1	B	206	LYS	CA-CB-CG	10.57	135.24	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	LYS	CA-CB-CG	10.57	135.24	114.10
1	B	600	PRO	CA-CB-CG	-10.56	84.43	104.50
1	C	600	PRO	CA-CB-CG	-10.55	84.45	104.50
1	B	304	LYS	N-CA-C	10.54	125.72	112.86
1	A	206	LYS	CA-CB-CG	10.53	135.17	114.10
1	C	304	LYS	N-CA-C	10.53	125.70	112.86
1	C	1071	GLN	CB-CG-CD	10.51	130.47	112.60
1	B	1071	GLN	CB-CG-CD	10.51	130.46	112.60
1	A	1071	GLN	CB-CG-CD	10.51	130.46	112.60
1	A	651	ILE	CB-CA-C	10.46	127.42	110.69
1	C	651	ILE	CB-CA-C	10.45	127.40	110.69
1	B	651	ILE	CB-CA-C	10.44	127.40	110.69
1	C	1005	GLN	CB-CG-CD	-10.38	94.95	112.60
1	B	187	LYS	CB-CA-C	-10.38	94.22	111.24
1	C	187	LYS	CB-CA-C	-10.37	94.23	111.24
1	A	1005	GLN	CB-CG-CD	-10.36	94.99	112.60
1	B	1005	GLN	CB-CG-CD	-10.36	94.99	112.60
1	A	187	LYS	CB-CA-C	-10.36	94.26	111.24
1	A	246	ARG	CD-NE-CZ	10.33	138.86	124.40
1	B	231	ILE	CB-CA-C	-10.31	99.63	111.80
1	B	246	ARG	CD-NE-CZ	10.31	138.84	124.40
1	C	246	ARG	CD-NE-CZ	10.30	138.82	124.40
1	B	947	LYS	CB-CA-C	10.23	130.31	110.67
1	C	947	LYS	CB-CA-C	10.22	130.29	110.67
1	A	947	LYS	CB-CA-C	10.22	130.28	110.67
1	C	1145	LEU	CD1-CG-CD2	-10.08	88.62	110.80
1	B	1145	LEU	CD1-CG-CD2	-10.07	88.64	110.80
1	A	1145	LEU	CD1-CG-CD2	-10.07	88.65	110.80
1	A	1101	HIS	CA-CB-CG	-10.03	103.77	113.80
1	C	1101	HIS	CA-CB-CG	-10.01	103.79	113.80
1	B	1101	HIS	CA-CB-CG	-10.01	103.79	113.80
1	C	901	GLN	CA-CB-CG	9.96	134.03	114.10
1	A	901	GLN	CA-CB-CG	9.96	134.02	114.10
1	B	113	LYS	CD-CE-NZ	9.95	143.75	111.90
1	B	901	GLN	CA-CB-CG	9.95	134.00	114.10
1	C	113	LYS	CD-CE-NZ	9.95	143.75	111.90
1	A	113	LYS	CD-CE-NZ	9.94	143.71	111.90
1	B	41	LYS	O-C-N	-9.86	109.78	122.20
1	A	41	LYS	O-C-N	-9.85	109.79	122.20
1	C	726	ILE	CB-CG1-CD1	-9.85	93.12	113.80
1	A	726	ILE	CB-CG1-CD1	-9.84	93.14	113.80
1	C	41	LYS	O-C-N	-9.84	109.81	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	726	ILE	CB-CG1-CD1	-9.83	93.17	113.80
1	A	723	THR	CA-CB-CG2	-9.71	93.99	110.50
1	B	723	THR	CA-CB-CG2	-9.70	94.01	110.50
1	C	723	THR	CA-CB-CG2	-9.70	94.02	110.50
1	B	767	LEU	CB-CG-CD2	-9.64	81.78	110.70
1	C	767	LEU	CB-CG-CD2	-9.64	81.79	110.70
1	A	767	LEU	CB-CG-CD2	-9.64	81.79	110.70
1	C	44	ARG	CB-CG-CD	9.60	133.37	111.30
1	A	44	ARG	CB-CG-CD	9.57	133.31	111.30
1	B	44	ARG	CB-CG-CD	9.57	133.31	111.30
1	B	43	PHE	N-CA-CB	9.56	124.09	110.04
1	C	43	PHE	N-CA-CB	9.56	124.09	110.04
1	A	1145	LEU	CB-CG-CD2	-9.55	82.06	110.70
1	A	43	PHE	N-CA-CB	9.54	124.06	110.04
1	B	1145	LEU	CB-CG-CD2	-9.54	82.08	110.70
1	A	1050	MET	CA-CB-CG	-9.53	95.03	114.10
1	C	1145	LEU	CB-CG-CD2	-9.53	82.10	110.70
1	B	1050	MET	CA-CB-CG	-9.53	95.05	114.10
1	C	1050	MET	CA-CB-CG	-9.52	95.06	114.10
1	C	811	LYS	CA-CB-CG	9.47	133.05	114.10
1	B	811	LYS	CA-CB-CG	9.47	133.04	114.10
1	A	811	LYS	CA-CB-CG	9.46	133.03	114.10
1	A	1083	HIS	CG-ND1-CE1	-9.41	93.30	109.30
1	B	651	ILE	CA-CB-CG2	-9.38	94.55	110.50
1	A	651	ILE	CA-CB-CG2	-9.38	94.55	110.50
1	C	1083	HIS	CG-ND1-CE1	-9.38	93.35	109.30
1	C	651	ILE	CA-CB-CG2	-9.38	94.56	110.50
1	C	195	LYS	CA-CB-CG	9.37	132.84	114.10
1	B	1083	HIS	CG-ND1-CE1	-9.37	93.37	109.30
1	A	195	LYS	CA-CB-CG	9.37	132.83	114.10
1	B	195	LYS	CA-CB-CG	9.37	132.83	114.10
1	B	765	ARG	CG-CD-NE	9.35	132.56	112.00
1	A	719	THR	OG1-CB-CG2	-9.34	90.62	109.30
1	A	765	ARG	CG-CD-NE	9.34	132.56	112.00
1	C	765	ARG	CG-CD-NE	9.33	132.53	112.00
1	C	329	PHE	N-CA-C	9.32	116.36	108.07
1	C	719	THR	OG1-CB-CG2	-9.32	90.66	109.30
1	B	719	THR	OG1-CB-CG2	-9.31	90.67	109.30
1	C	650	LEU	CB-CG-CD2	-9.25	82.94	110.70
1	B	650	LEU	CB-CG-CD2	-9.25	82.94	110.70
1	A	650	LEU	CB-CG-CD2	-9.25	82.96	110.70
1	A	947	LYS	CB-CG-CD	9.14	132.32	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	947	LYS	CB-CG-CD	9.13	132.30	111.30
1	C	947	LYS	CB-CG-CD	9.12	132.27	111.30
1	A	948	LEU	N-CA-C	-9.11	99.78	112.45
1	B	948	LEU	N-CA-C	-9.11	99.79	112.45
1	C	948	LEU	N-CA-C	-9.09	99.81	112.45
1	C	42	VAL	CA-CB-CG1	-9.03	95.04	110.40
1	A	42	VAL	CA-CB-CG1	-9.01	95.08	110.40
1	B	42	VAL	CA-CB-CG1	-9.01	95.09	110.40
1	A	1014	ARG	N-CA-CB	-8.99	96.98	110.01
1	C	233	ILE	N-CA-C	-8.96	95.72	108.80
1	B	1014	ARG	N-CA-CB	-8.95	97.03	110.01
1	C	1014	ARG	N-CA-CB	-8.95	97.04	110.01
1	A	233	ILE	N-CA-C	-8.92	95.78	108.80
1	B	233	ILE	N-CA-C	-8.91	95.79	108.80
1	C	767	LEU	CA-CB-CG	8.85	147.28	116.30
1	C	954	GLN	CB-CG-CD	8.85	127.64	112.60
1	A	767	LEU	CA-CB-CG	8.84	147.25	116.30
1	B	767	LEU	CA-CB-CG	8.84	147.25	116.30
1	A	954	GLN	CB-CG-CD	8.83	127.61	112.60
1	B	954	GLN	CB-CG-CD	8.83	127.61	112.60
1	B	233	ILE	CA-CB-CG1	8.81	125.38	110.40
1	B	318	PHE	CB-CG-CD2	-8.80	105.74	120.70
1	A	318	PHE	CB-CG-CD2	-8.80	105.74	120.70
1	A	233	ILE	CA-CB-CG1	8.79	125.34	110.40
1	C	318	PHE	CB-CG-CD2	-8.79	105.76	120.70
1	C	233	ILE	CA-CB-CG1	8.76	125.30	110.40
1	C	246	ARG	CG-CD-NE	8.70	131.13	112.00
1	A	246	ARG	CG-CD-NE	8.69	131.11	112.00
1	B	246	ARG	CG-CD-NE	8.69	131.11	112.00
1	B	78	ARG	CG-CD-NE	8.67	131.08	112.00
1	C	78	ARG	CG-CD-NE	8.67	131.08	112.00
1	A	78	ARG	CG-CD-NE	8.67	131.07	112.00
1	A	983	ARG	CG-CD-NE	8.63	130.99	112.00
1	B	983	ARG	CG-CD-NE	8.62	130.97	112.00
1	A	1013	ILE	CA-CB-CG1	8.62	125.05	110.40
1	C	905	ARG	CG-CD-NE	8.62	130.96	112.00
1	C	1113	GLN	CB-CA-C	8.62	127.57	110.42
1	B	905	ARG	CG-CD-NE	8.62	130.96	112.00
1	B	1013	ILE	CA-CB-CG1	8.61	125.04	110.40
1	A	905	ARG	CG-CD-NE	8.61	130.95	112.00
1	C	983	ARG	CG-CD-NE	8.61	130.94	112.00
1	A	1113	GLN	CB-CA-C	8.60	127.54	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1113	GLN	CB-CA-C	8.60	127.54	110.42
1	C	1013	ILE	CA-CB-CG1	8.60	125.02	110.40
1	B	1086	LYS	CD-CE-NZ	8.60	139.40	111.90
1	C	1086	LYS	CD-CE-NZ	8.59	139.39	111.90
1	A	1086	LYS	CD-CE-NZ	8.58	139.35	111.90
1	C	942	PRO	CA-N-CD	-8.55	100.03	112.00
1	A	942	PRO	CA-N-CD	-8.54	100.05	112.00
1	B	942	PRO	CA-N-CD	-8.53	100.05	112.00
1	A	774	GLN	CB-CA-C	8.52	124.80	109.29
1	B	774	GLN	CB-CA-C	8.52	124.80	109.29
1	A	723	THR	N-CA-CB	-8.52	96.86	111.69
1	C	723	THR	N-CA-CB	-8.52	96.87	111.69
1	C	774	GLN	CB-CA-C	8.49	124.74	109.29
1	B	723	THR	N-CA-CB	-8.48	96.93	111.69
1	A	1085	GLY	CA-C-N	8.42	136.76	121.94
1	A	1085	GLY	C-N-CA	8.42	136.76	121.94
1	B	1085	GLY	CA-C-N	8.40	136.73	121.94
1	B	1085	GLY	C-N-CA	8.40	136.73	121.94
1	C	1085	GLY	CA-C-N	8.40	136.72	121.94
1	C	1085	GLY	C-N-CA	8.40	136.72	121.94
1	B	922	LEU	N-CA-CB	8.37	123.95	109.72
1	C	922	LEU	N-CA-CB	8.35	123.92	109.72
1	A	922	LEU	N-CA-CB	8.35	123.91	109.72
1	C	925	ASN	OD1-CG-ND2	-8.35	114.25	122.60
1	C	983	ARG	N-CA-C	8.31	126.08	113.61
1	B	925	ASN	OD1-CG-ND2	-8.31	114.29	122.60
1	A	983	ARG	N-CA-C	8.29	126.04	113.61
1	A	925	ASN	OD1-CG-ND2	-8.28	114.32	122.60
1	A	42	VAL	CB-CA-C	-8.27	100.62	111.13
1	B	983	ARG	N-CA-C	8.27	126.02	113.61
1	A	312	ILE	CG1-CB-CG2	-8.27	85.90	110.70
1	B	312	ILE	CG1-CB-CG2	-8.27	85.90	110.70
1	C	312	ILE	CG1-CB-CG2	-8.25	85.95	110.70
1	B	1012	LEU	CA-CB-CG	8.24	145.14	116.30
1	C	1012	LEU	CA-CB-CG	8.23	145.12	116.30
1	A	1012	LEU	CA-CB-CG	8.23	145.11	116.30
1	A	712	ILE	CA-CB-CG1	8.23	124.39	110.40
1	C	42	VAL	CB-CA-C	-8.23	100.68	111.13
1	B	42	VAL	CB-CA-C	-8.22	100.68	111.13
1	B	712	ILE	CA-CB-CG1	8.22	124.37	110.40
1	C	44	ARG	NH1-CZ-NH2	-8.22	108.62	119.30
1	A	44	ARG	NH1-CZ-NH2	-8.21	108.62	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	712	ILE	CA-CB-CG1	8.21	124.36	110.40
1	B	44	ARG	NH1-CZ-NH2	-8.20	108.64	119.30
1	C	954	GLN	CG-CD-NE2	-8.20	104.10	116.40
1	B	954	GLN	CG-CD-NE2	-8.20	104.11	116.40
1	A	767	LEU	CB-CA-C	8.18	127.09	109.99
1	C	767	LEU	CB-CA-C	8.18	127.09	109.99
1	B	281	GLU	CB-CG-CD	8.17	126.50	112.60
1	A	281	GLU	CB-CG-CD	8.16	126.47	112.60
1	B	767	LEU	CB-CA-C	8.15	127.03	109.99
1	A	954	GLN	CG-CD-NE2	-8.14	104.19	116.40
1	C	281	GLU	CB-CG-CD	8.13	126.43	112.60
1	B	755	GLN	CG-CD-NE2	-8.12	104.22	116.40
1	C	1122	VAL	CG1-CB-CG2	-8.09	93.00	110.80
1	A	1122	VAL	CG1-CB-CG2	-8.09	93.01	110.80
1	C	755	GLN	CG-CD-NE2	-8.09	104.27	116.40
1	A	755	GLN	CG-CD-NE2	-8.08	104.28	116.40
1	B	1122	VAL	CG1-CB-CG2	-8.08	93.02	110.80
1	B	1072	GLU	CA-C-N	-8.00	108.04	121.64
1	B	1072	GLU	C-N-CA	-8.00	108.04	121.64
1	C	1072	GLU	CA-C-N	-7.97	108.09	121.64
1	C	1072	GLU	C-N-CA	-7.97	108.09	121.64
1	A	1072	GLU	CA-C-N	-7.96	108.10	121.64
1	A	1072	GLU	C-N-CA	-7.96	108.10	121.64
1	B	1145	LEU	CB-CG-CD1	7.87	134.32	110.70
1	C	1145	LEU	CB-CG-CD1	7.85	134.26	110.70
1	A	1145	LEU	CB-CG-CD1	7.85	134.25	110.70
1	B	611	LEU	CB-CG-CD2	-7.79	87.33	110.70
1	B	1073	LYS	N-CA-C	-7.79	95.55	108.32
1	C	611	LEU	CB-CG-CD2	-7.79	87.33	110.70
1	A	1073	LYS	N-CA-C	-7.79	95.55	108.32
1	A	611	LEU	CB-CG-CD2	-7.78	87.35	110.70
1	A	954	GLN	CA-CB-CG	7.78	129.66	114.10
1	A	153	MET	CB-CG-SD	7.76	135.99	112.70
1	C	1073	LYS	N-CA-C	-7.76	95.59	108.32
1	C	954	GLN	CA-CB-CG	7.75	129.61	114.10
1	C	153	MET	CB-CG-SD	7.75	135.94	112.70
1	B	153	MET	CB-CG-SD	7.75	135.93	112.70
1	B	231	ILE	N-CA-CB	-7.74	99.76	110.68
1	A	726	ILE	CA-C-N	-7.74	106.88	122.90
1	A	726	ILE	C-N-CA	-7.74	106.88	122.90
1	B	726	ILE	CA-C-N	-7.74	106.89	122.90
1	B	726	ILE	C-N-CA	-7.74	106.89	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	954	GLN	CA-CB-CG	7.73	129.56	114.10
1	C	726	ILE	CA-C-N	-7.72	106.91	122.90
1	C	726	ILE	C-N-CA	-7.72	106.91	122.90
1	A	303	LEU	CA-C-N	-7.72	110.94	123.05
1	A	303	LEU	C-N-CA	-7.72	110.94	123.05
1	C	1114	ILE	N-CA-C	-7.72	97.01	108.97
1	B	303	LEU	CA-C-N	-7.71	110.94	123.05
1	B	303	LEU	C-N-CA	-7.71	110.94	123.05
1	B	1114	ILE	N-CA-C	-7.70	97.03	108.97
1	A	1114	ILE	N-CA-C	-7.70	97.03	108.97
1	A	608	VAL	CA-CB-CG2	-7.69	97.33	110.40
1	C	608	VAL	CA-CB-CG2	-7.68	97.34	110.40
1	C	303	LEU	CA-C-N	-7.68	111.00	123.05
1	C	303	LEU	C-N-CA	-7.68	111.00	123.05
1	B	608	VAL	CA-CB-CG2	-7.68	97.35	110.40
1	B	790	LYS	CG-CD-CE	7.67	128.95	111.30
1	C	790	LYS	CG-CD-CE	7.66	128.93	111.30
1	A	790	LYS	CG-CD-CE	7.65	128.90	111.30
1	B	926	GLN	CG-CD-NE2	-7.62	104.98	116.40
1	A	926	GLN	CG-CD-NE2	-7.61	104.98	116.40
1	C	926	GLN	CG-CD-NE2	-7.61	104.98	116.40
1	B	905	ARG	NE-CZ-NH2	-7.58	112.38	119.20
1	A	905	ARG	NE-CZ-NH2	-7.56	112.39	119.20
1	B	1100	THR	CA-C-N	7.56	134.73	121.80
1	B	1100	THR	C-N-CA	7.56	134.73	121.80
1	C	905	ARG	NE-CZ-NH2	-7.56	112.40	119.20
1	A	1100	THR	CA-C-N	7.55	134.70	121.80
1	A	1100	THR	C-N-CA	7.55	134.70	121.80
1	C	1100	THR	CA-C-N	7.54	134.69	121.80
1	C	1100	THR	C-N-CA	7.54	134.69	121.80
1	A	947	LYS	CG-CD-CE	7.52	128.60	111.30
1	C	947	LYS	CG-CD-CE	7.52	128.59	111.30
1	A	44	ARG	NE-CZ-NH2	-7.51	112.44	119.20
1	B	947	LYS	CG-CD-CE	7.51	128.56	111.30
1	C	44	ARG	NE-CZ-NH2	-7.50	112.44	119.20
1	B	44	ARG	NE-CZ-NH2	-7.49	112.46	119.20
1	C	176	LEU	CA-C-N	-7.45	111.11	122.81
1	C	176	LEU	C-N-CA	-7.45	111.11	122.81
1	C	1113	GLN	CA-CB-CG	7.45	129.00	114.10
1	B	176	LEU	CA-C-N	-7.44	111.13	122.81
1	B	176	LEU	C-N-CA	-7.44	111.13	122.81
1	A	176	LEU	CA-C-N	-7.43	111.14	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	LEU	C-N-CA	-7.43	111.14	122.81
1	A	1113	GLN	CA-CB-CG	7.43	128.97	114.10
1	B	1113	GLN	CA-CB-CG	7.43	128.96	114.10
1	A	299	THR	OG1-CB-CG2	-7.37	94.55	109.30
1	B	299	THR	OG1-CB-CG2	-7.37	94.56	109.30
1	C	299	THR	OG1-CB-CG2	-7.36	94.57	109.30
1	B	208	THR	CA-CB-OG1	7.33	120.60	109.60
1	C	208	THR	CA-CB-OG1	7.32	120.58	109.60
1	B	41	LYS	CA-C-O	7.29	127.28	119.34
1	B	52	GLN	OE1-CD-NE2	-7.27	115.33	122.60
1	A	208	THR	CA-CB-OG1	7.27	120.50	109.60
1	C	41	LYS	CA-C-O	7.26	127.25	119.34
1	A	52	GLN	OE1-CD-NE2	-7.26	115.34	122.60
1	A	63	THR	CB-CA-C	-7.25	94.82	109.68
1	A	41	LYS	CA-C-O	7.24	127.23	119.34
1	B	63	THR	CB-CA-C	-7.24	94.83	109.68
1	C	52	GLN	OE1-CD-NE2	-7.24	115.36	122.60
1	C	63	THR	CB-CA-C	-7.24	94.84	109.68
1	B	246	ARG	N-CA-C	7.23	120.17	108.32
1	A	246	ARG	N-CA-C	7.21	120.14	108.32
1	A	711	SER	CA-C-N	7.21	133.25	122.58
1	A	711	SER	C-N-CA	7.21	133.25	122.58
1	C	246	ARG	N-CA-C	7.21	120.14	108.32
1	B	711	SER	CA-C-N	7.20	133.24	122.58
1	B	711	SER	C-N-CA	7.20	133.24	122.58
1	C	711	SER	CA-C-N	7.20	133.23	122.58
1	C	711	SER	C-N-CA	7.20	133.23	122.58
1	A	1129	VAL	CA-CB-CG2	-7.19	98.17	110.40
1	B	1129	VAL	CA-CB-CG2	-7.19	98.17	110.40
1	A	922	LEU	N-CA-C	7.19	123.16	111.37
1	B	187	LYS	N-CA-CB	-7.18	103.17	111.79
1	C	1129	VAL	CA-CB-CG2	-7.17	98.21	110.40
1	B	922	LEU	N-CA-C	7.17	123.13	111.37
1	C	922	LEU	N-CA-C	7.16	123.12	111.37
1	C	41	LYS	CA-CB-CG	7.16	128.42	114.10
1	B	41	LYS	CA-CB-CG	7.14	128.39	114.10
1	A	41	LYS	CA-CB-CG	7.14	128.37	114.10
1	A	187	LYS	N-CA-CB	-7.13	103.23	111.79
1	C	187	LYS	N-CA-CB	-7.12	103.25	111.79
1	C	231	ILE	CB-CA-C	-7.08	99.68	111.29
1	A	231	ILE	CB-CA-C	-7.07	99.70	111.29
1	B	872	GLN	CA-CB-CG	7.06	128.21	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	VAL	CG1-CB-CG2	-7.06	95.28	110.80
1	C	872	GLN	CA-CB-CG	7.05	128.21	114.10
1	A	872	GLN	CA-CB-CG	7.04	128.19	114.10
1	B	171	VAL	CG1-CB-CG2	-7.04	95.31	110.80
1	C	650	LEU	CB-CG-CD1	7.04	131.81	110.70
1	C	171	VAL	CG1-CB-CG2	-7.04	95.32	110.80
1	B	650	LEU	CB-CG-CD1	7.03	131.80	110.70
1	A	650	LEU	CB-CG-CD1	7.03	131.79	110.70
1	C	317	ASN	CA-C-N	-6.98	108.25	121.66
1	C	317	ASN	C-N-CA	-6.98	108.25	121.66
1	B	317	ASN	CA-C-N	-6.97	108.27	121.66
1	B	317	ASN	C-N-CA	-6.97	108.27	121.66
1	A	317	ASN	CA-C-N	-6.97	108.28	121.66
1	A	317	ASN	C-N-CA	-6.97	108.28	121.66
1	C	920	GLN	CG-CD-NE2	-6.95	105.98	116.40
1	B	920	GLN	CG-CD-NE2	-6.94	105.99	116.40
1	A	920	GLN	CG-CD-NE2	-6.92	106.01	116.40
1	C	231	ILE	N-CA-CB	-6.92	99.81	111.23
1	A	231	ILE	N-CA-CB	-6.91	99.83	111.23
1	A	1014	ARG	CB-CG-CD	-6.91	95.41	111.30
1	B	1014	ARG	CB-CG-CD	-6.90	95.43	111.30
1	A	1101	HIS	CB-CG-CD2	-6.88	122.25	131.20
1	C	1014	ARG	CB-CG-CD	-6.88	95.47	111.30
1	C	1101	HIS	CB-CG-CD2	-6.86	122.28	131.20
1	B	1101	HIS	CB-CG-CD2	-6.85	122.30	131.20
1	B	312	ILE	CA-CB-CG2	-6.82	98.90	110.50
1	A	312	ILE	CA-CB-CG2	-6.82	98.90	110.50
1	C	312	ILE	CA-CB-CG2	-6.80	98.94	110.50
1	A	1073	LYS	CA-CB-CG	6.80	127.70	114.10
1	B	1073	LYS	CA-CB-CG	6.80	127.70	114.10
1	C	1073	LYS	CA-CB-CG	6.79	127.68	114.10
1	A	1122	VAL	N-CA-C	6.76	117.81	108.89
1	A	947	LYS	CD-CE-NZ	-6.75	90.29	111.90
1	C	1122	VAL	N-CA-C	6.75	117.80	108.89
1	A	650	LEU	CD1-CG-CD2	-6.75	95.95	110.80
1	B	947	LYS	CD-CE-NZ	-6.75	90.31	111.90
1	C	947	LYS	CD-CE-NZ	-6.75	90.30	111.90
1	B	650	LEU	CD1-CG-CD2	-6.74	95.97	110.80
1	B	1114	ILE	CA-CB-CG1	6.73	121.84	110.40
1	C	1114	ILE	CA-CB-CG1	6.73	121.84	110.40
1	C	246	ARG	NE-CZ-NH1	6.72	128.22	121.50
1	A	1114	ILE	CA-CB-CG1	6.72	121.82	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1122	VAL	N-CA-C	6.72	117.76	108.89
1	C	650	LEU	CD1-CG-CD2	-6.71	96.03	110.80
1	A	63	THR	CA-C-N	6.71	132.26	123.00
1	A	63	THR	C-N-CA	6.71	132.26	123.00
1	C	63	THR	CA-C-N	6.69	132.24	123.00
1	C	63	THR	C-N-CA	6.69	132.24	123.00
1	B	1086	LYS	CB-CG-CD	6.69	126.69	111.30
1	B	63	THR	CA-C-N	6.69	132.23	123.00
1	B	63	THR	C-N-CA	6.69	132.23	123.00
1	C	1086	LYS	CB-CG-CD	6.69	126.68	111.30
1	C	113	LYS	CG-CD-CE	6.68	126.67	111.30
1	A	1086	LYS	CB-CG-CD	6.68	126.66	111.30
1	A	113	LYS	CG-CD-CE	6.67	126.65	111.30
1	A	246	ARG	NE-CZ-NH1	6.67	128.17	121.50
1	A	305	SER	N-CA-CB	6.67	123.51	111.37
1	B	113	LYS	CG-CD-CE	6.67	126.64	111.30
1	B	246	ARG	NE-CZ-NH1	6.67	128.17	121.50
1	B	305	SER	N-CA-CB	6.67	123.51	111.37
1	A	984	LEU	CA-C-N	6.66	132.58	121.92
1	A	984	LEU	C-N-CA	6.66	132.58	121.92
1	C	305	SER	N-CA-CB	6.66	123.49	111.37
1	B	825	LYS	N-CA-C	-6.66	104.73	112.92
1	C	984	LEU	CA-C-N	6.64	132.54	121.92
1	C	984	LEU	C-N-CA	6.64	132.54	121.92
1	A	304	LYS	CA-C-O	-6.62	112.51	120.32
1	B	984	LEU	CA-C-N	6.62	132.50	121.92
1	B	984	LEU	C-N-CA	6.62	132.50	121.92
1	C	1014	ARG	CD-NE-CZ	6.62	133.66	124.40
1	B	1014	ARG	CD-NE-CZ	6.61	133.66	124.40
1	C	237	ARG	NE-CZ-NH2	-6.61	113.25	119.20
1	A	825	LYS	N-CA-C	-6.61	104.79	112.92
1	B	237	ARG	NE-CZ-NH2	-6.60	113.26	119.20
1	C	825	LYS	N-CA-C	-6.59	104.81	112.92
1	A	1014	ARG	CD-NE-CZ	6.58	133.62	124.40
1	B	304	LYS	CA-C-O	-6.58	112.56	120.32
1	C	304	LYS	CA-C-O	-6.57	112.56	120.32
1	A	237	ARG	NE-CZ-NH2	-6.57	113.29	119.20
1	B	1086	LYS	CG-CD-CE	-6.55	96.23	111.30
1	A	1086	LYS	CG-CD-CE	-6.54	96.25	111.30
1	A	923	ILE	N-CA-C	6.54	118.07	110.62
1	C	1086	LYS	CG-CD-CE	-6.53	96.28	111.30
1	B	83	VAL	CA-C-N	6.53	137.58	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	VAL	C-N-CA	6.53	137.58	122.31
1	C	923	ILE	N-CA-C	6.52	118.06	110.62
1	A	83	VAL	CA-C-N	6.52	137.56	122.31
1	A	83	VAL	C-N-CA	6.52	137.56	122.31
1	C	83	VAL	CA-C-N	6.51	137.56	122.31
1	C	83	VAL	C-N-CA	6.51	137.56	122.31
1	B	1012	LEU	CB-CG-CD1	6.51	130.24	110.70
1	B	923	ILE	N-CA-C	6.51	118.04	110.62
1	A	1012	LEU	CB-CG-CD1	6.50	130.19	110.70
1	C	1012	LEU	CB-CG-CD1	6.50	130.19	110.70
1	A	278	LYS	N-CA-C	6.49	119.89	110.28
1	A	40	ASP	O-C-N	6.48	131.21	122.59
1	B	312	ILE	N-CA-C	-6.48	98.29	108.86
1	C	312	ILE	N-CA-C	-6.48	98.30	108.86
1	A	312	ILE	N-CA-C	-6.47	98.31	108.86
1	B	40	ASP	O-C-N	6.47	131.19	122.59
1	B	278	LYS	N-CA-C	6.47	119.85	110.28
1	B	600	PRO	N-CA-CB	-6.47	96.46	103.25
1	C	278	LYS	N-CA-C	6.47	119.85	110.28
1	A	134	GLN	CA-CB-CG	6.46	127.03	114.10
1	C	40	ASP	O-C-N	6.46	131.19	122.59
1	B	134	GLN	CA-CB-CG	6.46	127.02	114.10
1	B	1013	ILE	CB-CG1-CD1	6.46	127.36	113.80
1	A	1013	ILE	CB-CG1-CD1	6.45	127.34	113.80
1	C	1013	ILE	CB-CG1-CD1	6.45	127.34	113.80
1	C	134	GLN	CA-CB-CG	6.43	126.96	114.10
1	A	600	PRO	N-CA-CB	-6.43	96.50	103.25
1	A	727	LEU	N-CA-CB	6.43	122.76	111.19
1	C	233	ILE	CA-CB-CG2	-6.43	99.57	110.50
1	C	600	PRO	N-CA-CB	-6.43	96.50	103.25
1	B	727	LEU	N-CA-CB	6.41	122.72	111.19
1	C	171	VAL	CB-CA-C	6.41	120.69	110.82
1	B	233	ILE	CA-CB-CG2	-6.40	99.61	110.50
1	A	233	ILE	CA-CB-CG2	-6.40	99.61	110.50
1	C	727	LEU	N-CA-CB	6.40	122.71	111.19
1	B	869	MET	CG-SD-CE	6.40	114.98	100.90
1	B	651	ILE	N-CA-CB	-6.39	100.10	111.93
1	C	651	ILE	N-CA-CB	-6.39	100.10	111.93
1	B	171	VAL	CB-CA-C	6.39	120.66	110.82
1	A	869	MET	CG-SD-CE	6.38	114.94	100.90
1	A	171	VAL	CB-CA-C	6.38	120.64	110.82
1	C	869	MET	CG-SD-CE	6.38	114.93	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	651	ILE	N-CA-CB	-6.37	100.15	111.93
1	A	63	THR	N-CA-CB	6.35	119.44	110.36
1	B	63	THR	N-CA-CB	6.34	119.43	110.36
1	C	725	GLU	CA-C-N	-6.34	115.33	123.19
1	C	725	GLU	C-N-CA	-6.34	115.33	123.19
1	B	725	GLU	CA-C-N	-6.34	115.33	123.19
1	B	725	GLU	C-N-CA	-6.34	115.33	123.19
1	B	608	VAL	CB-CA-C	6.33	121.68	111.29
1	A	608	VAL	CB-CA-C	6.33	121.67	111.29
1	C	608	VAL	CB-CA-C	6.33	121.66	111.29
1	B	1038	LYS	CD-CE-NZ	6.31	132.10	111.90
1	C	63	THR	N-CA-CB	6.31	119.39	110.36
1	A	113	LYS	CB-CG-CD	6.31	125.81	111.30
1	C	1038	LYS	CD-CE-NZ	6.31	132.09	111.90
1	A	1038	LYS	CD-CE-NZ	6.30	132.07	111.90
1	C	113	LYS	CB-CG-CD	6.30	125.79	111.30
1	B	113	LYS	CB-CG-CD	6.30	125.79	111.30
1	B	739	THR	OG1-CB-CG2	6.30	121.90	109.30
1	A	725	GLU	CA-C-N	-6.29	115.39	123.19
1	A	725	GLU	C-N-CA	-6.29	115.39	123.19
1	A	1001	LEU	CA-C-N	-6.28	112.36	120.65
1	A	1001	LEU	C-N-CA	-6.28	112.36	120.65
1	A	306	PHE	CB-CA-C	-6.28	100.37	110.79
1	C	739	THR	OG1-CB-CG2	6.27	121.84	109.30
1	B	1001	LEU	CA-C-N	-6.26	112.38	120.65
1	B	1001	LEU	C-N-CA	-6.26	112.38	120.65
1	C	1001	LEU	CA-C-N	-6.26	112.39	120.65
1	C	1001	LEU	C-N-CA	-6.26	112.39	120.65
1	A	739	THR	OG1-CB-CG2	6.26	121.82	109.30
1	B	306	PHE	CB-CA-C	-6.25	100.41	110.79
1	B	670	ILE	CB-CG1-CD1	-6.25	100.67	113.80
1	C	306	PHE	CB-CA-C	-6.25	100.42	110.79
1	A	670	ILE	CB-CG1-CD1	-6.24	100.69	113.80
1	C	715	PRO	CA-N-CD	-6.24	103.27	112.00
1	A	715	PRO	CA-N-CD	-6.23	103.28	112.00
1	B	1101	HIS	N-CA-C	6.23	117.70	108.60
1	B	715	PRO	CA-N-CD	-6.23	103.28	112.00
1	C	670	ILE	CB-CG1-CD1	-6.22	100.74	113.80
1	A	56	LEU	CA-CB-CG	6.22	138.06	116.30
1	B	56	LEU	CA-CB-CG	6.22	138.06	116.30
1	B	17	ASN	CA-C-N	6.21	130.13	120.75
1	B	17	ASN	C-N-CA	6.21	130.13	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	933	LYS	CG-CD-CE	-6.21	97.03	111.30
1	C	278	LYS	CA-C-N	6.21	133.24	122.82
1	C	278	LYS	C-N-CA	6.21	133.24	122.82
1	C	933	LYS	CG-CD-CE	-6.20	97.03	111.30
1	C	56	LEU	CA-CB-CG	6.20	138.00	116.30
1	C	84	LEU	CB-CG-CD1	6.20	129.30	110.70
1	B	84	LEU	CB-CG-CD1	6.20	129.30	110.70
1	C	1101	HIS	N-CA-C	6.19	117.64	108.60
1	C	17	ASN	CA-C-N	6.19	130.09	120.75
1	C	17	ASN	C-N-CA	6.19	130.09	120.75
1	A	1101	HIS	N-CA-C	6.18	117.63	108.60
1	B	933	LYS	CG-CD-CE	-6.18	97.07	111.30
1	A	84	LEU	CB-CG-CD1	6.18	129.25	110.70
1	A	278	LYS	CA-C-N	6.18	133.20	122.82
1	A	278	LYS	C-N-CA	6.18	133.20	122.82
1	B	278	LYS	CA-C-N	6.18	133.20	122.82
1	B	278	LYS	C-N-CA	6.18	133.20	122.82
1	A	17	ASN	CA-C-N	6.18	130.08	120.75
1	A	17	ASN	C-N-CA	6.18	130.08	120.75
1	A	898	PHE	CB-CG-CD1	6.17	131.19	120.70
1	C	898	PHE	CB-CG-CD1	6.16	131.16	120.70
1	B	231	ILE	N-CA-C	-6.14	105.83	111.67
1	B	898	PHE	CB-CG-CD1	6.13	131.13	120.70
1	C	237	ARG	CA-CB-CG	6.13	126.37	114.10
1	B	774	GLN	N-CA-CB	-6.13	101.52	110.53
1	A	774	GLN	N-CA-CB	-6.13	101.52	110.53
1	A	995	ARG	N-CA-CB	-6.13	101.11	110.12
1	B	42	VAL	CA-C-O	-6.12	115.97	121.97
1	B	237	ARG	CA-CB-CG	6.12	126.33	114.10
1	A	237	ARG	CA-CB-CG	6.12	126.33	114.10
1	C	774	GLN	N-CA-CB	-6.11	101.54	110.53
1	B	901	GLN	N-CA-CB	6.10	119.29	110.20
1	C	42	VAL	CA-C-O	-6.10	115.99	121.97
1	B	995	ARG	N-CA-CB	-6.10	101.16	110.12
1	C	995	ARG	N-CA-CB	-6.10	101.15	110.12
1	A	901	GLN	N-CA-CB	6.10	119.28	110.20
1	A	995	ARG	CB-CA-C	6.09	120.90	110.79
1	A	42	VAL	CA-C-O	-6.09	116.00	121.97
1	C	901	GLN	N-CA-CB	6.09	119.27	110.20
1	C	995	ARG	CB-CA-C	6.08	120.89	110.79
1	B	995	ARG	CB-CA-C	6.08	120.88	110.79
1	A	1102	TRP	CB-CG-CD1	-6.02	117.86	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1102	TRP	CB-CG-CD1	-6.01	117.88	126.90
1	A	898	PHE	CB-CG-CD2	-6.00	110.50	120.70
1	B	898	PHE	CB-CG-CD2	-6.00	110.50	120.70
1	B	1102	TRP	CB-CG-CD1	-5.99	117.91	126.90
1	C	898	PHE	CB-CG-CD2	-5.99	110.52	120.70
1	A	1014	ARG	CB-CA-C	5.98	120.27	110.88
1	B	1014	ARG	CB-CA-C	5.98	120.27	110.88
1	B	905	ARG	CB-CG-CD	5.98	125.05	111.30
1	C	905	ARG	CB-CG-CD	5.97	125.04	111.30
1	A	905	ARG	CB-CG-CD	5.96	125.00	111.30
1	C	1014	ARG	CB-CA-C	5.95	120.23	110.88
1	C	51	THR	CA-C-N	-5.94	112.84	122.81
1	C	51	THR	C-N-CA	-5.94	112.84	122.81
1	B	51	THR	CA-C-N	-5.93	112.86	122.81
1	B	51	THR	C-N-CA	-5.93	112.86	122.81
1	A	51	THR	CA-C-N	-5.92	112.86	122.81
1	A	51	THR	C-N-CA	-5.92	112.86	122.81
1	A	187	LYS	O-C-N	-5.92	116.32	122.18
1	B	1013	ILE	CB-CA-C	5.91	121.79	112.16
1	A	1013	ILE	CB-CA-C	5.89	121.77	112.16
1	C	1083	HIS	CB-CG-CD2	-5.88	123.55	131.20
1	C	1013	ILE	CB-CA-C	5.87	121.73	112.16
1	B	56	LEU	N-CA-CB	5.87	117.88	109.78
1	B	602	THR	CA-C-N	-5.87	110.92	120.72
1	B	602	THR	C-N-CA	-5.87	110.92	120.72
1	A	602	THR	CA-C-N	-5.87	110.92	120.72
1	A	602	THR	C-N-CA	-5.87	110.92	120.72
1	B	187	LYS	O-C-N	-5.86	116.38	122.18
1	C	56	LEU	N-CA-CB	5.86	117.87	109.78
1	A	56	LEU	N-CA-CB	5.86	117.86	109.78
1	B	1083	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	A	1083	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	C	187	LYS	O-C-N	-5.86	116.38	122.18
1	A	926	GLN	N-CA-CB	-5.85	101.22	110.22
1	B	926	GLN	N-CA-CB	-5.84	101.22	110.22
1	C	926	GLN	N-CA-CB	-5.84	101.23	110.22
1	C	602	THR	CA-C-N	-5.84	110.97	120.72
1	C	602	THR	C-N-CA	-5.84	110.97	120.72
1	C	869	MET	CB-CG-SD	-5.80	95.31	112.70
1	B	611	LEU	CA-CB-CG	-5.79	96.02	116.30
1	C	602	THR	OG1-CB-CG2	5.79	120.88	109.30
1	A	869	MET	CB-CG-SD	-5.79	95.33	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	602	THR	OG1-CB-CG2	5.79	120.88	109.30
1	B	869	MET	CB-CG-SD	-5.79	95.33	112.70
1	A	611	LEU	CA-CB-CG	-5.79	96.05	116.30
1	C	611	LEU	CA-CB-CG	-5.78	96.05	116.30
1	A	602	THR	OG1-CB-CG2	5.78	120.86	109.30
1	B	611	LEU	CB-CG-CD1	5.74	127.93	110.70
1	A	611	LEU	CB-CG-CD1	5.74	127.91	110.70
1	C	127	VAL	CG1-CB-CG2	-5.74	98.18	110.80
1	C	611	LEU	CB-CG-CD1	5.73	127.90	110.70
1	C	20	THR	OG1-CB-CG2	5.73	120.75	109.30
1	B	1002	GLN	CG-CD-OE1	5.72	132.25	120.80
1	A	127	VAL	CG1-CB-CG2	-5.72	98.21	110.80
1	B	127	VAL	CG1-CB-CG2	-5.72	98.22	110.80
1	C	1002	GLN	CG-CD-OE1	5.72	132.24	120.80
1	A	20	THR	OG1-CB-CG2	5.71	120.72	109.30
1	C	1102	TRP	CB-CG-CD2	5.71	134.79	126.80
1	A	1002	GLN	CG-CD-OE1	5.70	132.21	120.80
1	B	20	THR	OG1-CB-CG2	5.70	120.71	109.30
1	B	158	ARG	CA-CB-CG	5.68	125.47	114.10
1	A	1102	TRP	CB-CG-CD2	5.67	134.74	126.80
1	C	1005	GLN	CA-CB-CG	5.67	125.44	114.10
1	C	158	ARG	CA-CB-CG	5.67	125.43	114.10
1	B	1102	TRP	CB-CG-CD2	5.66	134.72	126.80
1	A	995	ARG	CA-CB-CG	5.65	125.40	114.10
1	A	158	ARG	CA-CB-CG	5.65	125.39	114.10
1	A	1005	GLN	CA-CB-CG	5.64	125.39	114.10
1	C	869	MET	N-CA-C	5.64	120.62	111.37
1	A	933	LYS	N-CA-C	-5.64	104.75	111.69
1	B	869	MET	N-CA-C	5.64	120.62	111.37
1	B	1005	GLN	CA-CB-CG	5.64	125.37	114.10
1	A	208	THR	CA-CB-CG2	5.63	120.07	110.50
1	B	995	ARG	CA-CB-CG	5.63	125.36	114.10
1	A	869	MET	N-CA-C	5.62	120.59	111.37
1	B	933	LYS	N-CA-C	-5.62	104.78	111.69
1	A	922	LEU	CB-CG-CD1	-5.62	93.85	110.70
1	C	933	LYS	N-CA-C	-5.61	104.79	111.69
1	B	922	LEU	CB-CG-CD1	-5.61	93.88	110.70
1	A	312	ILE	CB-CA-C	-5.60	101.73	110.69
1	C	208	THR	CA-CB-CG2	5.60	120.03	110.50
1	C	922	LEU	CB-CG-CD1	-5.60	93.89	110.70
1	C	926	GLN	CB-CA-C	5.60	120.99	110.63
1	B	312	ILE	CB-CA-C	-5.60	101.73	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	983	ARG	CA-C-O	-5.60	112.57	119.18
1	C	995	ARG	CA-CB-CG	5.60	125.30	114.10
1	A	983	ARG	CA-C-O	-5.59	112.58	119.18
1	B	208	THR	CA-CB-CG2	5.59	120.01	110.50
1	A	171	VAL	CA-C-N	-5.59	113.42	122.81
1	A	171	VAL	C-N-CA	-5.59	113.42	122.81
1	C	312	ILE	CB-CA-C	-5.58	101.75	110.69
1	B	926	GLN	CB-CA-C	5.58	120.96	110.63
1	B	171	VAL	CA-C-N	-5.58	113.43	122.81
1	B	171	VAL	C-N-CA	-5.58	113.43	122.81
1	A	926	GLN	CB-CA-C	5.57	120.93	110.63
1	C	983	ARG	CA-C-O	-5.57	112.61	119.18
1	C	478	THR	OG1-CB-CG2	5.57	120.44	109.30
1	C	767	LEU	N-CA-CB	-5.57	101.33	110.40
1	A	767	LEU	N-CA-CB	-5.56	101.33	110.40
1	C	171	VAL	CA-C-N	-5.56	113.48	122.81
1	C	171	VAL	C-N-CA	-5.56	113.48	122.81
1	B	619	GLU	CB-CG-CD	5.55	122.04	112.60
1	A	619	GLU	CB-CG-CD	5.55	122.03	112.60
1	C	619	GLU	CB-CG-CD	5.55	122.04	112.60
1	C	202	LYS	CB-CG-CD	5.55	124.06	111.30
1	A	187	LYS	CA-C-O	5.54	126.01	121.02
1	B	712	ILE	N-CA-C	5.54	117.79	108.81
1	C	43	PHE	CA-CB-CG	5.54	119.34	113.80
1	A	202	LYS	CB-CG-CD	5.54	124.04	111.30
1	A	43	PHE	CA-CB-CG	5.53	119.33	113.80
1	C	187	LYS	CA-C-O	5.53	125.99	121.02
1	B	767	LEU	N-CA-CB	-5.52	101.40	110.40
1	B	202	LYS	CB-CG-CD	5.52	123.99	111.30
1	B	231	ILE	CA-C-O	5.51	126.48	120.69
1	B	187	LYS	CA-C-O	5.51	125.98	121.02
1	C	197	ILE	N-CA-CB	-5.51	102.29	112.43
1	C	727	LEU	CB-CG-CD2	5.51	127.23	110.70
1	A	719	THR	N-CA-C	-5.51	101.36	109.18
1	C	712	ILE	N-CA-C	5.50	117.72	108.81
1	A	712	ILE	N-CA-C	5.50	117.72	108.81
1	A	727	LEU	CB-CG-CD2	5.50	127.19	110.70
1	A	197	ILE	N-CA-CB	-5.50	102.32	112.43
1	B	197	ILE	N-CA-CB	-5.49	102.33	112.43
1	B	727	LEU	CB-CG-CD2	5.49	127.17	110.70
1	B	319	ARG	CA-C-N	-5.49	116.39	123.19
1	B	319	ARG	C-N-CA	-5.49	116.39	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	719	THR	N-CA-C	-5.49	101.39	109.18
1	B	43	PHE	CA-CB-CG	5.46	119.26	113.80
1	C	719	THR	N-CA-C	-5.46	101.43	109.18
1	A	603	ASN	CB-CG-ND2	-5.42	108.27	116.40
1	C	603	ASN	CB-CG-ND2	-5.40	108.29	116.40
1	B	603	ASN	CB-CG-ND2	-5.40	108.30	116.40
1	C	220	PHE	CB-CA-C	-5.40	100.90	109.80
1	A	1014	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	B	220	PHE	CB-CA-C	-5.36	100.96	109.80
1	A	220	PHE	CB-CA-C	-5.36	100.96	109.80
1	C	811	LYS	N-CA-CB	5.35	119.89	110.37
1	B	1014	ARG	NE-CZ-NH2	-5.35	114.39	119.20
1	C	1014	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	A	811	LYS	N-CA-CB	5.34	119.88	110.37
1	B	811	LYS	N-CA-CB	5.33	119.85	110.37
1	B	947	LYS	N-CA-C	5.32	117.99	111.82
1	B	63	THR	CA-CB-CG2	-5.31	101.48	110.50
1	B	1101	HIS	CG-ND1-CE1	-5.31	100.28	109.30
1	C	63	THR	CA-CB-CG2	-5.30	101.50	110.50
1	C	1101	HIS	CG-ND1-CE1	-5.30	100.30	109.30
1	A	63	THR	CA-CB-CG2	-5.29	101.51	110.50
1	A	947	LYS	N-CA-C	5.29	117.95	111.82
1	A	1101	HIS	CG-ND1-CE1	-5.29	100.31	109.30
1	C	947	LYS	N-CA-C	5.28	117.95	111.82
1	B	305	SER	N-CA-C	-5.28	101.16	109.50
1	C	312	ILE	CA-CB-CG1	5.28	119.38	110.40
1	A	312	ILE	CA-CB-CG1	5.27	119.36	110.40
1	C	305	SER	N-CA-C	-5.27	101.17	109.50
1	A	719	THR	N-CA-CB	5.26	119.53	111.22
1	A	305	SER	N-CA-C	-5.26	101.19	109.50
1	B	312	ILE	CA-CB-CG1	5.25	119.33	110.40
1	C	719	THR	N-CA-CB	5.25	119.51	111.22
1	B	719	THR	N-CA-CB	5.24	119.50	111.22
1	C	790	LYS	CA-CB-CG	-5.23	103.64	114.10
1	B	42	VAL	CA-C-N	-5.23	112.85	120.75
1	B	42	VAL	C-N-CA	-5.23	112.85	120.75
1	A	224	GLU	N-CA-CB	5.23	116.99	109.78
1	B	790	LYS	CA-CB-CG	-5.23	103.64	114.10
1	C	755	GLN	OE1-CD-NE2	5.22	127.83	122.60
1	A	42	VAL	CA-C-N	-5.22	112.87	120.75
1	A	42	VAL	C-N-CA	-5.22	112.87	120.75
1	B	755	GLN	OE1-CD-NE2	5.22	127.82	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	GLU	CA-CB-CG	5.22	124.54	114.10
1	A	790	LYS	CA-CB-CG	-5.22	103.67	114.10
1	C	755	GLN	N-CA-C	-5.22	106.59	113.17
1	B	246	ARG	CB-CA-C	5.22	118.70	109.89
1	A	743	CYS	CA-CB-SG	5.21	126.39	114.40
1	B	224	GLU	N-CA-CB	5.21	116.97	109.78
1	B	281	GLU	CA-CB-CG	5.21	124.53	114.10
1	B	311	GLY	CA-C-N	-5.21	114.40	122.69
1	B	311	GLY	C-N-CA	-5.21	114.40	122.69
1	C	246	ARG	CB-CA-C	5.21	118.70	109.89
1	A	246	ARG	CB-CA-C	5.21	118.69	109.89
1	C	42	VAL	CA-C-N	-5.21	112.89	120.75
1	C	42	VAL	C-N-CA	-5.21	112.89	120.75
1	A	755	GLN	N-CA-C	-5.20	106.62	113.17
1	B	743	CYS	CA-CB-SG	5.20	126.36	114.40
1	C	224	GLU	N-CA-CB	5.20	116.95	109.78
1	A	311	GLY	CA-C-N	-5.19	114.43	122.69
1	A	311	GLY	C-N-CA	-5.19	114.43	122.69
1	A	755	GLN	OE1-CD-NE2	5.19	127.79	122.60
1	C	42	VAL	N-CA-C	-5.19	102.31	110.09
1	A	281	GLU	CA-CB-CG	5.19	124.47	114.10
1	B	755	GLN	N-CA-C	-5.19	106.63	113.17
1	C	311	GLY	CA-C-N	-5.18	114.45	122.69
1	C	311	GLY	C-N-CA	-5.18	114.45	122.69
1	C	743	CYS	CA-CB-SG	5.18	126.32	114.40
1	B	78	ARG	NH1-CZ-NH2	-5.17	112.58	119.30
1	A	78	ARG	NH1-CZ-NH2	-5.17	112.58	119.30
1	A	1004	LEU	CA-C-N	-5.17	112.09	121.14
1	A	1004	LEU	C-N-CA	-5.17	112.09	121.14
1	A	602	THR	CA-CB-CG2	5.17	119.28	110.50
1	B	42	VAL	N-CA-C	-5.17	102.34	110.09
1	A	42	VAL	N-CA-C	-5.17	102.34	110.09
1	B	1004	LEU	CA-C-N	-5.16	112.11	121.14
1	B	1004	LEU	C-N-CA	-5.16	112.11	121.14
1	A	727	LEU	CB-CA-C	-5.16	100.39	108.91
1	B	727	LEU	CB-CA-C	-5.16	100.40	108.91
1	C	134	GLN	CG-CD-NE2	-5.16	108.67	116.40
1	C	39	PRO	CA-C-N	5.15	131.38	121.54
1	C	39	PRO	C-N-CA	5.15	131.38	121.54
1	A	811	LYS	CB-CA-C	-5.15	100.03	110.17
1	C	602	THR	CA-CB-CG2	5.15	119.25	110.50
1	B	39	PRO	CA-C-N	5.14	131.37	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	PRO	C-N-CA	5.14	131.37	121.54
1	C	1004	LEU	CA-C-N	-5.14	112.14	121.14
1	C	1004	LEU	C-N-CA	-5.14	112.14	121.14
1	B	811	LYS	CB-CA-C	-5.14	100.04	110.17
1	A	793	PRO	CA-C-N	5.13	129.32	122.95
1	A	793	PRO	C-N-CA	5.13	129.32	122.95
1	B	602	THR	CA-CB-CG2	5.13	119.23	110.50
1	C	811	LYS	CB-CA-C	-5.13	100.05	110.17
1	B	793	PRO	CA-C-N	5.13	129.31	122.95
1	B	793	PRO	C-N-CA	5.13	129.31	122.95
1	C	78	ARG	NH1-CZ-NH2	-5.13	112.63	119.30
1	C	727	LEU	CB-CA-C	-5.13	100.45	108.91
1	B	134	GLN	CG-CD-NE2	-5.12	108.73	116.40
1	C	793	PRO	CA-C-N	5.12	129.29	122.95
1	C	793	PRO	C-N-CA	5.12	129.29	122.95
1	A	39	PRO	CA-C-N	5.11	131.31	121.54
1	A	39	PRO	C-N-CA	5.11	131.31	121.54
1	A	1073	LYS	CB-CG-CD	-5.11	99.54	111.30
1	B	1073	LYS	CB-CG-CD	-5.11	99.54	111.30
1	A	134	GLN	CG-CD-NE2	-5.11	108.73	116.40
1	C	1073	LYS	CB-CG-CD	-5.10	99.57	111.30
1	B	1101	HIS	ND1-CE1-NE2	5.10	113.50	108.40
1	C	133	PHE	CG-CD2-CE2	5.10	129.37	120.70
1	C	920	GLN	N-CA-C	-5.10	106.16	112.38
1	A	133	PHE	CG-CD2-CE2	5.09	129.36	120.70
1	B	133	PHE	CG-CD2-CE2	5.09	129.35	120.70
1	C	195	LYS	CD-CE-NZ	5.08	128.16	111.90
1	B	195	LYS	CD-CE-NZ	5.08	128.15	111.90
1	B	920	GLN	N-CA-C	-5.08	106.19	112.38
1	A	195	LYS	CD-CE-NZ	5.07	128.14	111.90
1	A	920	GLN	N-CA-C	-5.07	106.20	112.38
1	B	727	LEU	O-C-N	-5.06	118.29	121.88
1	A	1101	HIS	ND1-CE1-NE2	5.06	113.46	108.40
1	C	1101	HIS	ND1-CE1-NE2	5.06	113.46	108.40
1	A	1083	HIS	CG-CD2-NE2	5.04	112.24	107.20
1	A	697	MET	CB-CG-SD	5.03	127.80	112.70
1	B	697	MET	CB-CG-SD	5.03	127.80	112.70
1	A	608	VAL	CA-CB-CG1	5.03	118.95	110.40
1	A	312	ILE	N-CA-CB	5.03	121.23	111.93
1	B	608	VAL	CA-CB-CG1	5.02	118.94	110.40
1	A	202	LYS	CB-CA-C	5.02	118.91	111.17
1	B	923	ILE	CB-CG1-CD1	5.02	124.35	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	697	MET	CB-CG-SD	5.02	127.77	112.70
1	C	608	VAL	CA-CB-CG1	5.02	118.94	110.40
1	A	923	ILE	CB-CG1-CD1	5.02	124.34	113.80
1	B	312	ILE	N-CA-CB	5.02	121.22	111.93
1	B	1083	HIS	CG-CD2-NE2	5.01	112.22	107.20
1	B	755	GLN	CA-CB-CG	5.01	124.13	114.10
1	C	755	GLN	CA-CB-CG	5.01	124.11	114.10
1	B	613	GLN	CA-CB-CG	5.01	124.11	114.10
1	C	613	GLN	CA-CB-CG	5.00	124.11	114.10
1	C	1083	HIS	CG-CD2-NE2	5.00	112.20	107.20

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	63	THR	CB
1	A	208	THR	CB
1	A	231	ILE	CB
1	A	712	ILE	CB
1	A	923	ILE	CB
1	B	63	THR	CB
1	B	208	THR	CB
1	B	231	ILE	CB
1	B	712	ILE	CB
1	B	923	ILE	CB
1	C	63	THR	CB
1	C	208	THR	CB
1	C	231	ILE	CB
1	C	712	ILE	CB
1	C	923	ILE	CB

All (161) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1002	GLN	Sidechain
1	A	1014	ARG	Sidechain
1	A	1071	GLN	Sidechain
1	A	1083	HIS	Sidechain
1	A	1089	PHE	Sidechain
1	A	1101	HIS	Peptide,Sidechain
1	A	1109	PHE	Sidechain
1	A	1112	PRO	Peptide
1	A	1113	GLN	Peptide,Sidechain

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Mol	Chain	Res	Type	Group
1	A	1129	VAL	Mainchain
1	A	133	PHE	Sidechain
1	A	134	GLN	Sidechain
1	A	201	PHE	Peptide
1	A	202	LYS	Peptide
1	A	220	PHE	Peptide
1	A	237	ARG	Sidechain
1	A	244	LEU	Peptide
1	A	246	ARG	Sidechain
1	A	266	TYR	Sidechain
1	A	277	LEU	Peptide
1	A	293	LEU	Peptide
1	A	304	LYS	Mainchain
1	A	306	PHE	Peptide
1	A	318	PHE	Peptide,Sidechain
1	A	319	ARG	Mainchain
1	A	34	ARG	Sidechain
1	A	37	TYR	Sidechain
1	A	41	LYS	Mainchain
1	A	42	VAL	Peptide
1	A	43	PHE	Sidechain
1	A	44	ARG	Sidechain
1	A	52	GLN	Sidechain
1	A	599	THR	Peptide
1	A	602	THR	Peptide
1	A	603	ASN	Sidechain
1	A	612	TYR	Peptide
1	A	725	GLU	Peptide
1	A	765	ARG	Sidechain
1	A	774	GLN	Sidechain
1	A	78	ARG	Sidechain
1	A	901	GLN	Sidechain
1	A	905	ARG	Sidechain
1	A	920	GLN	Sidechain
1	A	925	ASN	Sidechain
1	A	926	GLN	Sidechain
1	A	945	LEU	Peptide
1	A	947	LYS	Mainchain
1	A	954	GLN	Sidechain
1	A	983	ARG	Sidechain
1	A	99	ASN	Sidechain
1	B	1002	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	B	1014	ARG	Sidechain
1	B	1071	GLN	Sidechain
1	B	1083	HIS	Sidechain
1	B	1089	PHE	Sidechain
1	B	1101	HIS	Peptide,Sidechain
1	B	1109	PHE	Sidechain
1	B	1112	PRO	Peptide
1	B	1113	GLN	Peptide,Sidechain
1	B	1129	VAL	Mainchain
1	B	133	PHE	Sidechain
1	B	134	GLN	Sidechain
1	B	201	PHE	Peptide
1	B	202	LYS	Peptide
1	B	220	PHE	Peptide
1	B	237	ARG	Sidechain
1	B	244	LEU	Peptide
1	B	246	ARG	Sidechain
1	B	266	TYR	Sidechain
1	B	277	LEU	Peptide
1	B	293	LEU	Peptide
1	B	304	LYS	Mainchain
1	B	306	PHE	Peptide
1	B	318	PHE	Peptide,Sidechain
1	B	34	ARG	Sidechain
1	B	37	TYR	Sidechain
1	B	41	LYS	Mainchain
1	B	42	VAL	Peptide
1	B	43	PHE	Sidechain
1	B	44	ARG	Sidechain
1	B	488	CYS	Peptide
1	B	489	TYR	Peptide
1	B	52	GLN	Sidechain
1	B	599	THR	Peptide
1	B	602	THR	Peptide
1	B	603	ASN	Sidechain
1	B	612	TYR	Peptide
1	B	725	GLU	Peptide
1	B	765	ARG	Sidechain
1	B	774	GLN	Sidechain
1	B	78	ARG	Sidechain
1	B	901	GLN	Sidechain
1	B	905	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	920	GLN	Sidechain
1	B	925	ASN	Sidechain
1	B	926	GLN	Sidechain
1	B	945	LEU	Peptide
1	B	947	LYS	Mainchain
1	B	954	GLN	Sidechain
1	B	983	ARG	Sidechain
1	B	99	ASN	Sidechain
1	C	1002	GLN	Sidechain
1	C	1014	ARG	Sidechain
1	C	1071	GLN	Sidechain
1	C	1083	HIS	Sidechain
1	C	1089	PHE	Sidechain
1	C	1101	HIS	Peptide,Sidechain
1	C	1109	PHE	Sidechain
1	C	1112	PRO	Peptide
1	C	1113	GLN	Peptide,Sidechain
1	C	1129	VAL	Mainchain
1	C	133	PHE	Sidechain
1	C	134	GLN	Sidechain
1	C	201	PHE	Peptide
1	C	202	LYS	Peptide
1	C	220	PHE	Peptide
1	C	237	ARG	Sidechain
1	C	244	LEU	Peptide
1	C	246	ARG	Sidechain
1	C	266	TYR	Sidechain
1	C	277	LEU	Peptide
1	C	293	LEU	Peptide
1	C	304	LYS	Mainchain
1	C	306	PHE	Peptide
1	C	318	PHE	Peptide,Sidechain
1	C	331	ASN	Peptide
1	C	34	ARG	Sidechain
1	C	37	TYR	Sidechain
1	C	41	LYS	Mainchain
1	C	42	VAL	Peptide
1	C	43	PHE	Sidechain
1	C	44	ARG	Sidechain
1	C	52	GLN	Sidechain
1	C	579	PRO	Peptide
1	C	599	THR	Peptide

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Mol	Chain	Res	Type	Group
1	C	602	THR	Peptide
1	C	603	ASN	Sidechain
1	C	612	TYR	Peptide
1	C	725	GLU	Peptide
1	C	765	ARG	Sidechain
1	C	774	GLN	Sidechain
1	C	78	ARG	Sidechain
1	C	901	GLN	Sidechain
1	C	905	ARG	Sidechain
1	C	920	GLN	Sidechain
1	C	925	ASN	Sidechain
1	C	926	GLN	Sidechain
1	C	945	LEU	Peptide
1	C	947	LYS	Mainchain
1	C	954	GLN	Sidechain
1	C	983	ARG	Sidechain
1	C	99	ASN	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8292	8068	8072	1001	0
1	B	8253	8034	8040	1048	0
1	C	8292	8069	8068	1142	0
2	D	895	0	866	134	0
3	E	28	25	25	8	0
3	F	28	25	25	0	0
3	G	28	25	25	23	0
3	H	28	25	25	6	0
3	I	28	25	25	3	0
4	A	182	168	169	21	0
4	B	182	167	169	38	0
4	C	98	77	91	5	0
All	All	26334	24708	25600	3116	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 60.

All (3116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:948:LEU:CD1	1:B:948:LEU:CG	1.75	1.65
1:B:42:VAL:CG1	1:B:42:VAL:CB	1.76	1.61
1:C:948:LEU:CD1	1:C:948:LEU:CG	1.75	1.60
1:A:948:LEU:CG	1:A:948:LEU:CD1	1.75	1.58
1:B:42:VAL:CG1	1:B:42:VAL:CG2	1.74	1.56
1:B:611:LEU:CD2	1:B:611:LEU:CG	1.85	1.55
1:B:41:LYS:CA	1:B:41:LYS:C	1.76	1.55
1:A:41:LYS:C	1:A:41:LYS:CA	1.76	1.54
1:B:933:LYS:NZ	1:B:933:LYS:CE	1.68	1.54
1:C:611:LEU:CD2	1:C:611:LEU:CG	1.85	1.54
1:C:933:LYS:NZ	1:C:933:LYS:CE	1.68	1.53
1:C:1073:LYS:NZ	1:C:1073:LYS:CE	1.70	1.52
1:A:933:LYS:NZ	1:A:933:LYS:CE	1.68	1.52
1:A:611:LEU:CD2	1:A:611:LEU:CG	1.85	1.52
1:A:304:LYS:CG	1:A:304:LYS:CE	1.87	1.51
1:B:670:ILE:CB	1:B:670:ILE:CG2	1.87	1.51
1:B:1073:LYS:NZ	1:B:1073:LYS:CE	1.70	1.51
1:C:41:LYS:C	1:C:41:LYS:CA	1.76	1.51
1:C:670:ILE:CB	1:C:670:ILE:CG2	1.87	1.51
1:B:231:ILE:CG2	1:B:231:ILE:CG1	1.85	1.51
1:C:231:ILE:CG1	1:C:231:ILE:CG2	1.85	1.49
1:A:670:ILE:CB	1:A:670:ILE:CG2	1.87	1.49
1:A:231:ILE:CG1	1:A:231:ILE:CG2	1.85	1.49
1:A:1073:LYS:NZ	1:A:1073:LYS:CE	1.70	1.49
1:A:651:ILE:CD1	1:A:651:ILE:CG1	1.92	1.48
1:A:651:ILE:CG2	1:A:651:ILE:CB	1.92	1.47
1:B:304:LYS:CE	1:B:304:LYS:CG	1.87	1.47
1:B:651:ILE:CG1	1:B:651:ILE:CD1	1.92	1.47
1:C:304:LYS:CE	1:C:304:LYS:CG	1.87	1.47
1:C:1071:GLN:NE2	1:C:1071:GLN:CD	1.71	1.47
1:B:651:ILE:CB	1:B:651:ILE:CG2	1.92	1.46
1:C:651:ILE:CG1	1:C:651:ILE:CG2	1.93	1.46
1:A:1071:GLN:NE2	1:A:1071:GLN:CD	1.71	1.46
1:C:651:ILE:CG1	1:C:651:ILE:CD1	1.92	1.46
1:A:651:ILE:CG1	1:A:651:ILE:CG2	1.93	1.44
1:B:1071:GLN:CD	1:B:1071:GLN:NE2	1.71	1.44
1:C:651:ILE:CG2	1:C:651:ILE:CB	1.92	1.44
1:B:563:GLN:CA	1:C:41:LYS:HG2	1.44	1.43
1:B:651:ILE:CG1	1:B:651:ILE:CG2	1.93	1.43
1:C:651:ILE:CD1	1:C:651:ILE:HB	1.49	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:CG	1:B:41:LYS:CD	1.97	1.41
1:A:611:LEU:CD2	1:A:611:LEU:CD1	1.99	1.41
1:B:651:ILE:CD1	1:B:651:ILE:HB	1.49	1.40
1:C:611:LEU:CD2	1:C:611:LEU:HD13	1.51	1.40
1:C:41:LYS:CD	1:C:41:LYS:CG	1.97	1.40
1:C:651:ILE:CD1	1:C:651:ILE:CB	2.01	1.39
1:A:41:LYS:CG	1:A:41:LYS:CD	1.97	1.39
1:A:651:ILE:CD1	1:A:651:ILE:HB	1.49	1.39
1:C:611:LEU:CD2	1:C:611:LEU:CD1	1.99	1.39
1:B:611:LEU:CD2	1:B:611:LEU:CD1	1.99	1.39
1:B:611:LEU:CD2	1:B:611:LEU:HD13	1.51	1.39
1:A:611:LEU:CD2	1:A:611:LEU:HD13	1.51	1.38
1:B:651:ILE:CD1	1:B:651:ILE:CB	2.01	1.38
1:A:651:ILE:CD1	1:A:651:ILE:CB	2.01	1.36
1:A:562:PHE:O	1:B:41:LYS:HG3	1.23	1.33
1:A:231:ILE:CG2	1:A:231:ILE:CB	2.06	1.33
1:C:231:ILE:CG2	1:C:231:ILE:CB	2.06	1.32
1:B:231:ILE:CG2	1:B:231:ILE:CB	2.06	1.32
1:B:153:MET:HE2	4:B:1302:NAG:O4	1.28	1.31
1:C:452:LEU:HD13	2:D:33:ARG:CD	1.61	1.29
1:B:699:LEU:HD13	1:C:872:GLN:OE1	1.22	1.28
1:B:1130:ILE:HD11	1:C:920:GLN:OE1	1.26	1.28
1:B:231:ILE:CD1	1:B:231:ILE:HG21	1.66	1.25
1:C:231:ILE:HG21	1:C:231:ILE:CD1	1.66	1.25
1:B:563:GLN:CB	1:C:41:LYS:HG2	1.68	1.24
1:A:231:ILE:HG21	1:A:231:ILE:CD1	1.66	1.24
1:A:1071:GLN:NE2	1:A:1071:GLN:CG	1.99	1.24
1:B:1071:GLN:NE2	1:B:1071:GLN:CG	1.99	1.24
1:C:1071:GLN:NE2	1:C:1071:GLN:CG	1.99	1.24
1:B:231:ILE:CG2	1:B:231:ILE:HG13	1.55	1.23
1:C:231:ILE:CG2	1:C:231:ILE:HG13	1.55	1.22
1:C:905:ARG:NH2	1:C:1050:MET:HE2	1.56	1.21
1:B:905:ARG:NH2	1:B:1050:MET:HE2	1.56	1.20
1:A:231:ILE:CG2	1:A:231:ILE:HG13	1.55	1.19
1:B:42:VAL:CG1	1:B:42:VAL:HG23	1.69	1.19
1:B:281:GLU:OE1	4:B:1304:NAG:O7	1.59	1.19
1:A:905:ARG:NH2	1:A:1050:MET:HE2	1.56	1.18
1:C:304:LYS:CD	1:C:304:LYS:CB	2.22	1.18
1:B:231:ILE:HG21	1:B:231:ILE:HD12	1.26	1.17
1:A:304:LYS:CD	1:A:304:LYS:CB	2.22	1.17
1:B:41:LYS:CG	1:B:41:LYS:CE	2.23	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LYS:CG	1:C:41:LYS:CE	2.23	1.17
1:A:41:LYS:CG	1:A:41:LYS:CE	2.22	1.17
1:B:42:VAL:CG2	1:B:42:VAL:HG11	1.75	1.16
1:B:304:LYS:CD	1:B:304:LYS:CB	2.22	1.16
1:A:44:ARG:NH2	1:C:567:ARG:HB2	1.59	1.15
1:A:905:ARG:HH22	1:A:1050:MET:HE2	1.01	1.15
1:B:699:LEU:CD1	1:C:872:GLN:OE1	1.94	1.14
1:A:41:LYS:CG	1:C:562:PHE:O	1.95	1.13
1:B:699:LEU:HD11	1:C:872:GLN:NE2	1.61	1.13
1:A:41:LYS:CG	1:A:41:LYS:CB	2.28	1.12
1:B:41:LYS:CG	1:B:41:LYS:CB	2.28	1.12
1:A:1101:HIS:CE1	4:A:1312:NAG:C5	2.32	1.12
1:C:41:LYS:CG	1:C:41:LYS:CB	2.28	1.12
1:A:41:LYS:C	1:A:41:LYS:CB	2.23	1.11
1:B:42:VAL:CG1	1:B:42:VAL:HG22	1.64	1.11
1:C:1050:MET:HG3	1:C:1051:SER:N	1.56	1.11
1:C:41:LYS:C	1:C:41:LYS:CB	2.24	1.11
1:A:304:LYS:CE	1:A:304:LYS:HG3	1.67	1.11
1:B:41:LYS:C	1:B:41:LYS:CB	2.24	1.10
1:C:231:ILE:HG21	1:C:231:ILE:HD12	1.26	1.10
1:A:231:ILE:CG2	1:A:231:ILE:CD1	2.26	1.10
1:B:905:ARG:HH22	1:B:1050:MET:HE2	1.01	1.10
1:A:280:ASN:OD1	1:A:284:THR:OG1	1.68	1.09
2:D:71:GLN:HG2	2:D:78:VAL:HG12	1.34	1.09
1:A:564:GLN:HG2	1:B:41:LYS:HG2	1.34	1.09
1:B:386:LYS:NZ	1:C:981:LEU:O	1.84	1.09
1:A:231:ILE:HG21	1:A:231:ILE:HD12	1.26	1.09
1:B:280:ASN:OD1	1:B:284:THR:OG1	1.68	1.08
1:B:563:GLN:CA	1:C:41:LYS:CG	2.31	1.08
1:A:1101:HIS:HE1	4:A:1312:NAG:O5	1.36	1.08
1:C:280:ASN:OD1	1:C:284:THR:OG1	1.68	1.08
1:B:699:LEU:HD11	1:C:872:GLN:HE22	1.03	1.07
1:A:1130:ILE:HD11	1:B:920:GLN:OE1	1.53	1.07
1:C:452:LEU:CD1	2:D:33:ARG:CG	2.33	1.07
1:A:304:LYS:CG	1:A:304:LYS:HD2	1.55	1.06
1:A:794:ILE:HG13	1:A:796:ASP:OD2	1.55	1.06
1:B:563:GLN:HA	1:C:41:LYS:HG2	1.33	1.06
1:B:611:LEU:CD2	1:B:611:LEU:CB	2.33	1.06
1:C:651:ILE:HG21	1:C:651:ILE:HG12	1.37	1.06
1:B:794:ILE:HG13	1:B:796:ASP:OD2	1.55	1.06
1:A:611:LEU:CD2	1:A:611:LEU:CB	2.33	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:LEU:CD1	1:C:872:GLN:CD	2.29	1.06
1:C:651:ILE:CG2	1:C:651:ILE:HG12	1.86	1.06
1:C:611:LEU:CD2	1:C:611:LEU:CB	2.33	1.05
1:C:231:ILE:CG2	1:C:231:ILE:CA	2.34	1.05
1:C:304:LYS:CG	1:C:304:LYS:HD2	1.55	1.05
1:C:905:ARG:HH22	1:C:1050:MET:HE2	1.01	1.05
1:B:287:ASP:OD2	1:B:288:ALA:N	1.89	1.05
1:B:563:GLN:N	1:C:41:LYS:CG	2.19	1.05
1:C:794:ILE:HG13	1:C:796:ASP:OD2	1.55	1.05
1:C:304:LYS:CG	1:C:304:LYS:HD3	1.55	1.04
1:B:231:ILE:CG2	1:B:231:ILE:CD1	2.26	1.04
1:C:287:ASP:OD2	1:C:288:ALA:N	1.89	1.04
1:A:651:ILE:HG21	1:A:651:ILE:HG12	1.37	1.04
1:B:651:ILE:CG2	1:B:651:ILE:HG12	1.86	1.04
1:A:1050:MET:HG3	1:A:1051:SER:N	1.56	1.04
1:B:231:ILE:CG2	1:B:231:ILE:CA	2.34	1.04
1:A:133:PHE:CD1	1:A:160:TYR:HB2	1.93	1.03
1:A:1101:HIS:CE1	4:A:1312:NAG:O5	2.11	1.03
1:B:304:LYS:CG	1:B:304:LYS:HD2	1.55	1.03
1:A:41:LYS:HG2	1:C:562:PHE:O	1.56	1.03
1:A:1135:ASN:OD1	1:A:1136:THR:N	1.91	1.03
1:C:452:LEU:CD1	2:D:33:ARG:HG3	1.86	1.03
1:C:905:ARG:NH1	1:C:1049:LEU:O	1.92	1.03
1:A:231:ILE:CG2	1:A:231:ILE:CA	2.34	1.03
1:A:287:ASP:OD2	1:A:288:ALA:N	1.89	1.03
1:B:304:LYS:CE	1:B:304:LYS:HG3	1.66	1.03
1:B:651:ILE:HG12	1:B:651:ILE:HG21	1.37	1.03
1:B:1135:ASN:OD1	1:B:1136:THR:N	1.91	1.03
1:A:159:VAL:HG23	1:A:160:TYR:HD1	1.23	1.03
1:A:304:LYS:CG	1:A:304:LYS:HD3	1.55	1.03
1:A:651:ILE:CG2	1:A:651:ILE:HG12	1.86	1.03
1:B:304:LYS:CG	1:B:304:LYS:HD3	1.55	1.03
1:C:133:PHE:CD1	1:C:160:TYR:HB2	1.93	1.03
1:B:159:VAL:HG23	1:B:160:TYR:HD1	1.22	1.02
1:B:905:ARG:NH1	1:B:1049:LEU:O	1.92	1.02
1:C:231:ILE:CG2	1:C:231:ILE:CD1	2.26	1.02
1:B:133:PHE:CD1	1:B:160:TYR:HB2	1.93	1.02
1:B:563:GLN:CB	1:C:41:LYS:CG	2.36	1.02
1:C:1135:ASN:OD1	1:C:1136:THR:N	1.91	1.02
1:A:905:ARG:NH1	1:A:1049:LEU:O	1.92	1.02
1:B:1050:MET:HG3	1:B:1051:SER:N	1.56	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:VAL:HG23	1:C:160:TYR:HD1	1.23	1.01
1:C:560:LEU:O	1:C:577:ARG:NH2	1.94	1.01
1:C:1071:GLN:NE2	1:C:1071:GLN:HG3	1.75	1.01
1:A:562:PHE:O	1:B:41:LYS:CG	2.09	1.01
1:B:454:ARG:NH1	1:B:456:PHE:O	1.93	1.01
1:C:231:ILE:CG1	1:C:231:ILE:HG21	1.69	1.01
1:C:80:ASP:OD2	1:C:82:PRO:HD2	1.61	1.00
1:B:80:ASP:OD2	1:B:82:PRO:HD2	1.61	1.00
1:B:231:ILE:CG1	1:B:231:ILE:HG21	1.69	1.00
1:C:231:ILE:CG2	1:C:231:ILE:HD12	1.88	1.00
1:A:80:ASP:OD2	1:A:82:PRO:HD2	1.61	1.00
1:C:304:LYS:CE	1:C:304:LYS:HG3	1.67	1.00
1:C:452:LEU:HD13	2:D:33:ARG:CG	1.92	1.00
1:C:452:LEU:HD12	2:D:33:ARG:HG3	1.42	1.00
1:C:452:LEU:HD13	2:D:33:ARG:HD3	1.02	1.00
1:B:124:THR:HG23	4:B:1301:NAG:H83	1.37	0.99
1:B:1071:GLN:NE2	1:B:1071:GLN:HG3	1.75	0.99
1:B:705:VAL:HG21	1:C:883:THR:HG21	1.43	0.99
1:C:449:TYR:C	2:D:53:ALA:HB2	1.87	0.99
1:B:699:LEU:HD13	1:C:872:GLN:CD	1.85	0.99
1:A:1071:GLN:NE2	1:A:1071:GLN:HG3	1.75	0.98
1:A:738:CYS:SG	1:A:764:ASN:ND2	2.37	0.98
1:A:41:LYS:HG3	1:C:562:PHE:O	1.61	0.98
1:B:231:ILE:CG2	1:B:231:ILE:HD12	1.88	0.98
1:C:651:ILE:HB	1:C:651:ILE:HD13	1.44	0.98
1:B:699:LEU:CD1	1:C:872:GLN:NE2	2.26	0.97
1:B:738:CYS:SG	1:B:764:ASN:ND2	2.36	0.97
1:B:42:VAL:CG1	1:B:42:VAL:CA	2.42	0.97
1:B:231:ILE:HG21	1:B:231:ILE:HG13	1.29	0.97
1:C:738:CYS:SG	1:C:764:ASN:ND2	2.37	0.97
1:B:563:GLN:HB3	1:C:41:LYS:HG2	1.47	0.97
1:A:651:ILE:HB	1:A:651:ILE:HD13	1.44	0.96
1:B:153:MET:CE	4:B:1302:NAG:O4	2.13	0.96
1:C:905:ARG:HH22	1:C:1050:MET:CE	1.78	0.96
1:A:231:ILE:HG21	1:A:231:ILE:HG13	1.29	0.96
1:C:452:LEU:CD1	2:D:33:ARG:HD3	1.96	0.96
1:A:905:ARG:HH22	1:A:1050:MET:CE	1.78	0.96
1:B:563:GLN:N	1:C:41:LYS:HG3	1.81	0.95
1:B:905:ARG:HH22	1:B:1050:MET:CE	1.78	0.95
1:A:231:ILE:CG2	1:A:231:ILE:HD12	1.89	0.95
1:B:651:ILE:HB	1:B:651:ILE:HD13	1.44	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:CG1	1:A:231:ILE:HG21	1.69	0.95
1:C:651:ILE:CG1	1:C:651:ILE:HG21	1.90	0.95
1:A:41:LYS:HG3	1:C:562:PHE:C	1.91	0.95
1:C:452:LEU:CD1	2:D:33:ARG:CD	2.44	0.94
1:A:287:ASP:OD1	1:A:306:PHE:CE1	2.21	0.94
1:B:287:ASP:OD1	1:B:306:PHE:CE1	2.21	0.94
1:A:1101:HIS:CE1	4:A:1312:NAG:C6	2.50	0.94
1:B:563:GLN:HB3	1:C:41:LYS:CG	1.98	0.94
1:C:124:THR:N	3:G:1:NAG:H81	1.83	0.94
1:C:231:ILE:HG21	1:C:231:ILE:HG13	1.29	0.94
1:B:1083:HIS:ND1	1:B:1084:ASP:OD1	2.01	0.94
1:C:287:ASP:OD1	1:C:306:PHE:CE1	2.21	0.94
1:A:1101:HIS:HE1	4:A:1312:NAG:C5	1.75	0.93
1:B:563:GLN:NE2	1:C:41:LYS:O	2.01	0.93
1:A:1083:HIS:ND1	1:A:1084:ASP:OD1	2.01	0.93
1:C:1083:HIS:ND1	1:C:1084:ASP:OD1	2.01	0.93
1:A:41:LYS:O	1:A:41:LYS:HB2	1.69	0.93
1:C:41:LYS:O	1:C:41:LYS:HB2	1.69	0.93
1:A:304:LYS:CG	1:A:304:LYS:HE2	2.00	0.92
1:B:41:LYS:O	1:B:41:LYS:HB2	1.69	0.92
1:C:717:ASN:HB2	1:C:1071:GLN:OE1	1.70	0.92
1:A:44:ARG:HH22	1:C:567:ARG:HB2	1.28	0.92
1:B:304:LYS:CG	1:B:304:LYS:HE2	2.00	0.92
1:C:331:ASN:O	1:C:332:ILE:HG22	1.70	0.92
1:B:699:LEU:CD1	1:C:872:GLN:HE22	1.83	0.92
1:B:717:ASN:HB2	1:B:1071:GLN:OE1	1.69	0.91
1:A:304:LYS:CD	1:A:304:LYS:HG2	1.40	0.91
1:C:304:LYS:CD	1:C:304:LYS:HG3	1.40	0.91
1:C:304:LYS:CG	1:C:304:LYS:HE2	2.00	0.91
1:A:304:LYS:CD	1:A:304:LYS:HG3	1.40	0.91
1:A:717:ASN:HB2	1:A:1071:GLN:OE1	1.69	0.91
1:A:44:ARG:HH22	1:C:567:ARG:CB	1.83	0.91
1:C:450:ASN:O	2:D:33:ARG:HG3	1.69	0.91
1:B:41:LYS:CB	1:B:41:LYS:HE3	2.01	0.91
1:B:480:CYS:O	1:B:482:GLY:N	2.04	0.90
1:C:304:LYS:CD	1:C:304:LYS:HG2	1.40	0.90
1:A:41:LYS:C	1:A:41:LYS:HB2	1.95	0.90
1:C:41:LYS:CB	1:C:41:LYS:HE3	2.01	0.90
1:C:350:VAL:HG21	1:C:453:TYR:CD1	2.06	0.90
1:B:206:LYS:HD3	1:B:224:GLU:OE2	1.71	0.90
1:C:37:TYR:OH	1:C:53:ASP:OD1	1.89	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:THR:HG22	1:A:64:TRP:CE3	2.07	0.90
1:B:126:VAL:N	1:B:172:SER:OG	2.05	0.90
1:C:29:THR:HG22	1:C:64:TRP:CE3	2.07	0.90
1:C:41:LYS:CG	1:C:41:LYS:HE3	2.01	0.90
1:B:41:LYS:C	1:B:41:LYS:HB2	1.95	0.90
1:B:304:LYS:CD	1:B:304:LYS:HG3	1.40	0.90
1:C:206:LYS:HD3	1:C:224:GLU:OE2	1.72	0.90
1:A:41:LYS:CB	1:A:41:LYS:HE3	2.01	0.89
1:B:304:LYS:CD	1:B:304:LYS:HG2	1.40	0.89
1:A:304:LYS:CG	1:A:304:LYS:CD	0.90	0.89
1:C:304:LYS:CG	1:C:304:LYS:CD	0.90	0.89
1:C:611:LEU:HD13	1:C:611:LEU:HD21	1.55	0.89
1:B:29:THR:HG22	1:B:64:TRP:CE3	2.07	0.89
1:B:304:LYS:CG	1:B:304:LYS:CD	0.90	0.89
1:C:41:LYS:C	1:C:41:LYS:HB2	1.95	0.89
1:C:126:VAL:N	1:C:172:SER:OG	2.05	0.89
1:A:37:TYR:OH	1:A:53:ASP:OD1	1.89	0.89
1:A:611:LEU:HD13	1:A:611:LEU:HD22	1.54	0.89
1:A:206:LYS:HD3	1:A:224:GLU:OE2	1.72	0.89
1:B:37:TYR:OH	1:B:53:ASP:OD1	1.89	0.89
1:B:611:LEU:HD13	1:B:611:LEU:HD21	1.54	0.89
1:A:1049:LEU:HB2	1:A:1065:VAL:HG12	1.55	0.89
1:A:126:VAL:N	1:A:172:SER:OG	2.05	0.88
1:B:611:LEU:HD13	1:B:611:LEU:HD22	1.54	0.88
1:B:1049:LEU:HB2	1:B:1065:VAL:HG12	1.55	0.88
1:C:111:ASP:HB3	1:C:134:GLN:OE1	1.73	0.88
1:A:231:ILE:CG2	1:A:231:ILE:HA	2.03	0.88
1:A:111:ASP:HB3	1:A:134:GLN:OE1	1.73	0.88
1:B:231:ILE:CG2	1:B:231:ILE:HA	2.03	0.88
1:B:111:ASP:HB3	1:B:134:GLN:OE1	1.73	0.88
1:C:1049:LEU:HB2	1:C:1065:VAL:HG12	1.55	0.88
1:A:41:LYS:CG	1:A:41:LYS:HE3	2.01	0.88
1:A:792:PRO:O	1:A:795:LYS:NZ	2.07	0.87
1:B:41:LYS:CG	1:B:41:LYS:HE3	2.01	0.87
1:A:565:PHE:O	1:B:43:PHE:N	2.05	0.87
1:B:916:LEU:HD12	1:B:923:ILE:HD12	1.55	0.87
1:B:951:VAL:O	1:B:955:ASN:ND2	2.08	0.87
1:A:159:VAL:HG11	1:A:241:LEU:HD21	1.56	0.87
1:C:159:VAL:HG11	1:C:241:LEU:HD21	1.56	0.87
1:C:611:LEU:HD13	1:C:611:LEU:HD22	1.54	0.87
1:C:916:LEU:HD12	1:C:923:ILE:HD12	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:LEU:HD12	1:A:923:ILE:HD12	1.55	0.87
1:C:951:VAL:O	1:C:955:ASN:ND2	2.08	0.87
1:B:444:LYS:NZ	1:B:447:GLY:O	2.08	0.87
1:B:462:LYS:NZ	1:B:463:PRO:O	2.07	0.87
1:B:792:PRO:O	1:B:795:LYS:NZ	2.07	0.87
1:C:231:ILE:CG2	1:C:231:ILE:HA	2.03	0.87
1:C:651:ILE:CG2	1:C:651:ILE:CA	2.53	0.86
1:B:651:ILE:CG2	1:B:651:ILE:CA	2.53	0.86
1:C:792:PRO:O	1:C:795:LYS:NZ	2.07	0.86
1:A:111:ASP:CB	1:A:134:GLN:OE1	2.24	0.86
1:A:611:LEU:HD13	1:A:611:LEU:HD21	1.54	0.86
1:A:651:ILE:CG2	1:A:651:ILE:CA	2.53	0.86
1:C:120:VAL:HG13	1:C:127:VAL:HG23	1.57	0.86
1:A:120:VAL:HG13	1:A:127:VAL:HG23	1.57	0.86
1:A:304:LYS:HE2	1:A:304:LYS:HG2	1.55	0.86
1:B:111:ASP:CB	1:B:134:GLN:OE1	2.24	0.86
1:A:951:VAL:O	1:A:955:ASN:ND2	2.08	0.86
1:B:153:MET:HE2	4:B:1302:NAG:HO4	1.41	0.86
1:C:111:ASP:CB	1:C:134:GLN:OE1	2.24	0.85
1:B:159:VAL:HG11	1:B:241:LEU:HD21	1.56	0.85
1:B:42:VAL:HG11	1:B:42:VAL:HG22	1.43	0.85
1:B:120:VAL:HG13	1:B:127:VAL:HG23	1.57	0.85
1:B:563:GLN:N	1:C:41:LYS:HG2	1.87	0.84
1:C:651:ILE:HB	1:C:651:ILE:HD12	1.59	0.84
1:A:318:PHE:N	1:A:593:GLY:O	2.11	0.84
1:B:78:ARG:HH21	1:B:80:ASP:CA	1.90	0.84
1:C:78:ARG:HH21	1:C:80:ASP:CA	1.90	0.84
1:A:78:ARG:HH21	1:A:80:ASP:CA	1.90	0.84
1:C:937:SER:O	1:C:941:THR:N	2.11	0.84
1:B:55:PHE:O	1:B:271:GLN:N	2.11	0.84
1:B:304:LYS:HE2	1:B:304:LYS:HG2	1.56	0.84
1:A:353:TRP:O	1:A:466:ARG:NH1	2.11	0.83
1:A:773:GLU:O	1:A:777:ASN:OD1	1.96	0.83
1:C:951:VAL:HA	1:C:954:GLN:HG3	1.59	0.83
1:A:651:ILE:CG1	1:A:651:ILE:HG21	1.90	0.83
1:B:773:GLU:O	1:B:777:ASN:OD1	1.96	0.83
3:G:1:NAG:O3	3:G:2:NAG:O5	1.95	0.83
1:B:937:SER:O	1:B:941:THR:N	2.10	0.83
1:B:1049:LEU:HD21	1:B:1067:TYR:HB2	1.60	0.83
1:C:58:PHE:N	1:C:290:ASP:OD2	2.11	0.83
1:C:318:PHE:N	1:C:593:GLY:O	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1049:LEU:HD21	1:C:1067:TYR:HB2	1.60	0.83
1:A:1049:LEU:HD21	1:A:1067:TYR:HB2	1.60	0.83
1:C:55:PHE:O	1:C:271:GLN:N	2.11	0.83
1:A:699:LEU:HD11	1:B:872:GLN:HE22	1.42	0.83
1:C:124:THR:H	3:G:1:NAG:H81	1.41	0.83
1:C:773:GLU:O	1:C:777:ASN:OD1	1.96	0.83
1:A:422:ASN:OD1	1:A:454:ARG:N	2.11	0.83
1:B:318:PHE:N	1:B:593:GLY:O	2.11	0.83
1:C:304:LYS:HE2	1:C:304:LYS:HG2	1.55	0.83
1:C:120:VAL:CG1	1:C:127:VAL:HG23	2.09	0.83
1:A:559:PHE:CD1	1:B:43:PHE:CZ	2.67	0.82
1:B:58:PHE:N	1:B:290:ASP:OD2	2.11	0.82
1:A:937:SER:O	1:A:941:THR:N	2.11	0.82
1:A:58:PHE:N	1:A:290:ASP:OD2	2.11	0.82
1:A:120:VAL:CG1	1:A:127:VAL:HG23	2.09	0.82
1:C:529:LYS:O	1:C:529:LYS:NZ	2.13	0.82
1:A:318:PHE:CZ	1:A:615:VAL:HG11	2.15	0.82
1:A:730:SER:OG	1:A:1058:HIS:ND1	2.13	0.82
1:A:951:VAL:HA	1:A:954:GLN:HG3	1.59	0.82
1:C:457:ARG:NH1	1:C:471:GLU:O	2.12	0.82
1:A:405:ASP:O	1:A:409:GLN:NE2	2.13	0.82
1:A:350:VAL:HG21	1:A:418:ILE:HD12	1.62	0.82
1:C:318:PHE:CZ	1:C:615:VAL:HG11	2.15	0.81
1:B:120:VAL:CG1	1:B:127:VAL:HG23	2.09	0.81
1:B:1101:HIS:HE1	4:B:1312:NAG:O5	1.64	0.81
1:A:762:GLN:HA	1:A:765:ARG:HE	1.45	0.81
1:B:730:SER:OG	1:B:1058:HIS:ND1	2.13	0.81
1:B:951:VAL:HA	1:B:954:GLN:HG3	1.59	0.81
1:B:1073:LYS:NZ	1:B:1073:LYS:CD	2.44	0.81
4:B:1306:NAG:O3	4:B:1306:NAG:O7	1.98	0.81
1:C:46:SER:N	1:C:280:ASN:O	2.14	0.81
1:C:490:PHE:CE2	2:D:105:THR:HA	2.16	0.81
1:C:771:ALA:HA	1:C:774:GLN:OE1	1.81	0.81
1:C:1050:MET:HG3	1:C:1051:SER:H	1.46	0.81
1:B:318:PHE:CZ	1:B:615:VAL:HG11	2.15	0.81
1:B:444:LYS:O	1:B:498:GLN:NE2	2.14	0.81
1:A:1073:LYS:NZ	1:A:1073:LYS:CD	2.44	0.81
1:B:771:ALA:HA	1:B:774:GLN:OE1	1.81	0.81
1:C:498:GLN:O	1:C:501:ASN:ND2	2.14	0.81
1:B:46:SER:N	1:B:280:ASN:O	2.14	0.80
1:B:651:ILE:HB	1:B:651:ILE:HD12	1.59	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:794:ILE:CG1	1:C:796:ASP:OD2	2.29	0.80
2:D:33:ARG:N	2:D:98:SER:OG	2.12	0.80
1:A:564:GLN:CG	1:B:41:LYS:HG2	2.11	0.80
1:A:721:SER:OG	1:A:1066:THR:O	1.99	0.80
1:C:1083:HIS:HD1	1:C:1084:ASP:CG	1.89	0.80
1:B:762:GLN:HA	1:B:765:ARG:HE	1.45	0.80
1:B:1083:HIS:HD1	1:B:1084:ASP:CG	1.89	0.80
1:A:771:ALA:HA	1:A:774:GLN:OE1	1.81	0.80
1:B:1130:ILE:CD1	1:C:920:GLN:OE1	2.21	0.80
1:C:330:PRO:HA	1:C:580:GLN:HG3	1.63	0.80
1:C:730:SER:OG	1:C:1058:HIS:ND1	2.13	0.80
1:A:703:ASN:OD1	1:B:787:GLN:HG3	1.82	0.80
1:A:55:PHE:O	1:A:271:GLN:N	2.11	0.80
1:B:964:LYS:O	1:B:968:SER:OG	2.00	0.80
1:C:404:GLY:N	1:C:506:GLN:O	2.15	0.80
1:C:1073:LYS:NZ	1:C:1073:LYS:CD	2.44	0.80
1:A:964:LYS:O	1:A:968:SER:OG	2.00	0.80
1:B:794:ILE:CG1	1:B:796:ASP:OD2	2.29	0.80
1:B:721:SER:OG	1:B:1066:THR:O	1.99	0.79
1:C:304:LYS:HG3	1:C:304:LYS:HE3	1.64	0.79
1:C:330:PRO:HA	1:C:580:GLN:CG	2.12	0.79
1:A:349:SER:OG	1:A:452:LEU:O	1.99	0.79
1:A:553:THR:O	1:A:586:ASP:N	2.15	0.79
1:A:1083:HIS:HD1	1:A:1084:ASP:CG	1.89	0.79
1:B:85:PRO:HA	1:B:237:ARG:HA	1.63	0.79
1:C:721:SER:OG	1:C:1066:THR:O	1.99	0.79
1:C:762:GLN:HA	1:C:765:ARG:HE	1.45	0.79
1:B:304:LYS:HG3	1:B:304:LYS:HE3	1.64	0.79
1:A:46:SER:N	1:A:280:ASN:O	2.14	0.79
1:A:794:ILE:CG1	1:A:796:ASP:OD2	2.29	0.79
1:A:133:PHE:CE1	1:A:160:TYR:HD2	2.01	0.79
1:B:708:SER:OG	1:B:710:ASN:OD1	2.00	0.79
1:C:424:LYS:HB2	1:C:461:LEU:HD23	1.64	0.79
1:C:566:GLY:O	1:C:574:ASP:N	2.15	0.79
1:A:1050:MET:HG3	1:A:1051:SER:H	1.46	0.79
1:B:1005:GLN:C	1:B:1005:GLN:OE1	2.26	0.79
1:B:281:GLU:OE1	4:B:1304:NAG:C7	2.30	0.79
1:B:1050:MET:HG3	1:B:1051:SER:H	1.46	0.79
1:C:85:PRO:HA	1:C:237:ARG:HA	1.63	0.79
1:C:159:VAL:HG23	1:C:160:TYR:CD1	2.14	0.79
1:B:133:PHE:CE1	1:B:160:TYR:HD2	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1005:GLN:OE1	1:C:1005:GLN:C	2.26	0.79
1:A:1101:HIS:CE1	4:A:1312:NAG:H5	2.18	0.78
1:B:41:LYS:CE	1:B:41:LYS:CB	2.61	0.78
1:A:496:GLY:O	1:A:498:GLN:NE2	2.17	0.78
1:B:947:LYS:O	1:B:951:VAL:HG23	1.84	0.78
1:C:644:GLN:NE2	4:C:1305:NAG:O7	2.16	0.78
1:A:41:LYS:CE	1:A:41:LYS:CB	2.61	0.78
1:A:165:ASN:ND2	4:A:1302:NAG:H2	1.99	0.78
1:C:41:LYS:C	1:C:41:LYS:N	2.41	0.78
1:C:41:LYS:CE	1:C:41:LYS:HA	2.14	0.78
1:A:611:LEU:CD1	1:A:611:LEU:HD21	2.11	0.78
1:C:964:LYS:O	1:C:968:SER:OG	2.00	0.78
1:C:388:ASN:O	1:C:528:LYS:NZ	2.13	0.78
1:A:304:LYS:CE	1:A:304:LYS:HG2	1.82	0.78
1:A:661:GLU:O	1:A:695:TYR:OH	2.02	0.78
1:A:1005:GLN:C	1:A:1005:GLN:OE1	2.26	0.78
1:C:143:VAL:N	1:C:244:LEU:O	2.17	0.78
1:A:85:PRO:HA	1:A:237:ARG:HA	1.63	0.78
2:D:12:VAL:HG21	2:D:18:LEU:HG	1.65	0.78
1:C:41:LYS:CE	1:C:41:LYS:CB	2.61	0.78
1:C:661:GLU:O	1:C:695:TYR:OH	2.02	0.78
1:B:562:PHE:CE2	1:C:225:PRO:HG2	2.18	0.77
1:C:537:LYS:NZ	1:C:538:CYS:O	2.16	0.77
1:C:947:LYS:O	1:C:951:VAL:HG23	1.84	0.77
1:A:143:VAL:N	1:A:244:LEU:O	2.17	0.77
1:B:133:PHE:CG	1:B:160:TYR:HB2	2.20	0.77
1:A:41:LYS:CE	1:A:41:LYS:HA	2.14	0.77
1:B:153:MET:HE3	4:B:1302:NAG:O3	1.85	0.77
1:C:111:ASP:HA	1:C:134:GLN:OE1	1.85	0.77
1:A:37:TYR:HD1	1:A:55:PHE:CZ	2.03	0.77
1:B:111:ASP:HA	1:B:134:GLN:OE1	1.85	0.77
1:C:127:VAL:HG11	3:G:1:NAG:O5	1.84	0.77
1:B:143:VAL:N	1:B:244:LEU:O	2.17	0.77
1:B:159:VAL:HG23	1:B:160:TYR:CD1	2.14	0.77
1:C:666:ILE:HD12	1:C:670:ILE:HG22	1.66	0.77
1:A:408:ARG:O	1:A:414:GLN:NE2	2.17	0.77
1:A:38:TYR:O	1:A:204:TYR:OH	2.01	0.77
1:A:304:LYS:HG3	1:A:304:LYS:HE3	1.64	0.77
1:A:651:ILE:HB	1:A:651:ILE:HD12	1.59	0.77
1:B:37:TYR:HD1	1:B:55:PHE:CZ	2.03	0.77
1:B:41:LYS:CE	1:B:41:LYS:HA	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:PHE:CE1	1:C:160:TYR:HD2	2.01	0.77
1:B:905:ARG:NH2	1:B:1050:MET:CE	2.42	0.77
1:C:563:GLN:O	1:C:577:ARG:NE	2.18	0.77
1:A:106:PHE:HD1	1:A:238:PHE:HB2	1.50	0.77
1:A:111:ASP:O	1:A:134:GLN:NE2	2.18	0.77
1:A:133:PHE:CG	1:A:160:TYR:HB2	2.20	0.77
1:B:41:LYS:C	1:B:41:LYS:N	2.41	0.77
1:B:111:ASP:O	1:B:134:GLN:NE2	2.18	0.77
1:A:947:LYS:O	1:A:951:VAL:HG23	1.84	0.76
1:B:133:PHE:CE1	1:B:160:TYR:CD2	2.73	0.76
1:B:557:LYS:HB2	1:C:43:PHE:CE2	2.20	0.76
1:C:37:TYR:HD1	1:C:55:PHE:CZ	2.03	0.76
1:A:41:LYS:C	1:A:41:LYS:N	2.41	0.76
1:B:666:ILE:HD12	1:B:670:ILE:HG22	1.66	0.76
1:C:133:PHE:CE1	1:C:160:TYR:CD2	2.73	0.76
1:C:453:TYR:CZ	1:C:455:LEU:HG	2.20	0.76
1:A:111:ASP:HA	1:A:134:GLN:OE1	1.85	0.76
1:B:948:LEU:CD1	1:B:948:LEU:HG	2.13	0.76
1:A:133:PHE:CE1	1:A:160:TYR:CD2	2.73	0.76
1:A:1085:GLY:O	1:A:1086:LYS:HD2	1.86	0.76
1:B:1085:GLY:O	1:B:1086:LYS:HD2	1.86	0.76
1:C:106:PHE:HD1	1:C:238:PHE:HB2	1.50	0.76
1:C:350:VAL:HG21	1:C:453:TYR:HD1	1.50	0.76
1:B:304:LYS:CE	1:B:304:LYS:HG2	1.83	0.76
1:B:557:LYS:HB2	1:C:43:PHE:CZ	2.21	0.76
1:C:111:ASP:O	1:C:134:GLN:NE2	2.18	0.76
1:C:133:PHE:CG	1:C:160:TYR:HB2	2.20	0.76
1:B:106:PHE:HD1	1:B:238:PHE:HB2	1.50	0.76
1:A:666:ILE:HD12	1:A:670:ILE:HG22	1.66	0.76
2:D:67:LEU:HD11	2:D:80:LEU:HD11	1.68	0.76
1:A:502:GLY:O	1:A:506:GLN:N	2.17	0.76
1:C:1085:GLY:O	1:C:1086:LYS:HD2	1.86	0.76
1:B:109:THR:O	1:B:110:LEU:HD23	1.86	0.76
1:C:38:TYR:O	1:C:204:TYR:OH	2.01	0.76
1:A:920:GLN:HA	1:A:923:ILE:HG13	1.68	0.75
1:B:661:GLU:O	1:B:695:TYR:OH	2.02	0.75
1:A:44:ARG:NH2	1:C:567:ARG:CB	2.41	0.75
1:C:450:ASN:O	2:D:33:ARG:CG	2.34	0.75
1:C:920:GLN:HA	1:C:923:ILE:HG13	1.68	0.75
1:A:723:THR:O	1:A:1064:HIS:N	2.20	0.75
1:C:80:ASP:OD2	1:C:82:PRO:CD	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:O	1:A:110:LEU:HD23	1.86	0.75
1:A:866:THR:O	1:A:869:MET:HG2	1.86	0.75
1:B:31:SER:O	1:B:59:PHE:N	2.20	0.75
1:B:866:THR:O	1:B:869:MET:HG2	1.86	0.75
1:A:352:ALA:O	1:A:466:ARG:NH2	2.20	0.75
1:C:802:PHE:CD2	1:C:805:ILE:HD11	2.22	0.75
1:B:38:TYR:O	1:B:204:TYR:OH	2.01	0.74
1:B:802:PHE:CD2	1:B:805:ILE:HD11	2.22	0.74
1:C:905:ARG:NH2	1:C:1050:MET:CE	2.42	0.74
1:A:1085:GLY:C	1:A:1086:LYS:HD2	2.12	0.74
1:B:773:GLU:OE2	1:B:777:ASN:ND2	2.20	0.74
1:B:1085:GLY:C	1:B:1086:LYS:HD2	2.12	0.74
1:A:31:SER:O	1:A:59:PHE:N	2.20	0.74
1:A:802:PHE:CD2	1:A:805:ILE:HD11	2.22	0.74
1:C:109:THR:O	1:C:110:LEU:HD23	1.86	0.74
1:A:430:THR:O	1:A:515:PHE:N	2.20	0.74
1:A:551:VAL:HG13	1:A:588:THR:OG1	1.87	0.74
1:C:31:SER:O	1:C:59:PHE:N	2.20	0.74
1:C:490:PHE:CE2	1:C:492:LEU:HD11	2.22	0.74
1:A:331:ASN:OD1	4:A:1303:NAG:N2	2.21	0.74
1:B:920:GLN:HA	1:B:923:ILE:HG13	1.68	0.74
1:C:189:LEU:HD11	1:C:191:GLU:CD	2.12	0.74
1:A:328:ARG:NH2	1:A:531:THR:O	2.20	0.74
1:B:80:ASP:OD2	1:B:82:PRO:CD	2.35	0.74
1:C:106:PHE:O	1:C:116:SER:OG	2.05	0.74
1:A:80:ASP:OD2	1:A:82:PRO:CD	2.35	0.74
1:A:159:VAL:HG23	1:A:160:TYR:CD1	2.14	0.74
1:A:433:VAL:O	1:A:434:ILE:HD13	1.87	0.74
1:C:330:PRO:CA	1:C:580:GLN:HG3	2.17	0.73
1:C:1085:GLY:C	1:C:1086:LYS:HD2	2.12	0.73
1:A:350:VAL:CG2	1:A:418:ILE:HG23	2.18	0.73
1:B:325:SER:OG	1:B:540:ASN:O	2.04	0.73
1:C:444:LYS:HZ1	2:D:53:ALA:HB1	1.52	0.73
1:A:28:TYR:CE1	1:A:63:THR:HG22	2.24	0.73
1:A:361:CYS:O	1:A:524:VAL:HG23	1.88	0.73
1:C:28:TYR:CE1	1:C:63:THR:HG22	2.24	0.73
1:B:189:LEU:HD11	1:B:191:GLU:CD	2.13	0.73
1:B:723:THR:O	1:B:1064:HIS:N	2.20	0.73
1:C:559:PHE:CD1	1:C:584:ILE:HG21	2.24	0.73
1:A:773:GLU:OE2	1:A:777:ASN:ND2	2.20	0.73
1:C:117:LEU:HD11	1:C:128:ILE:CG2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:773:GLU:OE2	1:C:777:ASN:ND2	2.20	0.73
1:C:866:THR:O	1:C:869:MET:HG2	1.86	0.73
1:A:1050:MET:O	1:A:1065:VAL:N	2.14	0.73
1:B:611:LEU:CD2	1:B:611:LEU:HB3	2.18	0.73
1:B:117:LEU:HD11	1:B:128:ILE:CG2	2.19	0.73
1:B:375:SER:N	1:B:435:ALA:O	2.22	0.73
1:C:723:THR:O	1:C:1064:HIS:N	2.20	0.73
1:B:437:ASN:ND2	1:B:507:PRO:O	2.22	0.73
1:B:669:GLY:HA3	1:C:869:MET:HE1	1.71	0.73
1:A:106:PHE:O	1:A:116:SER:OG	2.05	0.73
1:A:189:LEU:HD11	1:A:191:GLU:CD	2.13	0.73
1:C:502:GLY:O	1:C:506:GLN:N	2.22	0.73
1:B:616:ASN:O	1:B:619:GLU:OE2	2.07	0.72
1:A:41:LYS:CA	1:A:41:LYS:HE3	2.19	0.72
1:B:41:LYS:CA	1:B:41:LYS:HE3	2.20	0.72
1:C:37:TYR:CD1	1:C:55:PHE:CZ	2.78	0.72
1:B:1089:PHE:N	1:B:1121:PHE:O	2.20	0.72
1:A:37:TYR:CD1	1:A:55:PHE:CZ	2.78	0.72
1:C:41:LYS:CA	1:C:41:LYS:HE3	2.20	0.72
1:A:29:THR:HB	1:A:216:LEU:HD11	1.72	0.72
1:A:117:LEU:HD11	1:A:128:ILE:CG2	2.19	0.72
1:B:28:TYR:CE1	1:B:63:THR:HG22	2.24	0.72
1:A:76:THR:OG1	1:A:77:LYS:N	2.22	0.72
1:B:29:THR:HB	1:B:216:LEU:HD11	1.72	0.72
1:C:579:PRO:HB2	1:C:580:GLN:NE2	2.05	0.72
1:B:1110:TYR:CE1	1:B:1112:PRO:HG3	2.25	0.72
1:C:922:LEU:HA	1:C:925:ASN:OD1	1.90	0.72
1:A:708:SER:OG	1:A:710:ASN:OD1	2.08	0.72
1:C:76:THR:OG1	1:C:77:LYS:N	2.22	0.72
1:C:77:LYS:NZ	1:C:258:TRP:O	2.15	0.72
1:C:350:VAL:HG21	1:C:453:TYR:CE1	2.24	0.72
1:C:616:ASN:O	1:C:619:GLU:OE2	2.07	0.72
1:B:492:LEU:H	1:B:492:LEU:HD12	1.54	0.72
1:B:922:LEU:HA	1:B:925:ASN:OD1	1.90	0.72
1:C:29:THR:HB	1:C:216:LEU:HD11	1.72	0.72
1:B:499:PRO:O	1:B:506:GLN:NE2	2.23	0.71
1:A:616:ASN:O	1:A:619:GLU:OE2	2.07	0.71
1:A:1110:TYR:CE1	1:A:1112:PRO:HG3	2.25	0.71
1:B:37:TYR:CD1	1:B:55:PHE:CZ	2.78	0.71
1:B:1089:PHE:CE1	1:C:914:ASN:HB3	2.25	0.71
1:B:1106:GLN:NE2	1:B:1109:PHE:HB3	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:LEU:HA	1:A:925:ASN:OD1	1.90	0.71
1:A:1089:PHE:N	1:A:1121:PHE:O	2.20	0.71
1:B:78:ARG:HH21	1:B:80:ASP:CB	2.04	0.71
1:C:1106:GLN:NE2	1:C:1109:PHE:HB3	2.05	0.71
1:A:905:ARG:NH2	1:A:1050:MET:CE	2.42	0.71
1:A:1106:GLN:NE2	1:A:1109:PHE:HB3	2.05	0.71
1:B:544:ASN:ND2	4:B:1305:NAG:O6	2.23	0.71
1:B:577:ARG:NE	4:B:1305:NAG:O4	2.20	0.71
1:C:78:ARG:HH21	1:C:80:ASP:CB	2.04	0.71
1:C:78:ARG:HH21	1:C:80:ASP:HB2	1.56	0.71
1:C:1110:TYR:CE1	1:C:1112:PRO:HG3	2.25	0.71
1:A:78:ARG:HH21	1:A:80:ASP:HB2	1.56	0.71
1:A:611:LEU:CD2	1:A:611:LEU:HB3	2.18	0.71
1:C:187:LYS:HB3	1:C:210:ILE:O	1.91	0.71
1:A:78:ARG:HH21	1:A:80:ASP:CB	2.04	0.71
1:B:76:THR:OG1	1:B:77:LYS:N	2.22	0.71
1:B:421:TYR:C	1:B:461:LEU:HD21	2.15	0.71
1:A:187:LYS:HB3	1:A:210:ILE:O	1.91	0.71
1:A:567:ARG:HB2	1:B:44:ARG:NH2	2.06	0.71
1:B:44:ARG:HB3	1:B:279:TYR:CD2	2.26	0.71
1:C:40:ASP:OD2	1:C:42:VAL:N	2.22	0.71
1:C:44:ARG:HB3	1:C:279:TYR:CD2	2.26	0.71
1:C:404:GLY:O	1:C:407:VAL:HG22	1.90	0.71
1:C:1089:PHE:N	1:C:1121:PHE:O	2.20	0.71
1:A:132:GLU:OE2	1:A:165:ASN:N	2.21	0.70
1:A:567:ARG:HB2	1:B:44:ARG:CZ	2.20	0.70
1:A:1073:LYS:HG3	1:A:1075:PHE:CZ	2.26	0.70
1:B:34:ARG:NH2	1:B:217:PRO:O	2.24	0.70
1:B:78:ARG:HH21	1:B:80:ASP:HA	1.56	0.70
1:B:562:PHE:CD2	1:C:41:LYS:HD3	2.27	0.70
1:C:651:ILE:CG2	1:C:651:ILE:HG13	2.18	0.70
1:C:17:ASN:HD21	3:H:1:NAG:H5	1.56	0.70
1:C:220:PHE:CE2	1:C:287:ASP:HA	2.26	0.70
1:B:187:LYS:HB3	1:B:210:ILE:O	1.91	0.70
1:C:453:TYR:HB3	1:C:494:SER:HA	1.74	0.70
1:B:78:ARG:HH21	1:B:80:ASP:HB2	1.56	0.70
2:D:33:ARG:NH2	2:D:58:TYR:OH	2.23	0.70
1:A:220:PHE:CE2	1:A:287:ASP:HA	2.26	0.70
1:C:323:THR:O	1:C:539:VAL:HG22	1.91	0.70
1:A:99:ASN:O	1:A:102:ARG:NE	2.23	0.70
1:A:570:ALA:HB1	1:B:963:VAL:HG11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LEU:HD13	1:B:872:GLN:OE1	1.91	0.70
1:C:34:ARG:NH2	1:C:217:PRO:O	2.24	0.70
1:C:330:PRO:HA	1:C:580:GLN:CD	2.15	0.70
1:C:132:GLU:OE2	1:C:165:ASN:N	2.21	0.70
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.74	0.70
1:C:453:TYR:CE2	1:C:455:LEU:HG	2.26	0.70
1:C:1073:LYS:HG3	1:C:1075:PHE:CZ	2.26	0.70
1:B:40:ASP:OD2	1:B:42:VAL:N	2.22	0.70
1:C:611:LEU:CD2	1:C:611:LEU:HB3	2.18	0.70
1:A:733:LYS:HE2	1:A:861:LEU:HB3	1.73	0.69
1:B:220:PHE:CE2	1:B:287:ASP:HA	2.26	0.69
1:A:78:ARG:HH21	1:A:80:ASP:HA	1.56	0.69
1:A:559:PHE:CE1	1:A:584:ILE:HG13	2.27	0.69
1:A:948:LEU:CD1	1:A:948:LEU:HG	2.13	0.69
1:B:611:LEU:CD1	1:B:611:LEU:HD21	2.11	0.69
1:C:111:ASP:CA	1:C:134:GLN:OE1	2.40	0.69
1:A:702:GLU:OE1	1:A:702:GLU:N	2.24	0.69
1:B:651:ILE:CG2	1:B:651:ILE:HG13	2.18	0.69
1:C:733:LYS:HE2	1:C:861:LEU:HB3	1.73	0.69
1:A:44:ARG:HB3	1:A:279:TYR:CD2	2.26	0.69
1:B:111:ASP:CA	1:B:134:GLN:OE1	2.40	0.69
1:B:1073:LYS:HG3	1:B:1075:PHE:CZ	2.26	0.69
1:A:563:GLN:O	1:A:577:ARG:NH1	2.25	0.69
1:C:78:ARG:HH21	1:C:80:ASP:HA	1.56	0.69
1:C:541:PHE:N	1:C:548:GLY:O	2.25	0.69
1:A:111:ASP:CA	1:A:134:GLN:OE1	2.40	0.69
1:B:733:LYS:HE2	1:B:861:LEU:HB3	1.73	0.69
1:A:34:ARG:NH2	1:A:217:PRO:O	2.24	0.69
1:A:77:LYS:NZ	1:A:258:TRP:O	2.15	0.69
1:A:618:THR:OG1	1:A:619:GLU:OE1	2.10	0.69
1:A:794:ILE:CD1	1:A:796:ASP:OD2	2.41	0.69
1:C:1050:MET:O	1:C:1065:VAL:N	2.14	0.69
1:A:41:LYS:CG	1:A:41:LYS:HE2	2.22	0.69
1:A:132:GLU:OE1	1:A:164:ASN:HB3	1.93	0.69
1:B:42:VAL:HG23	1:B:42:VAL:HG11	1.51	0.69
1:B:723:THR:N	1:B:1064:HIS:O	2.26	0.69
1:C:132:GLU:OE1	1:C:164:ASN:HB3	1.93	0.69
1:C:568:ASP:N	1:C:572:THR:O	2.26	0.69
1:C:618:THR:OG1	1:C:619:GLU:OE1	2.10	0.69
1:B:189:LEU:HB3	1:B:210:ILE:HD11	1.75	0.69
1:B:618:THR:OG1	1:B:619:GLU:OE1	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:ILE:CG1	1:B:651:ILE:HG21	1.90	0.69
1:B:900:MET:SD	1:B:917:TYR:OH	2.51	0.69
1:C:17:ASN:ND2	3:H:1:NAG:H5	2.08	0.69
1:A:189:LEU:HB3	1:A:210:ILE:HD11	1.75	0.69
1:B:794:ILE:CD1	1:B:796:ASP:OD2	2.41	0.69
1:B:913:GLN:O	1:B:917:TYR:HD1	1.76	0.69
1:C:41:LYS:HA	1:C:41:LYS:NZ	2.08	0.69
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.74	0.69
1:B:134:GLN:HB3	1:B:161:SER:OG	1.92	0.68
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.74	0.68
1:C:535:LYS:HA	1:C:552:LEU:HD23	1.75	0.68
1:A:134:GLN:HB3	1:A:161:SER:OG	1.93	0.68
1:B:472:ILE:HG23	1:B:489:TYR:O	1.93	0.68
1:C:794:ILE:CD1	1:C:796:ASP:OD2	2.41	0.68
1:C:913:GLN:O	1:C:917:TYR:HD1	1.76	0.68
1:B:132:GLU:O	1:B:132:GLU:HG2	1.93	0.68
1:B:132:GLU:OE2	1:B:165:ASN:N	2.21	0.68
1:B:705:VAL:HG21	1:C:883:THR:CG2	2.21	0.68
1:C:189:LEU:HB3	1:C:210:ILE:HD11	1.75	0.68
1:C:304:LYS:CE	1:C:304:LYS:HG2	1.82	0.68
1:A:132:GLU:HG2	1:A:132:GLU:O	1.93	0.68
1:B:106:PHE:O	1:B:116:SER:OG	2.05	0.68
1:B:111:ASP:HB3	1:B:134:GLN:CD	2.19	0.68
1:C:41:LYS:CG	1:C:41:LYS:HE2	2.22	0.68
1:B:1116:THR:HG23	1:B:1138:TYR:HD1	1.59	0.68
1:C:1102:TRP:CD1	1:C:1135:ASN:HD22	2.12	0.68
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.76	0.68
1:B:702:GLU:HB3	1:C:790:LYS:HD3	1.73	0.68
1:A:913:GLN:O	1:A:917:TYR:HD1	1.76	0.68
1:A:1102:TRP:CD1	1:A:1135:ASN:HD22	2.12	0.68
1:B:132:GLU:OE1	1:B:164:ASN:HB3	1.93	0.68
1:B:349:SER:OG	1:B:495:TYR:OH	2.12	0.68
1:B:1102:TRP:CD1	1:B:1135:ASN:HD22	2.12	0.68
1:A:41:LYS:HA	1:A:41:LYS:NZ	2.08	0.68
1:A:825:LYS:HD3	1:A:945:LEU:HD12	1.76	0.68
1:B:77:LYS:NZ	1:B:258:TRP:O	2.15	0.68
1:B:1050:MET:O	1:B:1065:VAL:N	2.14	0.68
1:C:948:LEU:CD1	1:C:948:LEU:HG	2.13	0.68
2:D:36:TRP:CD1	2:D:80:LEU:HD13	2.29	0.68
1:B:41:LYS:HA	1:B:41:LYS:NZ	2.08	0.68
1:B:393:THR:OG1	1:B:516:GLU:OE1	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:825:LYS:HD3	1:B:945:LEU:HD12	1.76	0.68
1:A:43:PHE:N	1:C:565:PHE:O	2.26	0.68
1:B:153:MET:HE2	4:B:1302:NAG:C4	2.23	0.68
1:C:340:GLU:OE1	1:C:340:GLU:N	2.26	0.68
1:C:492:LEU:O	2:D:103:THR:HG23	1.93	0.67
1:B:133:PHE:CE1	1:B:160:TYR:HB2	2.29	0.67
1:B:562:PHE:CE2	1:C:41:LYS:HE2	2.30	0.67
1:A:314:GLN:NE2	1:A:316:SER:O	2.28	0.67
1:C:111:ASP:HB3	1:C:134:GLN:CD	2.19	0.67
1:C:134:GLN:HB3	1:C:161:SER:OG	1.93	0.67
1:C:913:GLN:HB3	1:C:917:TYR:CE1	2.30	0.67
1:C:1116:THR:HG23	1:C:1138:TYR:HD1	1.59	0.67
1:A:913:GLN:HB3	1:A:917:TYR:CE1	2.30	0.67
1:B:314:GLN:NE2	1:B:316:SER:O	2.28	0.67
1:C:903:ALA:HB1	1:C:913:GLN:HG2	1.76	0.67
1:A:111:ASP:HB3	1:A:134:GLN:CD	2.19	0.67
1:A:594:GLY:HA3	1:A:613:GLN:HG2	1.77	0.67
1:A:1116:THR:HG23	1:A:1138:TYR:HD1	1.59	0.67
1:C:294:ASP:OD2	1:C:296:LEU:N	2.26	0.67
1:C:314:GLN:NE2	1:C:316:SER:O	2.28	0.67
1:A:1130:ILE:CD1	1:B:920:GLN:OE1	2.39	0.67
1:B:562:PHE:C	1:C:41:LYS:CG	2.68	0.67
1:B:577:ARG:CZ	4:B:1305:NAG:H83	2.25	0.67
1:B:913:GLN:HB3	1:B:917:TYR:CE1	2.30	0.67
1:C:594:GLY:HA3	1:C:613:GLN:HG2	1.77	0.67
1:A:452:LEU:HD12	1:A:492:LEU:HB2	1.76	0.67
1:B:367:VAL:O	1:B:371:SER:N	2.28	0.67
1:B:712:ILE:HD11	1:C:896:ILE:HG13	1.77	0.67
1:A:611:LEU:HG	1:A:612:TYR:N	2.09	0.67
1:C:132:GLU:O	1:C:132:GLU:HG2	1.93	0.67
1:C:802:PHE:HD2	1:C:805:ILE:HD11	1.58	0.67
1:A:41:LYS:HG2	1:C:564:GLN:HG3	1.76	0.67
1:A:381:GLY:HA3	1:A:430:THR:HG22	1.76	0.67
1:A:701:ALA:O	1:B:788:ILE:N	2.28	0.67
1:A:723:THR:N	1:A:1064:HIS:O	2.26	0.67
1:C:492:LEU:C	2:D:103:THR:HG23	2.20	0.67
1:A:49:HIS:CE1	1:A:51:THR:OG1	2.48	0.67
1:A:699:LEU:CD1	1:B:872:GLN:HE22	2.08	0.67
1:B:109:THR:C	1:B:110:LEU:HD23	2.20	0.67
1:B:802:PHE:HD2	1:B:805:ILE:HD11	1.58	0.67
1:B:702:GLU:HA	1:C:788:ILE:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:SER:O	1:B:761:THR:OG1	2.11	0.66
1:C:49:HIS:CE1	1:C:51:THR:OG1	2.48	0.66
1:A:883:THR:O	1:A:896:ILE:HG22	1.96	0.66
1:B:103:GLY:HA3	1:B:120:VAL:HA	1.77	0.66
1:B:594:GLY:HA3	1:B:613:GLN:HG2	1.77	0.66
1:C:330:PRO:HD2	1:C:332:ILE:HD12	1.75	0.66
1:C:733:LYS:CE	1:C:861:LEU:HB3	2.26	0.66
1:A:900:MET:SD	1:A:917:TYR:OH	2.51	0.66
1:B:49:HIS:CE1	1:B:51:THR:OG1	2.48	0.66
1:B:502:GLY:O	1:B:505:TYR:N	2.29	0.66
1:A:109:THR:C	1:A:110:LEU:HD23	2.20	0.66
1:A:350:VAL:HG21	1:A:418:ILE:HG23	1.76	0.66
1:C:185:ASN:ND2	1:C:212:LEU:O	2.28	0.66
1:C:900:MET:SD	1:C:917:TYR:OH	2.51	0.66
2:D:20:LEU:HG	2:D:82:MET:HE2	1.77	0.66
1:B:99:ASN:O	1:B:102:ARG:NE	2.23	0.66
1:C:327:VAL:O	1:C:531:THR:N	2.28	0.66
1:C:449:TYR:CE1	2:D:53:ALA:HA	2.31	0.66
1:A:40:ASP:OD2	1:A:42:VAL:N	2.22	0.66
1:A:84:LEU:CA	1:A:237:ARG:HH11	2.09	0.66
1:B:883:THR:O	1:B:896:ILE:HG22	1.96	0.66
1:B:903:ALA:HB1	1:B:913:GLN:HG2	1.76	0.66
1:A:133:PHE:CE1	1:A:160:TYR:HB2	2.30	0.66
1:A:133:PHE:HD1	1:A:162:SER:H	1.44	0.66
1:B:611:LEU:HG	1:B:612:TYR:N	2.09	0.66
1:C:28:TYR:CD1	4:C:1304:NAG:H5	2.30	0.66
1:C:452:LEU:HD23	2:D:104:CYS:O	1.94	0.66
1:C:473:TYR:HB2	1:C:491:PRO:HB3	1.78	0.66
1:A:145:TYR:CD1	1:A:152:TRP:CE3	2.84	0.66
1:B:145:TYR:CD1	1:B:152:TRP:CE3	2.84	0.66
1:A:792:PRO:HB2	1:A:794:ILE:HG23	1.77	0.66
1:A:948:LEU:CD1	1:A:948:LEU:CB	2.70	0.66
1:B:733:LYS:CE	1:B:861:LEU:HB3	2.26	0.66
1:C:29:THR:N	1:C:62:VAL:O	2.25	0.66
1:C:109:THR:C	1:C:110:LEU:HD23	2.20	0.66
1:A:91:TYR:HA	1:A:193:VAL:HG22	1.77	0.66
1:A:103:GLY:HA3	1:A:120:VAL:HA	1.77	0.66
1:A:143:VAL:HG11	1:A:245:HIS:CE1	2.31	0.66
1:A:733:LYS:CE	1:A:861:LEU:HB3	2.26	0.66
2:D:4:LEU:HD21	2:D:97:ALA:CB	2.25	0.66
1:A:100:ILE:HD12	1:A:263:ALA:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:VAL:HG22	1:B:514:SER:O	1.96	0.65
1:C:883:THR:O	1:C:896:ILE:HG22	1.96	0.65
1:A:402:ILE:O	1:A:508:TYR:N	2.28	0.65
1:A:802:PHE:HD2	1:A:805:ILE:HD11	1.58	0.65
1:C:84:LEU:CA	1:C:237:ARG:HH11	2.09	0.65
1:C:611:LEU:CD1	1:C:611:LEU:HD21	2.11	0.65
1:C:825:LYS:HD3	1:C:945:LEU:HD12	1.76	0.65
1:A:84:LEU:HA	1:A:237:ARG:NH1	2.12	0.65
1:A:434:ILE:O	1:A:510:VAL:HG13	1.97	0.65
1:B:100:ILE:HD12	1:B:263:ALA:HB2	1.77	0.65
1:B:106:PHE:CD1	1:B:238:PHE:HB2	2.31	0.65
1:C:133:PHE:CE1	1:C:160:TYR:HB2	2.30	0.65
1:C:327:VAL:H	1:C:531:THR:HG22	1.62	0.65
1:C:474:GLN:NE2	1:C:478:THR:O	2.29	0.65
2:D:103:THR:O	2:D:105:THR:N	2.29	0.65
1:A:294:ASP:OD2	1:A:296:LEU:N	2.26	0.65
1:A:41:LYS:CA	1:A:41:LYS:CE	2.75	0.65
1:B:185:ASN:ND2	1:B:212:LEU:O	2.28	0.65
4:B:1311:NAG:O3	4:B:1311:NAG:O7	2.13	0.65
1:C:93:ALA:O	1:C:266:TYR:N	2.25	0.65
1:C:100:ILE:HD12	1:C:263:ALA:HB2	1.77	0.65
1:C:145:TYR:CD1	1:C:152:TRP:CE3	2.84	0.65
2:D:4:LEU:HD21	2:D:97:ALA:HB2	1.77	0.65
1:A:185:ASN:ND2	1:A:212:LEU:O	2.28	0.65
1:A:758:SER:O	1:A:761:THR:OG1	2.11	0.65
1:B:84:LEU:HA	1:B:237:ARG:NH1	2.12	0.65
1:C:792:PRO:HB2	1:C:794:ILE:HG23	1.77	0.65
1:A:364:ASP:O	1:A:367:VAL:HG22	1.96	0.65
1:A:703:ASN:CG	1:B:787:GLN:HG3	2.21	0.65
1:A:1074:ASN:ND2	4:A:1311:NAG:O4	2.30	0.65
1:C:41:LYS:CA	1:C:41:LYS:CE	2.75	0.65
1:B:948:LEU:CD1	1:B:948:LEU:CB	2.69	0.65
1:C:91:TYR:HA	1:C:193:VAL:HG22	1.77	0.65
1:A:344:ALA:O	1:A:509:ARG:NH2	2.30	0.65
1:B:90:VAL:HG13	1:B:267:VAL:HG13	1.79	0.65
1:B:133:PHE:HD1	1:B:162:SER:H	1.44	0.65
1:B:318:PHE:HD2	1:B:318:PHE:C	2.05	0.65
1:B:433:VAL:HG13	1:B:512:VAL:HG22	1.77	0.65
1:C:310:LYS:NZ	1:C:663:ASP:O	2.27	0.65
1:A:310:LYS:NZ	1:A:663:ASP:O	2.27	0.65
1:C:103:GLY:HA3	1:C:120:VAL:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:PHE:HD1	1:C:162:SER:H	1.44	0.65
1:C:143:VAL:HG11	1:C:245:HIS:CE1	2.32	0.65
1:A:139:PRO:HB2	1:A:159:VAL:HG12	1.79	0.64
1:B:41:LYS:CG	1:B:41:LYS:HE2	2.22	0.64
1:B:83:VAL:O	1:B:237:ARG:NH1	2.31	0.64
1:B:143:VAL:HG11	1:B:245:HIS:CE1	2.31	0.64
1:C:723:THR:N	1:C:1064:HIS:O	2.26	0.64
1:C:758:SER:O	1:C:761:THR:OG1	2.11	0.64
1:B:41:LYS:CA	1:B:41:LYS:CE	2.75	0.64
1:B:78:ARG:NH2	1:B:80:ASP:HA	2.12	0.64
1:B:91:TYR:HA	1:B:193:VAL:HG22	1.77	0.64
1:B:792:PRO:HB2	1:B:794:ILE:HG23	1.78	0.64
1:C:651:ILE:CB	1:C:651:ILE:HD12	2.19	0.64
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.32	0.64
1:B:84:LEU:CA	1:B:237:ARG:HH11	2.09	0.64
1:B:120:VAL:HG13	1:B:127:VAL:CG2	2.28	0.64
1:B:310:LYS:NZ	1:B:663:ASP:O	2.27	0.64
1:C:83:VAL:O	1:C:237:ARG:NH1	2.31	0.64
1:C:330:PRO:O	1:C:332:ILE:HB	1.98	0.64
1:C:473:TYR:N	1:C:489:TYR:O	2.25	0.64
1:C:710:ASN:O	1:C:1076:THR:OG1	2.08	0.64
1:C:139:PRO:HB2	1:C:159:VAL:HG12	1.79	0.64
1:C:395:VAL:HG22	1:C:515:PHE:HA	1.78	0.64
1:B:332:ILE:HD12	1:B:333:THR:N	2.13	0.64
1:C:84:LEU:HA	1:C:237:ARG:NH1	2.12	0.64
1:C:366:SER:O	1:C:370:ASN:N	2.30	0.64
1:C:444:LYS:NZ	2:D:53:ALA:HB1	2.13	0.64
1:A:493:GLN:NE2	1:A:494:SER:O	2.28	0.64
1:C:90:VAL:HG13	1:C:267:VAL:HG13	1.79	0.64
1:C:99:ASN:O	1:C:102:ARG:NE	2.23	0.64
1:C:318:PHE:HD2	1:C:318:PHE:C	2.05	0.64
1:C:350:VAL:HG11	1:C:453:TYR:HA	1.79	0.64
1:A:323:THR:O	1:A:539:VAL:HG22	1.98	0.64
1:B:409:GLN:CD	1:B:418:ILE:HD12	2.23	0.64
1:C:145:TYR:N	1:C:246:ARG:O	2.30	0.64
1:A:197:ILE:O	1:A:200:TYR:N	2.31	0.64
1:A:329:PHE:O	1:A:580:GLN:NE2	2.29	0.64
1:A:651:ILE:CG2	1:A:651:ILE:HG13	2.18	0.64
1:B:152:TRP:CB	1:B:245:HIS:CE1	2.81	0.64
1:C:956:ALA:O	1:C:960:ASN:ND2	2.30	0.64
1:A:152:TRP:CB	1:A:245:HIS:CE1	2.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ASN:ND2	1:B:788:ILE:O	2.30	0.63
1:B:145:TYR:N	1:B:246:ARG:O	2.30	0.63
1:A:318:PHE:HD2	1:A:318:PHE:C	2.05	0.63
1:A:365:TYR:HB2	1:A:387:LEU:HD22	1.78	0.63
1:A:368:LEU:HD23	1:A:369:TYR:N	2.13	0.63
1:A:898:PHE:HA	1:A:901:GLN:HG3	1.79	0.63
1:A:905:ARG:CZ	1:A:1050:MET:HE2	2.28	0.63
1:A:1101:HIS:HE1	4:A:1312:NAG:C1	2.11	0.63
1:C:152:TRP:CB	1:C:245:HIS:CE1	2.81	0.63
1:C:329:PHE:C	1:C:580:GLN:HG3	2.24	0.63
1:A:78:ARG:NH2	1:A:80:ASP:HA	2.12	0.63
1:B:139:PRO:HB2	1:B:159:VAL:HG12	1.79	0.63
1:B:295:PRO:O	1:B:298:GLU:HG2	1.99	0.63
1:A:83:VAL:O	1:A:237:ARG:NH1	2.31	0.63
1:A:145:TYR:N	1:A:246:ARG:O	2.30	0.63
1:B:492:LEU:HD12	1:B:492:LEU:N	2.13	0.63
1:B:543:PHE:O	1:B:546:LEU:N	2.30	0.63
1:B:898:PHE:HA	1:B:901:GLN:HG3	1.79	0.63
2:D:32:CYS:SG	2:D:98:SER:OG	2.44	0.63
2:D:43:LYS:HE3	2:D:44:GLU:O	1.99	0.63
1:A:152:TRP:CE3	1:A:245:HIS:CG	2.86	0.63
1:A:865:LEU:HB3	1:A:869:MET:HG3	1.81	0.63
1:B:152:TRP:CE3	1:B:245:HIS:CG	2.86	0.63
1:B:878:LEU:O	1:B:882:ILE:HG23	1.99	0.63
1:C:197:ILE:O	1:C:200:TYR:N	2.31	0.63
1:A:342:PHE:O	1:A:509:ARG:NH2	2.32	0.63
1:A:1101:HIS:NE2	4:A:1312:NAG:H61	2.13	0.63
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.32	0.63
1:C:403:ARG:NE	1:C:504:GLY:O	2.29	0.63
1:A:90:VAL:HG13	1:A:267:VAL:HG13	1.79	0.63
1:A:93:ALA:O	1:A:266:TYR:N	2.25	0.63
1:A:120:VAL:HG13	1:A:127:VAL:CG2	2.28	0.63
1:A:407:VAL:HG11	1:A:508:TYR:CD2	2.33	0.63
1:A:563:GLN:HA	1:B:41:LYS:HB3	1.81	0.63
4:B:1304:NAG:C1	4:B:1304:NAG:H82	2.28	0.63
1:C:117:LEU:HD11	1:C:128:ILE:HG22	1.81	0.63
1:C:152:TRP:CE3	1:C:245:HIS:CG	2.86	0.63
1:C:865:LEU:HB3	1:C:869:MET:HG3	1.81	0.63
1:A:22:THR:HG23	1:A:76:THR:HB	1.81	0.63
1:A:295:PRO:O	1:A:298:GLU:HG2	1.99	0.63
1:B:865:LEU:HB3	1:B:869:MET:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:NH2	1:C:80:ASP:HA	2.12	0.63
1:C:295:PRO:O	1:C:298:GLU:HG2	1.99	0.63
1:C:318:PHE:HZ	1:C:615:VAL:HG11	1.64	0.63
1:C:898:PHE:HA	1:C:901:GLN:HG3	1.79	0.63
1:A:959:LEU:O	1:A:963:VAL:HG23	1.99	0.63
1:C:327:VAL:HG23	1:C:530:SER:C	2.24	0.63
1:C:403:ARG:HE	1:C:504:GLY:C	2.06	0.63
1:A:878:LEU:O	1:A:882:ILE:HG23	1.99	0.62
1:B:93:ALA:O	1:B:266:TYR:N	2.25	0.62
1:B:651:ILE:CB	1:B:651:ILE:HD12	2.19	0.62
1:C:959:LEU:O	1:C:963:VAL:HG23	1.99	0.62
1:A:578:ASP:OD2	1:A:581:THR:N	2.30	0.62
1:B:64:TRP:NE1	1:B:266:TYR:OH	2.33	0.62
1:C:495:TYR:O	1:C:505:TYR:OH	2.13	0.62
1:B:956:ALA:O	1:B:960:ASN:ND2	2.30	0.62
1:A:1009:THR:O	1:A:1013:ILE:HG13	2.00	0.62
1:B:143:VAL:HG22	1:B:154:GLU:HA	1.81	0.62
1:A:729:VAL:HG21	1:A:1060:VAL:HG12	1.82	0.62
1:B:1009:THR:O	1:B:1013:ILE:HG13	2.00	0.62
1:C:729:VAL:HG21	1:C:1060:VAL:HG12	1.82	0.62
1:A:64:TRP:NE1	1:A:266:TYR:OH	2.33	0.62
1:C:124:THR:HG23	3:G:1:NAG:H82	1.80	0.62
1:C:209:PRO:C	1:C:210:ILE:HD13	2.25	0.62
1:C:1014:ARG:N	1:C:1014:ARG:HD2	2.01	0.62
2:D:30:SER:O	2:D:100:LYS:HB2	1.98	0.62
1:B:959:LEU:O	1:B:963:VAL:HG23	1.99	0.62
1:C:143:VAL:HG13	1:C:153:MET:C	2.25	0.62
1:A:1071:GLN:NE2	1:A:1071:GLN:N	2.48	0.62
1:B:22:THR:HG23	1:B:76:THR:HB	1.81	0.62
1:B:357:ARG:C	1:B:358:ILE:HD13	2.23	0.62
1:B:699:LEU:CB	1:C:788:ILE:HD11	2.29	0.62
1:B:729:VAL:HG21	1:B:1060:VAL:HG12	1.82	0.62
1:B:1071:GLN:NE2	1:B:1071:GLN:N	2.48	0.62
1:B:1101:HIS:CE1	4:B:1312:NAG:O5	2.50	0.62
1:C:22:THR:HG23	1:C:76:THR:HB	1.81	0.62
1:C:327:VAL:HG23	1:C:530:SER:HA	1.82	0.62
1:C:1071:GLN:NE2	1:C:1071:GLN:N	2.48	0.62
2:D:67:LEU:HD21	2:D:80:LEU:HD11	1.82	0.62
1:A:143:VAL:HG22	1:A:154:GLU:HA	1.81	0.62
1:A:220:PHE:CZ	1:A:287:ASP:HA	2.35	0.62
1:B:117:LEU:HD11	1:B:128:ILE:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG13	1:A:153:MET:C	2.25	0.61
1:B:111:ASP:O	1:B:112:SER:OG	2.15	0.61
1:B:553:THR:O	1:B:586:ASP:N	2.25	0.61
1:B:751:ASN:O	1:B:755:GLN:HB3	1.99	0.61
1:C:64:TRP:NE1	1:C:266:TYR:OH	2.32	0.61
1:C:78:ARG:CD	1:C:78:ARG:C	2.64	0.61
1:C:220:PHE:CZ	1:C:287:ASP:HA	2.35	0.61
1:C:580:GLN:OE1	1:C:580:GLN:HA	1.99	0.61
1:C:1009:THR:O	1:C:1013:ILE:HG13	2.00	0.61
1:A:956:ALA:O	1:A:960:ASN:ND2	2.31	0.61
1:B:143:VAL:HG13	1:B:153:MET:C	2.25	0.61
1:B:197:ILE:O	1:B:200:TYR:N	2.31	0.61
1:C:64:TRP:CD1	1:C:66:HIS:CD2	2.88	0.61
1:C:86:PHE:N	1:C:236:THR:O	2.32	0.61
1:B:64:TRP:CD1	1:B:66:HIS:CD2	2.88	0.61
1:B:336:CYS:SG	1:B:363:ALA:HB2	2.40	0.61
1:B:341:VAL:O	1:B:344:ALA:HB2	2.00	0.61
1:C:130:VAL:CG1	1:C:168:PHE:H	2.13	0.61
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.33	0.61
1:A:712:ILE:HD13	1:B:895:GLN:O	1.99	0.61
1:B:969:ASN:HB2	1:C:755:GLN:O	2.00	0.61
1:C:449:TYR:O	2:D:32:CYS:O	2.19	0.61
1:C:751:ASN:O	1:C:755:GLN:HB3	1.99	0.61
1:C:878:LEU:O	1:C:882:ILE:HG23	1.99	0.61
2:D:6:GLU:OE2	2:D:110:GLY:HA3	2.01	0.61
2:D:50:SER:HB3	2:D:58:TYR:CZ	2.36	0.61
1:A:117:LEU:HD11	1:A:128:ILE:HG22	1.81	0.61
1:A:209:PRO:C	1:A:210:ILE:HD13	2.25	0.61
1:A:567:ARG:NE	1:A:571:ASP:O	2.33	0.61
1:A:1079:PRO:HA	1:B:900:MET:HE1	1.81	0.61
1:A:1101:HIS:CE1	4:A:1312:NAG:H62	2.34	0.61
1:A:318:PHE:HZ	1:A:615:VAL:HG11	1.64	0.61
1:A:551:VAL:HG13	1:A:588:THR:HG1	1.66	0.61
1:B:130:VAL:CG1	1:B:168:PHE:H	2.13	0.61
1:B:209:PRO:C	1:B:210:ILE:HD13	2.25	0.61
1:B:328:ARG:O	1:B:544:ASN:ND2	2.33	0.61
1:B:344:ALA:HB3	1:B:509:ARG:HE	1.65	0.61
1:B:710:ASN:O	1:B:1076:THR:OG1	2.08	0.61
1:A:1005:GLN:O	1:A:1009:THR:HG23	2.00	0.61
1:C:48:LEU:CD1	1:C:305:SER:HA	2.31	0.61
1:A:350:VAL:HG21	1:A:418:ILE:CD1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:O	1:A:407:VAL:N	2.34	0.61
1:C:145:TYR:CE1	1:C:152:TRP:CD2	2.89	0.61
1:C:448:ASN:OD1	2:D:53:ALA:HB3	2.00	0.61
1:C:779:GLN:OE1	1:C:783:ALA:HB3	2.01	0.61
1:A:145:TYR:CE1	1:A:152:TRP:CD2	2.89	0.61
1:B:48:LEU:CD1	1:B:305:SER:HA	2.31	0.61
1:B:294:ASP:OD2	1:B:296:LEU:N	2.26	0.61
1:B:1005:GLN:O	1:B:1009:THR:HG23	2.00	0.61
1:C:143:VAL:HG22	1:C:154:GLU:HA	1.81	0.61
1:C:1073:LYS:HG3	1:C:1075:PHE:CE1	2.36	0.61
1:A:64:TRP:CD1	1:A:66:HIS:CD2	2.88	0.61
1:A:278:LYS:O	1:A:285:ILE:HG23	2.01	0.61
1:A:602:THR:O	1:A:605:SER:N	2.34	0.61
1:B:619:GLU:OE2	1:B:619:GLU:N	2.34	0.61
1:C:112:SER:O	1:C:132:GLU:HG3	2.01	0.61
1:A:130:VAL:CG1	1:A:168:PHE:H	2.13	0.60
1:A:779:GLN:OE1	1:A:783:ALA:HB3	2.01	0.60
1:C:329:PHE:HA	1:C:580:GLN:HE21	1.65	0.60
1:A:376:THR:HG22	1:A:433:VAL:HG13	1.83	0.60
1:A:751:ASN:O	1:A:755:GLN:HB3	1.99	0.60
1:B:78:ARG:C	1:B:78:ARG:CD	2.64	0.60
1:B:278:LYS:O	1:B:285:ILE:HG23	2.01	0.60
1:B:699:LEU:HB2	1:C:788:ILE:HD11	1.81	0.60
1:B:905:ARG:CZ	1:B:1050:MET:HE2	2.27	0.60
1:C:619:GLU:OE2	1:C:619:GLU:N	2.34	0.60
1:A:48:LEU:CD1	1:A:305:SER:HA	2.31	0.60
1:A:574:ASP:O	1:A:587:ILE:N	2.34	0.60
1:B:145:TYR:CE1	1:B:152:TRP:CD2	2.89	0.60
1:B:220:PHE:CZ	1:B:287:ASP:HA	2.35	0.60
1:C:1005:GLN:O	1:C:1009:THR:HG23	2.00	0.60
1:A:619:GLU:OE2	1:A:619:GLU:N	2.34	0.60
1:A:670:ILE:CG2	1:A:670:ILE:CA	2.78	0.60
1:A:1073:LYS:HG3	1:A:1075:PHE:CE1	2.36	0.60
1:B:1071:GLN:HG3	1:B:1071:GLN:HE21	1.62	0.60
1:C:278:LYS:O	1:C:285:ILE:HG23	2.01	0.60
1:C:905:ARG:CZ	1:C:1050:MET:HE2	2.28	0.60
1:A:90:VAL:HG13	1:A:267:VAL:CG1	2.32	0.60
1:A:112:SER:O	1:A:132:GLU:HG3	2.01	0.60
1:C:120:VAL:HG13	1:C:127:VAL:CG2	2.28	0.60
1:C:817:PHE:CE2	1:C:821:LEU:HD21	2.37	0.60
1:A:567:ARG:HB2	1:B:44:ARG:HH22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:CYS:HB2	1:A:697:MET:HE2	1.83	0.60
1:C:406:GLU:OE1	1:C:406:GLU:N	2.33	0.60
1:C:452:LEU:HD21	2:D:98:SER:CB	2.32	0.60
1:C:602:THR:O	1:C:605:SER:N	2.34	0.60
1:A:111:ASP:O	1:A:112:SER:OG	2.15	0.60
1:B:112:SER:O	1:B:132:GLU:HG3	2.01	0.60
1:A:710:ASN:O	1:A:1076:THR:OG1	2.08	0.60
1:B:538:CYS:CA	1:B:551:VAL:HG22	2.32	0.60
1:C:90:VAL:HG13	1:C:267:VAL:CG1	2.32	0.60
1:C:662:CYS:HB2	1:C:697:MET:HE2	1.83	0.60
1:A:618:THR:HG1	1:A:619:GLU:CD	2.09	0.60
1:B:136:CYS:SG	1:B:137:ASN:N	2.75	0.60
1:B:779:GLN:OE1	1:B:783:ALA:HB3	2.01	0.60
1:C:127:VAL:HG11	3:G:1:NAG:C1	2.32	0.60
1:C:613:GLN:O	1:C:615:VAL:HG23	2.01	0.60
1:A:926:GLN:HA	1:A:929:SER:OG	2.02	0.60
1:B:817:PHE:CE2	1:B:821:LEU:HD21	2.37	0.60
1:B:926:GLN:HA	1:B:929:SER:OG	2.02	0.60
1:C:111:ASP:O	1:C:112:SER:OG	2.15	0.60
1:C:136:CYS:SG	1:C:137:ASN:N	2.75	0.60
1:C:948:LEU:CD1	1:C:948:LEU:CB	2.70	0.60
1:A:43:PHE:CE2	1:C:559:PHE:CE1	2.90	0.59
1:B:613:GLN:O	1:B:615:VAL:HG23	2.01	0.59
1:C:124:THR:OG1	3:G:1:NAG:O7	2.20	0.59
2:D:51:ILE:HG13	2:D:57:THR:HG22	1.83	0.59
1:A:78:ARG:C	1:A:78:ARG:CD	2.64	0.59
1:A:1056:ALA:N	1:A:1059:GLY:O	2.33	0.59
1:B:90:VAL:HG13	1:B:267:VAL:CG1	2.32	0.59
1:B:662:CYS:HB2	1:B:697:MET:HE2	1.83	0.59
1:B:1073:LYS:HG3	1:B:1075:PHE:CE1	2.36	0.59
1:C:84:LEU:O	1:C:238:PHE:N	2.31	0.59
1:C:490:PHE:CD2	1:C:492:LEU:HD11	2.37	0.59
1:C:553:THR:O	1:C:586:ASP:N	2.35	0.59
1:B:327:VAL:HG22	1:B:542:ASN:O	2.01	0.59
1:B:1054:GLN:N	1:B:1061:VAL:O	2.35	0.59
1:C:452:LEU:CD1	2:D:33:ARG:CB	2.80	0.59
1:C:750:SER:O	1:C:754:LEU:HG	2.02	0.59
1:C:1071:GLN:HG3	1:C:1071:GLN:HE21	1.62	0.59
1:A:566:GLY:CA	1:B:43:PHE:HB2	2.32	0.59
1:A:613:GLN:O	1:A:615:VAL:HG23	2.01	0.59
1:A:817:PHE:CE2	1:A:821:LEU:HD21	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:LYS:NZ	1:B:862:PRO:O	2.34	0.59
1:C:329:PHE:HA	1:C:580:GLN:NE2	2.17	0.59
1:C:578:ASP:OD1	1:C:580:GLN:HB2	2.02	0.59
1:C:926:GLN:HA	1:C:929:SER:OG	2.02	0.59
1:B:287:ASP:OD2	1:B:287:ASP:C	2.45	0.59
1:B:438:SER:O	1:B:442:ASP:N	2.34	0.59
1:B:602:THR:O	1:B:605:SER:N	2.34	0.59
1:B:705:VAL:CG2	1:C:883:THR:HG21	2.27	0.59
1:C:37:TYR:HB2	1:C:204:TYR:CD2	2.38	0.59
1:A:37:TYR:HB2	1:A:204:TYR:CD2	2.38	0.59
1:A:750:SER:O	1:A:754:LEU:HG	2.02	0.59
1:B:318:PHE:HZ	1:B:615:VAL:HG11	1.64	0.59
1:C:92:PHE:N	1:C:192:PHE:O	2.27	0.59
1:C:670:ILE:CG2	1:C:670:ILE:CA	2.78	0.59
1:C:1054:GLN:N	1:C:1061:VAL:O	2.35	0.59
1:A:78:ARG:NH2	1:A:80:ASP:CA	2.65	0.59
1:A:280:ASN:HB2	1:A:282:ASN:OD1	2.03	0.59
1:A:1054:GLN:N	1:A:1061:VAL:O	2.35	0.59
1:B:117:LEU:HD11	1:B:128:ILE:HG23	1.85	0.59
1:C:280:ASN:HB2	1:C:282:ASN:OD1	2.03	0.59
1:A:136:CYS:SG	1:A:137:ASN:N	2.75	0.59
1:A:651:ILE:CG2	1:A:651:ILE:C	2.76	0.59
1:A:933:LYS:NZ	1:A:933:LYS:CD	2.65	0.59
1:B:440:ASN:OD1	1:B:440:ASN:N	2.36	0.59
1:B:970:PHE:HA	1:C:756:TYR:O	2.02	0.59
1:B:37:TYR:HB2	1:B:204:TYR:CD2	2.38	0.59
1:B:92:PHE:N	1:B:192:PHE:O	2.27	0.59
1:B:1056:ALA:N	1:B:1059:GLY:O	2.33	0.59
1:C:277:LEU:HB3	1:C:279:TYR:CZ	2.38	0.59
1:C:452:LEU:HA	2:D:104:CYS:SG	2.43	0.59
1:C:611:LEU:HG	1:C:612:TYR:N	2.09	0.59
1:A:533:LEU:HD11	1:A:535:LYS:NZ	2.18	0.59
1:B:364:ASP:OD1	1:B:367:VAL:HG13	2.03	0.59
1:B:651:ILE:CG2	1:B:651:ILE:C	2.76	0.59
1:A:86:PHE:N	1:A:236:THR:O	2.32	0.58
1:A:165:ASN:HD21	4:A:1302:NAG:H2	1.68	0.58
1:A:403:ARG:NE	1:A:504:GLY:O	2.35	0.58
1:A:564:GLN:HG2	1:B:41:LYS:CG	2.22	0.58
1:B:280:ASN:HB2	1:B:282:ASN:OD1	2.03	0.58
1:C:127:VAL:CG1	3:G:1:NAG:C5	2.80	0.58
1:C:493:GLN:HA	2:D:103:THR:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:O	1:B:238:PHE:N	2.31	0.58
1:B:750:SER:O	1:B:754:LEU:HG	2.02	0.58
1:B:933:LYS:NZ	1:B:933:LYS:CD	2.65	0.58
1:B:951:VAL:CA	1:B:954:GLN:HG3	2.33	0.58
1:C:199:GLY:HA2	1:C:232:GLY:HA2	1.85	0.58
1:A:117:LEU:HD11	1:A:128:ILE:HG23	1.85	0.58
1:A:670:ILE:CG2	1:A:670:ILE:CG1	2.80	0.58
1:A:1014:ARG:N	1:A:1014:ARG:HD2	2.00	0.58
1:B:152:TRP:HB2	1:B:245:HIS:CE1	2.39	0.58
1:B:353:TRP:O	1:B:466:ARG:NH2	2.36	0.58
1:C:408:ARG:O	1:C:414:GLN:NE2	2.35	0.58
1:A:560:LEU:HD11	1:B:284:THR:HG22	1.84	0.58
1:A:719:THR:HG23	1:A:1068:VAL:HB	1.86	0.58
1:C:152:TRP:HB2	1:C:245:HIS:CE1	2.39	0.58
1:A:354:ASN:N	1:A:399:SER:O	2.37	0.58
1:B:281:GLU:CD	4:B:1304:NAG:C7	2.76	0.58
1:B:719:THR:HG23	1:B:1068:VAL:HB	1.86	0.58
1:C:117:LEU:HD11	1:C:128:ILE:HG23	1.85	0.58
1:C:529:LYS:O	1:C:530:SER:O	2.21	0.58
1:C:538:CYS:CA	1:C:551:VAL:HG22	2.32	0.58
1:C:1116:THR:O	1:C:1120:THR:HG22	2.04	0.58
1:A:29:THR:N	1:A:62:VAL:O	2.24	0.58
1:A:277:LEU:HB3	1:A:279:TYR:CZ	2.38	0.58
1:B:587:ILE:N	1:B:587:ILE:HD12	2.18	0.58
1:A:104:TRP:N	1:A:119:ILE:O	2.37	0.58
1:A:133:PHE:HE1	1:A:160:TYR:HD2	1.52	0.58
1:A:290:ASP:HB3	1:A:293:LEU:HB2	1.86	0.58
1:A:559:PHE:CD1	1:A:584:ILE:HG13	2.38	0.58
1:A:582:LEU:HD12	1:A:582:LEU:N	2.19	0.58
1:A:1116:THR:O	1:A:1120:THR:HG22	2.04	0.58
1:B:290:ASP:HB3	1:B:293:LEU:HB2	1.86	0.58
1:B:1102:TRP:CD1	1:B:1135:ASN:ND2	2.72	0.58
1:C:127:VAL:HG12	3:G:1:NAG:C5	2.33	0.58
1:C:453:TYR:OH	1:C:495:TYR:CZ	2.51	0.58
1:C:651:ILE:CG2	1:C:651:ILE:C	2.76	0.58
2:D:96:ALA:HB1	2:D:106:PHE:CD2	2.39	0.58
1:A:733:LYS:NZ	1:A:862:PRO:O	2.34	0.58
1:A:1102:TRP:CD1	1:A:1135:ASN:ND2	2.72	0.58
1:B:104:TRP:N	1:B:119:ILE:O	2.37	0.58
1:B:153:MET:CE	4:B:1302:NAG:C4	2.81	0.58
1:A:404:GLY:O	1:A:407:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PHE:CE1	1:B:43:PHE:CE2	2.91	0.58
1:A:741:TYR:OH	1:A:962:LEU:O	2.21	0.58
1:A:779:GLN:OE1	1:A:783:ALA:CB	2.52	0.58
1:C:644:GLN:CD	4:C:1305:NAG:O7	2.45	0.58
2:D:52:THR:OG1	2:D:56:ALA:N	2.37	0.58
1:B:120:VAL:CG2	1:B:241:LEU:HB3	2.34	0.58
1:B:277:LEU:HB3	1:B:279:TYR:CZ	2.38	0.58
1:C:37:TYR:HD1	1:C:55:PHE:HZ	1.52	0.58
1:C:104:TRP:N	1:C:119:ILE:O	2.37	0.58
1:C:127:VAL:CG1	3:G:1:NAG:O5	2.52	0.58
1:B:274:THR:O	1:B:291:CYS:HB2	2.04	0.57
1:C:290:ASP:HB3	1:C:293:LEU:HB2	1.86	0.57
1:C:1056:ALA:N	1:C:1059:GLY:O	2.33	0.57
1:A:942:PRO:HD2	1:A:942:PRO:O	2.04	0.57
1:A:951:VAL:HA	1:A:954:GLN:CG	2.33	0.57
1:B:334:ASN:O	1:B:362:VAL:HG22	2.04	0.57
1:B:994:ASP:O	1:B:998:THR:HG23	2.04	0.57
1:B:1116:THR:O	1:B:1120:THR:HG22	2.04	0.57
1:C:496:GLY:O	1:C:498:GLN:NE2	2.37	0.57
1:C:779:GLN:OE1	1:C:783:ALA:CB	2.52	0.57
1:A:206:LYS:HD3	1:A:224:GLU:CD	2.29	0.57
1:A:651:ILE:CB	1:A:651:ILE:HD12	2.19	0.57
1:A:994:ASP:O	1:A:998:THR:HG23	2.04	0.57
1:B:569:ILE:H	1:B:569:ILE:HD12	1.69	0.57
1:C:179:LEU:O	1:C:245:HIS:NE2	2.37	0.57
1:A:328:ARG:N	1:A:542:ASN:O	2.32	0.57
1:B:179:LEU:O	1:B:245:HIS:NE2	2.37	0.57
1:B:206:LYS:HD3	1:B:224:GLU:CD	2.30	0.57
1:B:393:THR:O	1:B:523:THR:OG1	2.12	0.57
1:C:136:CYS:HB3	1:C:139:PRO:HB3	1.87	0.57
1:C:994:ASP:O	1:C:998:THR:HG23	2.04	0.57
1:A:951:VAL:CA	1:A:954:GLN:HG3	2.33	0.57
1:B:48:LEU:HD21	1:B:278:LYS:HZ3	1.70	0.57
1:B:358:ILE:HD11	1:B:397:ALA:CB	2.33	0.57
1:B:779:GLN:OE1	1:B:783:ALA:CB	2.52	0.57
1:C:318:PHE:C	1:C:318:PHE:CD2	2.82	0.57
1:C:719:THR:HG23	1:C:1068:VAL:HB	1.86	0.57
1:C:1102:TRP:CD1	1:C:1135:ASN:ND2	2.71	0.57
1:A:749:CYS:O	1:A:752:LEU:N	2.38	0.57
1:B:199:GLY:HA2	1:B:232:GLY:HA2	1.85	0.57
1:A:274:THR:O	1:A:291:CYS:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:PHE:C	1:A:318:PHE:CD2	2.82	0.57
1:A:761:THR:HA	1:A:764:ASN:OD1	2.05	0.57
1:B:136:CYS:HB3	1:B:139:PRO:HB3	1.86	0.57
1:B:670:ILE:CG2	1:B:670:ILE:CA	2.78	0.57
1:C:327:VAL:HG12	1:C:542:ASN:HB3	1.84	0.57
1:C:741:TYR:OH	1:C:962:LEU:O	2.21	0.57
1:A:56:LEU:HD21	1:A:91:TYR:CD2	2.39	0.57
1:A:136:CYS:HB3	1:A:139:PRO:HB3	1.87	0.57
1:A:387:LEU:HD12	1:A:388:ASN:N	2.19	0.57
1:B:563:GLN:HB3	1:C:41:LYS:CB	2.35	0.57
1:C:329:PHE:C	1:C:580:GLN:CG	2.77	0.57
1:C:458:LYS:O	1:C:459:SER:O	2.22	0.57
1:A:152:TRP:HB2	1:A:245:HIS:CE1	2.39	0.57
1:A:1071:GLN:NE2	1:A:1071:GLN:CB	2.67	0.57
1:B:56:LEU:HD21	1:B:91:TYR:CD2	2.39	0.57
1:B:1083:HIS:ND1	1:B:1084:ASP:CG	2.59	0.57
1:C:56:LEU:HD21	1:C:91:TYR:CD2	2.39	0.57
1:C:78:ARG:NH2	1:C:80:ASP:CA	2.65	0.57
1:C:274:THR:O	1:C:291:CYS:HB2	2.04	0.57
1:C:933:LYS:NZ	1:C:933:LYS:CD	2.65	0.57
1:A:120:VAL:CG2	1:A:241:LEU:HB3	2.34	0.57
1:A:559:PHE:CE1	1:B:43:PHE:CZ	2.92	0.57
1:A:1002:GLN:O	1:A:1003:SER:C	2.48	0.57
1:B:133:PHE:CG	1:B:160:TYR:CB	2.88	0.57
1:B:318:PHE:C	1:B:318:PHE:CD2	2.82	0.57
1:B:741:TYR:OH	1:B:962:LEU:O	2.21	0.57
1:C:749:CYS:O	1:C:752:LEU:N	2.38	0.57
1:B:749:CYS:O	1:B:752:LEU:N	2.38	0.56
1:C:951:VAL:HA	1:C:954:GLN:CG	2.33	0.56
2:D:12:VAL:HG21	2:D:18:LEU:CG	2.32	0.56
1:A:246:ARG:HG3	1:A:257:GLY:O	2.05	0.56
1:A:1050:MET:CG	1:A:1051:SER:N	2.50	0.56
1:B:111:ASP:HA	1:B:134:GLN:HA	1.87	0.56
1:B:560:LEU:HD22	1:B:562:PHE:CE1	2.41	0.56
1:C:951:VAL:CA	1:C:954:GLN:HG3	2.33	0.56
1:A:120:VAL:HG12	1:A:127:VAL:HG23	1.87	0.56
1:A:143:VAL:HG13	1:A:153:MET:O	2.06	0.56
1:A:199:GLY:HA2	1:A:232:GLY:HA2	1.85	0.56
1:A:616:ASN:C	1:A:619:GLU:OE2	2.48	0.56
1:B:143:VAL:HG13	1:B:153:MET:O	2.06	0.56
1:B:761:THR:HA	1:B:764:ASN:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:942:PRO:HD2	1:B:942:PRO:O	2.04	0.56
1:B:951:VAL:HA	1:B:954:GLN:CG	2.33	0.56
1:C:143:VAL:HG13	1:C:153:MET:O	2.06	0.56
1:C:206:LYS:HD3	1:C:224:GLU:CD	2.30	0.56
1:C:437:ASN:ND2	1:C:507:PRO:O	2.37	0.56
1:C:761:THR:HA	1:C:764:ASN:OD1	2.05	0.56
1:C:1110:TYR:HE1	1:C:1112:PRO:HG3	1.71	0.56
1:A:354:ASN:O	1:A:399:SER:N	2.35	0.56
1:B:551:VAL:HG23	1:B:588:THR:HB	1.88	0.56
1:B:616:ASN:C	1:B:619:GLU:OE2	2.48	0.56
1:B:963:VAL:O	1:B:966:LEU:HD23	2.06	0.56
1:A:328:ARG:HA	1:A:530:SER:HA	1.87	0.56
1:B:117:LEU:HB2	1:B:130:VAL:HG23	1.87	0.56
1:B:310:LYS:C	1:B:310:LYS:HD3	2.31	0.56
1:B:511:VAL:HG12	1:B:513:LEU:HD13	1.85	0.56
1:B:1105:THR:OG1	1:B:1111:GLU:N	2.39	0.56
1:B:1110:TYR:HE1	1:B:1112:PRO:HG3	1.71	0.56
1:C:133:PHE:CG	1:C:160:TYR:CB	2.88	0.56
1:A:88:ASP:OD1	1:A:270:LEU:O	2.24	0.56
1:B:1002:GLN:O	1:B:1003:SER:C	2.48	0.56
1:C:942:PRO:HD2	1:C:942:PRO:O	2.04	0.56
1:A:17:ASN:OD1	3:E:2:NAG:H5	2.05	0.56
1:A:179:LEU:O	1:A:245:HIS:NE2	2.37	0.56
1:A:296:LEU:HA	1:A:299:THR:HG23	1.87	0.56
1:A:563:GLN:HA	1:B:41:LYS:CB	2.34	0.56
1:A:731:MET:N	1:A:1058:HIS:CE1	2.74	0.56
1:B:86:PHE:N	1:B:236:THR:O	2.32	0.56
1:B:455:LEU:HD12	1:B:491:PRO:O	2.06	0.56
1:B:942:PRO:O	1:B:943:SER:OG	2.19	0.56
1:C:367:VAL:HG23	1:C:368:LEU:HD23	1.85	0.56
1:C:544:ASN:N	1:C:544:ASN:OD1	2.38	0.56
1:C:618:THR:HG1	1:C:619:GLU:CD	2.13	0.56
1:C:963:VAL:O	1:C:966:LEU:HD23	2.06	0.56
1:A:1071:GLN:HG3	1:A:1071:GLN:HE21	1.62	0.56
1:A:1105:THR:OG1	1:A:1111:GLU:N	2.39	0.56
1:B:56:LEU:CD2	1:B:91:TYR:CD2	2.89	0.56
1:B:538:CYS:HA	1:B:551:VAL:HG22	1.87	0.56
1:C:246:ARG:HG3	1:C:257:GLY:O	2.05	0.56
1:C:731:MET:N	1:C:1058:HIS:CE1	2.74	0.56
1:A:403:ARG:O	1:A:407:VAL:HG13	2.06	0.56
1:A:699:LEU:HD11	1:B:872:GLN:NE2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ILE:HD11	1:B:896:ILE:HG13	1.87	0.56
1:B:710:ASN:OD1	1:B:710:ASN:N	2.38	0.56
1:B:731:MET:N	1:B:1058:HIS:CE1	2.74	0.56
1:C:310:LYS:HD3	1:C:310:LYS:C	2.31	0.56
1:C:354:ASN:O	1:C:399:SER:N	2.33	0.56
1:A:133:PHE:CG	1:A:160:TYR:CB	2.88	0.56
1:A:948:LEU:CD1	1:A:948:LEU:CD2	2.82	0.56
1:A:1014:ARG:O	1:A:1018:ILE:HG12	2.06	0.56
1:B:246:ARG:HG3	1:B:257:GLY:O	2.05	0.56
1:C:120:VAL:CG2	1:C:241:LEU:HB3	2.34	0.56
1:C:145:TYR:CD1	1:C:152:TRP:CD2	2.94	0.56
1:C:296:LEU:HA	1:C:299:THR:HG23	1.87	0.56
1:A:771:ALA:CA	1:A:774:GLN:OE1	2.52	0.55
1:B:145:TYR:CD1	1:B:152:TRP:CD2	2.94	0.55
1:B:364:ASP:O	1:B:367:VAL:HG22	2.06	0.55
1:C:41:LYS:CB	1:C:41:LYS:HE2	2.36	0.55
1:C:56:LEU:CD2	1:C:91:TYR:CD2	2.89	0.55
1:C:124:THR:HG23	3:G:1:NAG:C8	2.36	0.55
1:C:710:ASN:N	1:C:710:ASN:OD1	2.38	0.55
1:C:948:LEU:CD1	1:C:948:LEU:CD2	2.82	0.55
3:H:1:NAG:H61	3:H:2:NAG:C1	2.36	0.55
1:A:199:GLY:O	1:A:231:ILE:N	2.29	0.55
1:A:402:ILE:HD11	1:A:510:VAL:HG21	1.88	0.55
1:B:41:LYS:CB	1:B:41:LYS:HE2	2.36	0.55
1:B:92:PHE:HE1	1:B:265:TYR:HB2	1.71	0.55
1:C:92:PHE:HE1	1:C:265:TYR:HB2	1.72	0.55
1:C:616:ASN:C	1:C:619:GLU:OE2	2.48	0.55
1:C:1105:THR:OG1	1:C:1111:GLU:N	2.39	0.55
3:E:1:NAG:H82	3:E:1:NAG:C1	2.36	0.55
1:B:29:THR:N	1:B:62:VAL:O	2.25	0.55
1:B:586:ASP:N	1:B:586:ASP:OD1	2.39	0.55
1:C:450:ASN:ND2	2:D:53:ALA:HB3	2.20	0.55
1:A:559:PHE:HA	1:B:43:PHE:HE1	1.71	0.55
1:A:1083:HIS:ND1	1:A:1084:ASP:CG	2.59	0.55
1:B:296:LEU:HA	1:B:299:THR:HG23	1.87	0.55
1:B:1014:ARG:O	1:B:1018:ILE:HG12	2.06	0.55
1:C:111:ASP:HA	1:C:134:GLN:HA	1.87	0.55
1:C:393:THR:HG23	1:C:517:LEU:HD12	1.87	0.55
1:C:452:LEU:HD11	2:D:98:SER:OG	2.07	0.55
1:A:56:LEU:CD2	1:A:91:TYR:CD2	2.89	0.55
1:B:670:ILE:CG2	1:B:670:ILE:CG1	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1084:ASP:HB2	1:B:1086:LYS:HG2	1.88	0.55
1:C:117:LEU:HB2	1:C:130:VAL:HG23	1.87	0.55
1:C:133:PHE:HD1	1:C:162:SER:N	2.04	0.55
1:C:552:LEU:HD13	1:C:552:LEU:N	2.21	0.55
1:A:287:ASP:OD2	1:A:287:ASP:C	2.45	0.55
1:A:279:TYR:HA	1:A:284:THR:O	2.07	0.55
1:A:481:ASN:O	1:A:481:ASN:ND2	2.40	0.55
1:A:1110:TYR:HE1	1:A:1112:PRO:HG3	1.71	0.55
1:B:120:VAL:HG12	1:B:127:VAL:HG23	1.87	0.55
1:B:133:PHE:HD1	1:B:162:SER:N	2.04	0.55
1:B:1091:ARG:HE	1:B:1119:ASN:HA	1.72	0.55
1:C:453:TYR:CZ	1:C:495:TYR:CZ	2.94	0.55
1:C:1109:PHE:HD1	1:C:1110:TYR:H	1.53	0.55
2:D:31:THR:HG21	2:D:34:LYS:HE3	1.89	0.55
2:D:40:ALA:HB3	2:D:43:LYS:HG2	1.89	0.55
1:A:41:LYS:CB	1:A:41:LYS:HE2	2.36	0.55
1:A:41:LYS:CB	1:C:563:GLN:HA	2.37	0.55
1:A:310:LYS:C	1:A:310:LYS:HD3	2.31	0.55
1:B:353:TRP:O	1:B:466:ARG:NE	2.39	0.55
1:B:1014:ARG:HD2	1:B:1014:ARG:N	2.01	0.55
1:C:88:ASP:OD1	1:C:270:LEU:O	2.24	0.55
1:C:551:VAL:O	1:C:588:THR:OG1	2.16	0.55
1:C:1002:GLN:O	1:C:1003:SER:C	2.48	0.55
2:D:34:LYS:HD3	2:D:78:VAL:HG11	1.89	0.55
1:A:435:ALA:HA	1:A:510:VAL:HG22	1.89	0.55
1:A:963:VAL:O	1:A:966:LEU:HD23	2.06	0.55
1:A:1091:ARG:HE	1:A:1119:ASN:HA	1.72	0.55
1:B:78:ARG:NH2	1:B:80:ASP:CA	2.65	0.55
1:B:88:ASP:OD1	1:B:270:LEU:O	2.24	0.55
1:B:320:VAL:HB	1:B:590:CYS:SG	2.46	0.55
1:B:699:LEU:HB2	1:C:788:ILE:CD1	2.36	0.55
1:A:117:LEU:HB2	1:A:130:VAL:HG23	1.87	0.55
1:A:145:TYR:CD1	1:A:152:TRP:CD2	2.94	0.55
1:A:384:PRO:O	1:A:387:LEU:HD23	2.07	0.55
1:A:402:ILE:HG22	1:A:418:ILE:HG21	1.89	0.55
1:A:699:LEU:CD1	1:B:872:GLN:OE1	2.56	0.55
1:B:279:TYR:HA	1:B:284:THR:O	2.07	0.55
1:B:971:GLY:N	1:C:756:TYR:HA	2.22	0.55
1:A:64:TRP:CE2	1:A:266:TYR:OH	2.61	0.54
1:A:560:LEU:O	1:A:577:ARG:NH1	2.37	0.54
1:A:567:ARG:CG	1:B:44:ARG:HH22	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:SER:O	1:C:595:VAL:N	2.39	0.54
1:C:771:ALA:CA	1:C:774:GLN:OE1	2.52	0.54
1:A:79:PHE:CE2	1:A:244:LEU:HD22	2.43	0.54
1:A:699:LEU:CD1	1:B:872:GLN:NE2	2.70	0.54
1:B:433:VAL:CG1	1:B:512:VAL:HG22	2.37	0.54
1:B:897:PRO:CG	1:B:900:MET:HG2	2.37	0.54
1:C:79:PHE:CE2	1:C:244:LEU:HD22	2.43	0.54
1:C:84:LEU:HA	1:C:237:ARG:HH11	1.72	0.54
1:C:452:LEU:HB3	1:C:454:ARG:HH22	1.72	0.54
1:A:316:SER:O	1:A:595:VAL:N	2.39	0.54
1:A:710:ASN:OD1	1:A:710:ASN:N	2.38	0.54
1:A:718:PHE:HD2	1:A:719:THR:O	1.90	0.54
1:C:199:GLY:O	1:C:231:ILE:N	2.29	0.54
1:C:612:TYR:O	1:C:648:GLY:HA3	2.08	0.54
1:C:1084:ASP:HB2	1:C:1086:LYS:HG2	1.88	0.54
1:A:111:ASP:HA	1:A:134:GLN:HA	1.87	0.54
1:A:455:LEU:HD21	1:A:493:GLN:HB3	1.90	0.54
1:A:897:PRO:CG	1:A:900:MET:HG2	2.37	0.54
1:A:1084:ASP:HB2	1:A:1086:LYS:HG2	1.88	0.54
1:B:79:PHE:CE2	1:B:244:LEU:HD22	2.43	0.54
1:B:718:PHE:HD2	1:B:719:THR:O	1.90	0.54
1:C:327:VAL:HG23	1:C:530:SER:CA	2.37	0.54
1:C:670:ILE:CG2	1:C:670:ILE:CG1	2.80	0.54
1:C:1014:ARG:O	1:C:1018:ILE:HG12	2.06	0.54
1:A:37:TYR:HD1	1:A:55:PHE:HZ	1.52	0.54
1:A:44:ARG:HH22	1:C:567:ARG:HB3	1.70	0.54
1:A:816:SER:OG	1:A:819:GLU:HG3	2.08	0.54
1:B:726:ILE:HD12	1:B:1061:VAL:HG22	1.90	0.54
1:C:112:SER:HB2	1:C:132:GLU:HG2	1.90	0.54
1:C:569:ILE:O	1:C:570:ALA:HB3	2.08	0.54
1:C:796:ASP:OD2	1:C:796:ASP:N	2.40	0.54
1:C:942:PRO:O	1:C:943:SER:OG	2.19	0.54
1:A:112:SER:HB2	1:A:132:GLU:HG2	1.90	0.54
1:A:118:LEU:HD23	1:A:129:LYS:O	2.07	0.54
1:C:48:LEU:HD12	1:C:305:SER:HA	1.90	0.54
1:C:64:TRP:CE2	1:C:266:TYR:OH	2.60	0.54
1:C:279:TYR:HA	1:C:284:THR:O	2.07	0.54
1:C:726:ILE:HD12	1:C:1061:VAL:HG22	1.90	0.54
1:C:897:PRO:CG	1:C:900:MET:HG2	2.37	0.54
1:B:118:LEU:HD23	1:B:129:LYS:O	2.07	0.54
1:B:612:TYR:O	1:B:648:GLY:HA3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:GLY:HA2	1:C:407:VAL:HG13	1.88	0.54
1:C:555:SER:O	1:C:584:ILE:HD13	2.08	0.54
1:A:726:ILE:HD12	1:A:1061:VAL:HG22	1.90	0.54
1:A:1109:PHE:HD1	1:A:1110:TYR:H	1.53	0.54
1:B:48:LEU:HD12	1:B:305:SER:HA	1.90	0.54
1:B:1040:VAL:HG21	1:C:1035:GLY:HA3	1.90	0.54
1:B:1081:ILE:HG12	1:B:1135:ASN:HB3	1.89	0.54
1:C:118:LEU:HD23	1:C:129:LYS:O	2.07	0.54
1:C:287:ASP:OD2	1:C:287:ASP:C	2.45	0.54
1:C:472:ILE:HD12	1:C:488:CYS:HB3	1.89	0.54
2:D:90:THR:HG23	2:D:116:THR:HA	1.90	0.54
1:A:115:GLN:HE21	1:A:165:ASN:HB2	1.73	0.54
1:A:133:PHE:HD1	1:A:162:SER:N	2.04	0.54
1:A:365:TYR:CB	1:A:387:LEU:HD22	2.37	0.54
1:A:796:ASP:OD2	1:A:796:ASP:N	2.40	0.54
1:A:805:ILE:HG13	1:A:806:LEU:HD23	1.90	0.54
1:B:562:PHE:CD2	1:C:225:PRO:HG2	2.42	0.54
1:B:1109:PHE:HD1	1:B:1110:TYR:H	1.53	0.54
1:C:92:PHE:CE1	1:C:265:TYR:HB2	2.43	0.54
1:C:115:GLN:HE21	1:C:165:ASN:HB2	1.73	0.54
1:C:386:LYS:O	1:C:390:LEU:HD13	2.08	0.54
1:C:718:PHE:HD2	1:C:719:THR:O	1.90	0.54
1:C:1083:HIS:ND1	1:C:1084:ASP:CG	2.59	0.54
4:B:1304:NAG:C1	4:B:1304:NAG:C8	2.85	0.54
1:C:618:THR:OG1	1:C:619:GLU:CD	2.51	0.54
1:C:1047:TYR:HB3	1:C:1067:TYR:HB3	1.90	0.54
1:B:318:PHE:CD2	1:B:319:ARG:N	2.77	0.53
1:C:193:VAL:HG23	1:C:223:LEU:HD12	1.90	0.53
1:C:767:LEU:HA	1:C:770:ILE:HD12	1.91	0.53
1:C:930:ALA:O	1:C:934:ILE:HG12	2.08	0.53
1:A:36:VAL:HA	1:A:55:PHE:HE2	1.74	0.53
1:A:1038:LYS:HD3	1:A:1038:LYS:N	2.23	0.53
1:B:618:THR:OG1	1:B:619:GLU:CD	2.51	0.53
1:C:453:TYR:CD1	1:C:454:ARG:N	2.76	0.53
1:C:1038:LYS:N	1:C:1038:LYS:HD3	2.23	0.53
1:C:1083:HIS:O	1:C:1086:LYS:HB2	2.08	0.53
2:D:44:GLU:HG2	2:D:45:ARG:N	2.23	0.53
2:D:105:THR:HG22	2:D:106:PHE:H	1.73	0.53
1:A:92:PHE:CE1	1:A:265:TYR:HB2	2.43	0.53
1:A:253:ASP:OD2	1:A:256:SER:OG	2.26	0.53
1:A:1106:GLN:OE1	1:A:1111:GLU:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:GLN:CG	1:C:41:LYS:CG	2.87	0.53
1:C:282:ASN:OD1	1:C:284:THR:HG23	2.07	0.53
1:C:329:PHE:O	1:C:580:GLN:HG3	2.08	0.53
1:C:1091:ARG:HE	1:C:1119:ASN:HA	1.72	0.53
2:D:34:LYS:HD3	2:D:78:VAL:CG1	2.39	0.53
2:D:48:VAL:HG13	2:D:63:VAL:HG21	1.89	0.53
2:D:67:LEU:HD11	2:D:80:LEU:CD1	2.38	0.53
1:A:48:LEU:HD12	1:A:305:SER:HA	1.90	0.53
1:A:871:ALA:O	1:A:874:THR:OG1	2.23	0.53
1:A:1083:HIS:O	1:A:1086:LYS:HB2	2.08	0.53
1:B:112:SER:HB2	1:B:132:GLU:HG2	1.90	0.53
1:B:115:GLN:HE21	1:B:165:ASN:HB2	1.73	0.53
1:B:253:ASP:OD2	1:B:256:SER:OG	2.26	0.53
1:B:282:ASN:OD1	1:B:284:THR:HG23	2.07	0.53
1:B:316:SER:O	1:B:595:VAL:N	2.39	0.53
1:B:767:LEU:HA	1:B:770:ILE:HD12	1.90	0.53
1:B:1106:GLN:OE1	1:B:1111:GLU:HB3	2.08	0.53
1:C:450:ASN:HB3	2:D:53:ALA:H	1.73	0.53
1:C:452:LEU:HD21	2:D:98:SER:HB3	1.91	0.53
1:C:805:ILE:HG13	1:C:806:LEU:HD23	1.90	0.53
1:A:193:VAL:HG23	1:A:223:LEU:HD12	1.90	0.53
1:A:373:SER:OG	4:A:1304:NAG:O3	2.24	0.53
1:A:786:LYS:N	1:A:786:LYS:HD2	2.23	0.53
1:A:930:ALA:O	1:A:934:ILE:HG12	2.08	0.53
1:A:1081:ILE:HG12	1:A:1135:ASN:HB3	1.89	0.53
1:C:48:LEU:HD21	1:C:278:LYS:HZ3	1.74	0.53
1:C:64:TRP:CD1	1:C:266:TYR:CE1	2.97	0.53
1:C:328:ARG:NH2	1:C:329:PHE:O	2.42	0.53
1:A:64:TRP:CD1	1:A:266:TYR:CE1	2.97	0.53
1:A:318:PHE:CD2	1:A:319:ARG:N	2.77	0.53
1:A:566:GLY:HA3	1:B:43:PHE:HB2	1.91	0.53
1:A:612:TYR:O	1:A:648:GLY:HA3	2.08	0.53
1:A:767:LEU:HA	1:A:770:ILE:HD12	1.91	0.53
1:B:746:SER:O	1:B:749:CYS:HB2	2.09	0.53
1:B:816:SER:OG	1:B:819:GLU:HG3	2.07	0.53
1:B:930:ALA:O	1:B:934:ILE:HG12	2.08	0.53
1:C:84:LEU:CA	1:C:237:ARG:NH1	2.71	0.53
1:C:120:VAL:HG12	1:C:127:VAL:HG23	1.87	0.53
1:C:733:LYS:NZ	1:C:862:PRO:O	2.34	0.53
1:C:1071:GLN:NE2	1:C:1071:GLN:CB	2.67	0.53
2:D:34:LYS:CD	2:D:78:VAL:HG11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:HB3	1:C:563:GLN:NE2	2.24	0.53
1:A:140:PHE:CE2	1:A:244:LEU:HD21	2.44	0.53
1:A:282:ASN:OD1	1:A:284:THR:HG23	2.07	0.53
1:B:36:VAL:HA	1:B:55:PHE:HE2	1.74	0.53
1:B:48:LEU:HD21	1:B:278:LYS:NZ	2.24	0.53
1:B:78:ARG:CD	1:B:78:ARG:O	2.57	0.53
1:B:140:PHE:CE2	1:B:244:LEU:HD21	2.44	0.53
1:B:616:ASN:OD1	4:B:1308:NAG:C7	2.56	0.53
1:B:771:ALA:CA	1:B:774:GLN:OE1	2.52	0.53
1:B:796:ASP:OD2	1:B:796:ASP:N	2.40	0.53
1:C:318:PHE:CD2	1:C:319:ARG:N	2.77	0.53
1:C:344:ALA:O	1:C:509:ARG:NH1	2.42	0.53
1:C:495:TYR:O	1:C:505:TYR:CZ	2.61	0.53
1:A:84:LEU:CA	1:A:237:ARG:NH1	2.71	0.53
1:A:817:PHE:HD1	1:A:935:GLN:HE22	1.56	0.53
1:A:1047:TYR:HB3	1:A:1067:TYR:HB3	1.90	0.53
1:B:193:VAL:HG23	1:B:223:LEU:HD12	1.90	0.53
1:B:948:LEU:CD1	1:B:948:LEU:CD2	2.82	0.53
1:B:1038:LYS:HD3	1:B:1038:LYS:N	2.23	0.53
1:B:1047:TYR:HB3	1:B:1067:TYR:HB3	1.90	0.53
1:B:1083:HIS:O	1:B:1086:LYS:HB2	2.08	0.53
1:C:403:ARG:HD2	1:C:495:TYR:CD1	2.44	0.53
1:C:511:VAL:HG12	1:C:513:LEU:HD11	1.90	0.53
1:C:816:SER:OG	1:C:819:GLU:HG3	2.07	0.53
1:C:1081:ILE:HG12	1:C:1135:ASN:HB3	1.89	0.53
1:A:92:PHE:HE1	1:A:265:TYR:HB2	1.72	0.53
1:A:454:ARG:NH1	1:A:456:PHE:O	2.38	0.53
1:B:898:PHE:O	1:B:902:MET:HG3	2.09	0.53
1:C:140:PHE:CE2	1:C:244:LEU:HD21	2.44	0.53
1:C:717:ASN:N	1:C:1070:ALA:O	2.35	0.53
1:C:786:LYS:N	1:C:786:LYS:HD2	2.23	0.53
1:C:1109:PHE:CD1	1:C:1110:TYR:N	2.77	0.53
2:D:67:LEU:HD11	2:D:80:LEU:HD21	1.91	0.53
1:A:390:LEU:HD23	1:A:391:CYS:N	2.24	0.53
1:A:553:THR:HG23	1:A:586:ASP:HB3	1.91	0.53
1:B:92:PHE:CE1	1:B:265:TYR:HB2	2.43	0.53
1:C:452:LEU:CD1	2:D:33:ARG:HB2	2.39	0.53
1:C:528:LYS:HA	1:C:529:LYS:HB2	1.91	0.53
1:C:714:ILE:HG22	1:C:715:PRO:HD2	1.91	0.53
1:A:393:THR:HG22	1:A:522:ALA:HB2	1.90	0.52
1:A:560:LEU:HD21	1:B:284:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:CYS:N	1:A:1133:VAL:O	2.38	0.52
1:B:703:ASN:O	1:C:790:LYS:N	2.35	0.52
1:B:1101:HIS:CE1	4:B:1312:NAG:H4	2.44	0.52
1:C:97:LYS:NZ	1:C:185:ASN:O	2.41	0.52
1:C:401:VAL:HG13	1:C:442:ASP:OD2	2.09	0.52
1:C:948:LEU:CD1	1:C:948:LEU:HB2	2.39	0.52
1:A:78:ARG:CD	1:A:78:ARG:O	2.57	0.52
1:A:714:ILE:HG22	1:A:715:PRO:HD2	1.91	0.52
1:B:28:TYR:CD1	4:B:1307:NAG:H5	2.45	0.52
1:B:786:LYS:HD2	1:B:786:LYS:N	2.23	0.52
1:B:805:ILE:HG13	1:B:806:LEU:HD23	1.90	0.52
1:B:922:LEU:O	1:B:926:GLN:OE1	2.27	0.52
1:B:961:THR:O	1:B:965:GLN:HG2	2.10	0.52
1:B:1082:CYS:N	1:B:1133:VAL:O	2.38	0.52
1:C:78:ARG:CD	1:C:78:ARG:O	2.57	0.52
1:C:121:ASN:OD1	1:C:177:MET:HE1	2.10	0.52
2:D:99:VAL:HG11	2:D:102:PHE:HD2	1.75	0.52
1:A:559:PHE:CD1	1:A:584:ILE:CG1	2.93	0.52
1:A:559:PHE:N	1:A:559:PHE:HD1	2.07	0.52
1:A:594:GLY:H	1:A:613:GLN:HB3	1.74	0.52
1:A:1109:PHE:CD1	1:A:1110:TYR:N	2.77	0.52
1:B:37:TYR:HD1	1:B:55:PHE:HZ	1.52	0.52
1:B:64:TRP:CD1	1:B:266:TYR:CE1	2.97	0.52
1:B:449:TYR:O	1:B:494:SER:OG	2.27	0.52
1:B:1109:PHE:CD1	1:B:1110:TYR:N	2.77	0.52
1:C:253:ASP:OD2	1:C:256:SER:OG	2.26	0.52
1:A:92:PHE:N	1:A:192:PHE:O	2.27	0.52
1:A:97:LYS:NZ	1:A:185:ASN:O	2.41	0.52
1:A:746:SER:O	1:A:749:CYS:HB2	2.09	0.52
1:A:961:THR:O	1:A:965:GLN:HG2	2.09	0.52
1:B:153:MET:CE	4:B:1302:NAG:O3	2.56	0.52
1:B:577:ARG:CG	1:B:584:ILE:HD13	2.40	0.52
1:C:48:LEU:HD21	1:C:278:LYS:NZ	2.24	0.52
1:C:403:ARG:CD	1:C:495:TYR:CD1	2.92	0.52
1:C:922:LEU:O	1:C:926:GLN:OE1	2.27	0.52
1:C:961:THR:O	1:C:965:GLN:HG2	2.10	0.52
1:A:84:LEU:O	1:A:238:PHE:N	2.31	0.52
1:A:341:VAL:HG11	1:A:513:LEU:HD21	1.90	0.52
1:A:717:ASN:N	1:A:1070:ALA:O	2.35	0.52
1:A:1102:TRP:HD1	1:A:1135:ASN:ND2	2.08	0.52
1:B:501:ASN:O	1:B:506:GLN:NE2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:N	1:C:239:GLN:O	2.39	0.52
1:C:325:SER:OG	1:C:540:ASN:O	2.16	0.52
1:C:452:LEU:HD21	2:D:98:SER:HB2	1.92	0.52
1:C:715:PRO:CG	1:C:1069:PRO:HB2	2.40	0.52
1:C:746:SER:O	1:C:749:CYS:HB2	2.09	0.52
1:C:817:PHE:HD1	1:C:935:GLN:HE22	1.56	0.52
1:C:1088:HIS:HA	1:C:1122:VAL:HG23	1.91	0.52
1:A:17:ASN:O	3:E:2:NAG:H82	2.09	0.52
1:A:103:GLY:HA2	1:A:104:TRP:CE3	2.45	0.52
1:A:366:SER:OG	1:A:388:ASN:OD1	2.27	0.52
1:B:563:GLN:CD	1:C:41:LYS:HB2	2.35	0.52
1:B:714:ILE:HG22	1:B:715:PRO:HD2	1.91	0.52
1:C:36:VAL:HA	1:C:55:PHE:HE2	1.74	0.52
1:C:127:VAL:HG12	3:G:1:NAG:H5	1.91	0.52
1:C:452:LEU:HD23	2:D:104:CYS:C	2.33	0.52
1:C:594:GLY:H	1:C:613:GLN:HB3	1.74	0.52
1:A:48:LEU:HD21	1:A:278:LYS:NZ	2.24	0.52
1:B:83:VAL:C	1:B:237:ARG:HH11	2.18	0.52
1:B:103:GLY:HA2	1:B:104:TRP:CE3	2.45	0.52
1:B:568:ASP:N	1:B:568:ASP:OD1	2.43	0.52
1:B:701:ALA:O	1:C:788:ILE:N	2.42	0.52
1:C:454:ARG:NE	1:C:492:LEU:HD13	2.25	0.52
1:A:64:TRP:NE1	1:A:266:TYR:CZ	2.78	0.52
1:A:592:PHE:CZ	1:B:857:GLY:HA2	2.43	0.52
1:A:618:THR:OG1	1:A:619:GLU:CD	2.51	0.52
1:B:421:TYR:O	1:B:461:LEU:HD21	2.10	0.52
4:B:1306:NAG:HO3	4:B:1306:NAG:C7	2.16	0.52
1:C:306:PHE:HD2	1:C:306:PHE:O	1.93	0.52
1:A:581:THR:HG23	4:A:1303:NAG:H81	1.91	0.52
1:A:1084:ASP:C	1:A:1086:LYS:HG2	2.35	0.52
1:B:48:LEU:CD2	1:B:278:LYS:HD2	2.40	0.52
1:B:1084:ASP:C	1:B:1086:LYS:HG2	2.35	0.52
1:C:48:LEU:CD2	1:C:278:LYS:HD2	2.40	0.52
1:C:430:THR:O	1:C:515:PHE:N	2.35	0.52
1:C:449:TYR:N	2:D:53:ALA:HB2	2.25	0.52
1:A:83:VAL:C	1:A:237:ARG:HH11	2.18	0.52
1:A:246:ARG:HG3	1:A:257:GLY:C	2.35	0.52
1:A:416:GLY:O	1:A:420:ASP:N	2.40	0.52
1:A:711:SER:HA	1:A:1076:THR:HA	1.92	0.52
1:A:898:PHE:O	1:A:902:MET:HG3	2.09	0.52
1:B:776:LYS:O	1:B:780:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:TRP:NE1	1:C:266:TYR:CZ	2.78	0.52
1:C:102:ARG:O	1:C:121:ASN:N	2.43	0.52
1:C:131:CYS:SG	1:C:165:ASN:O	2.68	0.52
1:C:246:ARG:CZ	1:C:254:SER:HA	2.40	0.52
1:C:768:THR:O	1:C:772:VAL:HG22	2.10	0.52
1:C:776:LYS:O	1:C:780:GLU:HG2	2.10	0.52
1:A:246:ARG:CZ	1:A:254:SER:HA	2.40	0.51
1:A:433:VAL:C	1:A:434:ILE:HD13	2.34	0.51
1:A:566:GLY:HA2	1:B:43:PHE:HB2	1.92	0.51
1:A:580:GLN:O	4:A:1303:NAG:H82	2.09	0.51
1:A:717:ASN:O	1:A:1070:ALA:N	2.39	0.51
1:A:776:LYS:O	1:A:780:GLU:HG2	2.10	0.51
1:A:942:PRO:O	1:A:943:SER:OG	2.19	0.51
1:B:594:GLY:H	1:B:613:GLN:HB3	1.74	0.51
1:B:811:LYS:HD2	1:B:814:LYS:HG2	1.91	0.51
1:B:1051:SER:OG	1:B:1064:HIS:CG	2.63	0.51
1:B:1088:HIS:HA	1:B:1122:VAL:HG23	1.91	0.51
1:C:246:ARG:HG3	1:C:257:GLY:C	2.35	0.51
1:C:905:ARG:HH12	1:C:1050:MET:HB2	1.75	0.51
1:C:937:SER:O	1:C:941:THR:OG1	2.29	0.51
1:C:1106:GLN:OE1	1:C:1111:GLU:HB3	2.09	0.51
1:A:121:ASN:OD1	1:A:177:MET:HE1	2.10	0.51
1:A:131:CYS:SG	1:A:165:ASN:O	2.68	0.51
1:A:715:PRO:CG	1:A:1069:PRO:HB2	2.40	0.51
1:A:927:PHE:O	1:A:931:ILE:HG12	2.10	0.51
1:B:131:CYS:SG	1:B:165:ASN:O	2.68	0.51
1:B:768:THR:O	1:B:772:VAL:HG22	2.10	0.51
1:B:948:LEU:CD1	1:B:948:LEU:HB2	2.39	0.51
1:C:83:VAL:C	1:C:237:ARG:HH11	2.18	0.51
1:C:927:PHE:O	1:C:931:ILE:HG12	2.11	0.51
1:B:246:ARG:HG3	1:B:257:GLY:C	2.35	0.51
1:B:357:ARG:O	1:B:358:ILE:HD13	2.11	0.51
1:B:569:ILE:O	1:B:572:THR:HG22	2.10	0.51
1:B:711:SER:HA	1:B:1076:THR:HA	1.92	0.51
1:B:1102:TRP:HD1	1:B:1135:ASN:ND2	2.07	0.51
1:A:567:ARG:NH2	1:A:573:THR:OG1	2.43	0.51
1:A:578:ASP:N	1:A:583:GLU:O	2.41	0.51
1:A:768:THR:O	1:A:772:VAL:HG22	2.10	0.51
1:A:786:LYS:N	1:A:786:LYS:CD	2.74	0.51
1:A:933:LYS:NZ	1:A:933:LYS:HG2	2.26	0.51
1:A:1019:ARG:O	1:A:1023:ASN:OD1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:PHE:O	1:B:306:PHE:HD2	1.93	0.51
1:B:573:THR:HG21	1:B:576:VAL:HB	1.92	0.51
1:B:817:PHE:HD1	1:B:935:GLN:HE22	1.56	0.51
1:C:392:PHE:HA	1:C:517:LEU:HD13	1.91	0.51
1:C:403:ARG:HD3	1:C:495:TYR:CE1	2.46	0.51
1:C:494:SER:HB2	2:D:102:PHE:O	2.10	0.51
1:C:716:THR:HG22	1:C:1110:TYR:HB3	1.92	0.51
1:C:953:ASN:O	1:C:957:GLN:HG3	2.10	0.51
1:C:1050:MET:CG	1:C:1051:SER:N	2.50	0.51
1:A:306:PHE:HD2	1:A:306:PHE:O	1.93	0.51
1:A:1051:SER:OG	1:A:1064:HIS:CG	2.63	0.51
1:A:1074:ASN:OD1	1:A:1074:ASN:N	2.39	0.51
1:B:64:TRP:NE1	1:B:266:TYR:CZ	2.78	0.51
1:B:543:PHE:N	1:B:546:LEU:O	2.40	0.51
1:B:1074:ASN:OD1	1:B:1074:ASN:N	2.39	0.51
1:C:133:PHE:HE1	1:C:160:TYR:HD2	1.52	0.51
1:C:786:LYS:N	1:C:786:LYS:CD	2.74	0.51
1:C:1102:TRP:HD1	1:C:1135:ASN:ND2	2.07	0.51
1:A:544:ASN:ND2	1:A:544:ASN:O	2.44	0.51
1:A:559:PHE:CD1	1:A:559:PHE:N	2.78	0.51
1:A:922:LEU:O	1:A:926:GLN:OE1	2.27	0.51
1:A:948:LEU:CD1	1:A:948:LEU:HB2	2.39	0.51
1:A:1088:HIS:HA	1:A:1122:VAL:HG23	1.91	0.51
1:B:42:VAL:CG1	1:B:42:VAL:HA	2.37	0.51
1:B:102:ARG:O	1:B:121:ASN:N	2.43	0.51
1:B:454:ARG:HH11	1:B:454:ARG:HG3	1.76	0.51
1:B:716:THR:HG22	1:B:1110:TYR:HB3	1.92	0.51
1:B:933:LYS:NZ	1:B:933:LYS:HG2	2.26	0.51
1:C:988:GLU:HA	1:C:991:VAL:HG12	1.92	0.51
1:A:389:ASP:OD1	1:A:389:ASP:N	2.44	0.51
1:A:402:ILE:CG2	1:A:418:ILE:HG21	2.40	0.51
1:A:443:SER:OG	1:A:498:GLN:N	2.43	0.51
1:A:615:VAL:HG12	1:A:616:ASN:O	2.11	0.51
1:B:121:ASN:OD1	1:B:177:MET:HE1	2.10	0.51
1:B:717:ASN:N	1:B:1070:ALA:O	2.35	0.51
1:C:403:ARG:HG2	1:C:495:TYR:CZ	2.46	0.51
1:C:449:TYR:CA	2:D:53:ALA:HB2	2.39	0.51
1:C:535:LYS:CA	1:C:552:LEU:HD23	2.40	0.51
1:C:551:VAL:N	1:C:588:THR:O	2.37	0.51
1:C:717:ASN:O	1:C:1070:ALA:N	2.39	0.51
1:C:811:LYS:HD2	1:C:814:LYS:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:898:PHE:O	1:C:902:MET:HG3	2.09	0.51
1:C:1051:SER:OG	1:C:1064:HIS:CG	2.63	0.51
1:A:48:LEU:CD2	1:A:278:LYS:HD2	2.40	0.51
1:A:805:ILE:HA	1:A:816:SER:HB2	1.93	0.51
1:A:932:GLY:O	1:A:935:GLN:HB3	2.11	0.51
1:B:667:GLY:HA2	1:C:864:LEU:HD12	1.91	0.51
1:B:786:LYS:N	1:B:786:LYS:CD	2.74	0.51
1:B:896:ILE:HD13	1:B:901:GLN:HB3	1.92	0.51
1:B:1019:ARG:O	1:B:1023:ASN:OD1	2.29	0.51
1:C:103:GLY:HA2	1:C:104:TRP:CE3	2.45	0.51
1:C:552:LEU:H	1:C:552:LEU:HD22	1.75	0.51
1:C:565:PHE:HD1	1:C:565:PHE:H	1.57	0.51
1:A:388:ASN:O	1:A:528:LYS:NZ	2.44	0.51
1:A:564:GLN:H	1:B:41:LYS:HB2	1.76	0.51
1:A:896:ILE:HD13	1:A:901:GLN:HB3	1.92	0.51
1:A:905:ARG:HH12	1:A:1050:MET:HB2	1.75	0.51
1:B:562:PHE:O	1:C:41:LYS:CD	2.59	0.51
1:B:819:GLU:HA	1:B:822:LEU:HG	1.92	0.51
1:B:905:ARG:HH12	1:B:1050:MET:HB2	1.75	0.51
1:C:855:PHE:N	1:C:858:LEU:O	2.44	0.51
1:C:932:GLY:O	1:C:935:GLN:HB3	2.11	0.51
1:C:1084:ASP:C	1:C:1086:LYS:HG2	2.35	0.51
3:H:2:NAG:O7	3:H:2:NAG:O3	2.24	0.51
1:A:811:LYS:HD2	1:A:814:LYS:HG2	1.92	0.51
1:A:1012:LEU:HD13	1:C:1013:ILE:HD13	1.93	0.51
1:B:490:PHE:CE2	1:B:492:LEU:HD13	2.46	0.51
1:B:715:PRO:CG	1:B:1069:PRO:HB2	2.40	0.51
1:B:937:SER:O	1:B:941:THR:OG1	2.29	0.51
1:C:451:TYR:N	2:D:32:CYS:HB2	2.26	0.51
1:A:919:ASN:O	1:A:923:ILE:HG12	2.11	0.50
1:A:1014:ARG:N	1:A:1014:ARG:CD	2.70	0.50
1:B:49:HIS:O	1:B:277:LEU:HD23	2.11	0.50
1:B:199:GLY:O	1:B:231:ILE:N	2.29	0.50
1:B:927:PHE:O	1:B:931:ILE:HG12	2.10	0.50
1:C:449:TYR:C	2:D:32:CYS:O	2.54	0.50
1:C:538:CYS:HA	1:C:551:VAL:HG22	1.92	0.50
1:C:615:VAL:HG12	1:C:616:ASN:O	2.11	0.50
1:C:1082:CYS:N	1:C:1133:VAL:O	2.38	0.50
1:B:78:ARG:O	1:B:78:ARG:NE	2.44	0.50
1:B:871:ALA:O	1:B:874:THR:OG1	2.23	0.50
1:C:206:LYS:HZ1	1:C:221:SER:HG	1.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:ILE:HA	1:C:816:SER:HB2	1.93	0.50
1:A:565:PHE:HB3	1:A:576:VAL:HG23	1.93	0.50
1:A:819:GLU:HA	1:A:822:LEU:HG	1.92	0.50
1:B:615:VAL:HG12	1:B:616:ASN:O	2.11	0.50
1:B:988:GLU:HA	1:B:991:VAL:HG12	1.92	0.50
1:C:452:LEU:HD11	2:D:33:ARG:HB2	1.93	0.50
1:C:711:SER:HA	1:C:1076:THR:HA	1.92	0.50
1:C:896:ILE:HD13	1:C:901:GLN:HB3	1.92	0.50
1:C:916:LEU:O	1:C:920:GLN:N	2.45	0.50
1:A:78:ARG:O	1:A:78:ARG:NE	2.44	0.50
1:A:553:THR:N	1:A:586:ASP:O	2.44	0.50
1:A:902:MET:O	1:A:906:PHE:HD1	1.95	0.50
1:B:246:ARG:CZ	1:B:254:SER:HA	2.40	0.50
1:B:562:PHE:CE2	1:C:225:PRO:CG	2.91	0.50
1:B:855:PHE:N	1:B:858:LEU:O	2.44	0.50
1:B:932:GLY:O	1:B:935:GLN:HB3	2.11	0.50
1:B:953:ASN:O	1:B:957:GLN:HG3	2.10	0.50
1:C:65:PHE:HD2	1:C:265:TYR:O	1.94	0.50
1:C:933:LYS:NZ	1:C:933:LYS:HG2	2.26	0.50
1:A:49:HIS:O	1:A:277:LEU:HD23	2.11	0.50
1:A:102:ARG:O	1:A:121:ASN:N	2.43	0.50
1:B:228:ASP:OD1	1:B:228:ASP:N	2.44	0.50
1:B:919:ASN:O	1:B:923:ILE:HG12	2.11	0.50
1:B:1142:GLN:O	1:B:1145:LEU:HB3	2.12	0.50
1:C:49:HIS:O	1:C:277:LEU:HD23	2.11	0.50
1:C:1117:THR:OG1	1:C:1139:ASP:HA	2.12	0.50
1:A:92:PHE:CZ	1:A:265:TYR:HD2	2.30	0.50
1:A:100:ILE:O	1:A:242:LEU:HB2	2.12	0.50
1:A:881:THR:O	1:A:885:GLY:N	2.43	0.50
1:B:281:GLU:CD	4:B:1304:NAG:O7	2.47	0.50
1:B:802:PHE:CE2	1:B:805:ILE:HD11	2.47	0.50
1:C:453:TYR:CE2	1:C:455:LEU:CG	2.94	0.50
1:C:919:ASN:O	1:C:923:ILE:HG12	2.11	0.50
1:A:117:LEU:HD12	1:A:118:LEU:H	1.77	0.50
1:A:323:THR:O	1:A:539:VAL:HG13	2.11	0.50
1:A:855:PHE:N	1:A:858:LEU:O	2.44	0.50
1:A:913:GLN:HB3	1:A:917:TYR:HE1	1.77	0.50
1:A:1117:THR:OG1	1:A:1139:ASP:HA	2.12	0.50
1:B:902:MET:O	1:B:906:PHE:HD1	1.95	0.50
1:B:916:LEU:O	1:B:920:GLN:N	2.45	0.50
1:C:117:LEU:HD12	1:C:118:LEU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:819:GLU:HA	1:C:822:LEU:HG	1.92	0.50
1:C:1019:ARG:O	1:C:1023:ASN:OD1	2.29	0.50
2:D:51:ILE:CG1	2:D:57:THR:HG22	2.41	0.50
1:A:566:GLY:O	1:A:574:ASP:N	2.34	0.50
1:A:716:THR:HG22	1:A:1110:TYR:HB3	1.92	0.50
1:A:825:LYS:HD3	1:A:945:LEU:CD1	2.41	0.50
1:A:988:GLU:HA	1:A:991:VAL:HG12	1.92	0.50
1:B:233:ILE:CG2	1:B:234:ASN:N	2.74	0.50
1:C:330:PRO:HA	1:C:580:GLN:OE1	2.11	0.50
2:D:38:ARG:HG2	2:D:48:VAL:CG2	2.42	0.50
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.94	0.50
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.94	0.50
1:A:362:VAL:HG12	1:A:527:PRO:HD3	1.93	0.50
1:A:773:GLU:OE1	1:A:774:GLN:HB3	2.12	0.50
1:B:326:ILE:HD12	1:B:326:ILE:N	2.26	0.50
1:B:468:ILE:O	1:B:468:ILE:HG12	2.12	0.50
1:B:472:ILE:HG23	1:B:489:TYR:C	2.36	0.50
1:B:715:PRO:HA	1:B:1071:GLN:O	2.12	0.50
1:B:881:THR:O	1:B:885:GLY:N	2.43	0.50
1:B:1020:ALA:HA	1:B:1023:ASN:OD1	2.12	0.50
1:C:88:ASP:OD2	1:C:88:ASP:N	2.45	0.50
1:C:92:PHE:CZ	1:C:265:TYR:HD2	2.30	0.50
1:C:127:VAL:CG1	3:G:1:NAG:H5	2.41	0.50
1:C:130:VAL:HG12	1:C:168:PHE:H	1.77	0.50
1:C:449:TYR:CD1	2:D:53:ALA:HA	2.46	0.50
1:C:454:ARG:HA	1:C:492:LEU:HB2	1.94	0.50
1:C:490:PHE:CD2	2:D:105:THR:HG23	2.46	0.50
1:C:715:PRO:HA	1:C:1071:GLN:O	2.12	0.50
1:C:1135:ASN:OD1	1:C:1135:ASN:C	2.54	0.50
1:A:41:LYS:CB	1:A:41:LYS:O	2.43	0.49
1:A:730:SER:C	1:A:1058:HIS:CE1	2.90	0.49
1:A:953:ASN:O	1:A:957:GLN:HG3	2.11	0.49
1:A:1116:THR:HG23	1:A:1138:TYR:CD1	2.44	0.49
1:B:100:ILE:O	1:B:242:LEU:HB2	2.12	0.49
1:B:189:LEU:CB	1:B:210:ILE:HD11	2.41	0.49
1:B:562:PHE:C	1:C:41:LYS:CD	2.85	0.49
1:C:432:CYS:SG	1:C:434:ILE:HD11	2.52	0.49
1:C:884:SER:HG	1:C:887:THR:CB	2.24	0.49
1:C:902:MET:O	1:C:906:PHE:HD1	1.95	0.49
1:A:233:ILE:CG2	1:A:234:ASN:N	2.74	0.49
1:A:323:THR:OG1	1:A:324:GLU:OE1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:SER:OG	4:A:1304:NAG:N2	2.45	0.49
1:A:1142:GLN:O	1:A:1145:LEU:HB3	2.12	0.49
1:B:41:LYS:CB	1:B:41:LYS:O	2.43	0.49
1:B:88:ASP:OD2	1:B:88:ASP:N	2.45	0.49
1:B:117:LEU:HD12	1:B:118:LEU:H	1.77	0.49
1:B:120:VAL:HG23	1:B:241:LEU:HB3	1.94	0.49
1:B:130:VAL:HG12	1:B:168:PHE:H	1.77	0.49
1:B:206:LYS:NZ	1:B:221:SER:OG	2.25	0.49
1:B:395:VAL:HG12	1:B:396:TYR:N	2.28	0.49
1:C:40:ASP:O	1:C:41:LYS:NZ	2.42	0.49
1:C:481:ASN:O	1:C:481:ASN:ND2	2.45	0.49
1:C:577:ARG:HA	1:C:584:ILE:HA	1.93	0.49
1:C:949:GLN:O	1:C:953:ASN:ND2	2.41	0.49
1:C:1142:GLN:O	1:C:1145:LEU:HB3	2.12	0.49
1:A:57:PRO:HG3	1:A:273:ARG:HE	1.77	0.49
1:A:350:VAL:HG22	1:A:422:ASN:CB	2.42	0.49
1:A:542:ASN:HA	1:A:547:THR:HA	1.94	0.49
1:B:65:PHE:HD2	1:B:265:TYR:O	1.94	0.49
1:B:143:VAL:HG21	1:B:179:LEU:CD2	2.42	0.49
1:B:167:THR:OG1	1:B:168:PHE:N	2.45	0.49
1:B:393:THR:N	1:B:516:GLU:O	2.38	0.49
1:C:84:LEU:N	1:C:237:ARG:HH11	2.10	0.49
1:C:228:ASP:N	1:C:228:ASP:OD1	2.44	0.49
1:C:424:LYS:O	1:C:464:PHE:N	2.42	0.49
1:C:453:TYR:CD2	1:C:495:TYR:N	2.80	0.49
1:C:802:PHE:CE2	1:C:805:ILE:HD11	2.47	0.49
1:A:65:PHE:HD2	1:A:265:TYR:O	1.94	0.49
1:A:143:VAL:HG21	1:A:179:LEU:CD2	2.42	0.49
1:A:553:THR:HG22	1:A:588:THR:CG2	2.43	0.49
1:A:802:PHE:CE2	1:A:805:ILE:HD11	2.47	0.49
1:A:937:SER:O	1:A:941:THR:OG1	2.29	0.49
1:A:1020:ALA:HA	1:A:1023:ASN:OD1	2.12	0.49
1:A:1106:GLN:HE22	1:A:1109:PHE:HB3	1.76	0.49
1:B:197:ILE:O	1:B:198:ASP:OD2	2.31	0.49
1:B:805:ILE:HA	1:B:816:SER:HB2	1.93	0.49
1:B:825:LYS:HD3	1:B:945:LEU:CD1	2.41	0.49
1:B:1071:GLN:NE2	1:B:1071:GLN:CB	2.67	0.49
1:C:351:TYR:HB3	1:C:454:ARG:HB2	1.94	0.49
1:C:773:GLU:OE1	1:C:774:GLN:HB3	2.12	0.49
1:C:1020:ALA:HA	1:C:1023:ASN:OD1	2.12	0.49
1:A:393:THR:HG21	1:A:518:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:ILE:HD11	1:A:904:TYR:CE2	2.47	0.49
1:A:977:LEU:HA	1:A:980:ILE:HG12	1.94	0.49
1:B:92:PHE:CZ	1:B:265:TYR:HD2	2.30	0.49
1:B:560:LEU:HB3	1:B:562:PHE:HD1	1.77	0.49
1:B:730:SER:C	1:B:1058:HIS:CE1	2.90	0.49
1:B:1117:THR:OG1	1:B:1139:ASP:HA	2.12	0.49
1:C:78:ARG:O	1:C:78:ARG:NE	2.44	0.49
1:C:282:ASN:CG	1:C:284:THR:HG23	2.38	0.49
1:C:287:ASP:OD1	1:C:306:PHE:CD1	2.66	0.49
1:C:496:GLY:O	1:C:505:TYR:OH	2.31	0.49
1:C:568:ASP:HB3	1:C:572:THR:HG23	1.95	0.49
1:C:730:SER:C	1:C:1058:HIS:CE1	2.90	0.49
1:A:84:LEU:N	1:A:237:ARG:HH11	2.10	0.49
1:A:189:LEU:CB	1:A:210:ILE:HD11	2.41	0.49
1:A:197:ILE:O	1:A:198:ASP:OD2	2.31	0.49
1:A:282:ASN:CG	1:A:284:THR:HG23	2.38	0.49
1:A:1088:HIS:CG	1:A:1122:VAL:HG23	2.48	0.49
1:B:568:ASP:N	1:B:572:THR:O	2.35	0.49
1:B:1054:GLN:OE1	1:B:1054:GLN:HA	2.13	0.49
1:B:1088:HIS:CG	1:B:1122:VAL:HG23	2.48	0.49
1:B:1135:ASN:OD1	1:B:1135:ASN:C	2.54	0.49
1:C:100:ILE:O	1:C:242:LEU:HB2	2.12	0.49
1:C:233:ILE:CG2	1:C:234:ASN:N	2.74	0.49
1:C:1088:HIS:CG	1:C:1122:VAL:HG23	2.48	0.49
1:A:94:SER:N	1:A:190:ARG:O	2.42	0.49
1:A:228:ASP:OD1	1:A:228:ASP:N	2.44	0.49
1:A:603:ASN:C	1:A:603:ASN:OD1	2.56	0.49
1:A:715:PRO:HA	1:A:1071:GLN:O	2.12	0.49
1:A:1054:GLN:OE1	1:A:1054:GLN:HA	2.13	0.49
1:B:133:PHE:HA	1:B:162:SER:O	2.13	0.49
1:B:282:ASN:CG	1:B:284:THR:HG23	2.38	0.49
1:B:511:VAL:HG12	1:B:513:LEU:CD1	2.43	0.49
1:B:558:LYS:HG3	1:C:43:PHE:HE1	1.78	0.49
1:B:773:GLU:OE1	1:B:774:GLN:HB3	2.12	0.49
1:C:167:THR:OG1	1:C:168:PHE:N	2.45	0.49
1:C:197:ILE:O	1:C:198:ASP:OD2	2.31	0.49
1:C:397:ALA:HB1	1:C:511:VAL:HG13	1.94	0.49
1:C:603:ASN:C	1:C:603:ASN:OD1	2.56	0.49
1:C:741:TYR:CZ	1:C:966:LEU:HB3	2.48	0.49
1:A:985:ASP:OD2	1:A:985:ASP:C	2.55	0.49
1:A:1135:ASN:OD1	1:A:1135:ASN:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:SER:HA	1:B:265:TYR:HA	1.94	0.49
1:B:233:ILE:HG21	1:B:235:ILE:HG13	1.94	0.49
1:C:57:PRO:HG3	1:C:273:ARG:HE	1.77	0.49
1:C:726:ILE:O	1:C:726:ILE:HG22	2.12	0.49
1:C:906:PHE:HA	1:C:909:ILE:HG12	1.95	0.49
1:A:562:PHE:O	1:A:564:GLN:OE1	2.30	0.49
1:B:77:LYS:O	1:B:78:ARG:C	2.56	0.49
1:B:644:GLN:HA	1:B:649:CYS:HA	1.95	0.49
1:B:718:PHE:HA	1:B:1068:VAL:O	2.13	0.49
1:B:741:TYR:CZ	1:B:966:LEU:HB3	2.48	0.49
1:B:913:GLN:HB3	1:B:917:TYR:HE1	1.77	0.49
1:B:1010:GLN:O	1:B:1014:ARG:HD3	2.13	0.49
1:C:120:VAL:HG23	1:C:241:LEU:HB3	1.94	0.49
1:C:145:TYR:CE1	1:C:152:TRP:CE2	3.01	0.49
1:C:201:PHE:HB3	1:C:229:LEU:HB2	1.94	0.49
1:C:246:ARG:HD3	1:C:258:TRP:HB3	1.95	0.49
1:C:1049:LEU:HG	1:C:1066:THR:HA	1.95	0.49
2:D:40:ALA:HB3	2:D:43:LYS:CD	2.42	0.49
2:D:52:THR:CG2	2:D:56:ALA:HB3	2.43	0.49
2:D:75:LYS:O	2:D:77:THR:HG23	2.13	0.49
1:A:826:VAL:HG21	1:A:1057:PRO:HG2	1.95	0.49
1:A:916:LEU:O	1:A:920:GLN:N	2.45	0.49
1:B:84:LEU:CA	1:B:237:ARG:NH1	2.71	0.49
1:B:201:PHE:HB3	1:B:229:LEU:HB2	1.94	0.49
1:B:563:GLN:HA	1:C:41:LYS:CG	2.21	0.49
1:C:143:VAL:HG21	1:C:179:LEU:CD2	2.42	0.49
1:C:913:GLN:HB3	1:C:917:TYR:HE1	1.77	0.49
1:A:145:TYR:CE1	1:A:152:TRP:CE2	3.01	0.48
1:A:193:VAL:HG23	1:A:223:LEU:CD1	2.43	0.48
1:A:382:VAL:HG12	1:A:383:SER:H	1.77	0.48
1:A:390:LEU:HD22	1:A:392:PHE:CE2	2.47	0.48
1:A:703:ASN:ND2	1:B:787:GLN:CG	2.76	0.48
1:B:145:TYR:CE1	1:B:152:TRP:CE2	3.01	0.48
1:B:320:VAL:CG2	1:B:591:SER:O	2.60	0.48
1:B:896:ILE:HD11	1:B:904:TYR:CE2	2.47	0.48
1:C:453:TYR:CE2	1:C:495:TYR:CD1	3.01	0.48
1:C:977:LEU:HA	1:C:980:ILE:HG12	1.94	0.48
1:A:152:TRP:HB2	1:A:245:HIS:HE1	1.78	0.48
1:A:1010:GLN:O	1:A:1014:ARG:HD3	2.13	0.48
1:B:246:ARG:HD3	1:B:258:TRP:HB3	1.95	0.48
1:B:557:LYS:CB	1:C:43:PHE:CE2	2.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:ARG:O	1:C:44:ARG:NH2	2.46	0.48
1:B:726:ILE:HG22	1:B:726:ILE:O	2.13	0.48
1:B:1030:SER:HA	1:B:1034:LEU:HD12	1.96	0.48
1:C:234:ASN:C	1:C:234:ASN:OD1	2.56	0.48
1:C:330:PRO:CA	1:C:580:GLN:CD	2.84	0.48
1:C:438:SER:HA	1:C:441:LEU:HD12	1.95	0.48
1:A:103:GLY:HA3	1:A:119:ILE:O	2.14	0.48
1:A:167:THR:OG1	1:A:168:PHE:N	2.45	0.48
1:A:644:GLN:HA	1:A:649:CYS:HA	1.95	0.48
1:A:802:PHE:HB3	1:A:806:LEU:HG	1.95	0.48
1:A:906:PHE:HA	1:A:909:ILE:HG12	1.95	0.48
1:A:1110:TYR:CD1	1:A:1112:PRO:HD3	2.48	0.48
1:B:151:SER:CB	4:B:1302:NAG:H61	2.44	0.48
1:B:717:ASN:O	1:B:1070:ALA:N	2.39	0.48
1:B:826:VAL:HG21	1:B:1057:PRO:HG2	1.95	0.48
1:B:977:LEU:HA	1:B:980:ILE:HG12	1.94	0.48
1:B:1110:TYR:CD1	1:B:1112:PRO:HD3	2.48	0.48
1:C:666:ILE:HB	1:C:670:ILE:O	2.13	0.48
1:C:718:PHE:HA	1:C:1068:VAL:O	2.13	0.48
1:C:881:THR:O	1:C:885:GLY:N	2.43	0.48
1:C:985:ASP:OD2	1:C:985:ASP:C	2.55	0.48
1:A:726:ILE:O	1:A:726:ILE:HG22	2.12	0.48
1:A:741:TYR:CZ	1:A:966:LEU:HB3	2.48	0.48
1:B:111:ASP:OD1	1:B:113:LYS:NZ	2.47	0.48
1:B:143:VAL:HG22	1:B:154:GLU:CA	2.44	0.48
1:B:563:GLN:HB3	1:C:41:LYS:HB2	1.95	0.48
1:B:729:VAL:HB	1:B:1059:GLY:HA2	1.95	0.48
1:C:44:ARG:O	1:C:283:GLY:HA2	2.14	0.48
1:C:122:ASN:CG	3:G:1:NAG:C7	2.86	0.48
1:C:233:ILE:HG21	1:C:235:ILE:HG13	1.94	0.48
1:C:449:TYR:O	2:D:53:ALA:HB2	2.10	0.48
1:C:616:ASN:HB2	1:C:619:GLU:CD	2.39	0.48
1:C:896:ILE:HD11	1:C:904:TYR:CE2	2.48	0.48
1:C:1030:SER:HA	1:C:1034:LEU:HD12	1.96	0.48
1:C:1110:TYR:CD1	1:C:1112:PRO:HD3	2.48	0.48
3:E:1:NAG:C1	3:E:1:NAG:C8	2.92	0.48
1:A:234:ASN:C	1:A:234:ASN:OD1	2.56	0.48
1:A:457:ARG:NH2	1:A:467:ASP:OD2	2.46	0.48
1:A:616:ASN:HB2	1:A:619:GLU:CD	2.39	0.48
1:A:729:VAL:HB	1:A:1059:GLY:HA2	1.95	0.48
1:A:920:GLN:OE1	1:C:1130:ILE:HD11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:GLU:O	1:A:992:GLN:HG2	2.13	0.48
1:B:57:PRO:HG3	1:B:273:ARG:HE	1.77	0.48
1:B:105:ILE:N	1:B:239:GLN:O	2.39	0.48
1:B:985:ASP:C	1:B:985:ASP:OD2	2.55	0.48
1:C:111:ASP:OD1	1:C:113:LYS:NZ	2.47	0.48
1:C:133:PHE:HA	1:C:162:SER:O	2.13	0.48
1:C:312:ILE:HG22	1:C:598:ILE:HG23	1.96	0.48
1:C:490:PHE:CG	2:D:105:THR:HG23	2.48	0.48
1:C:1010:GLN:O	1:C:1014:ARG:HD3	2.13	0.48
1:A:77:LYS:O	1:A:78:ARG:C	2.56	0.48
1:A:120:VAL:HG23	1:A:241:LEU:HB3	1.94	0.48
1:A:552:LEU:HD23	1:A:552:LEU:H	1.78	0.48
1:A:567:ARG:CB	1:B:44:ARG:HH22	2.26	0.48
1:B:124:THR:CG2	4:B:1301:NAG:H83	2.27	0.48
1:B:193:VAL:HG23	1:B:223:LEU:CD1	2.43	0.48
1:B:234:ASN:C	1:B:234:ASN:OD1	2.56	0.48
1:B:357:ARG:NH2	1:C:231:ILE:HA	2.28	0.48
1:B:454:ARG:CZ	1:B:491:PRO:HB2	2.43	0.48
1:C:127:VAL:HG12	3:G:1:NAG:H62	1.95	0.48
1:C:143:VAL:HG22	1:C:154:GLU:CA	2.44	0.48
1:C:644:GLN:HA	1:C:649:CYS:HA	1.95	0.48
1:C:988:GLU:O	1:C:992:GLN:HG2	2.13	0.48
1:A:125:ASN:ND2	1:A:172:SER:O	2.46	0.48
1:A:287:ASP:OD1	1:A:306:PHE:CD1	2.66	0.48
1:B:118:LEU:HD22	1:B:135:PHE:HZ	1.78	0.48
1:B:312:ILE:HG22	1:B:598:ILE:HG23	1.96	0.48
1:B:748:GLU:O	1:B:752:LEU:HG	2.13	0.48
1:B:906:PHE:HA	1:B:909:ILE:HG12	1.95	0.48
1:C:436:TRP:O	1:C:509:ARG:N	2.42	0.48
1:C:537:LYS:O	1:C:539:VAL:HG23	2.13	0.48
1:C:1054:GLN:OE1	1:C:1054:GLN:HA	2.13	0.48
1:A:569:ILE:O	1:A:570:ALA:HB3	2.13	0.48
1:A:933:LYS:NZ	1:A:933:LYS:CG	2.77	0.48
1:A:1102:TRP:O	1:A:1115:ILE:HG13	2.14	0.48
1:B:220:PHE:HE2	1:B:287:ASP:HA	1.75	0.48
1:B:594:GLY:CA	1:B:613:GLN:HG2	2.43	0.48
1:B:1102:TRP:O	1:B:1115:ILE:HG13	2.14	0.48
1:C:77:LYS:O	1:C:78:ARG:C	2.56	0.48
1:C:94:SER:N	1:C:190:ARG:O	2.42	0.48
1:C:94:SER:HA	1:C:265:TYR:HA	1.94	0.48
1:C:329:PHE:CD2	1:C:527:PRO:O	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ALA:HB3	1:C:399:SER:O	2.14	0.48
1:C:565:PHE:N	1:C:565:PHE:CD1	2.81	0.48
1:A:78:ARG:C	1:A:78:ARG:NE	2.72	0.48
1:A:91:TYR:O	1:A:268:GLY:N	2.47	0.48
1:A:118:LEU:HD22	1:A:135:PHE:HZ	1.78	0.48
1:A:220:PHE:CZ	1:A:287:ASP:CA	2.97	0.48
1:A:718:PHE:HA	1:A:1068:VAL:O	2.13	0.48
1:A:856:ASN:OD1	1:A:858:LEU:N	2.38	0.48
1:B:78:ARG:C	1:B:78:ARG:NE	2.72	0.48
1:B:84:LEU:N	1:B:237:ARG:HH11	2.10	0.48
1:B:603:ASN:OD1	1:B:603:ASN:C	2.56	0.48
1:B:616:ASN:HB2	1:B:619:GLU:CD	2.39	0.48
1:B:902:MET:O	1:B:906:PHE:CD1	2.67	0.48
1:C:825:LYS:HD3	1:C:945:LEU:CD1	2.41	0.48
1:C:1106:GLN:HE22	1:C:1109:PHE:HB3	1.76	0.48
2:D:12:VAL:O	2:D:117:VAL:HA	2.14	0.48
1:A:133:PHE:HA	1:A:162:SER:O	2.13	0.48
1:A:233:ILE:HG21	1:A:235:ILE:HG13	1.94	0.48
1:A:533:LEU:HD11	1:A:535:LYS:HZ3	1.78	0.48
1:A:1016:ALA:HA	1:A:1019:ARG:NH1	2.29	0.48
1:B:37:TYR:OH	1:B:53:ASP:CG	2.57	0.48
1:B:48:LEU:HD12	1:B:304:LYS:O	2.14	0.48
1:B:1016:ALA:HA	1:B:1019:ARG:NH1	2.29	0.48
1:B:1049:LEU:HG	1:B:1066:THR:HA	1.95	0.48
1:B:1116:THR:HG23	1:B:1138:TYR:CD1	2.44	0.48
1:C:103:GLY:HA3	1:C:119:ILE:O	2.14	0.48
1:C:189:LEU:CB	1:C:210:ILE:HD11	2.41	0.48
1:C:1091:ARG:HE	1:C:1119:ASN:CA	2.27	0.48
1:A:40:ASP:C	1:A:41:LYS:HZ1	2.21	0.47
1:A:48:LEU:HD21	1:A:278:LYS:HZ3	1.79	0.47
1:A:88:ASP:OD2	1:A:88:ASP:N	2.45	0.47
1:A:111:ASP:OD1	1:A:113:LYS:NZ	2.47	0.47
1:A:130:VAL:HG11	1:A:168:PHE:H	1.79	0.47
1:A:130:VAL:HG12	1:A:168:PHE:H	1.77	0.47
1:A:143:VAL:HG22	1:A:154:GLU:CA	2.44	0.47
1:A:726:ILE:HD12	1:A:1061:VAL:CG2	2.44	0.47
1:A:902:MET:O	1:A:906:PHE:CD1	2.67	0.47
1:A:1013:ILE:HD13	1:B:1012:LEU:HD13	1.95	0.47
1:A:1091:ARG:HE	1:A:1119:ASN:CA	2.27	0.47
1:B:441:LEU:HD22	1:B:441:LEU:N	2.29	0.47
1:C:220:PHE:HE2	1:C:287:ASP:HA	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:729:VAL:HB	1:C:1059:GLY:HA2	1.95	0.47
1:C:871:ALA:O	1:C:874:THR:OG1	2.23	0.47
1:A:192:PHE:HB3	1:A:194:PHE:HE1	1.80	0.47
1:A:246:ARG:HD3	1:A:258:TRP:HB3	1.95	0.47
1:A:666:ILE:HB	1:A:670:ILE:O	2.13	0.47
1:A:1030:SER:HA	1:A:1034:LEU:HD12	1.96	0.47
1:B:96:GLU:OE2	1:B:101:ILE:HB	2.14	0.47
1:B:133:PHE:HE1	1:B:160:TYR:HD2	1.52	0.47
1:B:192:PHE:HB3	1:B:194:PHE:HE1	1.80	0.47
1:B:287:ASP:OD1	1:B:306:PHE:CD1	2.66	0.47
1:B:457:ARG:HD2	1:B:461:LEU:HD23	1.96	0.47
1:C:152:TRP:HB2	1:C:245:HIS:HE1	1.78	0.47
1:C:192:PHE:HB3	1:C:194:PHE:HE1	1.80	0.47
1:C:278:LYS:O	1:C:285:ILE:HA	2.14	0.47
1:C:402:ILE:O	1:C:507:PRO:HA	2.15	0.47
1:C:726:ILE:HD12	1:C:1061:VAL:CG2	2.44	0.47
1:C:802:PHE:HB3	1:C:806:LEU:HG	1.95	0.47
1:C:826:VAL:HG21	1:C:1057:PRO:HG2	1.95	0.47
1:A:37:TYR:OH	1:A:53:ASP:CG	2.57	0.47
1:A:48:LEU:HD12	1:A:304:LYS:O	2.14	0.47
1:A:278:LYS:O	1:A:285:ILE:HA	2.14	0.47
1:A:567:ARG:HG3	1:B:44:ARG:NH2	2.29	0.47
1:A:1024:LEU:HD11	1:A:1028:LYS:HE2	1.96	0.47
1:A:1049:LEU:HG	1:A:1066:THR:HA	1.95	0.47
1:A:1139:ASP:CG	1:A:1142:GLN:HE22	2.22	0.47
1:B:151:SER:OG	4:B:1302:NAG:C6	2.61	0.47
1:B:395:VAL:HG11	1:B:513:LEU:HG	1.95	0.47
1:B:704:SER:HA	1:C:790:LYS:O	2.14	0.47
1:B:726:ILE:HD12	1:B:1061:VAL:CG2	2.44	0.47
1:C:78:ARG:C	1:C:78:ARG:NE	2.72	0.47
1:C:200:TYR:N	1:C:200:TYR:CD1	2.82	0.47
1:C:560:LEU:N	1:C:560:LEU:HD23	2.28	0.47
1:C:707:TYR:CD1	1:C:708:SER:N	2.82	0.47
1:C:920:GLN:HA	1:C:923:ILE:CG1	2.42	0.47
1:C:1102:TRP:O	1:C:1115:ILE:HG13	2.14	0.47
1:A:41:LYS:O	1:C:563:GLN:HG3	2.14	0.47
1:A:594:GLY:CA	1:A:613:GLN:HG2	2.43	0.47
1:A:715:PRO:HG2	1:A:1069:PRO:CB	2.44	0.47
1:A:948:LEU:O	1:A:952:VAL:HG22	2.14	0.47
1:B:200:TYR:N	1:B:200:TYR:CD1	2.82	0.47
1:B:220:PHE:CZ	1:B:287:ASP:CA	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:PHE:HB3	1:B:806:LEU:HG	1.95	0.47
1:C:118:LEU:HD22	1:C:135:PHE:HZ	1.78	0.47
1:C:193:VAL:HG23	1:C:223:LEU:CD1	2.43	0.47
1:C:1081:ILE:CG1	1:C:1135:ASN:HB3	2.45	0.47
1:A:900:MET:HE1	1:C:1079:PRO:HA	1.97	0.47
1:B:91:TYR:O	1:B:268:GLY:N	2.47	0.47
1:B:203:ILE:HD12	1:B:227:VAL:HB	1.97	0.47
1:B:666:ILE:HB	1:B:670:ILE:O	2.13	0.47
1:B:977:LEU:O	1:B:981:LEU:HG	2.14	0.47
1:C:124:THR:HG1	3:G:1:NAG:C7	2.25	0.47
1:C:933:LYS:NZ	1:C:933:LYS:CG	2.77	0.47
1:C:1139:ASP:CG	1:C:1142:GLN:HE22	2.23	0.47
2:D:50:SER:HB3	2:D:58:TYR:CE2	2.48	0.47
1:A:94:SER:HA	1:A:265:TYR:HA	1.95	0.47
1:A:669:GLY:O	1:A:697:MET:HB3	2.14	0.47
1:A:949:GLN:O	1:A:953:ASN:ND2	2.41	0.47
1:B:475:ALA:HB2	1:B:489:TYR:HE2	1.79	0.47
1:B:515:PHE:N	1:B:515:PHE:CD1	2.83	0.47
1:B:669:GLY:O	1:B:697:MET:HB3	2.14	0.47
1:B:699:LEU:HD12	1:C:872:GLN:OE1	2.06	0.47
1:B:903:ALA:HB1	1:B:913:GLN:CG	2.44	0.47
1:B:1091:ARG:HE	1:B:1119:ASN:CA	2.27	0.47
1:C:37:TYR:OH	1:C:53:ASP:CG	2.57	0.47
1:C:91:TYR:O	1:C:268:GLY:N	2.47	0.47
1:C:361:CYS:H	1:C:524:VAL:HG22	1.80	0.47
1:C:454:ARG:NH2	1:C:492:LEU:HD13	2.29	0.47
1:C:669:GLY:O	1:C:697:MET:HB3	2.14	0.47
1:C:748:GLU:O	1:C:752:LEU:HG	2.14	0.47
1:C:818:ILE:O	1:C:822:LEU:HG	2.14	0.47
1:C:948:LEU:O	1:C:952:VAL:HG22	2.14	0.47
2:D:67:LEU:HD21	2:D:80:LEU:CD1	2.44	0.47
1:A:44:ARG:O	1:A:283:GLY:HA2	2.14	0.47
1:A:712:ILE:CD1	1:B:895:GLN:O	2.62	0.47
1:A:897:PRO:HG3	1:A:900:MET:HG2	1.97	0.47
1:B:278:LYS:O	1:B:285:ILE:HA	2.15	0.47
1:B:343:ASN:OD1	1:B:343:ASN:N	2.47	0.47
1:B:618:THR:HG1	1:B:619:GLU:CD	2.22	0.47
1:B:948:LEU:O	1:B:952:VAL:HG22	2.14	0.47
1:B:988:GLU:O	1:B:992:GLN:HG2	2.13	0.47
1:C:125:ASN:ND2	1:C:172:SER:O	2.46	0.47
1:C:130:VAL:HG11	1:C:168:PHE:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ILE:HD12	1:C:227:VAL:HB	1.97	0.47
1:C:715:PRO:HG2	1:C:1069:PRO:CB	2.44	0.47
1:C:902:MET:O	1:C:906:PHE:CD1	2.67	0.47
1:C:1116:THR:HG23	1:C:1138:TYR:CD1	2.44	0.47
1:A:31:SER:HB3	1:A:62:VAL:CG2	2.45	0.47
1:A:41:LYS:HA	1:A:41:LYS:HZ1	1.79	0.47
1:A:64:TRP:HZ2	1:A:214:ARG:HG3	1.80	0.47
1:A:105:ILE:HG22	1:A:118:LEU:HB3	1.97	0.47
1:A:312:ILE:HG22	1:A:598:ILE:HG23	1.96	0.47
1:A:559:PHE:CE1	1:A:584:ILE:CG1	2.97	0.47
1:A:748:GLU:O	1:A:752:LEU:HG	2.13	0.47
1:A:1091:ARG:NH2	1:A:1120:THR:O	2.48	0.47
1:B:103:GLY:HA3	1:B:119:ILE:O	2.14	0.47
1:B:870:ILE:O	1:B:874:THR:HG23	2.15	0.47
1:B:980:ILE:O	1:B:984:LEU:N	2.42	0.47
1:B:1081:ILE:CG1	1:B:1135:ASN:HB3	2.45	0.47
1:B:1107:ARG:HG2	1:C:904:TYR:CE1	2.50	0.47
1:C:450:ASN:ND2	2:D:54:ASP:H	2.12	0.47
1:C:450:ASN:HD22	2:D:54:ASP:H	1.63	0.47
1:C:533:LEU:HD22	1:C:578:ASP:OD2	2.15	0.47
1:C:578:ASP:C	1:C:580:GLN:H	2.23	0.47
1:C:578:ASP:N	1:C:583:GLU:O	2.29	0.47
1:C:897:PRO:HG3	1:C:900:MET:HG2	1.97	0.47
1:A:203:ILE:HD12	1:A:227:VAL:HB	1.97	0.47
1:A:994:ASP:O	1:A:997:ILE:HG22	2.15	0.47
1:B:40:ASP:O	1:B:41:LYS:NZ	2.42	0.47
1:B:44:ARG:O	1:B:283:GLY:HA2	2.14	0.47
1:B:933:LYS:NZ	1:B:933:LYS:CG	2.77	0.47
1:B:994:ASP:O	1:B:997:ILE:HG22	2.15	0.47
1:C:15:CYS:O	3:H:1:NAG:O7	2.33	0.47
1:C:111:ASP:HB3	1:C:134:GLN:NE2	2.30	0.47
1:C:330:PRO:C	1:C:332:ILE:N	2.73	0.47
1:C:454:ARG:CZ	1:C:492:LEU:HD13	2.45	0.47
1:C:1016:ALA:HA	1:C:1019:ARG:NH1	2.29	0.47
2:D:4:LEU:HD13	2:D:108:SER:HB3	1.96	0.47
2:D:99:VAL:HG11	2:D:102:PHE:CD2	2.49	0.47
1:A:96:GLU:OE2	1:A:101:ILE:HB	2.14	0.47
1:A:611:LEU:HB3	1:A:611:LEU:HD23	1.97	0.47
1:A:809:PRO:HA	1:A:814:LYS:HE2	1.97	0.47
1:A:884:SER:HG	1:A:887:THR:CB	2.25	0.47
1:B:31:SER:HB3	1:B:62:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ALA:HB3	1:B:414:GLN:HB2	1.96	0.47
1:B:702:GLU:OE1	1:B:702:GLU:N	2.48	0.47
1:B:1050:MET:CG	1:B:1051:SER:N	2.50	0.47
1:C:42:VAL:HG21	1:C:44:ARG:HE	1.80	0.47
1:C:96:GLU:OE2	1:C:101:ILE:HB	2.14	0.47
1:C:101:ILE:HD12	1:C:101:ILE:H	1.79	0.47
1:C:105:ILE:HG22	1:C:118:LEU:HB3	1.97	0.47
1:C:329:PHE:CE2	1:C:528:LYS:HB2	2.49	0.47
1:C:407:VAL:HG11	1:C:508:TYR:CD2	2.50	0.47
1:C:511:VAL:CG1	1:C:513:LEU:HD11	2.45	0.47
1:C:977:LEU:O	1:C:981:LEU:HG	2.14	0.47
3:G:1:NAG:HO3	3:G:2:NAG:C1	2.26	0.47
1:A:61:ASN:HD22	4:A:1306:NAG:H3	1.80	0.46
1:A:204:TYR:HA	1:A:224:GLU:O	2.15	0.46
1:A:403:ARG:H	1:A:406:GLU:HB2	1.80	0.46
1:A:977:LEU:O	1:A:981:LEU:HG	2.14	0.46
1:B:332:ILE:HD12	1:B:334:ASN:H	1.80	0.46
1:B:1024:LEU:HD11	1:B:1028:LYS:HE2	1.96	0.46
4:B:1312:NAG:O7	4:B:1312:NAG:C1	2.63	0.46
1:C:41:LYS:N	1:C:42:VAL:N	2.63	0.46
1:C:95:THR:N	1:C:264:ALA:O	2.36	0.46
1:C:327:VAL:CG2	1:C:530:SER:HA	2.45	0.46
1:C:350:VAL:HG13	1:C:351:TYR:N	2.30	0.46
1:C:531:THR:HG23	1:C:532:ASN:O	2.15	0.46
1:C:579:PRO:HG2	1:C:580:GLN:NE2	2.31	0.46
1:C:616:ASN:CG	4:C:1305:NAG:O7	2.59	0.46
1:C:770:ILE:O	1:C:774:GLN:OE1	2.33	0.46
1:C:1024:LEU:HD11	1:C:1028:LYS:HE2	1.96	0.46
1:A:44:ARG:HB3	1:A:279:TYR:CE2	2.50	0.46
1:A:101:ILE:H	1:A:101:ILE:HD12	1.79	0.46
1:A:818:ILE:O	1:A:822:LEU:HG	2.14	0.46
1:A:1081:ILE:CG1	1:A:1135:ASN:HB3	2.45	0.46
1:B:186:PHE:O	1:B:212:LEU:O	2.33	0.46
1:B:404:GLY:O	1:B:407:VAL:HG22	2.15	0.46
1:B:453:TYR:CE2	1:B:455:LEU:HD23	2.50	0.46
1:B:562:PHE:CG	1:C:41:LYS:HD3	2.50	0.46
1:B:715:PRO:HG2	1:B:1069:PRO:CB	2.44	0.46
1:B:1139:ASP:CG	1:B:1142:GLN:HE22	2.23	0.46
1:C:48:LEU:HD12	1:C:304:LYS:O	2.14	0.46
1:C:186:PHE:O	1:C:212:LEU:O	2.34	0.46
1:C:204:TYR:HA	1:C:224:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:900:MET:O	1:C:903:ALA:HB3	2.16	0.46
1:C:994:ASP:O	1:C:997:ILE:HG22	2.15	0.46
1:C:1050:MET:CG	1:C:1051:SER:H	2.21	0.46
1:A:213:VAL:HG13	1:A:214:ARG:H	1.80	0.46
1:A:312:ILE:HG21	1:A:312:ILE:HD13	1.64	0.46
1:A:743:CYS:HA	1:A:1000:ARG:NH1	2.31	0.46
1:B:44:ARG:HB3	1:B:279:TYR:CE2	2.50	0.46
1:C:31:SER:HB3	1:C:62:VAL:CG2	2.45	0.46
1:C:444:LYS:HB3	1:C:448:ASN:CA	2.45	0.46
1:C:473:TYR:HB2	1:C:491:PRO:CB	2.44	0.46
1:C:531:THR:HG23	1:C:532:ASN:N	2.30	0.46
1:C:594:GLY:CA	1:C:613:GLN:HG2	2.43	0.46
2:D:40:ALA:O	2:D:43:LYS:HG2	2.15	0.46
1:A:33:THR:H	1:A:58:PHE:HB3	1.80	0.46
1:A:111:ASP:HB3	1:A:134:GLN:NE2	2.30	0.46
1:A:143:VAL:HG21	1:A:179:LEU:HD23	1.98	0.46
1:A:572:THR:HG23	1:A:572:THR:O	2.13	0.46
1:A:870:ILE:O	1:A:874:THR:HG23	2.15	0.46
1:B:101:ILE:H	1:B:101:ILE:HD12	1.79	0.46
1:B:139:PRO:HB2	1:B:159:VAL:HA	1.98	0.46
1:B:143:VAL:HG21	1:B:179:LEU:HD23	1.98	0.46
1:B:381:GLY:O	1:B:382:VAL:HG13	2.15	0.46
1:C:320:VAL:CG2	1:C:590:CYS:SG	3.04	0.46
1:C:450:ASN:HD22	2:D:53:ALA:N	2.13	0.46
1:C:538:CYS:CB	1:C:551:VAL:HG22	2.45	0.46
1:C:656:VAL:HG12	1:C:657:ASN:H	1.80	0.46
1:C:965:GLN:O	1:C:968:SER:N	2.49	0.46
1:C:1091:ARG:NH2	1:C:1120:THR:O	2.48	0.46
1:A:17:ASN:N	3:E:2:NAG:O4	2.47	0.46
1:A:186:PHE:O	1:A:212:LEU:O	2.34	0.46
1:A:356:LYS:N	1:A:397:ALA:O	2.49	0.46
1:A:402:ILE:CD1	1:A:510:VAL:HG21	2.44	0.46
1:B:204:TYR:HA	1:B:224:GLU:O	2.15	0.46
1:B:358:ILE:HD11	1:B:397:ALA:HB3	1.96	0.46
1:B:714:ILE:HG22	1:B:715:PRO:CD	2.46	0.46
1:B:781:VAL:HG12	1:B:782:PHE:CG	2.51	0.46
1:B:809:PRO:HA	1:B:814:LYS:HE2	1.98	0.46
1:C:44:ARG:HB3	1:C:279:TYR:CE2	2.50	0.46
1:C:377:PHE:CD1	1:C:434:ILE:HD12	2.50	0.46
1:C:590:CYS:SG	1:C:590:CYS:O	2.74	0.46
1:C:903:ALA:HB1	1:C:913:GLN:CG	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:LYS:HB3	2:D:88:GLU:OE2	2.15	0.46
1:A:559:PHE:CE2	1:A:564:GLN:O	2.68	0.46
1:A:564:GLN:CD	1:B:41:LYS:HG2	2.41	0.46
1:A:656:VAL:HG12	1:A:657:ASN:H	1.80	0.46
1:A:703:ASN:CG	1:B:787:GLN:CG	2.88	0.46
1:A:770:ILE:O	1:A:774:GLN:OE1	2.33	0.46
1:B:33:THR:H	1:B:58:PHE:HB3	1.80	0.46
1:B:92:PHE:O	1:B:192:PHE:N	2.27	0.46
1:B:152:TRP:HB2	1:B:245:HIS:HE1	1.78	0.46
1:B:437:ASN:HA	1:B:508:TYR:HA	1.97	0.46
1:B:770:ILE:O	1:B:774:GLN:OE1	2.33	0.46
1:B:818:ILE:O	1:B:822:LEU:HG	2.14	0.46
1:B:897:PRO:HG3	1:B:900:MET:HG2	1.97	0.46
1:B:1106:GLN:HE22	1:B:1109:PHE:HB3	1.76	0.46
1:C:143:VAL:HG21	1:C:179:LEU:HD23	1.98	0.46
1:A:407:VAL:HG11	1:A:508:TYR:HD2	1.80	0.46
1:A:660:TYR:O	1:A:698:SER:N	2.47	0.46
1:A:759:PHE:HA	1:A:762:GLN:OE1	2.16	0.46
1:A:1076:THR:HG22	1:A:1097:SER:OG	2.16	0.46
1:A:1080:ALA:HB3	1:A:1132:ILE:HD12	1.98	0.46
1:B:64:TRP:HZ2	1:B:214:ARG:HG3	1.80	0.46
1:B:575:ALA:HA	1:B:585:LEU:O	2.15	0.46
1:B:1091:ARG:NH2	1:B:1120:THR:O	2.48	0.46
1:C:29:THR:HG22	1:C:64:TRP:HE3	1.76	0.46
1:C:220:PHE:CZ	1:C:287:ASP:CA	2.97	0.46
1:C:715:PRO:HB2	1:C:1070:ALA:O	2.15	0.46
1:C:781:VAL:HG12	1:C:782:PHE:CG	2.51	0.46
2:D:99:VAL:HG12	2:D:102:PHE:H	1.80	0.46
1:A:41:LYS:N	1:A:42:VAL:N	2.63	0.46
1:A:758:SER:HG	1:A:761:THR:HG1	1.62	0.46
1:B:42:VAL:HG21	1:B:44:ARG:HE	1.81	0.46
1:B:94:SER:N	1:B:190:ARG:O	2.42	0.46
1:B:97:LYS:NZ	1:B:185:ASN:O	2.41	0.46
1:B:111:ASP:C	1:B:134:GLN:HE22	2.21	0.46
1:B:213:VAL:HG13	1:B:214:ARG:H	1.80	0.46
1:B:486:PHE:HZ	1:C:377:PHE:O	1.98	0.46
1:B:715:PRO:HB2	1:B:1070:ALA:O	2.15	0.46
1:B:726:ILE:HD12	1:B:726:ILE:HA	1.54	0.46
1:B:1089:PHE:O	1:B:1121:PHE:N	2.42	0.46
1:C:30:ASN:C	1:C:30:ASN:OD1	2.59	0.46
1:C:490:PHE:CD1	2:D:105:THR:HG23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:HZ1	1:A:221:SER:HG	1.53	0.46
1:A:327:VAL:HG23	1:A:327:VAL:O	2.16	0.46
1:A:356:LYS:HG2	1:A:358:ILE:HD11	1.97	0.46
1:A:900:MET:O	1:A:903:ALA:HB3	2.16	0.46
1:B:127:VAL:HG11	4:B:1301:NAG:C1	2.46	0.46
1:B:723:THR:C	1:B:723:THR:CG2	2.87	0.46
1:B:884:SER:HG	1:B:887:THR:CB	2.26	0.46
1:B:983:ARG:O	1:B:984:LEU:HD23	2.16	0.46
1:B:1050:MET:CG	1:B:1051:SER:H	2.21	0.46
1:B:1076:THR:HG22	1:B:1097:SER:OG	2.16	0.46
1:C:22:THR:HG23	1:C:76:THR:CB	2.46	0.46
1:C:111:ASP:C	1:C:134:GLN:HE22	2.20	0.46
1:C:878:LEU:O	1:C:881:THR:OG1	2.33	0.46
1:C:1095:PHE:HB3	1:C:1115:ILE:CD1	2.46	0.46
1:A:49:HIS:NE2	1:A:51:THR:OG1	2.49	0.46
1:A:61:ASN:ND2	4:A:1306:NAG:H3	2.31	0.46
1:A:200:TYR:N	1:A:200:TYR:CD1	2.82	0.46
1:A:327:VAL:HG12	1:A:542:ASN:HB3	1.97	0.46
1:A:569:ILE:HG12	1:B:47:VAL:HG13	1.98	0.46
1:B:38:TYR:HD1	1:B:223:LEU:O	2.00	0.46
1:B:105:ILE:HG22	1:B:118:LEU:HB3	1.97	0.46
1:B:278:LYS:HB2	1:B:287:ASP:N	2.31	0.46
1:B:476:GLY:HA2	1:B:477[A]:SER:HB3	1.98	0.46
1:C:33:THR:H	1:C:58:PHE:HB3	1.80	0.46
1:C:38:TYR:HD1	1:C:223:LEU:O	1.99	0.46
1:C:119:ILE:HA	1:C:128:ILE:HG12	1.98	0.46
1:C:133:PHE:CD1	1:C:162:SER:N	2.84	0.46
1:C:213:VAL:HG13	1:C:214:ARG:H	1.80	0.46
1:C:759:PHE:HA	1:C:762:GLN:OE1	2.16	0.46
2:D:31:THR:HG21	2:D:34:LYS:CE	2.46	0.46
2:D:67:LEU:C	2:D:67:LEU:HD23	2.41	0.46
1:A:30:ASN:OD1	1:A:30:ASN:C	2.59	0.45
1:A:272:PRO:C	1:A:273:ARG:HD3	2.41	0.45
1:A:903:ALA:HB1	1:A:913:GLN:CG	2.44	0.45
1:A:1095:PHE:HB3	1:A:1115:ILE:CD1	2.46	0.45
1:B:119:ILE:HA	1:B:128:ILE:HG12	1.98	0.45
1:B:759:PHE:HA	1:B:762:GLN:OE1	2.16	0.45
1:B:900:MET:O	1:B:903:ALA:HB3	2.16	0.45
1:C:49:HIS:NE2	1:C:51:THR:OG1	2.49	0.45
1:C:124:THR:OG1	3:G:1:NAG:C7	2.64	0.45
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:TYR:O	1:C:698:SER:N	2.47	0.45
1:C:714:ILE:HG22	1:C:715:PRO:CD	2.46	0.45
1:C:870:ILE:O	1:C:874:THR:HG23	2.15	0.45
2:D:102:PHE:O	2:D:103:THR:C	2.59	0.45
3:G:2:NAG:O3	3:G:2:NAG:H82	2.17	0.45
1:A:42:VAL:HG21	1:A:44:ARG:HE	1.81	0.45
1:A:111:ASP:HB2	1:A:113:LYS:NZ	2.31	0.45
1:A:140:PHE:CD2	1:A:244:LEU:HD21	2.51	0.45
1:A:567:ARG:HG2	1:A:573:THR:HG23	1.97	0.45
1:A:715:PRO:HB2	1:A:1070:ALA:O	2.15	0.45
1:A:983:ARG:O	1:A:984:LEU:HD23	2.16	0.45
1:B:49:HIS:NE2	1:B:51:THR:OG1	2.49	0.45
1:C:450:ASN:HB3	2:D:52:THR:HB	1.98	0.45
1:C:1076:THR:HG22	1:C:1097:SER:OG	2.16	0.45
2:D:99:VAL:HG23	2:D:107:ASN:HB3	1.98	0.45
1:A:278:LYS:HB2	1:A:287:ASP:N	2.31	0.45
1:A:326:ILE:HD11	1:A:531:THR:OG1	2.16	0.45
1:A:455:LEU:HD11	1:A:493:GLN:HB2	1.98	0.45
1:A:551:VAL:HG12	1:A:590:CYS:HA	1.98	0.45
1:A:559:PHE:HA	1:B:43:PHE:CE1	2.49	0.45
1:A:1007:TYR:HA	1:A:1010:GLN:OE1	2.17	0.45
1:A:1052:PHE:CD1	1:A:1052:PHE:N	2.84	0.45
1:B:660:TYR:O	1:B:698:SER:N	2.47	0.45
1:C:48:LEU:CD2	1:C:278:LYS:CD	2.95	0.45
1:A:105:ILE:HG22	1:A:118:LEU:CB	2.47	0.45
1:A:748:GLU:HA	1:A:751:ASN:OD1	2.17	0.45
1:A:781:VAL:HG12	1:A:782:PHE:CG	2.51	0.45
1:A:1043:CYS:HA	1:A:1064:HIS:CE1	2.52	0.45
1:B:30:ASN:C	1:B:30:ASN:OD1	2.59	0.45
1:B:670:ILE:HD13	1:B:696:THR:HG23	1.99	0.45
1:B:1007:TYR:HA	1:B:1010:GLN:OE1	2.17	0.45
1:C:139:PRO:HB2	1:C:159:VAL:HA	1.98	0.45
1:C:233:ILE:HG23	1:C:234:ASN:N	2.32	0.45
1:C:916:LEU:HA	1:C:923:ILE:CD1	2.47	0.45
1:C:937:SER:C	1:C:941:THR:HG1	2.24	0.45
1:C:1080:ALA:HB3	1:C:1132:ILE:HD12	1.97	0.45
1:A:22:THR:HG23	1:A:76:THR:CB	2.46	0.45
1:A:233:ILE:HG23	1:A:234:ASN:N	2.32	0.45
1:A:310:LYS:HE2	1:A:664:ILE:HG12	1.99	0.45
1:A:350:VAL:HG23	1:A:418:ILE:HG23	1.98	0.45
1:A:670:ILE:HD13	1:A:696:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ILE:HG22	1:A:715:PRO:CD	2.46	0.45
1:B:34:ARG:NH2	1:B:218:GLN:C	2.74	0.45
1:B:41:LYS:N	1:B:42:VAL:N	2.63	0.45
1:B:49:HIS:O	1:B:277:LEU:HB2	2.16	0.45
1:B:111:ASP:HB3	1:B:134:GLN:NE2	2.30	0.45
1:B:272:PRO:C	1:B:273:ARG:HD3	2.41	0.45
1:B:567:ARG:H	1:C:42:VAL:HG12	1.81	0.45
1:B:1005:GLN:OE1	1:B:1005:GLN:O	2.34	0.45
1:C:310:LYS:HE2	1:C:664:ILE:HG12	1.99	0.45
1:C:461:LEU:H	1:C:461:LEU:HD22	1.82	0.45
2:D:3:GLN:C	2:D:4:LEU:HD12	2.42	0.45
1:A:34:ARG:NH2	1:A:218:GLN:C	2.74	0.45
1:A:220:PHE:HE2	1:A:287:ASP:HA	1.75	0.45
1:A:410:ILE:HD11	1:A:418:ILE:HB	1.98	0.45
1:A:461:LEU:HD23	1:A:462:LYS:O	2.17	0.45
1:A:965:GLN:O	1:A:968:SER:N	2.49	0.45
1:A:1005:GLN:OE1	1:A:1005:GLN:O	2.34	0.45
1:B:101:ILE:HG23	1:B:240:THR:OG1	2.17	0.45
1:B:326:ILE:HG23	1:B:531:THR:OG1	2.17	0.45
1:B:577:ARG:HE	4:B:1305:NAG:HO4	1.57	0.45
1:B:965:GLN:O	1:B:968:SER:N	2.49	0.45
1:B:1043:CYS:HA	1:B:1064:HIS:CE1	2.52	0.45
1:B:1095:PHE:HB3	1:B:1115:ILE:CD1	2.46	0.45
1:C:64:TRP:HZ2	1:C:214:ARG:HG3	1.80	0.45
1:C:726:ILE:HD12	1:C:726:ILE:HA	1.54	0.45
1:C:983:ARG:O	1:C:984:LEU:HD23	2.16	0.45
1:A:119:ILE:HA	1:A:128:ILE:HG12	1.99	0.45
1:A:747:THR:O	1:A:750:SER:OG	2.29	0.45
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.44	0.45
1:B:111:ASP:HB2	1:B:113:LYS:NZ	2.31	0.45
1:B:334:ASN:O	1:B:362:VAL:N	2.50	0.45
1:B:743:CYS:HA	1:B:1000:ARG:NH1	2.31	0.45
1:B:1052:PHE:N	1:B:1052:PHE:CD1	2.85	0.45
1:B:1080:ALA:HB3	1:B:1132:ILE:HD12	1.97	0.45
1:C:272:PRO:C	1:C:273:ARG:HD3	2.41	0.45
1:C:293:LEU:HD22	1:C:294:ASP:HB2	1.99	0.45
1:C:452:LEU:HD11	2:D:98:SER:CB	2.46	0.45
1:C:490:PHE:CE2	2:D:105:THR:HG23	2.52	0.45
1:C:774:GLN:NE2	1:C:774:GLN:C	2.74	0.45
1:A:48:LEU:CD2	1:A:278:LYS:CD	2.95	0.45
1:B:140:PHE:CD2	1:B:244:LEU:HD21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LYS:O	1:B:397:ALA:N	2.49	0.45
1:B:703:ASN:OD1	1:C:789:TYR:HA	2.16	0.45
1:B:740:MET:O	1:B:744:GLY:N	2.50	0.45
1:B:748:GLU:HA	1:B:751:ASN:OD1	2.17	0.45
1:B:916:LEU:HA	1:B:923:ILE:CD1	2.47	0.45
1:C:108:THR:HG23	1:C:235:ILE:HA	1.99	0.45
1:C:278:LYS:HB2	1:C:287:ASP:N	2.31	0.45
1:C:331:ASN:C	1:C:332:ILE:HG22	2.41	0.45
1:C:670:ILE:HD13	1:C:696:THR:HG23	1.99	0.45
1:C:906:PHE:O	1:C:910:GLY:N	2.50	0.45
1:C:1005:GLN:OE1	1:C:1005:GLN:O	2.34	0.45
1:A:49:HIS:O	1:A:277:LEU:HB2	2.17	0.45
1:A:139:PRO:HB2	1:A:159:VAL:HA	1.98	0.45
1:A:567:ARG:CB	1:B:44:ARG:NH2	2.79	0.45
1:A:906:PHE:O	1:A:910:GLY:N	2.50	0.45
1:A:916:LEU:HA	1:A:923:ILE:CD1	2.47	0.45
1:B:48:LEU:CD2	1:B:278:LYS:CD	2.95	0.45
1:B:130:VAL:HG11	1:B:168:PHE:H	1.79	0.45
1:B:293:LEU:HD22	1:B:294:ASP:HB2	1.99	0.45
1:B:310:LYS:HE2	1:B:664:ILE:HG12	1.99	0.45
1:B:567:ARG:N	1:C:42:VAL:HG12	2.32	0.45
1:B:701:ALA:O	1:C:788:ILE:O	2.35	0.45
1:C:34:ARG:NH2	1:C:218:GLN:C	2.74	0.45
1:C:41:LYS:CB	1:C:41:LYS:O	2.43	0.45
1:C:333:THR:HG23	1:C:362:VAL:CG1	2.47	0.45
1:C:409:GLN:HB3	1:C:418:ILE:HD12	1.98	0.45
1:C:451:TYR:O	2:D:32:CYS:SG	2.75	0.45
1:C:502:GLY:N	1:C:505:TYR:HB3	2.32	0.45
1:C:579:PRO:CB	1:C:580:GLN:NE2	2.77	0.45
1:C:1043:CYS:HA	1:C:1064:HIS:CE1	2.52	0.45
1:B:153:MET:CE	4:B:1302:NAG:C3	2.95	0.45
1:B:312:ILE:HD13	1:B:312:ILE:HG21	1.65	0.45
1:B:358:ILE:HD11	1:B:397:ALA:HB2	1.99	0.45
1:B:758:SER:HG	1:B:761:THR:HG1	1.62	0.45
1:C:111:ASP:HB2	1:C:113:LYS:NZ	2.31	0.45
1:C:452:LEU:HD13	2:D:33:ARG:CB	2.45	0.45
1:C:493:GLN:OE1	2:D:103:THR:OG1	2.20	0.45
1:C:723:THR:HG22	1:C:724:THR:N	2.32	0.45
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.41	0.45
1:C:794:ILE:HD11	1:C:796:ASP:CG	2.42	0.45
2:D:39:GLN:C	2:D:91:ALA:HB1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PHE:O	1:A:192:PHE:N	2.27	0.44
1:A:406:GLU:OE1	1:A:406:GLU:N	2.50	0.44
1:A:794:ILE:HD11	1:A:796:ASP:CG	2.42	0.44
1:B:105:ILE:HG22	1:B:118:LEU:CB	2.47	0.44
1:B:233:ILE:HG23	1:B:234:ASN:N	2.32	0.44
1:B:309:GLU:OE1	1:B:309:GLU:HA	2.17	0.44
1:B:656:VAL:HG12	1:B:657:ASN:H	1.80	0.44
1:B:723:THR:HG22	1:B:724:THR:N	2.32	0.44
1:B:906:PHE:O	1:B:910:GLY:N	2.50	0.44
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.44	0.44
1:C:49:HIS:O	1:C:277:LEU:HB2	2.17	0.44
1:C:92:PHE:O	1:C:192:PHE:N	2.27	0.44
1:C:131:CYS:HA	1:C:165:ASN:O	2.18	0.44
1:C:326:ILE:HG13	1:C:327:VAL:N	2.32	0.44
1:C:554:GLU:OE1	1:C:554:GLU:N	2.44	0.44
1:C:743:CYS:HA	1:C:1000:ARG:NH1	2.31	0.44
1:C:748:GLU:HA	1:C:751:ASN:OD1	2.17	0.44
1:A:105:ILE:N	1:A:239:GLN:O	2.39	0.44
1:A:246:ARG:HD3	1:A:258:TRP:CD1	2.53	0.44
1:A:291:CYS:SG	1:A:298:GLU:HA	2.57	0.44
1:A:861:LEU:HD22	1:A:861:LEU:H	1.83	0.44
1:A:980:ILE:O	1:A:984:LEU:N	2.42	0.44
1:B:80:ASP:OD2	1:B:80:ASP:C	2.60	0.44
1:B:611:LEU:HB3	1:B:611:LEU:HD23	1.97	0.44
1:B:703:ASN:N	1:C:788:ILE:O	2.49	0.44
1:B:856:ASN:OD1	1:B:858:LEU:N	2.38	0.44
1:C:444:LYS:HD3	1:C:445:VAL:O	2.17	0.44
1:C:747:THR:O	1:C:751:ASN:OD1	2.36	0.44
1:C:809:PRO:HA	1:C:814:LYS:HE2	1.98	0.44
1:C:1014:ARG:N	1:C:1014:ARG:CD	2.70	0.44
2:D:11:SER:HA	2:D:116:THR:HG22	1.98	0.44
1:A:38:TYR:HD1	1:A:223:LEU:O	1.99	0.44
1:A:914:ASN:O	1:A:918:GLU:N	2.50	0.44
1:B:102:ARG:HB3	1:B:121:ASN:O	2.17	0.44
1:B:143:VAL:HG11	1:B:245:HIS:HE1	1.82	0.44
1:B:246:ARG:HD3	1:B:258:TRP:CD1	2.53	0.44
1:B:731:MET:N	1:B:1058:HIS:HE1	2.15	0.44
1:B:794:ILE:HD11	1:B:796:ASP:CG	2.42	0.44
1:B:973:ILE:HG13	1:B:974:SER:N	2.32	0.44
1:B:1051:SER:C	1:B:1052:PHE:HD1	2.25	0.44
1:C:101:ILE:HG23	1:C:240:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:HG22	1:C:118:LEU:CB	2.47	0.44
1:C:140:PHE:CD2	1:C:244:LEU:HD21	2.51	0.44
1:C:275:PHE:CD1	1:C:289:VAL:O	2.70	0.44
1:C:511:VAL:HG12	1:C:513:LEU:CD1	2.46	0.44
1:A:68:ILE:O	1:A:77:LYS:HA	2.18	0.44
1:A:108:THR:HG23	1:A:235:ILE:HA	1.99	0.44
1:A:309:GLU:OE1	1:A:309:GLU:HA	2.17	0.44
1:A:444:LYS:O	1:A:497:PHE:O	2.36	0.44
1:A:517:LEU:HD23	1:A:518:LEU:N	2.32	0.44
1:A:723:THR:HG22	1:A:724:THR:N	2.32	0.44
1:A:1051:SER:C	1:A:1052:PHE:HD1	2.25	0.44
1:B:115:GLN:NE2	1:B:165:ASN:HB2	2.33	0.44
1:B:127:VAL:HG11	4:B:1301:NAG:O5	2.18	0.44
1:B:131:CYS:HA	1:B:165:ASN:O	2.18	0.44
1:C:102:ARG:HB3	1:C:121:ASN:O	2.17	0.44
1:C:206:LYS:NZ	1:C:221:SER:OG	2.25	0.44
1:C:449:TYR:N	2:D:53:ALA:CB	2.81	0.44
1:C:453:TYR:CD2	1:C:493:GLN:O	2.70	0.44
1:C:914:ASN:O	1:C:918:GLU:N	2.50	0.44
1:C:1007:TYR:HA	1:C:1010:GLN:OE1	2.17	0.44
1:C:1052:PHE:N	1:C:1052:PHE:CD1	2.85	0.44
1:A:275:PHE:CD1	1:A:289:VAL:O	2.70	0.44
1:A:368:LEU:HD23	1:A:368:LEU:C	2.41	0.44
1:A:723:THR:C	1:A:723:THR:CG2	2.87	0.44
1:A:740:MET:O	1:A:744:GLY:N	2.50	0.44
1:A:959:LEU:HA	1:A:1007:TYR:HE2	1.83	0.44
1:A:1071:GLN:NE2	1:A:1071:GLN:CA	2.81	0.44
1:B:64:TRP:CE2	1:B:266:TYR:OH	2.61	0.44
1:B:95:THR:N	1:B:264:ALA:O	2.36	0.44
1:B:108:THR:HG23	1:B:235:ILE:HA	1.99	0.44
1:B:747:THR:O	1:B:750:SER:OG	2.29	0.44
1:C:80:ASP:OD2	1:C:80:ASP:C	2.60	0.44
1:C:185:ASN:HB2	1:C:212:LEU:O	2.18	0.44
1:C:246:ARG:HD3	1:C:258:TRP:CD1	2.53	0.44
1:C:451:TYR:O	2:D:32:CYS:HB2	2.18	0.44
1:C:544:ASN:HB3	1:C:579:PRO:HB3	1.99	0.44
1:C:994:ASP:C	1:C:994:ASP:OD1	2.61	0.44
1:C:1107:ARG:HD2	1:C:1107:ARG:N	2.33	0.44
1:A:101:ILE:HG23	1:A:240:THR:OG1	2.17	0.44
1:A:185:ASN:HB2	1:A:212:LEU:O	2.18	0.44
1:A:298:GLU:O	1:A:302:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:PHE:CD1	1:B:162:SER:N	2.85	0.44
1:B:402:ILE:O	1:B:508:TYR:N	2.29	0.44
1:B:562:PHE:CZ	1:C:41:LYS:HE2	2.52	0.44
1:B:577:ARG:HG3	1:B:584:ILE:HD13	1.99	0.44
1:C:68:ILE:O	1:C:77:LYS:HA	2.18	0.44
1:C:298:GLU:O	1:C:302:THR:HG23	2.17	0.44
1:C:452:LEU:HD11	2:D:33:ARG:CB	2.47	0.44
1:C:515:PHE:N	1:C:515:PHE:CD1	2.82	0.44
1:C:559:PHE:HB3	1:C:577:ARG:NH2	2.32	0.44
1:C:740:MET:O	1:C:744:GLY:N	2.50	0.44
1:C:1051:SER:C	1:C:1052:PHE:HD1	2.25	0.44
1:C:1119:ASN:OD1	1:C:1119:ASN:N	2.51	0.44
2:D:38:ARG:HG2	2:D:48:VAL:HG23	2.00	0.44
1:A:565:PHE:CZ	1:B:42:VAL:HG12	2.52	0.44
1:B:1071:GLN:NE2	1:B:1071:GLN:CA	2.81	0.44
1:B:1119:ASN:OD1	1:B:1119:ASN:N	2.51	0.44
1:C:389:ASP:C	1:C:390:LEU:HD12	2.42	0.44
1:C:482:GLY:HA3	2:D:44:GLU:HG3	2.00	0.44
1:C:611:LEU:HB3	1:C:611:LEU:HD23	1.97	0.44
1:C:861:LEU:HD22	1:C:861:LEU:H	1.83	0.44
1:C:959:LEU:HA	1:C:1007:TYR:HE2	1.83	0.44
1:C:1071:GLN:NE2	1:C:1071:GLN:CA	2.81	0.44
1:A:102:ARG:HB3	1:A:121:ASN:O	2.17	0.44
1:B:40:ASP:C	1:B:41:LYS:HZ3	2.25	0.44
1:B:48:LEU:CD2	1:B:278:LYS:NZ	2.81	0.44
1:B:275:PHE:CD1	1:B:289:VAL:O	2.70	0.44
1:B:959:LEU:HA	1:B:1007:TYR:HE2	1.83	0.44
1:B:1107:ARG:N	1:B:1107:ARG:HD2	2.33	0.44
1:C:765:ARG:HH11	1:C:765:ARG:HD2	1.35	0.44
1:A:115:GLN:NE2	1:A:165:ASN:HB2	2.33	0.44
1:A:131:CYS:HA	1:A:165:ASN:O	2.18	0.44
1:A:1107:ARG:N	1:A:1107:ARG:HD2	2.33	0.44
1:B:22:THR:HG23	1:B:76:THR:CB	2.46	0.44
1:B:68:ILE:O	1:B:77:LYS:HA	2.18	0.44
1:B:151:SER:HB3	4:B:1302:NAG:H61	2.00	0.44
1:B:861:LEU:H	1:B:861:LEU:HD22	1.83	0.44
1:B:914:ASN:O	1:B:918:GLU:N	2.50	0.44
1:C:433:VAL:HG13	1:C:433:VAL:O	2.16	0.44
1:C:452:LEU:CB	2:D:104:CYS:HB3	2.48	0.44
1:A:48:LEU:CD2	1:A:278:LYS:NZ	2.81	0.43
1:A:293:LEU:HD22	1:A:294:ASP:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ASN:OD1	1:A:395:VAL:N	2.51	0.43
1:B:90:VAL:O	1:B:193:VAL:HA	2.18	0.43
1:B:185:ASN:HB2	1:B:212:LEU:O	2.18	0.43
1:B:291:CYS:SG	1:B:298:GLU:HA	2.57	0.43
1:B:490:PHE:CD2	1:B:492:LEU:HD13	2.53	0.43
1:B:1052:PHE:N	1:B:1052:PHE:HD1	2.16	0.43
1:C:209:PRO:O	1:C:210:ILE:HD13	2.18	0.43
1:C:291:CYS:SG	1:C:298:GLU:HA	2.57	0.43
1:C:581:THR:OG1	1:C:583:GLU:HG3	2.18	0.43
1:C:733:LYS:HG3	1:C:733:LYS:O	2.18	0.43
1:C:980:ILE:O	1:C:984:LEU:N	2.42	0.43
1:A:80:ASP:OD2	1:A:80:ASP:C	2.60	0.43
1:A:563:GLN:HE22	1:B:283:GLY:HA3	1.83	0.43
1:A:714:ILE:CG2	1:A:715:PRO:CD	2.96	0.43
1:A:731:MET:N	1:A:1058:HIS:HE1	2.15	0.43
1:A:973:ILE:HG13	1:A:974:SER:N	2.32	0.43
1:B:344:ALA:CB	1:B:509:ARG:HE	2.30	0.43
1:B:699:LEU:H	1:B:699:LEU:HG	1.66	0.43
1:B:730:SER:HB2	1:B:1058:HIS:CE1	2.53	0.43
1:B:747:THR:O	1:B:751:ASN:OD1	2.36	0.43
1:B:806:LEU:HB3	1:B:807:PRO:HD2	2.00	0.43
1:B:1050:MET:HB3	1:B:1065:VAL:HB	2.00	0.43
1:C:714:ILE:CG2	1:C:715:PRO:CD	2.96	0.43
2:D:67:LEU:HD11	2:D:80:LEU:CG	2.47	0.43
1:A:41:LYS:CG	1:C:562:PHE:C	2.65	0.43
1:A:920:GLN:HA	1:A:923:ILE:CG1	2.42	0.43
1:B:141:LEU:N	1:B:141:LEU:HD23	2.34	0.43
1:B:559:PHE:C	1:B:563:GLN:HG3	2.43	0.43
1:C:758:SER:HG	1:C:761:THR:HG1	1.61	0.43
1:C:1050:MET:HB3	1:C:1065:VAL:HB	2.00	0.43
1:A:41:LYS:HB2	1:C:563:GLN:HA	2.00	0.43
1:A:78:ARG:HD2	1:A:78:ARG:HA	1.10	0.43
1:A:90:VAL:O	1:A:193:VAL:HA	2.18	0.43
1:A:143:VAL:HG11	1:A:245:HIS:HE1	1.82	0.43
1:B:68:ILE:O	1:B:77:LYS:C	2.62	0.43
1:B:204:TYR:CE1	1:B:225:PRO:HB3	2.54	0.43
1:B:350:VAL:HG23	1:B:400:PHE:CD2	2.53	0.43
1:B:920:GLN:HA	1:B:923:ILE:CG1	2.42	0.43
1:B:984:LEU:HD22	1:B:988:GLU:OE2	2.18	0.43
1:C:657:ASN:CG	4:C:1306:NAG:H5	2.43	0.43
1:C:747:THR:O	1:C:750:SER:OG	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:856:ASN:OD1	1:C:858:LEU:N	2.38	0.43
1:C:925:ASN:O	1:C:928:ASN:OD1	2.37	0.43
1:C:1005:GLN:C	1:C:1005:GLN:CD	2.86	0.43
2:D:4:LEU:HD23	2:D:95:CYS:SG	2.58	0.43
2:D:22:CYS:HB3	2:D:78:VAL:HG23	1.99	0.43
1:A:61:ASN:ND2	4:A:1306:NAG:C1	2.81	0.43
1:A:209:PRO:O	1:A:210:ILE:HD13	2.18	0.43
1:A:379:CYS:HA	1:A:432:CYS:HA	1.99	0.43
1:A:553:THR:HG22	1:A:588:THR:HG21	2.01	0.43
1:A:925:ASN:O	1:A:928:ASN:OD1	2.37	0.43
1:B:356:LYS:N	1:B:397:ALA:O	2.49	0.43
1:B:538:CYS:N	1:B:551:VAL:HG22	2.34	0.43
1:C:68:ILE:O	1:C:77:LYS:C	2.62	0.43
1:C:309:GLU:OE1	1:C:309:GLU:HA	2.17	0.43
1:C:517:LEU:HD12	1:C:518:LEU:H	1.84	0.43
1:C:707:TYR:CG	1:C:708:SER:N	2.85	0.43
1:C:1052:PHE:N	1:C:1052:PHE:HD1	2.16	0.43
2:D:82:MET:HE1	2:D:115:VAL:HG11	2.01	0.43
1:A:22:THR:HG23	1:A:76:THR:CG2	2.48	0.43
1:A:35:GLY:O	1:A:55:PHE:CD2	2.71	0.43
1:A:68:ILE:O	1:A:77:LYS:C	2.62	0.43
1:A:560:LEU:HD12	1:A:562:PHE:HE1	1.84	0.43
1:A:578:ASP:O	1:A:582:LEU:N	2.50	0.43
1:A:747:THR:O	1:A:751:ASN:OD1	2.35	0.43
1:A:1050:MET:CG	1:A:1051:SER:H	2.21	0.43
1:A:1089:PHE:O	1:A:1121:PHE:N	2.42	0.43
1:B:22:THR:HG23	1:B:76:THR:CG2	2.48	0.43
1:B:199:GLY:O	1:B:229:LEU:O	2.37	0.43
1:B:324:GLU:H	1:B:539:VAL:HB	1.84	0.43
1:B:714:ILE:CG2	1:B:715:PRO:CD	2.96	0.43
1:C:48:LEU:CD2	1:C:278:LYS:NZ	2.81	0.43
1:C:115:GLN:NE2	1:C:165:ASN:HB2	2.33	0.43
1:C:255:SER:CA	1:C:258:TRP:HE1	2.32	0.43
1:C:591:SER:O	1:C:592:PHE:HB3	2.18	0.43
1:C:927:PHE:CD1	1:C:927:PHE:C	2.97	0.43
1:A:199:GLY:O	1:A:229:LEU:O	2.37	0.43
1:A:557:LYS:O	1:A:584:ILE:HG21	2.19	0.43
1:A:872:GLN:OE1	1:C:699:LEU:HD13	2.19	0.43
1:B:299:THR:HG22	1:B:597:VAL:HG21	2.01	0.43
1:B:865:LEU:O	1:B:870:ILE:HD11	2.19	0.43
1:B:994:ASP:C	1:B:994:ASP:OD1	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:VAL:O	1:C:193:VAL:HA	2.19	0.43
1:C:246:ARG:HD2	1:C:253:ASP:O	2.19	0.43
1:C:255:SER:C	1:C:258:TRP:HE1	2.26	0.43
1:C:454:ARG:HE	1:C:492:LEU:HD13	1.83	0.43
1:C:973:ILE:HG13	1:C:974:SER:N	2.32	0.43
1:A:255:SER:CA	1:A:258:TRP:HE1	2.32	0.43
1:A:358:ILE:HD12	1:A:395:VAL:O	2.18	0.43
1:A:367:VAL:O	1:A:371:SER:OG	2.32	0.43
1:A:567:ARG:CG	1:B:44:ARG:NH2	2.82	0.43
1:A:730:SER:HB2	1:A:1058:HIS:CE1	2.53	0.43
1:A:984:LEU:HD22	1:A:988:GLU:OE2	2.18	0.43
1:B:255:SER:C	1:B:258:TRP:HE1	2.26	0.43
1:B:298:GLU:O	1:B:302:THR:HG23	2.18	0.43
1:B:476:GLY:CA	1:B:477[A]:SER:HB3	2.49	0.43
1:B:568:ASP:HA	1:C:44:ARG:NH2	2.34	0.43
1:B:774:GLN:NE2	1:B:774:GLN:C	2.74	0.43
1:C:152:TRP:HE3	1:C:245:HIS:CG	2.34	0.43
1:C:580:GLN:OE1	1:C:580:GLN:CA	2.67	0.43
2:D:92:VAL:O	2:D:92:VAL:HG13	2.18	0.43
1:A:95:THR:N	1:A:264:ALA:O	2.36	0.43
1:A:352:ALA:O	1:A:353:TRP:C	2.61	0.43
1:A:533:LEU:HD12	1:A:534:VAL:N	2.34	0.43
1:A:573:THR:HB	1:A:587:ILE:HD13	2.01	0.43
1:A:733:LYS:HG3	1:A:733:LYS:O	2.18	0.43
1:A:805:ILE:CA	1:A:816:SER:HB2	2.49	0.43
1:A:927:PHE:CD1	1:A:927:PHE:C	2.97	0.43
1:C:22:THR:HG23	1:C:76:THR:CG2	2.48	0.43
1:C:143:VAL:CG1	1:C:245:HIS:ND1	2.82	0.43
1:C:449:TYR:O	1:C:449:TYR:CD1	2.72	0.43
1:C:699:LEU:H	1:C:699:LEU:HG	1.66	0.43
1:C:714:ILE:HG21	1:C:1109:PHE:O	2.19	0.43
1:C:723:THR:C	1:C:723:THR:CG2	2.87	0.43
1:C:730:SER:CB	1:C:1058:HIS:CE1	3.02	0.43
1:C:781:VAL:HG12	1:C:782:PHE:CD1	2.54	0.43
1:C:805:ILE:CA	1:C:816:SER:HB2	2.49	0.43
1:C:984:LEU:HD22	1:C:988:GLU:OE2	2.18	0.43
1:C:1116:THR:HB	1:C:1119:ASN:OD1	2.19	0.43
1:C:1142:GLN:N	1:C:1143:PRO:CD	2.82	0.43
1:A:44:ARG:O	1:A:279:TYR:CB	2.67	0.43
1:A:204:TYR:CE1	1:A:225:PRO:HB3	2.54	0.43
1:B:1014:ARG:N	1:B:1014:ARG:CD	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.82	0.43
1:C:35:GLY:O	1:C:55:PHE:CD2	2.72	0.43
1:C:78:ARG:HD2	1:C:78:ARG:HA	1.10	0.43
1:C:513:LEU:HD22	1:C:513:LEU:N	2.34	0.43
1:C:730:SER:HB2	1:C:1058:HIS:CE1	2.53	0.43
1:C:865:LEU:O	1:C:870:ILE:HD11	2.19	0.43
1:C:942:PRO:O	1:C:942:PRO:CD	2.67	0.43
1:A:564:GLN:O	1:A:577:ARG:N	2.48	0.42
1:A:781:VAL:HG12	1:A:782:PHE:CD1	2.54	0.42
1:A:1116:THR:HB	1:A:1119:ASN:OD1	2.19	0.42
1:A:1119:ASN:OD1	1:A:1119:ASN:N	2.51	0.42
1:A:1142:GLN:CD	1:A:1142:GLN:H	2.27	0.42
1:B:33:THR:O	1:B:34:ARG:HD3	2.19	0.42
1:B:255:SER:CA	1:B:258:TRP:HE1	2.32	0.42
1:B:332:ILE:HD11	1:B:362:VAL:HG13	2.01	0.42
1:B:434:ILE:O	1:B:510:VAL:HA	2.19	0.42
1:B:473:TYR:HB2	1:B:491:PRO:HB3	2.00	0.42
1:B:781:VAL:HG12	1:B:782:PHE:CD1	2.54	0.42
1:B:805:ILE:CA	1:B:816:SER:HB2	2.49	0.42
1:B:927:PHE:C	1:B:927:PHE:CD1	2.97	0.42
1:B:1039:ARG:NH2	1:B:1042:PHE:CD1	2.87	0.42
1:B:1143:PRO:O	1:B:1146:ASP:O	2.37	0.42
1:C:44:ARG:O	1:C:279:TYR:CB	2.67	0.42
1:C:143:VAL:HG11	1:C:245:HIS:HE1	1.82	0.42
1:C:199:GLY:O	1:C:229:LEU:O	2.37	0.42
1:A:109:THR:C	1:A:111:ASP:N	2.77	0.42
1:A:143:VAL:CG1	1:A:245:HIS:ND1	2.82	0.42
1:A:730:SER:CB	1:A:1058:HIS:CE1	3.02	0.42
1:A:806:LEU:HB3	1:A:807:PRO:HD2	2.00	0.42
1:A:1143:PRO:O	1:A:1146:ASP:O	2.38	0.42
1:B:35:GLY:O	1:B:55:PHE:CD2	2.71	0.42
1:B:486:PHE:CE2	1:C:377:PHE:HB2	2.54	0.42
1:B:942:PRO:O	1:B:942:PRO:CD	2.67	0.42
1:C:33:THR:O	1:C:34:ARG:HD3	2.19	0.42
1:C:299:THR:HG22	1:C:597:VAL:HG21	2.01	0.42
1:C:405:ASP:O	1:C:409:GLN:NE2	2.52	0.42
1:C:407:VAL:HG11	1:C:508:TYR:CG	2.54	0.42
1:A:56:LEU:HD13	1:A:269:TYR:O	2.20	0.42
1:A:141:LEU:N	1:A:141:LEU:HD23	2.34	0.42
1:A:152:TRP:HE3	1:A:245:HIS:CG	2.33	0.42
1:A:246:ARG:HD2	1:A:253:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:ASN:HA	1:A:644:GLN:HE22	1.84	0.42
1:A:808:ASP:HB3	1:A:812:PRO:HD2	2.02	0.42
1:A:1052:PHE:N	1:A:1052:PHE:HD1	2.16	0.42
1:B:44:ARG:O	1:B:279:TYR:CB	2.67	0.42
1:B:714:ILE:HG21	1:B:1109:PHE:O	2.19	0.42
1:B:971:GLY:H	1:C:756:TYR:HA	1.84	0.42
1:C:352:ALA:O	1:C:353:TRP:C	2.60	0.42
1:C:418:ILE:HG22	1:C:423:TYR:O	2.20	0.42
1:C:544:ASN:ND2	1:C:579:PRO:HB3	2.33	0.42
1:C:865:LEU:HA	1:C:869:MET:SD	2.60	0.42
2:D:59:TYR:CE1	2:D:69:ILE:HG22	2.54	0.42
1:A:33:THR:O	1:A:34:ARG:HD3	2.19	0.42
1:A:299:THR:HG22	1:A:597:VAL:HG21	2.01	0.42
1:A:457:ARG:HD3	1:A:457:ARG:HA	1.93	0.42
1:A:468:ILE:HG22	1:A:468:ILE:O	2.19	0.42
1:A:533:LEU:HD11	1:A:535:LYS:CE	2.50	0.42
1:A:1142:GLN:N	1:A:1143:PRO:CD	2.82	0.42
1:B:233:ILE:HG21	1:B:233:ILE:HD13	1.80	0.42
1:B:339:GLY:O	1:B:343:ASN:N	2.27	0.42
1:B:383:SER:HB3	1:B:386:LYS:CE	2.49	0.42
1:B:733:LYS:HG3	1:B:733:LYS:O	2.18	0.42
1:B:985:ASP:OD2	1:B:988:GLU:HG2	2.20	0.42
1:B:1110:TYR:CE1	1:B:1112:PRO:CG	3.00	0.42
1:B:1116:THR:HB	1:B:1119:ASN:OD1	2.19	0.42
4:B:1304:NAG:H83	4:B:1304:NAG:H3	2.01	0.42
1:C:141:LEU:HD23	1:C:141:LEU:N	2.34	0.42
1:C:204:TYR:CE1	1:C:225:PRO:HB3	2.54	0.42
1:C:941:THR:CG2	1:C:944:ALA:HB2	2.50	0.42
1:C:1039:ARG:NH2	1:C:1042:PHE:CD1	2.87	0.42
1:C:1083:HIS:HB3	1:C:1088:HIS:NE2	2.34	0.42
1:C:1097:SER:HA	1:C:1101:HIS:O	2.20	0.42
1:C:1110:TYR:CE1	1:C:1112:PRO:CG	3.00	0.42
2:D:105:THR:HG22	2:D:106:PHE:N	2.34	0.42
1:A:92:PHE:C	1:A:92:PHE:CD1	2.98	0.42
1:A:255:SER:C	1:A:258:TRP:HE1	2.26	0.42
1:A:1039:ARG:NH2	1:A:1042:PHE:CD1	2.87	0.42
1:B:125:ASN:ND2	1:B:172:SER:O	2.46	0.42
1:B:143:VAL:O	1:B:246:ARG:N	2.53	0.42
1:B:246:ARG:HD2	1:B:253:ASP:O	2.19	0.42
1:B:340:GLU:O	1:B:344:ALA:HA	2.19	0.42
1:B:1083:HIS:HB3	1:B:1088:HIS:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:HH12	1:C:580:GLN:HG2	1.84	0.42
1:C:390:LEU:HD12	1:C:390:LEU:N	2.35	0.42
1:C:451:TYR:CD2	2:D:100:LYS:NZ	2.86	0.42
1:C:577:ARG:O	1:C:578:ASP:C	2.63	0.42
1:C:731:MET:N	1:C:1058:HIS:HE1	2.15	0.42
1:C:923:ILE:HA	1:C:926:GLN:CD	2.45	0.42
1:C:1142:GLN:H	1:C:1142:GLN:CD	2.28	0.42
2:D:99:VAL:HB	2:D:107:ASN:CB	2.49	0.42
1:A:755:GLN:O	1:C:969:ASN:HB2	2.19	0.42
1:A:865:LEU:HA	1:A:869:MET:SD	2.60	0.42
1:A:933:LYS:HB2	1:A:933:LYS:HE3	1.82	0.42
1:A:942:PRO:O	1:A:942:PRO:CD	2.67	0.42
1:B:92:PHE:HD1	1:B:92:PHE:C	2.28	0.42
1:B:143:VAL:CG1	1:B:245:HIS:ND1	2.82	0.42
1:B:730:SER:CB	1:B:1058:HIS:CE1	3.02	0.42
1:B:941:THR:CG2	1:B:944:ALA:HB2	2.50	0.42
1:B:949:GLN:O	1:B:953:ASN:ND2	2.40	0.42
1:B:1097:SER:HA	1:B:1101:HIS:O	2.20	0.42
1:B:1138:TYR:CD1	1:B:1138:TYR:C	2.97	0.42
1:C:21:ARG:HG2	1:C:21:ARG:O	2.19	0.42
1:C:385:THR:O	1:C:386:LYS:HG2	2.20	0.42
1:C:450:ASN:O	1:C:452:LEU:HD12	2.20	0.42
1:C:453:TYR:CZ	1:C:495:TYR:CE1	3.07	0.42
1:C:715:PRO:HG2	1:C:1069:PRO:HB2	2.02	0.42
1:C:806:LEU:HB3	1:C:807:PRO:HD2	2.00	0.42
1:C:1143:PRO:O	1:C:1146:ASP:O	2.38	0.42
1:A:206:LYS:NZ	1:A:221:SER:OG	2.25	0.42
1:A:726:ILE:HD12	1:A:726:ILE:HA	1.54	0.42
1:A:1050:MET:HB3	1:A:1065:VAL:HB	2.00	0.42
1:B:454:ARG:HA	1:B:491:PRO:O	2.20	0.42
1:B:569:ILE:O	1:B:570:ALA:HB3	2.20	0.42
1:B:715:PRO:HG2	1:B:1069:PRO:HB2	2.02	0.42
1:B:817:PHE:O	1:B:821:LEU:HG	2.20	0.42
1:B:923:ILE:HA	1:B:926:GLN:CD	2.45	0.42
1:B:1005:GLN:C	1:B:1005:GLN:CD	2.86	0.42
1:C:50:SER:O	1:C:51:THR:OG1	2.34	0.42
1:C:530:SER:OG	1:C:531:THR:N	2.52	0.42
1:C:808:ASP:HB3	1:C:812:PRO:HD2	2.02	0.42
1:A:29:THR:HG22	1:A:64:TRP:HE3	1.76	0.42
1:A:199:GLY:HA2	1:A:232:GLY:CA	2.50	0.42
1:A:715:PRO:HG2	1:A:1069:PRO:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:LEU:O	1:A:870:ILE:HD11	2.19	0.42
1:A:994:ASP:C	1:A:994:ASP:OD1	2.61	0.42
1:B:21:ARG:O	1:B:21:ARG:HG2	2.20	0.42
1:B:56:LEU:HD13	1:B:269:TYR:O	2.20	0.42
1:B:92:PHE:C	1:B:92:PHE:CD1	2.98	0.42
1:B:109:THR:C	1:B:111:ASP:N	2.78	0.42
1:B:209:PRO:O	1:B:210:ILE:HD13	2.18	0.42
1:B:319:ARG:HH12	1:C:745:ASP:CG	2.28	0.42
1:B:352:ALA:HB2	1:B:468:ILE:HD12	2.01	0.42
1:B:925:ASN:O	1:B:928:ASN:OD1	2.37	0.42
1:C:30:ASN:HA	1:C:61:ASN:HA	2.02	0.42
1:C:127:VAL:CG1	3:G:1:NAG:C1	2.98	0.42
1:C:143:VAL:O	1:C:246:ARG:N	2.53	0.42
1:C:496:GLY:C	2:D:100:LYS:NZ	2.78	0.42
1:C:1056:ALA:HB3	1:C:1059:GLY:C	2.45	0.42
2:D:40:ALA:HB3	2:D:43:LYS:CG	2.50	0.42
1:A:30:ASN:HA	1:A:61:ASN:HA	2.02	0.42
1:A:61:ASN:HD22	4:A:1306:NAG:H5	1.85	0.42
1:A:187:LYS:HB3	1:A:187:LYS:HE3	1.85	0.42
1:A:565:PHE:C	1:B:43:PHE:H	2.19	0.42
1:A:1138:TYR:CD1	1:A:1138:TYR:C	2.97	0.42
1:B:146:HIS:ND1	1:B:151:SER:O	2.39	0.42
1:B:563:GLN:HG2	1:C:41:LYS:HG3	2.01	0.42
1:B:756:TYR:HD1	1:B:756:TYR:O	2.03	0.42
1:B:865:LEU:HA	1:B:869:MET:SD	2.60	0.42
1:C:122:ASN:OD1	3:G:1:NAG:O7	2.38	0.42
1:C:540:ASN:HA	1:C:549:THR:HG22	2.02	0.42
1:C:579:PRO:HG2	1:C:580:GLN:HE21	1.84	0.42
1:C:584:ILE:HD12	1:C:584:ILE:O	2.19	0.42
1:C:987:PRO:O	1:C:990:GLU:HG2	2.20	0.42
1:A:143:VAL:O	1:A:246:ARG:N	2.53	0.42
1:A:566:GLY:O	1:A:573:THR:HA	2.20	0.42
1:A:1097:SER:HA	1:A:1101:HIS:O	2.20	0.42
1:B:152:TRP:HB3	1:B:245:HIS:CE1	2.54	0.42
1:B:361:CYS:O	1:B:524:VAL:HG23	2.20	0.42
1:B:616:ASN:HA	1:B:644:GLN:HE22	1.85	0.42
1:B:1142:GLN:H	1:B:1142:GLN:CD	2.28	0.42
1:C:92:PHE:C	1:C:92:PHE:HD1	2.28	0.42
1:C:164:ASN:OD1	1:C:165:ASN:OD1	2.38	0.42
1:C:200:TYR:HA	1:C:229:LEU:O	2.20	0.42
1:C:343:ASN:N	1:C:343:ASN:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ILE:HG21	1:A:1109:PHE:O	2.19	0.41
1:A:922:LEU:O	1:A:925:ASN:HB2	2.19	0.41
1:B:453:TYR:CD1	1:B:493:GLN:O	2.73	0.41
1:B:563:GLN:CD	1:C:41:LYS:CB	2.92	0.41
1:B:922:LEU:O	1:B:925:ASN:HB2	2.19	0.41
1:B:937:SER:C	1:B:941:THR:HG1	2.27	0.41
1:C:1089:PHE:O	1:C:1121:PHE:N	2.42	0.41
2:D:52:THR:HG21	2:D:56:ALA:HB3	2.01	0.41
1:A:231:ILE:HA	1:A:231:ILE:HG23	1.96	0.41
1:A:393:THR:OG1	1:A:516:GLU:OE1	2.37	0.41
1:A:774:GLN:NE2	1:A:774:GLN:C	2.74	0.41
1:B:326:ILE:HG21	1:B:533:LEU:HA	2.01	0.41
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.41	0.41
1:C:756:TYR:O	1:C:756:TYR:HD1	2.03	0.41
2:D:38:ARG:NE	2:D:46:GLU:OE2	2.53	0.41
1:A:133:PHE:CD1	1:A:162:SER:N	2.84	0.41
1:A:453:TYR:HE2	1:A:495:TYR:N	2.18	0.41
1:A:565:PHE:O	1:B:42:VAL:CA	2.69	0.41
1:A:817:PHE:O	1:A:821:LEU:HG	2.20	0.41
1:A:987:PRO:O	1:A:990:GLU:HG2	2.20	0.41
1:B:30:ASN:HA	1:B:61:ASN:HA	2.02	0.41
1:B:152:TRP:HE3	1:B:245:HIS:CG	2.33	0.41
1:B:352:ALA:O	1:B:353:TRP:C	2.63	0.41
1:B:486:PHE:HE2	1:C:377:PHE:HB2	1.86	0.41
1:B:779:GLN:O	1:B:783:ALA:HB3	2.20	0.41
1:B:1107:ARG:CG	1:C:904:TYR:CE1	3.04	0.41
1:C:56:LEU:HD13	1:C:269:TYR:O	2.20	0.41
1:C:199:GLY:HA2	1:C:232:GLY:CA	2.50	0.41
1:C:539:VAL:HB	1:C:552:LEU:HD11	2.02	0.41
1:A:32:PHE:CZ	1:A:216:LEU:HB2	2.55	0.41
1:A:104:TRP:CZ2	1:A:192:PHE:CE2	3.09	0.41
1:A:195:LYS:HE3	1:A:202:LYS:HZ1	1.85	0.41
1:A:200:TYR:HA	1:A:229:LEU:O	2.20	0.41
1:A:443:SER:HG	1:A:498:GLN:C	2.26	0.41
1:A:699:LEU:CD1	1:B:872:GLN:CD	2.93	0.41
1:A:1056:ALA:HB3	1:A:1059:GLY:C	2.45	0.41
1:B:117:LEU:HD13	1:B:130:VAL:HB	2.03	0.41
1:B:574:ASP:CA	1:B:587:ILE:HD13	2.51	0.41
1:B:963:VAL:HA	1:B:966:LEU:HD22	2.03	0.41
1:B:1056:ALA:HB3	1:B:1059:GLY:C	2.45	0.41
1:C:92:PHE:C	1:C:92:PHE:CD1	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ASN:ND2	3:G:1:NAG:C7	2.82	0.41
1:C:444:LYS:HB3	1:C:448:ASN:HA	2.02	0.41
1:C:461:LEU:HD13	1:C:461:LEU:N	2.35	0.41
1:C:569:ILE:HD12	1:C:569:ILE:N	2.36	0.41
1:C:616:ASN:HA	1:C:644:GLN:HE22	1.85	0.41
1:C:922:LEU:O	1:C:925:ASN:HB2	2.19	0.41
1:C:985:ASP:OD2	1:C:988:GLU:HG2	2.19	0.41
1:A:21:ARG:O	1:A:21:ARG:HG2	2.20	0.41
1:A:43:PHE:CZ	1:C:559:PHE:CD1	3.08	0.41
1:A:43:PHE:CZ	1:C:559:PHE:CE1	3.09	0.41
1:A:92:PHE:C	1:A:92:PHE:HD1	2.28	0.41
1:A:164:ASN:OD1	1:A:165:ASN:OD1	2.38	0.41
1:A:353:TRP:O	1:A:353:TRP:CE3	2.74	0.41
1:A:576:VAL:HG22	1:A:577:ARG:N	2.35	0.41
1:A:941:THR:CG2	1:A:944:ALA:HB2	2.50	0.41
1:B:32:PHE:CZ	1:B:216:LEU:HB2	2.55	0.41
1:B:79:PHE:HE2	1:B:244:LEU:HD22	1.85	0.41
1:B:120:VAL:CG1	1:B:127:VAL:CG2	2.90	0.41
1:B:146:HIS:NE2	4:B:1302:NAG:H4	2.36	0.41
1:B:575:ALA:HB1	1:B:584:ILE:HB	2.02	0.41
1:B:584:ILE:HD13	1:B:584:ILE:N	2.35	0.41
1:B:1095:PHE:HB3	1:B:1115:ILE:HD13	2.03	0.41
1:C:359:SER:HA	1:C:524:VAL:HG21	2.02	0.41
1:C:405:ASP:HB3	1:C:406:GLU:OE1	2.21	0.41
1:C:451:TYR:O	2:D:32:CYS:CB	2.68	0.41
1:C:763:LEU:O	1:C:767:LEU:HG	2.21	0.41
2:D:33:ARG:NH2	2:D:58:TYR:CE2	2.88	0.41
2:D:99:VAL:HB	2:D:107:ASN:HB2	2.03	0.41
1:A:328:ARG:O	1:A:543:PHE:HA	2.21	0.41
1:A:592:PHE:CE2	1:B:857:GLY:HA2	2.55	0.41
1:A:756:TYR:OH	1:A:998:THR:HG22	2.21	0.41
1:A:872:GLN:HA	1:A:875:SER:HB3	2.02	0.41
1:A:963:VAL:HA	1:A:966:LEU:HD22	2.03	0.41
1:B:200:TYR:HA	1:B:229:LEU:O	2.20	0.41
1:B:353:TRP:O	1:B:466:ARG:CZ	2.69	0.41
1:B:658:ASN:HB3	1:B:660:TYR:CE1	2.56	0.41
1:B:763:LEU:O	1:B:767:LEU:HG	2.21	0.41
1:C:57:PRO:HB2	1:C:60:SER:OG	2.21	0.41
1:C:93:ALA:HA	1:C:191:GLU:OE1	2.21	0.41
1:C:448:ASN:C	1:C:450:ASN:H	2.28	0.41
1:C:817:PHE:O	1:C:821:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:872:GLN:HA	1:C:875:SER:HB3	2.02	0.41
1:C:1138:TYR:CD1	1:C:1138:TYR:C	2.97	0.41
2:D:2:VAL:HG12	2:D:4:LEU:CD1	2.50	0.41
2:D:36:TRP:CE2	2:D:80:LEU:HB2	2.55	0.41
1:A:130:VAL:CG1	1:A:130:VAL:O	2.69	0.41
1:A:152:TRP:HB3	1:A:245:HIS:CE1	2.55	0.41
1:A:577:ARG:HG3	1:A:582:LEU:HA	2.02	0.41
1:A:763:LEU:O	1:A:767:LEU:HG	2.21	0.41
1:A:804:GLN:HG3	1:A:935:GLN:HE21	1.85	0.41
1:A:1005:GLN:C	1:A:1005:GLN:CD	2.86	0.41
1:B:277:LEU:HB3	1:B:279:TYR:OH	2.21	0.41
1:B:563:GLN:CD	1:C:41:LYS:O	2.61	0.41
1:B:898:PHE:O	1:B:898:PHE:CD1	2.74	0.41
1:C:40:ASP:C	1:C:41:LYS:NZ	2.78	0.41
1:C:117:LEU:CB	1:C:130:VAL:HG23	2.51	0.41
1:C:123:ALA:C	3:G:1:NAG:H81	2.42	0.41
1:C:471:GLU:O	1:C:491:PRO:CD	2.68	0.41
1:C:708:SER:OG	1:C:710:ASN:OD1	2.38	0.41
1:C:963:VAL:HA	1:C:966:LEU:HD22	2.03	0.41
1:A:57:PRO:HB2	1:A:60:SER:OG	2.21	0.41
1:A:277:LEU:HB3	1:A:279:TYR:OH	2.21	0.41
1:A:565:PHE:O	1:B:42:VAL:HA	2.20	0.41
1:A:583:GLU:O	1:A:585:LEU:HD23	2.20	0.41
1:A:726:ILE:CD1	1:A:1061:VAL:CG2	2.99	0.41
1:A:779:GLN:O	1:A:783:ALA:HB3	2.20	0.41
1:A:985:ASP:OD2	1:A:988:GLU:HG2	2.20	0.41
1:A:1083:HIS:HB3	1:A:1088:HIS:NE2	2.35	0.41
1:A:1087:ALA:CB	1:A:1089:PHE:HE2	2.34	0.41
1:B:40:ASP:C	1:B:41:LYS:NZ	2.78	0.41
1:B:231:ILE:HA	1:B:231:ILE:HG23	1.96	0.41
1:B:346:ARG:HA	1:B:346:ARG:NE	2.35	0.41
1:B:395:VAL:HG21	1:B:515:PHE:CD2	2.55	0.41
1:B:577:ARG:HD3	1:B:584:ILE:N	2.35	0.41
1:B:794:ILE:HD11	1:B:796:ASP:OD2	2.20	0.41
1:C:17:ASN:OD1	3:H:1:NAG:H3	2.20	0.41
1:C:32:PHE:CZ	1:C:216:LEU:HB2	2.55	0.41
1:C:236:THR:HG21	3:I:1:NAG:C6	2.51	0.41
2:D:37:TYR:O	2:D:93:TYR:HA	2.21	0.41
1:A:40:ASP:OD2	1:A:41:LYS:N	2.53	0.41
1:A:40:ASP:C	1:A:41:LYS:NZ	2.78	0.41
1:A:64:TRP:CE2	1:A:266:TYR:CZ	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TRP:CE3	1:A:245:HIS:CD2	3.09	0.41
1:A:168:PHE:CG	1:A:169:GLU:N	2.89	0.41
1:A:190:ARG:HD3	1:A:207:HIS:HB2	2.03	0.41
1:A:417:LYS:HD2	1:A:453:TYR:CD1	2.55	0.41
1:A:432:CYS:O	1:A:512:VAL:HG13	2.21	0.41
1:A:658:ASN:HB3	1:A:660:TYR:CE1	2.56	0.41
1:A:794:ILE:HD11	1:A:796:ASP:OD2	2.20	0.41
1:A:923:ILE:HA	1:A:926:GLN:CD	2.45	0.41
1:B:64:TRP:CE2	1:B:266:TYR:CZ	3.09	0.41
1:B:93:ALA:HA	1:B:191:GLU:OE1	2.21	0.41
1:B:104:TRP:CZ2	1:B:192:PHE:CE2	3.09	0.41
1:B:152:TRP:CE3	1:B:245:HIS:CD2	3.09	0.41
1:B:199:GLY:HA2	1:B:232:GLY:CA	2.50	0.41
1:B:351:TYR:HB3	1:B:453:TYR:CB	2.51	0.41
1:B:560:LEU:N	1:B:563:GLN:HG3	2.36	0.41
1:B:697:MET:SD	1:B:698:SER:O	2.79	0.41
1:B:705:VAL:HG21	1:C:883:THR:CB	2.50	0.41
1:B:987:PRO:O	1:B:990:GLU:HG2	2.20	0.41
1:B:1087:ALA:CB	1:B:1089:PHE:HE2	2.34	0.41
1:C:40:ASP:OD2	1:C:41:LYS:N	2.53	0.41
1:C:141:LEU:HD12	1:C:154:GLU:CD	2.46	0.41
1:C:152:TRP:CE3	1:C:245:HIS:CD2	3.09	0.41
1:C:231:ILE:HB	1:C:232:GLY:H	1.60	0.41
1:C:490:PHE:CE1	2:D:105:THR:HG23	2.56	0.41
1:C:494:SER:CB	2:D:102:PHE:O	2.69	0.41
1:C:495:TYR:CD2	1:C:497:PHE:CZ	3.09	0.41
1:C:553:THR:HG23	1:C:586:ASP:HB3	2.03	0.41
1:C:756:TYR:OH	1:C:998:THR:HG22	2.21	0.41
1:C:779:GLN:O	1:C:783:ALA:HB3	2.20	0.41
1:C:976:VAL:HG12	1:C:979:ASP:H	1.86	0.41
2:D:43:LYS:NZ	2:D:43:LYS:HB2	2.36	0.41
3:I:2:NAG:O7	3:I:2:NAG:O3	2.36	0.41
1:A:14:GLN:HG3	1:A:15:CYS:N	2.36	0.41
1:A:141:LEU:HD12	1:A:154:GLU:CD	2.46	0.41
1:A:330:PRO:HD3	1:A:544:ASN:HA	2.03	0.41
1:B:28:TYR:CE1	4:B:1307:NAG:H5	2.56	0.41
1:B:164:ASN:OD1	1:B:165:ASN:OD1	2.38	0.41
1:B:383:SER:HB3	1:B:386:LYS:HE2	2.02	0.41
1:B:490:PHE:CG	1:B:492:LEU:CD1	3.04	0.41
1:B:756:TYR:OH	1:B:998:THR:HG22	2.21	0.41
1:C:104:TRP:CZ2	1:C:192:PHE:CE2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ARG:HD3	1:C:207:HIS:HB2	2.03	0.41
1:C:299:THR:HG21	1:C:597:VAL:HG11	2.04	0.41
1:C:726:ILE:CD1	1:C:1061:VAL:CG2	2.99	0.41
1:C:804:GLN:HG3	1:C:935:GLN:HE21	1.85	0.41
1:C:1006:THR:O	1:C:1010:GLN:CD	2.64	0.41
1:C:1043:CYS:C	1:C:1064:HIS:ND1	2.79	0.41
1:C:1074:ASN:OD1	1:C:1074:ASN:N	2.39	0.41
1:C:1095:PHE:HB3	1:C:1115:ILE:HD13	2.03	0.41
1:A:17:ASN:HD21	3:E:1:NAG:C3	2.34	0.40
1:A:117:LEU:HD13	1:A:130:VAL:HB	2.03	0.40
1:A:233:ILE:CG2	1:A:235:ILE:HG13	2.51	0.40
1:A:371:SER:O	1:A:372:ALA:HB3	2.21	0.40
1:A:406:GLU:HA	1:A:409:GLN:HB2	2.03	0.40
1:A:818:ILE:CD1	1:A:935:GLN:OE1	2.70	0.40
1:A:1089:PHE:O	1:A:1120:THR:OG1	2.38	0.40
1:B:104:TRP:HA	1:B:240:THR:HA	2.03	0.40
1:B:130:VAL:HG11	1:B:167:THR:OG1	2.21	0.40
1:B:190:ARG:HD3	1:B:207:HIS:HB2	2.03	0.40
1:B:773:GLU:O	1:B:777:ASN:CG	2.62	0.40
1:B:808:ASP:HB3	1:B:812:PRO:HD2	2.02	0.40
1:B:1006:THR:O	1:B:1010:GLN:CD	2.64	0.40
1:B:1117:THR:N	1:B:1138:TYR:O	2.50	0.40
4:B:1311:NAG:O3	4:B:1311:NAG:C7	2.69	0.40
1:C:236:THR:HG21	3:I:1:NAG:O6	2.20	0.40
1:C:697:MET:SD	1:C:698:SER:O	2.79	0.40
1:C:1062:PHE:N	1:C:1062:PHE:CD1	2.89	0.40
1:A:34:ARG:HD3	1:A:34:ARG:HA	1.87	0.40
1:A:295:PRO:O	1:A:299:THR:HG23	2.21	0.40
1:A:756:TYR:HD1	1:A:756:TYR:O	2.03	0.40
1:A:921:LYS:O	1:A:925:ASN:OD1	2.39	0.40
1:A:1095:PHE:HB3	1:A:1115:ILE:HD13	2.03	0.40
1:B:14:GLN:HG3	1:B:15:CYS:N	2.36	0.40
1:B:40:ASP:OD2	1:B:41:LYS:N	2.53	0.40
1:B:130:VAL:CG1	1:B:130:VAL:O	2.69	0.40
1:B:299:THR:HG21	1:B:597:VAL:HG11	2.04	0.40
1:B:562:PHE:CE2	1:C:41:LYS:CE	3.03	0.40
1:B:726:ILE:CD1	1:B:1061:VAL:CG2	2.99	0.40
1:B:1053:PRO:HA	1:B:1062:PHE:HA	2.04	0.40
1:C:152:TRP:HB3	1:C:245:HIS:CE1	2.54	0.40
1:C:363:ALA:HB3	1:C:365:TYR:CE1	2.56	0.40
1:C:422:ASN:CG	1:C:455:LEU:O	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:ILE:O	1:C:570:ALA:CB	2.70	0.40
1:C:1087:ALA:CB	1:C:1089:PHE:HE2	2.34	0.40
2:D:115:VAL:O	2:D:115:VAL:HG23	2.22	0.40
1:A:93:ALA:HA	1:A:191:GLU:OE1	2.21	0.40
1:A:195:LYS:HE3	1:A:202:LYS:NZ	2.36	0.40
1:A:233:ILE:HG21	1:A:233:ILE:HD13	1.80	0.40
1:A:752:LEU:O	1:A:755:GLN:OE1	2.39	0.40
1:A:898:PHE:O	1:A:898:PHE:CD1	2.74	0.40
1:B:804:GLN:HG3	1:B:935:GLN:HE21	1.85	0.40
1:C:18:LEU:HD13	1:C:258:TRP:CZ2	2.56	0.40
1:C:48:LEU:HD23	1:C:278:LYS:HD2	2.04	0.40
1:C:277:LEU:HB3	1:C:279:TYR:OH	2.21	0.40
1:C:924:ALA:O	1:C:928:ASN:OD1	2.39	0.40
1:C:1083:HIS:HB3	1:C:1088:HIS:CD2	2.57	0.40
3:E:1:NAG:H3	3:E:1:NAG:H83	2.03	0.40
1:A:359:SER:HA	1:A:524:VAL:HG11	2.02	0.40
1:A:528:LYS:HB3	1:A:529:LYS:HD2	2.04	0.40
1:A:716:THR:HG22	1:A:1110:TYR:CB	2.51	0.40
1:A:1053:PRO:HA	1:A:1062:PHE:HA	2.04	0.40
1:B:57:PRO:HB2	1:B:60:SER:OG	2.21	0.40
1:B:117:LEU:CB	1:B:130:VAL:HG23	2.51	0.40
1:B:168:PHE:CG	1:B:169:GLU:N	2.89	0.40
1:B:339:GLY:O	1:B:343:ASN:OD1	2.39	0.40
1:B:872:GLN:HA	1:B:875:SER:HB3	2.02	0.40
1:B:933:LYS:HB2	1:B:933:LYS:HE3	1.82	0.40
1:C:450:ASN:HA	2:D:32:CYS:O	2.22	0.40
1:C:538:CYS:O	1:C:538:CYS:SG	2.79	0.40
1:A:17:ASN:ND2	3:E:1:NAG:O3	2.55	0.40
1:A:365:TYR:HB2	1:A:387:LEU:HB2	2.03	0.40
1:A:503:VAL:HG13	1:A:508:TYR:OH	2.21	0.40
1:A:812:PRO:O	1:A:813:SER:HB3	2.22	0.40
1:B:558:LYS:NZ	1:B:560:LEU:HD12	2.36	0.40
1:B:562:PHE:CD2	1:C:41:LYS:CD	3.01	0.40
1:C:64:TRP:CE2	1:C:266:TYR:CZ	3.09	0.40
1:C:104:TRP:HA	1:C:240:THR:HA	2.03	0.40
1:C:115:GLN:NE2	1:C:165:ASN:O	2.51	0.40
1:C:117:LEU:HD13	1:C:130:VAL:HB	2.03	0.40
1:C:295:PRO:O	1:C:299:THR:HG23	2.21	0.40
1:C:339:GLY:O	1:C:344:ALA:N	2.54	0.40
1:C:452:LEU:HA	2:D:104:CYS:CB	2.51	0.40
1:C:473:TYR:HB2	1:C:491:PRO:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:818:ILE:CD1	1:C:935:GLN:OE1	2.70	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	1045/1264 (83%)	959 (92%)	85 (8%)	1 (0%)	48	80
1	B	1039/1264 (82%)	948 (91%)	90 (9%)	1 (0%)	48	80
1	C	1045/1264 (83%)	942 (90%)	98 (9%)	5 (0%)	24	59
2	D	117/124 (94%)	113 (97%)	4 (3%)	0	100	100
All	All	3246/3916 (83%)	2962 (91%)	277 (8%)	7 (0%)	44	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	332	ILE
1	C	459	SER
1	C	530	SER
1	C	591	SER
1	A	942	PRO
1	B	942	PRO
1	C	942	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	929/1100 (84%)	867 (93%)	62 (7%)	15	41
1	B	925/1100 (84%)	850 (92%)	75 (8%)	11	35
1	C	929/1100 (84%)	855 (92%)	74 (8%)	11	35
2	D	96/100 (96%)	89 (93%)	7 (7%)	13	39
All	All	2879/3400 (85%)	2661 (92%)	218 (8%)	14	37

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	42	VAL
1	A	49	HIS
1	A	53	ASP
1	A	78	ARG
1	A	99	ASN
1	A	133	PHE
1	A	152	TRP
1	A	231	ILE
1	A	320	VAL
1	A	323	THR
1	A	326	ILE
1	A	331	ASN
1	A	356	LYS
1	A	368	LEU
1	A	373	SER
1	A	377	PHE
1	A	382	VAL
1	A	389	ASP
1	A	402	ILE
1	A	410	ILE
1	A	425	LEU
1	A	432	CYS
1	A	434	ILE
1	A	443	SER
1	A	452	LEU
1	A	455	LEU
1	A	457	ARG
1	A	460[A]	ASN
1	A	460[B]	ASN

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Mol	Chain	Res	Type
1	A	461	LEU
1	A	462	LYS
1	A	464	PHE
1	A	492	LEU
1	A	497	PHE
1	A	524	VAL
1	A	531	THR
1	A	535	LYS
1	A	536	ASN
1	A	537	LYS
1	A	551	VAL
1	A	555	SER
1	A	557	LYS
1	A	558	LYS
1	A	559	PHE
1	A	562	PHE
1	A	573	THR
1	A	580	GLN
1	A	585	LEU
1	A	588	THR
1	A	603	ASN
1	A	619	GLU
1	A	651	ILE
1	A	703	ASN
1	A	794	ILE
1	A	882	ILE
1	A	902	MET
1	A	915	VAL
1	A	933	LYS
1	A	983	ARG
1	A	1095	PHE
1	A	1113	GLN
1	B	41	LYS
1	B	42	VAL
1	B	49	HIS
1	B	53	ASP
1	B	78	ARG
1	B	99	ASN
1	B	133	PHE
1	B	152	TRP
1	B	231	ILE
1	B	323	THR

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Mol	Chain	Res	Type
1	B	331	ASN
1	B	332	ILE
1	B	340	GLU
1	B	341	VAL
1	B	343	ASN
1	B	346	ARG
1	B	351	TYR
1	B	354	ASN
1	B	359	SER
1	B	374	PHE
1	B	378	LYS
1	B	386	LYS
1	B	390	LEU
1	B	391	CYS
1	B	396	TYR
1	B	403	ARG
1	B	409	GLN
1	B	430	THR
1	B	436	TRP
1	B	439	ASN
1	B	440	ASN
1	B	444	LYS
1	B	452	LEU
1	B	454	ARG
1	B	455	LEU
1	B	456	PHE
1	B	458	LYS
1	B	461	LEU
1	B	462	LYS
1	B	492	LEU
1	B	493	GLN
1	B	494	SER
1	B	495	TYR
1	B	498	GLN
1	B	509	ARG
1	B	515	PHE
1	B	516	GLU
1	B	524	VAL
1	B	525	CYS
1	B	529	LYS
1	B	535	LYS
1	B	536	ASN

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Mol	Chain	Res	Type
1	B	537	LYS
1	B	539	VAL
1	B	555	SER
1	B	557	LYS
1	B	558	LYS
1	B	563	GLN
1	B	568	ASP
1	B	569	ILE
1	B	576	VAL
1	B	584	ILE
1	B	586	ASP
1	B	590	CYS
1	B	603	ASN
1	B	619	GLU
1	B	651	ILE
1	B	794	ILE
1	B	882	ILE
1	B	902	MET
1	B	915	VAL
1	B	933	LYS
1	B	983	ARG
1	B	1095	PHE
1	B	1113	GLN
1	C	41	LYS
1	C	42	VAL
1	C	49	HIS
1	C	53	ASP
1	C	78	ARG
1	C	99	ASN
1	C	133	PHE
1	C	152	TRP
1	C	231	ILE
1	C	320	VAL
1	C	321	GLN
1	C	323	THR
1	C	326	ILE
1	C	328	ARG
1	C	329	PHE
1	C	333	THR
1	C	334	ASN
1	C	343	ASN
1	C	358	ILE

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Mol	Chain	Res	Type
1	C	364	ASP
1	C	368	LEU
1	C	377	PHE
1	C	391	CYS
1	C	392	PHE
1	C	399	SER
1	C	409	GLN
1	C	417	LYS
1	C	422	ASN
1	C	444	LYS
1	C	450	ASN
1	C	454	ARG
1	C	457	ARG
1	C	458	LYS
1	C	460[A]	ASN
1	C	460[B]	ASN
1	C	461	LEU
1	C	466	ARG
1	C	468	ILE
1	C	472	ILE
1	C	487	ASN
1	C	490	PHE
1	C	492	LEU
1	C	525	CYS
1	C	528	LYS
1	C	529	LYS
1	C	534	VAL
1	C	537	LYS
1	C	538	CYS
1	C	544	ASN
1	C	552	LEU
1	C	555	SER
1	C	558	LYS
1	C	560	LEU
1	C	562	PHE
1	C	563	GLN
1	C	565	PHE
1	C	572	THR
1	C	580	GLN
1	C	584	ILE
1	C	587	ILE
1	C	588	THR

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Mol	Chain	Res	Type
1	C	590	CYS
1	C	603	ASN
1	C	619	GLU
1	C	651	ILE
1	C	703	ASN
1	C	794	ILE
1	C	882	ILE
1	C	902	MET
1	C	915	VAL
1	C	933	LYS
1	C	983	ARG
1	C	1095	PHE
1	C	1113	GLN
2	D	32	CYS
2	D	43	LYS
2	D	88	GLU
2	D	99	VAL
2	D	100	LYS
2	D	104	CYS
2	D	116	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	61	ASN
1	A	66	HIS
1	A	115	GLN
1	A	196	ASN
1	A	388	ASN
1	A	437	ASN
1	A	655	HIS
1	A	703	ASN
1	A	764	ASN
1	A	784	GLN
1	A	955	ASN
1	A	1101	HIS
1	A	1142	GLN
1	B	23	GLN
1	B	66	HIS
1	B	115	GLN
1	B	196	ASN

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Mol	Chain	Res	Type
1	B	394	ASN
1	B	409	GLN
1	B	450	ASN
1	B	498	GLN
1	B	544	ASN
1	B	655	HIS
1	B	764	ASN
1	B	784	GLN
1	B	787	GLN
1	B	955	ASN
1	B	1101	HIS
1	B	1142	GLN
1	C	23	GLN
1	C	66	HIS
1	C	115	GLN
1	C	196	ASN
1	C	388	ASN
1	C	409	GLN
1	C	439	ASN
1	C	450	ASN
1	C	556	ASN
1	C	563	GLN
1	C	580	GLN
1	C	655	HIS
1	C	764	ASN
1	C	784	GLN
1	C	913	GLN
1	C	955	ASN
1	C	1142	GLN
2	D	73	ASN
2	D	114	GLN

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 ⓘ

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	3	14,14,15	0.60	1 (7%)	17,19,21	1.50	4 (23%)
3	NAG	E	2	3	14,14,15	0.43	0	17,19,21	0.45	0
3	NAG	F	1	3	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	F	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	G	1	3,1	14,14,15	1.27	2 (14%)	17,19,21	0.98	1 (5%)
3	NAG	G	2	3	14,14,15	0.35	0	17,19,21	0.89	1 (5%)
3	NAG	H	1	3	14,14,15	0.22	0	17,19,21	0.56	0
3	NAG	H	2	3	14,14,15	0.34	0	17,19,21	0.61	0
3	NAG	I	1	3,1	14,14,15	1.46	1 (7%)	17,19,21	0.47	0
3	NAG	I	2	3	14,14,15	1.03	2 (14%)	17,19,21	0.73	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3	-	6/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3	-	4/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	O5-C1	5.04	1.52	1.43
3	G	1	NAG	C1-C2	-3.06	1.48	1.52
3	I	2	NAG	O5-C1	2.87	1.48	1.43
3	G	1	NAG	O5-C1	2.60	1.48	1.43
3	I	2	NAG	C1-C2	2.46	1.55	1.52
3	E	1	NAG	O5-C1	-2.02	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C6-C5-C4	2.93	120.22	113.02
3	G	2	NAG	C1-O5-C5	2.75	115.87	112.19
3	E	1	NAG	O5-C5-C6	2.67	112.87	107.66
3	E	1	NAG	O5-C5-C4	2.64	117.26	110.83
3	E	1	NAG	C2-N2-C7	2.40	126.12	122.90
3	G	1	NAG	C1-C2-N2	-2.36	106.72	110.43
3	I	2	NAG	C1-O5-C5	2.09	114.99	112.19

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C1-C2-N2-C7
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6

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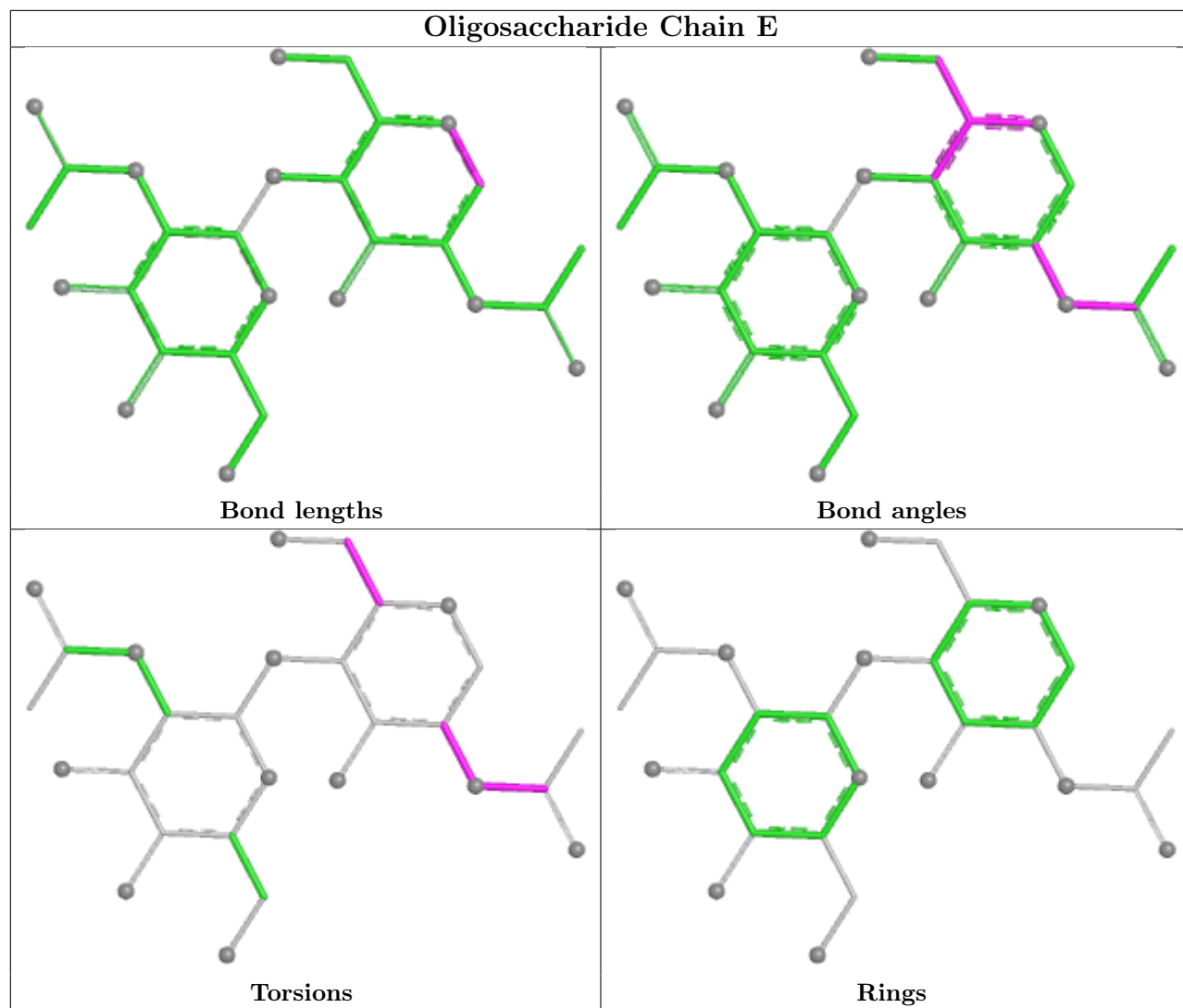
Mol	Chain	Res	Type	Atoms
3	I	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C1-C2-N2-C7
3	G	1	NAG	C3-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	H	2	NAG	C1-C2-N2-C7
3	E	1	NAG	C3-C2-N2-C7
3	I	1	NAG	C3-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7

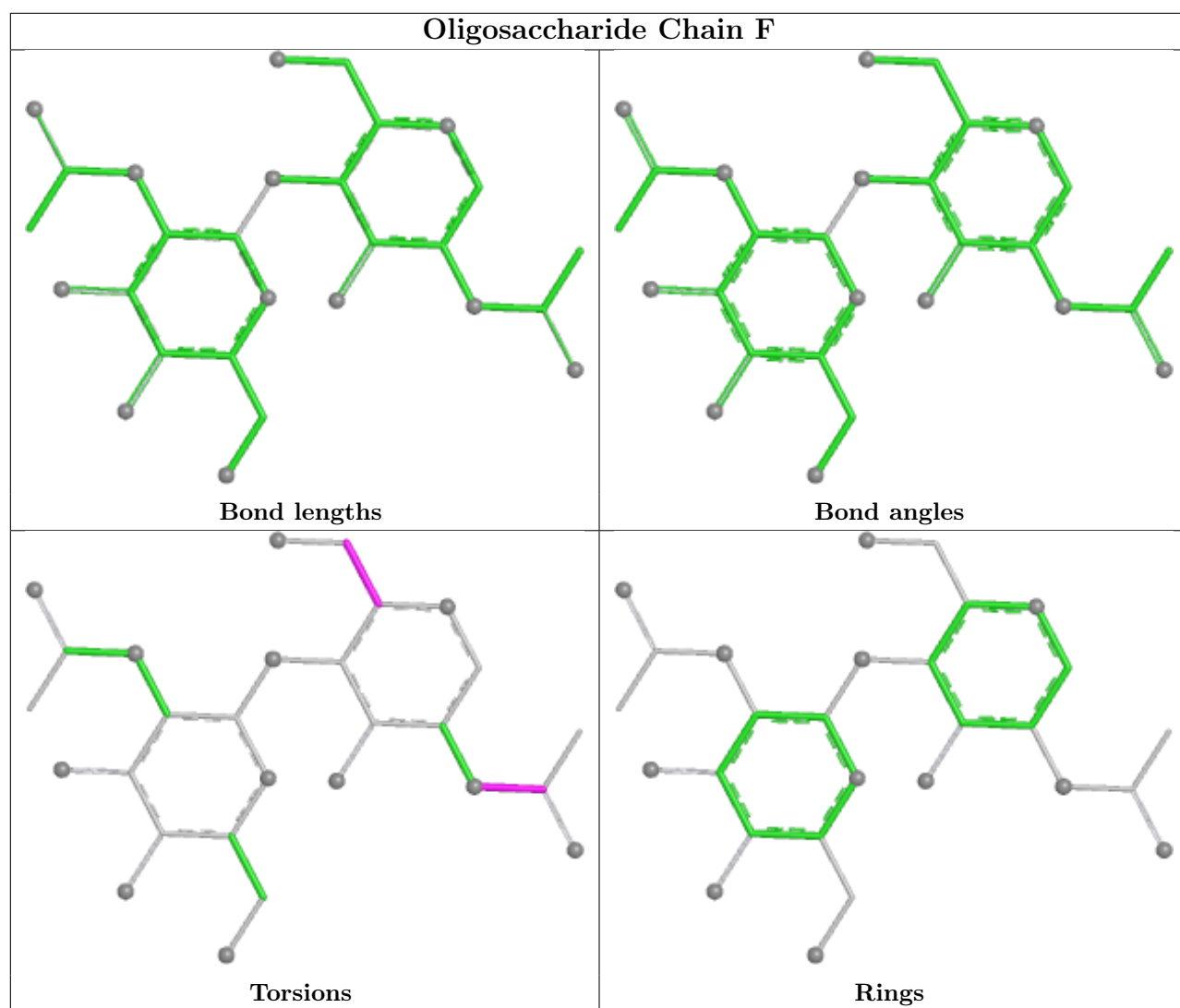
There are no ring outliers.

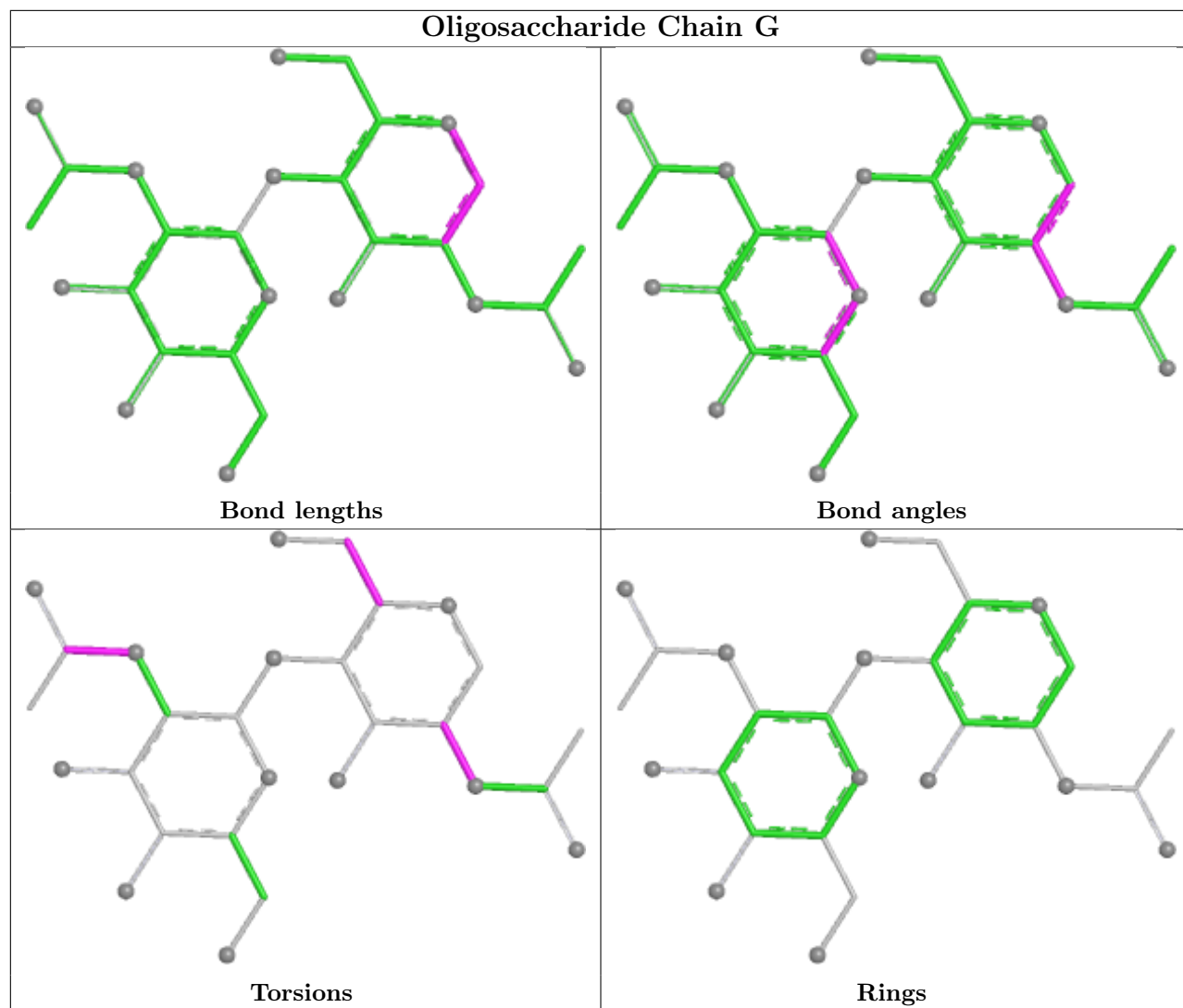
8 monomers are involved in 40 short contacts:

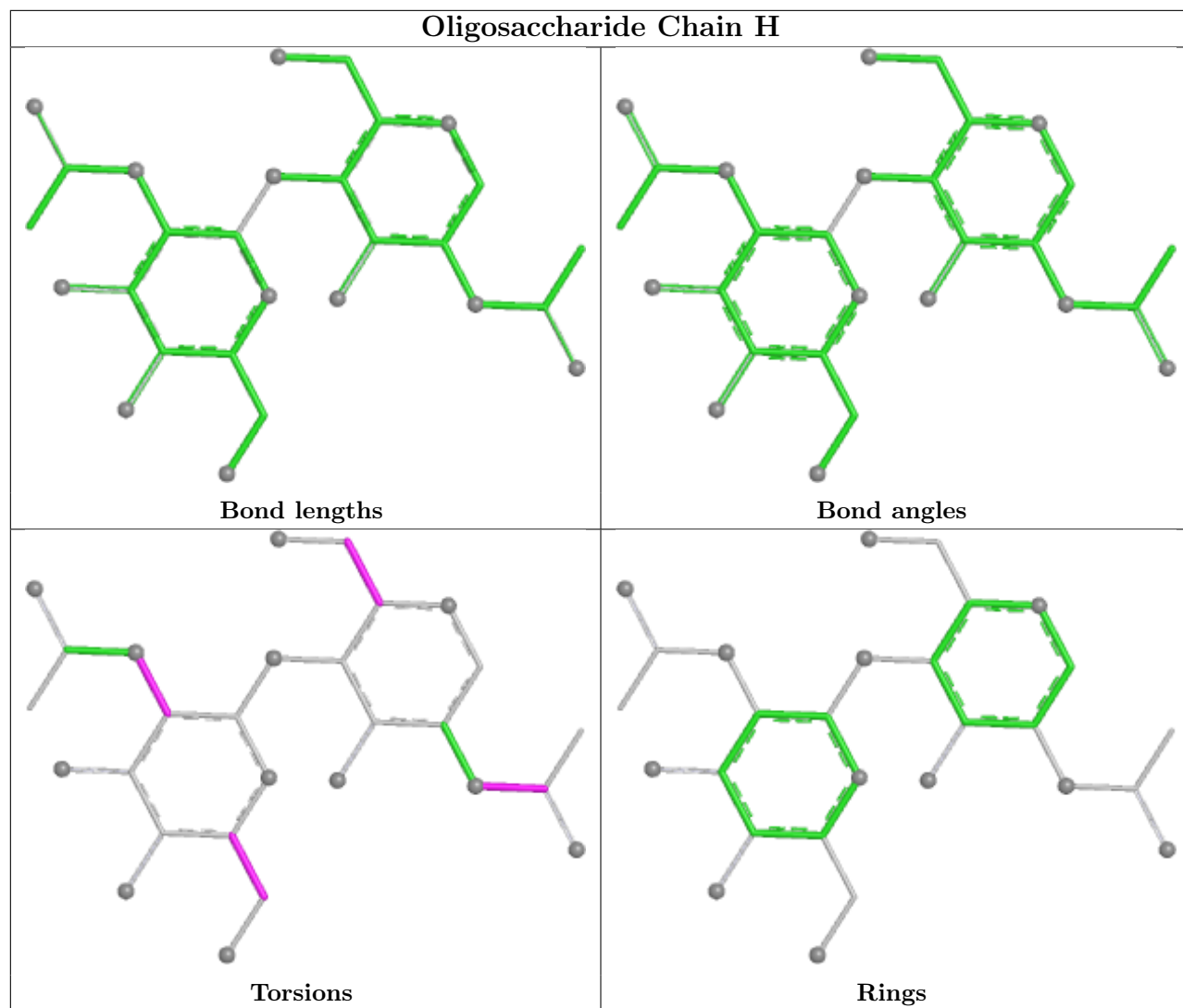
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	5	0
3	E	1	NAG	5	0
3	G	2	NAG	3	0
3	H	2	NAG	2	0
3	I	2	NAG	1	0
3	E	2	NAG	3	0
3	G	1	NAG	22	0
3	I	1	NAG	2	0

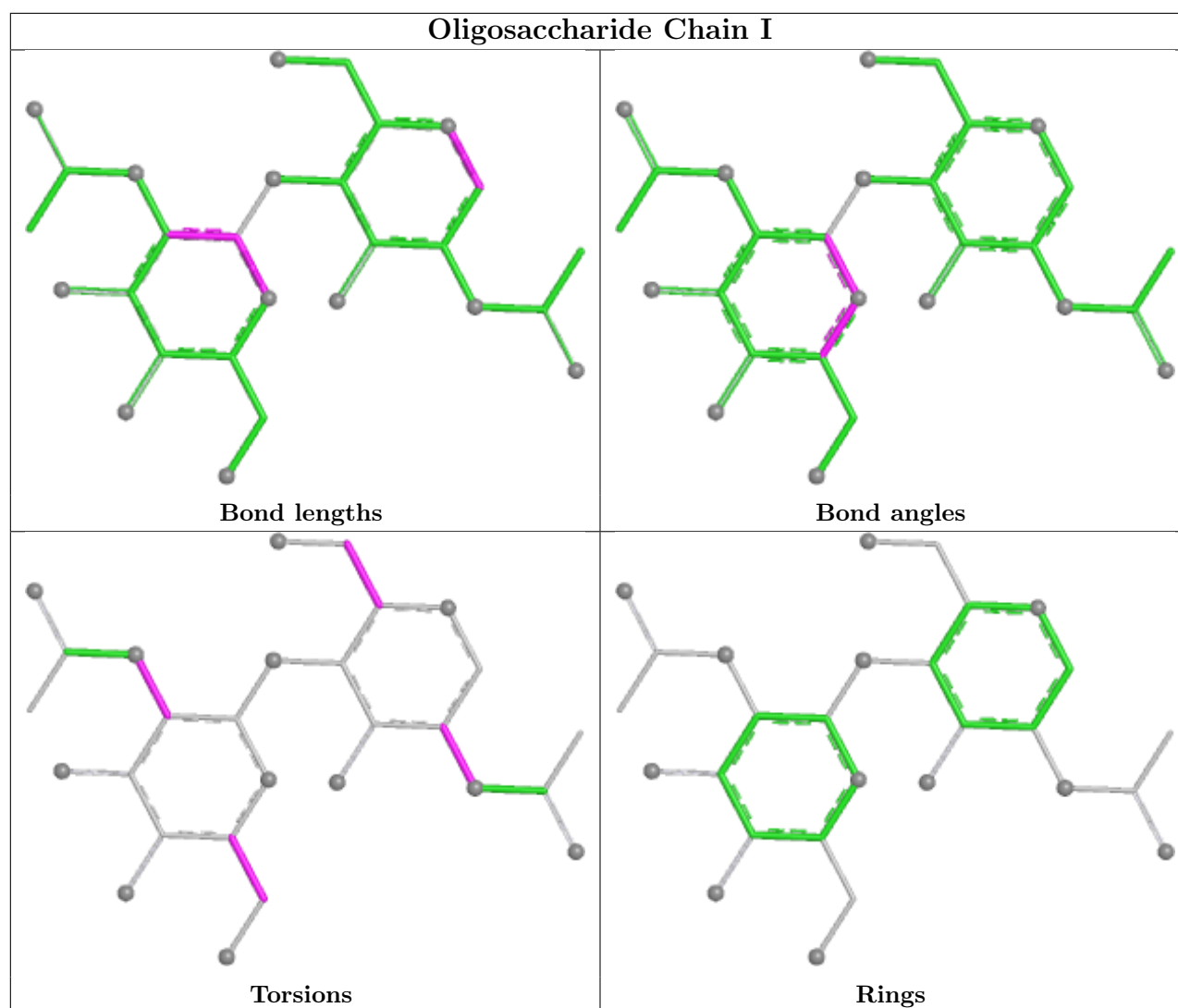
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

33 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	1307	1	14,14,15	0.22	0	17,19,21	0.95	1 (5%)
4	NAG	B	1303	-	14,14,15	0.20	0	17,19,21	0.47	0
4	NAG	C	1301	1	14,14,15	3.91	2 (14%)	17,19,21	2.21	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1306	1	14,14,15	2.59	2 (14%)	17,19,21	0.76	1 (5%)
4	NAG	B	1308	1	14,14,15	0.56	0	17,19,21	0.72	1 (5%)
4	NAG	C	1304	1	14,14,15	1.83	2 (14%)	17,19,21	1.24	2 (11%)
4	NAG	A	1303	1	14,14,15	0.43	0	17,19,21	0.52	0
4	NAG	A	1309	1	14,14,15	0.37	0	17,19,21	0.36	0
4	NAG	B	1310	1	14,14,15	0.18	0	17,19,21	0.51	0
4	NAG	C	1305	1	14,14,15	0.33	0	17,19,21	0.52	0
4	NAG	C	1302	-	14,14,15	0.19	0	17,19,21	0.46	0
4	NAG	A	1313	1	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	A	1308	-	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	A	1304	-	14,14,15	0.20	0	17,19,21	0.48	0
4	NAG	B	1312	1	14,14,15	1.68	2 (14%)	17,19,21	1.41	4 (23%)
4	NAG	A	1301	-	14,14,15	0.36	0	17,19,21	0.44	0
4	NAG	B	1307	1	14,14,15	0.38	0	17,19,21	1.07	2 (11%)
4	NAG	A	1305	1	14,14,15	1.52	1 (7%)	17,19,21	0.77	1 (5%)
4	NAG	C	1303	1	14,14,15	1.03	2 (14%)	17,19,21	0.81	0
4	NAG	A	1310	1	14,14,15	0.41	0	17,19,21	0.47	0
4	NAG	B	1302	-	14,14,15	0.64	1 (7%)	17,19,21	1.10	1 (5%)
4	NAG	A	1312	1	14,14,15	1.02	2 (14%)	17,19,21	1.10	1 (5%)
4	NAG	B	1301	1	14,14,15	1.07	1 (7%)	17,19,21	2.00	3 (17%)
4	NAG	B	1306	-	14,14,15	0.29	0	17,19,21	0.43	0
4	NAG	A	1302	-	14,14,15	0.27	0	17,19,21	0.75	0
4	NAG	A	1307	1	14,14,15	0.18	0	17,19,21	0.55	0
4	NAG	B	1313	1	14,14,15	0.17	0	17,19,21	0.55	0
4	NAG	B	1305	-	14,14,15	0.51	0	17,19,21	0.39	0
4	NAG	B	1304	-	14,14,15	0.38	0	17,19,21	0.83	1 (5%)
4	NAG	A	1306	-	14,14,15	0.63	0	17,19,21	0.52	0
4	NAG	B	1309	1	14,14,15	0.43	0	17,19,21	0.55	0
4	NAG	B	1311	1	14,14,15	3.08	2 (14%)	17,19,21	1.79	1 (5%)
4	NAG	A	1311	-	14,14,15	0.22	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	-	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1306	1	1/1/6/7	4/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1313	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1308	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1301	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	1	1/1/6/7	4/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1302	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	-	-	5/6/23/26	0/1/1/1
4	NAG	A	1306	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	-	-	4/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1301	NAG	C1-C2	13.57	1.70	1.52
4	C	1306	NAG	O5-C1	-8.83	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1311	NAG	O5-C1	8.41	1.57	1.43
4	B	1311	NAG	C1-C2	-7.71	1.41	1.52
4	C	1304	NAG	O5-C1	-6.37	1.33	1.43
4	A	1305	NAG	C1-C2	5.53	1.59	1.52
4	B	1312	NAG	C1-C2	5.38	1.59	1.52
4	C	1301	NAG	O5-C1	-5.17	1.35	1.43
4	C	1306	NAG	C1-C2	-3.91	1.47	1.52
4	B	1301	NAG	C1-C2	-3.17	1.48	1.52
4	B	1312	NAG	O5-C1	2.45	1.47	1.43
4	C	1303	NAG	O5-C1	2.42	1.47	1.43
4	A	1312	NAG	C1-C2	-2.42	1.49	1.52
4	C	1304	NAG	C1-C2	-2.32	1.49	1.52
4	C	1303	NAG	C1-C2	2.27	1.55	1.52
4	A	1312	NAG	C4-C5	-2.14	1.48	1.53
4	B	1302	NAG	O5-C1	-2.05	1.40	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1301	NAG	C1-O5-C5	7.45	122.17	112.19
4	B	1301	NAG	C1-O5-C5	6.72	121.19	112.19
4	B	1311	NAG	C1-O5-C5	6.47	120.85	112.19
4	C	1304	NAG	C1-O5-C5	-4.01	106.81	112.19
4	C	1301	NAG	C1-C2-N2	3.90	116.58	110.43
4	C	1307	NAG	C1-O5-C5	3.58	116.99	112.19
4	B	1302	NAG	O4-C4-C5	-3.43	100.89	109.32
4	B	1312	NAG	C1-C2-N2	-3.04	105.64	110.43
4	A	1312	NAG	C1-O5-C5	2.89	116.06	112.19
4	B	1312	NAG	C3-C4-C5	-2.77	105.20	110.23
4	B	1301	NAG	C4-C3-C2	-2.76	106.97	111.02
4	C	1306	NAG	C1-O5-C5	-2.51	108.82	112.19
4	B	1312	NAG	O5-C5-C4	-2.47	104.82	110.83
4	C	1301	NAG	O5-C5-C6	-2.41	102.97	107.66
4	B	1307	NAG	C1-C2-N2	2.33	114.10	110.43
4	B	1304	NAG	C2-N2-C7	2.31	126.00	122.90
4	B	1312	NAG	C4-C3-C2	2.23	114.28	111.02
4	B	1307	NAG	C1-O5-C5	2.20	115.14	112.19
4	C	1304	NAG	C3-C4-C5	2.12	114.08	110.23
4	B	1301	NAG	O5-C5-C4	2.04	115.80	110.83
4	B	1308	NAG	C1-O5-C5	2.03	114.90	112.19
4	A	1305	NAG	C1-C2-N2	2.02	113.62	110.43

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	1303	NAG	C1
4	C	1306	NAG	C1

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1304	NAG	C1-C2-N2-C7
4	B	1306	NAG	C3-C2-N2-C7
4	B	1307	NAG	C1-C2-N2-C7
4	B	1310	NAG	C1-C2-N2-C7
4	B	1312	NAG	C1-C2-N2-C7
4	C	1301	NAG	C1-C2-N2-C7
4	C	1303	NAG	C1-C2-N2-C7
4	B	1301	NAG	C4-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	A	1312	NAG	C4-C5-C6-O6
4	A	1312	NAG	O5-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	A	1309	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	A	1310	NAG	O5-C5-C6-O6
4	B	1309	NAG	C4-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	A	1309	NAG	C4-C5-C6-O6
4	B	1310	NAG	C4-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	A	1311	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	A	1311	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1313	NAG	O5-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	B	1303	NAG	C8-C7-N2-C2
4	B	1303	NAG	O7-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1308	NAG	C8-C7-N2-C2
4	B	1308	NAG	O7-C7-N2-C2
4	C	1306	NAG	C8-C7-N2-C2
4	C	1306	NAG	O7-C7-N2-C2
4	B	1306	NAG	C4-C5-C6-O6
4	B	1313	NAG	C4-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6
4	B	1311	NAG	O5-C5-C6-O6
4	A	1313	NAG	O5-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	A	1310	NAG	C4-C5-C6-O6
4	A	1311	NAG	C1-C2-N2-C7
4	B	1311	NAG	C3-C2-N2-C7
4	A	1304	NAG	C1-C2-N2-C7
4	B	1313	NAG	C1-C2-N2-C7
4	A	1301	NAG	C3-C2-N2-C7
4	A	1311	NAG	C3-C2-N2-C7
4	C	1303	NAG	C3-C2-N2-C7

There are no ring outliers.

18 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1306	NAG	1	0
4	B	1308	NAG	1	0
4	C	1304	NAG	1	0
4	A	1303	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1305	NAG	3	0
4	A	1304	NAG	2	0
4	B	1312	NAG	4	0
4	B	1307	NAG	2	0
4	B	1302	NAG	12	0
4	A	1312	NAG	9	0
4	B	1301	NAG	4	0
4	B	1306	NAG	2	0
4	A	1302	NAG	2	0
4	B	1305	NAG	4	0
4	B	1304	NAG	7	0
4	A	1306	NAG	4	0
4	B	1311	NAG	2	0
4	A	1311	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	528:LYS	C	529:LYS	N	6.70
1	A	527:PRO	C	528:LYS	N	4.58
1	B	481:ASN	C	482:GLY	N	3.18

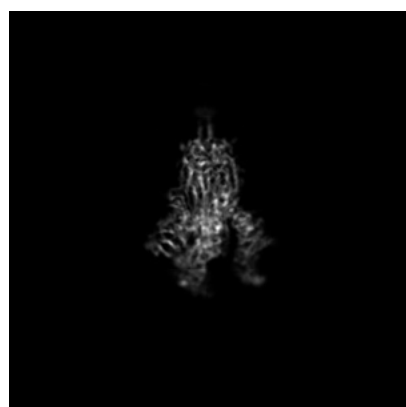
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14315. These allow visual inspection of the internal detail of the map and identification of artifacts.

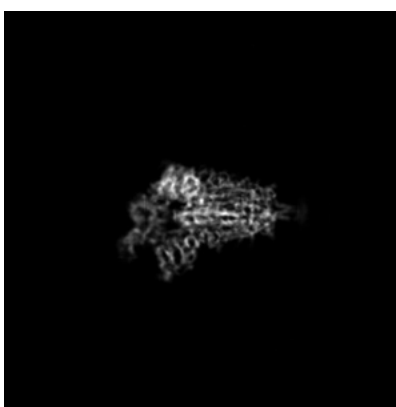
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

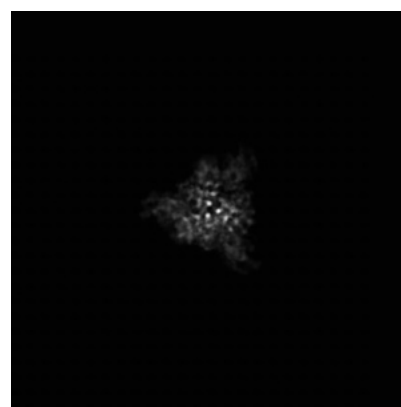
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

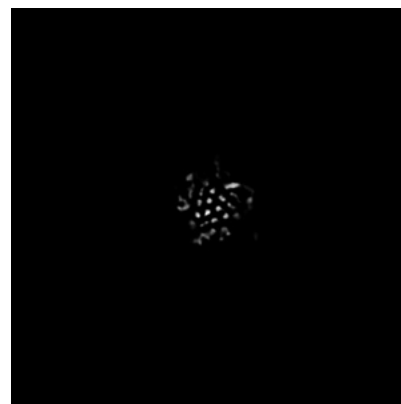
6.2.1 Primary map



X Index: 246



Y Index: 246



Z Index: 246

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: 241



Y Index: 238



Z Index: 224

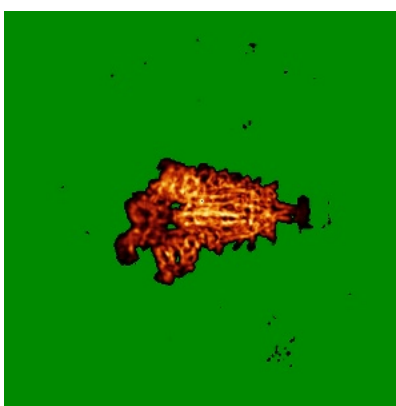
The images above show the largest variance slices of the map in three orthogonal directions.

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

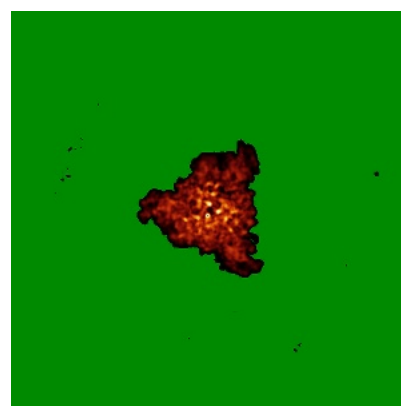
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

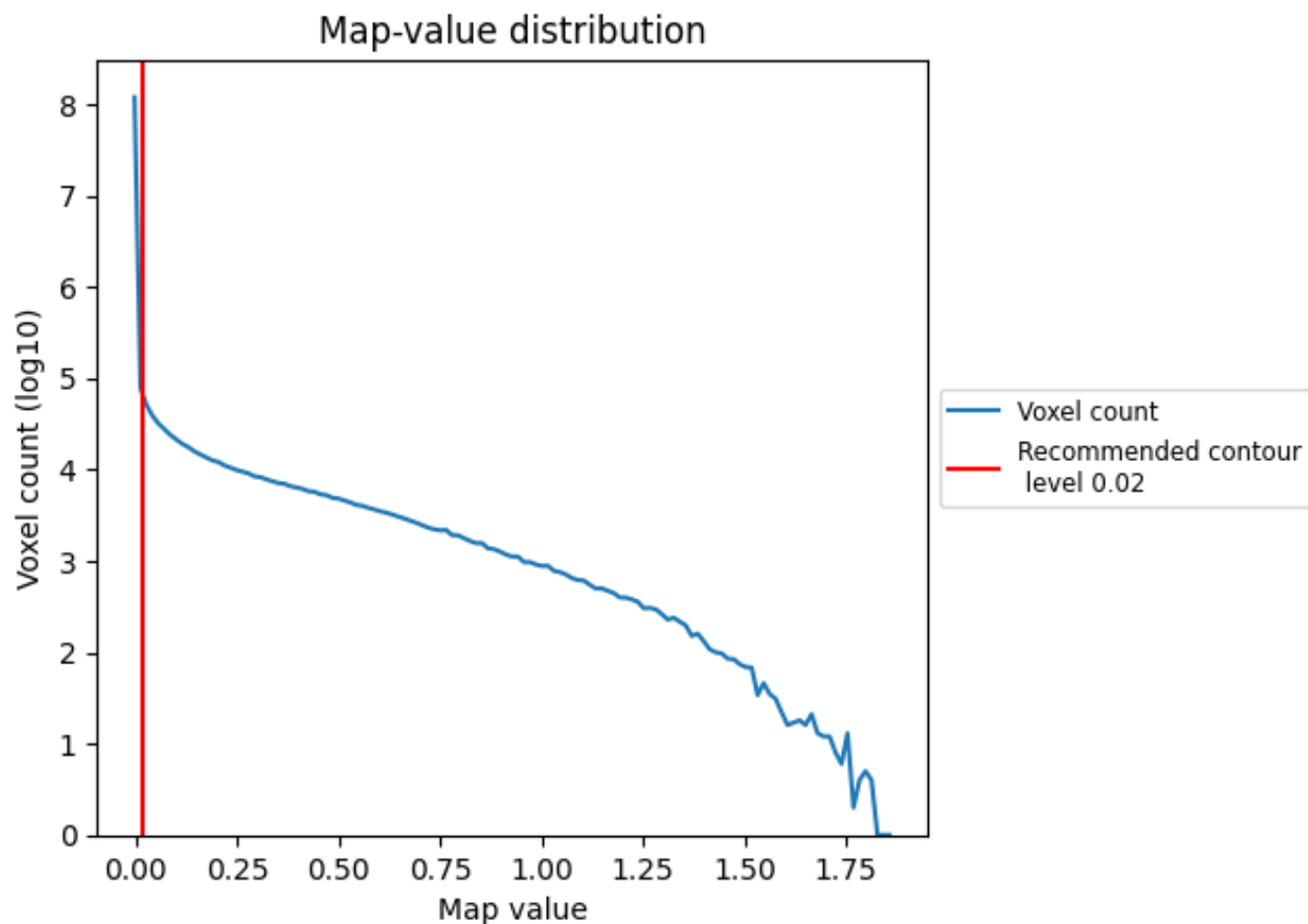
6.6 Mask visualisation

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

7 Map analysis [i](#)

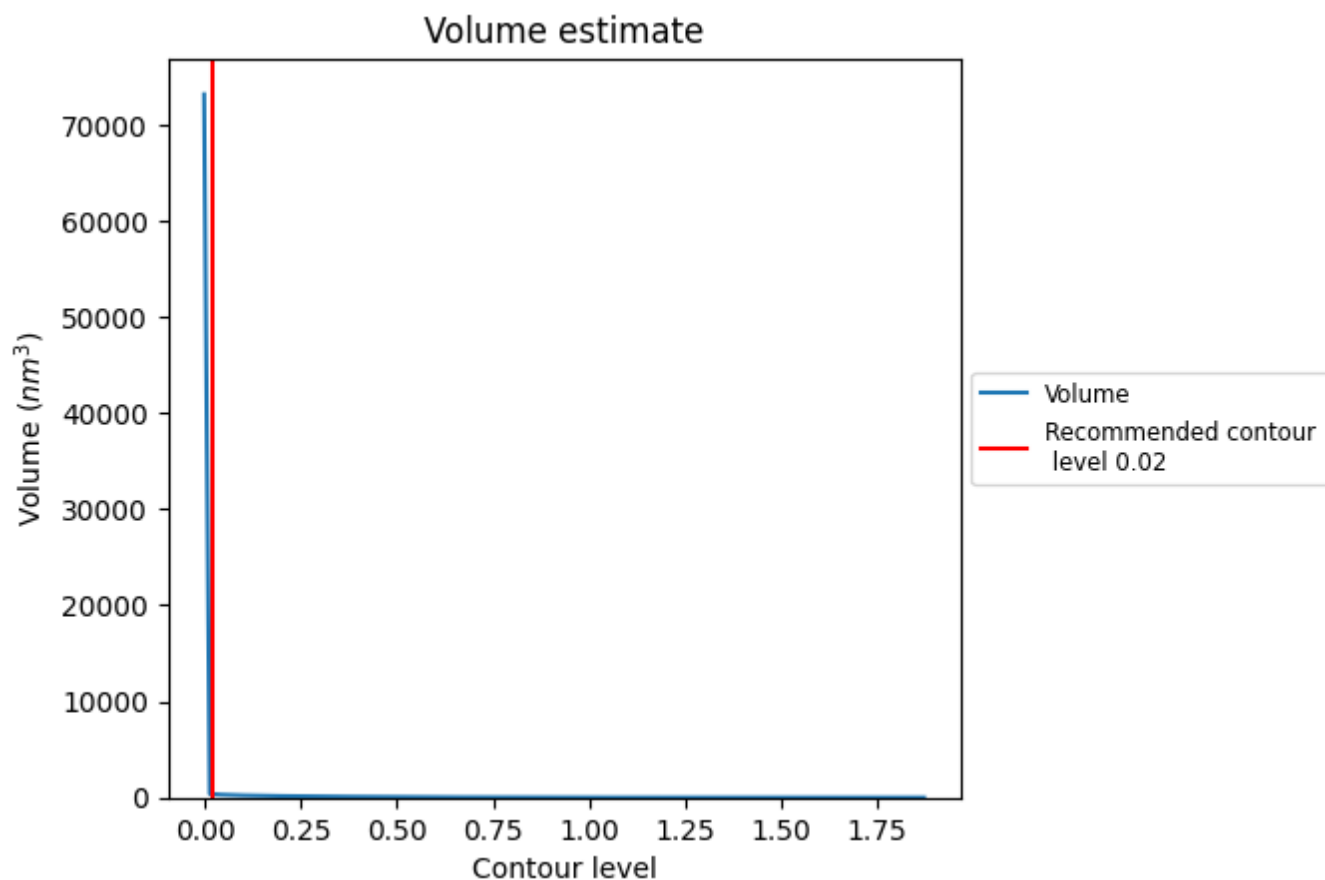
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

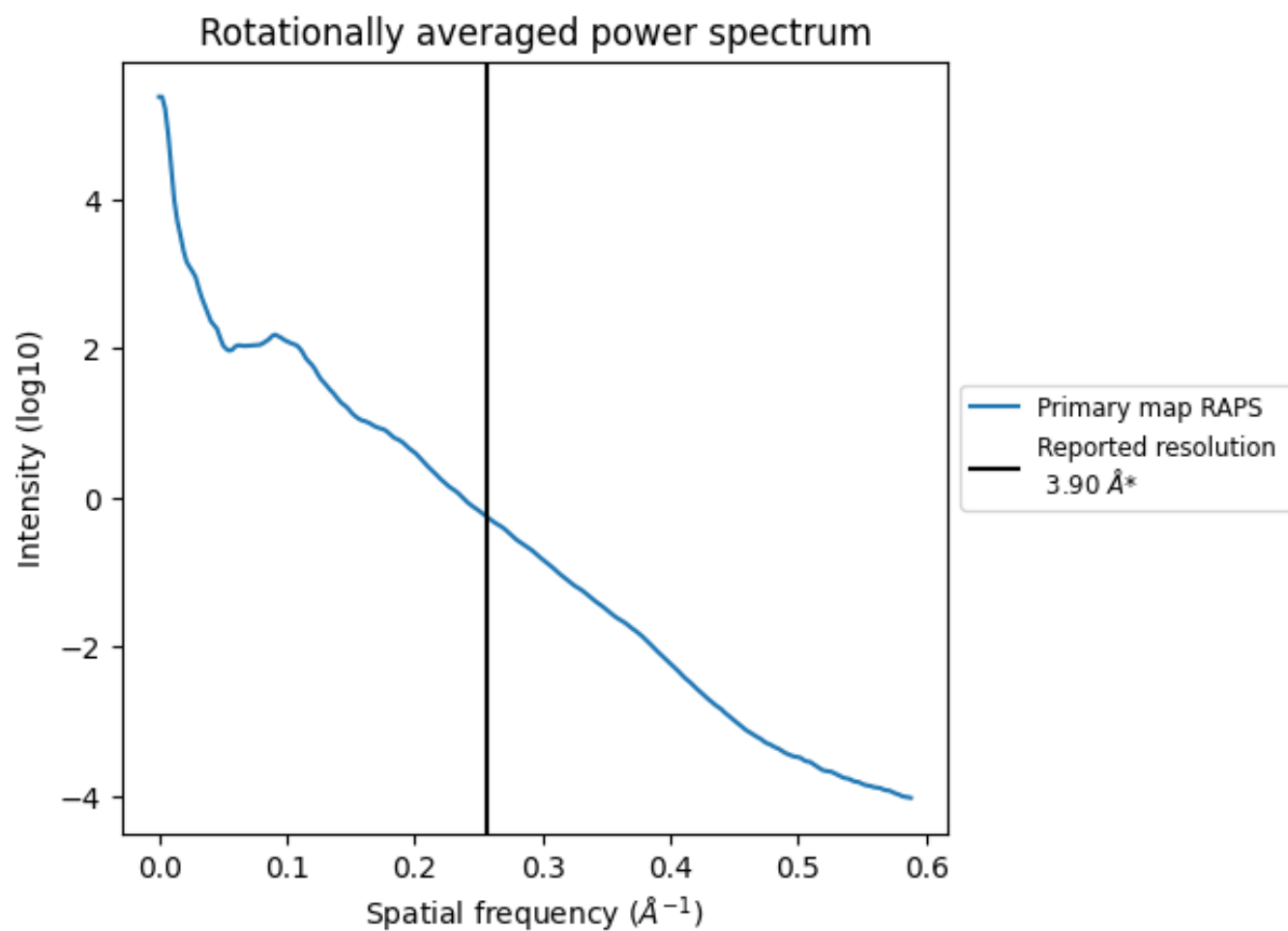
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 355 nm^3 ; this corresponds to an approximate mass of 321 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

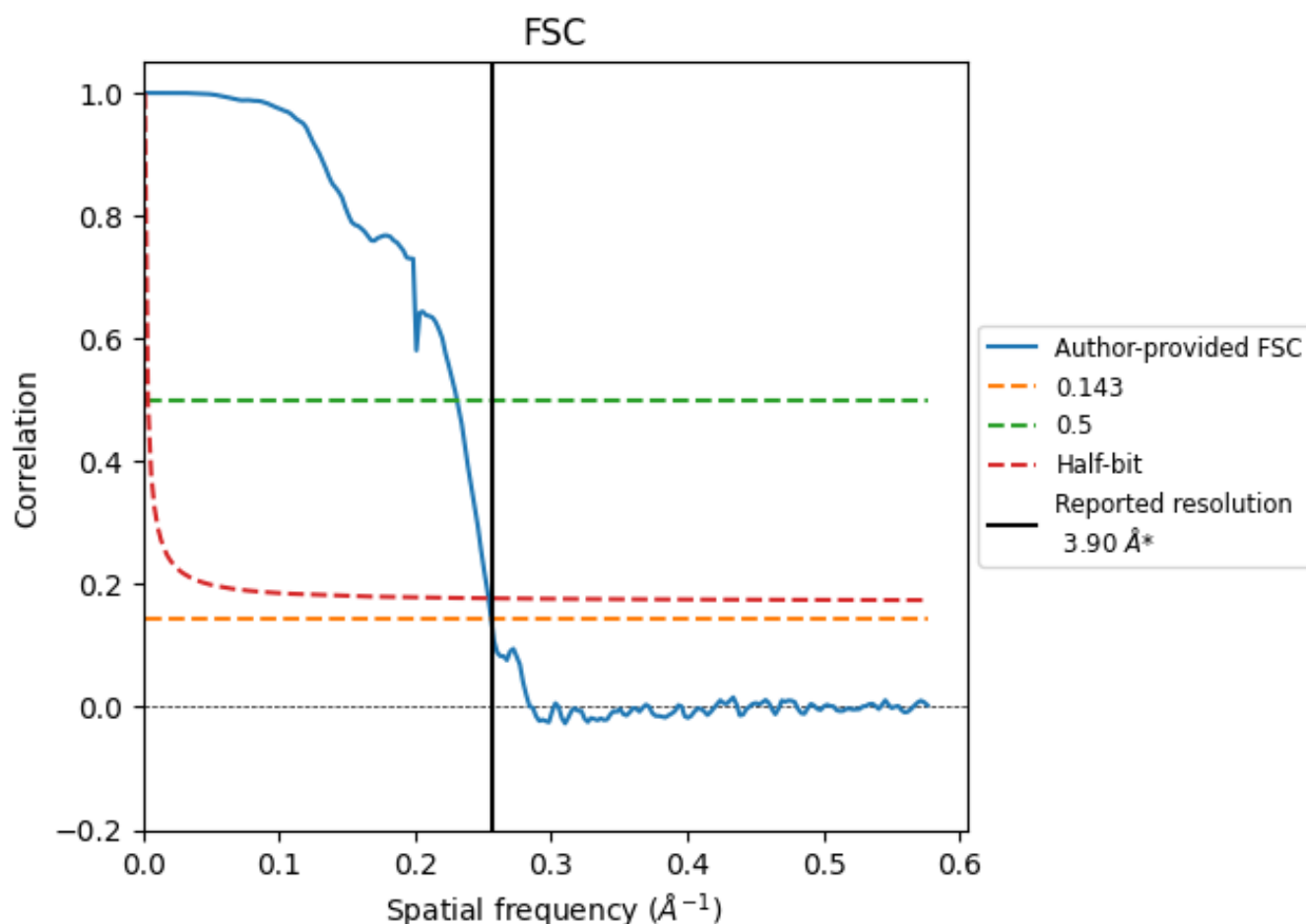


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

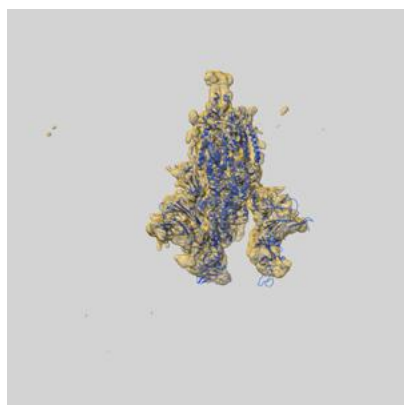
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.91	4.33	3.94
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

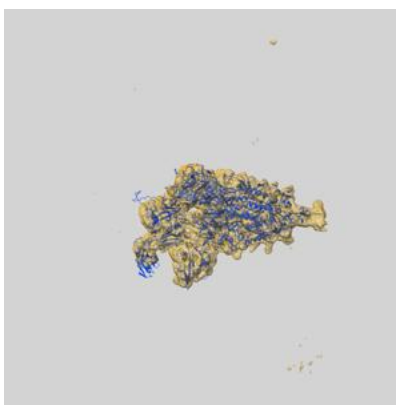
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14315 and PDB model 7R4R. Per-residue inclusion information can be found in section [3](#) on page [12](#).

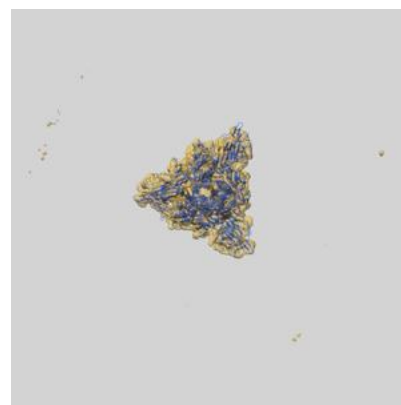
9.1 Map-model overlay [i](#)



X



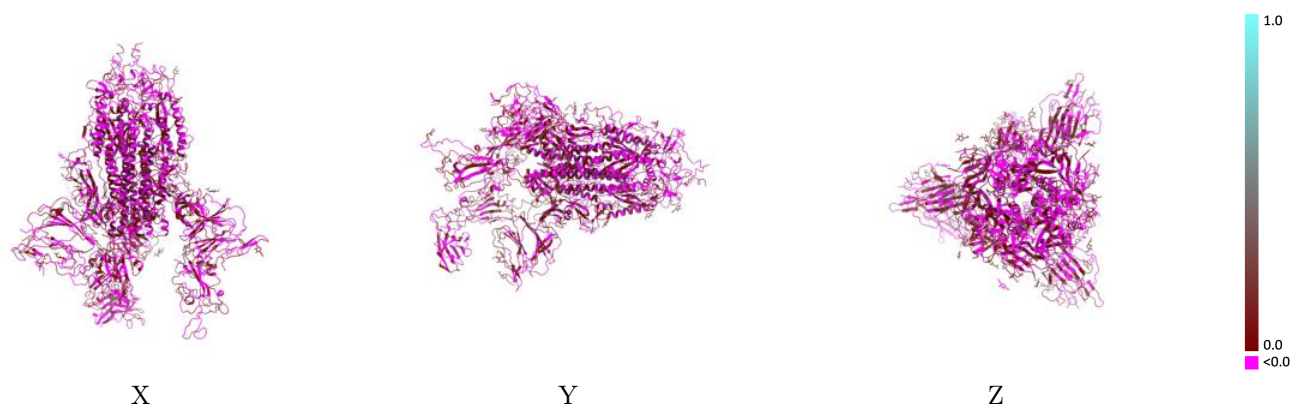
Y



Z

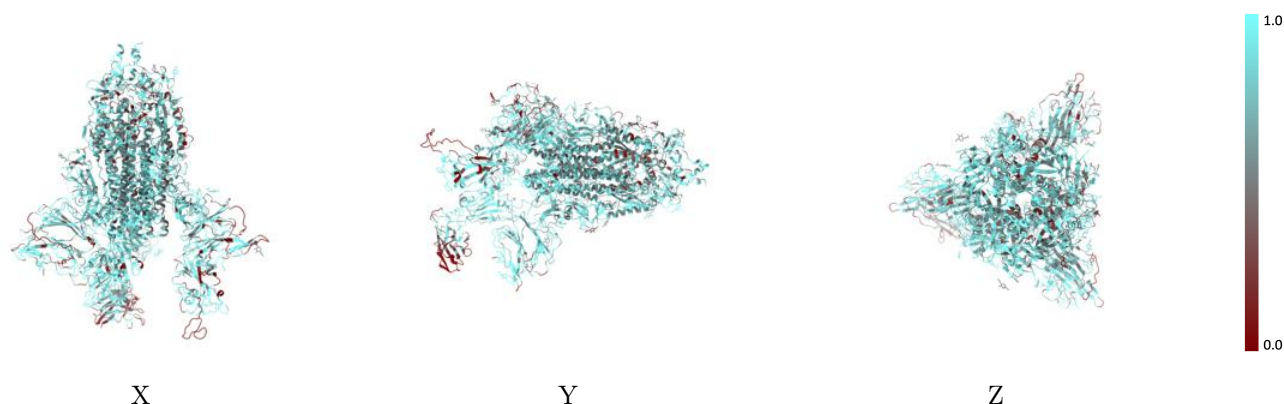
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



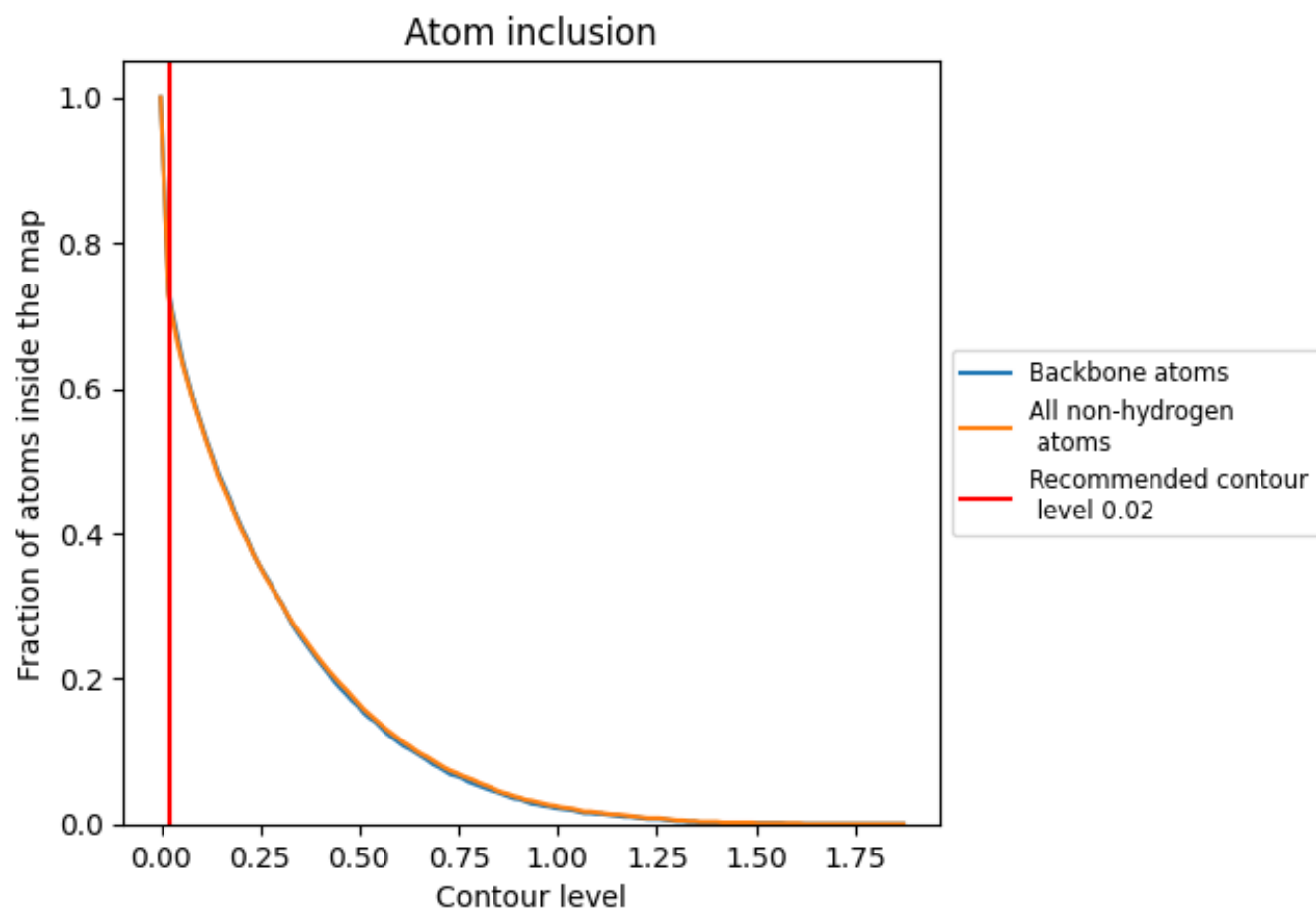
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.0300
A	0.7630	0.0470
B	0.7310	0.0220
C	0.7500	0.0290
D	0.3030	-0.0590
E	1.0000	0.2210
F	0.2500	-0.0160
G	0.5360	-0.0450
H	0.9640	0.2790
I	0.7860	0.2060

1.0

0.0

<0.0