



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:59 AM UTC

PDB ID : 1Q5C / pdb_00001q5c
EMDB ID : EMD-1052
Title : S-S-lambda-shaped TRANS and CIS interactions of cadherins model based on fitting C-cadherin (1L3W) to 3D map of desmosomes obtained by electron tomography
Authors : He, W.; Cowin, P.; Stokes, D.L.
Deposited on : 2003-08-06
Resolution : 30.00 Å (reported)
Based on initial model : 1L3W

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

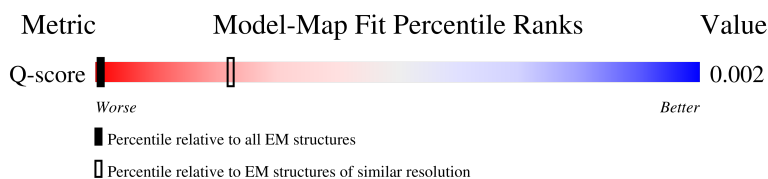
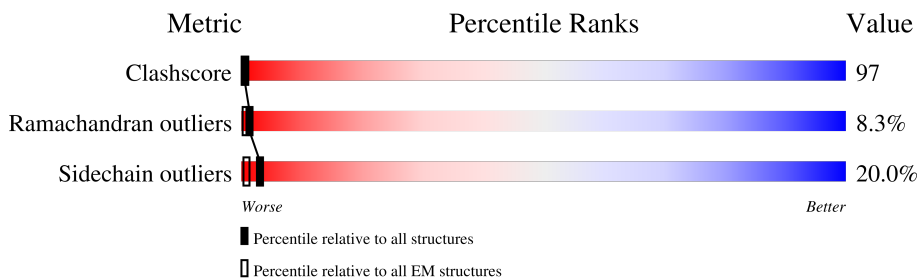
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 30.00 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	9 (30.00 - 30.30)

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	880	60% 14% 28% 14% 5% 39%
1	B	880	61% 14% 28% 15% 5% 39%
1	C	880	61% 13% 28% 15% 5% 39%
1	D	880	60% 13% 29% 15% 5% 39%

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
2	NAG	A	801	-	-	X	-
2	NAG	A	805	X	-	X	-
2	NAG	A	806	X	-	X	-
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-
2	NAG	A	902	X	-	X	-
2	NAG	A	903	X	-	-	-
2	NAG	B	801	-	-	X	-
2	NAG	B	805	X	-	X	-
2	NAG	B	806	X	-	X	-
2	NAG	B	807	-	-	X	-
2	NAG	B	809	-	-	X	-
2	NAG	B	810	-	-	X	-
2	NAG	B	902	X	-	X	-
2	NAG	B	903	X	-	-	-
2	NAG	C	801	-	-	X	-
2	NAG	C	805	X	-	-	-
2	NAG	C	806	X	-	X	-
2	NAG	C	807	-	-	X	-
2	NAG	C	809	-	-	X	-
2	NAG	C	810	-	-	X	-
2	NAG	C	902	X	-	X	-
2	NAG	C	903	X	-	-	-
2	NAG	D	801	-	-	X	-
2	NAG	D	805	X	-	X	-
2	NAG	D	806	X	-	X	-
2	NAG	D	807	-	-	X	-
2	NAG	D	809	-	-	X	-
2	NAG	D	810	-	-	X	-
2	NAG	D	902	X	-	X	-
2	NAG	D	903	X	-	-	-
3	NDG	A	811	-	-	X	-
3	NDG	B	811	-	-	X	-
3	NDG	D	811	-	-	X	-

2 Entry composition [i](#)

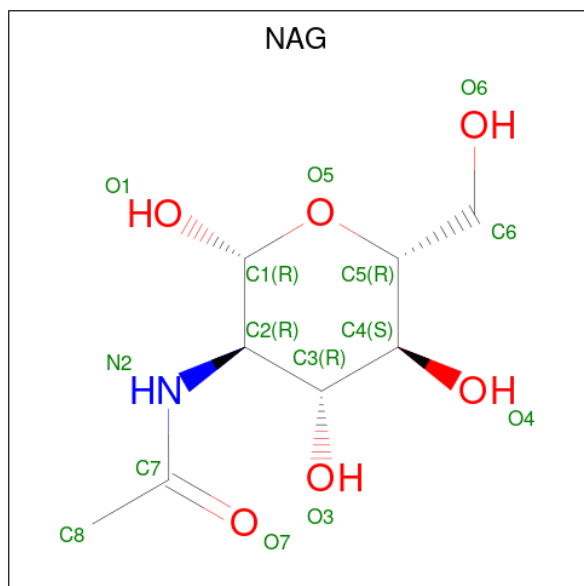
There are 4 unique types of molecules in this entry. The entry contains 17652 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called EP-cadherin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	B	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	C	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	D	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

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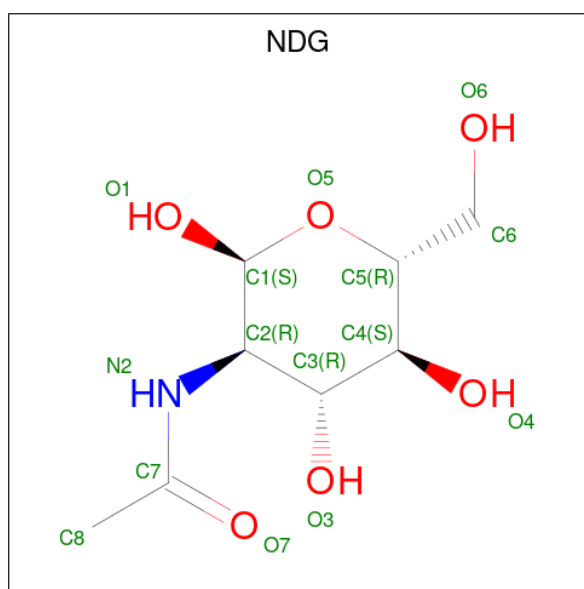
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

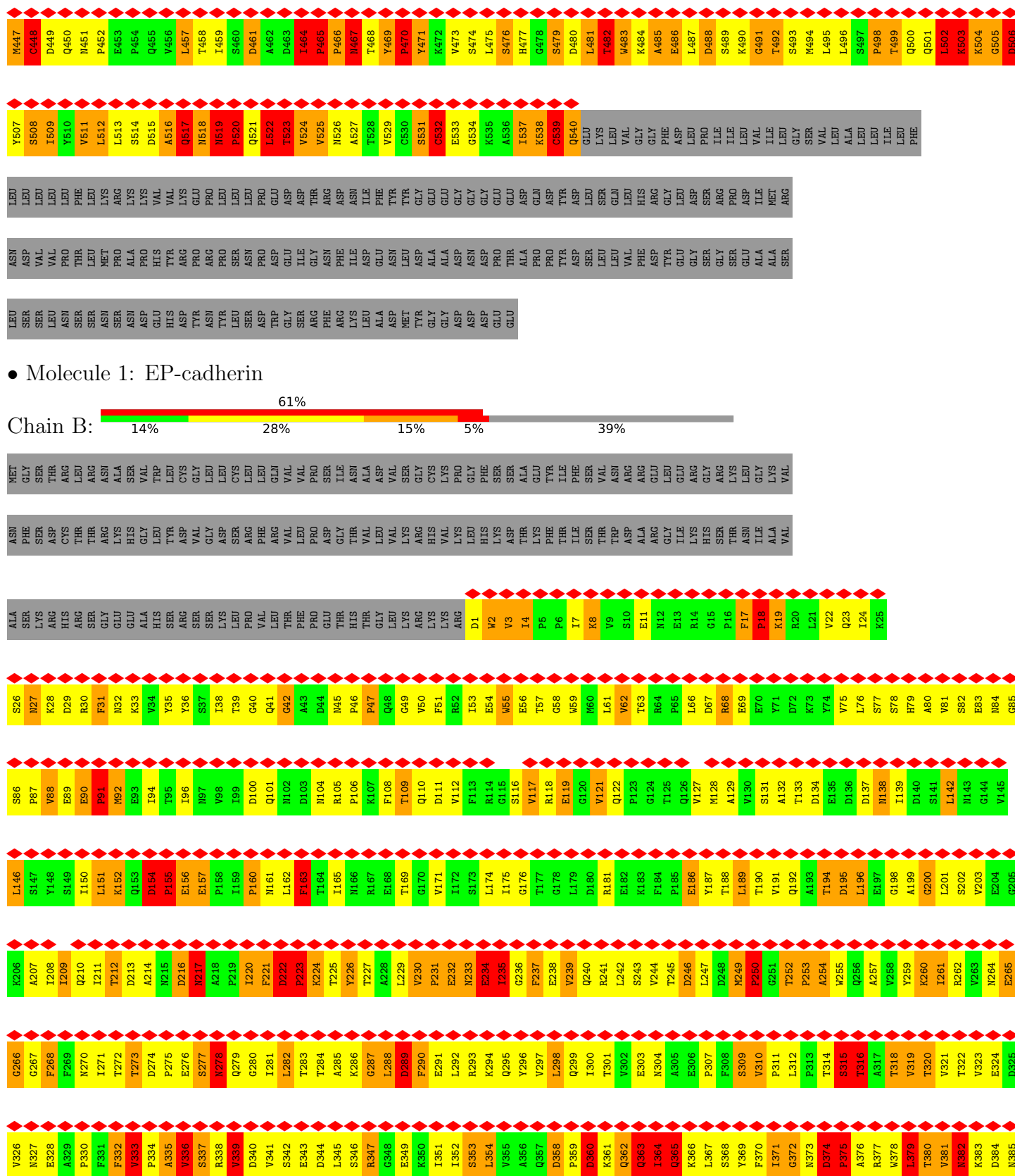
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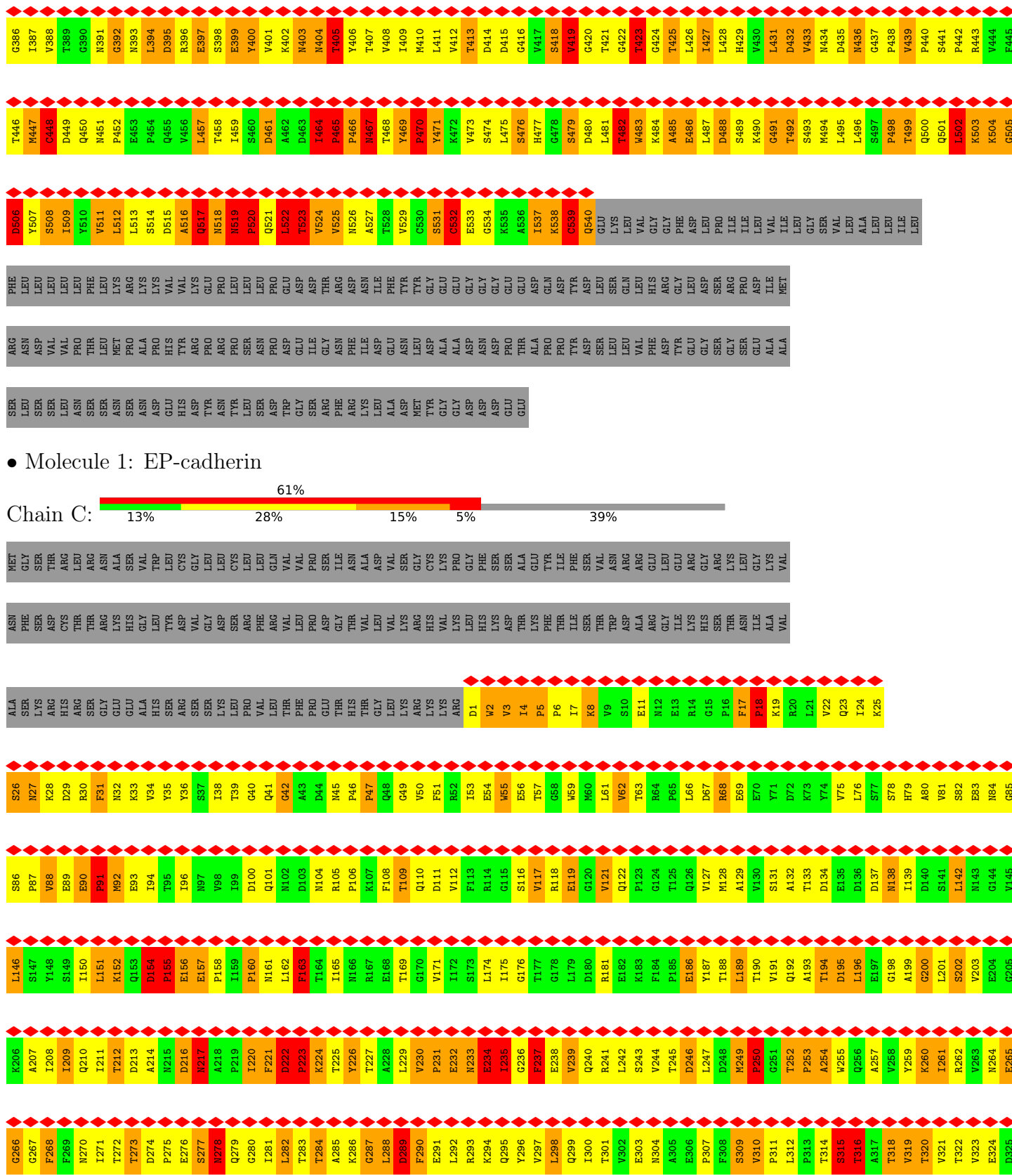
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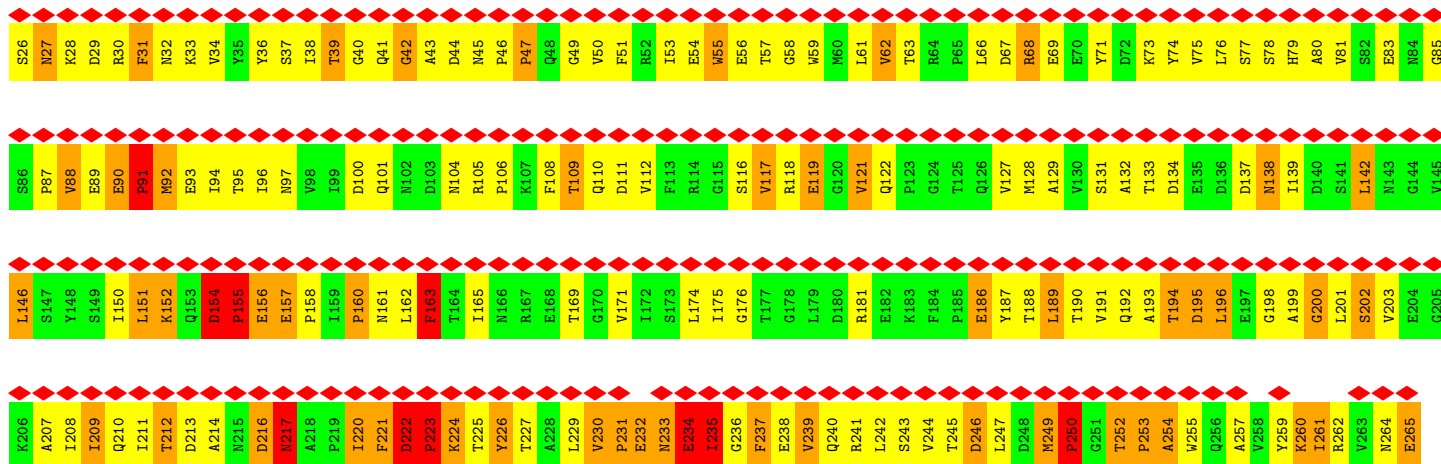
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	A	12	Total	Ca	0
			12	12	
4	B	12	Total	Ca	0
			12	12	
4	C	12	Total	Ca	0
			12	12	
4	D	12	Total	Ca	0
			12	12	







SER	ARG	PHE	D506	T446	G386	V326	G266
LEU	ASN	LEU	Y507	M447	T387	N327	G267
SER	ASP	LEU	S508	C448	V388	E328	G268
VAL	VAL	LEU	S508	D449	T389	A329	F269
LEU	PRO	LEU	V510	Q450	F331	P330	F269
SER	THR	PHE	V511	M451	N391	F332	N270
SER	LEU	LEU	S512	P452	G392	V333	T272
ASN	MET	LEU	S513	P452	G392	V333	T273
SER	PRO	ARG	S513	E453	N393	P334	T273
ASN	ALA	LYS	S514	P454	L394	A335	D274
ASP	PRO	LYS	D515	Q455	D395	V336	P275
GLU	HIS	VAL	D515	Q455	D395	V336	P275
HIS	TYR	VAL	A516	V456	R396	S337	E276
ASP	ARG	LYS	Q517	L457	E397	R338	S277
TYR	PRO	GLU	Q517	L457	E397	R338	S277
ASN	ARG	PRO	N518	T458	R398	V339	N278
PRO	PRO	LEU	N519	I459	E399	D340	Q279
SER	SER	LEU	F520	S460	Y400	D340	Q280
ASN	ASP	LEU	Q521	D461	V401	S342	I281
TRP	ASP	PRO	L522	A462	K402	E343	L282
GLY	ASP	GLU	S523	D463	N403	D344	T283
SER	ILE	ASP	V524	I464	N404	L345	T284
ARG	GLY	THR	V525	P465	T405	S346	A285
PHE	ASN	ARG	N526	P466	Y406	R347	K286
ARG	PHE	ASP	N526	P466	Y406	R347	K286
ILE	ILE	ASN	A527	M467	T407	G348	G287
LEU	ASP	ILE	A527	M467	T407	G348	G287
ALA	GLU	PHE	T528	T468	V408	E349	L288
ASP	ASN	TYR	V529	Y469	T409	K350	D289
LEU	LEU	TYR	F530	P470	M410	I351	F290
MET	ASP	GLY	S531	Y471	L411	T352	E291
TYR	GLY	GLU	S532	K472	V412	S353	L292
GLY	ALA	GLU	S532	K472	V412	S353	L292
ASP	ASP	GLY	E533	V473	T413	L354	R293
ASN	ASN	GLY	S534	S474	D414	V355	K294
ASP	ASP	GLY	K535	L475	D415	A356	Q295
ASP	PRO	GLU	K536	S476	G416	Q357	Y296
GLU	THR	GLU	A536	S476	G416	Q357	Y296
GLU	ALA	ASP	I537	H477	V417	D358	V297
PRO	PRO	GLN	K538	G478	S418	P359	L298
PRO	PRO	TYR	K539	S479	V419	D360	L298
ASP	ASP	ASP	C539	S479	G420	K361	Q299
LEU	LEU	LEU	Q540	D480	T421	Q362	I300
SER	SER	LEU	GLU	L481	T421	Q362	I300
LEU	LEU	SER	LYS	T482	G422	Q363	T301
LEU	GLN	LEU	LEU	M483	T423	I364	V302
VAL	VAL	LEU	VAL	M483	T423	I364	V302
PHE	PHE	HIS	GLY	K484	G424	Q365	E303
ASP	ASP	GLY	GLY	K484	G424	Q365	E303
ASP	ASP	GLY	GLY	K484	G424	Q365	E303
THR	THR	GLY	PHE	A485	L425	L367	N304
GLU	GLU	LEU	ASP	E486	L425	L367	A305
GLY	GLY	LEU	ASP	E486	L425	L367	A305
ASP	ASP	LEU	LEU	L487	I427	S368	E306
SER	SER	PRO	PRO	L487	I427	S368	E306
PRO	PRO	LEU	LEU	D488	L428	Y369	P307
ARG	ARG	ILE	ILE	D488	L428	Y369	P307
SER	SER	PRO	PRO	S489	V430	F370	F308
GLY	GLY	ASP	LEU	K490	I371	V310	S309
SER	SER	PRO	LEU	K490	I371	V310	S309
GLU	GLU	ASP	LEU	K490	I371	V310	S309
ALA	ALA	ILE	VAL	G491	G372	I371	P311
ALA	ALA	ILE	ILE	G491	G372	I371	P311
MET	MET	ILE	ILE	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
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		LEU	LEU	T492	D431	G372	P311
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		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
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		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
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		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
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		LEU	LEU	T492	D431	G372	P311
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		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311
		LEU	LEU	T492	D431	G372	P311

4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	no CTF correction. Imaging at underfocus 0.4 micron with CM200FEG microscope at 50,000 magnification	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1200	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	68276	Depositor
Image detector	GENERIC GATAN	Depositor
Maximum voxel value	6038.000	Depositor
Minimum voxel value	-5609.000	Depositor
Average voxel value	1381.050	Depositor
Voxel value standard deviation	380.764	Depositor
Recommended contour level	1950	Depositor
Tomogram size ($\text{\AA}$)	4765.7, 4765.7, 484.016	wwPDB
Tomogram dimensions	512, 512, 52	wwPDB
Tomogram angles ($^\circ$)	90, 90, 90	wwPDB
Grid spacing ($\text{\AA}$)	9.308, 9.308, 9.308	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.99	24/4276 (0.6%)	2.03	204/5839 (3.5%)
1	B	0.99	25/4276 (0.6%)	2.02	202/5839 (3.5%)
1	C	0.99	24/4276 (0.6%)	2.02	203/5839 (3.5%)
1	D	0.99	24/4276 (0.6%)	2.03	203/5839 (3.5%)
All	All	0.99	97/17104 (0.6%)	2.02	812/23356 (3.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	16

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	522	LEU	N-CA	-18.92	1.34	1.46
1	C	522	LEU	N-CA	-18.89	1.34	1.46
1	A	522	LEU	N-CA	-18.88	1.34	1.46
1	D	522	LEU	N-CA	-18.78	1.34	1.46
1	C	465	PRO	CA-C	12.00	1.58	1.51
1	B	465	PRO	CA-C	11.89	1.58	1.51
1	D	465	PRO	CA-C	11.89	1.58	1.51
1	A	465	PRO	CA-C	11.78	1.58	1.51
1	B	335	ALA	CA-CB	-11.08	1.34	1.52
1	A	335	ALA	CA-CB	-11.06	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	335	ALA	CA-CB	-11.03	1.34	1.52
1	C	335	ALA	CA-CB	-10.98	1.35	1.52
1	D	521	GLN	CA-C	-9.94	1.40	1.52
1	C	521	GLN	CA-C	-9.90	1.40	1.52
1	A	521	GLN	CA-C	-9.84	1.40	1.52
1	B	521	GLN	CA-C	-9.84	1.40	1.52
1	D	523	THR	N-CA	-9.56	1.33	1.46
1	B	523	THR	N-CA	-9.56	1.33	1.46
1	C	523	THR	N-CA	-9.52	1.33	1.46
1	A	523	THR	N-CA	-9.52	1.33	1.46
1	D	522	LEU	CA-C	-9.39	1.40	1.52
1	A	522	LEU	CA-C	-9.35	1.40	1.52
1	B	522	LEU	CA-C	-9.34	1.40	1.52
1	C	522	LEU	CA-C	-9.29	1.40	1.52
1	C	499	THR	CA-CB	7.68	1.66	1.53
1	B	499	THR	CA-CB	7.65	1.66	1.53
1	A	499	THR	CA-CB	7.65	1.66	1.53
1	D	499	THR	CA-CB	7.64	1.66	1.53
1	A	223	PRO	CG-CD	6.79	1.73	1.50
1	B	223	PRO	CG-CD	6.77	1.73	1.50
1	C	223	PRO	CG-CD	6.77	1.73	1.50
1	D	223	PRO	CG-CD	6.75	1.73	1.50
1	C	524	VAL	N-CA	-6.60	1.38	1.46
1	B	524	VAL	N-CA	-6.59	1.38	1.46
1	B	423	THR	CA-CB	-6.58	1.44	1.53
1	D	524	VAL	N-CA	-6.56	1.38	1.46
1	C	523	THR	CA-C	-6.56	1.44	1.52
1	A	423	THR	CA-CB	-6.55	1.44	1.53
1	D	523	THR	CA-C	-6.54	1.44	1.52
1	A	524	VAL	N-CA	-6.53	1.38	1.46
1	B	523	THR	CA-C	-6.53	1.44	1.52
1	C	423	THR	CA-CB	-6.52	1.44	1.53
1	D	423	THR	CA-CB	-6.52	1.44	1.53
1	A	523	THR	CA-C	-6.51	1.44	1.52
1	A	290	PHE	CA-C	-6.23	1.45	1.52
1	D	290	PHE	CA-C	-6.20	1.45	1.52
1	C	290	PHE	CA-C	-6.18	1.45	1.52
1	A	464	ILE	C-N	6.16	1.39	1.33
1	B	290	PHE	CA-C	-6.14	1.45	1.52
1	A	482	THR	CA-CB	-6.10	1.43	1.53
1	B	399	GLU	CA-C	-6.08	1.46	1.52
1	A	399	GLU	CA-C	-6.07	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	482	THR	CA-CB	-6.06	1.43	1.53
1	C	399	GLU	CA-C	-6.06	1.46	1.52
1	B	482	THR	CA-CB	-6.05	1.43	1.53
1	C	482	THR	CA-CB	-6.05	1.43	1.53
1	B	464	ILE	C-N	6.03	1.38	1.33
1	B	481	LEU	N-CA	6.02	1.51	1.46
1	D	481	LEU	N-CA	6.00	1.51	1.46
1	C	481	LEU	N-CA	6.00	1.51	1.46
1	C	464	ILE	C-N	5.99	1.38	1.33
1	D	464	ILE	C-N	5.97	1.38	1.33
1	D	18	PRO	N-CD	5.97	1.56	1.47
1	D	399	GLU	CA-C	-5.96	1.46	1.52
1	C	18	PRO	N-CD	5.95	1.56	1.47
1	B	18	PRO	N-CD	5.94	1.56	1.47
1	A	481	LEU	N-CA	5.93	1.51	1.46
1	A	18	PRO	N-CD	5.90	1.56	1.47
1	B	17	PHE	CA-C	5.83	1.60	1.53
1	D	17	PHE	CA-C	5.81	1.60	1.53
1	A	17	PHE	CA-C	5.79	1.60	1.53
1	C	17	PHE	CA-C	5.76	1.60	1.53
1	A	481	LEU	CA-C	-5.67	1.46	1.52
1	A	521	GLN	N-CA	-5.64	1.39	1.46
1	B	481	LEU	CA-C	-5.61	1.46	1.52
1	B	521	GLN	N-CA	-5.61	1.39	1.46
1	C	481	LEU	CA-C	-5.60	1.46	1.52
1	D	521	GLN	N-CA	-5.58	1.39	1.46
1	D	481	LEU	CA-C	-5.55	1.46	1.52
1	C	521	GLN	N-CA	-5.54	1.39	1.46
1	D	18	PRO	CA-CB	-5.52	1.43	1.53
1	C	18	PRO	CA-CB	-5.51	1.43	1.53
1	A	18	PRO	CA-CB	-5.50	1.43	1.53
1	B	18	PRO	CA-CB	-5.49	1.43	1.53
1	C	320	THR	CA-CB	-5.45	1.45	1.53
1	D	320	THR	CA-CB	-5.41	1.45	1.53
1	C	483	TRP	N-CA	-5.39	1.40	1.46
1	B	320	THR	CA-CB	-5.39	1.46	1.53
1	B	483	TRP	N-CA	-5.37	1.40	1.46
1	D	483	TRP	N-CA	-5.34	1.40	1.46
1	A	483	TRP	N-CA	-5.33	1.40	1.46
1	A	320	THR	CA-CB	-5.33	1.46	1.53
1	C	17	PHE	C-O	-5.23	1.16	1.24
1	A	17	PHE	C-O	-5.18	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	PHE	C-O	-5.17	1.17	1.24
1	D	17	PHE	C-O	-5.17	1.17	1.24
1	B	522	LEU	C-O	5.00	1.27	1.23

All (812) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	290	PHE	N-CA-C	27.42	145.39	108.38
1	A	290	PHE	N-CA-C	27.41	145.38	108.38
1	C	290	PHE	N-CA-C	25.18	145.37	108.60
1	B	290	PHE	N-CA-C	25.17	145.35	108.60
1	C	516	ALA	N-CA-C	-20.89	88.42	114.75
1	B	516	ALA	N-CA-C	-20.88	88.45	114.75
1	A	516	ALA	N-CA-C	-20.88	88.45	114.75
1	D	516	ALA	N-CA-C	-20.86	88.46	114.75
1	B	376	ALA	N-CA-C	19.04	137.09	110.24
1	C	376	ALA	N-CA-C	19.03	137.07	110.24
1	D	376	ALA	N-CA-C	19.03	137.07	110.24
1	A	376	ALA	N-CA-C	19.01	137.05	110.24
1	D	374	ASP	CA-C-N	-17.34	98.17	119.84
1	D	374	ASP	C-N-CA	-17.34	98.17	119.84
1	D	235	ILE	N-CA-C	17.33	145.39	109.34
1	C	235	ILE	N-CA-C	17.33	145.38	109.34
1	B	235	ILE	N-CA-C	17.32	145.37	109.34
1	C	374	ASP	CA-C-N	-17.32	98.19	119.84
1	C	374	ASP	C-N-CA	-17.32	98.19	119.84
1	B	374	ASP	CA-C-N	-17.31	98.21	119.84
1	B	374	ASP	C-N-CA	-17.31	98.21	119.84
1	A	374	ASP	CA-C-N	-17.30	98.21	119.84
1	A	374	ASP	C-N-CA	-17.30	98.21	119.84
1	A	235	ILE	N-CA-C	17.30	145.32	109.34
1	D	481	LEU	N-CA-C	-16.72	85.92	113.50
1	B	481	LEU	N-CA-C	-16.70	85.95	113.50
1	C	481	LEU	N-CA-C	-16.69	85.96	113.50
1	A	481	LEU	N-CA-C	-16.67	85.99	113.50
1	A	520	PRO	N-CA-C	15.92	136.31	111.15
1	C	520	PRO	N-CA-C	15.92	136.30	111.15
1	D	336	VAL	N-CA-C	15.91	132.09	108.54
1	A	336	VAL	N-CA-C	15.91	132.09	108.54
1	B	520	PRO	N-CA-C	15.90	136.27	111.15
1	B	336	VAL	N-CA-C	15.89	132.05	108.54
1	C	336	VAL	N-CA-C	15.87	132.03	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	520	PRO	N-CA-C	15.87	136.23	111.15
1	C	519	ASN	CA-C-N	-15.50	104.09	119.90
1	C	519	ASN	C-N-CA	-15.50	104.09	119.90
1	B	519	ASN	CA-C-N	-15.49	104.10	119.90
1	B	519	ASN	C-N-CA	-15.49	104.10	119.90
1	A	519	ASN	CA-C-N	-15.48	104.11	119.90
1	A	519	ASN	C-N-CA	-15.48	104.11	119.90
1	D	519	ASN	CA-C-N	-15.46	104.13	119.90
1	D	519	ASN	C-N-CA	-15.46	104.13	119.90
1	A	277	SER	N-CA-C	-15.26	91.53	110.61
1	D	277	SER	N-CA-C	-15.24	91.56	110.61
1	B	277	SER	N-CA-C	-15.21	91.59	110.61
1	C	277	SER	N-CA-C	-15.21	91.59	110.61
1	A	492	THR	N-CA-C	14.86	129.31	111.33
1	C	492	THR	N-CA-C	14.83	129.27	111.33
1	D	492	THR	N-CA-C	14.82	129.26	111.33
1	B	492	THR	N-CA-C	14.80	129.24	111.33
1	B	374	ASP	N-CA-C	14.72	142.35	109.81
1	C	374	ASP	N-CA-C	14.71	142.33	109.81
1	D	374	ASP	N-CA-C	14.71	142.33	109.81
1	A	374	ASP	N-CA-C	14.71	142.32	109.81
1	D	398	SER	N-CA-C	14.51	141.71	110.80
1	B	398	SER	N-CA-C	14.51	141.71	110.80
1	A	398	SER	N-CA-C	14.50	141.69	110.80
1	C	398	SER	N-CA-C	14.49	141.66	110.80
1	C	521	GLN	CA-C-N	-13.11	103.22	121.84
1	C	521	GLN	C-N-CA	-13.11	103.22	121.84
1	A	521	GLN	CA-C-N	-13.11	103.23	121.84
1	A	521	GLN	C-N-CA	-13.11	103.23	121.84
1	B	521	GLN	CA-C-N	-13.07	103.28	121.84
1	B	521	GLN	C-N-CA	-13.07	103.28	121.84
1	D	521	GLN	CA-C-N	-13.06	103.30	121.84
1	D	521	GLN	C-N-CA	-13.06	103.30	121.84
1	D	289	ASP	CA-C-N	-12.95	100.61	122.10
1	D	289	ASP	C-N-CA	-12.95	100.61	122.10
1	A	289	ASP	CA-C-N	-12.92	100.65	122.10
1	A	289	ASP	C-N-CA	-12.92	100.65	122.10
1	B	289	ASP	CA-C-N	-12.38	100.63	121.80
1	B	289	ASP	C-N-CA	-12.38	100.63	121.80
1	C	289	ASP	CA-C-N	-12.38	100.64	121.80
1	C	289	ASP	C-N-CA	-12.38	100.64	121.80
1	C	233	ASN	N-CA-C	12.03	132.27	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASN	N-CA-C	12.02	132.26	107.37
1	D	233	ASN	N-CA-C	12.00	132.22	107.37
1	B	233	ASN	N-CA-C	12.00	132.21	107.37
1	A	223	PRO	N-CA-C	-11.92	87.92	112.47
1	C	223	PRO	N-CA-C	-11.91	87.93	112.47
1	D	223	PRO	N-CA-C	-11.91	87.93	112.47
1	B	223	PRO	N-CA-C	-11.91	87.94	112.47
1	B	17	PHE	C-N-CD	-11.54	95.21	120.60
1	C	17	PHE	C-N-CD	-11.54	95.22	120.60
1	A	17	PHE	C-N-CD	-11.53	95.24	120.60
1	D	17	PHE	C-N-CD	-11.53	95.25	120.60
1	B	465	PRO	C-N-CD	-11.04	96.31	120.60
1	C	465	PRO	C-N-CD	-11.04	96.31	120.60
1	D	465	PRO	C-N-CD	-11.04	96.32	120.60
1	A	465	PRO	C-N-CD	-11.01	96.38	120.60
1	B	471	TYR	N-CA-C	10.82	126.50	110.17
1	A	222	ASP	CA-C-N	-10.80	106.34	119.84
1	A	222	ASP	C-N-CA	-10.80	106.34	119.84
1	B	222	ASP	CA-C-N	-10.80	106.34	119.84
1	B	222	ASP	C-N-CA	-10.80	106.34	119.84
1	C	471	TYR	N-CA-C	10.80	126.47	110.17
1	D	222	ASP	CA-C-N	-10.80	106.34	119.84
1	D	222	ASP	C-N-CA	-10.80	106.34	119.84
1	A	471	TYR	N-CA-C	10.78	126.45	110.17
1	D	471	TYR	N-CA-C	10.79	126.45	110.17
1	C	222	ASP	CA-C-N	-10.74	106.41	119.84
1	C	222	ASP	C-N-CA	-10.74	106.41	119.84
1	A	236	GLY	N-CA-C	-10.57	88.13	113.18
1	B	236	GLY	N-CA-C	-10.57	88.14	113.18
1	D	236	GLY	N-CA-C	-10.55	88.17	113.18
1	C	236	GLY	N-CA-C	-10.55	88.18	113.18
1	A	234	GLU	CA-C-N	10.17	140.28	121.97
1	A	234	GLU	C-N-CA	10.17	140.28	121.97
1	D	234	GLU	CA-C-N	10.14	140.22	121.97
1	D	234	GLU	C-N-CA	10.14	140.22	121.97
1	C	234	GLU	CA-C-N	10.13	140.21	121.97
1	C	234	GLU	C-N-CA	10.13	140.21	121.97
1	B	234	GLU	CA-C-N	10.13	140.20	121.97
1	B	234	GLU	C-N-CA	10.13	140.20	121.97
1	C	522	LEU	CA-C-N	-10.12	102.21	121.54
1	C	522	LEU	C-N-CA	-10.12	102.21	121.54
1	A	522	LEU	CA-C-N	-10.11	102.23	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	LEU	C-N-CA	-10.11	102.23	121.54
1	D	522	LEU	CA-C-N	-10.11	102.23	121.54
1	D	522	LEU	C-N-CA	-10.11	102.23	121.54
1	B	522	LEU	CA-C-N	-10.10	102.25	121.54
1	B	522	LEU	C-N-CA	-10.10	102.25	121.54
1	C	230	VAL	CA-C-N	10.07	132.43	119.84
1	C	230	VAL	C-N-CA	10.07	132.43	119.84
1	B	230	VAL	CA-C-N	10.07	132.43	119.84
1	B	230	VAL	C-N-CA	10.07	132.43	119.84
1	A	230	VAL	CA-C-N	10.07	132.43	119.84
1	A	230	VAL	C-N-CA	10.07	132.43	119.84
1	D	230	VAL	CA-C-N	10.06	132.42	119.84
1	D	230	VAL	C-N-CA	10.06	132.42	119.84
1	C	332	PHE	N-CA-C	-9.93	97.42	110.53
1	D	332	PHE	N-CA-C	-9.93	97.42	110.53
1	A	332	PHE	N-CA-C	-9.93	97.42	110.53
1	B	332	PHE	N-CA-C	-9.92	97.43	110.53
1	C	221	PHE	N-CA-C	9.81	124.57	109.96
1	B	221	PHE	N-CA-C	9.80	124.56	109.96
1	A	221	PHE	N-CA-C	9.79	124.55	109.96
1	D	221	PHE	N-CA-C	9.78	124.53	109.96
1	A	362	GLN	N-CA-C	-9.70	90.13	110.80
1	D	362	GLN	N-CA-C	-9.70	90.14	110.80
1	A	374	ASP	CB-CA-C	-9.69	91.08	110.17
1	C	362	GLN	N-CA-C	-9.69	90.16	110.80
1	C	374	ASP	CB-CA-C	-9.69	91.08	110.17
1	B	362	GLN	N-CA-C	-9.69	90.17	110.80
1	B	374	ASP	CB-CA-C	-9.69	91.08	110.17
1	D	374	ASP	CB-CA-C	-9.69	91.08	110.17
1	C	405	THR	N-CA-C	9.68	125.36	110.36
1	A	405	THR	N-CA-C	9.68	125.36	110.36
1	B	405	THR	N-CA-C	9.67	125.35	110.36
1	D	405	THR	N-CA-C	9.67	125.35	110.36
1	A	249	MET	CA-C-N	9.59	131.83	119.84
1	A	249	MET	C-N-CA	9.59	131.83	119.84
1	C	249	MET	CA-C-N	9.57	131.80	119.84
1	C	249	MET	C-N-CA	9.57	131.80	119.84
1	D	398	SER	CA-C-N	-9.57	105.24	122.46
1	D	398	SER	C-N-CA	-9.57	105.24	122.46
1	A	221	PHE	CA-C-N	-9.56	98.46	121.80
1	A	221	PHE	C-N-CA	-9.56	98.46	121.80
1	B	221	PHE	CA-C-N	-9.56	98.47	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	PHE	C-N-CA	-9.56	98.47	121.80
1	C	221	PHE	CA-C-N	-9.56	98.46	121.80
1	C	221	PHE	C-N-CA	-9.56	98.46	121.80
1	D	221	PHE	CA-C-N	-9.56	98.46	121.80
1	D	221	PHE	C-N-CA	-9.56	98.46	121.80
1	A	398	SER	CA-C-N	-9.56	105.25	122.46
1	A	398	SER	C-N-CA	-9.56	105.25	122.46
1	C	398	SER	CA-C-N	-9.56	105.25	122.46
1	C	398	SER	C-N-CA	-9.56	105.25	122.46
1	B	398	SER	CA-C-N	-9.55	105.26	122.46
1	B	398	SER	C-N-CA	-9.55	105.26	122.46
1	C	234	GLU	N-CA-C	-9.54	90.48	110.80
1	A	234	GLU	N-CA-C	-9.54	90.48	110.80
1	B	249	MET	CA-C-N	9.54	131.76	119.84
1	B	249	MET	C-N-CA	9.54	131.76	119.84
1	D	249	MET	CA-C-N	9.53	131.76	119.84
1	D	249	MET	C-N-CA	9.53	131.76	119.84
1	B	234	GLU	N-CA-C	-9.51	90.55	110.80
1	D	234	GLU	N-CA-C	-9.50	90.56	110.80
1	A	319	VAL	N-CA-C	9.43	122.51	108.46
1	C	319	VAL	N-CA-C	9.42	122.50	108.46
1	B	319	VAL	N-CA-C	9.42	122.50	108.46
1	D	319	VAL	N-CA-C	9.41	122.49	108.46
1	D	479	SER	N-CA-C	-9.20	101.75	113.16
1	C	337	SER	N-CA-C	-9.20	91.59	108.24
1	D	337	SER	N-CA-C	-9.19	91.60	108.24
1	A	479	SER	N-CA-C	-9.19	101.77	113.16
1	C	479	SER	N-CA-C	-9.18	101.77	113.16
1	A	337	SER	N-CA-C	-9.18	91.62	108.24
1	B	337	SER	N-CA-C	-9.17	91.64	108.24
1	B	479	SER	N-CA-C	-9.16	101.80	113.16
1	D	503	LYS	N-CA-C	9.00	129.97	110.80
1	C	503	LYS	N-CA-C	8.99	129.94	110.80
1	A	403	ASN	N-CA-C	-8.98	95.78	109.79
1	B	503	LYS	N-CA-C	8.97	129.92	110.80
1	B	403	ASN	N-CA-C	-8.97	95.80	109.79
1	A	503	LYS	N-CA-C	8.97	129.90	110.80
1	D	403	ASN	N-CA-C	-8.97	95.80	109.79
1	C	403	ASN	N-CA-C	-8.96	95.81	109.79
1	D	382	ASN	N-CA-C	-8.64	95.22	108.96
1	B	382	ASN	N-CA-C	-8.63	95.24	108.96
1	A	382	ASN	N-CA-C	-8.61	95.27	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	382	ASN	N-CA-C	-8.61	95.27	108.96
1	B	521	GLN	N-CA-C	-8.48	96.94	109.15
1	D	521	GLN	N-CA-C	-8.48	96.94	109.15
1	C	521	GLN	N-CA-C	-8.47	96.95	109.15
1	A	521	GLN	N-CA-C	-8.47	96.95	109.15
1	C	476	SER	N-CA-C	8.44	128.78	110.80
1	D	476	SER	N-CA-C	8.44	128.78	110.80
1	A	476	SER	N-CA-C	8.44	128.77	110.80
1	B	476	SER	N-CA-C	8.43	128.75	110.80
1	A	397	GLU	N-CA-C	8.38	123.24	112.34
1	B	397	GLU	N-CA-C	8.37	123.22	112.34
1	D	397	GLU	N-CA-C	8.36	123.20	112.34
1	C	397	GLU	N-CA-C	8.36	123.20	112.34
1	A	520	PRO	CA-C-N	8.33	134.65	121.66
1	A	520	PRO	C-N-CA	8.33	134.65	121.66
1	B	520	PRO	CA-C-N	8.31	134.62	121.66
1	B	520	PRO	C-N-CA	8.31	134.62	121.66
1	C	520	PRO	CA-C-N	8.30	134.61	121.66
1	C	520	PRO	C-N-CA	8.30	134.61	121.66
1	A	291	GLU	N-CA-C	-8.28	101.26	112.94
1	D	520	PRO	CA-C-N	8.26	134.54	121.66
1	D	520	PRO	C-N-CA	8.26	134.54	121.66
1	B	291	GLU	N-CA-C	-8.26	101.30	112.94
1	D	291	GLU	N-CA-C	-8.24	101.32	112.94
1	C	291	GLU	N-CA-C	-8.24	101.32	112.94
1	C	532	CYS	N-CA-C	8.11	128.06	110.80
1	A	254	ALA	N-CA-C	-8.10	102.43	112.88
1	D	532	CYS	N-CA-C	8.09	128.03	110.80
1	D	254	ALA	N-CA-C	-8.08	102.45	112.88
1	A	532	CYS	N-CA-C	8.08	128.00	110.80
1	C	254	ALA	N-CA-C	-8.08	102.46	112.88
1	B	222	ASP	N-CA-C	8.07	127.64	109.81
1	B	532	CYS	N-CA-C	8.07	127.98	110.80
1	A	222	ASP	N-CA-C	8.06	127.63	109.81
1	C	31	PHE	N-CA-C	8.06	121.24	111.40
1	D	222	ASP	N-CA-C	8.06	127.62	109.81
1	B	254	ALA	N-CA-C	-8.06	102.48	112.88
1	C	222	ASP	N-CA-C	8.06	127.62	109.81
1	A	31	PHE	N-CA-C	8.05	121.22	111.40
1	B	46	PRO	C-N-CD	-8.05	102.89	120.60
1	D	31	PHE	N-CA-C	8.04	121.21	111.40
1	B	31	PHE	N-CA-C	8.03	121.20	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PRO	C-N-CD	-8.03	102.94	120.60
1	D	46	PRO	C-N-CD	-8.03	102.94	120.60
1	C	46	PRO	C-N-CD	-8.02	102.95	120.60
1	B	290	PHE	CA-C-O	7.96	129.82	121.38
1	C	290	PHE	CA-C-O	7.95	129.81	121.38
1	C	397	GLU	CA-C-N	-7.95	106.36	121.54
1	C	397	GLU	C-N-CA	-7.95	106.36	121.54
1	A	397	GLU	CA-C-N	-7.95	106.36	121.54
1	A	397	GLU	C-N-CA	-7.95	106.36	121.54
1	B	397	GLU	CA-C-N	-7.94	106.38	121.54
1	B	397	GLU	C-N-CA	-7.94	106.38	121.54
1	A	523	THR	N-CA-CB	-7.93	97.10	110.49
1	D	397	GLU	CA-C-N	-7.92	106.40	121.54
1	D	397	GLU	C-N-CA	-7.92	106.40	121.54
1	A	290	PHE	CA-C-O	7.92	129.79	121.31
1	B	523	THR	N-CA-CB	-7.92	97.11	110.49
1	C	523	THR	N-CA-CB	-7.91	97.12	110.49
1	D	290	PHE	CA-C-O	7.91	129.77	121.31
1	D	523	THR	N-CA-CB	-7.90	97.14	110.49
1	B	222	ASP	CA-CB-CG	-7.88	104.72	112.60
1	C	222	ASP	CA-CB-CG	-7.85	104.75	112.60
1	B	381	VAL	N-CA-C	7.83	119.88	108.53
1	C	381	VAL	N-CA-C	7.82	119.87	108.53
1	D	222	ASP	CA-CB-CG	-7.82	104.78	112.60
1	A	222	ASP	CA-CB-CG	-7.81	104.79	112.60
1	A	381	VAL	N-CA-C	7.81	119.85	108.53
1	D	381	VAL	N-CA-C	7.79	119.83	108.53
1	D	502	LEU	N-CA-C	7.78	127.38	110.80
1	C	502	LEU	N-CA-C	7.78	127.36	110.80
1	B	502	LEU	N-CA-C	7.76	127.33	110.80
1	A	502	LEU	N-CA-C	7.76	127.33	110.80
1	D	432	ASP	N-CA-C	7.72	122.43	109.76
1	C	432	ASP	N-CA-C	7.72	122.43	109.76
1	B	432	ASP	N-CA-C	7.72	122.42	109.76
1	C	246	ASP	N-CA-C	-7.71	99.11	110.52
1	A	432	ASP	N-CA-C	7.71	122.40	109.76
1	D	246	ASP	N-CA-C	-7.71	99.12	110.52
1	B	246	ASP	N-CA-C	-7.70	99.13	110.52
1	A	246	ASP	N-CA-C	-7.69	99.14	110.52
1	A	315	SER	N-CA-C	7.68	120.93	108.41
1	B	17	PHE	CA-C-O	-7.68	113.69	120.60
1	C	525	VAL	N-CA-C	-7.67	93.38	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	525	VAL	N-CA-C	-7.65	93.42	109.34
1	B	315	SER	N-CA-C	7.64	120.87	108.41
1	C	315	SER	N-CA-C	7.64	120.87	108.41
1	A	525	VAL	N-CA-C	-7.64	93.45	109.34
1	A	17	PHE	CA-C-O	-7.64	113.72	120.60
1	D	17	PHE	CA-C-O	-7.63	113.73	120.60
1	D	315	SER	N-CA-C	7.63	120.86	108.41
1	B	525	VAL	N-CA-C	-7.63	93.47	109.34
1	C	522	LEU	N-CA-C	-7.59	97.18	108.34
1	C	17	PHE	CA-C-O	-7.59	113.77	120.60
1	A	522	LEU	N-CA-C	-7.59	97.19	108.34
1	B	522	LEU	N-CA-C	-7.58	97.19	108.34
1	A	320	THR	N-CA-C	7.58	120.87	108.52
1	D	522	LEU	N-CA-C	-7.57	97.21	108.34
1	B	320	THR	N-CA-C	7.56	120.85	108.52
1	C	320	THR	N-CA-C	7.56	120.85	108.52
1	C	290	PHE	CA-C-N	7.56	134.01	122.37
1	C	290	PHE	C-N-CA	7.56	134.01	122.37
1	D	320	THR	N-CA-C	7.55	120.83	108.52
1	B	290	PHE	CA-C-N	7.54	133.98	122.37
1	B	290	PHE	C-N-CA	7.54	133.98	122.37
1	D	290	PHE	CA-C-N	7.54	133.98	122.37
1	D	290	PHE	C-N-CA	7.54	133.98	122.37
1	A	290	PHE	CA-C-N	7.53	133.97	122.37
1	A	290	PHE	C-N-CA	7.53	133.97	122.37
1	C	522	LEU	N-CA-CB	7.51	118.57	111.59
1	D	290	PHE	O-C-N	7.50	131.01	122.99
1	A	290	PHE	O-C-N	7.49	131.00	122.99
1	B	339	VAL	N-CA-C	7.45	124.83	109.34
1	C	339	VAL	N-CA-C	7.44	124.82	109.34
1	A	339	VAL	N-CA-C	7.44	124.81	109.34
1	A	522	LEU	N-CA-CB	7.42	118.50	111.59
1	D	339	VAL	N-CA-C	7.42	124.77	109.34
1	D	522	LEU	N-CA-CB	7.41	118.48	111.59
1	B	522	LEU	N-CA-CB	7.40	118.47	111.59
1	C	252	THR	CA-C-N	7.40	129.09	119.84
1	C	252	THR	C-N-CA	7.40	129.09	119.84
1	B	217	ASN	N-CA-C	7.38	121.68	109.95
1	D	217	ASN	N-CA-C	7.38	121.68	109.95
1	D	62	VAL	N-CA-C	-7.37	97.81	108.36
1	C	217	ASN	N-CA-C	7.37	121.67	109.95
1	B	290	PHE	O-C-N	7.35	130.98	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	VAL	N-CA-C	-7.35	97.85	108.36
1	B	252	THR	CA-C-N	7.35	129.03	119.84
1	B	252	THR	C-N-CA	7.35	129.03	119.84
1	A	252	THR	CA-C-N	7.35	129.02	119.84
1	A	252	THR	C-N-CA	7.35	129.02	119.84
1	A	217	ASN	N-CA-C	7.34	121.63	109.95
1	D	252	THR	CA-C-N	7.34	129.02	119.84
1	D	252	THR	C-N-CA	7.34	129.02	119.84
1	B	62	VAL	N-CA-C	-7.34	97.87	108.36
1	C	290	PHE	O-C-N	7.34	130.97	123.26
1	C	62	VAL	N-CA-C	-7.33	97.88	108.36
1	B	379	LEU	N-CA-C	7.21	119.61	110.24
1	C	379	LEU	N-CA-C	7.20	119.60	110.24
1	A	266	GLY	N-CA-C	-7.20	103.28	115.80
1	D	379	LEU	N-CA-C	7.18	119.58	110.24
1	B	266	GLY	N-CA-C	-7.18	103.31	115.80
1	A	379	LEU	N-CA-C	7.17	119.56	110.24
1	D	266	GLY	N-CA-C	-7.16	103.35	115.80
1	C	266	GLY	N-CA-C	-7.14	103.37	115.80
1	A	90	GLU	N-CA-C	-7.13	99.21	109.48
1	D	90	GLU	N-CA-C	-7.13	99.22	109.48
1	C	90	GLU	N-CA-C	-7.12	99.22	109.48
1	B	90	GLU	N-CA-C	-7.12	99.23	109.48
1	B	519	ASN	N-CA-C	7.09	125.49	109.81
1	D	519	ASN	N-CA-C	7.09	125.48	109.81
1	A	358	ASP	CA-C-N	7.08	128.68	119.84
1	A	358	ASP	C-N-CA	7.08	128.68	119.84
1	C	519	ASN	N-CA-C	7.07	125.44	109.81
1	B	485	ALA	N-CA-C	7.07	120.47	110.50
1	D	485	ALA	N-CA-C	7.07	120.46	110.50
1	A	519	ASN	N-CA-C	7.06	125.42	109.81
1	D	358	ASP	CA-C-N	7.06	128.67	119.84
1	D	358	ASP	C-N-CA	7.06	128.67	119.84
1	A	485	ALA	N-CA-C	7.05	120.45	110.50
1	C	358	ASP	CA-C-N	7.05	128.65	119.84
1	C	358	ASP	C-N-CA	7.05	128.65	119.84
1	B	358	ASP	CA-C-N	7.05	128.65	119.84
1	B	358	ASP	C-N-CA	7.05	128.65	119.84
1	D	194	THR	N-CA-C	7.03	120.60	109.50
1	C	485	ALA	N-CA-C	7.02	120.40	110.50
1	C	399	GLU	N-CA-C	7.01	121.69	112.72
1	B	194	THR	N-CA-C	7.00	120.56	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	THR	N-CA-C	7.00	120.56	109.50
1	C	439	VAL	CA-C-N	7.00	126.76	119.76
1	C	439	VAL	C-N-CA	7.00	126.76	119.76
1	B	399	GLU	N-CA-C	7.00	121.67	112.72
1	B	439	VAL	CA-C-N	6.99	126.75	119.76
1	B	439	VAL	C-N-CA	6.99	126.75	119.76
1	D	399	GLU	N-CA-C	6.98	121.65	112.72
1	A	399	GLU	N-CA-C	6.98	121.65	112.72
1	D	439	VAL	CA-C-N	6.98	126.74	119.76
1	D	439	VAL	C-N-CA	6.98	126.74	119.76
1	C	194	THR	N-CA-C	6.97	120.52	109.50
1	A	104	ASN	N-CA-C	6.95	120.25	109.07
1	B	104	ASN	N-CA-C	6.94	120.25	109.07
1	A	439	VAL	CA-C-N	6.94	126.70	119.76
1	A	439	VAL	C-N-CA	6.94	126.70	119.76
1	D	104	ASN	N-CA-C	6.93	120.22	109.07
1	C	104	ASN	N-CA-C	6.92	120.21	109.07
1	A	481	LEU	CA-C-O	6.92	126.05	118.65
1	B	481	LEU	CA-C-O	6.91	126.05	118.65
1	C	481	LEU	CA-C-O	6.90	126.03	118.65
1	C	364	ILE	N-CA-C	-6.89	95.00	109.34
1	C	252	THR	N-CA-C	6.88	119.34	110.39
1	A	364	ILE	N-CA-C	-6.88	95.03	109.34
1	B	491	GLY	N-CA-C	6.88	129.47	113.18
1	D	252	THR	N-CA-C	6.88	119.33	110.39
1	D	364	ILE	N-CA-C	-6.87	95.04	109.34
1	B	364	ILE	N-CA-C	-6.87	95.05	109.34
1	A	252	THR	N-CA-C	6.87	119.32	110.39
1	D	481	LEU	CA-C-O	6.87	126.00	118.65
1	D	491	GLY	N-CA-C	6.86	129.44	113.18
1	B	252	THR	N-CA-C	6.86	119.30	110.39
1	B	221	PHE	CA-C-O	-6.85	112.82	120.70
1	A	491	GLY	N-CA-C	6.85	129.41	113.18
1	A	520	PRO	CA-C-O	6.84	129.09	121.36
1	C	491	GLY	N-CA-C	6.84	129.38	113.18
1	C	520	PRO	CA-C-O	6.84	129.09	121.36
1	A	221	PHE	CA-C-O	-6.83	112.84	120.70
1	B	520	PRO	CA-C-O	6.83	129.08	121.36
1	C	119	GLU	N-CA-C	6.82	118.71	111.28
1	D	520	PRO	CA-C-O	6.80	129.05	121.36
1	C	221	PHE	CA-C-O	-6.80	112.88	120.70
1	D	119	GLU	N-CA-C	6.79	118.69	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	PHE	CA-C-O	-6.79	112.89	120.70
1	B	119	GLU	N-CA-C	6.78	118.67	111.28
1	A	119	GLU	N-CA-C	6.76	118.65	111.28
1	C	484	LYS	CA-C-N	6.74	131.51	120.94
1	C	484	LYS	C-N-CA	6.74	131.51	120.94
1	A	484	LYS	CA-C-N	6.68	131.43	120.94
1	A	484	LYS	C-N-CA	6.68	131.43	120.94
1	B	484	LYS	CA-C-N	6.68	131.42	120.94
1	B	484	LYS	C-N-CA	6.68	131.42	120.94
1	D	484	LYS	CA-C-N	6.66	131.40	120.94
1	D	484	LYS	C-N-CA	6.66	131.40	120.94
1	A	2	TRP	N-CA-C	-6.63	94.71	107.57
1	D	2	TRP	N-CA-C	-6.62	94.73	107.57
1	B	2	TRP	N-CA-C	-6.60	94.76	107.57
1	C	2	TRP	N-CA-C	-6.60	94.76	107.57
1	B	46	PRO	CA-C-N	6.58	142.79	127.00
1	B	46	PRO	C-N-CA	6.58	142.79	127.00
1	A	232	GLU	N-CA-C	6.57	119.03	111.02
1	D	486	GLU	N-CA-C	6.56	118.49	108.52
1	C	46	PRO	CA-C-N	6.54	142.71	127.00
1	C	46	PRO	C-N-CA	6.54	142.71	127.00
1	A	46	PRO	CA-C-N	6.54	142.69	127.00
1	A	46	PRO	C-N-CA	6.54	142.69	127.00
1	D	437	GLY	CA-C-N	6.54	128.01	119.84
1	D	437	GLY	C-N-CA	6.54	128.01	119.84
1	A	486	GLU	N-CA-C	6.53	118.45	108.52
1	D	46	PRO	CA-C-N	6.53	142.68	127.00
1	D	46	PRO	C-N-CA	6.53	142.68	127.00
1	C	486	GLU	N-CA-C	6.53	118.45	108.52
1	A	437	GLY	CA-C-N	6.53	128.00	119.84
1	A	437	GLY	C-N-CA	6.53	128.00	119.84
1	B	486	GLU	N-CA-C	6.52	118.43	108.52
1	D	232	GLU	N-CA-C	6.52	118.97	111.02
1	B	335	ALA	N-CA-C	-6.51	93.90	107.37
1	C	232	GLU	N-CA-C	6.51	118.96	111.02
1	A	335	ALA	N-CA-C	-6.50	93.91	107.37
1	C	335	ALA	N-CA-C	-6.50	93.91	107.37
1	B	437	GLY	CA-C-N	6.50	127.97	119.84
1	B	437	GLY	C-N-CA	6.50	127.97	119.84
1	D	335	ALA	N-CA-C	-6.50	93.92	107.37
1	C	437	GLY	CA-C-N	6.48	127.94	119.84
1	C	437	GLY	C-N-CA	6.48	127.94	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	GLU	N-CA-C	6.48	118.92	111.02
1	A	539	CYS	N-CA-C	6.45	124.55	110.80
1	B	522	LEU	CA-CB-CG	-6.45	93.73	116.30
1	B	539	CYS	N-CA-C	6.45	124.54	110.80
1	D	539	CYS	N-CA-C	6.45	124.54	110.80
1	A	522	LEU	CA-CB-CG	-6.45	93.74	116.30
1	D	522	LEU	CA-CB-CG	-6.44	93.75	116.30
1	C	539	CYS	N-CA-C	6.44	124.52	110.80
1	D	121	VAL	N-CA-C	6.44	117.48	110.21
1	B	400	TYR	N-CA-C	-6.43	103.55	111.40
1	C	522	LEU	CA-CB-CG	-6.43	93.78	116.30
1	D	400	TYR	N-CA-C	-6.43	103.55	111.40
1	A	400	TYR	N-CA-C	-6.43	103.56	111.40
1	B	230	VAL	C-N-CD	-6.42	98.66	125.00
1	C	230	VAL	C-N-CD	-6.41	98.72	125.00
1	A	121	VAL	N-CA-C	6.41	117.45	110.21
1	D	230	VAL	C-N-CD	-6.41	98.74	125.00
1	A	230	VAL	C-N-CD	-6.40	98.74	125.00
1	C	121	VAL	N-CA-C	6.40	117.44	110.21
1	B	121	VAL	N-CA-C	6.39	117.44	110.21
1	D	531	SER	N-CA-C	6.39	124.42	110.80
1	C	531	SER	N-CA-C	6.39	124.41	110.80
1	C	400	TYR	N-CA-C	-6.38	103.61	111.40
1	A	531	SER	N-CA-C	6.37	124.38	110.80
1	B	531	SER	N-CA-C	6.37	124.38	110.80
1	D	42	GLY	N-CA-C	-6.37	107.50	115.08
1	A	42	GLY	N-CA-C	-6.35	107.52	115.08
1	B	42	GLY	N-CA-C	-6.35	107.52	115.08
1	A	328	GLU	N-CA-C	6.34	120.25	110.42
1	C	328	GLU	N-CA-C	6.34	120.25	110.42
1	C	42	GLY	N-CA-C	-6.34	107.54	115.08
1	D	328	GLU	N-CA-C	6.34	120.24	110.42
1	C	26	SER	N-CA-C	-6.34	99.37	109.76
1	B	431	LEU	N-CA-C	6.33	119.02	109.41
1	A	431	LEU	N-CA-C	6.32	119.02	109.41
1	B	26	SER	N-CA-C	-6.32	99.40	109.76
1	D	26	SER	N-CA-C	-6.32	99.40	109.76
1	C	431	LEU	N-CA-C	6.31	119.01	109.41
1	A	26	SER	N-CA-C	-6.30	99.43	109.76
1	B	328	GLU	N-CA-C	6.30	120.19	110.42
1	D	431	LEU	N-CA-C	6.29	118.98	109.41
1	C	380	THR	N-CA-C	6.26	118.70	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	ASN	N-CA-C	-6.25	100.95	110.14
1	D	304	ASN	N-CA-C	-6.25	100.95	110.14
1	B	380	THR	N-CA-C	6.24	118.67	108.55
1	D	122	GLN	N-CA-C	6.24	118.91	110.29
1	D	380	THR	N-CA-C	6.24	118.66	108.55
1	A	304	ASN	N-CA-C	-6.24	100.97	110.14
1	A	380	THR	N-CA-C	6.23	118.64	108.55
1	C	413	THR	N-CA-C	6.23	119.05	108.90
1	C	122	GLN	N-CA-C	6.22	118.88	110.29
1	B	304	ASN	N-CA-C	-6.22	101.00	110.14
1	A	122	GLN	N-CA-C	6.22	118.87	110.29
1	B	413	THR	N-CA-C	6.21	119.03	108.90
1	A	233	ASN	CB-CA-C	-6.21	103.25	111.82
1	A	413	THR	N-CA-C	6.20	119.01	108.90
1	D	233	ASN	CB-CA-C	-6.20	103.26	111.82
1	B	233	ASN	CB-CA-C	-6.20	103.26	111.82
1	D	413	THR	N-CA-C	6.20	119.00	108.90
1	B	122	GLN	N-CA-C	6.19	118.84	110.29
1	C	233	ASN	CB-CA-C	-6.19	103.27	111.82
1	A	186	GLU	N-CA-C	6.18	118.37	107.61
1	C	186	GLU	N-CA-C	6.17	118.35	107.61
1	C	470	PRO	N-CA-C	6.17	125.19	112.47
1	A	222	ASP	N-CA-CB	6.17	121.35	110.37
1	B	470	PRO	N-CA-C	6.17	125.17	112.47
1	B	163	PHE	N-CA-C	6.16	118.31	109.14
1	D	222	ASP	N-CA-CB	6.15	121.33	110.37
1	D	470	PRO	N-CA-C	6.15	125.15	112.47
1	D	503	LYS	CB-CA-C	-6.15	98.19	110.42
1	D	163	PHE	N-CA-C	6.14	118.29	109.14
1	C	222	ASP	N-CA-CB	6.14	121.30	110.37
1	A	163	PHE	N-CA-C	6.14	118.29	109.14
1	B	222	ASP	N-CA-CB	6.14	121.29	110.37
1	B	39	THR	N-CA-C	6.13	119.03	109.52
1	C	163	PHE	N-CA-C	6.13	118.28	109.14
1	A	39	THR	N-CA-C	6.13	119.02	109.52
1	B	503	LYS	CB-CA-C	-6.13	98.22	110.42
1	C	503	LYS	CB-CA-C	-6.13	98.22	110.42
1	A	470	PRO	N-CA-C	6.13	125.09	112.47
1	A	503	LYS	CB-CA-C	-6.12	98.24	110.42
1	D	39	THR	N-CA-C	6.12	119.00	109.52
1	C	39	THR	N-CA-C	6.11	119.00	109.52
1	B	186	GLU	N-CA-C	6.11	118.36	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	PRO	CA-N-CD	-6.10	102.96	111.50
1	C	234	GLU	O-C-N	6.10	130.70	122.59
1	D	186	GLU	N-CA-C	6.09	118.34	107.80
1	B	234	GLU	O-C-N	6.09	130.69	122.59
1	C	18	PRO	CA-N-CD	-6.09	102.97	111.50
1	D	18	PRO	CA-N-CD	-6.08	102.99	111.50
1	A	18	PRO	CA-N-CD	-6.08	102.99	111.50
1	D	234	GLU	O-C-N	6.07	130.67	122.59
1	A	234	GLU	O-C-N	6.06	130.65	122.59
1	C	488	ASP	N-CA-C	-6.05	101.97	110.50
1	D	157	GLU	CA-C-N	6.05	141.52	127.00
1	D	157	GLU	C-N-CA	6.05	141.52	127.00
1	D	481	LEU	CA-CB-CG	-6.04	95.14	116.30
1	B	481	LEU	CA-CB-CG	-6.04	95.15	116.30
1	C	157	GLU	CA-C-N	6.04	141.50	127.00
1	C	157	GLU	C-N-CA	6.04	141.50	127.00
1	A	481	LEU	CA-CB-CG	-6.04	95.16	116.30
1	A	157	GLU	CA-C-N	6.03	141.48	127.00
1	A	157	GLU	C-N-CA	6.03	141.48	127.00
1	C	481	LEU	CA-CB-CG	-6.03	95.19	116.30
1	B	376	ALA	CA-C-N	6.03	133.05	121.54
1	B	376	ALA	C-N-CA	6.03	133.05	121.54
1	A	376	ALA	CA-C-N	6.02	133.04	121.54
1	A	376	ALA	C-N-CA	6.02	133.04	121.54
1	A	488	ASP	N-CA-C	-6.02	102.01	110.50
1	D	488	ASP	N-CA-C	-6.02	102.01	110.50
1	B	157	GLU	CA-C-N	6.02	141.44	127.00
1	B	157	GLU	C-N-CA	6.02	141.44	127.00
1	B	488	ASP	N-CA-C	-6.02	102.01	110.50
1	D	376	ALA	CA-C-N	6.01	133.02	121.54
1	D	376	ALA	C-N-CA	6.01	133.02	121.54
1	C	376	ALA	CA-C-N	5.99	132.98	121.54
1	C	376	ALA	C-N-CA	5.99	132.98	121.54
1	A	504	LYS	N-CA-C	5.94	119.39	108.58
1	D	504	LYS	N-CA-C	5.93	119.38	108.58
1	A	245	THR	N-CA-C	5.91	117.10	107.23
1	B	504	LYS	N-CA-C	5.91	119.34	108.58
1	C	504	LYS	N-CA-C	5.90	119.32	108.58
1	C	245	THR	N-CA-C	5.88	117.05	107.23
1	B	245	THR	N-CA-C	5.86	117.01	107.23
1	D	245	THR	N-CA-C	5.86	117.01	107.23
1	D	505	GLY	N-CA-C	5.84	127.03	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	505	GLY	N-CA-C	5.84	127.03	113.18
1	B	314	THR	CA-C-N	-5.84	114.77	123.00
1	B	314	THR	C-N-CA	-5.84	114.77	123.00
1	A	314	THR	CA-C-N	-5.83	114.78	123.00
1	A	314	THR	C-N-CA	-5.83	114.78	123.00
1	B	505	GLY	N-CA-C	5.82	126.98	113.18
1	D	314	THR	CA-C-N	-5.82	114.79	123.00
1	D	314	THR	C-N-CA	-5.82	114.79	123.00
1	A	505	GLY	N-CA-C	5.81	126.95	113.18
1	C	314	THR	CA-C-N	-5.80	114.81	123.00
1	C	314	THR	C-N-CA	-5.80	114.81	123.00
1	A	469	TYR	CA-C-N	5.78	127.06	119.84
1	A	469	TYR	C-N-CA	5.78	127.06	119.84
1	D	481	LEU	O-C-N	5.78	128.66	121.84
1	C	481	LEU	O-C-N	5.76	128.64	121.84
1	B	481	LEU	O-C-N	5.75	128.63	121.84
1	A	465	PRO	CA-C-N	5.75	140.80	127.00
1	A	465	PRO	C-N-CA	5.75	140.80	127.00
1	C	465	PRO	CA-C-N	5.75	140.80	127.00
1	C	465	PRO	C-N-CA	5.75	140.80	127.00
1	B	465	PRO	CA-C-N	5.75	140.80	127.00
1	B	465	PRO	C-N-CA	5.75	140.80	127.00
1	D	326	VAL	N-CA-C	-5.74	100.00	108.85
1	D	465	PRO	CA-C-N	5.74	140.78	127.00
1	D	465	PRO	C-N-CA	5.74	140.78	127.00
1	D	469	TYR	CA-C-N	5.74	127.02	119.84
1	D	469	TYR	C-N-CA	5.74	127.02	119.84
1	A	481	LEU	O-C-N	5.73	128.60	121.84
1	B	326	VAL	N-CA-C	-5.73	100.02	108.85
1	A	326	VAL	N-CA-C	-5.73	100.03	108.85
1	C	326	VAL	N-CA-C	-5.72	100.03	108.85
1	D	520	PRO	O-C-N	5.72	130.16	122.89
1	C	469	TYR	CA-C-N	5.72	126.99	119.84
1	C	469	TYR	C-N-CA	5.72	126.99	119.84
1	B	469	TYR	CA-C-N	5.70	126.97	119.84
1	B	469	TYR	C-N-CA	5.70	126.97	119.84
1	C	353	SER	N-CA-C	-5.68	99.87	108.67
1	A	520	PRO	O-C-N	5.67	130.09	122.89
1	B	353	SER	N-CA-C	-5.67	99.88	108.67
1	B	520	PRO	O-C-N	5.66	130.07	122.89
1	C	520	PRO	O-C-N	5.66	130.07	122.89
1	C	376	ALA	CA-C-O	5.65	127.37	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	353	SER	N-CA-C	-5.65	99.91	108.67
1	D	376	ALA	CA-C-O	5.65	127.37	121.15
1	D	235	ILE	N-CA-CB	-5.64	101.92	111.23
1	A	376	ALA	CA-C-O	5.64	127.36	121.15
1	B	235	ILE	N-CA-CB	-5.64	101.92	111.23
1	A	235	ILE	N-CA-CB	-5.64	101.93	111.23
1	A	353	SER	N-CA-C	-5.63	99.94	108.67
1	B	376	ALA	CA-C-O	5.62	127.33	121.15
1	C	235	ILE	N-CA-CB	-5.62	101.96	111.23
1	D	365	GLN	CA-C-N	-5.60	112.91	123.27
1	D	365	GLN	C-N-CA	-5.60	112.91	123.27
1	B	365	GLN	CA-C-N	-5.59	112.94	123.27
1	B	365	GLN	C-N-CA	-5.59	112.94	123.27
1	D	237	PHE	N-CA-C	5.59	117.59	108.76
1	A	237	PHE	N-CA-C	5.58	117.58	108.76
1	C	365	GLN	CA-C-N	-5.58	112.94	123.27
1	C	365	GLN	C-N-CA	-5.58	112.94	123.27
1	D	133	THR	N-CA-C	5.58	117.56	109.07
1	B	418	SER	N-CA-C	5.57	122.67	110.80
1	A	365	GLN	CA-C-N	-5.57	112.97	123.27
1	A	365	GLN	C-N-CA	-5.57	112.97	123.27
1	B	133	THR	N-CA-C	5.56	117.53	109.07
1	D	418	SER	N-CA-C	5.56	122.65	110.80
1	A	418	SER	N-CA-C	5.56	122.64	110.80
1	B	237	PHE	N-CA-C	5.55	117.54	108.76
1	A	133	THR	N-CA-C	5.55	117.50	109.07
1	C	133	THR	N-CA-C	5.54	117.50	109.07
1	C	237	PHE	N-CA-C	5.54	117.52	108.76
1	C	418	SER	N-CA-C	5.54	122.60	110.80
1	B	538	LYS	N-CA-C	-5.49	102.16	110.28
1	A	538	LYS	N-CA-C	-5.48	102.17	110.28
1	B	224	LYS	N-CA-C	-5.47	107.15	113.88
1	C	222	ASP	C-N-CD	-5.47	102.56	125.00
1	A	222	ASP	C-N-CD	-5.47	102.56	125.00
1	C	538	LYS	N-CA-C	-5.47	102.18	110.28
1	D	157	GLU	C-N-CD	-5.47	108.56	120.60
1	D	538	LYS	N-CA-C	-5.47	102.18	110.28
1	A	157	GLU	C-N-CD	-5.47	108.57	120.60
1	B	222	ASP	C-N-CD	-5.47	102.58	125.00
1	C	157	GLU	C-N-CD	-5.47	108.57	120.60
1	D	222	ASP	C-N-CD	-5.47	102.58	125.00
1	C	224	LYS	N-CA-C	-5.47	107.16	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	GLU	C-N-CD	-5.45	108.60	120.60
1	D	4	ILE	CA-C-N	5.45	126.00	120.38
1	D	4	ILE	C-N-CA	5.45	126.00	120.38
1	A	480	ASP	CA-C-N	5.45	128.56	120.17
1	A	480	ASP	C-N-CA	5.45	128.56	120.17
1	A	224	LYS	N-CA-C	-5.44	107.19	113.88
1	C	532	CYS	N-CA-CB	-5.44	101.29	110.49
1	D	224	LYS	N-CA-C	-5.44	107.19	113.88
1	C	235	ILE	CA-C-N	5.43	132.06	121.41
1	C	235	ILE	C-N-CA	5.43	132.06	121.41
1	D	392	GLY	N-CA-C	5.43	122.07	112.83
1	D	532	CYS	N-CA-CB	-5.43	101.31	110.49
1	B	4	ILE	CA-C-N	5.43	125.97	120.38
1	B	4	ILE	C-N-CA	5.43	125.97	120.38
1	B	480	ASP	CA-C-N	5.43	128.54	120.17
1	B	480	ASP	C-N-CA	5.43	128.54	120.17
1	D	235	ILE	CA-C-N	5.43	132.05	121.41
1	D	235	ILE	C-N-CA	5.43	132.05	121.41
1	C	392	GLY	N-CA-C	5.43	122.05	112.83
1	C	480	ASP	CA-C-N	5.43	128.53	120.17
1	C	480	ASP	C-N-CA	5.43	128.53	120.17
1	A	392	GLY	N-CA-C	5.42	122.05	112.83
1	D	480	ASP	CA-C-N	5.42	128.52	120.17
1	D	480	ASP	C-N-CA	5.42	128.52	120.17
1	B	235	ILE	CA-C-N	5.42	132.04	121.41
1	B	235	ILE	C-N-CA	5.42	132.04	121.41
1	B	392	GLY	N-CA-C	5.42	122.05	112.83
1	D	448	CYS	CA-CB-SG	-5.42	101.93	114.40
1	A	4	ILE	CA-C-N	5.42	125.96	120.38
1	A	4	ILE	C-N-CA	5.42	125.96	120.38
1	A	532	CYS	N-CA-CB	-5.42	101.33	110.49
1	A	235	ILE	CA-C-N	5.42	132.03	121.41
1	A	235	ILE	C-N-CA	5.42	132.03	121.41
1	C	4	ILE	CA-C-N	5.42	125.96	120.38
1	C	4	ILE	C-N-CA	5.42	125.96	120.38
1	A	448	CYS	CA-CB-SG	-5.41	101.96	114.40
1	D	502	LEU	CB-CA-C	-5.41	99.67	110.42
1	B	448	CYS	CA-CB-SG	-5.40	101.98	114.40
1	C	448	CYS	CA-CB-SG	-5.40	101.97	114.40
1	B	502	LEU	CB-CA-C	-5.40	99.68	110.42
1	B	532	CYS	N-CA-CB	-5.39	101.37	110.49
1	C	502	LEU	CB-CA-C	-5.39	99.69	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	LEU	CB-CA-C	-5.39	99.69	110.42
1	A	209	ILE	N-CA-C	5.38	115.70	108.17
1	C	209	ILE	N-CA-C	5.37	115.69	108.17
1	B	209	ILE	N-CA-C	5.35	115.66	108.17
1	D	209	ILE	N-CA-C	5.34	115.65	108.17
1	A	527	ALA	N-CA-C	5.34	117.03	107.80
1	B	142	LEU	N-CA-C	-5.34	105.99	112.88
1	A	142	LEU	N-CA-C	-5.33	106.00	112.88
1	B	527	ALA	N-CA-C	5.33	117.02	107.80
1	C	527	ALA	N-CA-C	5.32	117.00	107.80
1	A	465	PRO	N-CA-C	5.31	115.57	110.47
1	D	527	ALA	N-CA-C	5.31	116.98	107.80
1	D	142	LEU	N-CA-C	-5.30	106.04	112.88
1	D	295	GLN	N-CA-C	5.29	118.44	109.76
1	D	250	PRO	N-CA-C	5.29	123.36	112.47
1	D	465	PRO	N-CA-C	5.29	115.55	110.47
1	C	142	LEU	N-CA-C	-5.29	106.06	112.88
1	A	295	GLN	N-CA-C	5.28	118.42	109.76
1	A	423	THR	N-CA-C	5.28	116.91	108.41
1	B	250	PRO	N-CA-C	5.27	123.33	112.47
1	C	250	PRO	N-CA-C	5.27	123.33	112.47
1	B	465	PRO	N-CA-C	5.26	115.52	110.47
1	B	423	THR	N-CA-C	5.26	116.87	108.41
1	C	295	GLN	N-CA-C	5.26	118.38	109.76
1	C	465	PRO	N-CA-C	5.26	115.52	110.47
1	C	221	PHE	CB-CA-C	-5.25	102.60	110.16
1	C	423	THR	N-CA-C	5.25	116.86	108.41
1	A	250	PRO	N-CA-C	5.25	123.28	112.47
1	D	520	PRO	CA-CB-CG	-5.25	94.53	104.50
1	A	316	THR	N-CA-C	5.25	117.63	110.55
1	C	537	ILE	N-CA-C	5.24	117.33	109.20
1	D	423	THR	N-CA-C	5.24	116.85	108.41
1	B	537	ILE	N-CA-C	5.24	117.32	109.20
1	B	295	GLN	N-CA-C	5.24	118.35	109.76
1	A	520	PRO	CA-CB-CG	-5.23	94.56	104.50
1	A	465	PRO	CA-C-O	5.23	124.67	120.90
1	C	520	PRO	CA-CB-CG	-5.23	94.57	104.50
1	D	467	ASN	N-CA-C	5.23	121.93	110.80
1	D	537	ILE	N-CA-C	5.23	117.30	109.20
1	C	316	THR	N-CA-C	5.23	117.61	110.55
1	A	235	ILE	CA-C-O	5.22	127.31	120.78
1	A	467	ASN	N-CA-C	5.22	121.93	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	467	ASN	N-CA-C	5.22	121.93	110.80
1	B	520	PRO	CA-CB-CG	-5.22	94.58	104.50
1	B	467	ASN	N-CA-C	5.22	121.91	110.80
1	B	506	ASP	N-CA-C	5.22	121.91	110.80
1	B	316	THR	N-CA-C	5.21	117.59	110.55
1	B	465	PRO	CA-C-O	5.21	124.65	120.90
1	D	221	PHE	CB-CA-C	-5.21	102.66	110.16
1	D	506	ASP	N-CA-C	5.21	121.90	110.80
1	A	502	LEU	CA-C-N	5.21	131.49	121.54
1	A	502	LEU	C-N-CA	5.21	131.49	121.54
1	C	506	ASP	N-CA-C	5.21	121.89	110.80
1	C	502	LEU	CA-C-N	5.21	131.49	121.54
1	C	502	LEU	C-N-CA	5.21	131.49	121.54
1	D	235	ILE	CA-C-O	5.20	127.28	120.78
1	A	221	PHE	CB-CA-C	-5.20	102.67	110.16
1	A	506	ASP	N-CA-C	5.20	121.88	110.80
1	A	537	ILE	N-CA-C	5.20	117.26	109.20
1	D	502	LEU	CA-C-N	5.20	131.47	121.54
1	D	502	LEU	C-N-CA	5.20	131.47	121.54
1	C	235	ILE	CA-C-O	5.20	127.27	120.78
1	B	502	LEU	CA-C-N	5.19	131.46	121.54
1	B	502	LEU	C-N-CA	5.19	131.46	121.54
1	B	235	ILE	CA-C-O	5.19	127.27	120.78
1	B	221	PHE	CB-CA-C	-5.19	102.69	110.16
1	D	316	THR	N-CA-C	5.18	117.55	110.55
1	D	465	PRO	CA-C-O	5.17	124.62	120.90
1	A	336	VAL	N-CA-CB	-5.17	105.17	110.95
1	B	294	LYS	N-CA-C	-5.14	107.67	114.04
1	C	465	PRO	CA-C-O	5.14	124.60	120.90
1	C	336	VAL	N-CA-CB	-5.14	105.19	110.95
1	A	249	MET	N-CA-C	5.14	121.16	109.81
1	D	336	VAL	N-CA-CB	-5.14	105.20	110.95
1	D	249	MET	N-CA-C	5.13	121.15	109.81
1	A	154	ASP	CA-C-N	-5.13	113.43	119.84
1	A	154	ASP	C-N-CA	-5.13	113.43	119.84
1	C	294	LYS	N-CA-C	-5.13	107.68	114.04
1	A	394	LEU	N-CA-C	-5.13	102.57	109.95
1	B	18	PRO	CA-CB-CG	-5.13	94.26	104.00
1	B	249	MET	N-CA-C	5.13	121.14	109.81
1	A	18	PRO	CA-CB-CG	-5.12	94.27	104.00
1	A	294	LYS	N-CA-C	-5.12	107.69	114.04
1	D	18	PRO	CA-CB-CG	-5.12	94.27	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	ASP	CA-C-N	-5.12	113.44	119.84
1	D	154	ASP	C-N-CA	-5.12	113.44	119.84
1	B	336	VAL	N-CA-CB	-5.12	105.22	110.95
1	C	249	MET	N-CA-C	5.12	121.12	109.81
1	C	154	ASP	CA-C-N	-5.11	113.45	119.84
1	C	154	ASP	C-N-CA	-5.11	113.45	119.84
1	B	154	ASP	CA-C-N	-5.10	113.46	119.84
1	B	154	ASP	C-N-CA	-5.10	113.46	119.84
1	D	294	LYS	N-CA-C	-5.10	107.71	114.04
1	C	18	PRO	CA-CB-CG	-5.09	94.32	104.00
1	B	508	SER	N-CA-C	5.07	118.22	110.36
1	A	508	SER	N-CA-C	5.07	118.21	110.36
1	D	508	SER	N-CA-C	5.06	118.20	110.36
1	C	508	SER	N-CA-C	5.05	118.19	110.36
1	D	290	PHE	CB-CA-C	-5.05	101.51	111.91
1	B	419	VAL	N-CA-C	5.05	114.92	107.75
1	A	290	PHE	CB-CA-C	-5.04	101.52	111.91
1	C	419	VAL	N-CA-C	5.04	114.90	107.75
1	A	419	VAL	N-CA-C	5.04	114.90	107.75
1	D	419	VAL	N-CA-C	5.03	114.90	107.75
1	C	5	PRO	N-CA-C	5.01	116.82	110.70

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	PHE	Sidechain
1	A	18	PRO	Mainchain
1	A	222	ASP	Mainchain
1	A	520	PRO	Mainchain
1	B	17	PHE	Sidechain
1	B	18	PRO	Mainchain
1	B	222	ASP	Mainchain
1	B	520	PRO	Mainchain
1	C	17	PHE	Sidechain
1	C	18	PRO	Mainchain
1	C	222	ASP	Mainchain
1	C	520	PRO	Mainchain
1	D	17	PHE	Sidechain
1	D	18	PRO	Mainchain
1	D	222	ASP	Mainchain
1	D	520	PRO	Mainchain

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	4191	0	4089	818	0
1	B	4191	0	4081	893	0
1	C	4191	0	4078	1144	0
1	D	4191	0	4082	1147	0
2	A	182	0	168	89	0
2	B	182	0	168	86	0
2	C	182	0	169	86	0
2	D	182	0	169	88	0
3	A	28	0	24	9	0
3	B	28	0	24	10	0
3	C	28	0	24	8	0
3	D	28	0	24	9	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
4	C	12	0	0	0	0
4	D	12	0	0	0	0
All	All	17652	0	17100	3367	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 97.

All (3367) 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:A:24:ILE:HB	1:D:2:TRP:CE2	1.18	1.70
1:C:87:PRO:HG3	1:D:43:ALA:CB	1.22	1.65
1:C:87:PRO:CG	1:D:43:ALA:CB	1.77	1.61
1:C:87:PRO:HG3	1:D:43:ALA:CA	1.16	1.58
1:C:83:GLU:HA	1:D:41:GLN:CD	1.24	1.58
1:D:464:ILE:HD12	1:D:465:PRO:CD	1.29	1.58
1:C:81:VAL:HG21	1:D:45:ASN:CB	1.32	1.55
1:C:87:PRO:CA	1:D:43:ALA:HB2	1.12	1.55
1:C:81:VAL:CG2	1:D:45:ASN:CB	1.80	1.54
1:A:24:ILE:CB	1:D:2:TRP:CE2	1.91	1.54
1:B:83:GLU:HB2	1:C:25:LYS:CD	1.10	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.54
1:C:464:ILE:HD12	1:C:465:PRO:CD	1.30	1.54
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.53
1:C:81:VAL:HG12	1:D:43:ALA:CB	1.33	1.53
1:C:1:ASP:HA	1:D:89:GLU:CD	1.21	1.53
1:C:81:VAL:CG1	1:D:43:ALA:HB3	1.40	1.52
1:B:31:PHE:HE1	1:D:75:VAL:CG1	1.22	1.50
1:B:83:GLU:CB	1:C:25:LYS:CD	1.87	1.48
1:B:33:LYS:N	1:C:25:LYS:HE2	1.26	1.47
1:A:24:ILE:CB	1:D:2:TRP:NE1	1.77	1.46
1:C:27:ASN:HD22	1:D:93:GLU:CB	1.26	1.46
1:A:1:ASP:N	1:B:94:ILE:HD11	1.18	1.45
1:C:32:ASN:H	1:D:75:VAL:CG2	1.24	1.45
1:C:79:HIS:CA	1:D:39:THR:HG21	1.24	1.45
1:C:87:PRO:CG	1:D:43:ALA:HA	1.38	1.43
1:B:31:PHE:N	1:C:30:ARG:HB2	1.31	1.42
1:C:464:ILE:CD1	1:C:465:PRO:HD2	1.50	1.42
1:C:79:HIS:HA	1:D:39:THR:CG2	1.09	1.41
1:A:2:TRP:CE2	1:B:80:ALA:CB	1.76	1.41
1:B:464:ILE:CD1	1:B:465:PRO:HD2	1.50	1.40
1:A:464:ILE:CD1	1:A:465:PRO:HD2	1.50	1.40
1:D:464:ILE:CD1	1:D:465:PRO:HD2	1.50	1.40
1:A:9:VAL:C	1:D:30:ARG:HD3	1.44	1.40
1:C:1:ASP:CA	1:D:89:GLU:CD	1.96	1.38
1:A:90:GLU:HB3	1:B:3:VAL:C	1.46	1.38
1:C:85:GLY:CA	1:D:42:GLY:N	1.83	1.38
1:B:31:PHE:HA	1:C:30:ARG:CA	1.54	1.38
1:C:81:VAL:CG2	1:D:45:ASN:HB2	0.91	1.37
1:C:83:GLU:HA	1:D:41:GLN:NE2	1.06	1.37
1:C:87:PRO:CD	1:D:43:ALA:HA	1.55	1.37
1:B:89:GLU:HA	1:D:1:ASP:CB	1.34	1.36
1:C:87:PRO:CA	1:D:43:ALA:CB	2.02	1.36
1:B:31:PHE:HA	1:C:30:ARG:N	1.38	1.35
1:C:1:ASP:N	1:D:28:LYS:HD3	1.37	1.34
1:C:83:GLU:CA	1:D:41:GLN:NE2	1.90	1.33
1:A:2:TRP:CD2	1:B:80:ALA:HB2	1.29	1.33
1:B:31:PHE:CE1	1:D:75:VAL:CG1	2.12	1.33
1:B:31:PHE:CE1	1:D:75:VAL:HG11	1.64	1.33
1:B:89:GLU:CA	1:D:1:ASP:CB	1.87	1.32
1:A:24:ILE:HB	1:D:2:TRP:NE1	1.02	1.32
1:C:90:GLU:HB3	1:D:79:HIS:O	1.28	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ASP:O	1:D:28:LYS:NZ	1.63	1.31
1:C:87:PRO:CB	1:D:43:ALA:CB	2.09	1.31
1:C:27:ASN:ND2	1:D:93:GLU:CB	1.91	1.31
1:C:81:VAL:HG22	1:D:45:ASN:ND2	1.42	1.30
1:C:32:ASN:N	1:D:75:VAL:HG21	1.43	1.30
1:B:89:GLU:HA	1:D:1:ASP:CG	0.94	1.29
1:C:79:HIS:CB	1:D:44:ASP:OD1	1.81	1.29
1:C:85:GLY:HA2	1:D:42:GLY:N	1.40	1.28
1:B:30:ARG:C	1:C:30:ARG:HB2	1.58	1.27
1:C:32:ASN:N	1:D:75:VAL:CG2	1.92	1.27
1:A:2:TRP:CE2	1:B:80:ALA:HB2	0.95	1.27
1:A:4:ILE:HA	1:B:90:GLU:C	1.59	1.26
1:A:4:ILE:CA	1:B:91:PRO:N	1.97	1.26
1:C:84:ASN:HB2	1:D:74:TYR:CE1	1.44	1.25
1:B:540:GLN:O	1:B:540:GLN:CD	1.79	1.24
1:C:28:LYS:O	1:D:75:VAL:HG13	1.07	1.24
1:C:540:GLN:O	1:C:540:GLN:CD	1.79	1.24
1:A:540:GLN:O	1:A:540:GLN:CD	1.79	1.24
1:C:28:LYS:O	1:D:75:VAL:CG1	1.86	1.24
1:A:4:ILE:HA	1:B:91:PRO:N	1.20	1.23
1:A:91:PRO:N	1:B:3:VAL:HG22	1.51	1.23
1:B:83:GLU:HB2	1:C:25:LYS:CG	1.53	1.23
1:C:4:ILE:CG2	1:D:87:PRO:HG2	1.69	1.23
1:D:540:GLN:O	1:D:540:GLN:CD	1.79	1.23
1:C:87:PRO:N	1:D:43:ALA:HB2	1.52	1.22
1:B:33:LYS:H	1:C:25:LYS:CE	1.52	1.22
1:C:83:GLU:CA	1:D:41:GLN:CD	2.11	1.22
1:C:90:GLU:OE1	1:D:53:ILE:CD1	1.85	1.22
1:A:2:TRP:CD2	1:B:80:ALA:CB	2.04	1.22
1:C:1:ASP:HA	1:D:89:GLU:OE2	1.37	1.21
1:B:86:SER:CA	1:D:90:GLU:HG3	1.62	1.20
1:C:87:PRO:CG	1:D:43:ALA:CA	1.85	1.20
1:C:84:ASN:HB2	1:D:74:TYR:CZ	1.43	1.20
1:C:31:PHE:HB2	1:D:95:THR:CG2	1.72	1.19
1:C:90:GLU:CA	1:D:79:HIS:H	1.53	1.19
1:B:32:ASN:HB2	1:C:29:ASP:OD2	1.41	1.19
1:B:83:GLU:N	1:C:25:LYS:HD3	1.56	1.19
1:C:84:ASN:CB	1:D:74:TYR:CE1	2.15	1.19
1:C:31:PHE:CB	1:D:95:THR:HG23	1.72	1.18
1:C:79:HIS:HB2	1:D:44:ASP:OD1	1.40	1.18
1:B:31:PHE:HE2	1:C:26:SER:O	1.25	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:GLN:HG2	1:D:532:CYS:O	1.43	1.18
1:B:30:ARG:C	1:C:30:ARG:CB	2.16	1.18
1:C:450:GLN:HG2	1:C:532:CYS:O	1.43	1.18
1:D:8:LYS:H	1:D:8:LYS:HD2	1.04	1.18
1:A:9:VAL:C	1:D:30:ARG:CD	2.18	1.17
1:C:89:GLU:OE1	1:D:78:SER:OG	1.56	1.17
1:D:474:SER:HB2	1:D:512:LEU:HG	1.25	1.17
1:A:482:THR:HG23	1:A:499:THR:CG2	1.75	1.17
1:B:154:ASP:C	2:B:801:NAG:H82	1.70	1.16
1:A:469:TYR:CG	1:A:470:PRO:HD2	1.81	1.16
1:B:89:GLU:CA	1:D:1:ASP:HB2	1.41	1.16
1:B:482:THR:HG23	1:B:499:THR:CG2	1.75	1.16
1:D:423:THR:HB	2:D:810:NAG:C7	1.76	1.16
1:D:482:THR:HG23	1:D:499:THR:CG2	1.75	1.16
1:B:423:THR:HB	2:B:810:NAG:C7	1.76	1.16
1:B:469:TYR:CG	1:B:470:PRO:HD2	1.81	1.16
1:B:83:GLU:CB	1:C:25:LYS:HD2	1.55	1.16
1:C:87:PRO:CD	1:D:43:ALA:CA	2.16	1.16
1:A:154:ASP:C	2:A:801:NAG:H82	1.70	1.16
1:A:338:ARG:HD3	1:A:352:ILE:HG22	1.26	1.16
1:C:1:ASP:N	1:D:88:VAL:HG12	1.61	1.16
1:C:482:THR:HG23	1:C:499:THR:CG2	1.75	1.16
1:D:154:ASP:C	2:D:801:NAG:H82	1.70	1.16
1:D:234:GLU:H	1:D:235:ILE:HG23	1.08	1.16
1:C:35:TYR:O	1:D:45:ASN:ND2	1.76	1.15
1:D:338:ARG:HD3	1:D:352:ILE:HG22	1.26	1.15
1:B:234:GLU:H	1:B:235:ILE:HG23	1.08	1.15
1:C:469:TYR:CG	1:C:470:PRO:HD2	1.81	1.15
1:A:450:GLN:HG2	1:A:532:CYS:O	1.43	1.15
1:D:469:TYR:CG	1:D:470:PRO:HD2	1.80	1.15
1:C:91:PRO:CB	1:D:37:SER:OG	1.93	1.15
1:B:31:PHE:CA	1:C:30:ARG:N	2.08	1.14
1:C:87:PRO:CB	1:D:43:ALA:HB1	1.72	1.14
1:C:87:PRO:CB	1:D:43:ALA:HB2	1.75	1.14
1:B:450:GLN:HG2	1:B:532:CYS:O	1.43	1.14
1:C:154:ASP:C	2:C:801:NAG:H82	1.70	1.14
1:C:423:THR:HB	2:C:810:NAG:C7	1.76	1.14
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.13
1:C:8:LYS:H	1:C:8:LYS:HD2	1.04	1.13
1:C:403:ASN:HB2	2:C:902:NAG:H83	1.30	1.13
1:B:32:ASN:CB	1:C:29:ASP:OD2	1.96	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:VAL:HG23	1:D:45:ASN:HB2	1.28	1.13
1:C:84:ASN:CB	1:D:74:TYR:CZ	2.23	1.13
1:B:84:ASN:OD1	1:C:26:SER:CA	1.85	1.12
1:C:93:GLU:OE2	1:D:85:GLY:HA2	1.43	1.12
1:A:1:ASP:H3	1:B:94:ILE:CD1	1.63	1.12
1:C:27:ASN:ND2	1:D:93:GLU:HB3	1.58	1.12
1:C:79:HIS:CA	1:D:39:THR:CG2	1.84	1.12
1:D:32:ASN:HD21	1:D:83:GLU:HB2	0.98	1.12
1:A:8:LYS:H	1:A:8:LYS:HD2	1.04	1.12
1:C:31:PHE:HB2	1:D:95:THR:HG21	1.32	1.12
1:D:403:ASN:HB2	2:D:902:NAG:H83	1.30	1.12
1:B:89:GLU:N	1:D:1:ASP:HB2	1.65	1.11
1:B:301:THR:HG21	2:B:805:NAG:H82	1.29	1.11
1:C:85:GLY:CA	1:D:42:GLY:CA	1.77	1.11
1:A:403:ASN:HB2	2:A:902:NAG:H83	1.30	1.11
1:C:31:PHE:HB3	1:D:75:VAL:HG22	1.23	1.11
1:C:81:VAL:HG22	1:D:45:ASN:CG	1.74	1.11
1:C:338:ARG:HD3	1:C:352:ILE:HG22	1.26	1.11
1:B:83:GLU:H	1:C:25:LYS:HD3	0.97	1.11
1:A:1:ASP:N	1:B:94:ILE:CD1	2.13	1.11
1:A:90:GLU:HB3	1:B:3:VAL:CA	1.70	1.10
1:B:222:ASP:O	1:B:222:ASP:OD1	1.69	1.10
1:C:474:SER:HB2	1:C:512:LEU:HG	1.25	1.10
1:B:83:GLU:CG	1:C:25:LYS:HD2	1.82	1.10
1:A:90:GLU:HG3	1:B:3:VAL:HG23	1.24	1.10
1:A:222:ASP:OD1	1:A:222:ASP:O	1.69	1.10
1:A:234:GLU:H	1:A:235:ILE:HG23	1.08	1.10
1:C:84:ASN:C	1:D:74:TYR:CE2	2.28	1.10
1:B:474:SER:HB2	1:B:512:LEU:HG	1.25	1.09
1:C:90:GLU:OE2	1:D:53:ILE:CG2	2.00	1.09
1:C:91:PRO:CA	1:D:37:SER:OG	1.81	1.09
1:A:227:THR:HG21	2:A:807:NAG:C8	1.82	1.09
1:C:31:PHE:HE2	1:D:73:LYS:C	1.50	1.09
1:C:222:ASP:OD1	1:C:222:ASP:O	1.69	1.09
1:C:227:THR:HG21	2:C:807:NAG:C8	1.82	1.09
1:D:482:THR:HG23	1:D:499:THR:HG22	1.09	1.09
1:A:9:VAL:CA	1:D:30:ARG:HD3	1.83	1.09
1:C:482:THR:HG23	1:C:499:THR:HG22	1.09	1.09
1:A:32:ASN:HD21	1:A:83:GLU:HB2	0.98	1.09
1:B:227:THR:HG21	2:B:807:NAG:C8	1.82	1.08
1:C:32:ASN:HD21	1:C:83:GLU:HB2	0.98	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:THR:HG21	2:D:807:NAG:C8	1.82	1.08
1:C:234:GLU:H	1:C:235:ILE:HG23	1.08	1.08
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.08
1:B:8:LYS:H	1:B:8:LYS:HD2	1.04	1.08
1:C:31:PHE:CB	1:D:95:THR:CG2	2.29	1.08
1:D:222:ASP:OD1	1:D:222:ASP:O	1.69	1.08
1:D:301:THR:HG21	2:D:805:NAG:H82	1.29	1.08
1:B:33:LYS:N	1:C:25:LYS:CE	2.13	1.08
1:A:301:THR:HG21	2:A:805:NAG:H82	1.29	1.07
1:B:84:ASN:OD1	1:C:26:SER:C	1.96	1.07
1:C:31:PHE:CE2	1:D:74:TYR:N	2.21	1.07
1:C:87:PRO:HA	1:D:43:ALA:HB2	1.11	1.07
1:C:90:GLU:OE1	1:D:53:ILE:HD13	0.90	1.07
1:C:301:THR:HG21	2:C:805:NAG:H82	1.29	1.07
1:B:31:PHE:CA	1:C:30:ARG:HB2	1.85	1.07
1:A:290:PHE:HB2	1:A:292:LEU:N	1.69	1.07
1:B:335:ALA:HB1	3:B:811:NDG:O6	1.54	1.07
1:B:482:THR:HG23	1:B:499:THR:HG22	1.09	1.07
1:C:29:ASP:HA	1:D:75:VAL:HG11	1.31	1.07
1:C:450:GLN:CG	1:C:532:CYS:O	2.03	1.07
1:C:89:GLU:N	1:D:38:ILE:HG13	1.69	1.07
1:A:450:GLN:CG	1:A:532:CYS:O	2.02	1.06
1:C:87:PRO:HD3	1:D:43:ALA:HA	1.32	1.06
1:C:290:PHE:HB2	1:C:292:LEU:N	1.69	1.06
1:B:450:GLN:CG	1:B:532:CYS:O	2.03	1.06
1:C:1:ASP:H2	1:D:88:VAL:CG1	1.66	1.06
1:A:337:SER:HA	1:A:427:ILE:HG23	1.38	1.06
1:B:290:PHE:HB2	1:B:292:LEU:N	1.69	1.06
1:C:4:ILE:HG22	1:D:87:PRO:HB2	1.38	1.06
1:C:485:ALA:O	1:C:486:GLU:HG2	1.54	1.06
1:A:482:THR:HG23	1:A:499:THR:HG22	1.09	1.06
1:A:485:ALA:O	1:A:486:GLU:HG2	1.55	1.06
1:B:403:ASN:HB2	2:B:902:NAG:H83	1.30	1.06
1:D:290:PHE:HB2	1:D:292:LEU:N	1.69	1.06
1:A:335:ALA:HB1	3:A:811:NDG:O6	1.54	1.06
1:B:338:ARG:HD3	1:B:352:ILE:HG22	1.26	1.06
1:D:469:TYR:CD1	1:D:470:PRO:HD2	1.91	1.06
1:A:24:ILE:CA	1:D:2:TRP:CE2	2.23	1.05
1:B:469:TYR:CD1	1:B:470:PRO:HD2	1.92	1.05
1:D:335:ALA:HB1	3:D:811:NDG:O6	1.54	1.05
1:D:450:GLN:CG	1:D:532:CYS:O	2.03	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ALA:O	1:B:486:GLU:HG2	1.55	1.05
1:A:464:ILE:CD1	1:A:465:PRO:CD	2.20	1.05
1:B:337:SER:HA	1:B:427:ILE:HG23	1.38	1.05
1:C:81:VAL:HG21	1:D:45:ASN:CA	1.87	1.05
1:C:335:ALA:HB1	3:C:811:NDG:O6	1.54	1.05
1:A:3:VAL:HG22	1:B:78:SER:H	1.21	1.04
1:A:8:LYS:HE3	1:D:28:LYS:HG3	1.39	1.04
1:C:82:SER:CB	1:D:75:VAL:H	1.70	1.04
1:C:522:LEU:HD22	1:C:523:THR:HB	1.39	1.04
1:D:485:ALA:O	1:D:486:GLU:HG2	1.54	1.04
1:B:31:PHE:CE2	1:C:26:SER:O	2.09	1.04
1:B:84:ASN:ND2	1:D:91:PRO:HB2	1.71	1.04
1:C:31:PHE:CG	1:D:95:THR:HG23	1.92	1.04
1:C:87:PRO:HG3	1:D:43:ALA:HB1	1.17	1.04
1:C:90:GLU:OE2	1:D:53:ILE:HG21	1.57	1.04
1:C:90:GLU:CB	1:D:79:HIS:O	2.05	1.04
1:C:469:TYR:CD1	1:C:470:PRO:HD2	1.92	1.04
1:A:24:ILE:HA	1:D:2:TRP:CG	1.60	1.04
1:A:290:PHE:HB2	1:A:292:LEU:H	0.88	1.04
1:B:31:PHE:HE2	1:C:26:SER:C	1.65	1.04
1:B:464:ILE:CD1	1:B:465:PRO:CD	2.20	1.04
1:C:87:PRO:CG	1:D:43:ALA:HB1	1.61	1.04
1:D:464:ILE:CD1	1:D:465:PRO:CD	2.20	1.04
1:D:522:LEU:HD22	1:D:523:THR:HB	1.39	1.04
1:A:469:TYR:CD1	1:A:470:PRO:HD2	1.92	1.04
1:C:482:THR:HG21	1:C:499:THR:H	1.23	1.04
1:A:2:TRP:C	1:B:92:MET:HB2	1.79	1.03
1:C:81:VAL:HG11	1:D:45:ASN:H	1.21	1.03
1:A:482:THR:CG2	1:A:499:THR:N	2.22	1.03
1:C:464:ILE:CD1	1:C:465:PRO:CD	2.20	1.03
1:C:482:THR:CG2	1:C:499:THR:N	2.22	1.03
1:D:482:THR:CG2	1:D:499:THR:N	2.22	1.02
1:B:83:GLU:CB	1:C:25:LYS:HD3	1.76	1.02
1:A:482:THR:HG21	1:A:499:THR:H	1.23	1.02
1:C:90:GLU:N	1:D:79:HIS:N	2.07	1.02
1:C:450:GLN:HB2	1:C:533:GLU:HA	1.41	1.02
1:C:337:SER:HA	1:C:427:ILE:HG23	1.38	1.02
1:C:403:ASN:HB2	2:C:902:NAG:C8	1.90	1.02
1:B:482:THR:CG2	1:B:499:THR:N	2.22	1.02
1:C:81:VAL:HG22	1:D:45:ASN:HD22	1.02	1.02
1:C:90:GLU:N	1:D:79:HIS:H	1.54	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:PHE:HB2	1:C:292:LEU:H	0.88	1.02
1:A:432:ASP:OD2	1:A:464:ILE:HG22	1.60	1.01
1:C:1:ASP:N	1:D:88:VAL:CG1	2.21	1.01
1:C:81:VAL:CG1	1:D:44:ASP:H	1.73	1.01
1:B:403:ASN:HB2	2:B:902:NAG:C8	1.90	1.01
1:B:290:PHE:HB2	1:B:292:LEU:H	0.88	1.01
1:B:432:ASP:OD2	1:B:464:ILE:HG22	1.60	1.01
1:C:81:VAL:HG11	1:D:44:ASP:N	1.75	1.01
1:C:82:SER:HB3	1:D:75:VAL:H	1.23	1.01
1:A:24:ILE:HB	1:D:2:TRP:CZ2	1.96	1.01
1:A:522:LEU:HD22	1:A:523:THR:HB	1.39	1.01
1:B:274:ASP:O	1:B:278:ASN:HA	1.61	1.01
1:D:290:PHE:HB2	1:D:292:LEU:H	0.88	1.01
1:A:403:ASN:HB2	2:A:902:NAG:C8	1.90	1.01
1:C:79:HIS:CB	1:D:39:THR:CG2	2.37	1.01
1:C:89:GLU:OE1	1:D:78:SER:N	1.75	1.01
1:C:93:GLU:H	1:D:81:VAL:HG11	1.25	1.01
1:C:274:ASP:O	1:C:278:ASN:HA	1.61	1.01
1:D:274:ASP:O	1:D:278:ASN:HA	1.61	1.01
1:C:4:ILE:HG22	1:D:87:PRO:CB	1.90	1.00
1:B:31:PHE:N	1:C:30:ARG:CB	2.24	1.00
1:B:522:LEU:HD22	1:B:523:THR:HB	1.39	1.00
1:C:32:ASN:N	1:D:75:VAL:HG23	1.76	1.00
1:D:337:SER:HA	1:D:427:ILE:HG23	1.38	1.00
1:A:188:THR:HG23	1:A:208:ILE:HG12	1.43	1.00
1:A:274:ASP:O	1:A:278:ASN:HA	1.61	1.00
1:C:81:VAL:HG22	1:D:45:ASN:HB2	1.32	1.00
1:C:86:SER:HA	1:D:42:GLY:C	1.83	1.00
1:D:403:ASN:HB2	2:D:902:NAG:C8	1.90	1.00
1:A:523:THR:HG23	1:A:524:VAL:H	1.27	1.00
1:B:86:SER:HA	1:D:90:GLU:CA	1.39	1.00
1:C:432:ASP:OD2	1:C:464:ILE:HG22	1.60	1.00
1:C:81:VAL:HB	1:D:41:GLN:C	1.86	1.00
1:C:523:THR:HG23	1:C:524:VAL:H	1.26	1.00
1:A:90:GLU:CB	1:B:3:VAL:C	2.35	1.00
1:D:432:ASP:OD2	1:D:464:ILE:HG22	1.60	1.00
1:A:450:GLN:HB2	1:A:533:GLU:HA	1.41	0.99
1:C:1:ASP:H2	1:D:88:VAL:HG12	0.84	0.99
1:C:93:GLU:CB	1:D:81:VAL:HG11	1.92	0.99
1:C:79:HIS:CB	1:D:39:THR:HG22	1.93	0.99
1:C:90:GLU:CB	1:D:79:HIS:H	1.74	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:THR:HG23	1:C:208:ILE:HG12	1.43	0.99
1:B:482:THR:HG21	1:B:499:THR:H	1.23	0.99
1:C:87:PRO:C	1:D:76:LEU:HD22	1.88	0.99
1:B:320:THR:HG21	2:B:807:NAG:N2	1.78	0.99
1:C:4:ILE:CG2	1:D:87:PRO:CG	2.41	0.99
1:D:188:THR:HG23	1:D:208:ILE:HG12	1.43	0.99
1:D:450:GLN:HB2	1:D:533:GLU:HA	1.41	0.99
1:A:4:ILE:CA	1:B:90:GLU:C	2.33	0.99
1:D:482:THR:HG21	1:D:499:THR:H	1.23	0.99
1:B:523:THR:HG23	1:B:524:VAL:H	1.26	0.98
1:C:90:GLU:HB3	1:D:79:HIS:C	1.87	0.98
1:B:31:PHE:HA	1:C:30:ARG:CB	1.92	0.98
1:B:450:GLN:HB2	1:B:533:GLU:HA	1.41	0.98
1:A:482:THR:CG2	1:A:499:THR:H	1.76	0.98
1:C:2:TRP:H	1:D:89:GLU:HA	1.23	0.98
1:A:320:THR:HG21	2:A:807:NAG:N2	1.78	0.98
1:B:82:SER:HB3	1:C:27:ASN:HB3	1.44	0.98
1:C:1:ASP:N	1:D:28:LYS:CD	2.25	0.98
1:D:482:THR:CG2	1:D:499:THR:H	1.76	0.98
1:A:10:SER:N	1:D:30:ARG:CD	2.27	0.98
1:C:91:PRO:HA	1:D:79:HIS:CD2	1.96	0.98
1:C:482:THR:CG2	1:C:499:THR:H	1.76	0.98
1:B:30:ARG:O	1:C:30:ARG:HG3	1.64	0.97
1:C:320:THR:HG21	2:C:807:NAG:N2	1.78	0.97
1:D:523:THR:HG23	1:D:524:VAL:H	1.26	0.97
1:C:31:PHE:CG	1:D:95:THR:CG2	2.47	0.97
1:D:8:LYS:H	1:D:8:LYS:CD	1.74	0.97
1:B:366:LYS:HG3	1:B:367:LEU:H	1.28	0.97
1:B:86:SER:CA	1:D:90:GLU:CG	2.20	0.97
1:C:8:LYS:H	1:C:8:LYS:CD	1.74	0.97
1:A:90:GLU:C	1:B:3:VAL:HG22	1.85	0.97
1:B:188:THR:HG23	1:B:208:ILE:HG12	1.43	0.97
1:A:366:LYS:HG3	1:A:367:LEU:H	1.28	0.97
1:B:87:PRO:HG2	1:C:2:TRP:HB2	1.45	0.97
1:D:320:THR:HG21	2:D:807:NAG:N2	1.78	0.97
1:C:80:ALA:HB3	1:D:77:SER:HB3	1.45	0.97
1:D:366:LYS:HG3	1:D:367:LEU:H	1.28	0.97
1:C:4:ILE:HG23	1:D:87:PRO:HG2	1.45	0.96
1:C:81:VAL:HG22	1:D:45:ASN:CB	1.78	0.96
1:A:32:ASN:HD21	1:A:83:GLU:CB	1.79	0.96
1:C:27:ASN:HD22	1:D:93:GLU:HB2	0.80	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:PRO:HA	1:D:43:ALA:CB	1.77	0.96
1:B:235:ILE:CG1	1:B:287:GLY:HA2	1.96	0.96
1:C:32:ASN:HD21	1:C:83:GLU:CB	1.79	0.96
1:C:81:VAL:HG13	1:D:44:ASP:OD2	1.64	0.96
1:D:482:THR:HG21	1:D:499:THR:N	1.81	0.96
1:B:482:THR:CG2	1:B:499:THR:H	1.76	0.96
1:A:3:VAL:HG22	1:B:78:SER:N	1.79	0.96
1:A:227:THR:HG21	2:A:807:NAG:H83	1.48	0.96
1:A:235:ILE:CG1	1:A:287:GLY:HA2	1.96	0.96
1:A:482:THR:HG21	1:A:499:THR:N	1.81	0.96
1:C:81:VAL:CG1	1:D:44:ASP:N	2.27	0.96
1:B:31:PHE:CA	1:C:30:ARG:H	1.75	0.96
1:C:27:ASN:ND2	1:D:93:GLU:H	1.62	0.96
1:C:85:GLY:C	1:D:41:GLN:C	2.34	0.96
1:C:320:THR:HG21	2:C:807:NAG:HN2	1.31	0.96
1:C:90:GLU:CD	1:D:53:ILE:HG21	1.89	0.95
1:B:83:GLU:HB2	1:C:25:LYS:HD2	0.96	0.95
1:C:31:PHE:HE2	1:D:74:TYR:N	1.59	0.95
1:C:235:ILE:CG1	1:C:287:GLY:HA2	1.96	0.95
1:A:24:ILE:HB	1:D:2:TRP:HE1	1.28	0.95
1:B:31:PHE:CB	1:C:30:ARG:H	1.79	0.95
1:C:88:VAL:HG12	1:D:94:ILE:HB	1.47	0.95
1:B:31:PHE:CE2	1:C:26:SER:C	2.45	0.95
1:C:88:VAL:O	1:D:94:ILE:HD12	1.65	0.95
1:B:320:THR:HG21	2:B:807:NAG:HN2	1.31	0.95
1:A:2:TRP:NE1	1:B:80:ALA:HB2	1.82	0.95
1:A:24:ILE:CA	1:D:2:TRP:CG	2.39	0.95
1:B:86:SER:N	1:D:90:GLU:HG3	1.44	0.95
1:C:1:ASP:H2	1:D:28:LYS:HD3	0.96	0.95
1:A:90:GLU:CG	1:B:3:VAL:HG23	1.96	0.95
1:B:227:THR:HG21	2:B:807:NAG:H83	1.48	0.95
1:B:31:PHE:HE1	1:D:75:VAL:HG11	0.78	0.94
1:C:374:ASP:O	1:C:375:PRO:C	2.06	0.94
1:D:235:ILE:CG1	1:D:287:GLY:HA2	1.96	0.94
1:A:24:ILE:HA	1:D:2:TRP:CD1	2.02	0.94
1:A:290:PHE:CB	1:A:292:LEU:H	1.79	0.94
1:B:366:LYS:CG	1:B:367:LEU:H	1.80	0.94
1:B:482:THR:HG21	1:B:499:THR:N	1.81	0.94
1:A:89:GLU:OE1	1:B:2:TRP:HB3	1.65	0.94
1:C:289:ASP:O	1:C:290:PHE:HB3	1.67	0.94
1:D:366:LYS:CG	1:D:367:LEU:H	1.80	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLU:CA	1:C:25:LYS:HD3	1.97	0.94
1:C:91:PRO:CA	1:D:79:HIS:CD2	2.50	0.94
1:D:227:THR:HG21	2:D:807:NAG:H83	1.48	0.94
1:D:290:PHE:CB	1:D:292:LEU:H	1.79	0.94
1:A:8:LYS:H	1:A:8:LYS:CD	1.74	0.94
1:B:86:SER:CA	1:D:90:GLU:CA	2.30	0.94
1:C:290:PHE:CB	1:C:292:LEU:H	1.79	0.94
1:D:32:ASN:HD21	1:D:83:GLU:CB	1.79	0.94
1:C:366:LYS:HG3	1:C:367:LEU:H	1.28	0.94
1:A:99:ILE:HG21	1:D:30:ARG:HH12	1.29	0.93
1:C:27:ASN:HD22	1:C:28:LYS:N	1.66	0.93
1:C:91:PRO:HB2	1:D:37:SER:OG	1.65	0.93
1:B:85:GLY:C	1:D:91:PRO:HD2	1.92	0.93
1:A:195:ASP:HB2	1:A:201:LEU:H	1.34	0.93
1:B:396:ARG:HH22	1:B:464:ILE:HB	1.33	0.93
1:C:352:ILE:HG13	1:C:388:VAL:HB	1.51	0.93
1:D:352:ILE:HG13	1:D:388:VAL:HB	1.51	0.93
1:B:227:THR:HG21	2:B:807:NAG:C7	1.99	0.93
1:C:87:PRO:HD3	1:D:43:ALA:CA	1.92	0.93
1:C:366:LYS:CG	1:C:367:LEU:H	1.80	0.93
1:A:27:ASN:HD22	1:A:28:LYS:N	1.66	0.93
1:C:32:ASN:ND2	1:C:83:GLU:HB2	1.83	0.93
1:C:227:THR:HG21	2:C:807:NAG:H83	1.48	0.93
1:C:464:ILE:HD12	1:C:465:PRO:HD2	0.94	0.93
1:A:366:LYS:CG	1:A:367:LEU:H	1.80	0.93
1:A:374:ASP:O	1:A:375:PRO:C	2.06	0.93
1:A:396:ARG:HH22	1:A:464:ILE:HB	1.33	0.93
1:B:27:ASN:HD22	1:B:28:LYS:N	1.66	0.93
1:B:30:ARG:C	1:C:30:ARG:CG	2.31	0.93
1:A:1:ASP:HA	1:B:24:ILE:HG21	1.51	0.93
1:A:24:ILE:CB	1:D:2:TRP:CD1	2.52	0.93
1:A:24:ILE:CG2	1:D:2:TRP:NE1	2.32	0.92
1:B:89:GLU:CA	1:D:1:ASP:CG	1.90	0.92
1:B:290:PHE:CB	1:B:292:LEU:H	1.79	0.92
1:B:464:ILE:HD12	1:B:465:PRO:HD2	0.94	0.92
1:D:195:ASP:HB2	1:D:201:LEU:H	1.34	0.92
1:A:320:THR:HG21	2:A:807:NAG:HN2	1.31	0.92
1:A:446:THR:HG23	1:A:539:CYS:SG	2.09	0.92
1:A:464:ILE:HD12	1:A:465:PRO:HD2	0.94	0.92
1:B:32:ASN:CA	1:C:29:ASP:OD2	2.17	0.92
1:B:404:ASN:ND2	1:B:404:ASN:O	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ASN:ND2	1:D:93:GLU:HB2	1.65	0.92
1:D:464:ILE:HD12	1:D:465:PRO:HD2	0.94	0.92
1:A:227:THR:HG21	2:A:807:NAG:C7	1.99	0.92
1:C:404:ASN:O	1:C:404:ASN:ND2	2.03	0.92
1:D:289:ASP:O	1:D:290:PHE:HB3	1.67	0.92
1:D:320:THR:HG21	2:D:807:NAG:HN2	1.31	0.92
1:B:403:ASN:HB2	2:B:902:NAG:C7	2.00	0.92
1:C:86:SER:N	1:D:41:GLN:O	2.01	0.92
1:C:1:ASP:CB	1:D:89:GLU:CD	2.37	0.92
1:D:27:ASN:HD22	1:D:28:LYS:N	1.66	0.92
1:D:446:THR:HG23	1:D:539:CYS:SG	2.10	0.92
1:B:31:PHE:CA	1:C:30:ARG:CB	2.48	0.92
1:A:32:ASN:ND2	1:A:83:GLU:HB2	1.84	0.92
1:C:88:VAL:HG22	1:D:76:LEU:HD23	1.47	0.92
1:C:90:GLU:CD	1:D:53:ILE:HD13	1.95	0.92
1:C:195:ASP:HB2	1:C:201:LEU:H	1.34	0.92
2:C:805:NAG:H62	2:C:806:NAG:C7	2.00	0.92
1:D:227:THR:HG21	2:D:807:NAG:C7	1.99	0.92
1:D:396:ARG:HH22	1:D:464:ILE:HB	1.33	0.92
1:C:87:PRO:HD3	1:D:42:GLY:O	1.69	0.92
1:C:227:THR:HG21	2:C:807:NAG:C7	1.99	0.92
1:C:446:THR:HG23	1:C:539:CYS:SG	2.10	0.92
2:A:805:NAG:H62	2:A:806:NAG:C7	1.99	0.91
1:B:446:THR:HG23	1:B:539:CYS:SG	2.10	0.91
1:C:1:ASP:H3	1:D:88:VAL:HB	1.35	0.91
1:C:340:ASP:HA	1:C:429:HIS:HB3	1.53	0.91
1:D:32:ASN:ND2	1:D:83:GLU:HB2	1.84	0.91
1:A:403:ASN:HB2	2:A:902:NAG:C7	2.00	0.91
1:A:404:ASN:O	1:A:404:ASN:ND2	2.03	0.91
1:C:86:SER:H	1:D:74:TYR:HD2	1.16	0.91
1:C:517:GLN:O	1:C:519:ASN:N	2.03	0.91
1:D:335:ALA:CB	3:D:811:NDG:O6	2.18	0.91
1:D:374:ASP:O	1:D:375:PRO:C	2.06	0.91
1:B:234:GLU:N	1:B:235:ILE:HG23	1.86	0.91
1:A:335:ALA:CB	3:A:811:NDG:O6	2.18	0.91
1:B:83:GLU:H	1:C:25:LYS:CD	1.84	0.91
1:B:335:ALA:CB	3:B:811:NDG:O6	2.18	0.91
1:C:1:ASP:O	1:D:28:LYS:CE	2.19	0.91
1:A:340:ASP:HA	1:A:429:HIS:HB3	1.53	0.91
1:B:289:ASP:O	1:B:290:PHE:HB3	1.67	0.91
1:B:374:ASP:O	1:B:375:PRO:C	2.06	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:805:NAG:O5	2:C:806:NAG:H83	1.71	0.91
1:A:10:SER:N	1:D:30:ARG:HD3	1.86	0.91
1:C:396:ARG:HH22	1:C:464:ILE:HB	1.33	0.91
1:C:403:ASN:HB2	2:C:902:NAG:C7	2.00	0.91
1:D:403:ASN:HB2	2:D:902:NAG:C7	2.00	0.91
1:B:83:GLU:CG	1:C:25:LYS:CD	2.45	0.91
2:B:805:NAG:H62	2:B:806:NAG:C7	2.00	0.91
1:C:81:VAL:HB	1:D:41:GLN:CA	1.86	0.91
1:A:289:ASP:O	1:A:290:PHE:HB3	1.67	0.90
1:B:352:ILE:HG13	1:B:388:VAL:HB	1.51	0.90
1:B:378:TRP:HB2	1:B:379:LEU:HD23	1.53	0.90
1:A:378:TRP:HB2	1:A:379:LEU:HD23	1.53	0.90
1:D:234:GLU:N	1:D:235:ILE:HG23	1.86	0.90
2:D:805:NAG:O5	2:D:806:NAG:H83	1.71	0.90
1:C:79:HIS:HB3	1:D:44:ASP:OD1	1.70	0.90
1:D:8:LYS:HD2	1:D:8:LYS:N	1.87	0.90
1:D:517:GLN:O	1:D:519:ASN:N	2.03	0.90
1:A:154:ASP:HB3	1:A:155:PRO:HD2	1.54	0.90
1:C:1:ASP:HA	1:D:89:GLU:OE1	1.68	0.90
1:C:87:PRO:CD	1:D:43:ALA:CB	2.48	0.90
2:D:805:NAG:H62	2:D:806:NAG:C7	1.99	0.90
1:A:24:ILE:CB	1:D:2:TRP:CZ2	2.54	0.90
1:B:464:ILE:HD11	1:B:465:PRO:HD2	1.53	0.90
1:B:517:GLN:O	1:B:519:ASN:N	2.03	0.90
1:C:396:ARG:NH2	1:C:464:ILE:CG2	2.35	0.90
1:D:340:ASP:HA	1:D:429:HIS:HB3	1.53	0.90
1:D:404:ASN:O	1:D:404:ASN:ND2	2.03	0.90
1:C:378:TRP:HB2	1:C:379:LEU:HD23	1.53	0.90
1:A:396:ARG:NH2	1:A:464:ILE:CG2	2.35	0.90
2:A:805:NAG:O5	2:A:806:NAG:H83	1.71	0.90
1:B:154:ASP:HB3	1:B:155:PRO:HD2	1.54	0.90
1:C:234:GLU:N	1:C:235:ILE:HG23	1.86	0.90
1:A:234:GLU:N	1:A:235:ILE:HG23	1.86	0.90
1:C:335:ALA:CB	3:C:811:NDG:O6	2.18	0.90
1:C:90:GLU:OE2	1:D:53:ILE:HG23	1.72	0.89
1:B:396:ARG:NH2	1:B:464:ILE:CG2	2.35	0.89
1:B:518:ASN:O	1:B:520:PRO:HD3	1.72	0.89
1:A:523:THR:HG23	1:A:524:VAL:CG2	2.03	0.89
1:B:8:LYS:H	1:B:8:LYS:CD	1.74	0.89
1:B:195:ASP:HB2	1:B:201:LEU:H	1.34	0.89
1:C:8:LYS:HD2	1:C:8:LYS:N	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:VAL:CG2	1:D:45:ASN:HD22	1.85	0.89
1:D:449:ASP:H	1:D:532:CYS:HB3	1.37	0.89
1:A:338:ARG:HD3	1:A:352:ILE:CG2	2.02	0.89
1:C:87:PRO:CA	1:D:76:LEU:HD22	1.96	0.89
1:C:93:GLU:H	1:D:81:VAL:CG1	1.86	0.89
2:B:805:NAG:O5	2:B:806:NAG:H83	1.71	0.89
1:C:371:ILE:CD1	1:C:381:VAL:HG11	2.03	0.89
1:C:518:ASN:O	1:C:520:PRO:HD3	1.72	0.89
1:D:154:ASP:HB3	1:D:155:PRO:HD2	1.54	0.89
1:D:523:THR:HG23	1:D:524:VAL:CG2	2.03	0.89
1:D:338:ARG:HD3	1:D:352:ILE:CG2	2.02	0.89
1:A:517:GLN:O	1:A:519:ASN:N	2.03	0.89
1:A:8:LYS:CE	1:D:28:LYS:HG3	2.03	0.89
1:D:464:ILE:HD12	1:D:465:PRO:HD3	1.53	0.89
1:D:518:ASN:O	1:D:520:PRO:HD3	1.72	0.89
1:A:4:ILE:HA	1:B:91:PRO:CD	1.94	0.89
1:A:8:LYS:HD2	1:A:8:LYS:N	1.87	0.89
1:B:464:ILE:HD12	1:B:465:PRO:HD3	1.53	0.89
1:A:221:PHE:HE1	1:A:315:SER:O	1.56	0.89
1:B:31:PHE:CA	1:C:30:ARG:CA	2.49	0.89
1:B:221:PHE:HE1	1:B:315:SER:O	1.56	0.89
1:C:154:ASP:HB3	1:C:155:PRO:HD2	1.54	0.89
1:D:221:PHE:HE1	1:D:315:SER:O	1.56	0.89
1:A:24:ILE:HG22	1:D:2:TRP:CD1	2.08	0.88
1:A:352:ILE:HG13	1:A:388:VAL:HB	1.51	0.88
1:B:449:ASP:H	1:B:532:CYS:HB3	1.37	0.88
1:C:318:THR:HG21	2:C:806:NAG:H5	1.55	0.88
1:B:371:ILE:CD1	1:B:381:VAL:HG11	2.03	0.88
1:C:89:GLU:OE1	1:D:78:SER:CB	2.21	0.88
1:A:449:ASP:H	1:A:532:CYS:HB3	1.37	0.88
1:B:8:LYS:HD2	1:B:8:LYS:N	1.87	0.88
1:C:31:PHE:HB3	1:D:75:VAL:CG2	2.02	0.88
1:C:81:VAL:HG13	1:D:40:GLY:H	1.38	0.88
1:C:464:ILE:HD12	1:C:465:PRO:HD3	1.53	0.88
1:C:486:GLU:HB2	1:C:495:LEU:HB2	1.56	0.88
1:D:396:ARG:NH2	1:D:464:ILE:CG2	2.35	0.88
1:A:3:VAL:HG23	1:B:91:PRO:HB3	1.55	0.88
1:C:338:ARG:HD3	1:C:352:ILE:CG2	2.02	0.88
1:B:523:THR:HG23	1:B:524:VAL:CG2	2.03	0.88
1:A:91:PRO:HA	1:B:1:ASP:O	1.73	0.88
1:B:338:ARG:HD3	1:B:352:ILE:CG2	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:ILE:HD11	1:C:465:PRO:HD2	1.53	0.88
1:C:482:THR:HG21	1:C:499:THR:N	1.81	0.88
1:D:378:TRP:HB2	1:D:379:LEU:HD23	1.53	0.88
1:A:464:ILE:HD11	1:A:465:PRO:HD2	1.53	0.88
1:C:449:ASP:H	1:C:532:CYS:HB3	1.37	0.88
1:A:343:GLU:HB3	1:A:433:VAL:HG21	1.55	0.88
1:A:486:GLU:HB2	1:A:495:LEU:HB2	1.56	0.88
1:C:483:TRP:CZ3	1:C:498:PRO:HG3	2.09	0.88
1:C:523:THR:HG23	1:C:524:VAL:CG2	2.03	0.88
1:B:483:TRP:CZ3	1:B:498:PRO:HG3	2.09	0.88
1:C:89:GLU:OE1	1:D:78:SER:CA	2.22	0.88
1:D:371:ILE:CD1	1:D:381:VAL:HG11	2.03	0.88
1:D:464:ILE:HD11	1:D:465:PRO:HD2	1.53	0.88
1:A:518:ASN:O	1:A:520:PRO:HD3	1.72	0.88
1:C:343:GLU:HB3	1:C:433:VAL:HG21	1.55	0.87
1:D:333:VAL:HB	1:D:334:PRO:HD3	1.56	0.87
1:D:483:TRP:CZ3	1:D:498:PRO:HG3	2.09	0.87
1:B:340:ASP:HA	1:B:429:HIS:HB3	1.53	0.87
1:C:87:PRO:HD3	1:D:42:GLY:C	2.00	0.87
1:B:257:ALA:O	1:B:273:THR:HG21	1.74	0.87
1:C:440:PRO:CD	1:C:522:LEU:HD12	2.05	0.87
1:A:371:ILE:CD1	1:A:381:VAL:HG11	2.03	0.87
1:C:86:SER:CA	1:D:42:GLY:C	2.46	0.87
1:D:441:SER:OG	1:D:442:PRO:HD3	1.75	0.87
1:A:440:PRO:CD	1:A:522:LEU:HD12	2.05	0.87
1:C:257:ALA:O	1:C:273:THR:HG21	1.74	0.87
1:B:318:THR:HG21	2:B:806:NAG:H5	1.56	0.86
1:C:35:TYR:HD2	1:D:45:ASN:OD1	1.55	0.86
1:A:318:THR:HG21	2:A:806:NAG:H5	1.56	0.86
1:A:320:THR:HG21	2:A:807:NAG:C2	2.05	0.86
1:B:277:SER:C	1:B:278:ASN:HD22	1.83	0.86
1:B:333:VAL:HB	1:B:334:PRO:HD3	1.56	0.86
1:B:343:GLU:HB3	1:B:433:VAL:HG21	1.55	0.86
1:C:81:VAL:CG1	1:D:45:ASN:H	1.87	0.86
1:C:221:PHE:HE1	1:C:315:SER:O	1.56	0.86
1:C:320:THR:HG21	2:C:807:NAG:C2	2.05	0.86
1:B:320:THR:HG21	2:B:807:NAG:C2	2.05	0.86
1:A:257:ALA:O	1:A:273:THR:HG21	1.74	0.86
1:B:486:GLU:HB2	1:B:495:LEU:HB2	1.56	0.86
1:C:333:VAL:HB	1:C:334:PRO:HD3	1.56	0.86
1:D:277:SER:C	1:D:278:ASN:HD22	1.83	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TRP:CZ3	1:A:498:PRO:HG3	2.09	0.86
1:C:82:SER:HB3	1:D:75:VAL:N	1.89	0.86
1:C:85:GLY:CA	1:D:41:GLN:C	2.47	0.86
1:C:87:PRO:HG3	1:D:43:ALA:C	2.00	0.86
1:B:440:PRO:CD	1:B:522:LEU:HD12	2.05	0.86
1:B:441:SER:OG	1:B:442:PRO:HD3	1.75	0.86
1:A:99:ILE:HG21	1:D:30:ARG:NH1	1.90	0.86
1:A:441:SER:OG	1:A:442:PRO:HD3	1.75	0.86
1:C:91:PRO:CA	1:D:79:HIS:HD2	1.89	0.86
1:D:486:GLU:HB2	1:D:495:LEU:HB2	1.56	0.86
1:A:1:ASP:H1	1:B:94:ILE:HD11	1.40	0.86
1:C:87:PRO:HD2	1:D:51:PHE:HB2	1.57	0.86
1:C:235:ILE:HG13	1:C:287:GLY:HA2	1.57	0.86
1:C:31:PHE:HE1	1:D:97:ASN:OD1	1.58	0.86
1:C:523:THR:HG23	1:C:524:VAL:N	1.90	0.86
1:A:440:PRO:HD2	1:A:522:LEU:HD12	1.58	0.85
1:C:441:SER:OG	1:C:442:PRO:HD3	1.75	0.85
1:C:517:GLN:C	1:C:519:ASN:H	1.84	0.85
1:A:277:SER:C	1:A:278:ASN:HD22	1.84	0.85
1:B:464:ILE:HD12	1:B:465:PRO:N	1.91	0.85
1:A:464:ILE:HD12	1:A:465:PRO:HD3	1.53	0.85
1:B:30:ARG:C	1:C:30:ARG:HG3	1.96	0.85
1:D:440:PRO:CD	1:D:522:LEU:HD12	2.05	0.85
1:D:523:THR:HG23	1:D:524:VAL:N	1.90	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:CE1	1.95	0.85
1:B:523:THR:HG23	1:B:524:VAL:N	1.90	0.85
1:C:85:GLY:CA	1:D:42:GLY:HA2	1.70	0.85
1:D:257:ALA:O	1:D:273:THR:HG21	1.74	0.85
1:D:517:GLN:C	1:D:519:ASN:H	1.84	0.85
1:A:235:ILE:HG13	1:A:287:GLY:HA2	1.58	0.85
1:C:91:PRO:HA	1:D:79:HIS:HD2	1.40	0.85
1:C:483:TRP:HZ2	1:C:507:TYR:CE1	1.95	0.85
1:D:423:THR:CB	2:D:810:NAG:C7	2.54	0.85
1:A:4:ILE:HG22	1:B:91:PRO:O	1.76	0.85
1:A:464:ILE:HD12	1:A:465:PRO:N	1.91	0.85
1:A:483:TRP:HZ2	1:A:507:TYR:CE1	1.95	0.85
1:C:451:ASN:N	1:C:533:GLU:O	2.10	0.85
1:D:318:THR:HG21	2:D:806:NAG:H5	1.56	0.85
1:D:343:GLU:HB3	1:D:433:VAL:HG21	1.55	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:HE1	1.24	0.85
1:C:81:VAL:HG12	1:D:43:ALA:CA	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLU:CA	1:D:79:HIS:N	2.38	0.85
1:A:438:PRO:HB3	1:A:471:TYR:HE2	1.41	0.85
1:A:517:GLN:C	1:A:519:ASN:H	1.84	0.85
1:B:30:ARG:O	1:C:30:ARG:HA	1.77	0.85
1:C:31:PHE:O	1:D:73:LYS:HD3	1.77	0.85
1:C:87:PRO:HB3	1:D:43:ALA:HB1	1.56	0.85
1:D:464:ILE:HD12	1:D:465:PRO:N	1.91	0.85
1:D:483:TRP:HZ2	1:D:507:TYR:CE1	1.95	0.85
1:A:333:VAL:HB	1:A:334:PRO:HD3	1.56	0.85
1:A:423:THR:CB	2:A:810:NAG:C7	2.54	0.85
1:D:320:THR:HG21	2:D:807:NAG:C2	2.05	0.85
1:B:438:PRO:HB3	1:B:471:TYR:HE2	1.41	0.85
1:B:423:THR:CB	2:B:810:NAG:C7	2.54	0.84
1:B:517:GLN:C	1:B:519:ASN:H	1.84	0.84
1:C:222:ASP:OD1	1:C:222:ASP:C	2.20	0.84
1:A:396:ARG:HD3	1:A:431:LEU:C	2.02	0.84
1:B:375:PRO:HB3	1:B:400:TYR:CE2	2.12	0.84
1:C:423:THR:CB	2:C:810:NAG:C7	2.54	0.84
1:B:451:ASN:N	1:B:533:GLU:O	2.10	0.84
1:C:277:SER:C	1:C:278:ASN:HD22	1.84	0.84
1:D:155:PRO:HB2	2:D:801:NAG:H81	1.60	0.84
1:B:155:PRO:C	1:B:157:GLU:H	1.86	0.84
1:B:230:VAL:O	1:B:324:GLU:N	2.11	0.84
1:B:235:ILE:HG13	1:B:287:GLY:HA2	1.58	0.84
1:C:438:PRO:HB3	1:C:471:TYR:HE2	1.41	0.84
1:D:375:PRO:HB3	1:D:400:TYR:CE2	2.12	0.84
1:A:396:ARG:NE	1:A:432:ASP:HB2	1.93	0.84
1:B:396:ARG:HD3	1:B:431:LEU:C	2.03	0.84
1:C:1:ASP:H2	1:D:28:LYS:CD	1.86	0.84
1:C:375:PRO:HB3	1:C:400:TYR:CE2	2.12	0.84
1:D:396:ARG:NE	1:D:432:ASP:HB2	1.93	0.84
1:A:155:PRO:HB2	2:A:801:NAG:H81	1.59	0.84
1:B:27:ASN:HD22	1:B:27:ASN:C	1.85	0.84
1:C:230:VAL:O	1:C:324:GLU:N	2.11	0.84
1:C:440:PRO:HD2	1:C:522:LEU:HD12	1.59	0.84
1:D:230:VAL:O	1:D:324:GLU:N	2.11	0.84
1:A:423:THR:HB	2:A:810:NAG:N2	1.93	0.84
1:C:1:ASP:CA	1:D:28:LYS:HD3	2.08	0.84
1:C:27:ASN:HD22	1:C:27:ASN:C	1.85	0.84
1:C:396:ARG:NE	1:C:432:ASP:HB2	1.93	0.84
1:A:375:PRO:HB3	1:A:400:TYR:CE2	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:OG	1:A:167:ARG:HD2	1.78	0.83
1:C:464:ILE:HD12	1:C:465:PRO:N	1.92	0.83
1:D:438:PRO:HB3	1:D:471:TYR:HE2	1.41	0.83
1:A:423:THR:CB	2:A:810:NAG:N2	2.42	0.83
1:A:451:ASN:N	1:A:533:GLU:O	2.10	0.83
1:B:423:THR:CB	2:B:810:NAG:N2	2.42	0.83
1:A:87:PRO:O	1:B:2:TRP:CZ2	2.30	0.83
1:A:222:ASP:OD1	1:A:222:ASP:C	2.20	0.83
1:B:32:ASN:ND2	1:B:83:GLU:H	1.77	0.83
1:D:423:THR:CB	2:D:810:NAG:N2	2.42	0.83
1:B:32:ASN:CB	1:C:27:ASN:HA	2.07	0.83
1:B:448:CYS:O	1:B:452:PRO:HG3	1.79	0.83
1:C:92:MET:HE2	1:D:91:PRO:CG	2.07	0.83
1:C:448:CYS:O	1:C:452:PRO:HG3	1.79	0.83
1:D:155:PRO:C	1:D:157:GLU:H	1.86	0.83
1:D:448:CYS:O	1:D:452:PRO:HG3	1.78	0.83
1:A:230:VAL:O	1:A:324:GLU:N	2.11	0.83
1:C:396:ARG:HD3	1:C:431:LEU:C	2.03	0.83
1:C:423:THR:CB	2:C:810:NAG:N2	2.42	0.83
1:A:523:THR:HG23	1:A:524:VAL:N	1.90	0.83
1:C:28:LYS:HD3	1:C:88:VAL:HG12	1.61	0.83
1:C:483:TRP:HZ2	1:C:507:TYR:HE1	1.24	0.83
1:B:222:ASP:OD1	1:B:222:ASP:C	2.20	0.83
1:B:396:ARG:NE	1:B:432:ASP:HB2	1.93	0.83
1:D:28:LYS:HD3	1:D:88:VAL:HG12	1.61	0.83
1:D:396:ARG:HD3	1:D:431:LEU:C	2.03	0.83
1:D:440:PRO:HD2	1:D:522:LEU:HD12	1.59	0.83
1:D:469:TYR:CG	1:D:470:PRO:CD	2.61	0.83
1:A:32:ASN:ND2	1:A:83:GLU:H	1.77	0.83
1:B:423:THR:HB	2:B:810:NAG:N2	1.93	0.83
1:B:446:THR:HG21	1:B:537:ILE:O	1.79	0.83
1:C:32:ASN:ND2	1:C:83:GLU:H	1.77	0.83
1:C:80:ALA:CB	1:D:39:THR:OG1	2.25	0.83
1:D:446:THR:HG21	1:D:537:ILE:O	1.79	0.83
1:A:289:ASP:O	1:A:289:ASP:OD2	1.97	0.82
1:B:154:ASP:HB3	2:B:801:NAG:HN2	1.44	0.82
1:B:482:THR:HG21	1:B:500:GLN:N	1.94	0.82
1:D:222:ASP:OD1	1:D:222:ASP:C	2.20	0.82
1:A:469:TYR:CG	1:A:470:PRO:CD	2.61	0.82
1:A:540:GLN:O	1:A:540:GLN:OE1	1.97	0.82
1:B:540:GLN:O	1:B:540:GLN:OE1	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:ASN:N	1:D:533:GLU:O	2.10	0.82
1:A:448:CYS:O	1:A:452:PRO:HG3	1.79	0.82
1:D:482:THR:HG21	1:D:500:GLN:N	1.94	0.82
1:C:482:THR:HG21	1:C:500:GLN:N	1.94	0.82
1:C:540:GLN:O	1:C:540:GLN:OE1	1.97	0.82
1:D:27:ASN:HD22	1:D:27:ASN:C	1.85	0.82
1:D:235:ILE:HG13	1:D:287:GLY:HA2	1.58	0.82
1:A:482:THR:HG21	1:A:500:GLN:N	1.94	0.82
1:B:469:TYR:CG	1:B:470:PRO:CD	2.61	0.82
1:D:423:THR:HB	2:D:810:NAG:N2	1.93	0.82
1:C:35:TYR:HD2	1:D:45:ASN:CG	1.86	0.82
1:B:28:LYS:HD3	1:B:88:VAL:HG12	1.61	0.82
1:B:440:PRO:HD2	1:B:522:LEU:HD12	1.59	0.82
1:C:469:TYR:CG	1:C:470:PRO:CD	2.61	0.82
1:B:155:PRO:HB2	2:B:801:NAG:H81	1.59	0.82
1:B:234:GLU:H	1:B:235:ILE:CG2	1.92	0.82
1:C:423:THR:HB	2:C:810:NAG:N2	1.93	0.82
1:D:483:TRP:HZ2	1:D:507:TYR:HE1	1.24	0.82
1:C:90:GLU:OE2	1:D:36:TYR:C	2.17	0.81
1:D:32:ASN:ND2	1:D:83:GLU:H	1.77	0.81
1:D:289:ASP:O	1:D:289:ASP:OD2	1.97	0.81
1:A:3:VAL:N	1:B:78:SER:O	2.12	0.81
1:A:154:ASP:HB3	2:A:801:NAG:N2	1.95	0.81
1:C:155:PRO:HB2	2:C:801:NAG:H81	1.60	0.81
1:A:154:ASP:HB3	2:A:801:NAG:HN2	1.45	0.81
1:A:432:ASP:CG	1:A:464:ILE:HG22	2.05	0.81
1:A:446:THR:HG21	1:A:537:ILE:O	1.79	0.81
1:A:505:GLY:C	1:A:506:ASP:OD1	2.23	0.81
1:B:289:ASP:O	1:B:289:ASP:OD2	1.97	0.81
1:C:85:GLY:HA3	1:D:42:GLY:HA2	1.62	0.81
1:C:154:ASP:HB3	2:C:801:NAG:HN2	1.44	0.81
1:C:446:THR:HG21	1:C:537:ILE:O	1.79	0.81
1:A:483:TRP:HZ2	1:A:507:TYR:HE1	1.24	0.81
1:C:289:ASP:O	1:C:289:ASP:OD2	1.97	0.81
1:C:432:ASP:CG	1:C:464:ILE:HG22	2.05	0.81
1:C:31:PHE:CE1	1:D:97:ASN:OD1	2.33	0.81
1:C:154:ASP:HB3	2:C:801:NAG:N2	1.95	0.81
1:A:27:ASN:HD22	1:A:27:ASN:C	1.85	0.81
1:B:496:LEU:HD21	1:B:509:ILE:HD13	1.63	0.81
1:D:154:ASP:HB3	2:D:801:NAG:N2	1.95	0.81
1:D:496:LEU:HD21	1:D:509:ILE:HD13	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:GLY:C	1:D:506:ASP:OD1	2.23	0.81
1:D:540:GLN:O	1:D:540:GLN:OE1	1.97	0.81
1:A:90:GLU:HB3	1:B:3:VAL:O	1.80	0.81
1:B:265:GLU:HB3	1:B:268:PHE:HE2	1.46	0.81
1:A:396:ARG:HH21	1:A:464:ILE:HG22	1.46	0.81
1:B:290:PHE:CE2	1:B:293:ARG:HB2	2.16	0.81
1:B:432:ASP:CG	1:B:464:ILE:HG22	2.05	0.81
1:C:496:LEU:HD21	1:C:509:ILE:HD13	1.63	0.81
1:C:505:GLY:C	1:C:506:ASP:OD1	2.23	0.81
1:D:469:TYR:CD2	1:D:470:PRO:HD2	2.16	0.81
1:A:28:LYS:HD3	1:A:88:VAL:HG12	1.61	0.81
1:B:469:TYR:CD2	1:B:470:PRO:HD2	2.16	0.81
1:B:505:GLY:C	1:B:506:ASP:OD1	2.23	0.81
1:C:290:PHE:CE2	1:C:293:ARG:HB2	2.16	0.81
1:A:486:GLU:O	1:A:494:MET:HA	1.81	0.81
1:B:127:VAL:HG13	1:B:128:MET:H	1.46	0.81
1:B:486:GLU:O	1:B:494:MET:HA	1.81	0.81
1:C:486:GLU:O	1:C:494:MET:HA	1.81	0.81
1:B:32:ASN:C	1:C:25:LYS:HE2	2.06	0.80
1:C:88:VAL:C	1:D:38:ILE:HG13	2.05	0.80
1:C:155:PRO:C	1:C:157:GLU:H	1.86	0.80
1:D:432:ASP:CG	1:D:464:ILE:HG22	2.05	0.80
1:A:265:GLU:HB3	1:A:268:PHE:HE2	1.46	0.80
1:B:86:SER:N	1:D:91:PRO:HD2	1.96	0.80
1:B:154:ASP:HB3	2:B:801:NAG:N2	1.95	0.80
1:C:79:HIS:HB3	1:D:39:THR:HG22	1.63	0.80
1:C:84:ASN:HA	1:D:71:TYR:CD2	2.16	0.80
1:D:486:GLU:O	1:D:494:MET:HA	1.81	0.80
1:A:155:PRO:C	1:A:157:GLU:H	1.86	0.80
1:A:290:PHE:CE2	1:A:293:ARG:HB2	2.16	0.80
1:A:469:TYR:CD2	1:A:470:PRO:HD2	2.16	0.80
1:B:30:ARG:O	1:C:30:ARG:CG	2.29	0.80
1:C:432:ASP:OD2	1:C:464:ILE:CG2	2.30	0.80
1:A:127:VAL:HG13	1:A:128:MET:H	1.46	0.80
1:C:93:GLU:N	1:D:81:VAL:HG11	1.96	0.80
1:C:299:GLN:HG2	1:C:318:THR:HG23	1.62	0.80
1:D:265:GLU:HB3	1:D:268:PHE:HE2	1.46	0.80
1:D:406:TYR:CD1	2:D:808:NAG:H83	2.17	0.80
1:C:265:GLU:HB3	1:C:268:PHE:HE2	1.46	0.80
1:C:540:GLN:O	1:C:540:GLN:CG	2.30	0.80
1:A:234:GLU:H	1:A:235:ILE:CG2	1.92	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLN:HG2	1:A:318:THR:HG23	1.62	0.80
1:A:482:THR:OG1	1:A:500:GLN:HG2	1.82	0.80
1:A:496:LEU:HD21	1:A:509:ILE:HD13	1.63	0.80
1:C:396:ARG:HH21	1:C:464:ILE:HG22	1.46	0.80
1:C:469:TYR:CD2	1:C:470:PRO:HD2	2.16	0.80
1:D:371:ILE:HD11	1:D:381:VAL:HG11	1.64	0.80
1:A:406:TYR:CD1	2:A:808:NAG:H83	2.17	0.80
1:C:1:ASP:H3	1:D:88:VAL:CB	1.95	0.80
1:D:234:GLU:H	1:D:235:ILE:CG2	1.92	0.80
1:A:232:GLU:HG3	1:A:290:PHE:N	1.98	0.79
1:A:290:PHE:HD2	1:A:293:ARG:H	1.28	0.79
1:B:232:GLU:HG3	1:B:290:PHE:N	1.98	0.79
1:B:406:TYR:CD1	2:B:808:NAG:H83	2.17	0.79
1:C:35:TYR:CD2	1:D:45:ASN:OD1	2.35	0.79
1:C:87:PRO:CD	1:D:43:ALA:HB2	2.12	0.79
1:C:234:GLU:H	1:C:235:ILE:CG2	1.92	0.79
1:D:396:ARG:HH21	1:D:464:ILE:HG22	1.46	0.79
1:B:396:ARG:HH21	1:B:464:ILE:HG22	1.46	0.79
1:D:449:ASP:HB3	1:D:532:CYS:H	1.47	0.79
1:A:365:GLN:HG3	1:A:365:GLN:O	1.82	0.79
1:C:127:VAL:HG13	1:C:128:MET:H	1.46	0.79
1:D:290:PHE:CE2	1:D:293:ARG:HB2	2.16	0.79
1:A:523:THR:CG2	1:A:524:VAL:H	1.94	0.79
1:C:371:ILE:HD11	1:C:381:VAL:HG11	1.64	0.79
1:C:85:GLY:HA2	1:D:42:GLY:H	1.45	0.79
1:D:127:VAL:HG13	1:D:128:MET:H	1.46	0.79
1:A:7:ILE:HG23	1:D:27:ASN:OD1	1.83	0.79
1:A:195:ASP:HB3	1:A:200:GLY:HA3	1.65	0.79
1:C:406:TYR:CD1	2:C:808:NAG:H83	2.17	0.79
1:D:154:ASP:HB3	2:D:801:NAG:HN2	1.44	0.79
1:D:482:THR:OG1	1:D:500:GLN:HG2	1.82	0.79
2:D:809:NAG:H61	2:D:810:NAG:H62	1.65	0.79
1:A:24:ILE:CG1	1:D:2:TRP:CZ2	2.66	0.79
1:B:32:ASN:HB3	1:C:27:ASN:HA	1.64	0.79
1:B:449:ASP:HB3	1:B:532:CYS:H	1.47	0.79
1:C:27:ASN:ND2	1:D:93:GLU:N	2.30	0.79
1:C:154:ASP:CB	1:C:155:PRO:HD2	2.13	0.79
1:A:154:ASP:CB	1:A:155:PRO:HD2	2.13	0.79
1:A:301:THR:HG21	2:A:805:NAG:C8	2.12	0.79
1:A:485:ALA:O	1:A:486:GLU:CG	2.31	0.79
1:B:299:GLN:HG2	1:B:318:THR:HG23	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLU:C	1:D:79:HIS:H	1.78	0.79
1:C:485:ALA:O	1:C:486:GLU:CG	2.30	0.79
1:D:154:ASP:CB	1:D:155:PRO:HD2	2.13	0.79
1:D:299:GLN:HG2	1:D:318:THR:HG23	1.62	0.79
1:A:1:ASP:HA	1:B:24:ILE:HD13	1.63	0.79
1:A:432:ASP:OD2	1:A:464:ILE:CG2	2.30	0.78
1:A:540:GLN:O	1:A:540:GLN:CG	2.30	0.78
1:B:485:ALA:O	1:B:486:GLU:CG	2.31	0.78
1:C:87:PRO:C	1:D:76:LEU:CD2	2.53	0.78
1:A:238:GLU:HA	1:A:283:THR:HG22	1.66	0.78
1:B:154:ASP:CB	1:B:155:PRO:HD2	2.13	0.78
1:C:238:GLU:HA	1:C:283:THR:HG22	1.66	0.78
1:B:371:ILE:HD11	1:B:381:VAL:HG11	1.64	0.78
1:C:90:GLU:CB	1:D:79:HIS:N	2.45	0.78
1:D:232:GLU:HG3	1:D:290:PHE:N	1.98	0.78
1:C:232:GLU:HG3	1:C:290:PHE:N	1.98	0.78
1:A:24:ILE:CA	1:D:2:TRP:CD1	2.61	0.78
1:A:501:GLN:HG2	1:A:501:GLN:O	1.84	0.78
1:B:88:VAL:O	1:D:1:ASP:CB	2.32	0.78
2:B:809:NAG:H61	2:B:810:NAG:H62	1.65	0.78
1:D:432:ASP:OD2	1:D:464:ILE:CG2	2.30	0.78
2:C:809:NAG:H61	2:C:810:NAG:H62	1.65	0.78
1:A:156:GLU:HG3	1:A:160:PRO:HB3	1.66	0.78
1:A:524:VAL:CG2	2:A:904:NAG:H81	2.14	0.78
1:C:93:GLU:HB2	1:D:81:VAL:HG11	1.64	0.78
1:C:156:GLU:HG3	1:C:160:PRO:HB3	1.66	0.78
1:C:449:ASP:HB3	1:C:532:CYS:H	1.47	0.78
1:D:365:GLN:HG3	1:D:365:GLN:O	1.82	0.78
1:B:156:GLU:HG3	1:B:160:PRO:HB3	1.66	0.78
1:C:91:PRO:C	1:D:37:SER:OG	2.26	0.78
1:C:482:THR:OG1	1:C:500:GLN:HG2	1.82	0.78
1:B:432:ASP:OD2	1:B:464:ILE:CG2	2.30	0.78
1:B:482:THR:OG1	1:B:500:GLN:HG2	1.82	0.78
1:C:81:VAL:HG13	1:D:40:GLY:N	1.98	0.78
1:D:238:GLU:HA	1:D:283:THR:HG22	1.66	0.78
1:A:10:SER:HB2	1:D:30:ARG:HG3	1.64	0.78
1:A:449:ASP:HB3	1:A:532:CYS:H	1.47	0.78
1:B:238:GLU:HA	1:B:283:THR:HG22	1.66	0.78
1:A:147:SER:OG	1:A:167:ARG:CG	2.32	0.77
1:A:371:ILE:HD11	1:A:381:VAL:HG11	1.64	0.77
1:B:524:VAL:CG2	2:B:904:NAG:H81	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:SER:N	1:D:41:GLN:O	2.17	0.77
1:B:290:PHE:HD2	1:B:293:ARG:H	1.28	0.77
1:B:335:ALA:HB1	3:B:811:NDG:H6	1.49	0.77
1:C:365:GLN:HG3	1:C:365:GLN:O	1.82	0.77
1:C:523:THR:CG2	1:C:524:VAL:H	1.94	0.77
1:A:2:TRP:CG	1:B:80:ALA:HB2	2.16	0.77
1:A:147:SER:OG	1:A:167:ARG:CD	2.32	0.77
1:C:524:VAL:CG2	2:C:904:NAG:H81	2.14	0.77
1:D:223:PRO:HD2	1:D:226:TYR:OH	1.85	0.77
1:D:485:ALA:O	1:D:486:GLU:CG	2.30	0.77
1:A:24:ILE:HG13	1:D:2:TRP:CZ2	2.19	0.77
1:A:223:PRO:HD2	1:A:226:TYR:OH	1.85	0.77
1:D:194:THR:HB	1:D:198:GLY:HA2	1.66	0.77
1:D:524:VAL:CG2	2:D:904:NAG:H81	2.14	0.77
1:A:2:TRP:O	1:B:92:MET:HB2	1.83	0.77
1:C:86:SER:HA	1:D:42:GLY:O	1.84	0.77
1:C:195:ASP:HB3	1:C:200:GLY:HA3	1.65	0.77
1:C:223:PRO:HD2	1:C:226:TYR:OH	1.85	0.77
2:A:809:NAG:H61	2:A:810:NAG:H62	1.65	0.77
1:B:31:PHE:HZ	1:C:34:VAL:HG21	1.49	0.77
1:C:86:SER:HB3	1:D:76:LEU:HD11	1.66	0.77
1:C:194:THR:HB	1:C:198:GLY:HA2	1.67	0.77
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.77
1:D:195:ASP:HB3	1:D:200:GLY:HA3	1.65	0.77
1:B:30:ARG:O	1:C:30:ARG:CB	2.31	0.77
1:B:362:GLN:O	1:B:364:ILE:HG23	1.85	0.77
1:C:81:VAL:HG11	1:D:45:ASN:N	1.99	0.77
1:A:194:THR:HB	1:A:198:GLY:HA2	1.67	0.77
1:B:540:GLN:O	1:B:540:GLN:CG	2.30	0.77
1:A:196:LEU:HB2	1:A:199:ALA:HB3	1.67	0.76
1:B:86:SER:HA	1:D:90:GLU:HA	1.62	0.76
1:C:31:PHE:HA	1:D:73:LYS:NZ	2.00	0.76
1:D:272:THR:HG22	1:D:273:THR:H	1.51	0.76
1:D:540:GLN:O	1:D:540:GLN:CG	2.30	0.76
1:B:88:VAL:C	1:D:1:ASP:HB2	2.09	0.76
1:B:440:PRO:HB3	1:B:457:LEU:HD21	1.67	0.76
1:D:290:PHE:HD2	1:D:293:ARG:H	1.28	0.76
1:B:195:ASP:HB3	1:B:200:GLY:HA3	1.65	0.76
1:C:186:GLU:O	2:C:801:NAG:O7	2.03	0.76
1:C:362:GLN:O	1:C:364:ILE:HG23	1.85	0.76
1:D:186:GLU:O	2:D:801:NAG:O7	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:SER:HG	1:D:370:PHE:HE1	1.33	0.76
1:A:4:ILE:C	1:B:91:PRO:HB2	2.10	0.76
1:B:365:GLN:O	1:B:365:GLN:HG3	1.82	0.76
1:B:366:LYS:CG	1:B:367:LEU:N	2.48	0.76
1:C:396:ARG:HH21	1:C:464:ILE:CG2	1.98	0.76
1:D:241:ARG:HE	1:D:281:ILE:HD12	1.51	0.76
1:A:90:GLU:N	1:B:2:TRP:HE3	1.83	0.76
1:B:186:GLU:O	2:B:801:NAG:O7	2.04	0.76
1:C:88:VAL:CG1	1:D:94:ILE:HB	2.15	0.76
1:D:440:PRO:HB3	1:D:457:LEU:HD21	1.67	0.76
1:A:186:GLU:O	2:A:801:NAG:O7	2.03	0.76
1:A:396:ARG:HH21	1:A:464:ILE:CG2	1.98	0.76
1:A:24:ILE:CG2	1:D:2:TRP:CD1	2.67	0.76
1:A:290:PHE:HZ	1:A:296:TYR:HH	1.33	0.76
1:B:196:LEU:HB2	1:B:199:ALA:HB3	1.67	0.76
1:B:523:THR:HG23	1:B:524:VAL:HG22	1.67	0.76
1:C:4:ILE:HG21	1:D:87:PRO:HG2	1.68	0.76
1:D:362:GLN:O	1:D:364:ILE:HG23	1.85	0.76
1:B:501:GLN:O	1:B:501:GLN:HG2	1.84	0.76
1:C:196:LEU:HB2	1:C:199:ALA:HB3	1.67	0.76
1:D:156:GLU:HG3	1:D:160:PRO:HB3	1.66	0.76
1:D:290:PHE:HZ	1:D:296:TYR:HH	1.31	0.76
1:A:440:PRO:HB3	1:A:457:LEU:HD21	1.67	0.76
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.76
1:B:82:SER:CB	1:C:27:ASN:HB3	2.15	0.76
1:B:223:PRO:HD2	1:B:226:TYR:OH	1.85	0.76
1:D:371:ILE:HD12	1:D:410:MET:HB3	1.68	0.76
1:A:91:PRO:CA	1:B:1:ASP:O	2.34	0.76
1:A:289:ASP:O	1:A:289:ASP:CG	2.29	0.76
1:C:83:GLU:OE1	1:D:41:GLN:NE2	2.12	0.76
1:C:501:GLN:HG2	1:C:501:GLN:O	1.84	0.76
1:D:196:LEU:HB2	1:D:199:ALA:HB3	1.67	0.76
1:D:448:CYS:SG	1:D:537:ILE:HG22	2.26	0.76
1:B:301:THR:HG21	2:B:805:NAG:C8	2.12	0.75
1:A:371:ILE:HD12	1:A:410:MET:HB3	1.68	0.75
1:B:84:ASN:HD22	1:D:91:PRO:HB2	1.49	0.75
1:C:301:THR:HG21	2:C:805:NAG:C8	2.13	0.75
1:C:371:ILE:HD12	1:C:410:MET:HB3	1.68	0.75
1:A:90:GLU:C	1:B:3:VAL:CG2	2.57	0.75
1:A:188:THR:HG23	1:A:208:ILE:CG1	2.16	0.75
1:B:88:VAL:HG13	1:C:27:ASN:OD1	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:THR:HG22	1:B:273:THR:H	1.51	0.75
1:B:364:ILE:HG13	1:B:364:ILE:O	1.87	0.75
1:C:272:THR:HG22	1:C:273:THR:H	1.50	0.75
1:D:501:GLN:O	1:D:501:GLN:HG2	1.84	0.75
1:B:448:CYS:SG	1:B:537:ILE:HG22	2.27	0.75
1:A:362:GLN:O	1:A:364:ILE:HG23	1.85	0.75
1:A:396:ARG:NH2	1:A:464:ILE:HB	2.02	0.75
1:B:31:PHE:CE2	1:C:29:ASP:CB	2.68	0.75
1:B:194:THR:HB	1:B:198:GLY:HA2	1.67	0.75
1:B:482:THR:CG2	1:B:499:THR:CG2	2.62	0.75
1:C:92:MET:HE2	1:D:91:PRO:HG2	1.66	0.75
1:C:448:CYS:SG	1:C:537:ILE:HG22	2.27	0.75
1:D:290:PHE:CD2	1:D:293:ARG:N	2.55	0.75
1:B:396:ARG:NH2	1:B:464:ILE:HB	2.02	0.75
1:C:289:ASP:O	1:C:289:ASP:CG	2.29	0.75
1:C:440:PRO:HB3	1:C:457:LEU:HD21	1.67	0.75
1:D:449:ASP:HB3	1:D:532:CYS:N	2.02	0.75
1:C:290:PHE:HD2	1:C:293:ARG:H	1.28	0.75
1:A:5:PRO:HD2	1:B:90:GLU:OE2	1.87	0.75
1:A:448:CYS:SG	1:A:537:ILE:HG22	2.27	0.74
1:D:366:LYS:CG	1:D:367:LEU:N	2.48	0.74
1:A:449:ASP:HB3	1:A:532:CYS:N	2.02	0.74
1:A:485:ALA:C	1:A:486:GLU:HG2	2.12	0.74
1:B:371:ILE:HD12	1:B:410:MET:HB3	1.68	0.74
1:A:523:THR:HG23	1:A:524:VAL:HG22	1.67	0.74
1:C:396:ARG:NH2	1:C:464:ILE:HB	2.02	0.74
1:D:523:THR:HG23	1:D:524:VAL:HG22	1.67	0.74
1:A:241:ARG:HE	1:A:281:ILE:HD12	1.51	0.74
1:A:272:THR:HG22	1:A:273:THR:H	1.50	0.74
1:C:2:TRP:N	1:D:89:GLU:HA	2.01	0.74
1:C:188:THR:HG23	1:C:208:ILE:CG1	2.16	0.74
1:A:3:VAL:HG23	1:B:91:PRO:CB	2.17	0.74
1:B:368:SER:HG	1:B:370:PHE:HE1	1.36	0.74
1:C:241:ARG:HE	1:C:281:ILE:HD12	1.51	0.74
1:D:188:THR:HG23	1:D:208:ILE:CG1	2.16	0.74
1:D:450:GLN:HG3	1:D:533:GLU:OE2	1.88	0.74
1:D:485:ALA:C	1:D:486:GLU:HG2	2.11	0.74
1:A:79:HIS:HA	1:B:1:ASP:H2	1.53	0.74
1:B:84:ASN:O	1:C:24:ILE:HB	1.87	0.74
1:B:84:ASN:HD21	1:D:91:PRO:HB2	1.53	0.74
1:B:396:ARG:HH21	1:B:464:ILE:CG2	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ASP:HB3	1:B:532:CYS:N	2.02	0.74
1:B:450:GLN:HG3	1:B:533:GLU:OE2	1.88	0.74
1:C:1:ASP:C	1:D:28:LYS:NZ	2.44	0.74
1:A:364:ILE:O	1:A:364:ILE:HG13	1.87	0.74
1:C:80:ALA:HB3	1:D:39:THR:OG1	1.88	0.74
1:C:88:VAL:HG22	1:D:76:LEU:CD2	1.96	0.74
1:C:482:THR:CG2	1:C:499:THR:CG2	2.62	0.74
1:D:1:ASP:CG	1:D:2:TRP:H	1.96	0.74
1:D:451:ASN:O	1:D:534:GLY:HA2	1.88	0.74
1:A:79:HIS:HA	1:B:1:ASP:N	2.03	0.74
1:A:298:LEU:N	1:A:298:LEU:HD23	2.03	0.74
1:B:485:ALA:C	1:B:486:GLU:HG2	2.11	0.74
1:C:290:PHE:HZ	1:C:296:TYR:HH	1.35	0.74
1:D:523:THR:CG2	1:D:524:VAL:N	2.46	0.74
1:A:450:GLN:HG3	1:A:533:GLU:OE2	1.88	0.74
1:C:31:PHE:CB	1:D:75:VAL:HG22	2.13	0.74
1:C:35:TYR:CD2	1:D:45:ASN:CG	2.65	0.74
1:C:523:THR:HG23	1:C:524:VAL:HG22	1.67	0.74
1:B:188:THR:HG23	1:B:208:ILE:CG1	2.16	0.73
1:B:290:PHE:HZ	1:B:296:TYR:HH	1.33	0.73
1:B:320:THR:CG2	2:B:807:NAG:HN2	2.01	0.73
1:C:90:GLU:OE2	1:D:37:SER:CA	2.30	0.73
1:C:366:LYS:CG	1:C:367:LEU:N	2.48	0.73
1:C:450:GLN:HG3	1:C:533:GLU:OE2	1.88	0.73
1:D:289:ASP:O	1:D:289:ASP:CG	2.29	0.73
1:A:223:PRO:HB2	1:A:226:TYR:CE2	2.23	0.73
1:B:1:ASP:CG	1:B:2:TRP:H	1.96	0.73
1:B:31:PHE:HA	1:C:30:ARG:HA	1.67	0.73
1:C:1:ASP:H1	1:D:28:LYS:HB2	1.53	0.73
1:C:26:SER:OG	1:D:77:SER:CB	2.36	0.73
1:C:449:ASP:HB3	1:C:532:CYS:N	2.02	0.73
1:D:320:THR:CG2	2:D:807:NAG:HN2	2.02	0.73
1:A:320:THR:CG2	2:A:807:NAG:N2	2.52	0.73
1:A:482:THR:CG2	1:A:499:THR:CG2	2.62	0.73
1:B:31:PHE:CE2	1:C:29:ASP:HB3	2.14	0.73
1:B:451:ASN:O	1:B:534:GLY:HA2	1.88	0.73
1:C:4:ILE:HG22	1:D:87:PRO:CG	2.16	0.73
1:C:88:VAL:HG12	1:D:94:ILE:CB	2.18	0.73
1:C:223:PRO:HB2	1:C:226:TYR:CE2	2.23	0.73
1:C:364:ILE:O	1:C:364:ILE:HG13	1.87	0.73
1:C:485:ALA:C	1:C:486:GLU:HG2	2.11	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ASN:O	1:A:534:GLY:HA2	1.88	0.73
1:B:241:ARG:HE	1:B:281:ILE:HD12	1.51	0.73
1:C:79:HIS:CG	1:D:44:ASP:OD1	2.41	0.73
1:D:223:PRO:HB2	1:D:226:TYR:CE2	2.23	0.73
1:D:364:ILE:O	1:D:364:ILE:HG13	1.87	0.73
1:A:276:GLU:HG3	1:A:277:SER:H	1.54	0.73
1:B:298:LEU:N	1:B:298:LEU:HD23	2.03	0.73
1:C:1:ASP:H1	1:D:28:LYS:HD3	1.47	0.73
1:C:84:ASN:O	1:D:47:PRO:HG2	1.88	0.73
1:D:333:VAL:CB	1:D:334:PRO:HD3	2.18	0.73
1:B:289:ASP:O	1:B:289:ASP:CG	2.29	0.73
1:C:451:ASN:O	1:C:534:GLY:HA2	1.88	0.73
1:D:373:ASN:ND2	1:D:374:ASP:H	1.87	0.73
1:A:333:VAL:CB	1:A:334:PRO:HD3	2.18	0.73
1:B:276:GLU:HG3	1:B:277:SER:H	1.54	0.73
1:C:290:PHE:HE2	1:C:293:ARG:HB2	1.52	0.73
1:A:27:ASN:C	1:A:27:ASN:ND2	2.46	0.73
1:B:223:PRO:HB2	1:B:226:TYR:CE2	2.23	0.73
1:B:273:THR:O	2:B:803:NAG:H82	1.89	0.73
1:B:290:PHE:HE2	1:B:293:ARG:HB2	1.52	0.73
1:B:320:THR:CG2	2:B:807:NAG:N2	2.52	0.73
1:B:373:ASN:ND2	1:B:374:ASP:H	1.87	0.73
1:D:298:LEU:N	1:D:298:LEU:HD23	2.03	0.73
1:D:301:THR:HG21	2:D:805:NAG:C8	2.12	0.73
1:A:342:SER:HA	1:A:431:LEU:HB2	1.71	0.73
1:B:364:ILE:O	1:B:364:ILE:CG1	2.37	0.73
1:D:364:ILE:O	1:D:364:ILE:CG1	2.37	0.73
1:D:396:ARG:HH21	1:D:464:ILE:CG2	1.98	0.73
1:A:373:ASN:ND2	1:A:374:ASP:H	1.87	0.72
1:B:88:VAL:C	1:D:1:ASP:CB	2.62	0.72
1:C:273:THR:O	2:C:803:NAG:H82	1.89	0.72
1:C:511:VAL:HG23	1:C:523:THR:O	1.89	0.72
1:A:90:GLU:CB	1:B:3:VAL:O	2.34	0.72
1:A:273:THR:O	2:A:803:NAG:H82	1.89	0.72
1:A:320:THR:CG2	2:A:807:NAG:HN2	2.01	0.72
1:B:32:ASN:HA	1:C:29:ASP:OD2	1.87	0.72
1:B:33:LYS:HB3	1:B:83:GLU:HG2	1.71	0.72
1:C:1:ASP:N	1:D:88:VAL:CB	2.52	0.72
1:C:298:LEU:HD23	1:C:298:LEU:N	2.03	0.72
1:D:33:LYS:HB3	1:D:83:GLU:HG2	1.71	0.72
1:D:290:PHE:HE2	1:D:293:ARG:HB2	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:THR:CG2	2:D:807:NAG:N2	2.52	0.72
1:C:320:THR:CG2	2:C:807:NAG:N2	2.52	0.72
1:D:482:THR:CG2	1:D:499:THR:CG2	2.62	0.72
1:A:99:ILE:CG2	1:D:30:ARG:NH1	2.50	0.72
1:A:511:VAL:HG23	1:A:523:THR:O	1.89	0.72
1:C:373:ASN:ND2	1:C:374:ASP:H	1.87	0.72
1:D:273:THR:O	2:D:803:NAG:H82	1.89	0.72
1:D:511:VAL:HG23	1:D:523:THR:O	1.89	0.72
1:A:1:ASP:CG	1:A:2:TRP:H	1.96	0.72
1:C:222:ASP:O	1:C:222:ASP:CG	2.32	0.72
1:D:222:ASP:O	1:D:222:ASP:CG	2.32	0.72
1:A:364:ILE:O	1:A:364:ILE:CG1	2.37	0.72
1:B:511:VAL:HG23	1:B:523:THR:O	1.89	0.72
1:C:333:VAL:CB	1:C:334:PRO:HD3	2.18	0.72
1:C:32:ASN:H	1:D:75:VAL:HG21	0.57	0.72
1:C:91:PRO:C	1:D:79:HIS:CD2	2.66	0.72
1:C:276:GLU:HG3	1:C:277:SER:H	1.54	0.72
1:A:24:ILE:C	1:D:2:TRP:CZ2	2.48	0.72
1:A:394:LEU:HD12	1:A:394:LEU:N	2.05	0.72
1:B:333:VAL:CB	1:B:334:PRO:HD3	2.18	0.72
1:C:1:ASP:CA	1:D:89:GLU:OE2	2.16	0.72
1:C:366:LYS:HG3	1:C:367:LEU:N	2.04	0.72
1:C:82:SER:HB2	1:D:75:VAL:H	1.52	0.72
1:D:276:GLU:HG3	1:D:277:SER:H	1.54	0.72
1:A:474:SER:CB	1:A:512:LEU:HG	2.14	0.71
1:D:396:ARG:NH2	1:D:464:ILE:HB	2.02	0.71
1:B:394:LEU:N	1:B:394:LEU:HD12	2.05	0.71
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.71
1:D:27:ASN:C	1:D:27:ASN:ND2	2.46	0.71
1:D:342:SER:HA	1:D:431:LEU:HB2	1.71	0.71
1:A:517:GLN:C	1:A:519:ASN:N	2.47	0.71
1:B:222:ASP:O	1:B:222:ASP:CG	2.32	0.71
1:C:90:GLU:HB3	1:D:79:HIS:N	2.05	0.71
1:C:227:THR:O	2:C:812:NAG:O5	2.09	0.71
1:C:342:SER:HA	1:C:431:LEU:HB2	1.71	0.71
1:C:364:ILE:O	1:C:364:ILE:CG1	2.37	0.71
1:B:316:THR:O	2:B:806:NAG:H82	1.91	0.71
1:C:229:LEU:HD23	1:C:322:THR:HB	1.73	0.71
1:C:394:LEU:HD12	1:C:394:LEU:N	2.05	0.71
1:D:229:LEU:HD23	1:D:322:THR:HB	1.73	0.71
1:D:414:ASP:HB3	1:D:420:GLY:HA3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:CG	1:A:277:SER:H	2.03	0.71
1:C:32:ASN:CG	1:C:33:LYS:H	1.98	0.71
1:C:434:ASN:OD1	1:C:467:ASN:HB3	1.91	0.71
1:D:32:ASN:CG	1:D:33:LYS:H	1.99	0.71
1:D:438:PRO:HB3	1:D:471:TYR:CE2	2.26	0.71
1:B:434:ASN:OD1	1:B:467:ASN:HB3	1.91	0.71
1:C:90:GLU:HB3	1:D:79:HIS:CA	2.20	0.71
1:A:335:ALA:HB1	3:A:811:NDG:H6	1.55	0.71
1:A:403:ASN:CB	2:A:902:NAG:N2	2.54	0.71
1:B:187:TYR:HA	2:B:801:NAG:C7	2.21	0.71
1:B:30:ARG:O	1:C:30:ARG:CA	2.39	0.71
1:B:290:PHE:CD2	1:B:293:ARG:N	2.55	0.71
1:C:81:VAL:CG1	1:D:40:GLY:N	2.49	0.71
1:C:187:TYR:HA	2:C:801:NAG:C7	2.21	0.71
1:D:337:SER:CA	1:D:427:ILE:HG23	2.19	0.71
1:A:91:PRO:CA	1:B:3:VAL:HG22	2.21	0.71
1:B:517:GLN:C	1:B:519:ASN:N	2.47	0.71
1:C:93:GLU:OE2	1:D:85:GLY:CA	2.30	0.71
1:D:276:GLU:CG	1:D:277:SER:H	2.03	0.71
1:A:187:TYR:HA	2:A:801:NAG:C7	2.21	0.70
1:A:414:ASP:HB3	1:A:420:GLY:HA3	1.73	0.70
1:B:483:TRP:CZ2	1:B:507:TYR:HE1	2.09	0.70
1:C:26:SER:OG	1:D:77:SER:HB2	1.90	0.70
1:C:33:LYS:HB3	1:C:83:GLU:HG2	1.71	0.70
1:C:320:THR:CG2	2:C:807:NAG:HN2	2.02	0.70
1:D:394:LEU:HD12	1:D:394:LEU:N	2.05	0.70
1:A:290:PHE:HE2	1:A:293:ARG:HB2	1.52	0.70
1:A:290:PHE:CD2	1:A:293:ARG:N	2.54	0.70
1:B:33:LYS:H	1:C:25:LYS:HE2	0.84	0.70
1:B:227:THR:O	2:B:812:NAG:O5	2.09	0.70
1:B:229:LEU:HD23	1:B:322:THR:HB	1.73	0.70
1:B:342:SER:HA	1:B:431:LEU:HB2	1.71	0.70
1:C:85:GLY:N	1:D:74:TYR:CE2	2.59	0.70
1:D:187:TYR:HA	2:D:801:NAG:C7	2.21	0.70
1:A:32:ASN:CG	1:A:33:LYS:H	1.99	0.70
1:B:414:ASP:HB3	1:B:420:GLY:HA3	1.73	0.70
1:D:434:ASN:OD1	1:D:467:ASN:HB3	1.91	0.70
1:A:33:LYS:HB3	1:A:83:GLU:HG2	1.71	0.70
1:A:222:ASP:O	1:A:222:ASP:CG	2.32	0.70
1:B:405:THR:OG1	1:B:406:TYR:N	2.22	0.70
1:D:227:THR:O	2:D:812:NAG:O5	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:THR:O	2:D:806:NAG:H82	1.91	0.70
1:A:1:ASP:HB3	1:B:92:MET:HB3	1.72	0.70
1:A:3:VAL:CG2	1:B:78:SER:H	2.01	0.70
1:A:316:THR:O	2:A:806:NAG:H82	1.91	0.70
1:C:276:GLU:CG	1:C:277:SER:H	2.03	0.70
1:D:403:ASN:CB	2:D:902:NAG:N2	2.54	0.70
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.73	0.70
1:C:31:PHE:CD1	1:D:95:THR:CG2	2.75	0.70
1:C:80:ALA:HB3	1:D:77:SER:CB	2.21	0.70
1:A:434:ASN:OD1	1:A:467:ASN:HB3	1.91	0.70
1:A:229:LEU:HD23	1:A:322:THR:HB	1.73	0.70
1:B:83:GLU:N	1:C:25:LYS:CD	2.43	0.70
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.74	0.70
1:C:4:ILE:CG2	1:D:87:PRO:CB	2.68	0.69
1:C:396:ARG:HE	1:C:432:ASP:HB2	1.57	0.69
1:C:414:ASP:HB3	1:C:420:GLY:HA3	1.73	0.69
1:D:474:SER:HB2	1:D:512:LEU:CG	2.15	0.69
1:A:227:THR:O	2:A:812:NAG:O5	2.09	0.69
1:A:438:PRO:HB3	1:A:471:TYR:CE2	2.26	0.69
1:C:1:ASP:H3	1:D:88:VAL:CG1	2.03	0.69
1:C:290:PHE:CD2	1:C:293:ARG:N	2.55	0.69
1:C:316:THR:O	2:C:806:NAG:H82	1.91	0.69
1:C:337:SER:CA	1:C:427:ILE:HG23	2.20	0.69
1:C:403:ASN:CB	2:C:902:NAG:N2	2.54	0.69
1:D:405:THR:OG1	1:D:406:TYR:N	2.22	0.69
1:A:483:TRP:CZ2	1:A:507:TYR:HE1	2.09	0.69
1:B:540:GLN:CD	1:B:540:GLN:C	2.60	0.69
1:A:128:MET:HE1	1:A:207:ALA:HB1	1.74	0.69
1:B:276:GLU:CG	1:B:277:SER:H	2.03	0.69
1:B:438:PRO:HB3	1:B:471:TYR:CE2	2.26	0.69
1:C:82:SER:HB3	1:D:75:VAL:O	1.92	0.69
1:C:186:GLU:OE1	2:C:801:NAG:H62	1.93	0.69
1:A:53:ILE:HG13	1:A:59:TRP:O	1.93	0.69
1:A:366:LYS:CG	1:A:367:LEU:N	2.48	0.69
1:B:83:GLU:HG2	1:C:25:LYS:CD	2.20	0.69
1:C:128:MET:HE1	1:C:207:ALA:HB1	1.74	0.69
1:C:483:TRP:CZ2	1:C:507:TYR:HE1	2.09	0.69
1:D:53:ILE:HG13	1:D:59:TRP:O	1.93	0.69
1:D:186:GLU:OE1	2:D:801:NAG:H62	1.93	0.69
1:A:10:SER:N	1:D:30:ARG:HG3	2.08	0.69
1:A:242:LEU:HD12	1:A:280:GLY:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ASN:CB	2:B:902:NAG:N2	2.54	0.69
1:B:474:SER:CB	1:B:512:LEU:HG	2.14	0.69
1:C:79:HIS:HB3	1:D:39:THR:CG2	2.20	0.69
1:C:90:GLU:HG2	1:D:36:TYR:CB	2.08	0.69
1:C:289:ASP:O	1:C:290:PHE:CB	2.25	0.69
1:D:128:MET:HE1	1:D:207:ALA:HB1	1.74	0.69
1:B:83:GLU:O	1:C:25:LYS:N	2.17	0.69
1:B:242:LEU:HD12	1:B:280:GLY:O	1.93	0.69
1:C:83:GLU:CB	1:D:41:GLN:NE2	2.56	0.69
1:C:523:THR:HG23	1:C:524:VAL:HG23	1.74	0.69
1:C:405:THR:OG1	1:C:406:TYR:N	2.22	0.69
1:D:523:THR:HG23	1:D:524:VAL:HG23	1.74	0.69
1:A:1:ASP:HA	1:B:24:ILE:CD1	2.22	0.68
1:A:186:GLU:OE1	2:A:801:NAG:H62	1.93	0.68
1:A:282:LEU:HD23	1:A:283:THR:N	2.08	0.68
1:B:282:LEU:HD23	1:B:283:THR:N	2.08	0.68
1:B:81:VAL:HB	1:D:90:GLU:HG2	1.74	0.68
1:C:31:PHE:HB3	1:D:95:THR:HG23	1.72	0.68
1:C:242:LEU:HD12	1:C:280:GLY:O	1.93	0.68
1:C:474:SER:HB2	1:C:512:LEU:CG	2.15	0.68
1:A:290:PHE:HZ	1:A:296:TYR:OH	1.76	0.68
1:A:320:THR:HG21	2:A:807:NAG:H2	1.76	0.68
1:C:90:GLU:CD	1:D:36:TYR:HB3	2.18	0.68
1:C:272:THR:HG22	1:C:273:THR:N	2.09	0.68
1:C:290:PHE:HZ	1:C:296:TYR:OH	1.77	0.68
1:D:272:THR:HG22	1:D:273:THR:N	2.09	0.68
1:A:396:ARG:HD3	1:A:431:LEU:O	1.93	0.68
1:B:282:LEU:HD23	1:B:283:THR:H	1.59	0.68
1:B:320:THR:HG21	2:B:807:NAG:H2	1.76	0.68
1:C:87:PRO:N	1:D:43:ALA:CB	2.35	0.68
1:C:282:LEU:HD23	1:C:283:THR:N	2.08	0.68
1:D:242:LEU:HD12	1:D:280:GLY:O	1.93	0.68
1:C:87:PRO:HD3	1:D:43:ALA:N	2.08	0.68
1:C:195:ASP:HB2	1:C:201:LEU:N	2.08	0.68
1:C:282:LEU:HD23	1:C:283:THR:H	1.58	0.68
1:A:482:THR:HG21	1:A:500:GLN:H	1.59	0.68
1:B:396:ARG:HD3	1:B:431:LEU:O	1.94	0.68
1:C:84:ASN:HA	1:D:71:TYR:CG	2.28	0.68
1:C:154:ASP:O	1:C:155:PRO:C	2.36	0.68
1:B:53:ILE:HG13	1:B:59:TRP:O	1.93	0.68
1:B:155:PRO:HB2	2:B:801:NAG:C8	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:VAL:HB	1:B:334:PRO:CD	2.24	0.68
1:B:337:SER:CA	1:B:427:ILE:HG23	2.20	0.68
1:C:89:GLU:CA	1:D:38:ILE:HG13	2.24	0.68
1:A:368:SER:HG	1:A:370:PHE:HE1	1.42	0.68
1:A:371:ILE:CG2	1:A:372:GLY:N	2.57	0.68
1:B:128:MET:HE1	1:B:207:ALA:HB1	1.74	0.68
1:B:347:ARG:CD	1:B:392:GLY:H	2.07	0.68
1:C:4:ILE:HG23	1:D:87:PRO:CG	2.17	0.68
1:C:53:ILE:HG13	1:C:59:TRP:O	1.93	0.68
1:D:396:ARG:HE	1:D:432:ASP:HB2	1.57	0.68
1:B:87:PRO:HG2	1:C:2:TRP:CB	2.21	0.68
1:B:221:PHE:CE1	1:B:315:SER:O	2.45	0.68
1:B:396:ARG:HE	1:B:432:ASP:CB	2.07	0.68
1:C:396:ARG:HD3	1:C:431:LEU:O	1.94	0.68
1:B:371:ILE:CG2	1:B:372:GLY:N	2.57	0.68
1:C:1:ASP:CA	1:D:89:GLU:CG	2.57	0.68
1:C:93:GLU:HB3	1:D:81:VAL:HG11	1.73	0.68
1:C:137:ASP:OD2	1:C:139:ILE:HG22	1.94	0.68
1:C:155:PRO:HB2	2:C:801:NAG:C8	2.24	0.68
1:C:371:ILE:CG2	1:C:372:GLY:N	2.57	0.68
1:C:440:PRO:HA	1:C:458:THR:O	1.94	0.68
1:D:154:ASP:O	1:D:155:PRO:C	2.36	0.68
1:D:347:ARG:CD	1:D:392:GLY:H	2.07	0.68
1:A:272:THR:HG22	1:A:273:THR:N	2.09	0.67
1:A:282:LEU:HD23	1:A:283:THR:H	1.58	0.67
1:B:186:GLU:OE1	2:B:801:NAG:H62	1.93	0.67
1:B:289:ASP:O	1:B:290:PHE:CB	2.25	0.67
1:D:282:LEU:HD23	1:D:283:THR:H	1.58	0.67
1:D:333:VAL:HB	1:D:334:PRO:CD	2.24	0.67
1:D:440:PRO:HA	1:D:458:THR:O	1.94	0.67
1:A:347:ARG:CD	1:A:392:GLY:H	2.07	0.67
1:B:32:ASN:HB2	1:C:27:ASN:HA	1.74	0.67
1:B:84:ASN:OD1	1:C:27:ASN:N	2.25	0.67
1:C:333:VAL:HB	1:C:334:PRO:CD	2.24	0.67
1:D:195:ASP:HB2	1:D:201:LEU:N	2.08	0.67
1:D:396:ARG:HE	1:D:432:ASP:CB	2.07	0.67
1:D:423:THR:HB	2:D:810:NAG:C8	2.24	0.67
1:B:137:ASP:OD2	1:B:139:ILE:HG22	1.94	0.67
1:B:154:ASP:O	1:B:155:PRO:C	2.36	0.67
1:D:137:ASP:OD2	1:D:139:ILE:HG22	1.94	0.67
1:A:155:PRO:HB2	2:A:801:NAG:C8	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ARG:CD	1:C:392:GLY:H	2.07	0.67
1:C:474:SER:CB	1:C:512:LEU:HG	2.14	0.67
1:B:272:THR:HG22	1:B:273:THR:N	2.09	0.67
1:B:440:PRO:HA	1:B:458:THR:O	1.94	0.67
1:B:482:THR:HG21	1:B:500:GLN:H	1.59	0.67
1:C:90:GLU:HG2	1:D:36:TYR:HB3	1.75	0.67
1:D:282:LEU:HD23	1:D:283:THR:N	2.08	0.67
1:D:474:SER:CB	1:D:512:LEU:HG	2.14	0.67
1:D:483:TRP:CZ2	1:D:507:TYR:HE1	2.09	0.67
1:D:524:VAL:HG21	2:D:904:NAG:H81	1.77	0.67
1:B:290:PHE:HZ	1:B:296:TYR:OH	1.76	0.67
1:C:482:THR:HG21	1:C:500:GLN:H	1.58	0.67
1:D:396:ARG:NH2	1:D:464:ILE:CB	2.58	0.67
1:B:474:SER:HB2	1:B:512:LEU:CG	2.15	0.67
1:B:524:VAL:HG21	2:B:904:NAG:H81	1.76	0.67
1:D:187:TYR:HA	2:D:801:NAG:C8	2.25	0.67
1:A:396:ARG:HE	1:A:432:ASP:CB	2.07	0.67
1:B:396:ARG:HE	1:B:432:ASP:HB2	1.57	0.67
1:B:401:VAL:HG13	1:B:405:THR:O	1.95	0.67
1:C:224:LYS:HE3	1:C:316:THR:O	1.95	0.67
1:C:396:ARG:HE	1:C:432:ASP:CB	2.07	0.67
1:C:401:VAL:HG13	1:C:405:THR:O	1.95	0.67
1:A:10:SER:N	1:D:30:ARG:CG	2.58	0.67
1:A:137:ASP:OD2	1:A:139:ILE:HG22	1.94	0.67
1:A:423:THR:HB	2:A:810:NAG:C8	2.24	0.67
1:C:187:TYR:HA	2:C:801:NAG:C8	2.25	0.67
1:C:221:PHE:CE1	1:C:315:SER:O	2.45	0.67
1:B:195:ASP:HB2	1:B:201:LEU:N	2.08	0.67
1:D:347:ARG:CG	1:D:392:GLY:H	2.08	0.67
1:D:373:ASN:ND2	1:D:374:ASP:N	2.43	0.67
1:D:446:THR:CG2	1:D:537:ILE:O	2.43	0.67
1:A:396:ARG:NH2	1:A:464:ILE:CB	2.58	0.66
1:B:446:THR:CG2	1:B:537:ILE:O	2.43	0.66
1:D:401:VAL:HG13	1:D:405:THR:O	1.95	0.66
1:C:82:SER:CB	1:D:75:VAL:N	2.49	0.66
1:C:423:THR:HB	2:C:810:NAG:C8	2.24	0.66
1:A:405:THR:OG1	1:A:406:TYR:N	2.22	0.66
1:B:187:TYR:HA	2:B:801:NAG:C8	2.25	0.66
1:C:27:ASN:ND2	1:D:93:GLU:CA	2.58	0.66
1:C:232:GLU:HG3	1:C:290:PHE:H	1.61	0.66
1:C:524:VAL:HG21	2:C:904:NAG:H81	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:THR:HG21	2:D:807:NAG:H2	1.76	0.66
1:A:187:TYR:HA	2:A:801:NAG:C8	2.25	0.66
1:A:482:THR:OG1	1:A:500:GLN:CG	2.44	0.66
1:C:81:VAL:HG11	1:D:43:ALA:C	2.21	0.66
1:A:347:ARG:HD2	1:A:392:GLY:H	1.60	0.66
1:A:440:PRO:HA	1:A:458:THR:O	1.94	0.66
1:C:86:SER:CB	1:D:76:LEU:HD11	2.26	0.66
1:C:396:ARG:NH2	1:C:464:ILE:CB	2.58	0.66
1:D:232:GLU:HG2	1:D:289:ASP:HA	1.77	0.66
1:D:290:PHE:HZ	1:D:296:TYR:OH	1.77	0.66
1:D:371:ILE:CG2	1:D:372:GLY:N	2.57	0.66
1:D:403:ASN:HB2	2:D:902:NAG:N2	2.10	0.66
1:D:440:PRO:HD2	1:D:522:LEU:CD1	2.26	0.66
1:A:36:TYR:CE2	1:D:2:TRP:HH2	2.13	0.66
1:A:347:ARG:CG	1:A:392:GLY:H	2.08	0.66
1:B:27:ASN:C	1:B:27:ASN:ND2	2.46	0.66
1:B:347:ARG:HD2	1:B:392:GLY:H	1.60	0.66
1:B:396:ARG:NH2	1:B:464:ILE:CB	2.58	0.66
1:B:403:ASN:HB2	2:B:902:NAG:N2	2.10	0.66
1:B:423:THR:HB	2:B:810:NAG:C8	2.24	0.66
1:B:482:THR:OG1	1:B:500:GLN:CG	2.44	0.66
1:C:440:PRO:HD2	1:C:522:LEU:CD1	2.26	0.66
1:A:154:ASP:O	1:A:155:PRO:C	2.36	0.66
1:A:224:LYS:HE3	1:A:316:THR:O	1.95	0.66
1:A:524:VAL:HG21	2:A:904:NAG:H81	1.77	0.66
1:C:90:GLU:OE1	1:D:53:ILE:HG21	1.95	0.66
1:C:373:ASN:ND2	1:C:374:ASP:N	2.43	0.66
1:C:438:PRO:HB3	1:C:471:TYR:CE2	2.26	0.66
1:D:347:ARG:HD2	1:D:392:GLY:H	1.60	0.66
1:D:396:ARG:HD3	1:D:431:LEU:O	1.94	0.66
1:D:464:ILE:O	1:D:467:ASN:HB2	1.96	0.66
1:A:8:LYS:HB2	1:D:30:ARG:HE	1.61	0.66
1:A:195:ASP:HB2	1:A:201:LEU:N	2.08	0.66
1:A:373:ASN:ND2	1:A:374:ASP:N	2.43	0.66
1:C:232:GLU:HG2	1:C:289:ASP:HA	1.77	0.66
1:A:396:ARG:HE	1:A:432:ASP:HB2	1.57	0.66
1:A:401:VAL:HG13	1:A:405:THR:O	1.95	0.66
1:A:440:PRO:HD2	1:A:522:LEU:CD1	2.26	0.66
1:B:440:PRO:HD3	1:B:522:LEU:HD12	1.78	0.66
2:B:805:NAG:C6	2:B:806:NAG:C7	2.74	0.66
1:B:232:GLU:HG3	1:B:290:PHE:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:CG	1:B:392:GLY:H	2.08	0.66
1:B:464:ILE:O	1:B:467:ASN:HB2	1.95	0.66
1:C:347:ARG:CG	1:C:392:GLY:H	2.08	0.66
1:C:482:THR:OG1	1:C:500:GLN:CG	2.44	0.66
1:D:366:LYS:HG3	1:D:367:LEU:HG	1.77	0.66
1:A:337:SER:CA	1:A:427:ILE:HG23	2.20	0.65
1:A:403:ASN:HB2	2:A:902:NAG:N2	2.10	0.65
1:B:265:GLU:HB3	1:B:268:PHE:CE2	2.31	0.65
2:C:805:NAG:C6	2:C:806:NAG:C7	2.74	0.65
1:D:482:THR:HG21	1:D:500:GLN:H	1.59	0.65
1:B:224:LYS:HE3	1:B:316:THR:O	1.95	0.65
1:B:373:ASN:ND2	1:B:374:ASP:N	2.43	0.65
1:B:524:VAL:HG23	2:B:904:NAG:H81	1.78	0.65
1:C:88:VAL:HG12	1:D:94:ILE:N	2.10	0.65
1:C:320:THR:HG21	2:C:807:NAG:H2	1.76	0.65
1:A:10:SER:HB2	1:D:30:ARG:CG	2.26	0.65
1:A:232:GLU:HG2	1:A:289:ASP:HA	1.77	0.65
1:A:446:THR:CG2	1:A:537:ILE:O	2.44	0.65
1:A:464:ILE:O	1:A:467:ASN:HB2	1.96	0.65
1:C:1:ASP:H1	1:D:28:LYS:CD	2.03	0.65
1:C:366:LYS:HG3	1:C:367:LEU:HG	1.77	0.65
1:D:32:ASN:ND2	1:D:83:GLU:N	2.45	0.65
1:D:155:PRO:HB2	2:D:801:NAG:C8	2.24	0.65
1:D:482:THR:OG1	1:D:500:GLN:CG	2.44	0.65
1:B:30:ARG:HH11	1:C:30:ARG:HG2	1.60	0.65
1:C:347:ARG:HD2	1:C:392:GLY:H	1.60	0.65
1:D:488:ASP:HB2	1:D:493:SER:OG	1.97	0.65
1:A:90:GLU:HG3	1:B:3:VAL:CG2	2.14	0.65
1:A:333:VAL:HB	1:A:334:PRO:CD	2.24	0.65
1:B:440:PRO:HD2	1:B:522:LEU:CD1	2.26	0.65
1:A:32:ASN:ND2	1:A:83:GLU:N	2.44	0.65
1:B:84:ASN:OD1	1:C:26:SER:HA	1.71	0.65
1:B:232:GLU:HG2	1:B:289:ASP:HA	1.77	0.65
1:B:406:TYR:CE1	2:B:808:NAG:H83	2.32	0.65
1:C:464:ILE:O	1:C:467:ASN:HB2	1.96	0.65
1:C:488:ASP:HB2	1:C:493:SER:OG	1.97	0.65
1:C:524:VAL:HG23	2:C:904:NAG:H81	1.78	0.65
2:C:809:NAG:C6	2:C:810:NAG:H62	2.26	0.65
2:A:805:NAG:C6	2:A:806:NAG:C7	2.74	0.65
2:B:809:NAG:C6	2:B:810:NAG:H62	2.26	0.65
1:C:79:HIS:CG	1:D:39:THR:HG22	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:SER:OG	1:C:349:GLU:HG3	1.97	0.65
1:D:224:LYS:HE3	1:D:316:THR:O	1.95	0.65
1:A:89:GLU:OE1	1:B:2:TRP:CB	2.26	0.65
1:A:212:THR:HG22	1:A:213:ASP:H	1.62	0.65
1:B:31:PHE:CZ	1:C:34:VAL:HG21	2.32	0.65
1:C:403:ASN:HB2	2:C:902:NAG:N2	2.10	0.65
1:C:446:THR:CG2	1:C:537:ILE:O	2.44	0.65
1:A:2:TRP:CE2	1:B:79:HIS:O	2.43	0.65
1:A:327:ASN:HA	1:A:360:ASP:OD2	1.97	0.65
1:A:364:ILE:O	1:A:364:ILE:HD12	1.97	0.65
1:B:346:SER:OG	1:B:349:GLU:HG3	1.97	0.65
1:B:488:ASP:HB2	1:B:493:SER:OG	1.97	0.65
1:C:88:VAL:HG23	1:D:39:THR:O	1.97	0.65
1:A:2:TRP:CE2	1:B:80:ALA:HB1	2.16	0.65
1:A:440:PRO:HD3	1:A:522:LEU:HD12	1.78	0.65
1:B:366:LYS:HG3	1:B:367:LEU:HG	1.77	0.65
1:B:482:THR:HG21	1:B:499:THR:CA	2.27	0.65
1:C:81:VAL:CG1	1:D:43:ALA:CA	2.70	0.65
1:C:440:PRO:HD3	1:C:522:LEU:HD12	1.78	0.65
2:D:809:NAG:C6	2:D:810:NAG:H62	2.26	0.65
1:A:9:VAL:C	1:D:30:ARG:HD2	2.16	0.64
1:B:212:THR:HG22	1:B:213:ASP:H	1.62	0.64
1:B:327:ASN:HA	1:B:360:ASP:OD2	1.97	0.64
1:B:364:ILE:O	1:B:364:ILE:HD12	1.97	0.64
1:C:32:ASN:ND2	1:C:83:GLU:N	2.45	0.64
1:A:366:LYS:HG3	1:A:367:LEU:HG	1.77	0.64
1:C:31:PHE:HD2	1:D:75:VAL:HG23	1.62	0.64
1:A:155:PRO:C	1:A:157:GLU:N	2.56	0.64
1:A:482:THR:HG21	1:A:499:THR:CA	2.27	0.64
1:B:341:VAL:HG21	1:B:345:LEU:HD12	1.79	0.64
1:A:469:TYR:CD2	1:A:470:PRO:CD	2.81	0.64
1:C:1:ASP:C	1:D:28:LYS:HZ3	1.97	0.64
1:D:212:THR:HG22	1:D:213:ASP:H	1.62	0.64
1:D:232:GLU:HG3	1:D:290:PHE:H	1.61	0.64
1:D:265:GLU:HB3	1:D:268:PHE:CE2	2.31	0.64
1:D:482:THR:HG21	1:D:499:THR:CA	2.27	0.64
1:A:346:SER:OG	1:A:349:GLU:HG3	1.97	0.64
1:A:482:THR:HG22	1:A:499:THR:N	2.13	0.64
1:B:88:VAL:O	1:D:1:ASP:CG	2.40	0.64
1:C:364:ILE:O	1:C:364:ILE:HD12	1.97	0.64
1:D:406:TYR:CE1	2:D:808:NAG:H83	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:524:VAL:HG23	2:D:904:NAG:H81	1.78	0.64
1:A:154:ASP:O	2:A:801:NAG:H82	1.98	0.64
1:A:347:ARG:HG3	1:A:392:GLY:H	1.62	0.64
1:A:406:TYR:CE1	2:A:808:NAG:H83	2.32	0.64
2:A:809:NAG:C6	2:A:810:NAG:H62	2.26	0.64
1:C:504:LYS:NZ	1:C:531:SER:OG	2.31	0.64
1:D:341:VAL:HG21	1:D:345:LEU:HD12	1.79	0.64
1:D:346:SER:OG	1:D:349:GLU:HG3	1.97	0.64
1:D:409:ILE:HG12	1:D:425:THR:HG23	1.80	0.64
1:C:90:GLU:OE2	1:D:37:SER:HA	1.98	0.64
1:C:409:ILE:HG12	1:C:425:THR:HG23	1.80	0.64
1:A:343:GLU:HB3	1:A:433:VAL:CG2	2.28	0.64
1:A:524:VAL:HG23	2:A:904:NAG:H81	1.78	0.64
1:C:81:VAL:HG21	1:D:45:ASN:HB2	0.64	0.64
1:C:347:ARG:HG3	1:C:392:GLY:H	1.62	0.64
1:A:364:ILE:O	1:A:364:ILE:CD1	2.46	0.64
1:A:419:VAL:HG13	2:A:809:NAG:O7	1.98	0.64
1:A:540:GLN:CD	1:A:540:GLN:C	2.60	0.64
1:B:409:ILE:HG12	1:B:425:THR:HG23	1.80	0.64
1:C:341:VAL:HG21	1:C:345:LEU:HD12	1.79	0.64
1:C:517:GLN:C	1:C:519:ASN:N	2.46	0.64
1:D:347:ARG:HG3	1:D:392:GLY:H	1.62	0.64
1:D:375:PRO:HB3	1:D:400:TYR:CD2	2.33	0.64
1:A:474:SER:HB2	1:A:512:LEU:CG	2.15	0.64
1:C:327:ASN:HA	1:C:360:ASP:OD2	1.97	0.64
1:C:364:ILE:O	1:C:364:ILE:CD1	2.46	0.64
1:C:486:GLU:O	1:C:494:MET:CA	2.46	0.64
1:A:488:ASP:HB2	1:A:493:SER:OG	1.97	0.63
1:C:406:TYR:CE1	2:C:808:NAG:H83	2.32	0.63
1:D:327:ASN:HA	1:D:360:ASP:OD2	1.97	0.63
1:A:22:VAL:HG22	1:A:23:GLN:N	2.14	0.63
1:A:341:VAL:HG21	1:A:345:LEU:HD12	1.79	0.63
1:A:486:GLU:O	1:A:494:MET:CA	2.46	0.63
1:A:504:LYS:NZ	1:A:531:SER:OG	2.31	0.63
1:B:419:VAL:HG13	2:B:809:NAG:O7	1.98	0.63
1:C:343:GLU:HB3	1:C:433:VAL:CG2	2.28	0.63
1:D:221:PHE:CE1	1:D:315:SER:O	2.45	0.63
1:D:440:PRO:HD3	1:D:522:LEU:HD12	1.78	0.63
1:B:155:PRO:C	1:B:157:GLU:N	2.56	0.63
1:B:343:GLU:HB3	1:B:433:VAL:CG2	2.28	0.63
1:B:375:PRO:HB3	1:B:400:TYR:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:PRO:C	1:D:38:ILE:HD11	2.24	0.63
1:C:142:LEU:HB3	1:C:196:LEU:HA	1.81	0.63
1:A:10:SER:HA	1:D:30:ARG:HD2	1.81	0.63
1:A:299:GLN:C	1:A:300:ILE:HD12	2.24	0.63
1:B:87:PRO:HD2	1:D:90:GLU:O	1.97	0.63
1:B:142:LEU:HB3	1:B:196:LEU:HA	1.81	0.63
1:B:469:TYR:CD2	1:B:470:PRO:CD	2.81	0.63
1:C:84:ASN:HB3	1:D:73:LYS:O	1.98	0.63
1:C:265:GLU:HB3	1:C:268:PHE:CE2	2.31	0.63
1:C:375:PRO:HB3	1:C:400:TYR:CD2	2.33	0.63
1:C:419:VAL:HG13	2:C:809:NAG:O7	1.98	0.63
1:D:154:ASP:C	2:D:801:NAG:C8	2.62	0.63
1:D:504:LYS:NZ	1:D:531:SER:OG	2.31	0.63
1:A:221:PHE:CE1	1:A:315:SER:O	2.45	0.63
1:B:371:ILE:HG22	1:B:372:GLY:N	2.14	0.63
1:C:371:ILE:HG22	1:C:372:GLY:N	2.14	0.63
1:A:91:PRO:HA	1:B:1:ASP:C	2.23	0.63
1:A:154:ASP:CA	2:A:801:NAG:H82	2.29	0.63
1:A:232:GLU:HG3	1:A:290:PHE:H	1.61	0.63
1:A:486:GLU:O	1:A:495:LEU:N	2.31	0.63
1:B:127:VAL:HG22	1:B:128:MET:N	2.14	0.63
1:B:504:LYS:NZ	1:B:531:SER:OG	2.31	0.63
1:C:1:ASP:N	1:D:88:VAL:HB	2.11	0.63
1:C:446:THR:CG2	1:C:539:CYS:SG	2.86	0.63
1:D:142:LEU:HB3	1:D:196:LEU:HA	1.81	0.63
1:D:364:ILE:O	1:D:364:ILE:CD1	2.46	0.63
1:C:469:TYR:CD2	1:C:470:PRO:CD	2.81	0.63
1:C:482:THR:HG21	1:C:499:THR:CA	2.27	0.63
1:D:469:TYR:CE1	1:D:470:PRO:HD2	2.34	0.63
1:D:486:GLU:O	1:D:494:MET:CA	2.46	0.63
1:B:347:ARG:HG3	1:B:392:GLY:H	1.62	0.63
1:C:403:ASN:CB	2:C:902:NAG:C7	2.76	0.63
1:D:364:ILE:O	1:D:364:ILE:HD12	1.97	0.63
1:D:419:VAL:HG13	2:D:809:NAG:O7	1.98	0.63
1:B:364:ILE:O	1:B:364:ILE:CD1	2.46	0.63
1:C:127:VAL:HG22	1:C:128:MET:N	2.14	0.63
1:C:154:ASP:CA	2:C:801:NAG:H82	2.29	0.63
1:C:212:THR:HG22	1:C:213:ASP:H	1.62	0.63
1:D:371:ILE:HG22	1:D:372:GLY:N	2.14	0.63
1:A:3:VAL:CG2	1:B:78:SER:N	2.60	0.62
1:A:142:LEU:HB3	1:A:196:LEU:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASP:C	2:A:801:NAG:C8	2.62	0.62
1:A:409:ILE:HG12	1:A:425:THR:HG23	1.80	0.62
1:C:81:VAL:CG1	1:D:43:ALA:CB	2.26	0.62
1:D:411:LEU:HD22	1:D:421:THR:HG23	1.81	0.62
1:A:127:VAL:HG22	1:A:128:MET:N	2.14	0.62
1:A:375:PRO:HB3	1:A:400:TYR:CD2	2.33	0.62
1:B:22:VAL:HG22	1:B:23:GLN:N	2.14	0.62
1:C:27:ASN:ND2	1:C:27:ASN:C	2.46	0.62
1:C:374:ASP:O	1:C:375:PRO:O	2.17	0.62
1:C:449:ASP:H	1:C:532:CYS:CB	2.12	0.62
1:D:22:VAL:HG22	1:D:23:GLN:N	2.14	0.62
1:A:89:GLU:CD	1:B:2:TRP:CD1	2.51	0.62
1:B:154:ASP:O	2:B:801:NAG:H82	1.98	0.62
1:C:90:GLU:OE2	1:D:36:TYR:O	2.15	0.62
1:C:227:THR:CG2	2:C:807:NAG:C7	2.76	0.62
1:C:411:LEU:HD22	1:C:421:THR:HG23	1.81	0.62
1:D:343:GLU:HB3	1:D:433:VAL:CG2	2.27	0.62
1:D:508:SER:HB3	1:D:526:ASN:OD1	2.00	0.62
1:B:374:ASP:O	1:B:375:PRO:O	2.17	0.62
1:C:299:GLN:C	1:C:300:ILE:HD12	2.24	0.62
1:C:524:VAL:HG23	2:C:904:NAG:C8	2.29	0.62
1:D:127:VAL:HG22	1:D:128:MET:N	2.14	0.62
1:D:524:VAL:HG23	2:D:904:NAG:C8	2.29	0.62
1:A:1:ASP:H2	1:B:94:ILE:HD11	1.51	0.62
1:A:68:ARG:HD3	1:A:100:ASP:HA	1.82	0.62
1:A:89:GLU:O	1:B:1:ASP:O	2.18	0.62
1:B:154:ASP:CA	2:B:801:NAG:H82	2.29	0.62
1:B:299:GLN:C	1:B:300:ILE:HD12	2.24	0.62
1:C:87:PRO:O	1:D:38:ILE:HD11	2.00	0.62
1:C:524:VAL:CG2	2:C:904:NAG:C8	2.78	0.62
1:D:155:PRO:C	1:D:157:GLU:N	2.56	0.62
1:A:227:THR:CG2	2:A:807:NAG:C7	2.76	0.62
1:A:403:ASN:CB	2:A:902:NAG:C7	2.76	0.62
1:B:88:VAL:O	1:D:1:ASP:OD2	2.17	0.62
1:B:524:VAL:CG2	2:B:904:NAG:C8	2.78	0.62
1:C:154:ASP:O	2:C:801:NAG:H82	1.98	0.62
1:C:469:TYR:CE1	1:C:470:PRO:HD2	2.34	0.62
1:D:371:ILE:CG2	1:D:372:GLY:H	2.13	0.62
1:D:518:ASN:O	1:D:520:PRO:CD	2.46	0.62
2:D:805:NAG:C6	2:D:806:NAG:C7	2.74	0.62
1:A:147:SER:OG	1:A:167:ARG:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LYS:H	1:C:25:LYS:NZ	1.97	0.62
1:B:83:GLU:HG2	1:C:25:LYS:HD2	1.79	0.62
1:B:154:ASP:C	2:B:801:NAG:C8	2.62	0.62
1:B:508:SER:HB3	1:B:526:ASN:OD1	1.99	0.62
1:C:508:SER:HB3	1:C:526:ASN:OD1	2.00	0.62
1:C:518:ASN:O	1:C:520:PRO:CD	2.46	0.62
1:D:299:GLN:C	1:D:300:ILE:HD12	2.24	0.62
1:A:212:THR:HG22	1:A:213:ASP:N	2.15	0.62
1:A:371:ILE:HG22	1:A:372:GLY:N	2.14	0.62
1:A:449:ASP:H	1:A:532:CYS:CB	2.12	0.62
1:A:524:VAL:HG23	2:A:904:NAG:C8	2.29	0.62
1:B:486:GLU:O	1:B:495:LEU:N	2.31	0.62
1:C:79:HIS:HB3	1:D:44:ASP:CG	2.25	0.62
1:C:482:THR:HG22	1:C:499:THR:N	2.13	0.62
1:B:371:ILE:CG2	1:B:372:GLY:H	2.13	0.62
1:B:411:LEU:HD22	1:B:421:THR:HG23	1.81	0.62
1:B:518:ASN:O	1:B:520:PRO:CD	2.46	0.62
1:B:469:TYR:CE1	1:B:470:PRO:HD2	2.34	0.62
1:C:212:THR:HG22	1:C:213:ASP:N	2.15	0.62
1:D:154:ASP:CA	2:D:801:NAG:H82	2.29	0.62
1:A:91:PRO:CD	1:B:3:VAL:HG22	2.28	0.61
1:B:446:THR:CG2	1:B:539:CYS:SG	2.86	0.61
1:C:68:ARG:HD3	1:C:100:ASP:HA	1.82	0.61
1:C:155:PRO:C	1:C:157:GLU:N	2.56	0.61
1:C:393:ASN:C	1:C:394:LEU:HD12	2.25	0.61
1:C:486:GLU:O	1:C:495:LEU:N	2.31	0.61
1:D:68:ARG:HD3	1:D:100:ASP:HA	1.82	0.61
1:D:235:ILE:HG12	1:D:287:GLY:HA2	1.82	0.61
1:D:415:ASP:OD1	1:D:416:GLY:N	2.26	0.61
1:A:508:SER:HB3	1:A:526:ASN:OD1	2.00	0.61
1:A:524:VAL:CG2	2:A:904:NAG:C8	2.78	0.61
1:B:486:GLU:O	1:B:494:MET:CA	2.46	0.61
1:C:1:ASP:H1	1:D:28:LYS:CB	2.13	0.61
1:C:22:VAL:HG22	1:C:23:GLN:N	2.14	0.61
1:D:403:ASN:O	1:D:405:THR:N	2.33	0.61
1:A:374:ASP:O	1:A:375:PRO:O	2.17	0.61
1:C:181:ARG:NE	1:C:213:ASP:OD1	2.34	0.61
1:A:393:ASN:C	1:A:394:LEU:HD12	2.25	0.61
1:B:212:THR:HG22	1:B:213:ASP:N	2.15	0.61
1:C:27:ASN:HD21	1:D:93:GLU:H	1.45	0.61
1:C:85:GLY:HA3	1:D:47:PRO:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:ASP:O	1:D:375:PRO:O	2.17	0.61
1:A:2:TRP:CD1	1:B:80:ALA:HB2	2.35	0.61
1:A:411:LEU:HD22	1:A:421:THR:HG23	1.81	0.61
1:C:379:LEU:HD23	1:C:379:LEU:H	1.66	0.61
1:D:403:ASN:CB	2:D:902:NAG:C7	2.76	0.61
1:D:154:ASP:O	2:D:801:NAG:H82	1.98	0.61
1:D:524:VAL:CG2	2:D:904:NAG:C8	2.78	0.61
1:A:91:PRO:N	1:B:1:ASP:O	2.33	0.61
1:B:181:ARG:NE	1:B:213:ASP:OD1	2.34	0.61
1:B:393:ASN:C	1:B:394:LEU:HD12	2.25	0.61
1:B:403:ASN:O	1:B:405:THR:N	2.33	0.61
1:C:403:ASN:O	1:C:405:THR:N	2.33	0.61
1:D:469:TYR:CD2	1:D:470:PRO:CD	2.80	0.61
1:D:475:LEU:O	1:D:479:SER:HB3	2.01	0.61
1:A:9:VAL:N	1:D:30:ARG:HD3	2.15	0.61
1:A:403:ASN:O	1:A:405:THR:N	2.33	0.61
1:A:415:ASP:OD1	1:A:416:GLY:N	2.27	0.61
1:B:524:VAL:HG23	2:B:904:NAG:C8	2.29	0.61
1:C:31:PHE:O	1:D:73:LYS:CD	2.47	0.61
1:C:85:GLY:HA2	1:D:41:GLN:C	2.13	0.61
1:D:32:ASN:CG	1:D:33:LYS:N	2.59	0.61
1:D:212:THR:HG22	1:D:213:ASP:N	2.15	0.61
1:A:181:ARG:NE	1:A:213:ASP:OD1	2.34	0.61
1:A:379:LEU:HD23	1:A:379:LEU:H	1.66	0.61
1:A:469:TYR:CE1	1:A:470:PRO:HD2	2.34	0.61
1:B:475:LEU:O	1:B:479:SER:HB3	2.01	0.61
1:D:181:ARG:NE	1:D:213:ASP:OD1	2.34	0.61
1:D:379:LEU:HD23	1:D:379:LEU:H	1.66	0.61
1:A:475:LEU:O	1:A:479:SER:HB3	2.01	0.61
1:D:449:ASP:H	1:D:532:CYS:CB	2.12	0.61
1:A:232:GLU:CG	1:A:290:PHE:N	2.64	0.60
1:B:68:ARG:HD3	1:B:100:ASP:HA	1.82	0.60
1:C:371:ILE:CG2	1:C:372:GLY:H	2.13	0.60
1:C:88:VAL:CA	1:D:38:ILE:HD11	2.31	0.60
1:C:189:LEU:N	1:C:189:LEU:HD23	2.16	0.60
1:D:189:LEU:N	1:D:189:LEU:HD23	2.16	0.60
1:D:393:ASN:C	1:D:394:LEU:HD12	2.25	0.60
1:B:379:LEU:HD23	1:B:379:LEU:H	1.66	0.60
1:B:450:GLN:HB2	1:B:533:GLU:CA	2.26	0.60
1:C:232:GLU:CG	1:C:290:PHE:N	2.64	0.60
1:C:81:VAL:H	1:D:45:ASN:HD22	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLU:CG	1:D:36:TYR:HB3	2.32	0.60
1:C:482:THR:HG21	1:C:499:THR:C	2.27	0.60
1:D:432:ASP:CG	1:D:464:ILE:CG2	2.74	0.60
1:D:523:THR:CG2	1:D:524:VAL:H	1.94	0.60
1:B:189:LEU:N	1:B:189:LEU:HD23	2.17	0.60
1:D:403:ASN:CB	2:D:902:NAG:H83	2.21	0.60
1:C:336:VAL:HB	1:C:426:LEU:HD23	1.84	0.60
1:C:514:SER:HA	1:C:517:GLN:O	2.02	0.60
1:A:189:LEU:HD23	1:A:189:LEU:N	2.16	0.60
1:A:265:GLU:HB3	1:A:268:PHE:CE2	2.31	0.60
1:A:371:ILE:CG2	1:A:372:GLY:H	2.13	0.60
1:A:432:ASP:CG	1:A:464:ILE:CG2	2.74	0.60
1:B:336:VAL:HB	1:B:426:LEU:HD23	1.84	0.60
1:C:89:GLU:C	1:D:38:ILE:HG13	2.26	0.60
1:D:227:THR:CG2	2:D:807:NAG:C7	2.76	0.60
1:A:2:TRP:CZ2	1:B:36:TYR:CD2	2.75	0.60
1:A:482:THR:HG21	1:A:499:THR:C	2.27	0.60
1:C:146:LEU:HA	1:C:194:THR:O	2.02	0.60
1:C:475:LEU:O	1:C:479:SER:HB3	2.01	0.60
1:D:446:THR:CG2	1:D:539:CYS:SG	2.86	0.60
1:D:517:GLN:C	1:D:519:ASN:N	2.47	0.60
1:A:32:ASN:CG	1:A:33:LYS:N	2.59	0.60
1:B:227:THR:CG2	2:B:807:NAG:C7	2.76	0.60
1:B:396:ARG:NH2	1:B:464:ILE:HG21	2.17	0.60
1:C:32:ASN:CB	1:D:75:VAL:HG23	2.31	0.60
1:C:508:SER:HA	1:C:526:ASN:HA	1.84	0.60
1:C:116:SER:HA	1:C:210:GLN:O	2.02	0.60
1:C:154:ASP:C	2:C:801:NAG:C8	2.62	0.60
1:C:450:GLN:HB2	1:C:533:GLU:CA	2.26	0.59
1:A:154:ASP:CG	1:A:155:PRO:CD	2.75	0.59
1:B:482:THR:HG21	1:B:499:THR:C	2.27	0.59
1:B:508:SER:HA	1:B:526:ASN:HA	1.84	0.59
1:C:81:VAL:HG13	1:D:44:ASP:H	1.63	0.59
1:D:154:ASP:CG	1:D:155:PRO:CD	2.75	0.59
1:D:367:LEU:CB	1:D:413:THR:O	2.51	0.59
1:A:363:GLN:C	1:A:364:ILE:CG2	2.76	0.59
1:B:514:SER:HA	1:B:517:GLN:O	2.02	0.59
1:D:116:SER:HA	1:D:210:GLN:O	2.02	0.59
1:D:232:GLU:CG	1:D:290:PHE:N	2.64	0.59
1:D:514:SER:HA	1:D:517:GLN:O	2.02	0.59
1:A:446:THR:CG2	1:A:539:CYS:SG	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:SER:HA	1:B:210:GLN:O	2.02	0.59
1:B:154:ASP:CG	1:B:155:PRO:CD	2.75	0.59
1:C:90:GLU:CD	1:D:37:SER:C	2.66	0.59
1:C:154:ASP:CG	1:C:155:PRO:CD	2.75	0.59
1:D:49:GLY:O	1:D:63:THR:HG21	2.02	0.59
1:D:146:LEU:HA	1:D:194:THR:O	2.02	0.59
1:D:239:VAL:HG13	1:D:240:GLN:H	1.67	0.59
1:D:363:GLN:C	1:D:364:ILE:CG2	2.75	0.59
1:D:482:THR:HG21	1:D:499:THR:C	2.27	0.59
1:B:32:ASN:C	1:C:25:LYS:CE	2.68	0.59
1:B:239:VAL:HG13	1:B:240:GLN:H	1.67	0.59
1:B:268:PHE:HA	1:B:285:ALA:HB3	1.84	0.59
1:B:432:ASP:CG	1:B:464:ILE:CG2	2.74	0.59
1:C:31:PHE:CB	1:D:95:THR:HG21	2.10	0.59
1:D:396:ARG:NH2	1:D:464:ILE:HG21	2.17	0.59
1:A:239:VAL:HG13	1:A:240:GLN:H	1.67	0.59
1:B:363:GLN:C	1:B:364:ILE:CG2	2.76	0.59
1:B:449:ASP:H	1:B:532:CYS:CB	2.12	0.59
1:C:92:MET:HE2	1:D:91:PRO:HG3	1.83	0.59
1:C:443:ARG:HG3	1:C:443:ARG:HH11	1.67	0.59
1:D:336:VAL:HB	1:D:426:LEU:HD23	1.84	0.59
1:B:49:GLY:O	1:B:63:THR:HG21	2.02	0.59
1:B:286:LYS:O	1:B:287:GLY:O	2.21	0.59
1:C:32:ASN:CG	1:C:33:LYS:N	2.59	0.59
1:C:235:ILE:HG12	1:C:287:GLY:HA2	1.82	0.59
1:C:239:VAL:HG13	1:C:240:GLN:H	1.67	0.59
1:A:49:GLY:O	1:A:63:THR:HG21	2.02	0.59
1:A:116:SER:HA	1:A:210:GLN:O	2.02	0.59
1:A:450:GLN:HB2	1:A:533:GLU:CA	2.26	0.59
1:A:514:SER:HA	1:A:517:GLN:O	2.02	0.59
1:A:518:ASN:O	1:A:520:PRO:CD	2.46	0.59
1:C:268:PHE:HA	1:C:285:ALA:HB3	1.84	0.59
1:C:286:LYS:O	1:C:287:GLY:O	2.21	0.59
1:C:367:LEU:C	1:C:367:LEU:HD12	2.28	0.59
1:A:90:GLU:CB	1:B:3:VAL:HG23	2.33	0.59
1:A:367:LEU:CB	1:A:413:THR:O	2.51	0.59
1:A:396:ARG:NH2	1:A:464:ILE:HG21	2.17	0.59
1:B:38:ILE:HG22	1:B:53:ILE:HG22	1.85	0.59
1:B:146:LEU:HA	1:B:194:THR:O	2.02	0.59
1:B:367:LEU:CB	1:B:413:THR:O	2.51	0.59
1:B:482:THR:HG22	1:B:499:THR:N	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LYS:HB3	1:D:76:LEU:O	2.03	0.59
1:C:335:ALA:HB1	3:C:811:NDG:C6	2.33	0.59
1:D:363:GLN:O	1:D:364:ILE:HG22	2.03	0.59
1:D:486:GLU:O	1:D:495:LEU:N	2.31	0.59
1:D:508:SER:HA	1:D:526:ASN:HA	1.84	0.59
1:A:38:ILE:HG22	1:A:53:ILE:HG22	1.85	0.59
1:A:195:ASP:CB	1:A:200:GLY:HA3	2.33	0.59
1:C:49:GLY:O	1:C:63:THR:HG21	2.02	0.59
1:D:367:LEU:C	1:D:367:LEU:HD12	2.28	0.59
1:A:4:ILE:CG2	1:B:91:PRO:O	2.33	0.58
1:B:88:VAL:O	1:D:1:ASP:HB3	2.01	0.58
1:B:473:VAL:HA	1:B:513:LEU:HD23	1.85	0.58
1:C:443:ARG:HA	1:C:525:VAL:HG13	1.85	0.58
1:A:146:LEU:HA	1:A:194:THR:O	2.02	0.58
1:B:367:LEU:C	1:B:367:LEU:HD12	2.28	0.58
1:C:367:LEU:CB	1:C:413:THR:O	2.51	0.58
1:D:38:ILE:HG22	1:D:53:ILE:HG22	1.85	0.58
1:A:286:LYS:O	1:A:287:GLY:O	2.21	0.58
1:B:232:GLU:HG2	1:B:289:ASP:CA	2.33	0.58
1:B:335:ALA:HB1	3:B:811:NDG:C6	2.33	0.58
1:B:403:ASN:CB	2:B:902:NAG:C7	2.76	0.58
1:C:86:SER:N	1:D:74:TYR:HD2	1.94	0.58
1:C:88:VAL:CG2	1:D:76:LEU:HD23	2.25	0.58
1:D:443:ARG:HA	1:D:525:VAL:HG13	1.85	0.58
1:A:367:LEU:HD12	1:A:367:LEU:C	2.28	0.58
1:A:443:ARG:HH11	1:A:443:ARG:HG3	1.67	0.58
1:B:537:ILE:HG12	1:B:538:LYS:N	2.19	0.58
1:C:309:SER:O	1:C:310:VAL:HG23	2.03	0.58
1:C:363:GLN:C	1:C:364:ILE:CG2	2.75	0.58
1:D:232:GLU:HG2	1:D:289:ASP:CA	2.33	0.58
1:D:286:LYS:O	1:D:287:GLY:O	2.21	0.58
1:D:366:LYS:HG3	1:D:367:LEU:N	2.04	0.58
1:B:522:LEU:CD2	1:B:523:THR:HB	2.26	0.58
1:C:28:LYS:HD3	1:D:76:LEU:O	2.02	0.58
1:C:406:TYR:HB3	1:C:428:LEU:CD2	2.33	0.58
1:C:432:ASP:CG	1:C:464:ILE:CG2	2.74	0.58
1:A:336:VAL:HB	1:A:426:LEU:HD23	1.84	0.58
1:A:366:LYS:HG3	1:A:367:LEU:N	2.04	0.58
1:B:403:ASN:C	1:B:405:THR:H	2.12	0.58
1:C:31:PHE:HA	1:D:73:LYS:HZ1	1.69	0.58
1:C:226:TYR:CE2	1:C:242:LEU:HD23	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:MET:HB2	1:C:529:VAL:HG22	1.84	0.58
1:D:221:PHE:HA	1:D:244:VAL:HG12	1.85	0.58
1:D:226:TYR:CE2	1:D:242:LEU:HD23	2.39	0.58
1:A:1:ASP:CA	1:B:24:ILE:HD13	2.33	0.58
1:B:42:GLY:HA2	1:B:47:PRO:O	2.04	0.58
1:B:232:GLU:CG	1:B:290:PHE:N	2.64	0.58
1:B:235:ILE:HG12	1:B:287:GLY:HA2	1.82	0.58
1:D:406:TYR:HB3	1:D:428:LEU:CD2	2.33	0.58
1:D:443:ARG:HH11	1:D:443:ARG:HG3	1.67	0.58
1:D:522:LEU:CD2	1:D:523:THR:HB	2.26	0.58
1:D:537:ILE:HG12	1:D:538:LYS:N	2.19	0.58
1:A:363:GLN:O	1:A:364:ILE:HG22	2.03	0.58
1:A:473:VAL:HA	1:A:513:LEU:HD23	1.85	0.58
1:C:42:GLY:HA2	1:C:47:PRO:O	2.04	0.58
1:C:232:GLU:HG2	1:C:289:ASP:CA	2.33	0.58
1:C:396:ARG:NH2	1:C:464:ILE:HG21	2.17	0.58
1:D:473:VAL:HA	1:D:513:LEU:HD23	1.85	0.58
1:A:232:GLU:HG2	1:A:289:ASP:CA	2.33	0.58
1:A:537:ILE:HG12	1:A:538:LYS:N	2.19	0.58
1:B:406:TYR:HB3	1:B:428:LEU:CD2	2.33	0.58
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.67	0.58
1:C:79:HIS:ND1	1:D:39:THR:HG22	2.19	0.58
1:C:83:GLU:C	1:D:41:GLN:NE2	2.61	0.58
1:C:88:VAL:C	1:D:38:ILE:CG1	2.76	0.58
1:D:296:TYR:HB2	1:D:321:VAL:HB	1.86	0.58
1:A:154:ASP:CB	1:A:155:PRO:CD	2.82	0.58
1:A:221:PHE:HA	1:A:244:VAL:HG12	1.85	0.58
1:A:309:SER:O	1:A:310:VAL:HG23	2.03	0.58
1:A:406:TYR:HB3	1:A:428:LEU:CD2	2.33	0.58
1:A:508:SER:HA	1:A:526:ASN:HA	1.84	0.58
1:B:415:ASP:OD1	1:B:416:GLY:N	2.27	0.58
1:B:443:ARG:HA	1:B:525:VAL:HG13	1.85	0.58
1:C:38:ILE:HG22	1:C:53:ILE:HG22	1.85	0.58
1:C:332:PHE:CD2	1:C:424:GLY:HA3	2.39	0.58
1:D:42:GLY:HA2	1:D:47:PRO:O	2.04	0.58
1:A:42:GLY:HA2	1:A:47:PRO:O	2.04	0.57
1:A:406:TYR:HB3	1:A:428:LEU:HD21	1.86	0.57
1:B:87:PRO:CG	1:C:2:TRP:HB2	2.29	0.57
1:B:309:SER:O	1:B:310:VAL:HG23	2.03	0.57
1:C:90:GLU:CG	1:D:79:HIS:O	2.51	0.57
1:A:268:PHE:HA	1:A:285:ALA:HB3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:MET:HB2	1:A:529:VAL:HG22	1.84	0.57
1:B:332:PHE:CD2	1:B:424:GLY:HA3	2.39	0.57
1:B:406:TYR:HB3	1:B:428:LEU:HD21	1.87	0.57
1:C:88:VAL:CG1	1:D:94:ILE:O	2.52	0.57
1:D:268:PHE:HA	1:D:285:ALA:HB3	1.84	0.57
1:A:332:PHE:CD2	1:A:424:GLY:HA3	2.39	0.57
1:A:403:ASN:C	1:A:405:THR:H	2.12	0.57
1:B:154:ASP:CB	1:B:155:PRO:CD	2.82	0.57
1:B:221:PHE:HA	1:B:244:VAL:HG12	1.85	0.57
1:B:226:TYR:CE2	1:B:242:LEU:HD23	2.39	0.57
1:B:523:THR:CG2	1:B:524:VAL:H	1.94	0.57
1:C:296:TYR:HB2	1:C:321:VAL:HB	1.86	0.57
1:C:473:VAL:HA	1:C:513:LEU:HD23	1.85	0.57
1:D:447:MET:HB2	1:D:529:VAL:HG22	1.84	0.57
1:B:447:MET:HB2	1:B:529:VAL:HG22	1.84	0.57
1:C:154:ASP:CB	2:C:801:NAG:HN2	2.16	0.57
1:C:240:GLN:HG3	1:C:241:ARG:N	2.19	0.57
1:D:154:ASP:CB	1:D:155:PRO:CD	2.82	0.57
1:D:330:PRO:HD3	1:D:414:ASP:HB2	1.86	0.57
1:D:403:ASN:C	1:D:405:THR:H	2.12	0.57
1:A:336:VAL:HG12	1:A:338:ARG:HB2	1.87	0.57
1:B:28:LYS:NZ	1:D:2:TRP:O	2.33	0.57
1:C:83:GLU:CB	1:D:41:GLN:HE22	2.16	0.57
1:A:2:TRP:CZ2	1:B:79:HIS:O	2.38	0.57
1:A:4:ILE:CB	1:B:90:GLU:C	2.76	0.57
1:B:68:ARG:HG3	1:B:69:GLU:N	2.19	0.57
1:B:330:PRO:HD3	1:B:414:ASP:HB2	1.86	0.57
1:C:87:PRO:CD	1:D:43:ALA:N	2.65	0.57
1:C:363:GLN:O	1:C:364:ILE:HG22	2.03	0.57
1:D:32:ASN:HD22	1:D:83:GLU:H	1.51	0.57
1:D:195:ASP:CB	1:D:200:GLY:HA3	2.33	0.57
1:D:482:THR:HG22	1:D:499:THR:N	2.13	0.57
1:A:10:SER:CA	1:D:30:ARG:HD2	2.35	0.57
1:A:235:ILE:HG12	1:A:287:GLY:HA2	1.82	0.57
1:B:195:ASP:CB	1:B:200:GLY:HA3	2.33	0.57
1:B:363:GLN:O	1:B:364:ILE:HG22	2.03	0.57
1:D:332:PHE:CD2	1:D:424:GLY:HA3	2.39	0.57
1:D:406:TYR:HB3	1:D:428:LEU:HD21	1.87	0.57
1:A:330:PRO:HD3	1:A:414:ASP:HB2	1.86	0.57
1:C:195:ASP:CB	1:C:200:GLY:HA3	2.33	0.57
1:C:505:GLY:HA2	1:C:529:VAL:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:ASP:CB	2:D:801:NAG:HN2	2.16	0.57
1:A:108:PHE:CE1	1:A:203:VAL:HG23	2.40	0.57
1:A:296:TYR:HB2	1:A:321:VAL:HB	1.86	0.57
1:A:335:ALA:HB1	3:A:811:NDG:C6	2.33	0.57
1:A:369:TYR:HD1	1:A:383:LYS:O	1.88	0.57
1:B:189:LEU:HD21	1:B:209:ILE:HD12	1.87	0.57
1:B:222:ASP:N	1:B:243:SER:O	2.38	0.57
1:B:240:GLN:HG3	1:B:241:ARG:N	2.19	0.57
1:B:259:TYR:O	1:B:260:LYS:HB3	2.05	0.57
1:B:336:VAL:HG12	1:B:338:ARG:HB2	1.87	0.57
1:C:89:GLU:N	1:D:38:ILE:CG1	2.58	0.57
1:C:268:PHE:C	1:C:285:ALA:HB3	2.30	0.57
1:C:403:ASN:C	1:C:405:THR:H	2.12	0.57
1:D:240:GLN:HG3	1:D:241:ARG:N	2.19	0.57
1:D:369:TYR:HD1	1:D:383:LYS:O	1.88	0.57
1:C:26:SER:CB	1:D:77:SER:HB2	2.34	0.57
1:C:154:ASP:CB	1:C:155:PRO:CD	2.82	0.57
1:C:221:PHE:HA	1:C:244:VAL:HG12	1.85	0.57
1:C:537:ILE:HG12	1:C:538:LYS:N	2.19	0.57
1:A:138:ASN:HD22	1:A:138:ASN:C	2.13	0.56
1:A:240:GLN:HG3	1:A:241:ARG:N	2.19	0.56
1:B:118:ARG:HA	1:B:212:THR:HB	1.87	0.56
1:D:335:ALA:HB1	3:D:811:NDG:C6	2.33	0.56
1:A:118:ARG:HA	1:A:212:THR:HB	1.87	0.56
1:A:443:ARG:HA	1:A:525:VAL:HG13	1.85	0.56
1:B:85:GLY:O	1:D:90:GLU:HA	2.05	0.56
1:B:378:TRP:O	1:B:391:ASN:HB2	2.06	0.56
1:D:68:ARG:HG3	1:D:69:GLU:N	2.19	0.56
1:A:68:ARG:HG3	1:A:69:GLU:N	2.19	0.56
1:A:226:TYR:CE2	1:A:242:LEU:HD23	2.39	0.56
1:A:505:GLY:HA2	1:A:529:VAL:H	1.69	0.56
1:B:369:TYR:HD1	1:B:383:LYS:O	1.88	0.56
1:C:27:ASN:HD21	1:D:93:GLU:HB3	1.60	0.56
1:C:82:SER:OG	1:D:74:TYR:HB3	2.05	0.56
1:C:155:PRO:N	2:C:801:NAG:H82	2.20	0.56
1:C:369:TYR:HD1	1:C:383:LYS:O	1.88	0.56
1:D:138:ASN:C	1:D:138:ASN:HD22	2.13	0.56
1:D:189:LEU:HD21	1:D:209:ILE:HD12	1.87	0.56
1:D:309:SER:O	1:D:310:VAL:HG23	2.03	0.56
1:B:154:ASP:CB	2:B:801:NAG:HN2	2.16	0.56
1:B:296:TYR:HB2	1:B:321:VAL:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ALA:HB1	3:C:811:NDG:H6	1.66	0.56
1:C:336:VAL:HG12	1:C:338:ARG:HB2	1.87	0.56
1:D:378:TRP:O	1:D:391:ASN:HB2	2.06	0.56
1:A:5:PRO:N	1:B:91:PRO:HB2	2.21	0.56
1:B:83:GLU:CG	1:C:25:LYS:HD3	2.25	0.56
1:B:394:LEU:N	1:B:394:LEU:CD1	2.69	0.56
1:D:222:ASP:N	1:D:243:SER:O	2.38	0.56
1:A:1:ASP:H3	1:B:94:ILE:HD11	0.74	0.56
1:A:189:LEU:HD21	1:A:209:ILE:HD12	1.87	0.56
1:A:222:ASP:N	1:A:243:SER:O	2.38	0.56
1:B:30:ARG:NH1	1:C:30:ARG:HB3	2.21	0.56
1:B:138:ASN:C	1:B:138:ASN:HD22	2.13	0.56
1:B:268:PHE:C	1:B:285:ALA:HB3	2.30	0.56
1:C:108:PHE:CE1	1:C:203:VAL:HG23	2.40	0.56
1:C:378:TRP:O	1:C:391:ASN:HB2	2.06	0.56
1:C:415:ASP:OD1	1:C:416:GLY:N	2.26	0.56
1:D:155:PRO:N	2:D:801:NAG:H82	2.20	0.56
1:A:268:PHE:C	1:A:285:ALA:HB3	2.30	0.56
1:A:403:ASN:CB	2:A:902:NAG:H83	2.21	0.56
1:B:108:PHE:CE1	1:B:203:VAL:HG23	2.40	0.56
1:C:189:LEU:HD21	1:C:209:ILE:HD12	1.87	0.56
1:A:4:ILE:CA	1:B:91:PRO:CD	2.69	0.56
1:C:68:ARG:HG3	1:C:69:GLU:N	2.19	0.56
1:C:84:ASN:C	1:D:74:TYR:HE2	2.07	0.56
1:C:138:ASN:HD22	1:C:138:ASN:C	2.13	0.56
1:C:162:LEU:O	1:C:174:LEU:HD12	2.06	0.56
1:C:365:GLN:O	1:C:365:GLN:CG	2.54	0.56
1:D:108:PHE:CE1	1:D:203:VAL:HG23	2.40	0.56
1:D:162:LEU:O	1:D:174:LEU:HD12	2.06	0.56
1:D:450:GLN:HB2	1:D:533:GLU:CA	2.26	0.56
1:B:505:GLY:HA2	1:B:529:VAL:H	1.69	0.56
1:C:118:ARG:HA	1:C:212:THR:HB	1.87	0.56
1:C:406:TYR:HB3	1:C:428:LEU:HD21	1.86	0.56
1:C:31:PHE:O	1:D:73:LYS:CE	2.54	0.56
1:C:88:VAL:HG13	1:D:94:ILE:O	2.05	0.56
1:C:222:ASP:N	1:C:243:SER:O	2.38	0.56
1:D:336:VAL:HG12	1:D:338:ARG:HB2	1.87	0.56
1:A:2:TRP:CH2	1:B:35:TYR:O	2.58	0.55
1:A:394:LEU:N	1:A:394:LEU:CD1	2.69	0.55
1:C:84:ASN:O	1:D:74:TYR:CE2	2.57	0.55
1:C:87:PRO:C	1:D:38:ILE:CD1	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:VAL:HG21	1:D:351:ILE:CG2	2.36	0.55
1:B:162:LEU:O	1:B:174:LEU:HD12	2.06	0.55
1:C:35:TYR:HB3	1:D:45:ASN:ND2	2.22	0.55
1:C:330:PRO:HD3	1:C:414:ASP:HB2	1.86	0.55
1:D:259:TYR:O	1:D:260:LYS:HB3	2.05	0.55
1:D:268:PHE:C	1:D:285:ALA:HB3	2.30	0.55
1:B:318:THR:CG2	2:B:806:NAG:H5	2.34	0.55
1:C:1:ASP:N	1:D:89:GLU:OE2	2.38	0.55
1:C:352:ILE:HG13	1:C:388:VAL:CB	2.33	0.55
1:C:403:ASN:CB	2:C:902:NAG:H83	2.21	0.55
1:D:155:PRO:HG2	2:D:801:NAG:O7	2.07	0.55
1:D:505:GLY:HA2	1:D:529:VAL:H	1.70	0.55
1:A:333:VAL:CG2	1:A:334:PRO:HD3	2.36	0.55
1:B:339:VAL:HG21	1:B:351:ILE:CG2	2.37	0.55
1:C:79:HIS:HB3	1:D:39:THR:CB	2.36	0.55
1:C:259:TYR:O	1:C:260:LYS:HB3	2.05	0.55
1:C:339:VAL:HG21	1:C:351:ILE:CG2	2.37	0.55
1:D:118:ARG:HA	1:D:212:THR:HB	1.87	0.55
1:D:268:PHE:CD2	1:D:268:PHE:N	2.75	0.55
1:D:394:LEU:N	1:D:394:LEU:CD1	2.69	0.55
1:A:365:GLN:O	1:A:365:GLN:CG	2.54	0.55
1:B:30:ARG:NH1	1:C:30:ARG:CG	2.69	0.55
1:C:278:ASN:HD22	1:C:278:ASN:N	2.05	0.55
1:D:28:LYS:HB3	1:D:88:VAL:HG11	1.89	0.55
1:A:162:LEU:O	1:A:174:LEU:HD12	2.06	0.55
1:A:318:THR:CG2	2:A:806:NAG:H5	2.34	0.55
1:C:31:PHE:CE2	1:D:73:LYS:C	2.36	0.55
1:C:79:HIS:N	1:D:39:THR:HG21	2.10	0.55
1:C:459:ILE:HG21	1:C:471:TYR:CE2	2.42	0.55
1:D:419:VAL:CG1	1:D:420:GLY:N	2.70	0.55
1:B:330:PRO:HB3	1:B:358:ASP:HB2	1.89	0.55
1:C:333:VAL:CG2	1:C:334:PRO:HD3	2.36	0.55
1:C:394:LEU:N	1:C:394:LEU:CD1	2.69	0.55
1:C:439:VAL:HG13	1:C:522:LEU:HD11	1.88	0.55
1:A:419:VAL:CG1	1:A:420:GLY:N	2.70	0.55
1:B:28:LYS:HE3	1:D:4:ILE:N	2.13	0.55
1:B:226:TYR:O	1:B:227:THR:CG2	2.55	0.55
1:B:419:VAL:CG1	1:B:420:GLY:N	2.70	0.55
1:C:81:VAL:HG21	1:D:45:ASN:N	2.20	0.55
1:C:86:SER:O	1:D:41:GLN:O	2.25	0.55
1:D:363:GLN:C	1:D:364:ILE:HG23	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:N	2:A:801:NAG:H82	2.20	0.55
1:A:226:TYR:O	1:A:227:THR:CG2	2.55	0.55
1:B:83:GLU:CB	1:C:25:LYS:CG	2.37	0.55
1:B:333:VAL:CG2	1:B:334:PRO:HD3	2.36	0.55
1:C:82:SER:OG	1:D:74:TYR:CD2	2.60	0.55
1:C:83:GLU:CA	1:D:41:GLN:HE22	2.06	0.55
1:C:155:PRO:HG2	2:C:801:NAG:O7	2.07	0.55
1:D:278:ASN:HD22	1:D:278:ASN:N	2.05	0.55
1:D:459:ILE:HG21	1:D:471:TYR:CE2	2.42	0.55
1:D:466:PRO:O	1:D:468:THR:N	2.40	0.55
1:A:10:SER:N	1:D:30:ARG:HD2	2.20	0.55
1:A:378:TRP:O	1:A:391:ASN:HB2	2.06	0.55
1:A:438:PRO:HB2	1:A:513:LEU:HD12	1.89	0.55
1:A:459:ILE:HG21	1:A:471:TYR:CE2	2.42	0.55
1:B:155:PRO:HG2	2:B:801:NAG:O7	2.07	0.55
1:B:363:GLN:C	1:B:364:ILE:HG23	2.32	0.55
1:C:31:PHE:CB	1:D:75:VAL:CG2	2.80	0.55
1:D:333:VAL:CG2	1:D:334:PRO:HD3	2.36	0.55
1:A:75:VAL:O	1:A:76:LEU:HD23	2.07	0.54
1:A:259:TYR:O	1:A:260:LYS:HB3	2.05	0.54
1:B:28:LYS:HB3	1:B:88:VAL:HG11	1.89	0.54
1:B:466:PRO:O	1:B:468:THR:N	2.40	0.54
1:C:31:PHE:CD2	1:D:74:TYR:O	2.60	0.54
1:D:439:VAL:HG13	1:D:522:LEU:HD11	1.88	0.54
1:A:339:VAL:HG21	1:A:351:ILE:CG2	2.37	0.54
1:C:226:TYR:HB2	1:C:319:VAL:HG22	1.89	0.54
1:D:272:THR:CG2	1:D:273:THR:H	2.19	0.54
1:A:90:GLU:HB2	1:B:3:VAL:O	2.06	0.54
1:A:330:PRO:HB3	1:A:358:ASP:HB2	1.89	0.54
1:A:466:PRO:O	1:A:468:THR:N	2.40	0.54
1:A:490:LYS:O	1:A:490:LYS:HG2	2.08	0.54
1:B:169:THR:OG1	1:B:171:VAL:HG23	2.07	0.54
1:C:32:ASN:HD22	1:C:83:GLU:H	1.51	0.54
1:C:169:THR:OG1	1:C:171:VAL:HG23	2.08	0.54
1:D:226:TYR:O	1:D:227:THR:CG2	2.55	0.54
1:D:330:PRO:HB3	1:D:358:ASP:HB2	1.89	0.54
1:B:439:VAL:HG13	1:B:522:LEU:HD11	1.88	0.54
1:B:450:GLN:CB	1:B:532:CYS:O	2.56	0.54
1:C:419:VAL:CG1	1:C:420:GLY:N	2.70	0.54
1:B:226:TYR:HB2	1:B:319:VAL:HG22	1.89	0.54
1:C:28:LYS:HB3	1:C:88:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:VAL:O	1:D:211:ILE:HA	2.07	0.54
1:A:10:SER:CB	1:D:30:ARG:HG3	2.36	0.54
1:A:268:PHE:CD2	1:A:268:PHE:N	2.75	0.54
1:A:332:PHE:HD2	1:A:424:GLY:HA3	1.73	0.54
1:A:439:VAL:HG13	1:A:522:LEU:HD11	1.88	0.54
1:C:87:PRO:CG	1:D:43:ALA:HB2	1.86	0.54
1:C:88:VAL:CG2	1:D:75:VAL:O	2.43	0.54
1:C:268:PHE:CD2	1:C:268:PHE:N	2.75	0.54
1:C:466:PRO:O	1:C:468:THR:N	2.40	0.54
1:D:226:TYR:C	1:D:227:THR:HG23	2.33	0.54
1:D:490:LYS:O	1:D:490:LYS:HG2	2.08	0.54
1:A:90:GLU:N	1:B:2:TRP:CE3	2.60	0.54
1:B:217:ASN:N	1:B:217:ASN:ND2	2.56	0.54
1:C:1:ASP:N	1:D:28:LYS:CB	2.71	0.54
1:D:169:THR:OG1	1:D:171:VAL:HG23	2.07	0.54
1:A:28:LYS:HB3	1:A:88:VAL:HG11	1.89	0.54
1:A:155:PRO:HG2	2:A:801:NAG:O7	2.07	0.54
1:A:226:TYR:C	1:A:227:THR:HG23	2.33	0.54
1:B:459:ILE:HG21	1:B:471:TYR:CE2	2.42	0.54
1:C:93:GLU:HB3	1:D:81:VAL:CG1	2.37	0.54
1:C:117:VAL:O	1:C:211:ILE:HA	2.07	0.54
1:C:226:TYR:O	1:C:227:THR:CG2	2.55	0.54
1:C:330:PRO:HB3	1:C:358:ASP:HB2	1.89	0.54
1:D:217:ASN:N	1:D:217:ASN:ND2	2.56	0.54
1:D:332:PHE:HD2	1:D:424:GLY:HA3	1.73	0.54
1:A:272:THR:CG2	1:A:273:THR:H	2.18	0.54
1:A:402:LYS:C	1:A:403:ASN:O	2.46	0.54
1:B:403:ASN:CB	2:B:902:NAG:H83	2.21	0.54
1:D:241:ARG:NE	1:D:281:ILE:HD12	2.22	0.54
1:D:438:PRO:HB2	1:D:513:LEU:HD12	1.89	0.54
1:B:154:ASP:CG	1:B:155:PRO:HD2	2.33	0.54
1:B:252:THR:HG23	1:B:253:PRO:HD2	1.90	0.54
1:B:490:LYS:O	1:B:490:LYS:HG2	2.08	0.54
1:C:90:GLU:H	1:D:79:HIS:N	1.91	0.54
1:C:217:ASN:N	1:C:217:ASN:ND2	2.56	0.54
1:C:252:THR:HG23	1:C:253:PRO:HD2	1.90	0.54
1:D:443:ARG:HG3	1:D:443:ARG:NH1	2.24	0.54
1:A:32:ASN:HD22	1:A:83:GLU:H	1.51	0.53
1:B:75:VAL:O	1:B:76:LEU:HD23	2.08	0.53
1:B:81:VAL:CB	1:D:90:GLU:HG2	2.37	0.53
1:B:86:SER:N	1:D:91:PRO:CD	2.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:VAL:O	1:B:211:ILE:HA	2.07	0.53
1:B:249:MET:O	1:B:252:THR:HB	2.08	0.53
1:B:272:THR:CG2	1:B:273:THR:H	2.19	0.53
1:C:226:TYR:C	1:C:227:THR:HG23	2.33	0.53
1:A:217:ASN:N	1:A:217:ASN:ND2	2.56	0.53
1:A:249:MET:O	1:A:252:THR:HB	2.09	0.53
1:A:373:ASN:HB3	1:A:409:ILE:H	1.74	0.53
1:B:438:PRO:HB2	1:B:513:LEU:HD12	1.89	0.53
1:B:458:THR:HG22	1:B:493:SER:HB3	1.91	0.53
1:C:85:GLY:N	1:D:74:TYR:CD2	2.77	0.53
1:C:154:ASP:CG	1:C:155:PRO:HD2	2.33	0.53
1:A:117:VAL:O	1:A:211:ILE:HA	2.07	0.53
1:A:443:ARG:HG3	1:A:443:ARG:NH1	2.23	0.53
1:C:75:VAL:O	1:C:76:LEU:HD23	2.08	0.53
1:C:79:HIS:CB	1:D:39:THR:CB	2.80	0.53
1:C:438:PRO:HB2	1:C:513:LEU:HD12	1.89	0.53
1:C:522:LEU:CD2	1:C:523:THR:HB	2.26	0.53
1:D:105:ARG:HG3	1:D:106:PRO:HD2	1.91	0.53
1:D:373:ASN:HB3	1:D:409:ILE:H	1.73	0.53
1:D:450:GLN:CB	1:D:532:CYS:O	2.56	0.53
1:A:22:VAL:HG22	1:A:23:GLN:H	1.73	0.53
1:A:458:THR:HG22	1:A:493:SER:HB3	1.91	0.53
1:C:363:GLN:C	1:C:364:ILE:HG23	2.32	0.53
1:C:443:ARG:HG3	1:C:443:ARG:NH1	2.23	0.53
1:C:450:GLN:CB	1:C:532:CYS:O	2.56	0.53
1:D:458:THR:HG22	1:D:493:SER:HB3	1.91	0.53
1:B:332:PHE:HD2	1:B:424:GLY:HA3	1.73	0.53
1:B:373:ASN:HB3	1:B:409:ILE:H	1.74	0.53
1:C:490:LYS:HG2	1:C:490:LYS:O	2.08	0.53
1:D:22:VAL:HG22	1:D:23:GLN:H	1.73	0.53
1:D:367:LEU:HD13	1:D:412:VAL:HG23	1.91	0.53
1:A:320:THR:CG2	2:A:807:NAG:C2	2.77	0.53
1:C:105:ARG:HG3	1:C:106:PRO:HD2	1.91	0.53
1:C:272:THR:CG2	1:C:273:THR:H	2.18	0.53
1:D:75:VAL:O	1:D:76:LEU:HD23	2.08	0.53
1:A:154:ASP:CG	1:A:155:PRO:HD2	2.33	0.53
1:A:169:THR:OG1	1:A:171:VAL:HG23	2.07	0.53
1:B:27:ASN:C	1:B:29:ASP:H	2.15	0.53
1:B:415:ASP:CG	1:B:416:GLY:H	2.16	0.53
1:C:81:VAL:CG1	1:D:43:ALA:C	2.80	0.53
1:C:312:LEU:O	3:C:804:NDG:C8	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:TYR:O	1:C:383:LYS:HG2	2.09	0.53
1:D:154:ASP:CG	1:D:155:PRO:HD2	2.33	0.53
1:D:242:LEU:O	1:D:279:GLN:HB3	2.09	0.53
1:D:249:MET:O	1:D:252:THR:HB	2.08	0.53
1:B:379:LEU:H	1:B:379:LEU:CD2	2.22	0.53
1:C:318:THR:CG2	2:C:806:NAG:H5	2.34	0.53
1:C:332:PHE:HD2	1:C:424:GLY:HA3	1.73	0.53
1:A:27:ASN:C	1:A:29:ASP:H	2.15	0.53
1:A:154:ASP:CB	2:A:801:NAG:HN2	2.16	0.53
1:A:242:LEU:O	1:A:279:GLN:HB3	2.09	0.53
1:A:312:LEU:O	3:A:804:NDG:C8	2.57	0.53
1:A:347:ARG:HG3	1:A:391:ASN:HA	1.91	0.53
1:B:369:TYR:O	1:B:383:LYS:HG2	2.09	0.53
1:A:252:THR:HG23	1:A:253:PRO:HD2	1.90	0.53
1:A:278:ASN:HD22	1:A:278:ASN:N	2.05	0.53
1:C:249:MET:O	1:C:252:THR:HB	2.08	0.53
1:A:289:ASP:O	1:A:290:PHE:CB	2.25	0.52
1:B:226:TYR:C	1:B:227:THR:HG23	2.33	0.52
1:B:347:ARG:HG3	1:B:391:ASN:HA	1.91	0.52
1:C:1:ASP:O	1:D:28:LYS:CD	2.57	0.52
1:D:31:PHE:CD2	1:D:32:ASN:HB2	2.44	0.52
1:D:227:THR:CG2	2:D:807:NAG:H83	2.32	0.52
1:A:226:TYR:HB2	1:A:319:VAL:HG22	1.89	0.52
1:A:363:GLN:C	1:A:364:ILE:HG23	2.32	0.52
1:A:369:TYR:O	1:A:383:LYS:HG2	2.09	0.52
1:A:2:TRP:CZ2	1:B:36:TYR:HA	2.43	0.52
1:A:4:ILE:CA	1:B:91:PRO:CB	2.81	0.52
1:A:24:ILE:HA	1:D:2:TRP:CB	2.33	0.52
1:A:24:ILE:CG2	1:D:2:TRP:HE1	2.18	0.52
1:A:31:PHE:CD2	1:A:32:ASN:HB2	2.45	0.52
1:A:352:ILE:HG13	1:A:388:VAL:CB	2.33	0.52
1:A:450:GLN:CB	1:A:532:CYS:O	2.56	0.52
1:A:512:LEU:HD11	1:A:519:ASN:HD21	1.75	0.52
1:B:31:PHE:CD2	1:B:32:ASN:HB2	2.44	0.52
1:C:81:VAL:CG1	1:D:43:ALA:H	2.22	0.52
1:C:83:GLU:N	1:D:41:GLN:CD	2.66	0.52
1:C:533:GLU:HA	1:C:533:GLU:OE2	2.09	0.52
1:D:312:LEU:O	3:D:804:NDG:C8	2.57	0.52
1:D:496:LEU:HD21	1:D:509:ILE:CD1	2.38	0.52
1:D:512:LEU:HD11	1:D:519:ASN:HD21	1.74	0.52
1:D:513:LEU:C	1:D:514:SER:HG	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:GLU:HA	1:D:533:GLU:OE2	2.09	0.52
1:A:2:TRP:HH2	1:B:35:TYR:O	1.92	0.52
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.23	0.52
1:C:31:PHE:CD2	1:C:32:ASN:HB2	2.45	0.52
1:C:91:PRO:N	1:D:79:HIS:HD2	2.03	0.52
1:C:379:LEU:H	1:C:379:LEU:CD2	2.22	0.52
1:D:272:THR:CG2	2:D:803:NAG:HN2	2.23	0.52
1:A:367:LEU:HD13	1:A:412:VAL:HG23	1.91	0.52
1:B:22:VAL:HG22	1:B:23:GLN:H	1.73	0.52
1:B:312:LEU:O	3:B:804:NDG:C8	2.57	0.52
1:B:496:LEU:HD21	1:B:509:ILE:CD1	2.38	0.52
1:C:373:ASN:CG	1:C:374:ASP:H	2.18	0.52
1:D:226:TYR:HB2	1:D:319:VAL:HG22	1.89	0.52
1:A:513:LEU:C	1:A:514:SER:HG	2.17	0.52
1:B:30:ARG:NH1	1:C:30:ARG:HG2	2.25	0.52
1:B:512:LEU:HD11	1:B:519:ASN:HD21	1.75	0.52
1:C:28:LYS:CB	1:D:76:LEU:O	2.57	0.52
1:C:512:LEU:HD11	1:C:519:ASN:HD21	1.74	0.52
1:D:318:THR:CG2	2:D:806:NAG:H5	2.34	0.52
1:D:396:ARG:NH2	1:D:464:ILE:HG22	2.12	0.52
1:A:338:ARG:HB3	1:A:339:VAL:HG22	1.92	0.52
1:A:371:ILE:HG23	1:A:372:GLY:H	1.73	0.52
1:B:246:ASP:C	1:B:247:LEU:HD12	2.35	0.52
1:C:93:GLU:CA	1:D:81:VAL:HG11	2.38	0.52
1:C:242:LEU:O	1:C:279:GLN:HB3	2.09	0.52
1:C:336:VAL:O	1:C:426:LEU:HD22	2.10	0.52
1:C:338:ARG:HB3	1:C:339:VAL:HG22	1.92	0.52
1:C:367:LEU:HD13	1:C:412:VAL:HG23	1.91	0.52
1:C:371:ILE:HG23	1:C:372:GLY:H	1.73	0.52
1:C:458:THR:HG22	1:C:493:SER:HB3	1.90	0.52
1:D:246:ASP:C	1:D:247:LEU:HD12	2.35	0.52
1:D:338:ARG:HB3	1:D:339:VAL:HG22	1.92	0.52
1:A:496:LEU:HD21	1:A:509:ILE:CD1	2.38	0.52
1:A:505:GLY:O	1:A:506:ASP:OD1	2.28	0.52
1:B:155:PRO:N	2:B:801:NAG:H82	2.20	0.52
1:B:272:THR:CG2	2:B:803:NAG:HN2	2.23	0.52
1:B:371:ILE:HG23	1:B:372:GLY:H	1.73	0.52
1:B:426:LEU:O	1:B:426:LEU:HD13	2.10	0.52
1:C:27:ASN:HD21	1:D:93:GLU:N	2.04	0.52
1:C:347:ARG:HG3	1:C:391:ASN:HA	1.91	0.52
1:C:373:ASN:HB3	1:C:409:ILE:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:GLN:CB	1:C:533:GLU:HA	2.29	0.52
1:D:365:GLN:O	1:D:365:GLN:CG	2.54	0.52
1:D:373:ASN:CG	1:D:374:ASP:H	2.18	0.52
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.91	0.52
1:B:89:GLU:N	1:D:1:ASP:CB	2.46	0.52
1:B:194:THR:HG22	1:B:195:ASP:N	2.25	0.52
1:C:246:ASP:C	1:C:247:LEU:HD12	2.35	0.52
1:D:482:THR:CG2	1:D:499:THR:CA	2.87	0.52
1:B:105:ARG:HG3	1:B:106:PRO:HD2	1.91	0.52
1:B:221:PHE:HB3	1:B:223:PRO:O	2.10	0.52
1:B:367:LEU:HD13	1:B:412:VAL:HG23	1.91	0.52
1:D:27:ASN:C	1:D:29:ASP:H	2.15	0.52
1:D:221:PHE:HB3	1:D:223:PRO:O	2.10	0.52
1:D:252:THR:HG23	1:D:253:PRO:HD2	1.90	0.52
1:D:347:ARG:HD2	1:D:392:GLY:N	2.25	0.52
1:D:371:ILE:HG23	1:D:372:GLY:H	1.73	0.52
1:D:482:THR:HG22	1:D:482:THR:O	2.09	0.52
1:D:505:GLY:O	1:D:506:ASP:OD1	2.28	0.52
1:A:246:ASP:C	1:A:247:LEU:HD12	2.35	0.51
1:A:272:THR:CG2	2:A:803:NAG:HN2	2.23	0.51
1:A:482:THR:CG2	1:A:499:THR:CA	2.87	0.51
1:B:533:GLU:HA	1:B:533:GLU:OE2	2.09	0.51
1:C:30:ARG:NH2	1:D:6:PRO:HG3	2.25	0.51
1:D:234:GLU:HB2	1:D:235:ILE:HG22	1.93	0.51
1:D:369:TYR:O	1:D:383:LYS:HG2	2.09	0.51
1:A:3:VAL:HG21	1:B:77:SER:OG	2.10	0.51
1:A:221:PHE:HB3	1:A:223:PRO:O	2.10	0.51
1:A:514:SER:HB3	1:A:517:GLN:O	2.10	0.51
1:A:533:GLU:HA	1:A:533:GLU:OE2	2.09	0.51
1:B:142:LEU:O	1:B:196:LEU:HD23	2.11	0.51
1:B:242:LEU:O	1:B:279:GLN:HB3	2.09	0.51
1:B:266:GLY:N	1:B:268:PHE:CE2	2.76	0.51
1:B:373:ASN:CG	1:B:374:ASP:H	2.18	0.51
1:C:22:VAL:HG22	1:C:23:GLN:H	1.73	0.51
1:C:272:THR:CG2	2:C:803:NAG:HN2	2.23	0.51
1:C:482:THR:CG2	1:C:499:THR:CA	2.87	0.51
1:C:514:SER:HB3	1:C:517:GLN:O	2.11	0.51
1:A:234:GLU:HB2	1:A:235:ILE:HG22	1.93	0.51
1:B:81:VAL:CG1	1:D:90:GLU:HG2	2.40	0.51
1:B:333:VAL:CB	1:B:334:PRO:CD	2.88	0.51
1:C:33:LYS:HB3	1:C:83:GLU:CG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:VAL:HG22	1:D:75:VAL:O	2.03	0.51
1:C:426:LEU:O	1:C:426:LEU:HD13	2.10	0.51
1:D:333:VAL:CB	1:D:334:PRO:CD	2.88	0.51
1:D:347:ARG:HG3	1:D:391:ASN:HA	1.91	0.51
1:D:426:LEU:O	1:D:426:LEU:HD13	2.09	0.51
1:D:514:SER:HB3	1:D:517:GLN:O	2.10	0.51
1:A:4:ILE:C	1:B:91:PRO:CB	2.82	0.51
1:A:90:GLU:CB	1:B:3:VAL:CA	2.60	0.51
1:A:373:ASN:CG	1:A:374:ASP:H	2.18	0.51
1:A:396:ARG:CZ	1:A:432:ASP:HB2	2.41	0.51
1:A:426:LEU:O	1:A:426:LEU:HD13	2.09	0.51
1:B:514:SER:HB3	1:B:517:GLN:O	2.10	0.51
1:C:88:VAL:CG1	1:D:94:ILE:N	2.73	0.51
1:C:155:PRO:CD	2:C:801:NAG:H82	2.40	0.51
1:C:194:THR:HG22	1:C:195:ASP:N	2.25	0.51
1:C:347:ARG:HD2	1:C:392:GLY:N	2.25	0.51
1:D:33:LYS:HB3	1:D:83:GLU:CG	2.40	0.51
1:D:336:VAL:O	1:D:426:LEU:HD22	2.10	0.51
1:B:402:LYS:C	1:B:403:ASN:O	2.46	0.51
1:B:471:TYR:N	1:B:471:TYR:CD1	2.79	0.51
1:C:82:SER:HB2	1:D:74:TYR:HA	1.92	0.51
1:C:142:LEU:O	1:C:196:LEU:HD23	2.11	0.51
1:C:151:LEU:HD12	1:C:190:THR:O	2.11	0.51
1:D:151:LEU:HD12	1:D:190:THR:O	2.11	0.51
1:D:155:PRO:CD	2:D:801:NAG:H82	2.40	0.51
1:D:402:LYS:C	1:D:403:ASN:O	2.46	0.51
1:A:297:VAL:CG2	2:A:807:NAG:H62	2.41	0.51
1:A:458:THR:HA	1:A:493:SER:HA	1.93	0.51
1:B:297:VAL:CG2	2:B:807:NAG:H62	2.41	0.51
1:B:336:VAL:O	1:B:426:LEU:HD22	2.10	0.51
1:C:31:PHE:C	1:D:73:LYS:CE	2.83	0.51
1:C:82:SER:OG	1:D:74:TYR:HD2	1.93	0.51
1:C:90:GLU:H	1:D:78:SER:CB	1.92	0.51
1:C:90:GLU:H	1:D:78:SER:HB2	1.74	0.51
1:A:333:VAL:CB	1:A:334:PRO:CD	2.88	0.51
1:A:428:LEU:O	1:A:428:LEU:HD23	2.11	0.51
1:B:482:THR:CG2	1:B:499:THR:CA	2.87	0.51
1:B:505:GLY:O	1:B:506:ASP:OD1	2.28	0.51
1:C:266:GLY:N	1:C:268:PHE:CE2	2.76	0.51
1:C:505:GLY:O	1:C:506:ASP:OD1	2.28	0.51
1:A:4:ILE:HA	1:B:90:GLU:CA	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HD12	1:A:190:THR:O	2.11	0.51
1:A:450:GLN:CG	1:A:533:GLU:OE2	2.58	0.51
1:B:155:PRO:CD	2:B:801:NAG:H82	2.40	0.51
1:B:458:THR:HA	1:B:493:SER:HA	1.93	0.51
1:C:333:VAL:CB	1:C:334:PRO:CD	2.88	0.51
1:A:194:THR:HG22	1:A:195:ASP:N	2.25	0.51
1:B:76:LEU:O	1:B:94:ILE:N	2.44	0.51
1:B:352:ILE:HG13	1:B:388:VAL:CB	2.33	0.51
1:B:428:LEU:HD23	1:B:428:LEU:O	2.11	0.51
1:C:25:LYS:NZ	1:C:29:ASP:OD2	2.40	0.51
1:C:31:PHE:CD1	1:D:95:THR:HG21	2.44	0.51
1:C:234:GLU:HB2	1:C:235:ILE:HG22	1.93	0.51
1:C:368:SER:OG	1:C:370:PHE:HE1	1.94	0.51
2:C:809:NAG:H61	2:C:810:NAG:C6	2.39	0.51
1:D:396:ARG:CZ	1:D:432:ASP:HB2	2.41	0.51
2:D:809:NAG:H61	2:D:810:NAG:C6	2.39	0.51
1:A:336:VAL:O	1:A:426:LEU:HD22	2.10	0.51
1:A:458:THR:HG22	1:A:493:SER:CB	2.41	0.51
1:A:471:TYR:CD1	1:A:471:TYR:N	2.79	0.51
1:B:151:LEU:HD12	1:B:190:THR:O	2.11	0.51
1:B:338:ARG:HB3	1:B:339:VAL:HG22	1.92	0.51
1:C:88:VAL:HG12	1:D:94:ILE:CA	2.40	0.51
1:C:241:ARG:NE	1:C:281:ILE:HD12	2.22	0.51
1:C:415:ASP:CG	1:C:416:GLY:H	2.16	0.51
1:D:76:LEU:O	1:D:94:ILE:N	2.44	0.51
1:D:276:GLU:HG3	1:D:277:SER:N	2.25	0.51
1:D:352:ILE:HG13	1:D:388:VAL:CB	2.33	0.51
1:B:32:ASN:HB2	1:C:26:SER:O	2.11	0.50
1:C:31:PHE:CA	1:D:73:LYS:NZ	2.72	0.50
1:C:155:PRO:HG2	2:C:801:NAG:C7	2.42	0.50
1:C:458:THR:HA	1:C:493:SER:HA	1.93	0.50
1:D:80:ALA:O	1:D:88:VAL:HG23	2.11	0.50
1:D:194:THR:HG22	1:D:195:ASP:N	2.25	0.50
1:D:458:THR:HA	1:D:493:SER:HA	1.93	0.50
1:B:432:ASP:CB	1:B:464:ILE:CG2	2.90	0.50
1:B:450:GLN:CG	1:B:533:GLU:OE2	2.58	0.50
1:C:90:GLU:N	1:D:78:SER:C	2.30	0.50
1:C:221:PHE:HB3	1:C:223:PRO:O	2.10	0.50
1:C:286:LYS:C	1:C:287:GLY:O	2.55	0.50
1:C:428:LEU:O	1:C:428:LEU:HD23	2.11	0.50
1:D:217:ASN:N	1:D:217:ASN:HD22	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:THR:HG22	1:D:493:SER:CB	2.42	0.50
1:A:80:ALA:O	1:A:88:VAL:HG23	2.11	0.50
1:A:155:PRO:CD	2:A:801:NAG:H82	2.40	0.50
1:A:241:ARG:NE	1:A:281:ILE:HD12	2.22	0.50
1:A:286:LYS:C	1:A:287:GLY:O	2.55	0.50
1:A:290:PHE:CE2	1:A:293:ARG:CB	2.92	0.50
1:A:374:ASP:C	1:A:375:PRO:O	2.54	0.50
1:A:419:VAL:HG22	2:A:809:NAG:H81	1.93	0.50
1:C:28:LYS:CD	1:C:88:VAL:HG12	2.38	0.50
1:C:261:ILE:HD11	1:C:264:ASN:HD22	1.77	0.50
1:C:352:ILE:CG1	1:C:388:VAL:HB	2.33	0.50
1:C:450:GLN:CG	1:C:533:GLU:OE2	2.58	0.50
1:D:142:LEU:O	1:D:196:LEU:HD23	2.11	0.50
1:D:297:VAL:CG2	2:D:807:NAG:H62	2.41	0.50
1:A:2:TRP:CD2	1:B:80:ALA:HB3	2.30	0.50
1:A:142:LEU:O	1:A:196:LEU:HD23	2.11	0.50
1:B:227:THR:CG2	2:B:807:NAG:H83	2.32	0.50
1:B:268:PHE:CD2	1:B:268:PHE:N	2.75	0.50
1:B:419:VAL:HG22	2:B:809:NAG:H81	1.93	0.50
1:C:297:VAL:CG2	2:C:807:NAG:H62	2.41	0.50
1:C:382:ASN:OD1	1:C:385:ASN:N	2.45	0.50
1:C:396:ARG:CZ	1:C:432:ASP:HB2	2.41	0.50
1:C:402:LYS:C	1:C:403:ASN:O	2.46	0.50
1:D:382:ASN:OD1	1:D:385:ASN:N	2.45	0.50
1:D:415:ASP:CG	1:D:416:GLY:H	2.16	0.50
1:D:432:ASP:CB	1:D:464:ILE:CG2	2.89	0.50
1:A:11:GLU:OE2	1:A:69:GLU:OE1	2.30	0.50
1:A:76:LEU:O	1:A:94:ILE:N	2.44	0.50
1:A:89:GLU:O	1:B:1:ASP:C	2.54	0.50
1:B:217:ASN:N	1:B:217:ASN:HD22	2.09	0.50
1:B:327:ASN:OD1	1:B:360:ASP:OD1	2.30	0.50
1:B:458:THR:HG22	1:B:493:SER:CB	2.42	0.50
1:C:290:PHE:CE2	1:C:293:ARG:CB	2.92	0.50
1:C:458:THR:HG22	1:C:493:SER:CB	2.42	0.50
1:D:428:LEU:O	1:D:428:LEU:HD23	2.11	0.50
1:D:471:TYR:CD1	1:D:471:TYR:N	2.79	0.50
1:A:382:ASN:OD1	1:A:385:ASN:N	2.44	0.50
1:B:155:PRO:HG2	2:B:801:NAG:C7	2.42	0.50
1:B:216:ASP:HB2	1:B:217:ASN:ND2	2.27	0.50
1:B:366:LYS:HG3	1:B:367:LEU:N	2.04	0.50
1:B:373:ASN:ND2	1:B:374:ASP:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ASP:HB2	1:C:217:ASN:ND2	2.27	0.50
1:C:471:TYR:N	1:C:471:TYR:CD1	2.79	0.50
1:C:482:THR:HG22	1:C:482:THR:O	2.09	0.50
1:D:11:GLU:OE2	1:D:69:GLU:OE1	2.30	0.50
1:D:261:ILE:HD11	1:D:264:ASN:HD22	1.77	0.50
1:D:450:GLN:CB	1:D:533:GLU:HA	2.29	0.50
1:A:1:ASP:HB3	1:B:92:MET:CB	2.40	0.50
1:A:109:THR:HG22	1:A:110:GLN:HG3	1.94	0.50
1:A:155:PRO:HG2	2:A:801:NAG:C7	2.42	0.50
1:A:423:THR:HB	2:A:810:NAG:H83	1.93	0.50
1:B:80:ALA:O	1:B:88:VAL:HG23	2.11	0.50
1:B:286:LYS:C	1:B:287:GLY:O	2.55	0.50
1:B:423:THR:HB	2:B:810:NAG:H83	1.93	0.50
2:B:809:NAG:H61	2:B:810:NAG:C6	2.39	0.50
1:C:1:ASP:C	1:D:28:LYS:HD3	2.37	0.50
1:C:88:VAL:HG21	1:D:75:VAL:O	2.07	0.50
1:C:496:LEU:HD21	1:C:509:ILE:CD1	2.38	0.50
1:D:155:PRO:HG2	2:D:801:NAG:C7	2.42	0.50
1:D:320:THR:CG2	2:D:807:NAG:C2	2.77	0.50
1:A:347:ARG:HD2	1:A:392:GLY:N	2.25	0.50
1:A:352:ILE:CG1	1:A:388:VAL:HB	2.34	0.50
1:B:290:PHE:CE2	1:B:293:ARG:CB	2.93	0.50
1:B:449:ASP:CB	1:B:532:CYS:H	2.22	0.50
1:C:87:PRO:N	1:D:43:ALA:CA	2.69	0.50
1:A:327:ASN:OD1	1:A:360:ASP:OD1	2.30	0.50
1:B:366:LYS:HG2	1:B:367:LEU:H	1.74	0.50
1:B:367:LEU:HB2	1:B:413:THR:O	2.12	0.50
1:C:217:ASN:N	1:C:217:ASN:HD22	2.09	0.50
1:C:432:ASP:CB	1:C:464:ILE:CG2	2.90	0.50
1:D:352:ILE:CG1	1:D:388:VAL:HB	2.33	0.50
1:D:373:ASN:ND2	1:D:374:ASP:OD1	2.45	0.50
1:A:1:ASP:CA	1:B:24:ILE:HG21	2.32	0.49
1:A:426:LEU:HD13	1:A:426:LEU:C	2.37	0.49
1:B:11:GLU:OE2	1:B:69:GLU:OE1	2.30	0.49
1:B:347:ARG:HD2	1:B:392:GLY:N	2.25	0.49
1:B:449:ASP:CB	1:B:532:CYS:N	2.74	0.49
1:B:457:LEU:HD23	1:B:494:MET:SD	2.52	0.49
1:C:11:GLU:OE2	1:C:69:GLU:OE1	2.30	0.49
1:C:33:LYS:NZ	1:C:56:GLU:OE1	2.42	0.49
1:C:81:VAL:HB	1:D:43:ALA:H	1.76	0.49
1:C:327:ASN:OD1	1:C:360:ASP:OD1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ALA:CB	3:C:811:NDG:C6	2.90	0.49
1:D:367:LEU:HB2	1:D:413:THR:O	2.12	0.49
1:D:457:LEU:HD23	1:D:494:MET:SD	2.52	0.49
1:B:276:GLU:CG	1:B:277:SER:N	2.71	0.49
1:B:352:ILE:CG1	1:B:388:VAL:HB	2.34	0.49
1:B:426:LEU:HD13	1:B:426:LEU:C	2.37	0.49
1:C:373:ASN:ND2	1:C:374:ASP:OD1	2.45	0.49
1:C:426:LEU:HD13	1:C:426:LEU:C	2.37	0.49
1:D:154:ASP:O	2:D:801:NAG:C8	2.60	0.49
1:A:10:SER:CA	1:D:30:ARG:CD	2.89	0.49
1:B:33:LYS:HB3	1:B:83:GLU:CG	2.40	0.49
1:D:273:THR:H	2:D:803:NAG:HN2	1.60	0.49
1:D:335:ALA:CB	3:D:811:NDG:C6	2.90	0.49
1:D:419:VAL:HG22	2:D:809:NAG:H81	1.93	0.49
1:B:68:ARG:HD3	1:B:100:ASP:CA	2.43	0.49
1:B:234:GLU:HB2	1:B:235:ILE:HG22	1.92	0.49
1:B:396:ARG:CZ	1:B:432:ASP:HB2	2.41	0.49
1:C:68:ARG:HD3	1:C:100:ASP:CA	2.43	0.49
1:C:86:SER:N	1:D:74:TYR:CD2	2.73	0.49
1:C:151:LEU:HD12	1:C:151:LEU:H	1.77	0.49
1:C:336:VAL:CG1	1:C:338:ARG:HB2	2.43	0.49
1:C:367:LEU:HB2	1:C:413:THR:O	2.12	0.49
1:D:286:LYS:C	1:D:287:GLY:O	2.55	0.49
1:D:397:GLU:OE1	1:D:397:GLU:N	2.45	0.49
1:D:451:ASN:O	1:D:534:GLY:CA	2.60	0.49
1:A:252:THR:CG2	1:A:253:PRO:HD2	2.43	0.49
1:B:192:GLN:HA	1:B:203:VAL:O	2.13	0.49
1:C:109:THR:HG22	1:C:110:GLN:HG3	1.94	0.49
1:C:423:THR:HB	2:C:810:NAG:H83	1.94	0.49
1:D:68:ARG:HD3	1:D:100:ASP:CA	2.43	0.49
1:D:252:THR:CG2	1:D:253:PRO:HD2	2.43	0.49
1:A:87:PRO:O	1:B:2:TRP:CH2	2.66	0.49
1:A:217:ASN:N	1:A:217:ASN:HD22	2.09	0.49
1:A:272:THR:CG2	1:A:273:THR:N	2.76	0.49
1:B:109:THR:HG22	1:B:110:GLN:CG	2.42	0.49
1:B:224:LYS:HE3	2:B:806:NAG:H82	1.95	0.49
1:B:365:GLN:HA	1:B:416:GLY:HA3	1.95	0.49
1:B:382:ASN:OD1	1:B:385:ASN:N	2.45	0.49
1:D:224:LYS:HE3	2:D:806:NAG:H82	1.95	0.49
1:D:276:GLU:CG	1:D:277:SER:N	2.71	0.49
1:D:336:VAL:CG1	1:D:338:ARG:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:THR:HB	2:D:810:NAG:H83	1.94	0.49
1:A:373:ASN:ND2	1:A:374:ASP:OD1	2.45	0.49
1:A:415:ASP:CG	1:A:416:GLY:H	2.16	0.49
1:A:432:ASP:CB	1:A:464:ILE:CG2	2.89	0.49
1:A:457:LEU:HD23	1:A:494:MET:SD	2.52	0.49
1:B:151:LEU:HD12	1:B:151:LEU:H	1.77	0.49
1:B:261:ILE:HD11	1:B:264:ASN:HD22	1.77	0.49
1:B:276:GLU:HG3	1:B:277:SER:N	2.25	0.49
1:C:109:THR:HG22	1:C:110:GLN:CG	2.42	0.49
1:D:310:VAL:HG12	1:D:312:LEU:HG	1.95	0.49
1:A:89:GLU:OE1	1:B:2:TRP:CG	2.62	0.49
1:A:186:GLU:OE1	2:A:801:NAG:C6	2.59	0.49
1:B:365:GLN:O	1:B:365:GLN:CG	2.54	0.49
1:C:26:SER:HG	1:D:77:SER:CB	2.23	0.49
1:C:31:PHE:CD2	1:D:75:VAL:HG23	2.44	0.49
1:C:252:THR:CG2	1:C:253:PRO:HD2	2.43	0.49
1:C:281:ILE:HG23	1:C:281:ILE:O	2.13	0.49
1:C:468:THR:C	1:C:469:TYR:O	2.54	0.49
1:C:512:LEU:HD11	1:C:519:ASN:ND2	2.28	0.49
1:D:216:ASP:HB2	1:D:217:ASN:ND2	2.27	0.49
1:A:216:ASP:HB2	1:A:217:ASN:ND2	2.27	0.49
1:A:367:LEU:HD13	1:A:412:VAL:CG2	2.43	0.49
1:B:28:LYS:CD	1:B:88:VAL:HG12	2.38	0.49
1:B:109:THR:HG22	1:B:110:GLN:HG3	1.94	0.49
1:B:335:ALA:CB	3:B:811:NDG:C6	2.90	0.49
1:B:336:VAL:CG1	1:B:338:ARG:HB2	2.43	0.49
1:B:451:ASN:O	1:B:534:GLY:CA	2.60	0.49
1:C:282:LEU:CD2	1:C:283:THR:N	2.76	0.49
1:C:397:GLU:OE1	1:C:397:GLU:N	2.45	0.49
1:D:374:ASP:C	1:D:375:PRO:O	2.54	0.49
2:D:809:NAG:H62	2:D:810:NAG:O6	2.13	0.49
1:A:224:LYS:HE3	2:A:806:NAG:H82	1.95	0.49
1:A:261:ILE:HD11	1:A:264:ASN:HD22	1.77	0.49
1:A:365:GLN:HA	1:A:416:GLY:HA3	1.95	0.49
1:A:432:ASP:CB	1:A:464:ILE:HG21	2.43	0.49
1:B:31:PHE:O	1:C:29:ASP:C	2.56	0.49
1:B:87:PRO:HG2	1:C:2:TRP:CD1	2.47	0.49
1:B:154:ASP:O	2:B:801:NAG:C8	2.60	0.49
1:B:273:THR:H	2:B:803:NAG:HN2	1.60	0.49
1:C:310:VAL:HG12	1:C:312:LEU:HG	1.95	0.49
1:C:419:VAL:HG22	2:C:809:NAG:H81	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:ASP:CB	1:C:532:CYS:H	2.22	0.49
1:D:151:LEU:HD12	1:D:151:LEU:H	1.78	0.49
1:D:186:GLU:OE1	2:D:801:NAG:C6	2.59	0.49
1:D:250:PRO:O	1:D:255:TRP:CE3	2.66	0.49
1:D:449:ASP:CB	1:D:532:CYS:H	2.22	0.49
1:A:273:THR:H	2:A:803:NAG:HN2	1.60	0.48
1:B:32:ASN:HA	1:C:29:ASP:CG	2.36	0.48
1:B:67:ASP:OD2	1:B:69:GLU:HB2	2.13	0.48
1:B:84:ASN:O	1:C:24:ILE:CB	2.57	0.48
1:B:250:PRO:O	1:B:255:TRP:CE3	2.66	0.48
1:B:278:ASN:HD22	1:B:278:ASN:N	2.05	0.48
1:C:67:ASP:OD2	1:C:69:GLU:HB2	2.13	0.48
1:C:151:LEU:O	1:C:152:LYS:HB2	2.13	0.48
1:C:457:LEU:HD23	1:C:494:MET:SD	2.52	0.48
1:D:109:THR:HG22	1:D:110:GLN:HG3	1.94	0.48
1:D:432:ASP:CB	1:D:464:ILE:HG21	2.43	0.48
1:D:519:ASN:CG	1:D:519:ASN:O	2.55	0.48
1:A:28:LYS:CD	1:A:88:VAL:HG12	2.38	0.48
1:A:151:LEU:HD12	1:A:151:LEU:H	1.78	0.48
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.95	0.48
1:A:335:ALA:CB	3:A:811:NDG:C6	2.90	0.48
1:A:522:LEU:CD2	1:A:523:THR:HB	2.26	0.48
1:B:32:ASN:ND2	1:B:83:GLU:N	2.44	0.48
1:B:150:ILE:HD11	1:B:165:ILE:HB	1.96	0.48
1:B:241:ARG:NE	1:B:281:ILE:HD12	2.22	0.48
1:C:80:ALA:O	1:C:88:VAL:HG23	2.11	0.48
1:C:154:ASP:O	2:C:801:NAG:C8	2.60	0.48
1:C:432:ASP:CB	1:C:464:ILE:HG21	2.43	0.48
1:D:224:LYS:CE	2:D:806:NAG:C8	2.91	0.48
1:A:266:GLY:N	1:A:268:PHE:CE2	2.76	0.48
1:B:186:GLU:OE1	2:B:801:NAG:C6	2.59	0.48
1:B:482:THR:HG22	1:B:482:THR:O	2.09	0.48
1:C:192:GLN:HA	1:C:203:VAL:O	2.13	0.48
1:C:250:PRO:O	1:C:255:TRP:CE3	2.66	0.48
1:C:367:LEU:HD13	1:C:412:VAL:CG2	2.43	0.48
1:D:151:LEU:O	1:D:152:LYS:HB2	2.13	0.48
1:D:327:ASN:OD1	1:D:360:ASP:OD1	2.30	0.48
1:D:367:LEU:HD13	1:D:412:VAL:CG2	2.43	0.48
1:D:368:SER:OG	1:D:370:PHE:HE1	1.94	0.48
1:A:8:LYS:CB	1:D:30:ARG:HH21	2.26	0.48
1:A:192:GLN:HA	1:A:203:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LEU:HD11	1:A:519:ASN:ND2	2.28	0.48
1:B:119:GLU:OE2	1:B:216:ASP:OD1	2.32	0.48
1:B:272:THR:CG2	1:B:273:THR:N	2.76	0.48
1:B:512:LEU:HD11	1:B:519:ASN:ND2	2.28	0.48
2:B:809:NAG:C6	2:B:810:NAG:C6	2.92	0.48
1:C:32:ASN:HB3	1:D:75:VAL:HG23	1.94	0.48
1:C:374:ASP:C	1:C:375:PRO:O	2.54	0.48
1:D:468:THR:C	1:D:469:TYR:O	2.54	0.48
1:A:41:GLN:HA	1:A:45:ASN:HB2	1.95	0.48
1:A:109:THR:HG22	1:A:110:GLN:CG	2.42	0.48
1:A:468:THR:C	1:A:469:TYR:O	2.54	0.48
2:A:809:NAG:H62	2:A:810:NAG:O6	2.13	0.48
1:B:151:LEU:O	1:B:152:LYS:HB2	2.13	0.48
1:B:374:ASP:C	1:B:375:PRO:O	2.54	0.48
2:B:809:NAG:H62	2:B:810:NAG:O6	2.13	0.48
1:C:119:GLU:OE2	1:C:216:ASP:OD1	2.32	0.48
2:C:809:NAG:C6	2:C:810:NAG:C6	2.92	0.48
1:D:117:VAL:O	1:D:212:THR:N	2.46	0.48
1:D:448:CYS:SG	1:D:537:ILE:CG2	3.01	0.48
1:A:282:LEU:CD2	1:A:283:THR:N	2.76	0.48
1:A:483:TRP:CZ2	1:A:507:TYR:CE1	2.87	0.48
1:B:261:ILE:CD1	1:B:264:ASN:ND2	2.77	0.48
1:B:432:ASP:CB	1:B:464:ILE:HG21	2.43	0.48
1:C:276:GLU:CG	1:C:277:SER:N	2.71	0.48
1:D:192:GLN:HA	1:D:203:VAL:O	2.13	0.48
1:D:426:LEU:HD13	1:D:426:LEU:C	2.37	0.48
1:A:1:ASP:CG	1:A:2:TRP:N	2.70	0.48
1:A:10:SER:H	1:D:30:ARG:HG3	1.75	0.48
1:A:155:PRO:O	1:A:157:GLU:N	2.43	0.48
1:A:336:VAL:CG1	1:A:338:ARG:HB2	2.43	0.48
1:A:397:GLU:OE1	1:A:397:GLU:N	2.44	0.48
1:B:31:PHE:CG	1:C:30:ARG:N	2.57	0.48
1:B:241:ARG:HE	1:B:281:ILE:CD1	2.24	0.48
1:B:513:LEU:C	1:B:514:SER:HG	2.22	0.48
1:C:261:ILE:CD1	1:C:264:ASN:ND2	2.77	0.48
1:C:518:ASN:C	1:C:520:PRO:CD	2.87	0.48
1:A:5:PRO:N	1:B:91:PRO:CB	2.75	0.48
1:A:154:ASP:O	2:A:801:NAG:C8	2.60	0.48
1:A:367:LEU:HB2	1:A:413:THR:O	2.12	0.48
1:A:449:ASP:CB	1:A:532:CYS:H	2.22	0.48
1:B:252:THR:CG2	1:B:253:PRO:HD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ILE:HG23	1:B:281:ILE:O	2.13	0.48
1:B:397:GLU:N	1:B:397:GLU:OE1	2.45	0.48
1:C:224:LYS:HE3	2:C:806:NAG:H82	1.95	0.48
1:C:225:THR:HA	1:C:318:THR:O	2.14	0.48
1:A:225:THR:HA	1:A:318:THR:O	2.14	0.48
1:B:224:LYS:CE	2:B:806:NAG:C8	2.91	0.48
1:B:225:THR:HA	1:B:318:THR:O	2.14	0.48
1:B:282:LEU:CD2	1:B:283:THR:N	2.76	0.48
1:B:367:LEU:HD13	1:B:412:VAL:CG2	2.43	0.48
1:B:448:CYS:SG	1:B:537:ILE:CG2	3.01	0.48
1:B:537:ILE:CG1	1:B:538:LYS:N	2.77	0.48
1:C:1:ASP:CA	1:D:89:GLU:OE1	2.39	0.48
1:C:31:PHE:C	1:D:75:VAL:CG2	2.79	0.48
1:C:273:THR:H	2:C:803:NAG:HN2	1.60	0.48
1:C:418:SER:O	1:C:419:VAL:HG23	2.14	0.48
1:D:41:GLN:HA	1:D:45:ASN:HB2	1.95	0.48
1:D:119:GLU:OE2	1:D:216:ASP:OD1	2.32	0.48
1:C:41:GLN:HA	1:C:45:ASN:HB2	1.96	0.48
2:C:809:NAG:H62	2:C:810:NAG:O6	2.13	0.48
1:D:150:ILE:HD11	1:D:165:ILE:HB	1.96	0.48
1:D:241:ARG:HE	1:D:281:ILE:CD1	2.24	0.48
1:D:281:ILE:O	1:D:281:ILE:HG23	2.13	0.48
1:D:512:LEU:HD11	1:D:519:ASN:ND2	2.28	0.48
2:A:809:NAG:C6	2:A:810:NAG:C6	2.92	0.47
1:C:88:VAL:C	1:D:76:LEU:C	2.62	0.47
1:C:227:THR:CG2	2:C:807:NAG:H83	2.32	0.47
1:C:344:ASP:CG	1:C:344:ASP:O	2.57	0.47
1:D:225:THR:HA	1:D:318:THR:O	2.14	0.47
1:D:450:GLN:CG	1:D:533:GLU:OE2	2.58	0.47
1:A:67:ASP:OD2	1:A:69:GLU:HB2	2.13	0.47
1:A:151:LEU:O	1:A:152:LYS:HB2	2.13	0.47
1:A:224:LYS:CE	2:A:806:NAG:C8	2.91	0.47
1:A:268:PHE:CA	1:A:285:ALA:HB3	2.45	0.47
1:A:368:SER:OG	1:A:370:PHE:HE1	1.94	0.47
1:A:482:THR:HG22	1:A:482:THR:O	2.09	0.47
1:B:41:GLN:HA	1:B:45:ASN:HB2	1.95	0.47
1:C:76:LEU:O	1:C:94:ILE:N	2.44	0.47
1:C:150:ILE:HD11	1:C:165:ILE:HB	1.96	0.47
1:D:138:ASN:C	1:D:138:ASN:ND2	2.73	0.47
1:D:261:ILE:CD1	1:D:264:ASN:ND2	2.77	0.47
1:D:282:LEU:CD2	1:D:283:THR:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:GLN:HA	1:D:416:GLY:HA3	1.95	0.47
1:D:537:ILE:CG1	1:D:538:LYS:N	2.77	0.47
1:A:33:LYS:HB3	1:A:83:GLU:CG	2.40	0.47
1:A:138:ASN:C	1:A:138:ASN:ND2	2.73	0.47
1:A:150:ILE:HD11	1:A:165:ILE:HB	1.96	0.47
1:A:418:SER:O	1:A:419:VAL:HG23	2.14	0.47
1:A:518:ASN:C	1:A:520:PRO:CD	2.87	0.47
1:C:155:PRO:O	1:C:157:GLU:N	2.43	0.47
1:C:301:THR:CG2	1:C:316:THR:HG23	2.45	0.47
1:D:109:THR:HG22	1:D:110:GLN:CG	2.42	0.47
1:D:344:ASP:O	1:D:344:ASP:CG	2.57	0.47
1:D:514:SER:CA	1:D:517:GLN:O	2.62	0.47
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.32	0.47
1:A:344:ASP:O	1:A:344:ASP:CG	2.57	0.47
1:B:27:ASN:ND2	1:B:28:LYS:N	2.50	0.47
1:B:28:LYS:HG3	1:D:3:VAL:HG21	1.87	0.47
1:B:268:PHE:CA	1:B:285:ALA:HB3	2.45	0.47
1:C:32:ASN:CA	1:D:75:VAL:CG2	2.88	0.47
1:C:50:VAL:HB	1:C:51:PHE:CD1	2.50	0.47
1:C:226:TYR:O	1:C:227:THR:HG23	2.15	0.47
1:C:320:THR:CB	2:C:807:NAG:N2	2.78	0.47
1:C:365:GLN:HA	1:C:416:GLY:HA3	1.95	0.47
1:D:8:LYS:CD	1:D:8:LYS:N	2.51	0.47
1:D:67:ASP:OD2	1:D:69:GLU:HB2	2.13	0.47
1:A:250:PRO:O	1:A:255:TRP:CE3	2.67	0.47
1:A:450:GLN:CB	1:A:533:GLU:HA	2.29	0.47
1:A:514:SER:CA	1:A:517:GLN:O	2.62	0.47
1:A:519:ASN:CG	1:A:519:ASN:O	2.55	0.47
1:A:537:ILE:CG1	1:A:538:LYS:N	2.77	0.47
1:B:300:ILE:HD12	1:B:300:ILE:N	2.30	0.47
1:C:81:VAL:HG21	1:D:45:ASN:C	2.40	0.47
1:C:92:MET:HG3	1:D:79:HIS:ND1	2.29	0.47
1:C:224:LYS:CE	2:C:806:NAG:C8	2.91	0.47
1:C:449:ASP:CB	1:C:532:CYS:N	2.74	0.47
1:D:320:THR:CB	2:D:807:NAG:N2	2.78	0.47
1:D:518:ASN:C	1:D:520:PRO:CD	2.87	0.47
1:A:50:VAL:HB	1:A:51:PHE:CD1	2.50	0.47
1:A:261:ILE:CD1	1:A:264:ASN:ND2	2.77	0.47
1:B:33:LYS:N	1:C:25:LYS:NZ	2.61	0.47
1:B:226:TYR:O	1:B:227:THR:HG23	2.14	0.47
1:B:310:VAL:HG12	1:B:312:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:SER:O	1:B:419:VAL:HG23	2.14	0.47
1:C:36:TYR:O	1:C:55:TRP:HA	2.15	0.47
1:A:68:ARG:HD3	1:A:100:ASP:CA	2.43	0.47
1:B:468:THR:C	1:B:469:TYR:O	2.54	0.47
1:B:518:ASN:C	1:B:520:PRO:CD	2.87	0.47
1:B:519:ASN:O	1:B:519:ASN:CG	2.55	0.47
1:C:186:GLU:OE1	2:C:801:NAG:C6	2.59	0.47
1:C:440:PRO:HB3	1:C:457:LEU:CD2	2.43	0.47
1:D:448:CYS:C	1:D:452:PRO:HG3	2.40	0.47
2:D:809:NAG:C6	2:D:810:NAG:C6	2.92	0.47
1:A:90:GLU:CB	1:B:3:VAL:CG2	2.93	0.47
1:A:320:THR:CB	2:A:807:NAG:N2	2.78	0.47
1:B:50:VAL:HB	1:B:51:PHE:CD1	2.50	0.47
1:C:23:GLN:HB2	1:C:59:TRP:CE3	2.50	0.47
1:C:300:ILE:HD12	1:C:300:ILE:N	2.30	0.47
1:C:537:ILE:CG1	1:C:538:LYS:N	2.77	0.47
1:D:23:GLN:HB2	1:D:59:TRP:CE3	2.50	0.47
1:A:226:TYR:O	1:A:227:THR:HG23	2.15	0.47
1:A:281:ILE:HG23	1:A:281:ILE:O	2.13	0.47
1:A:301:THR:CG2	1:A:316:THR:HG23	2.45	0.47
1:B:271:ILE:O	1:B:271:ILE:HG23	2.15	0.47
1:B:539:CYS:HB3	1:B:540:GLN:H	1.46	0.47
1:C:67:ASP:CG	1:C:69:GLU:HB2	2.40	0.47
1:C:81:VAL:HG12	1:D:43:ALA:HB3	0.53	0.47
1:C:81:VAL:CG1	1:D:43:ALA:N	2.77	0.47
1:C:89:GLU:CD	1:D:92:MET:H	2.22	0.47
1:D:33:LYS:NZ	1:D:56:GLU:OE1	2.42	0.47
1:D:50:VAL:HB	1:D:51:PHE:CD1	2.50	0.47
1:A:8:LYS:HB3	1:D:30:ARG:HH21	1.79	0.47
1:A:23:GLN:HB2	1:A:59:TRP:CE3	2.50	0.47
1:A:108:PHE:HE1	1:A:203:VAL:HG23	1.80	0.47
1:B:88:VAL:CG1	1:C:27:ASN:OD1	2.60	0.47
1:B:320:THR:CB	2:B:807:NAG:N2	2.78	0.47
1:B:344:ASP:CG	1:B:344:ASP:O	2.57	0.47
1:C:82:SER:OG	1:D:41:GLN:O	2.12	0.47
1:C:272:THR:CG2	1:C:273:THR:N	2.76	0.47
1:C:514:SER:CA	1:C:517:GLN:O	2.62	0.47
1:D:67:ASP:CG	1:D:69:GLU:HB2	2.40	0.47
1:D:226:TYR:O	1:D:227:THR:HG23	2.15	0.47
1:D:418:SER:O	1:D:419:VAL:HG23	2.14	0.47
1:A:270:ASN:OD1	1:A:271:ILE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ILE:HD12	1:A:300:ILE:N	2.30	0.46
1:C:519:ASN:CG	1:C:519:ASN:O	2.55	0.46
1:D:268:PHE:CA	1:D:285:ALA:HB3	2.45	0.46
1:D:301:THR:CG2	1:D:316:THR:HG23	2.45	0.46
1:D:482:THR:HG22	1:D:499:THR:H	1.70	0.46
1:A:33:LYS:NZ	1:A:56:GLU:OE1	2.42	0.46
1:B:67:ASP:CG	1:B:69:GLU:HB2	2.40	0.46
1:B:155:PRO:O	1:B:157:GLU:N	2.43	0.46
1:B:310:VAL:HG12	1:B:311:PRO:O	2.15	0.46
1:B:408:VAL:O	1:B:426:LEU:N	2.48	0.46
1:C:3:VAL:HB	1:C:4:ILE:H	1.51	0.46
1:C:88:VAL:N	1:D:38:ILE:HG12	2.30	0.46
1:C:138:ASN:C	1:C:138:ASN:ND2	2.73	0.46
1:C:310:VAL:HG12	1:C:311:PRO:O	2.15	0.46
1:D:36:TYR:O	1:D:55:TRP:HA	2.15	0.46
1:D:272:THR:HG23	2:D:803:NAG:HN2	1.81	0.46
1:D:289:ASP:O	1:D:290:PHE:CB	2.25	0.46
1:D:300:ILE:HD12	1:D:300:ILE:N	2.29	0.46
1:D:363:GLN:O	1:D:364:ILE:CG2	2.63	0.46
1:A:227:THR:CG2	2:A:807:NAG:H83	2.32	0.46
1:A:271:ILE:HG23	1:A:271:ILE:O	2.15	0.46
1:A:449:ASP:N	1:A:532:CYS:HB3	2.19	0.46
1:B:23:GLN:HB2	1:B:59:TRP:CE3	2.50	0.46
1:B:31:PHE:CD2	1:C:29:ASP:OD2	2.69	0.46
1:B:301:THR:CG2	1:B:316:THR:HG23	2.45	0.46
1:C:1:ASP:CG	1:C:2:TRP:H	1.96	0.46
1:D:194:THR:CG2	1:D:195:ASP:N	2.79	0.46
1:A:194:THR:CG2	1:A:195:ASP:N	2.79	0.46
1:A:262:ARG:HG3	1:A:299:GLN:HB2	1.98	0.46
1:A:511:VAL:N	1:A:523:THR:O	2.46	0.46
1:B:368:SER:OG	1:B:370:PHE:HE1	1.94	0.46
1:A:67:ASP:CG	1:A:69:GLU:HB2	2.40	0.46
1:A:87:PRO:O	1:B:2:TRP:HZ2	1.83	0.46
1:A:227:THR:N	2:A:812:NAG:H2	2.31	0.46
1:A:506:ASP:OD1	1:A:506:ASP:N	2.49	0.46
1:B:36:TYR:O	1:B:55:TRP:HA	2.15	0.46
1:C:54:GLU:HB2	1:C:57:THR:OG1	2.16	0.46
1:C:81:VAL:H	1:D:45:ASN:ND2	2.10	0.46
1:C:108:PHE:HE1	1:C:203:VAL:HG23	1.80	0.46
1:C:262:ARG:HG3	1:C:299:GLN:HB2	1.97	0.46
1:C:539:CYS:HB3	1:C:540:GLN:H	1.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:GLU:HB2	1:D:57:THR:OG1	2.16	0.46
1:D:155:PRO:O	1:D:157:GLU:N	2.43	0.46
1:D:506:ASP:OD1	1:D:506:ASP:N	2.49	0.46
1:A:36:TYR:O	1:A:55:TRP:HA	2.15	0.46
1:A:310:VAL:HG12	1:A:311:PRO:O	2.15	0.46
1:A:440:PRO:HB3	1:A:457:LEU:CD2	2.43	0.46
2:A:809:NAG:H61	2:A:810:NAG:C6	2.39	0.46
1:C:459:ILE:HD12	1:C:459:ILE:N	2.31	0.46
1:D:310:VAL:HG12	1:D:311:PRO:O	2.15	0.46
1:D:459:ILE:N	1:D:459:ILE:HD12	2.31	0.46
1:A:8:LYS:HE2	1:D:28:LYS:HG3	1.94	0.46
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.16	0.46
1:A:79:HIS:CA	1:B:1:ASP:N	2.70	0.46
1:B:117:VAL:O	1:B:212:THR:N	2.46	0.46
1:B:155:PRO:CB	2:B:801:NAG:C8	2.94	0.46
1:B:194:THR:CG2	1:B:195:ASP:N	2.79	0.46
1:B:272:THR:HG23	2:B:803:NAG:HN2	1.80	0.46
1:B:459:ILE:HD12	1:B:459:ILE:N	2.31	0.46
1:C:3:VAL:HB	1:D:87:PRO:HB2	1.97	0.46
1:C:272:THR:HG23	2:C:803:NAG:HN2	1.80	0.46
1:C:421:THR:HG21	2:C:809:NAG:H61	1.98	0.46
1:D:187:TYR:HE1	1:D:211:ILE:HD11	1.81	0.46
1:D:374:ASP:N	1:D:374:ASP:OD1	2.49	0.46
1:B:109:THR:CB	1:B:131:SER:HB2	2.46	0.46
1:B:138:ASN:C	1:B:138:ASN:ND2	2.73	0.46
1:B:461:ASP:HB3	1:B:468:THR:CG2	2.46	0.46
1:B:514:SER:CA	1:B:517:GLN:O	2.62	0.46
1:C:100:ASP:OD1	1:C:101:GLN:N	2.49	0.46
1:C:194:THR:CG2	1:C:195:ASP:N	2.79	0.46
1:C:374:ASP:N	1:C:374:ASP:OD1	2.49	0.46
1:C:448:CYS:SG	1:C:537:ILE:CG2	3.01	0.46
1:D:100:ASP:OD1	1:D:101:GLN:N	2.49	0.46
1:D:339:VAL:HG11	1:D:351:ILE:HG23	1.98	0.46
1:A:4:ILE:HB	1:B:90:GLU:C	2.39	0.46
1:A:363:GLN:O	1:A:364:ILE:CG2	2.63	0.46
1:B:450:GLN:CB	1:B:533:GLU:HA	2.29	0.46
1:B:506:ASP:OD1	1:B:506:ASP:N	2.49	0.46
1:C:227:THR:N	2:C:812:NAG:H2	2.31	0.46
1:C:241:ARG:HE	1:C:281:ILE:CD1	2.24	0.46
1:C:408:VAL:O	1:C:426:LEU:N	2.49	0.46
1:D:270:ASN:OD1	1:D:271:ILE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:CG2	1:A:381:VAL:N	2.79	0.46
1:A:448:CYS:C	1:A:452:PRO:HG3	2.40	0.46
1:A:449:ASP:CB	1:A:532:CYS:N	2.74	0.46
1:B:100:ASP:OD1	1:B:101:GLN:N	2.49	0.46
1:B:227:THR:N	2:B:812:NAG:H2	2.31	0.46
1:B:363:GLN:O	1:B:364:ILE:CG2	2.63	0.46
1:B:380:THR:CG2	1:B:381:VAL:N	2.79	0.46
1:B:432:ASP:CG	1:B:433:VAL:N	2.74	0.46
1:C:1:ASP:CA	1:D:28:LYS:CD	2.88	0.46
1:C:276:GLU:HG3	1:C:277:SER:N	2.25	0.46
2:C:805:NAG:C5	2:C:806:NAG:H83	2.46	0.46
1:D:109:THR:CB	1:D:131:SER:HB2	2.46	0.46
1:D:290:PHE:CE2	1:D:293:ARG:CB	2.92	0.46
1:D:432:ASP:CG	1:D:433:VAL:N	2.74	0.46
1:D:524:VAL:HG21	2:D:904:NAG:C8	2.44	0.46
1:A:8:LYS:CD	1:A:8:LYS:N	2.51	0.45
1:A:432:ASP:CG	1:A:433:VAL:N	2.74	0.45
1:B:30:ARG:NH1	1:C:30:ARG:CB	2.78	0.45
1:B:33:LYS:NZ	1:B:56:GLU:OE1	2.42	0.45
1:B:262:ARG:HG3	1:B:299:GLN:HB2	1.98	0.45
1:B:374:ASP:N	1:B:374:ASP:OD1	2.49	0.45
1:B:473:VAL:CG2	1:B:487:LEU:HD21	2.47	0.45
1:C:32:ASN:CA	1:D:75:VAL:HG23	2.44	0.45
1:C:109:THR:CB	1:C:131:SER:HB2	2.46	0.45
1:C:227:THR:HG22	1:C:320:THR:HB	1.98	0.45
1:C:271:ILE:HG23	1:C:271:ILE:O	2.15	0.45
1:C:451:ASN:O	1:C:534:GLY:CA	2.60	0.45
1:D:227:THR:HG22	1:D:320:THR:HB	1.99	0.45
1:D:461:ASP:HB3	1:D:468:THR:CG2	2.46	0.45
2:D:805:NAG:C5	2:D:806:NAG:H83	2.46	0.45
1:A:117:VAL:O	1:A:212:THR:N	2.46	0.45
1:A:155:PRO:CB	2:A:801:NAG:C8	2.94	0.45
1:A:241:ARG:HE	1:A:281:ILE:CD1	2.24	0.45
1:A:276:GLU:HG3	1:A:277:SER:N	2.25	0.45
1:A:298:LEU:N	1:A:298:LEU:CD2	2.75	0.45
1:A:312:LEU:O	3:A:804:NDG:H8C1	2.17	0.45
1:A:373:ASN:CG	1:A:374:ASP:N	2.75	0.45
1:A:408:VAL:O	1:A:426:LEU:N	2.48	0.45
1:A:459:ILE:N	1:A:459:ILE:HD12	2.31	0.45
1:B:227:THR:HG22	1:B:320:THR:HB	1.98	0.45
1:B:381:VAL:HA	1:B:387:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ASP:O	1:D:28:LYS:HD3	2.16	0.45
1:C:28:LYS:CG	1:D:93:GLU:HG2	2.11	0.45
1:C:268:PHE:CA	1:C:285:ALA:HB3	2.45	0.45
1:C:371:ILE:HD12	1:C:371:ILE:HA	1.65	0.45
1:C:432:ASP:CG	1:C:433:VAL:N	2.74	0.45
1:C:450:GLN:CB	1:C:533:GLU:OE2	2.64	0.45
1:D:108:PHE:HE1	1:D:203:VAL:HG23	1.80	0.45
1:D:271:ILE:HG23	1:D:271:ILE:O	2.15	0.45
1:D:408:VAL:O	1:D:426:LEU:N	2.49	0.45
1:A:421:THR:HG21	2:A:809:NAG:H61	1.98	0.45
1:B:85:GLY:N	1:C:25:LYS:O	2.47	0.45
1:B:261:ILE:HD11	1:B:264:ASN:ND2	2.32	0.45
1:C:506:ASP:OD1	1:C:506:ASP:N	2.49	0.45
1:D:152:LYS:O	1:D:189:LEU:HA	2.17	0.45
1:D:473:VAL:CG2	1:D:487:LEU:HD21	2.47	0.45
1:A:374:ASP:N	1:A:374:ASP:OD1	2.49	0.45
1:A:381:VAL:HA	1:A:387:ILE:O	2.17	0.45
1:B:8:LYS:CD	1:B:8:LYS:N	2.51	0.45
1:B:187:TYR:HE1	1:B:211:ILE:HD11	1.81	0.45
1:B:270:ASN:OD1	1:B:271:ILE:N	2.49	0.45
1:B:373:ASN:CG	1:B:374:ASP:N	2.75	0.45
1:B:400:TYR:O	1:B:401:VAL:C	2.59	0.45
1:B:450:GLN:CB	1:B:533:GLU:OE2	2.64	0.45
1:C:187:TYR:HE1	1:C:211:ILE:HD11	1.81	0.45
1:D:381:VAL:HA	1:D:387:ILE:O	2.17	0.45
1:D:440:PRO:HB3	1:D:457:LEU:CD2	2.43	0.45
1:A:187:TYR:HE1	1:A:211:ILE:HD11	1.81	0.45
1:A:336:VAL:HG11	1:A:338:ARG:HD2	1.99	0.45
1:A:380:THR:HG22	1:A:381:VAL:N	2.32	0.45
1:B:152:LYS:O	1:B:189:LEU:HA	2.17	0.45
1:B:421:THR:HG21	2:B:809:NAG:H61	1.98	0.45
1:B:524:VAL:HG21	2:B:904:NAG:C8	2.44	0.45
1:C:93:GLU:CB	1:D:81:VAL:CG1	2.79	0.45
1:C:373:ASN:CG	1:C:374:ASP:N	2.75	0.45
1:C:400:TYR:O	1:C:401:VAL:C	2.59	0.45
1:D:266:GLY:N	1:D:268:PHE:CE2	2.76	0.45
1:D:421:THR:HG21	2:D:809:NAG:H61	1.98	0.45
1:A:100:ASP:OD1	1:A:101:GLN:N	2.49	0.45
1:A:261:ILE:HD11	1:A:264:ASN:ND2	2.32	0.45
1:A:339:VAL:HG11	1:A:351:ILE:HG23	1.98	0.45
1:A:367:LEU:H	1:A:367:LEU:HG	1.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ASN:O	1:A:534:GLY:CA	2.60	0.45
1:A:461:ASP:HB3	1:A:468:THR:CG2	2.46	0.45
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.50	0.45
2:A:805:NAG:C5	2:A:806:NAG:H83	2.46	0.45
1:B:1:ASP:CG	1:B:2:TRP:N	2.70	0.45
1:B:371:ILE:HD12	1:B:371:ILE:HA	1.65	0.45
1:B:469:TYR:CD2	1:B:470:PRO:N	2.85	0.45
1:C:84:ASN:C	1:D:74:TYR:CZ	2.90	0.45
1:C:339:VAL:HG11	1:C:351:ILE:HG23	1.98	0.45
1:C:381:VAL:HA	1:C:387:ILE:O	2.17	0.45
1:C:449:ASP:N	1:C:532:CYS:HB3	2.19	0.45
1:C:461:ASP:HB3	1:C:468:THR:CG2	2.46	0.45
1:D:449:ASP:CB	1:D:532:CYS:N	2.74	0.45
1:B:187:TYR:CE1	1:B:211:ILE:HD11	2.52	0.45
1:B:482:THR:O	1:B:483:TRP:CD2	2.70	0.45
2:B:805:NAG:H62	2:B:806:NAG:N2	2.31	0.45
1:C:298:LEU:N	1:C:298:LEU:CD2	2.75	0.45
1:C:371:ILE:HD13	1:C:381:VAL:HG11	1.95	0.45
1:C:396:ARG:HH21	1:C:432:ASP:CG	2.25	0.45
1:C:519:ASN:O	1:C:520:PRO:C	2.59	0.45
1:D:336:VAL:HG11	1:D:338:ARG:HD2	1.99	0.45
1:D:450:GLN:CB	1:D:533:GLU:OE2	2.64	0.45
1:A:272:THR:HG23	2:A:803:NAG:HN2	1.80	0.45
1:A:396:ARG:HH21	1:A:432:ASP:CG	2.25	0.45
1:A:448:CYS:SG	1:A:537:ILE:CG2	3.01	0.45
1:A:482:THR:O	1:A:483:TRP:CD2	2.70	0.45
1:B:54:GLU:HB2	1:B:57:THR:OG1	2.16	0.45
1:B:128:MET:HB3	1:B:129:ALA:H	1.62	0.45
1:B:134:ASP:HB2	1:B:146:LEU:HD11	1.99	0.45
1:B:162:LEU:HB2	1:B:163:PHE:CE1	2.52	0.45
1:B:312:LEU:O	3:B:804:NDG:H8C1	2.17	0.45
1:C:117:VAL:O	1:C:212:THR:N	2.46	0.45
1:C:187:TYR:CE1	1:C:211:ILE:HD11	2.52	0.45
1:C:336:VAL:HG11	1:C:338:ARG:HD2	1.99	0.45
1:D:109:THR:HB	1:D:131:SER:HB2	1.99	0.45
1:D:162:LEU:HB2	1:D:163:PHE:CE1	2.52	0.45
1:A:1:ASP:OD1	1:B:24:ILE:HB	2.17	0.45
1:A:232:GLU:HA	1:A:288:LEU:HD12	1.99	0.45
1:A:450:GLN:CB	1:A:533:GLU:OE2	2.64	0.45
1:A:469:TYR:CE2	1:A:470:PRO:HB2	2.52	0.45
1:B:380:THR:HG22	1:B:381:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:SER:O	1:D:39:THR:HG21	2.17	0.45
1:D:262:ARG:HG3	1:D:299:GLN:HB2	1.97	0.45
1:D:482:THR:O	1:D:483:TRP:CD2	2.70	0.45
1:A:162:LEU:HB2	1:A:163:PHE:CE1	2.52	0.45
1:A:473:VAL:CG2	1:A:487:LEU:HD21	2.47	0.45
1:A:485:ALA:O	1:A:486:GLU:OE1	2.35	0.45
1:B:108:PHE:HE1	1:B:203:VAL:HG23	1.80	0.45
1:C:31:PHE:O	1:D:73:LYS:NZ	2.47	0.45
1:C:134:ASP:HB2	1:C:146:LEU:HD11	1.99	0.45
1:C:270:ASN:OD1	1:C:271:ILE:N	2.49	0.45
1:C:380:THR:HG22	1:C:381:VAL:N	2.32	0.45
1:D:187:TYR:CE1	1:D:211:ILE:HD11	2.52	0.45
1:D:396:ARG:HH21	1:D:432:ASP:CG	2.25	0.45
1:D:469:TYR:CD2	1:D:470:PRO:N	2.85	0.45
1:D:485:ALA:O	1:D:486:GLU:OE1	2.35	0.45
1:A:36:TYR:CE2	1:D:2:TRP:CH2	3.00	0.44
1:A:109:THR:CB	1:A:131:SER:HB2	2.46	0.44
1:B:441:SER:CB	1:B:442:PRO:HD3	2.47	0.44
1:C:3:VAL:CB	1:D:87:PRO:HB2	2.47	0.44
1:C:79:HIS:HB3	1:D:39:THR:HB	1.96	0.44
1:C:109:THR:HB	1:C:131:SER:HB2	1.99	0.44
1:C:403:ASN:C	1:C:405:THR:N	2.76	0.44
1:C:448:CYS:C	1:C:452:PRO:HG3	2.40	0.44
1:D:227:THR:N	2:D:812:NAG:H2	2.31	0.44
1:B:30:ARG:CZ	1:C:30:ARG:HB3	2.47	0.44
1:B:31:PHE:CE1	1:D:75:VAL:HG12	2.38	0.44
1:C:482:THR:O	1:C:483:TRP:CD2	2.70	0.44
1:A:109:THR:HB	1:A:131:SER:HB2	1.99	0.44
1:A:134:ASP:HB2	1:A:146:LEU:HD11	1.99	0.44
1:B:31:PHE:CD2	1:B:31:PHE:C	2.95	0.44
1:B:339:VAL:HG11	1:B:351:ILE:HG23	1.98	0.44
1:B:396:ARG:HH21	1:B:432:ASP:CG	2.25	0.44
1:C:469:TYR:CE2	1:C:470:PRO:HB2	2.52	0.44
1:C:473:VAL:CG2	1:C:487:LEU:HD21	2.47	0.44
1:D:312:LEU:O	3:D:804:NDG:H8C1	2.17	0.44
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.44
1:A:469:TYR:CD2	1:A:470:PRO:N	2.85	0.44
1:B:336:VAL:HG11	1:B:338:ARG:HD2	1.99	0.44
1:B:439:VAL:HA	1:B:440:PRO:HD3	1.81	0.44
1:C:461:ASP:HB3	1:C:468:THR:HG22	2.00	0.44
1:D:250:PRO:C	1:D:252:THR:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:SER:HA	1:A:87:PRO:HD3	1.83	0.44
1:A:152:LYS:O	1:A:189:LEU:HA	2.17	0.44
1:A:224:LYS:HE3	2:A:806:NAG:C8	2.48	0.44
1:B:224:LYS:HE3	2:B:806:NAG:C8	2.48	0.44
1:B:442:PRO:HD2	1:B:457:LEU:HD12	2.00	0.44
2:B:805:NAG:C5	2:B:806:NAG:H83	2.46	0.44
1:C:261:ILE:HD11	1:C:264:ASN:ND2	2.32	0.44
1:D:28:LYS:CD	1:D:88:VAL:HG12	2.38	0.44
1:D:511:VAL:N	1:D:523:THR:O	2.46	0.44
1:A:22:VAL:CG2	1:A:23:GLN:N	2.81	0.44
1:A:252:THR:HA	1:A:253:PRO:HD3	1.81	0.44
1:A:441:SER:CB	1:A:442:PRO:HD3	2.47	0.44
1:B:485:ALA:O	1:B:486:GLU:OE1	2.35	0.44
1:C:85:GLY:CA	1:D:47:PRO:HD2	2.48	0.44
1:C:181:ARG:NH1	1:C:249:MET:HE3	2.33	0.44
1:D:67:ASP:OD1	1:D:69:GLU:HB2	2.18	0.44
1:D:224:LYS:HE3	2:D:806:NAG:C8	2.48	0.44
1:D:232:GLU:HA	1:D:288:LEU:HD12	1.99	0.44
1:D:380:THR:CG2	1:D:381:VAL:N	2.79	0.44
1:A:489:SER:C	1:A:491:GLY:H	2.26	0.44
1:B:194:THR:HG23	1:B:201:LEU:O	2.18	0.44
1:B:290:PHE:CD2	1:B:293:ARG:O	2.71	0.44
1:B:320:THR:CG2	2:B:807:NAG:C2	2.76	0.44
1:C:22:VAL:CG2	1:C:23:GLN:N	2.81	0.44
1:C:67:ASP:OD1	1:C:69:GLU:HB2	2.18	0.44
1:C:152:LYS:O	1:C:189:LEU:HA	2.17	0.44
1:C:220:ILE:O	1:C:220:ILE:HG22	2.18	0.44
1:C:489:SER:C	1:C:491:GLY:H	2.26	0.44
1:D:290:PHE:CD2	1:D:293:ARG:O	2.71	0.44
1:D:421:THR:CG2	1:D:422:GLY:N	2.81	0.44
1:A:227:THR:HG22	1:A:320:THR:HB	1.98	0.44
1:A:442:PRO:HD2	1:A:457:LEU:HD12	2.00	0.44
1:A:524:VAL:HG21	2:A:904:NAG:C8	2.44	0.44
1:B:448:CYS:C	1:B:452:PRO:HG3	2.40	0.44
1:C:88:VAL:HA	1:D:38:ILE:HD11	1.99	0.44
1:C:90:GLU:CD	1:D:53:ILE:CG2	2.68	0.44
1:C:250:PRO:C	1:C:252:THR:H	2.26	0.44
1:C:380:THR:CG2	1:C:381:VAL:N	2.79	0.44
1:D:155:PRO:CB	2:D:801:NAG:C8	2.94	0.44
1:D:261:ILE:HD11	1:D:264:ASN:ND2	2.32	0.44
1:D:435:ASP:HB2	1:D:436:ASN:H	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:VAL:HG21	1:B:77:SER:HA	2.00	0.44
1:A:92:MET:HB2	1:B:1:ASP:CB	2.48	0.44
1:A:290:PHE:CD2	1:A:293:ARG:O	2.71	0.44
1:B:22:VAL:CG2	1:B:23:GLN:N	2.81	0.44
1:B:368:SER:CB	1:B:370:PHE:HE1	2.31	0.44
1:B:469:TYR:CE2	1:B:470:PRO:HB2	2.52	0.44
1:C:32:ASN:HD22	1:C:83:GLU:N	2.13	0.44
1:C:90:GLU:CD	1:D:36:TYR:CB	2.90	0.44
1:C:151:LEU:HD12	1:C:151:LEU:N	2.33	0.44
1:C:162:LEU:HB2	1:C:163:PHE:CE1	2.52	0.44
1:A:419:VAL:HG13	1:A:420:GLY:N	2.33	0.43
1:B:3:VAL:HB	1:B:4:ILE:H	1.51	0.43
1:B:109:THR:HB	1:B:131:SER:HB2	1.99	0.43
1:B:151:LEU:HD12	1:B:151:LEU:N	2.33	0.43
1:B:421:THR:CG2	1:B:422:GLY:N	2.81	0.43
1:B:522:LEU:HA	1:B:522:LEU:HD23	1.36	0.43
1:C:78:SER:C	1:D:39:THR:HG21	2.43	0.43
1:C:82:SER:HB3	1:D:75:VAL:C	2.43	0.43
1:C:363:GLN:O	1:C:364:ILE:CG2	2.63	0.43
1:C:469:TYR:CD2	1:C:470:PRO:N	2.85	0.43
1:C:485:ALA:O	1:C:486:GLU:OE1	2.35	0.43
1:D:31:PHE:CD2	1:D:31:PHE:C	2.95	0.43
1:D:469:TYR:CE2	1:D:470:PRO:HB2	2.52	0.43
1:A:8:LYS:CB	1:D:30:ARG:HE	2.30	0.43
1:A:92:MET:CG	1:B:3:VAL:HG12	2.47	0.43
1:A:181:ARG:NH1	1:A:249:MET:HE3	2.33	0.43
1:A:421:THR:CG2	1:A:422:GLY:N	2.81	0.43
1:A:519:ASN:O	1:A:520:PRO:C	2.59	0.43
1:B:419:VAL:HG13	1:B:420:GLY:N	2.33	0.43
1:B:482:THR:C	1:B:483:TRP:CG	2.96	0.43
1:C:312:LEU:O	3:C:804:NDG:H8C1	2.17	0.43
1:D:220:ILE:O	1:D:220:ILE:HG22	2.18	0.43
1:D:403:ASN:C	1:D:405:THR:N	2.76	0.43
2:D:805:NAG:H62	2:D:806:NAG:N2	2.31	0.43
1:A:299:GLN:CG	1:A:318:THR:HG23	2.42	0.43
1:A:335:ALA:HB3	3:A:811:NDG:O6	2.15	0.43
1:A:385:ASN:O	1:A:386:GLY:C	2.62	0.43
1:B:232:GLU:HA	1:B:288:LEU:HD12	2.00	0.43
1:B:450:GLN:HG3	1:B:532:CYS:O	2.10	0.43
1:C:89:GLU:HB3	1:D:78:SER:O	2.01	0.43
1:C:232:GLU:HA	1:C:288:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:VAL:N	1:C:523:THR:O	2.46	0.43
1:D:441:SER:CB	1:D:442:PRO:HD3	2.47	0.43
1:A:194:THR:HG23	1:A:201:LEU:O	2.18	0.43
1:A:247:LEU:HD12	1:A:247:LEU:N	2.33	0.43
1:A:400:TYR:O	1:A:401:VAL:C	2.59	0.43
1:A:482:THR:C	1:A:483:TRP:CG	2.96	0.43
1:B:252:THR:HA	1:B:253:PRO:HD3	1.81	0.43
1:B:297:VAL:HG21	2:B:807:NAG:H62	2.01	0.43
1:C:128:MET:HB3	1:C:129:ALA:H	1.62	0.43
1:C:289:ASP:C	1:C:290:PHE:CD1	2.97	0.43
1:C:290:PHE:CD2	1:C:293:ARG:O	2.71	0.43
1:C:385:ASN:O	1:C:386:GLY:C	2.62	0.43
1:C:441:SER:CB	1:C:442:PRO:HD3	2.47	0.43
1:D:128:MET:HB3	1:D:129:ALA:H	1.62	0.43
1:A:187:TYR:CE1	1:A:211:ILE:HD11	2.52	0.43
1:A:368:SER:CB	1:A:370:PHE:HE1	2.31	0.43
1:C:224:LYS:HE3	2:C:806:NAG:C8	2.48	0.43
1:C:442:PRO:HD2	1:C:457:LEU:HD12	2.00	0.43
1:C:458:THR:C	1:C:459:ILE:HD12	2.44	0.43
1:C:482:THR:C	1:C:483:TRP:CG	2.96	0.43
1:D:247:LEU:HD12	1:D:247:LEU:N	2.33	0.43
1:D:380:THR:HG22	1:D:381:VAL:N	2.32	0.43
1:D:419:VAL:HG13	1:D:420:GLY:N	2.33	0.43
1:D:458:THR:C	1:D:459:ILE:HD12	2.44	0.43
1:D:461:ASP:HB3	1:D:468:THR:HG22	2.00	0.43
1:A:4:ILE:HB	1:B:90:GLU:HB3	1.48	0.43
1:B:354:LEU:HD12	1:B:386:GLY:O	2.18	0.43
1:C:421:THR:CG2	1:C:422:GLY:N	2.81	0.43
1:D:3:VAL:HB	1:D:4:ILE:H	1.51	0.43
1:D:181:ARG:NH1	1:D:249:MET:HE3	2.33	0.43
1:D:194:THR:HG23	1:D:201:LEU:O	2.18	0.43
1:D:249:MET:HA	1:D:250:PRO:HD3	1.85	0.43
1:D:289:ASP:C	1:D:290:PHE:CD1	2.97	0.43
1:D:335:ALA:HB3	3:D:811:NDG:O6	2.15	0.43
1:D:368:SER:CB	1:D:370:PHE:HE1	2.31	0.43
1:D:442:PRO:HD2	1:D:457:LEU:HD12	2.00	0.43
1:A:250:PRO:C	1:A:252:THR:H	2.26	0.43
1:B:83:GLU:HB3	1:C:25:LYS:HB2	1.45	0.43
1:B:333:VAL:HG23	1:B:334:PRO:HD3	2.01	0.43
1:B:458:THR:C	1:B:459:ILE:HD12	2.44	0.43
1:C:155:PRO:CB	2:C:801:NAG:C8	2.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:ASP:HB2	1:D:146:LEU:HD11	1.99	0.43
1:D:450:GLN:HG3	1:D:532:CYS:O	2.10	0.43
1:D:482:THR:C	1:D:483:TRP:CG	2.96	0.43
1:A:1:ASP:CA	1:B:24:ILE:CD1	2.95	0.43
1:A:9:VAL:O	1:D:30:ARG:CD	2.62	0.43
1:A:32:ASN:HD22	1:A:83:GLU:N	2.13	0.43
1:A:79:HIS:CA	1:B:1:ASP:H1	2.30	0.43
1:A:90:GLU:O	1:B:1:ASP:C	2.62	0.43
1:A:195:ASP:HB3	1:A:196:LEU:HG	2.01	0.43
1:B:343:GLU:CD	1:B:395:ASP:HA	2.44	0.43
1:C:154:ASP:HB3	2:C:801:NAG:C7	2.48	0.43
1:C:194:THR:HG23	1:C:201:LEU:O	2.18	0.43
1:D:22:VAL:CG2	1:D:23:GLN:N	2.81	0.43
1:D:32:ASN:HD22	1:D:83:GLU:N	2.13	0.43
1:D:175:ILE:CG2	1:D:176:GLY:N	2.82	0.43
1:A:297:VAL:HG21	2:A:807:NAG:H62	2.01	0.43
1:A:333:VAL:HG23	1:A:334:PRO:HD3	2.01	0.43
1:A:354:LEU:HD12	1:A:386:GLY:O	2.18	0.43
1:B:67:ASP:OD1	1:B:69:GLU:HB2	2.18	0.43
1:B:181:ARG:NH1	1:B:249:MET:HE3	2.33	0.43
1:B:247:LEU:HD12	1:B:247:LEU:N	2.33	0.43
1:B:385:ASN:O	1:B:386:GLY:C	2.62	0.43
1:B:489:SER:C	1:B:491:GLY:H	2.26	0.43
1:C:40:GLY:O	1:C:45:ASN:HB2	2.19	0.43
1:C:354:LEU:HD12	1:C:386:GLY:O	2.18	0.43
1:C:368:SER:CB	1:C:370:PHE:HE1	2.31	0.43
1:D:367:LEU:H	1:D:367:LEU:HG	1.41	0.43
1:D:371:ILE:HG13	1:D:410:MET:SD	2.59	0.43
1:D:489:SER:C	1:D:491:GLY:H	2.26	0.43
1:A:24:ILE:O	1:D:2:TRP:CH2	2.58	0.43
1:A:289:ASP:C	1:A:290:PHE:CD1	2.97	0.43
1:B:232:GLU:CG	1:B:289:ASP:C	2.92	0.43
1:B:289:ASP:C	1:B:290:PHE:CD1	2.97	0.43
1:B:371:ILE:HG13	1:B:410:MET:SD	2.59	0.43
1:C:343:GLU:CD	1:C:395:ASP:HA	2.44	0.43
1:D:343:GLU:CD	1:D:395:ASP:HA	2.44	0.43
1:D:354:LEU:HD12	1:D:386:GLY:O	2.18	0.43
1:A:188:THR:H	2:A:801:NAG:H83	1.84	0.42
1:A:409:ILE:HD13	3:A:811:NDG:H8C3	2.01	0.42
1:B:220:ILE:O	1:B:220:ILE:HG22	2.18	0.42
1:B:250:PRO:C	1:B:252:THR:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:VAL:HG23	1:C:334:PRO:HD3	2.01	0.42
1:C:524:VAL:HG21	2:C:904:NAG:C8	2.44	0.42
1:D:298:LEU:N	1:D:298:LEU:CD2	2.75	0.42
1:D:339:VAL:HG21	1:D:351:ILE:HG22	2.01	0.42
1:A:90:GLU:O	1:A:91:PRO:O	2.37	0.42
1:A:226:TYR:C	1:A:227:THR:CG2	2.92	0.42
1:A:230:VAL:O	1:A:323:VAL:HA	2.20	0.42
1:A:461:ASP:HB3	1:A:468:THR:HG22	2.00	0.42
1:B:435:ASP:HB2	1:B:436:ASN:H	1.58	0.42
1:B:461:ASP:HB3	1:B:468:THR:HG22	2.00	0.42
1:C:261:ILE:H	1:C:261:ILE:HD13	1.85	0.42
1:C:277:SER:O	1:C:278:ASN:C	2.62	0.42
1:C:490:LYS:O	1:C:490:LYS:CG	2.67	0.42
1:A:343:GLU:CD	1:A:395:ASP:HA	2.44	0.42
1:A:371:ILE:HG13	1:A:410:MET:SD	2.59	0.42
1:B:175:ILE:CG2	1:B:176:GLY:N	2.82	0.42
1:C:4:ILE:HA	1:C:5:PRO:HD3	1.72	0.42
1:C:88:VAL:C	1:D:38:ILE:CD1	2.92	0.42
1:C:450:GLN:HG3	1:C:532:CYS:O	2.10	0.42
1:D:232:GLU:CG	1:D:289:ASP:C	2.92	0.42
1:D:277:SER:O	1:D:278:ASN:C	2.62	0.42
1:D:400:TYR:O	1:D:401:VAL:C	2.59	0.42
1:A:92:MET:HG2	1:B:3:VAL:HG12	2.01	0.42
1:A:151:LEU:HD12	1:A:151:LEU:N	2.33	0.42
1:A:347:ARG:HD2	1:A:392:GLY:CA	2.50	0.42
1:A:403:ASN:C	1:A:405:THR:N	2.75	0.42
1:B:40:GLY:O	1:B:45:ASN:HB2	2.19	0.42
1:B:226:TYR:C	1:B:227:THR:CG2	2.93	0.42
1:B:277:SER:O	1:B:278:ASN:C	2.62	0.42
1:B:409:ILE:HD13	3:B:811:NDG:H8C3	2.01	0.42
1:C:5:PRO:HA	1:C:6:PRO:HD3	1.85	0.42
1:C:88:VAL:O	1:D:94:ILE:CD1	2.50	0.42
1:C:247:LEU:HD12	1:C:247:LEU:N	2.33	0.42
1:C:371:ILE:HA	1:C:410:MET:HB3	2.02	0.42
1:C:515:ASP:OD1	1:C:516:ALA:N	2.53	0.42
1:D:333:VAL:HG23	1:D:334:PRO:HD3	2.01	0.42
1:D:409:ILE:HD13	3:D:811:NDG:H8C3	2.01	0.42
1:A:5:PRO:HA	1:A:6:PRO:HD3	1.85	0.42
1:A:175:ILE:CG2	1:A:176:GLY:N	2.82	0.42
1:A:239:VAL:HG11	1:A:282:LEU:HD22	2.02	0.42
1:A:250:PRO:HA	1:A:255:TRP:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:VAL:N	1:D:38:ILE:CG1	2.82	0.42
1:C:232:GLU:CG	1:C:289:ASP:C	2.92	0.42
1:C:339:VAL:HG21	1:C:351:ILE:HG22	2.01	0.42
1:D:347:ARG:HD2	1:D:392:GLY:CA	2.49	0.42
1:D:482:THR:HG23	1:D:499:THR:HG23	1.88	0.42
1:A:220:ILE:O	1:A:220:ILE:HG22	2.18	0.42
2:A:805:NAG:H62	2:A:806:NAG:N2	2.31	0.42
1:B:339:VAL:HG21	1:B:351:ILE:HG22	2.01	0.42
1:B:469:TYR:CE2	1:B:470:PRO:HD2	2.54	0.42
1:C:35:TYR:HB3	1:D:45:ASN:CG	2.44	0.42
1:C:226:TYR:C	1:C:227:THR:CG2	2.92	0.42
1:C:252:THR:HA	1:C:253:PRO:HD3	1.81	0.42
1:D:195:ASP:HB3	1:D:196:LEU:HG	2.01	0.42
1:D:261:ILE:HD13	1:D:261:ILE:H	1.85	0.42
1:D:264:ASN:HB3	1:D:267:GLY:HA2	2.01	0.42
1:D:469:TYR:CE2	1:D:470:PRO:HD2	2.54	0.42
1:A:232:GLU:CG	1:A:289:ASP:C	2.92	0.42
1:A:505:GLY:H	1:A:529:VAL:HB	1.85	0.42
1:B:31:PHE:CD2	1:C:29:ASP:CG	2.98	0.42
1:B:502:LEU:HA	1:B:502:LEU:HD23	1.82	0.42
1:C:83:GLU:CA	1:D:41:GLN:OE1	2.59	0.42
1:C:175:ILE:CG2	1:C:176:GLY:N	2.82	0.42
1:C:367:LEU:H	1:C:367:LEU:HG	1.41	0.42
1:D:7:ILE:O	1:D:96:ILE:HG23	2.20	0.42
1:D:188:THR:H	2:D:801:NAG:H83	1.84	0.42
1:D:250:PRO:HA	1:D:255:TRP:CG	2.54	0.42
1:D:297:VAL:HG21	2:D:807:NAG:H62	2.01	0.42
1:A:108:PHE:HA	1:A:132:ALA:CB	2.50	0.42
1:A:264:ASN:HB3	1:A:267:GLY:HA2	2.01	0.42
1:B:84:ASN:O	1:C:24:ILE:CA	2.68	0.42
1:B:87:PRO:HG2	1:D:90:GLU:H	1.82	0.42
1:B:87:PRO:CG	1:C:2:TRP:CB	2.94	0.42
1:B:108:PHE:HA	1:B:132:ALA:CB	2.50	0.42
1:B:188:THR:H	2:B:801:NAG:H83	1.84	0.42
1:B:230:VAL:O	1:B:323:VAL:HA	2.20	0.42
1:B:298:LEU:N	1:B:298:LEU:CD2	2.75	0.42
1:C:239:VAL:HG11	1:C:282:LEU:HD22	2.02	0.42
1:C:371:ILE:HG13	1:C:410:MET:SD	2.59	0.42
1:D:151:LEU:HD12	1:D:151:LEU:N	2.33	0.42
1:D:373:ASN:CG	1:D:374:ASP:N	2.75	0.42
1:D:483:TRP:CZ2	1:D:507:TYR:CE1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:PRO:CG	1:C:2:TRP:CD1	3.03	0.42
1:C:7:ILE:O	1:C:96:ILE:HG23	2.20	0.42
1:C:188:THR:H	2:C:801:NAG:H83	1.84	0.42
1:C:347:ARG:HD2	1:C:392:GLY:CA	2.50	0.42
1:C:409:ILE:HD13	3:C:811:NDG:H8C3	2.01	0.42
1:D:226:TYR:C	1:D:227:THR:CG2	2.93	0.42
1:D:231:PRO:O	1:D:288:LEU:HD12	2.20	0.42
1:B:31:PHE:CE2	1:C:27:ASN:N	2.78	0.42
1:B:195:ASP:HB3	1:B:196:LEU:HG	2.01	0.42
1:B:264:ASN:HB3	1:B:267:GLY:HA2	2.01	0.42
1:B:335:ALA:HB3	3:B:811:NDG:O6	2.15	0.42
1:B:347:ARG:HD2	1:B:392:GLY:CA	2.50	0.42
1:B:515:ASP:OD1	1:B:516:ALA:N	2.52	0.42
1:C:8:LYS:CD	1:C:8:LYS:N	2.51	0.42
1:C:23:GLN:HB2	1:C:59:TRP:CD2	2.55	0.42
1:C:90:GLU:HG2	1:D:36:TYR:HA	1.43	0.42
1:C:237:PHE:N	1:C:284:THR:OG1	2.42	0.42
1:C:366:LYS:HG2	1:C:367:LEU:H	1.74	0.42
1:C:419:VAL:HG13	1:C:420:GLY:N	2.33	0.42
1:D:490:LYS:O	1:D:490:LYS:CG	2.67	0.42
1:A:5:PRO:HG3	1:B:91:PRO:HG2	1.22	0.41
1:A:23:GLN:HB2	1:A:59:TRP:CD2	2.55	0.41
1:A:212:THR:CG2	1:A:213:ASP:H	2.32	0.41
1:B:7:ILE:O	1:B:96:ILE:HG23	2.20	0.41
1:B:81:VAL:HG12	1:D:90:GLU:HG2	2.02	0.41
1:C:250:PRO:HA	1:C:255:TRP:CG	2.54	0.41
1:D:252:THR:C	1:D:254:ALA:H	2.28	0.41
1:D:522:LEU:HB3	1:D:523:THR:H	1.57	0.41
1:A:127:VAL:HG22	1:A:128:MET:HG3	2.03	0.41
1:A:230:VAL:HG23	1:A:323:VAL:HA	2.03	0.41
1:A:458:THR:C	1:A:459:ILE:HD12	2.44	0.41
1:A:502:LEU:HD22	1:A:503:LYS:H	1.85	0.41
1:B:23:GLN:HB2	1:B:59:TRP:CD2	2.55	0.41
1:B:250:PRO:HA	1:B:255:TRP:CG	2.54	0.41
1:B:367:LEU:H	1:B:367:LEU:HG	1.41	0.41
1:C:252:THR:C	1:C:254:ALA:H	2.28	0.41
1:D:4:ILE:HA	1:D:5:PRO:HD3	1.72	0.41
1:D:272:THR:CG2	1:D:273:THR:N	2.76	0.41
1:D:385:ASN:O	1:D:386:GLY:C	2.62	0.41
1:A:7:ILE:O	1:A:96:ILE:HG23	2.20	0.41
1:A:31:PHE:CD2	1:A:31:PHE:C	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ASP:OD1	1:A:516:ALA:N	2.52	0.41
1:B:212:THR:CG2	1:B:213:ASP:H	2.32	0.41
1:B:231:PRO:O	1:B:288:LEU:HD12	2.20	0.41
1:B:511:VAL:N	1:B:523:THR:O	2.46	0.41
1:C:231:PRO:O	1:C:235:ILE:HD13	2.21	0.41
1:C:264:ASN:HB3	1:C:267:GLY:HA2	2.01	0.41
1:C:297:VAL:HG21	2:C:807:NAG:H62	2.01	0.41
1:C:347:ARG:HG3	1:C:392:GLY:N	2.33	0.41
1:C:423:THR:CG2	2:C:810:NAG:N2	2.84	0.41
1:C:502:LEU:HD22	1:C:503:LYS:H	1.85	0.41
1:D:230:VAL:O	1:D:323:VAL:HA	2.20	0.41
1:D:474:SER:N	1:D:512:LEU:O	2.53	0.41
1:A:277:SER:O	1:A:278:ASN:C	2.62	0.41
1:A:339:VAL:HG21	1:A:351:ILE:HG22	2.01	0.41
1:A:469:TYR:CE2	1:A:470:PRO:HD2	2.54	0.41
1:B:23:GLN:HA	1:B:58:GLY:O	2.21	0.41
1:B:347:ARG:HG3	1:B:392:GLY:N	2.33	0.41
1:B:371:ILE:HA	1:B:410:MET:HB3	2.02	0.41
1:C:1:ASP:HB2	1:D:89:GLU:HG2	1.11	0.41
1:C:231:PRO:O	1:C:288:LEU:HD12	2.20	0.41
1:C:522:LEU:HA	1:C:522:LEU:HD23	1.36	0.41
1:D:108:PHE:HA	1:D:132:ALA:CB	2.50	0.41
1:A:23:GLN:HA	1:A:58:GLY:O	2.21	0.41
1:A:40:GLY:O	1:A:45:ASN:HB2	2.19	0.41
1:A:154:ASP:HB3	2:A:801:NAG:C7	2.48	0.41
1:B:127:VAL:HG22	1:B:128:MET:HG3	2.03	0.41
1:B:231:PRO:O	1:B:235:ILE:HD13	2.21	0.41
1:C:32:ASN:ND2	1:C:83:GLU:CB	2.62	0.41
1:C:108:PHE:HA	1:C:132:ALA:CB	2.50	0.41
1:D:23:GLN:HB2	1:D:59:TRP:CD2	2.55	0.41
1:D:108:PHE:HA	1:D:132:ALA:HB2	2.03	0.41
1:D:111:ASP:O	1:D:112:VAL:HG13	2.21	0.41
1:D:231:PRO:O	1:D:235:ILE:HD13	2.21	0.41
1:D:347:ARG:HG3	1:D:392:GLY:N	2.33	0.41
1:D:371:ILE:HA	1:D:410:MET:HB3	2.02	0.41
1:D:515:ASP:OD1	1:D:516:ALA:N	2.52	0.41
1:A:4:ILE:HD12	1:B:90:GLU:HB3	1.53	0.41
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.51	0.41
1:A:423:THR:CG2	2:A:810:NAG:N2	2.84	0.41
1:B:19:LYS:HB3	1:B:62:VAL:HG12	2.03	0.41
1:B:108:PHE:CZ	1:B:191:VAL:HG23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASP:O	1:B:112:VAL:HG13	2.21	0.41
1:B:118:ARG:CA	1:B:212:THR:HB	2.51	0.41
1:B:474:SER:N	1:B:512:LEU:O	2.53	0.41
1:C:111:ASP:O	1:C:112:VAL:HG13	2.21	0.41
1:C:195:ASP:HB3	1:C:196:LEU:HG	2.01	0.41
1:D:68:ARG:HD3	1:D:100:ASP:CB	2.51	0.41
1:D:118:ARG:CA	1:D:212:THR:HB	2.51	0.41
1:D:227:THR:C	2:D:812:NAG:O5	2.64	0.41
1:A:62:VAL:O	1:A:62:VAL:HG13	2.21	0.41
1:C:31:PHE:CD2	1:D:74:TYR:C	2.99	0.41
1:C:68:ARG:HD3	1:C:100:ASP:CB	2.51	0.41
1:C:88:VAL:N	1:D:38:ILE:HD11	2.36	0.41
1:C:108:PHE:HA	1:C:132:ALA:HB2	2.03	0.41
1:C:108:PHE:CZ	1:C:191:VAL:HG23	2.56	0.41
1:C:474:SER:N	1:C:512:LEU:O	2.54	0.41
1:D:297:VAL:HG22	2:D:807:NAG:H62	2.03	0.41
1:A:36:TYR:CZ	1:D:2:TRP:HH2	2.39	0.41
1:A:90:GLU:C	1:B:1:ASP:O	2.64	0.41
1:A:111:ASP:O	1:A:112:VAL:HG13	2.21	0.41
1:B:490:LYS:O	1:B:490:LYS:CG	2.67	0.41
1:B:505:GLY:H	1:B:529:VAL:HB	1.85	0.41
1:C:212:THR:CG2	1:C:213:ASP:H	2.32	0.41
1:C:274:ASP:HA	1:C:275:PRO:HD3	1.93	0.41
1:C:540:GLN:O	1:C:540:GLN:NE2	2.47	0.41
1:A:371:ILE:HA	1:A:410:MET:HB3	2.02	0.41
1:A:474:SER:N	1:A:512:LEU:O	2.54	0.41
1:B:27:ASN:C	1:B:29:ASP:N	2.79	0.41
1:B:108:PHE:HA	1:B:132:ALA:HB2	2.03	0.41
1:B:261:ILE:HD13	1:B:261:ILE:H	1.85	0.41
1:B:316:THR:OG1	2:B:806:NAG:H83	2.21	0.41
1:B:403:ASN:C	1:B:405:THR:N	2.76	0.41
1:B:409:ILE:HD13	3:B:811:NDG:C8	2.51	0.41
1:B:440:PRO:HB3	1:B:457:LEU:CD2	2.43	0.41
1:C:42:GLY:CA	1:C:47:PRO:O	2.69	0.41
1:C:62:VAL:O	1:C:62:VAL:HG13	2.21	0.41
1:C:118:ARG:CA	1:C:212:THR:HB	2.51	0.41
1:C:230:VAL:O	1:C:323:VAL:HA	2.20	0.41
1:C:239:VAL:HG13	1:C:240:GLN:N	2.33	0.41
1:C:297:VAL:HG22	2:C:807:NAG:H62	2.03	0.41
1:D:119:GLU:CG	1:D:214:ALA:HB3	2.51	0.41
1:D:127:VAL:HG22	1:D:128:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:VAL:HG11	1:D:282:LEU:HD22	2.02	0.41
1:D:449:ASP:HB2	1:D:531:SER:HA	2.03	0.41
1:A:193:ALA:O	1:A:202:SER:HA	2.21	0.41
1:B:249:MET:O	1:B:252:THR:CB	2.69	0.41
1:B:252:THR:C	1:B:254:ALA:H	2.28	0.41
1:B:519:ASN:O	1:B:520:PRO:C	2.59	0.41
1:C:89:GLU:CD	1:D:92:MET:N	2.78	0.41
1:C:252:THR:O	1:C:255:TRP:N	2.54	0.41
1:D:62:VAL:O	1:D:62:VAL:HG13	2.21	0.41
1:A:231:PRO:O	1:A:288:LEU:HD12	2.20	0.40
1:A:239:VAL:HG13	1:A:240:GLN:N	2.33	0.40
1:A:319:VAL:CG1	1:A:320:THR:N	2.84	0.40
1:A:409:ILE:C	1:A:410:MET:HG2	2.46	0.40
1:A:490:LYS:O	1:A:490:LYS:CG	2.67	0.40
1:B:119:GLU:CG	1:B:214:ALA:HB3	2.51	0.40
1:B:230:VAL:HG23	1:B:323:VAL:HA	2.03	0.40
1:B:409:ILE:C	1:B:410:MET:HG2	2.46	0.40
1:C:119:GLU:CG	1:C:214:ALA:HB3	2.51	0.40
1:C:193:ALA:O	1:C:202:SER:HA	2.21	0.40
1:C:320:THR:CG2	2:C:807:NAG:C2	2.76	0.40
1:D:27:ASN:C	1:D:29:ASP:N	2.79	0.40
1:D:138:ASN:HD22	1:D:138:ASN:N	2.19	0.40
1:D:259:TYR:O	1:D:260:LYS:CB	2.69	0.40
1:D:502:LEU:HD22	1:D:503:LYS:H	1.85	0.40
1:D:505:GLY:H	1:D:529:VAL:HB	1.85	0.40
1:D:522:LEU:HA	1:D:522:LEU:HD23	1.36	0.40
1:A:19:LYS:HB3	1:A:62:VAL:HG12	2.03	0.40
1:A:108:PHE:CZ	1:A:191:VAL:HG23	2.56	0.40
1:A:119:GLU:CG	1:A:214:ALA:HB3	2.51	0.40
1:A:316:THR:OG1	2:A:806:NAG:H83	2.21	0.40
1:B:19:LYS:HB3	1:B:62:VAL:CG1	2.52	0.40
1:B:227:THR:C	2:B:812:NAG:O5	2.64	0.40
1:D:108:PHE:CZ	1:D:191:VAL:HG23	2.56	0.40
1:D:252:THR:HA	1:D:253:PRO:HD3	1.81	0.40
1:D:316:THR:OG1	2:D:806:NAG:H83	2.21	0.40
1:D:451:ASN:C	1:D:534:GLY:HA2	2.46	0.40
1:A:272:THR:O	1:A:281:ILE:HG22	2.22	0.40
1:C:26:SER:OG	1:D:77:SER:OG	2.35	0.40
1:C:79:HIS:CB	1:D:39:THR:HB	2.35	0.40
1:C:230:VAL:HG23	1:C:323:VAL:HA	2.03	0.40
1:C:249:MET:O	1:C:252:THR:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:MET:HA	1:C:250:PRO:HD3	1.85	0.40
1:C:290:PHE:CG	1:C:292:LEU:HB2	2.56	0.40
1:C:505:GLY:H	1:C:529:VAL:HB	1.85	0.40
1:D:23:GLN:HA	1:D:58:GLY:O	2.21	0.40
1:D:154:ASP:HB3	2:D:801:NAG:C7	2.48	0.40
1:D:249:MET:O	1:D:252:THR:CB	2.69	0.40
1:D:299:GLN:CG	1:D:318:THR:HG23	2.42	0.40
1:A:261:ILE:HD13	1:A:261:ILE:H	1.85	0.40
1:A:297:VAL:HG22	2:A:807:NAG:H62	2.03	0.40
1:B:68:ARG:HD3	1:B:100:ASP:CB	2.51	0.40
1:B:274:ASP:HA	1:B:275:PRO:HD3	1.93	0.40
1:B:449:ASP:N	1:B:532:CYS:HB3	2.19	0.40
1:C:34:VAL:CG1	1:C:80:ALA:HB1	2.52	0.40
1:C:90:GLU:HB3	1:D:79:HIS:H	1.59	0.40
1:C:329:ALA:HA	1:C:330:PRO:HD3	1.87	0.40
1:C:385:ASN:O	1:C:385:ASN:ND2	2.55	0.40
1:C:469:TYR:CE2	1:C:470:PRO:HD2	2.54	0.40
1:D:11:GLU:O	1:D:12:ASN:C	2.65	0.40
1:D:19:LYS:HB3	1:D:62:VAL:HG12	2.03	0.40
1:D:34:VAL:CG1	1:D:80:ALA:HB1	2.52	0.40
1:D:193:ALA:O	1:D:202:SER:HA	2.21	0.40
1:D:222:ASP:H	1:D:243:SER:C	2.30	0.40
1:D:230:VAL:HG23	1:D:323:VAL:HA	2.03	0.40
1:D:345:LEU:HD22	1:D:349:GLU:HB2	2.03	0.40
1:D:385:ASN:O	1:D:385:ASN:ND2	2.55	0.40
1:D:409:ILE:HD13	3:D:811:NDG:C8	2.51	0.40
1:A:227:THR:C	2:A:812:NAG:O5	2.64	0.40
1:A:231:PRO:O	1:A:235:ILE:HD13	2.21	0.40
1:A:249:MET:O	1:A:252:THR:CB	2.69	0.40
1:A:482:THR:HG22	1:A:499:THR:H	1.70	0.40
1:B:378:TRP:HB2	1:B:379:LEU:H	1.64	0.40
1:B:385:ASN:O	1:B:385:ASN:ND2	2.55	0.40
1:C:259:TYR:O	1:C:260:LYS:CB	2.69	0.40
1:C:445:PHE:CD2	1:C:445:PHE:N	2.89	0.40
1:D:19:LYS:HB3	1:D:62:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	538/880 (61%)	402 (75%)	91 (17%)	45 (8%)	0	9
1	B	538/880 (61%)	401 (74%)	93 (17%)	44 (8%)	0	9
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	0	9
1	D	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	0	9
All	All	2152/3520 (61%)	1605 (75%)	368 (17%)	179 (8%)	1	9

All (179) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	155	PRO
1	A	235	ILE
1	A	347	ARG
1	A	363	GLN
1	A	364	ILE
1	A	374	ASP
1	A	404	ASN
1	A	467	ASN
1	A	476	SER
1	A	502	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	B	91	PRO
1	B	155	PRO
1	B	235	ILE
1	B	347	ARG
1	B	363	GLN
1	B	364	ILE
1	B	374	ASP
1	B	404	ASN

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Mol	Chain	Res	Type
1	B	467	ASN
1	B	476	SER
1	B	502	LEU
1	B	517	GLN
1	B	518	ASN
1	B	519	ASN
1	C	91	PRO
1	C	155	PRO
1	C	235	ILE
1	C	347	ARG
1	C	363	GLN
1	C	364	ILE
1	C	374	ASP
1	C	404	ASN
1	C	467	ASN
1	C	476	SER
1	C	502	LEU
1	C	517	GLN
1	C	518	ASN
1	C	519	ASN
1	D	91	PRO
1	D	155	PRO
1	D	235	ILE
1	D	347	ARG
1	D	363	GLN
1	D	364	ILE
1	D	374	ASP
1	D	404	ASN
1	D	467	ASN
1	D	476	SER
1	D	502	LEU
1	D	517	GLN
1	D	518	ASN
1	D	519	ASN
1	A	3	VAL
1	A	156	GLU
1	A	260	LYS
1	A	287	GLY
1	A	470	PRO
1	A	503	LYS
1	B	3	VAL
1	B	156	GLU

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Mol	Chain	Res	Type
1	B	260	LYS
1	B	287	GLY
1	B	470	PRO
1	B	503	LYS
1	C	3	VAL
1	C	156	GLU
1	C	260	LYS
1	C	287	GLY
1	C	470	PRO
1	C	503	LYS
1	D	3	VAL
1	D	156	GLU
1	D	260	LYS
1	D	287	GLY
1	D	470	PRO
1	D	503	LYS
1	A	55	TRP
1	A	212	THR
1	A	250	PRO
1	A	333	VAL
1	A	360	ASP
1	A	372	GLY
1	A	377	ARG
1	A	506	ASP
1	B	55	TRP
1	B	212	THR
1	B	250	PRO
1	B	333	VAL
1	B	360	ASP
1	B	372	GLY
1	B	377	ARG
1	B	506	ASP
1	C	55	TRP
1	C	212	THR
1	C	250	PRO
1	C	333	VAL
1	C	360	ASP
1	C	372	GLY
1	C	377	ARG
1	C	506	ASP
1	D	55	TRP
1	D	212	THR

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Mol	Chain	Res	Type
1	D	250	PRO
1	D	333	VAL
1	D	360	ASP
1	D	372	GLY
1	D	377	ARG
1	D	506	ASP
1	A	152	LYS
1	A	223	PRO
1	A	359	PRO
1	A	375	PRO
1	B	152	LYS
1	B	223	PRO
1	B	359	PRO
1	B	375	PRO
1	C	152	LYS
1	C	223	PRO
1	C	359	PRO
1	C	375	PRO
1	D	152	LYS
1	D	223	PRO
1	D	359	PRO
1	D	375	PRO
1	A	160	PRO
1	A	265	GLU
1	A	278	ASN
1	A	289	ASP
1	A	482	THR
1	B	160	PRO
1	B	265	GLU
1	B	278	ASN
1	B	289	ASP
1	B	482	THR
1	C	160	PRO
1	C	265	GLU
1	C	278	ASN
1	C	289	ASP
1	C	482	THR
1	D	160	PRO
1	D	265	GLU
1	D	278	ASN
1	D	289	ASP
1	D	482	THR

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Mol	Chain	Res	Type
1	A	498	PRO
1	A	523	THR
1	B	498	PRO
1	B	523	THR
1	C	498	PRO
1	C	523	THR
1	D	498	PRO
1	D	523	THR
1	A	154	ASP
1	A	307	PRO
1	B	154	ASP
1	B	307	PRO
1	C	154	ASP
1	C	307	PRO
1	D	154	ASP
1	D	307	PRO
1	A	222	ASP
1	B	222	ASP
1	C	222	ASP
1	D	222	ASP
1	A	200	GLY
1	B	200	GLY
1	C	200	GLY
1	D	200	GLY
1	A	47	PRO
1	A	158	PRO
1	B	47	PRO
1	C	47	PRO
1	C	158	PRO
1	D	47	PRO
1	D	158	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	480/779 (62%)	384 (80%)	96 (20%)	1	7
1	B	480/779 (62%)	384 (80%)	96 (20%)	1	7
1	C	480/779 (62%)	384 (80%)	96 (20%)	1	7
1	D	480/779 (62%)	384 (80%)	96 (20%)	1	7
All	All	1920/3116 (62%)	1536 (80%)	384 (20%)	3	7

All (384) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	18	PRO
1	A	19	LYS
1	A	27	ASN
1	A	61	LEU
1	A	66	LEU
1	A	68	ARG
1	A	88	VAL
1	A	91	PRO
1	A	92	MET
1	A	109	THR
1	A	117	VAL
1	A	121	VAL
1	A	138	ASN
1	A	146	LEU
1	A	151	LEU
1	A	155	PRO
1	A	161	ASN
1	A	163	PHE
1	A	189	LEU
1	A	195	ASP
1	A	196	LEU
1	A	202	SER
1	A	216	ASP
1	A	217	ASN
1	A	220	ILE
1	A	223	PRO
1	A	226	TYR
1	A	231	PRO
1	A	233	ASN

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Mol	Chain	Res	Type
1	A	234	GLU
1	A	235	ILE
1	A	237	PHE
1	A	239	VAL
1	A	250	PRO
1	A	253	PRO
1	A	261	ILE
1	A	268	PHE
1	A	273	THR
1	A	278	ASN
1	A	282	LEU
1	A	284	THR
1	A	288	LEU
1	A	298	LEU
1	A	303	GLU
1	A	309	SER
1	A	310	VAL
1	A	315	SER
1	A	316	THR
1	A	318	THR
1	A	333	VAL
1	A	336	VAL
1	A	339	VAL
1	A	353	SER
1	A	354	LEU
1	A	360	ASP
1	A	361	LYS
1	A	363	GLN
1	A	364	ILE
1	A	365	GLN
1	A	371	ILE
1	A	375	PRO
1	A	379	LEU
1	A	382	ASN
1	A	384	ASP
1	A	394	LEU
1	A	395	ASP
1	A	399	GLU
1	A	405	THR
1	A	407	THR
1	A	419	VAL
1	A	423	THR

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Mol	Chain	Res	Type
1	A	425	THR
1	A	427	ILE
1	A	433	VAL
1	A	436	ASN
1	A	447	MET
1	A	448	CYS
1	A	457	LEU
1	A	461	ASP
1	A	464	ILE
1	A	465	PRO
1	A	466	PRO
1	A	470	PRO
1	A	477	HIS
1	A	492	THR
1	A	509	ILE
1	A	511	VAL
1	A	512	LEU
1	A	517	GLN
1	A	520	PRO
1	A	522	LEU
1	A	523	THR
1	A	532	CYS
1	A	539	CYS
1	A	540	GLN
1	B	8	LYS
1	B	18	PRO
1	B	19	LYS
1	B	27	ASN
1	B	61	LEU
1	B	66	LEU
1	B	68	ARG
1	B	88	VAL
1	B	91	PRO
1	B	92	MET
1	B	109	THR
1	B	117	VAL
1	B	121	VAL
1	B	138	ASN
1	B	146	LEU
1	B	151	LEU
1	B	155	PRO
1	B	161	ASN

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Mol	Chain	Res	Type
1	B	163	PHE
1	B	189	LEU
1	B	195	ASP
1	B	196	LEU
1	B	202	SER
1	B	216	ASP
1	B	217	ASN
1	B	220	ILE
1	B	223	PRO
1	B	226	TYR
1	B	231	PRO
1	B	233	ASN
1	B	234	GLU
1	B	235	ILE
1	B	237	PHE
1	B	239	VAL
1	B	250	PRO
1	B	253	PRO
1	B	261	ILE
1	B	268	PHE
1	B	273	THR
1	B	278	ASN
1	B	282	LEU
1	B	284	THR
1	B	288	LEU
1	B	298	LEU
1	B	303	GLU
1	B	309	SER
1	B	310	VAL
1	B	315	SER
1	B	316	THR
1	B	318	THR
1	B	333	VAL
1	B	336	VAL
1	B	339	VAL
1	B	353	SER
1	B	354	LEU
1	B	360	ASP
1	B	361	LYS
1	B	363	GLN
1	B	364	ILE
1	B	365	GLN

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Mol	Chain	Res	Type
1	B	371	ILE
1	B	375	PRO
1	B	379	LEU
1	B	382	ASN
1	B	384	ASP
1	B	394	LEU
1	B	395	ASP
1	B	399	GLU
1	B	405	THR
1	B	407	THR
1	B	419	VAL
1	B	423	THR
1	B	425	THR
1	B	427	ILE
1	B	433	VAL
1	B	436	ASN
1	B	447	MET
1	B	448	CYS
1	B	457	LEU
1	B	461	ASP
1	B	464	ILE
1	B	465	PRO
1	B	466	PRO
1	B	470	PRO
1	B	477	HIS
1	B	492	THR
1	B	509	ILE
1	B	511	VAL
1	B	512	LEU
1	B	517	GLN
1	B	520	PRO
1	B	522	LEU
1	B	523	THR
1	B	532	CYS
1	B	539	CYS
1	B	540	GLN
1	C	8	LYS
1	C	18	PRO
1	C	19	LYS
1	C	27	ASN
1	C	61	LEU
1	C	66	LEU

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Mol	Chain	Res	Type
1	C	68	ARG
1	C	88	VAL
1	C	91	PRO
1	C	92	MET
1	C	109	THR
1	C	117	VAL
1	C	121	VAL
1	C	138	ASN
1	C	146	LEU
1	C	151	LEU
1	C	155	PRO
1	C	161	ASN
1	C	163	PHE
1	C	189	LEU
1	C	195	ASP
1	C	196	LEU
1	C	202	SER
1	C	216	ASP
1	C	217	ASN
1	C	220	ILE
1	C	223	PRO
1	C	226	TYR
1	C	231	PRO
1	C	233	ASN
1	C	234	GLU
1	C	235	ILE
1	C	237	PHE
1	C	239	VAL
1	C	250	PRO
1	C	253	PRO
1	C	261	ILE
1	C	268	PHE
1	C	273	THR
1	C	278	ASN
1	C	282	LEU
1	C	284	THR
1	C	288	LEU
1	C	298	LEU
1	C	303	GLU
1	C	309	SER
1	C	310	VAL
1	C	315	SER

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Mol	Chain	Res	Type
1	C	316	THR
1	C	318	THR
1	C	333	VAL
1	C	336	VAL
1	C	339	VAL
1	C	353	SER
1	C	354	LEU
1	C	360	ASP
1	C	361	LYS
1	C	363	GLN
1	C	364	ILE
1	C	365	GLN
1	C	371	ILE
1	C	375	PRO
1	C	379	LEU
1	C	382	ASN
1	C	384	ASP
1	C	394	LEU
1	C	395	ASP
1	C	399	GLU
1	C	405	THR
1	C	407	THR
1	C	419	VAL
1	C	423	THR
1	C	425	THR
1	C	427	ILE
1	C	433	VAL
1	C	436	ASN
1	C	447	MET
1	C	448	CYS
1	C	457	LEU
1	C	461	ASP
1	C	464	ILE
1	C	465	PRO
1	C	466	PRO
1	C	470	PRO
1	C	477	HIS
1	C	492	THR
1	C	509	ILE
1	C	511	VAL
1	C	512	LEU
1	C	517	GLN

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Mol	Chain	Res	Type
1	C	520	PRO
1	C	522	LEU
1	C	523	THR
1	C	532	CYS
1	C	539	CYS
1	C	540	GLN
1	D	8	LYS
1	D	18	PRO
1	D	19	LYS
1	D	27	ASN
1	D	61	LEU
1	D	66	LEU
1	D	68	ARG
1	D	88	VAL
1	D	91	PRO
1	D	92	MET
1	D	109	THR
1	D	117	VAL
1	D	121	VAL
1	D	138	ASN
1	D	146	LEU
1	D	151	LEU
1	D	155	PRO
1	D	161	ASN
1	D	163	PHE
1	D	189	LEU
1	D	195	ASP
1	D	196	LEU
1	D	202	SER
1	D	216	ASP
1	D	217	ASN
1	D	220	ILE
1	D	223	PRO
1	D	226	TYR
1	D	231	PRO
1	D	233	ASN
1	D	234	GLU
1	D	235	ILE
1	D	237	PHE
1	D	239	VAL
1	D	250	PRO
1	D	253	PRO

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Mol	Chain	Res	Type
1	D	261	ILE
1	D	268	PHE
1	D	273	THR
1	D	278	ASN
1	D	282	LEU
1	D	284	THR
1	D	288	LEU
1	D	298	LEU
1	D	303	GLU
1	D	309	SER
1	D	310	VAL
1	D	315	SER
1	D	316	THR
1	D	318	THR
1	D	333	VAL
1	D	336	VAL
1	D	339	VAL
1	D	353	SER
1	D	354	LEU
1	D	360	ASP
1	D	361	LYS
1	D	363	GLN
1	D	364	ILE
1	D	365	GLN
1	D	371	ILE
1	D	375	PRO
1	D	379	LEU
1	D	382	ASN
1	D	384	ASP
1	D	394	LEU
1	D	395	ASP
1	D	399	GLU
1	D	405	THR
1	D	407	THR
1	D	419	VAL
1	D	423	THR
1	D	425	THR
1	D	427	ILE
1	D	433	VAL
1	D	436	ASN
1	D	447	MET
1	D	448	CYS

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Mol	Chain	Res	Type
1	D	457	LEU
1	D	461	ASP
1	D	464	ILE
1	D	465	PRO
1	D	466	PRO
1	D	470	PRO
1	D	477	HIS
1	D	492	THR
1	D	509	ILE
1	D	511	VAL
1	D	512	LEU
1	D	517	GLN
1	D	520	PRO
1	D	522	LEU
1	D	523	THR
1	D	532	CYS
1	D	539	CYS
1	D	540	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	27	ASN
1	A	32	ASN
1	A	45	ASN
1	A	97	ASN
1	A	104	ASN
1	A	110	GLN
1	A	122	GLN
1	A	138	ASN
1	A	217	ASN
1	A	240	GLN
1	A	264	ASN
1	A	278	ASN
1	A	299	GLN
1	A	373	ASN
1	A	385	ASN
1	A	391	ASN
1	A	393	ASN
1	A	404	ASN
1	A	455	GLN

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Mol	Chain	Res	Type
1	A	467	ASN
1	A	517	GLN
1	A	519	ASN
1	B	12	ASN
1	B	27	ASN
1	B	45	ASN
1	B	97	ASN
1	B	102	ASN
1	B	104	ASN
1	B	110	GLN
1	B	122	GLN
1	B	138	ASN
1	B	192	GLN
1	B	217	ASN
1	B	240	GLN
1	B	264	ASN
1	B	278	ASN
1	B	299	GLN
1	B	373	ASN
1	B	385	ASN
1	B	391	ASN
1	B	404	ASN
1	B	455	GLN
1	B	467	ASN
1	B	517	GLN
1	B	519	ASN
1	C	12	ASN
1	C	27	ASN
1	C	32	ASN
1	C	45	ASN
1	C	97	ASN
1	C	102	ASN
1	C	104	ASN
1	C	110	GLN
1	C	122	GLN
1	C	138	ASN
1	C	217	ASN
1	C	240	GLN
1	C	264	ASN
1	C	278	ASN
1	C	299	GLN
1	C	373	ASN

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Mol	Chain	Res	Type
1	C	385	ASN
1	C	391	ASN
1	C	404	ASN
1	C	455	GLN
1	C	467	ASN
1	C	517	GLN
1	C	519	ASN
1	D	12	ASN
1	D	27	ASN
1	D	32	ASN
1	D	45	ASN
1	D	104	ASN
1	D	110	GLN
1	D	122	GLN
1	D	138	ASN
1	D	192	GLN
1	D	217	ASN
1	D	233	ASN
1	D	240	GLN
1	D	264	ASN
1	D	278	ASN
1	D	299	GLN
1	D	373	ASN
1	D	385	ASN
1	D	391	ASN
1	D	404	ASN
1	D	455	GLN
1	D	467	ASN
1	D	477	HIS
1	D	517	GLN
1	D	519	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 48 are monoatomic - leaving 60 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	B	902	1	14,14,15	1.12	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	B	808	1	14,14,15	0.66	0	17,19,21	0.70	0
3	NDG	A	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	D	904	1	14,14,15	0.78	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	A	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	B	904	1	14,14,15	0.76	1 (7%)	17,19,21	0.69	0
2	NAG	D	807	1	14,14,15	0.65	0	17,19,21	1.18	2 (11%)
2	NAG	D	902	1	14,14,15	1.13	1 (7%)	17,19,21	1.08	1 (5%)
2	NAG	A	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	D	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.75	1 (5%)
2	NAG	B	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	A	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
2	NAG	A	805	1	14,14,15	0.72	0	17,19,21	1.06	1 (5%)
3	NDG	D	804	1	14,14,15	0.64	0	17,19,21	0.77	0
2	NAG	B	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	D	903	1	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	A	902	1	14,14,15	1.15	1 (7%)	17,19,21	1.08	2 (11%)
2	NAG	B	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	D	806	1	14,14,15	0.55	0	17,19,21	1.38	3 (17%)
2	NAG	A	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	C	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	C	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	C	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	C	806	1	14,14,15	0.57	0	17,19,21	1.39	3 (17%)
2	NAG	C	810	1	14,14,15	0.66	0	17,19,21	1.33	4 (23%)
3	NDG	B	804	1	14,14,15	0.64	0	17,19,21	0.78	0
2	NAG	D	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
3	NDG	B	811	1	14,14,15	0.86	0	17,19,21	1.96	1 (5%)
2	NAG	A	806	1	14,14,15	0.55	0	17,19,21	1.39	3 (17%)
3	NDG	C	804	1	14,14,15	0.64	0	17,19,21	0.78	0
2	NAG	C	807	1	14,14,15	0.63	0	17,19,21	1.19	2 (11%)
2	NAG	C	902	1	14,14,15	1.13	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	D	808	1	14,14,15	0.66	0	17,19,21	0.70	0
2	NAG	C	808	1	14,14,15	0.68	0	17,19,21	0.70	0
2	NAG	B	809	1	14,14,15	0.76	0	17,19,21	0.94	0
2	NAG	A	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
3	NDG	D	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	C	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	A	801	1	14,14,15	0.71	0	17,19,21	0.99	1 (5%)
2	NAG	A	808	1	14,14,15	0.67	0	17,19,21	0.70	0
3	NDG	A	804	1	14,14,15	0.65	0	17,19,21	0.78	0
2	NAG	D	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	B	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	C	903	1	14,14,15	0.55	0	17,19,21	0.78	0
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	C	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.93	0
2	NAG	D	809	1	14,14,15	0.78	1 (7%)	17,19,21	0.94	0
2	NAG	B	903	1	14,14,15	0.56	0	17,19,21	0.79	0
2	NAG	C	805	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
2	NAG	D	802	1	14,14,15	0.79	1 (7%)	17,19,21	0.85	0
2	NAG	B	806	1	14,14,15	0.56	0	17,19,21	1.39	3 (17%)
2	NAG	D	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	B	801	1	14,14,15	0.70	0	17,19,21	0.97	1 (5%)
2	NAG	A	903	1	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	B	805	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
3	NDG	C	811	1	14,14,15	0.86	0	17,19,21	1.96	1 (5%)
2	NAG	C	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	A	812	1	14,14,15	0.84	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	B	807	1	14,14,15	0.65	0	17,19,21	1.20	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	808	1	-	3/6/23/26	0/1/1/1
3	NDG	A	811	1	-	2/6/23/26	0/1/1/1
2	NAG	D	904	1	-	3/6/23/26	0/1/1/1
2	NAG	A	809	1	-	2/6/23/26	0/1/1/1
2	NAG	B	904	1	-	3/6/23/26	0/1/1/1
2	NAG	D	807	1	-	5/6/23/26	0/1/1/1
2	NAG	D	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	810	1	-	3/6/23/26	0/1/1/1
2	NAG	D	812	1	-	4/6/23/26	0/1/1/1
2	NAG	B	810	1	-	3/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NDG	D	804	1	-	0/6/23/26	0/1/1/1
2	NAG	B	812	1	-	4/6/23/26	0/1/1/1
2	NAG	D	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	802	1	-	2/6/23/26	0/1/1/1
2	NAG	A	803	1	-	2/6/23/26	0/1/1/1
2	NAG	C	801	1	-	4/6/23/26	0/1/1/1
2	NAG	C	803	1	-	2/6/23/26	0/1/1/1
2	NAG	C	802	1	-	2/6/23/26	0/1/1/1
2	NAG	D	801	1	-	4/6/23/26	0/1/1/1
2	NAG	C	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	810	1	-	3/6/23/26	0/1/1/1
3	NDG	B	804	1	-	0/6/23/26	0/1/1/1
2	NAG	D	805	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NDG	B	811	1	-	2/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NDG	C	804	1	-	0/6/23/26	0/1/1/1
2	NAG	C	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	807	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	808	1	-	3/6/23/26	0/1/1/1
2	NAG	C	808	1	-	3/6/23/26	0/1/1/1
2	NAG	B	809	1	-	2/6/23/26	0/1/1/1
2	NAG	A	802	1	-	2/6/23/26	0/1/1/1
3	NDG	D	811	1	-	2/6/23/26	0/1/1/1
2	NAG	C	812	1	-	4/6/23/26	0/1/1/1
2	NAG	A	801	1	-	4/6/23/26	0/1/1/1
2	NAG	A	808	1	-	3/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	D	803	1	-	2/6/23/26	0/1/1/1
2	NAG	B	803	1	-	2/6/23/26	0/1/1/1
2	NAG	C	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	904	1	-	3/6/23/26	0/1/1/1
2	NAG	C	809	1	-	2/6/23/26	0/1/1/1
2	NAG	A	812	1	-	4/6/23/26	0/1/1/1
2	NAG	D	809	1	-	2/6/23/26	0/1/1/1
2	NAG	B	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	802	1	-	2/6/23/26	0/1/1/1
2	NAG	B	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	810	1	-	3/6/23/26	0/1/1/1
2	NAG	B	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	805	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	903	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NDG	C	811	1	-	2/6/23/26	0/1/1/1
2	NAG	C	904	1	-	3/6/23/26	0/1/1/1
2	NAG	A	807	1	-	5/6/23/26	0/1/1/1
2	NAG	B	807	1	-	5/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NAG	C1-C2	3.43	1.57	1.52
2	C	902	NAG	C1-C2	3.37	1.56	1.52
2	B	902	NAG	C1-C2	3.35	1.56	1.52
2	D	902	NAG	C1-C2	3.34	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	803	NAG	O5-C5	2.65	1.48	1.43
2	D	803	NAG	O5-C5	2.64	1.48	1.43
2	A	803	NAG	O5-C5	2.62	1.48	1.43
2	B	803	NAG	O5-C5	2.62	1.48	1.43
2	D	904	NAG	C1-C2	-2.45	1.49	1.52
2	C	904	NAG	C1-C2	-2.42	1.49	1.52
2	A	904	NAG	C1-C2	-2.42	1.49	1.52
2	B	904	NAG	C1-C2	-2.39	1.49	1.52
2	A	812	NAG	C1-C2	-2.36	1.49	1.52
2	C	812	NAG	C1-C2	-2.32	1.49	1.52
2	D	812	NAG	C1-C2	-2.29	1.49	1.52
2	B	812	NAG	C1-C2	-2.27	1.49	1.52
2	A	802	NAG	C1-C2	2.12	1.55	1.52
2	D	802	NAG	C1-C2	2.11	1.55	1.52
2	B	802	NAG	C1-C2	2.11	1.55	1.52
2	D	809	NAG	C1-C2	-2.08	1.49	1.52
2	C	802	NAG	C1-C2	2.06	1.55	1.52
2	C	809	NAG	C1-C2	-2.05	1.49	1.52
2	A	809	NAG	C1-C2	-2.04	1.49	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	811	NDG	C2-N2-C7	-7.43	112.94	122.90
3	A	811	NDG	C2-N2-C7	-7.43	112.94	122.90
3	B	811	NDG	C2-N2-C7	-7.42	112.96	122.90
3	C	811	NDG	C2-N2-C7	-7.41	112.97	122.90
2	B	806	NAG	C2-N2-C7	-3.65	118.00	122.90
2	C	806	NAG	C2-N2-C7	-3.63	118.04	122.90
2	A	806	NAG	C2-N2-C7	-3.59	118.08	122.90
2	D	806	NAG	C2-N2-C7	-3.58	118.11	122.90
2	C	805	NAG	C2-N2-C7	-3.19	118.63	122.90
2	A	805	NAG	C2-N2-C7	-3.18	118.64	122.90
2	B	805	NAG	C2-N2-C7	-3.16	118.67	122.90
2	D	805	NAG	C2-N2-C7	-3.15	118.68	122.90
2	B	807	NAG	C2-N2-C7	-3.09	118.76	122.90
2	D	807	NAG	C2-N2-C7	-3.07	118.79	122.90
2	A	807	NAG	C2-N2-C7	-3.05	118.81	122.90
2	C	807	NAG	C2-N2-C7	-3.05	118.82	122.90
2	C	803	NAG	C2-N2-C7	-3.01	118.87	122.90
2	B	803	NAG	C2-N2-C7	-3.00	118.88	122.90
2	D	803	NAG	C2-N2-C7	-2.99	118.90	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	803	NAG	C2-N2-C7	-2.97	118.92	122.90
2	C	810	NAG	C1-C2-N2	2.53	114.42	110.43
2	B	810	NAG	C1-C2-N2	2.52	114.41	110.43
2	A	810	NAG	C1-C2-N2	2.51	114.40	110.43
2	D	810	NAG	C1-C2-N2	2.50	114.37	110.43
2	B	810	NAG	C4-C3-C2	-2.46	107.41	111.02
2	B	803	NAG	C1-O5-C5	2.46	115.49	112.19
2	C	803	NAG	C1-O5-C5	2.46	115.49	112.19
2	C	810	NAG	C4-C3-C2	-2.46	107.41	111.02
2	A	806	NAG	C4-C3-C2	-2.46	107.42	111.02
2	A	810	NAG	C4-C3-C2	-2.46	107.42	111.02
2	D	810	NAG	C4-C3-C2	-2.45	107.42	111.02
2	A	803	NAG	C1-O5-C5	2.45	115.47	112.19
2	B	806	NAG	C4-C3-C2	-2.45	107.43	111.02
2	D	806	NAG	C4-C3-C2	-2.44	107.44	111.02
2	C	806	NAG	C4-C3-C2	-2.43	107.46	111.02
2	D	803	NAG	C1-O5-C5	2.42	115.43	112.19
2	D	810	NAG	O5-C1-C2	-2.39	107.60	111.29
2	A	810	NAG	O5-C1-C2	-2.37	107.62	111.29
2	C	810	NAG	O5-C1-C2	-2.35	107.65	111.29
2	B	810	NAG	O5-C1-C2	-2.35	107.66	111.29
2	B	810	NAG	C1-O5-C5	-2.27	109.15	112.19
2	C	810	NAG	C1-O5-C5	-2.24	109.18	112.19
2	D	810	NAG	C1-O5-C5	-2.23	109.20	112.19
2	A	810	NAG	C1-O5-C5	-2.22	109.21	112.19
2	A	812	NAG	C2-N2-C7	-2.18	119.98	122.90
2	C	902	NAG	O5-C1-C2	2.18	114.66	111.29
2	C	812	NAG	C2-N2-C7	-2.17	119.99	122.90
2	B	812	NAG	C2-N2-C7	-2.16	120.00	122.90
2	A	801	NAG	C1-C2-N2	-2.16	107.03	110.43
2	B	902	NAG	O5-C1-C2	2.14	114.61	111.29
2	D	801	NAG	C1-C2-N2	-2.14	107.06	110.43
2	C	801	NAG	C1-C2-N2	-2.14	107.06	110.43
2	D	902	NAG	O5-C1-C2	2.13	114.59	111.29
2	B	801	NAG	C1-C2-N2	-2.13	107.08	110.43
2	D	812	NAG	C2-N2-C7	-2.12	120.06	122.90
2	A	902	NAG	O5-C1-C2	2.12	114.57	111.29
2	A	807	NAG	O5-C1-C2	-2.08	108.07	111.29
2	C	807	NAG	O5-C1-C2	-2.06	108.10	111.29
2	B	807	NAG	O5-C1-C2	-2.05	108.11	111.29
2	B	902	NAG	C1-O5-C5	2.05	114.93	112.19
2	A	806	NAG	O5-C1-C2	-2.04	108.13	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	904	NAG	C2-N2-C7	-2.04	120.17	122.90
2	C	904	NAG	C2-N2-C7	-2.04	120.17	122.90
2	D	904	NAG	C2-N2-C7	-2.03	120.18	122.90
2	D	807	NAG	O5-C1-C2	-2.03	108.16	111.29
2	C	902	NAG	C1-O5-C5	2.02	114.89	112.19
2	D	806	NAG	O5-C1-C2	-2.01	108.17	111.29
2	B	806	NAG	O5-C1-C2	-2.01	108.18	111.29
2	C	806	NAG	O5-C1-C2	-2.01	108.19	111.29
2	A	902	NAG	C1-O5-C5	2.00	114.87	112.19

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	805	NAG	C1
2	A	806	NAG	C1
2	A	902	NAG	C1
2	A	903	NAG	C1
2	B	805	NAG	C1
2	B	806	NAG	C1
2	B	902	NAG	C1
2	B	903	NAG	C1
2	C	805	NAG	C1
2	C	806	NAG	C1
2	C	902	NAG	C1
2	C	903	NAG	C1
2	D	805	NAG	C1
2	D	806	NAG	C1
2	D	902	NAG	C1
2	D	903	NAG	C1

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	807	NAG	C3-C2-N2-C7
2	A	808	NAG	C1-C2-N2-C7
2	A	810	NAG	C1-C2-N2-C7
2	A	812	NAG	C1-C2-N2-C7
2	A	902	NAG	C3-C2-N2-C7
2	A	904	NAG	C3-C2-N2-C7
2	B	807	NAG	C3-C2-N2-C7
2	B	808	NAG	C1-C2-N2-C7
2	B	810	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	B	812	NAG	C1-C2-N2-C7
2	B	902	NAG	C3-C2-N2-C7
2	B	904	NAG	C3-C2-N2-C7
2	C	807	NAG	C3-C2-N2-C7
2	C	808	NAG	C1-C2-N2-C7
2	C	810	NAG	C1-C2-N2-C7
2	C	812	NAG	C1-C2-N2-C7
2	C	902	NAG	C3-C2-N2-C7
2	C	904	NAG	C3-C2-N2-C7
2	D	807	NAG	C3-C2-N2-C7
2	D	808	NAG	C1-C2-N2-C7
2	D	810	NAG	C1-C2-N2-C7
2	D	812	NAG	C1-C2-N2-C7
2	D	902	NAG	C3-C2-N2-C7
2	D	904	NAG	C3-C2-N2-C7
3	A	811	NDG	C4-C5-C6-O6
3	B	811	NDG	C4-C5-C6-O6
3	C	811	NDG	C4-C5-C6-O6
3	D	811	NDG	C4-C5-C6-O6
2	A	802	NAG	C4-C5-C6-O6
2	A	807	NAG	C4-C5-C6-O6
2	B	802	NAG	C4-C5-C6-O6
2	B	807	NAG	C4-C5-C6-O6
2	C	802	NAG	C4-C5-C6-O6
2	C	807	NAG	C4-C5-C6-O6
2	D	807	NAG	C4-C5-C6-O6
3	A	811	NDG	O5-C5-C6-O6
3	B	811	NDG	O5-C5-C6-O6
3	C	811	NDG	O5-C5-C6-O6
3	D	811	NDG	O5-C5-C6-O6
2	D	802	NAG	C4-C5-C6-O6
2	A	809	NAG	O5-C5-C6-O6
2	B	809	NAG	O5-C5-C6-O6
2	C	809	NAG	O5-C5-C6-O6
2	D	809	NAG	O5-C5-C6-O6
2	A	809	NAG	C4-C5-C6-O6
2	B	809	NAG	C4-C5-C6-O6
2	C	809	NAG	C4-C5-C6-O6
2	D	809	NAG	C4-C5-C6-O6
2	A	807	NAG	O5-C5-C6-O6
2	B	807	NAG	O5-C5-C6-O6
2	C	807	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	807	NAG	O5-C5-C6-O6
2	A	807	NAG	C8-C7-N2-C2
2	B	807	NAG	C8-C7-N2-C2
2	C	807	NAG	C8-C7-N2-C2
2	D	807	NAG	C8-C7-N2-C2
2	A	805	NAG	O5-C5-C6-O6
2	B	805	NAG	O5-C5-C6-O6
2	C	805	NAG	O5-C5-C6-O6
2	D	805	NAG	O5-C5-C6-O6
2	A	802	NAG	O5-C5-C6-O6
2	B	802	NAG	O5-C5-C6-O6
2	C	802	NAG	O5-C5-C6-O6
2	D	802	NAG	O5-C5-C6-O6
2	B	904	NAG	C4-C5-C6-O6
2	A	904	NAG	C4-C5-C6-O6
2	C	904	NAG	C4-C5-C6-O6
2	D	904	NAG	C4-C5-C6-O6
2	A	805	NAG	C4-C5-C6-O6
2	C	805	NAG	C4-C5-C6-O6
2	D	805	NAG	C4-C5-C6-O6
2	B	805	NAG	C4-C5-C6-O6
2	A	810	NAG	C4-C5-C6-O6
2	B	810	NAG	C4-C5-C6-O6
2	C	810	NAG	C4-C5-C6-O6
2	D	810	NAG	C4-C5-C6-O6
2	A	812	NAG	O5-C5-C6-O6
2	B	812	NAG	O5-C5-C6-O6
2	C	812	NAG	O5-C5-C6-O6
2	D	812	NAG	O5-C5-C6-O6
2	A	807	NAG	O7-C7-N2-C2
2	B	807	NAG	O7-C7-N2-C2
2	C	807	NAG	O7-C7-N2-C2
2	D	807	NAG	O7-C7-N2-C2
2	A	803	NAG	C4-C5-C6-O6
2	B	803	NAG	C4-C5-C6-O6
2	C	803	NAG	C4-C5-C6-O6
2	D	803	NAG	C4-C5-C6-O6
2	A	810	NAG	O5-C5-C6-O6
2	B	810	NAG	O5-C5-C6-O6
2	C	810	NAG	O5-C5-C6-O6
2	D	810	NAG	O5-C5-C6-O6
2	B	904	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	904	NAG	O5-C5-C6-O6
2	A	904	NAG	O5-C5-C6-O6
2	D	904	NAG	O5-C5-C6-O6
2	B	801	NAG	C4-C5-C6-O6
2	D	801	NAG	C4-C5-C6-O6
2	A	801	NAG	C4-C5-C6-O6
2	C	801	NAG	C4-C5-C6-O6
2	A	803	NAG	O5-C5-C6-O6
2	B	803	NAG	O5-C5-C6-O6
2	C	803	NAG	O5-C5-C6-O6
2	D	803	NAG	O5-C5-C6-O6
2	C	903	NAG	C4-C5-C6-O6
2	D	903	NAG	C4-C5-C6-O6
2	A	903	NAG	C4-C5-C6-O6
2	B	903	NAG	C4-C5-C6-O6
2	A	808	NAG	C4-C5-C6-O6
2	A	806	NAG	C4-C5-C6-O6
2	C	808	NAG	C4-C5-C6-O6
2	D	806	NAG	C4-C5-C6-O6
2	B	808	NAG	C4-C5-C6-O6
2	D	808	NAG	C4-C5-C6-O6
2	B	806	NAG	C4-C5-C6-O6
2	A	801	NAG	C3-C2-N2-C7
2	A	903	NAG	C3-C2-N2-C7
2	B	801	NAG	C3-C2-N2-C7
2	B	903	NAG	C3-C2-N2-C7
2	C	801	NAG	C3-C2-N2-C7
2	C	903	NAG	C3-C2-N2-C7
2	D	801	NAG	C3-C2-N2-C7
2	D	903	NAG	C3-C2-N2-C7
2	C	806	NAG	C4-C5-C6-O6
2	B	801	NAG	O5-C5-C6-O6
2	A	801	NAG	O5-C5-C6-O6
2	C	801	NAG	O5-C5-C6-O6
2	D	801	NAG	O5-C5-C6-O6
2	A	801	NAG	C1-C2-N2-C7
2	A	902	NAG	C1-C2-N2-C7
2	B	801	NAG	C1-C2-N2-C7
2	B	902	NAG	C1-C2-N2-C7
2	C	801	NAG	C1-C2-N2-C7
2	C	902	NAG	C1-C2-N2-C7
2	D	801	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	D	902	NAG	C1-C2-N2-C7
2	A	806	NAG	O5-C5-C6-O6
2	D	806	NAG	O5-C5-C6-O6
2	C	806	NAG	O5-C5-C6-O6
2	B	806	NAG	O5-C5-C6-O6
2	A	808	NAG	C3-C2-N2-C7
2	A	812	NAG	C3-C2-N2-C7
2	B	808	NAG	C3-C2-N2-C7
2	B	812	NAG	C3-C2-N2-C7
2	C	808	NAG	C3-C2-N2-C7
2	C	812	NAG	C3-C2-N2-C7
2	D	808	NAG	C3-C2-N2-C7
2	D	812	NAG	C3-C2-N2-C7
2	C	812	NAG	C4-C5-C6-O6
2	B	812	NAG	C4-C5-C6-O6
2	D	812	NAG	C4-C5-C6-O6
2	A	812	NAG	C4-C5-C6-O6

There are no ring outliers.

52 monomers are involved in 385 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	902	NAG	7	0
2	B	808	NAG	2	0
3	A	811	NDG	7	0
2	D	904	NAG	6	0
2	A	809	NAG	8	0
2	B	904	NAG	6	0
2	D	807	NAG	16	0
2	D	902	NAG	7	0
2	A	810	NAG	12	0
2	D	812	NAG	3	0
2	B	810	NAG	11	0
2	A	807	NAG	16	0
2	A	805	NAG	7	0
3	D	804	NDG	2	0
2	B	812	NAG	3	0
2	A	902	NAG	7	0
2	D	806	NAG	12	0
2	A	803	NAG	4	0
2	C	801	NAG	22	0
2	C	803	NAG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	NAG	22	0
2	C	806	NAG	10	0
2	C	810	NAG	12	0
3	B	804	NDG	2	0
2	D	805	NAG	7	0
3	B	811	NDG	8	0
2	A	806	NAG	12	0
3	C	804	NDG	2	0
2	C	807	NAG	16	0
2	C	902	NAG	7	0
2	D	808	NAG	2	0
2	C	808	NAG	2	0
2	B	809	NAG	8	0
3	D	811	NDG	7	0
2	C	812	NAG	2	0
2	A	801	NAG	22	0
2	A	808	NAG	2	0
3	A	804	NDG	2	0
2	D	803	NAG	4	0
2	B	803	NAG	4	0
2	A	904	NAG	6	0
2	C	809	NAG	8	0
2	D	809	NAG	8	0
2	C	805	NAG	6	0
2	B	806	NAG	12	0
2	D	810	NAG	11	0
2	B	801	NAG	21	0
2	B	805	NAG	7	0
3	C	811	NDG	6	0
2	C	904	NAG	6	0
2	A	812	NAG	3	0
2	B	807	NAG	15	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

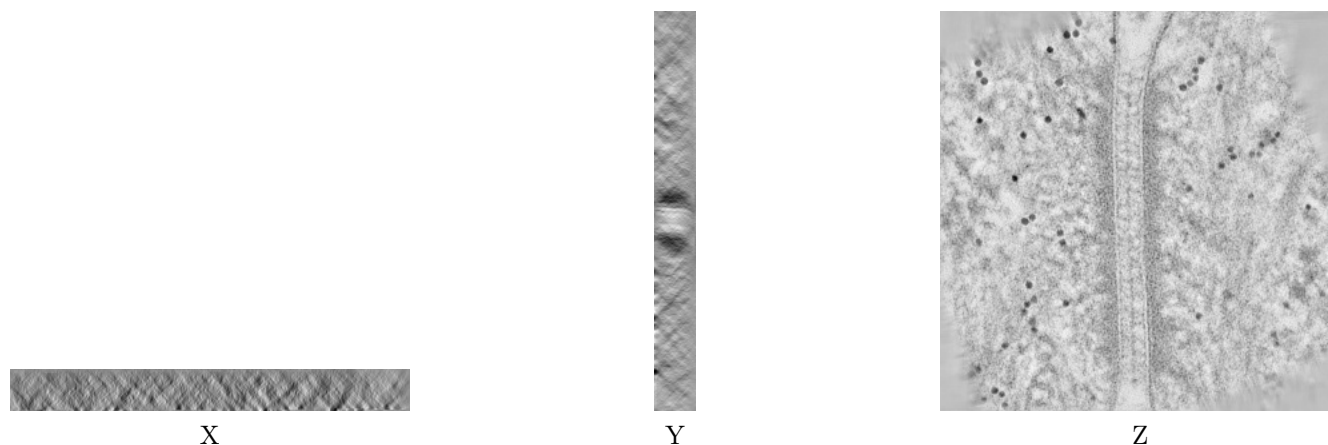
5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Tomogram visualisation [i](#)

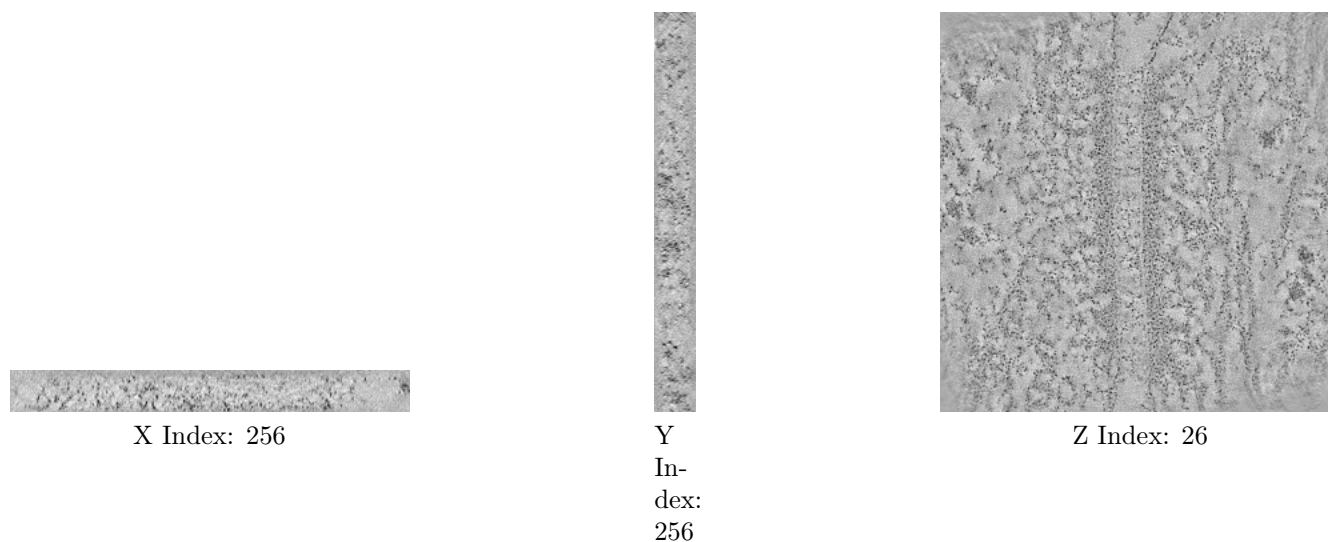
This section contains visualisations of the EMDB entry EMD-1052. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



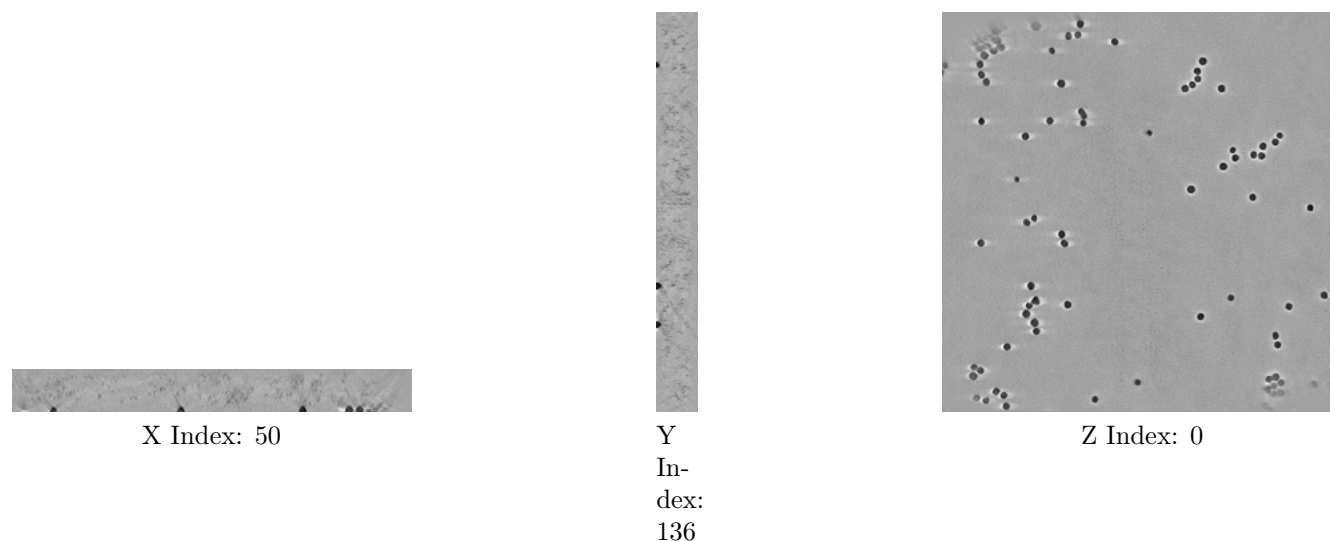
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



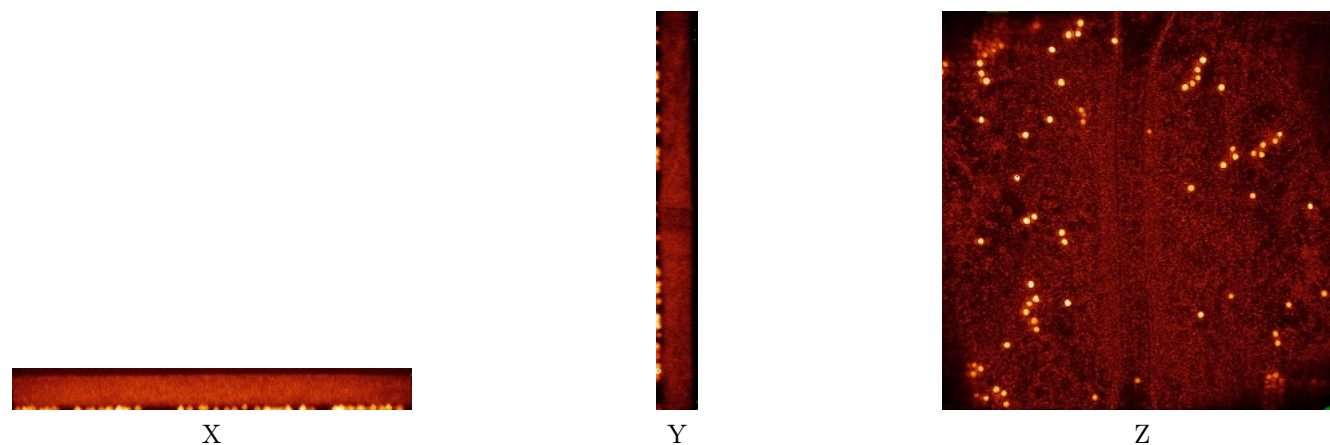
The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices [i](#)



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

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



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

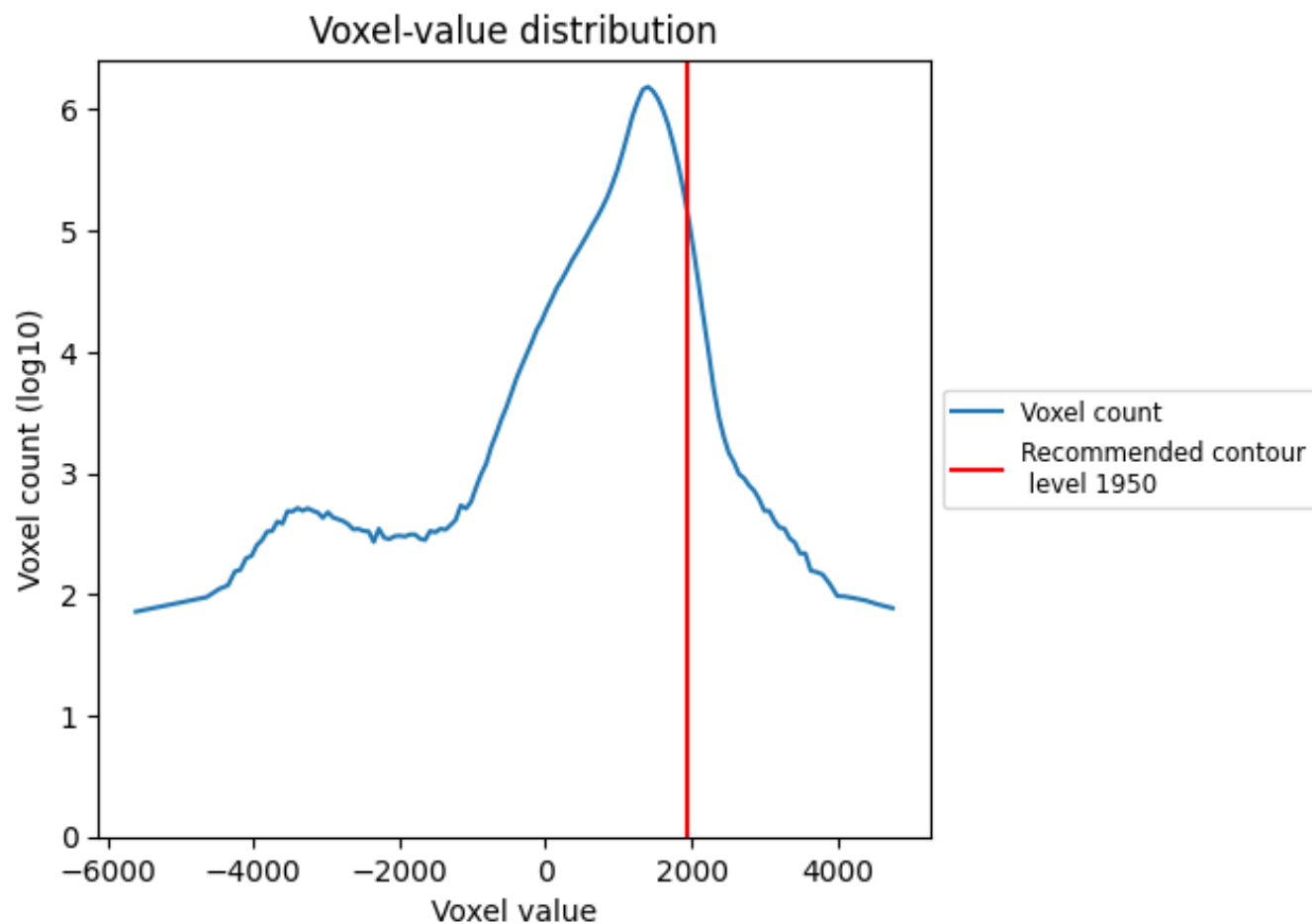
6.5 Mask visualisation [i](#)

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

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

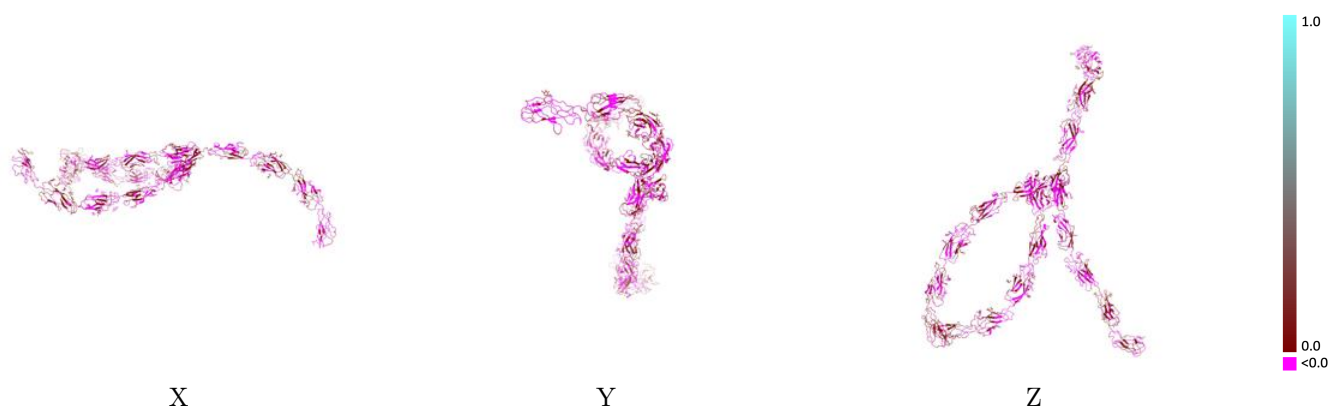
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1052 and PDB model 1Q5C. Per-residue inclusion information can be found in section 3 on page 9.

8.1 Map-model overlay [i](#)

This section was not generated.

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

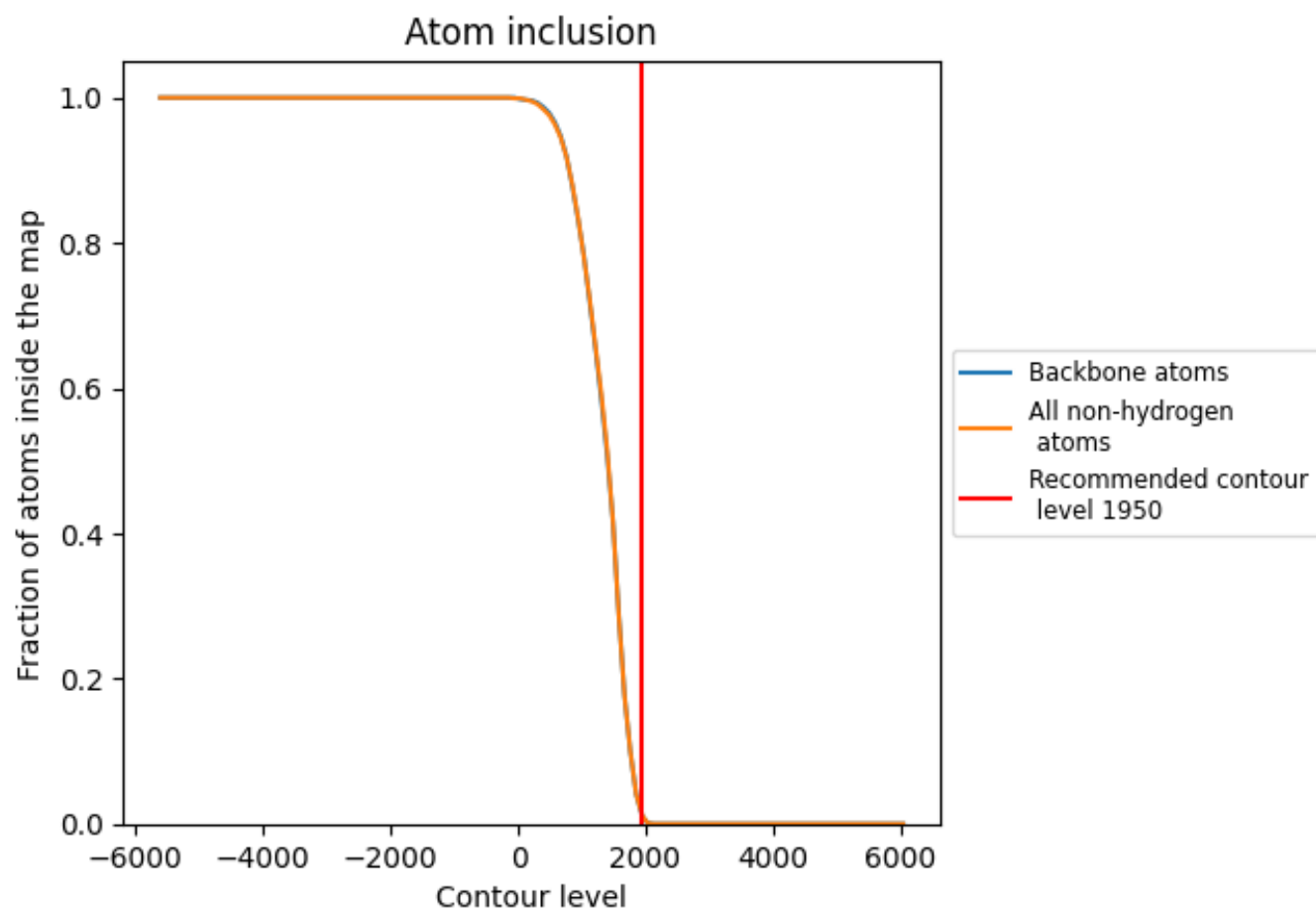


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 1% of all backbone atoms, 1% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1950) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0110	0.0020
A	0.0140	0.0090
B	0.0060	0.0060
C	0.0000	-0.0030
D	0.0240	-0.0030

