



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:21 AM UTC

PDB ID : 1Q55 / pdb_00001q55
EMDB ID : EMD-1052
Title : W-shaped trans 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

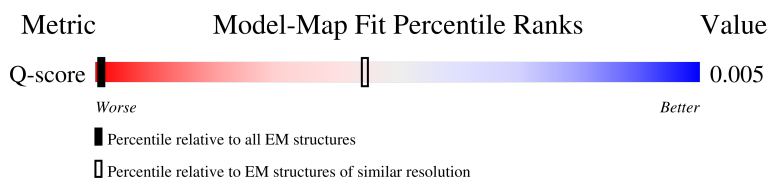
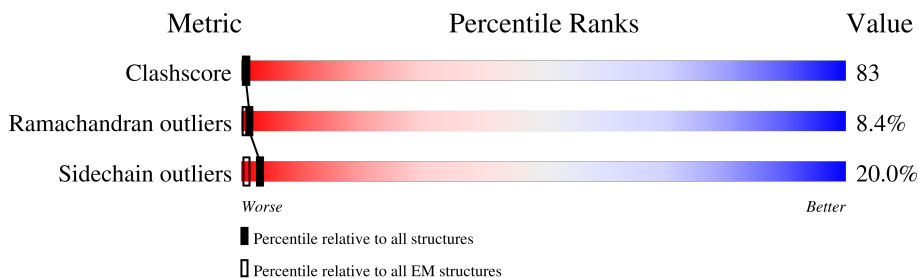
1 Overall quality at a glance i

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% 27% 15% 5% 39%
1	C	880	61% 14% 27% 15% 5% 39%
1	D	880	61% 15% 27% 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	-	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	C	811	-	-	X	-

2 Entry composition [i](#)

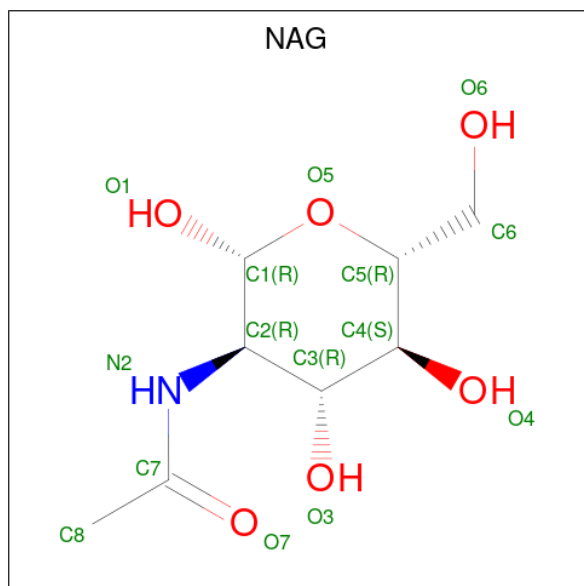
There are 4 unique types of molecules in this entry. The entry contains 17652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	A	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0
2	B	1	Total 14	C 8	N 1	O 5	0

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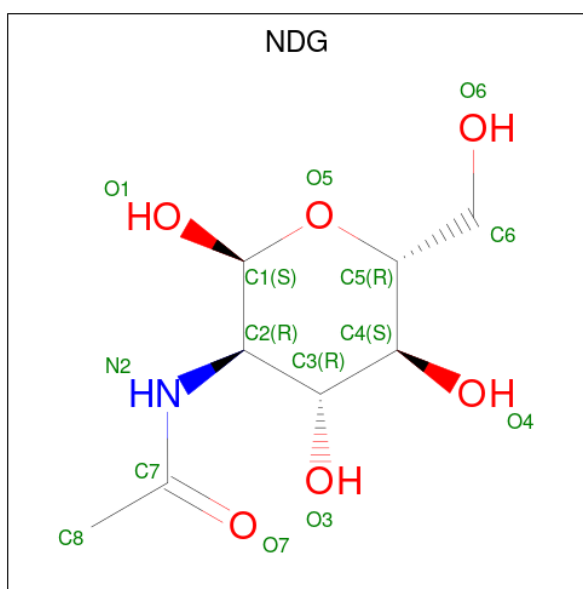
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2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

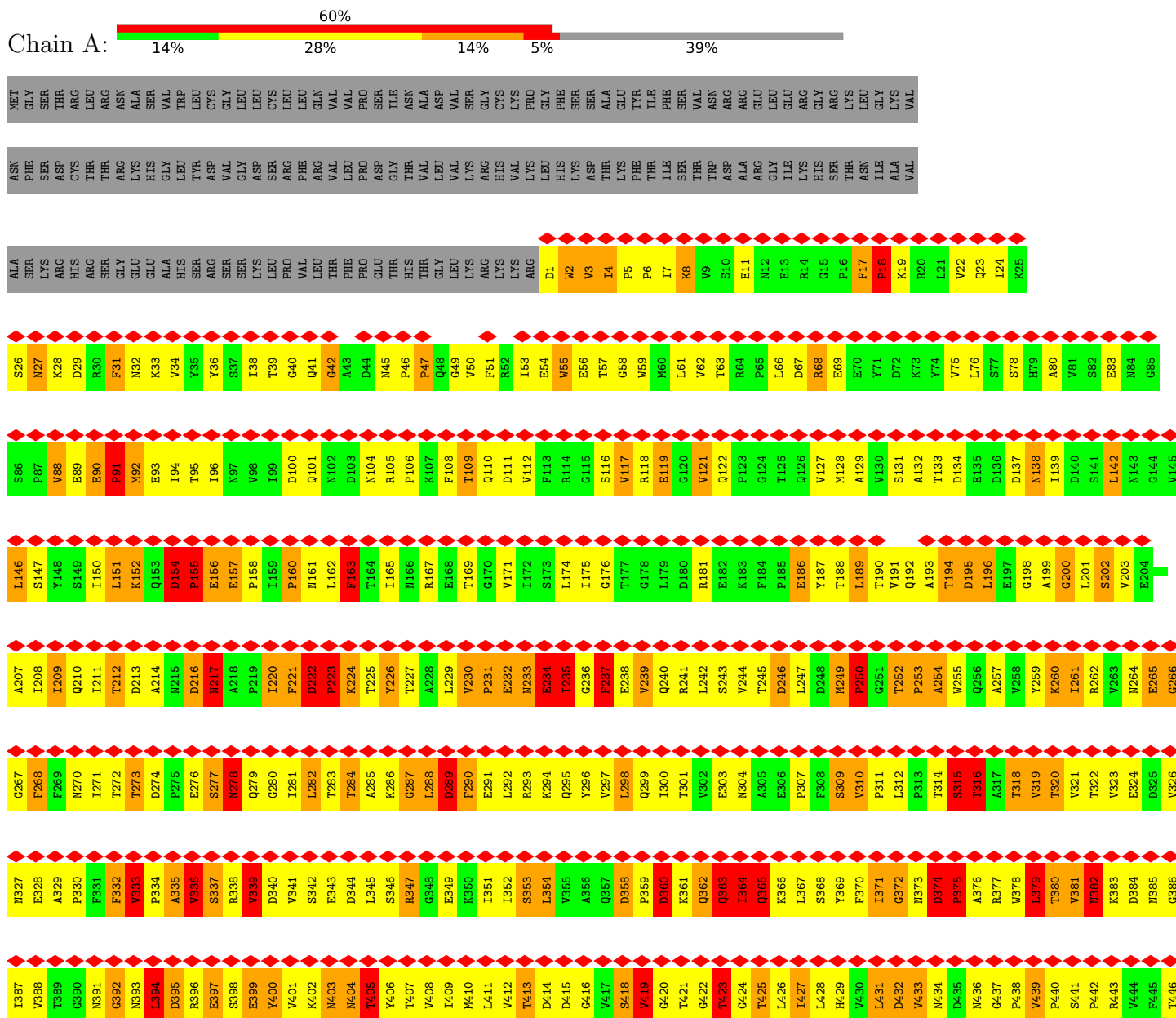
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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	

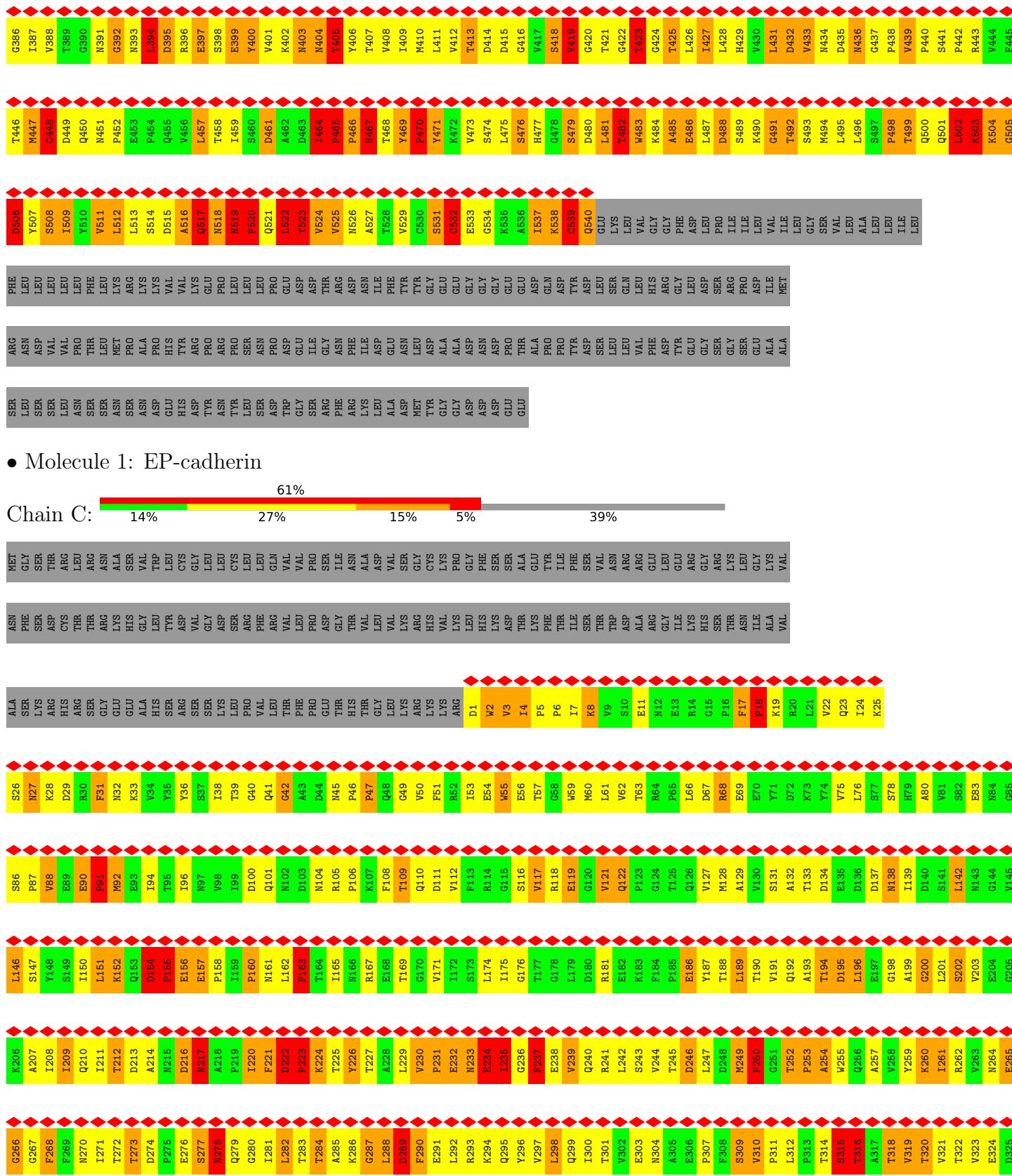
3 Residue-property plots

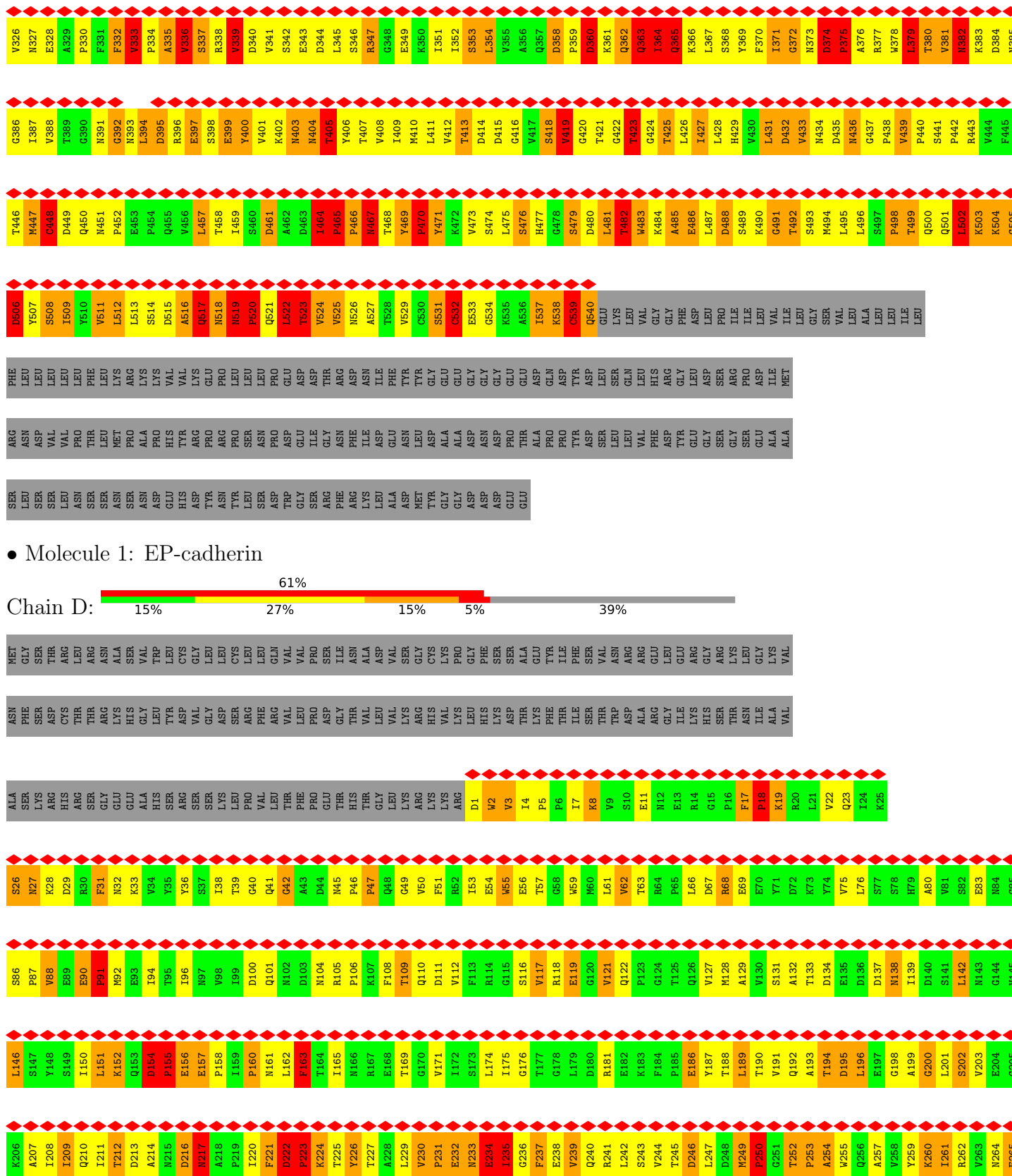
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: EP-cadherin









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
ASN	PRO	LEU	Y510	Q450	G390	P330	N270
SER	THR	PHE	Y511	M451	R391	F331	I271
SER	SER	LEU	Y512	P452	G392	F332	T272
ASN	MET	ARG	Y513	P453	R393	V333	T273
ASN	ALA	LYS	S514	L394	L394	P334	D274
ASP	PRO	LYS	S514	Q455	D395	A335	P275
GLU	HIS	VAL	D515	Q455	R396	V336	E276
HIS	TYR	VAL	A516	V456	E397	S337	S277
ASP	ARG	LYS	Q517	L457	E397	R338	N278
TYR	PRO	GLU	M518	T458	R398	V339	Q279
ASN	ARG	PRO	M519	I459	E399	D340	Q280
TYR	PRO	LEU	P520	S460	Y400	V341	I281
LEU	SER	LEU	Q521	D461	V401	S342	L282
ASN	ASN	LEU	L522	A462	K402	E343	T283
TRP	ASP	GLU	Q523	D463	N403	D344	T284
GLY	GLU	ASP	T523	P465	N404	L345	A285
SER	ILE	ASP	Y524	I464	T405	S346	K286
ARG	GLY	THR	V524	P465	Y406	R347	G287
PHE	ASN	ASP	M526	P466	T407	G348	L288
ARG	PHE	ASP	A527	M467	V408	E349	D289
LYS	ILE	ASN	L528	T468	T409	K350	F290
LEU	ASP	ILE	T528	Y469	M410	I351	E291
ALA	GLU	PHE	Y529	P470	L411	L352	L292
ASP	ASN	TYR	C530	Y471	V412	S353	R293
MET	LEU	TYR	S531	G472	D413	L354	K294
TYR	ASP	GLY	L532	K472	D414	V355	Q295
GLY	ALA	GLU	C532	L473	D415	A356	Y296
ASP	ASP	GLY	E533	S474	G416	Q357	V297
ASP	ASN	GLY	C534	L475	V417	D358	L298
ASP	ASP	GLY	K536	L475	G417	P359	Q299
GLU	PRO	GLU	A536	S476	V417	D360	I300
GLU	ALA	ASP	L537	H477	S418	K361	T301
PRO	PRO	GLN	K538	G478	V419	Q362	V302
PRO	TYR	ASP	C539	S479	G420	Q363	E303
ASP	ASP	LEU	Q540	D480	G421	I364	N304
SER	SER	LEU	GLU	L481	T421	V369	S309
LEU	LEU	SER	LYS	T482	G422	F370	V310
LEU	GLN	LEU	LEU	T482	T423	I371	P311
VAL	VAL	LEU	VAL	M483	G424	G372	L312
PHE	ASP	HIS	GLY	K484	T424	N373	P313
ASP	PHE	ARG	GLY	L485	T425	D374	T314
TYR	TYR	GLY	PHE	E486	L426	P375	S315
GLU	GLU	LEU	ASP	L487	T427	A376	T316
GLY	GLY	ASP	LEU	L487	L428	R377	A317
SER	SER	SER	PRO	D488	L428	M378	T318
GLY	ARG	ARG	ILE	S489	H429	L379	V319
SER	PRO	PRO	ILE	K490	V430	T380	V320
GLU	GLU	ASP	LEU	K490	V430	V381	V321
ALA	ALA	ILE	VAL	G491	L431	N382	T322
ALA	ALA	MET	ILE	T492	D432	K383	V323
			LEU	S493	V433	D384	E324
			LEU	M494	N434	N385	D325
			SER	L495	D435		
			LEU	L496	N436		
			ALA	S497	G437		
			LEU	P498	P438		
			LEU	T499	V439		
			ILE	Q500	P440		
			LEU	Q501	S441		
			LEU	L502	P442		
			LEU	K503	R443		
			LEU	S504	V444		
			LEU	C505	F445		

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/UT	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%)	2.02	203/5839 (3.5%)
1	B	0.99	24/4276 (0.6%)	2.02	204/5839 (3.5%)
1	C	0.99	24/4276 (0.6%)	2.02	202/5839 (3.5%)
1	D	0.99	24/4276 (0.6%)	2.02	202/5839 (3.5%)
All	All	0.99	96/17104 (0.6%)	2.02	811/23356 (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 (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	LEU	N-CA	-18.92	1.34	1.46
1	C	522	LEU	N-CA	-18.91	1.34	1.46
1	D	522	LEU	N-CA	-18.89	1.34	1.46
1	B	522	LEU	N-CA	-18.81	1.34	1.46
1	A	465	PRO	CA-C	12.07	1.58	1.51
1	B	465	PRO	CA-C	11.97	1.58	1.51
1	D	465	PRO	CA-C	11.92	1.58	1.51
1	C	465	PRO	CA-C	11.83	1.58	1.51
1	B	335	ALA	CA-CB	-11.07	1.34	1.52
1	C	335	ALA	CA-CB	-11.03	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ALA	CA-CB	-11.03	1.34	1.52
1	D	335	ALA	CA-CB	-11.03	1.34	1.52
1	C	521	GLN	CA-C	-9.90	1.40	1.52
1	D	521	GLN	CA-C	-9.88	1.40	1.52
1	B	521	GLN	CA-C	-9.88	1.40	1.52
1	A	521	GLN	CA-C	-9.80	1.40	1.52
1	D	523	THR	N-CA	-9.56	1.33	1.46
1	C	523	THR	N-CA	-9.56	1.33	1.46
1	A	523	THR	N-CA	-9.53	1.33	1.46
1	B	523	THR	N-CA	-9.50	1.33	1.46
1	A	522	LEU	CA-C	-9.34	1.40	1.52
1	C	522	LEU	CA-C	-9.32	1.40	1.52
1	B	522	LEU	CA-C	-9.32	1.40	1.52
1	D	522	LEU	CA-C	-9.30	1.40	1.52
1	B	499	THR	CA-CB	7.69	1.66	1.53
1	A	499	THR	CA-CB	7.68	1.66	1.53
1	C	499	THR	CA-CB	7.67	1.66	1.53
1	D	499	THR	CA-CB	7.65	1.66	1.53
1	C	223	PRO	CG-CD	6.78	1.73	1.50
1	D	223	PRO	CG-CD	6.78	1.73	1.50
1	A	223	PRO	CG-CD	6.76	1.73	1.50
1	B	223	PRO	CG-CD	6.76	1.73	1.50
1	D	423	THR	CA-CB	-6.63	1.44	1.53
1	B	423	THR	CA-CB	-6.59	1.44	1.53
1	A	524	VAL	N-CA	-6.58	1.38	1.46
1	D	524	VAL	N-CA	-6.56	1.38	1.46
1	C	423	THR	CA-CB	-6.55	1.44	1.53
1	D	523	THR	CA-C	-6.55	1.44	1.52
1	B	524	VAL	N-CA	-6.54	1.38	1.46
1	C	524	VAL	N-CA	-6.54	1.38	1.46
1	C	523	THR	CA-C	-6.53	1.44	1.52
1	A	423	THR	CA-CB	-6.51	1.44	1.53
1	A	523	THR	CA-C	-6.49	1.44	1.52
1	B	523	THR	CA-C	-6.47	1.44	1.52
1	A	290	PHE	CA-C	-6.20	1.45	1.52
1	D	290	PHE	CA-C	-6.18	1.45	1.52
1	C	290	PHE	CA-C	-6.17	1.45	1.52
1	A	464	ILE	C-N	6.12	1.39	1.33
1	B	290	PHE	CA-C	-6.11	1.45	1.52
1	D	399	GLU	CA-C	-6.10	1.46	1.52
1	A	399	GLU	CA-C	-6.09	1.46	1.52
1	B	399	GLU	CA-C	-6.09	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	482	THR	CA-CB	-6.08	1.43	1.53
1	C	464	ILE	C-N	6.08	1.38	1.33
1	B	482	THR	CA-CB	-6.07	1.43	1.53
1	C	399	GLU	CA-C	-6.05	1.46	1.52
1	C	481	LEU	N-CA	6.04	1.51	1.46
1	D	482	THR	CA-CB	-6.04	1.43	1.53
1	B	464	ILE	C-N	6.03	1.38	1.33
1	C	482	THR	CA-CB	-6.03	1.43	1.53
1	D	464	ILE	C-N	6.01	1.38	1.33
1	B	481	LEU	N-CA	5.98	1.51	1.46
1	C	18	PRO	N-CD	5.97	1.56	1.47
1	A	481	LEU	N-CA	5.95	1.51	1.46
1	D	18	PRO	N-CD	5.93	1.56	1.47
1	D	481	LEU	N-CA	5.92	1.51	1.46
1	B	18	PRO	N-CD	5.91	1.56	1.47
1	C	17	PHE	CA-C	5.88	1.60	1.53
1	A	18	PRO	N-CD	5.88	1.56	1.47
1	A	17	PHE	CA-C	5.83	1.60	1.53
1	D	17	PHE	CA-C	5.80	1.60	1.53
1	B	17	PHE	CA-C	5.80	1.60	1.53
1	A	521	GLN	N-CA	-5.64	1.39	1.46
1	B	521	GLN	N-CA	-5.63	1.39	1.46
1	D	521	GLN	N-CA	-5.63	1.39	1.46
1	A	481	LEU	CA-C	-5.62	1.46	1.52
1	C	481	LEU	CA-C	-5.61	1.46	1.52
1	C	521	GLN	N-CA	-5.61	1.39	1.46
1	D	481	LEU	CA-C	-5.59	1.46	1.52
1	B	481	LEU	CA-C	-5.58	1.46	1.52
1	B	18	PRO	CA-CB	-5.54	1.43	1.53
1	A	18	PRO	CA-CB	-5.52	1.43	1.53
1	C	18	PRO	CA-CB	-5.52	1.43	1.53
1	D	18	PRO	CA-CB	-5.50	1.43	1.53
1	D	320	THR	CA-CB	-5.44	1.45	1.53
1	A	320	THR	CA-CB	-5.42	1.45	1.53
1	C	320	THR	CA-CB	-5.41	1.45	1.53
1	D	483	TRP	N-CA	-5.38	1.40	1.46
1	B	320	THR	CA-CB	-5.37	1.46	1.53
1	A	483	TRP	N-CA	-5.36	1.40	1.46
1	C	483	TRP	N-CA	-5.36	1.40	1.46
1	B	483	TRP	N-CA	-5.32	1.40	1.46
1	C	17	PHE	C-O	-5.25	1.16	1.24
1	A	17	PHE	C-O	-5.21	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	PHE	C-O	-5.20	1.16	1.24
1	D	17	PHE	C-O	-5.15	1.17	1.24

All (811) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	PHE	N-CA-C	25.20	145.40	108.60
1	A	290	PHE	N-CA-C	25.19	145.38	108.60
1	D	290	PHE	N-CA-C	25.19	145.38	108.60
1	B	290	PHE	N-CA-C	25.17	145.35	108.60
1	A	516	ALA	N-CA-C	-20.89	88.42	114.75
1	D	516	ALA	N-CA-C	-20.88	88.44	114.75
1	B	516	ALA	N-CA-C	-20.87	88.45	114.75
1	C	516	ALA	N-CA-C	-20.86	88.47	114.75
1	C	376	ALA	N-CA-C	19.06	137.12	110.24
1	B	376	ALA	N-CA-C	19.05	137.11	110.24
1	D	376	ALA	N-CA-C	19.04	137.09	110.24
1	A	376	ALA	N-CA-C	18.99	137.01	110.24
1	C	235	ILE	N-CA-C	17.34	145.40	109.34
1	A	374	ASP	CA-C-N	-17.33	98.17	119.84
1	A	374	ASP	C-N-CA	-17.33	98.17	119.84
1	B	235	ILE	N-CA-C	17.33	145.39	109.34
1	B	374	ASP	CA-C-N	-17.32	98.19	119.84
1	B	374	ASP	C-N-CA	-17.32	98.19	119.84
1	A	235	ILE	N-CA-C	17.31	145.34	109.34
1	D	235	ILE	N-CA-C	17.30	145.32	109.34
1	C	374	ASP	CA-C-N	-17.28	98.24	119.84
1	C	374	ASP	C-N-CA	-17.28	98.24	119.84
1	D	374	ASP	CA-C-N	-17.27	98.25	119.84
1	D	374	ASP	C-N-CA	-17.27	98.25	119.84
1	C	481	LEU	N-CA-C	-16.72	85.91	113.50
1	D	481	LEU	N-CA-C	-16.71	85.92	113.50
1	B	481	LEU	N-CA-C	-16.71	85.92	113.50
1	A	481	LEU	N-CA-C	-16.70	85.94	113.50
1	A	336	VAL	N-CA-C	15.93	132.12	108.54
1	D	520	PRO	N-CA-C	15.93	136.32	111.15
1	B	336	VAL	N-CA-C	15.91	132.09	108.54
1	A	520	PRO	N-CA-C	15.90	136.27	111.15
1	D	336	VAL	N-CA-C	15.90	132.07	108.54
1	C	336	VAL	N-CA-C	15.89	132.05	108.54
1	B	520	PRO	N-CA-C	15.88	136.25	111.15
1	C	520	PRO	N-CA-C	15.87	136.23	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	519	ASN	CA-C-N	-15.53	104.06	119.90
1	D	519	ASN	C-N-CA	-15.53	104.06	119.90
1	A	519	ASN	CA-C-N	-15.52	104.07	119.90
1	A	519	ASN	C-N-CA	-15.52	104.07	119.90
1	B	519	ASN	CA-C-N	-15.46	104.13	119.90
1	B	519	ASN	C-N-CA	-15.46	104.13	119.90
1	C	519	ASN	CA-C-N	-15.43	104.16	119.90
1	C	519	ASN	C-N-CA	-15.43	104.16	119.90
1	A	277	SER	N-CA-C	-15.25	91.54	110.61
1	D	277	SER	N-CA-C	-15.22	91.58	110.61
1	B	277	SER	N-CA-C	-15.22	91.58	110.61
1	C	277	SER	N-CA-C	-15.22	91.58	110.61
1	D	492	THR	N-CA-C	14.89	129.35	111.33
1	A	492	THR	N-CA-C	14.85	129.29	111.33
1	C	492	THR	N-CA-C	14.84	129.29	111.33
1	B	492	THR	N-CA-C	14.82	129.27	111.33
1	B	374	ASP	N-CA-C	14.74	142.38	109.81
1	D	374	ASP	N-CA-C	14.74	142.38	109.81
1	A	374	ASP	N-CA-C	14.71	142.32	109.81
1	C	374	ASP	N-CA-C	14.70	142.29	109.81
1	C	398	SER	N-CA-C	14.52	141.74	110.80
1	D	398	SER	N-CA-C	14.50	141.69	110.80
1	B	398	SER	N-CA-C	14.50	141.69	110.80
1	A	398	SER	N-CA-C	14.49	141.67	110.80
1	A	521	GLN	CA-C-N	-13.08	103.27	121.84
1	A	521	GLN	C-N-CA	-13.08	103.27	121.84
1	B	521	GLN	CA-C-N	-13.08	103.27	121.84
1	B	521	GLN	C-N-CA	-13.08	103.27	121.84
1	D	521	GLN	CA-C-N	-13.07	103.28	121.84
1	D	521	GLN	C-N-CA	-13.07	103.28	121.84
1	C	521	GLN	CA-C-N	-13.03	103.33	121.84
1	C	521	GLN	C-N-CA	-13.03	103.33	121.84
1	B	289	ASP	CA-C-N	-12.38	100.62	121.80
1	B	289	ASP	C-N-CA	-12.38	100.62	121.80
1	A	289	ASP	CA-C-N	-12.37	100.65	121.80
1	A	289	ASP	C-N-CA	-12.37	100.65	121.80
1	C	289	ASP	CA-C-N	-12.37	100.66	121.80
1	C	289	ASP	C-N-CA	-12.37	100.66	121.80
1	D	289	ASP	CA-C-N	-12.35	100.68	121.80
1	D	289	ASP	C-N-CA	-12.35	100.68	121.80
1	A	233	ASN	N-CA-C	12.02	132.26	107.37
1	D	233	ASN	N-CA-C	12.02	132.24	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	ASN	N-CA-C	12.01	132.23	107.37
1	C	233	ASN	N-CA-C	12.01	132.23	107.37
1	B	223	PRO	N-CA-C	-11.92	87.91	112.47
1	D	223	PRO	N-CA-C	-11.92	87.91	112.47
1	C	223	PRO	N-CA-C	-11.92	87.91	112.47
1	A	223	PRO	N-CA-C	-11.90	87.96	112.47
1	A	17	PHE	C-N-CD	-11.53	95.24	120.60
1	C	17	PHE	C-N-CD	-11.53	95.24	120.60
1	D	17	PHE	C-N-CD	-11.53	95.24	120.60
1	B	17	PHE	C-N-CD	-11.52	95.26	120.60
1	B	465	PRO	C-N-CD	-11.02	96.35	120.60
1	A	465	PRO	C-N-CD	-11.02	96.35	120.60
1	D	465	PRO	C-N-CD	-11.02	96.36	120.60
1	C	465	PRO	C-N-CD	-11.02	96.37	120.60
1	B	471	TYR	N-CA-C	10.82	126.50	110.17
1	C	471	TYR	N-CA-C	10.80	126.47	110.17
1	D	471	TYR	N-CA-C	10.78	126.45	110.17
1	B	222	ASP	CA-C-N	-10.78	106.37	119.84
1	B	222	ASP	C-N-CA	-10.78	106.37	119.84
1	C	222	ASP	CA-C-N	-10.78	106.37	119.84
1	C	222	ASP	C-N-CA	-10.78	106.37	119.84
1	D	222	ASP	CA-C-N	-10.77	106.37	119.84
1	D	222	ASP	C-N-CA	-10.77	106.37	119.84
1	A	222	ASP	CA-C-N	-10.76	106.39	119.84
1	A	222	ASP	C-N-CA	-10.76	106.39	119.84
1	A	471	TYR	N-CA-C	10.76	126.42	110.17
1	C	236	GLY	N-CA-C	-10.57	88.12	113.18
1	A	236	GLY	N-CA-C	-10.57	88.13	113.18
1	B	236	GLY	N-CA-C	-10.55	88.17	113.18
1	D	236	GLY	N-CA-C	-10.55	88.17	113.18
1	D	234	GLU	CA-C-N	10.16	140.27	121.97
1	D	234	GLU	C-N-CA	10.16	140.27	121.97
1	A	234	GLU	CA-C-N	10.16	140.26	121.97
1	A	234	GLU	C-N-CA	10.16	140.26	121.97
1	C	234	GLU	CA-C-N	10.16	140.25	121.97
1	C	234	GLU	C-N-CA	10.16	140.25	121.97
1	B	522	LEU	CA-C-N	-10.13	102.18	121.54
1	B	522	LEU	C-N-CA	-10.13	102.18	121.54
1	C	522	LEU	CA-C-N	-10.13	102.19	121.54
1	C	522	LEU	C-N-CA	-10.13	102.19	121.54
1	A	522	LEU	CA-C-N	-10.13	102.19	121.54
1	A	522	LEU	C-N-CA	-10.13	102.19	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	522	LEU	CA-C-N	-10.13	102.19	121.54
1	D	522	LEU	C-N-CA	-10.13	102.19	121.54
1	B	234	GLU	CA-C-N	10.11	140.17	121.97
1	B	234	GLU	C-N-CA	10.11	140.17	121.97
1	A	230	VAL	CA-C-N	10.10	132.47	119.84
1	A	230	VAL	C-N-CA	10.10	132.47	119.84
1	C	230	VAL	CA-C-N	10.06	132.42	119.84
1	C	230	VAL	C-N-CA	10.06	132.42	119.84
1	D	230	VAL	CA-C-N	10.05	132.40	119.84
1	D	230	VAL	C-N-CA	10.05	132.40	119.84
1	B	230	VAL	CA-C-N	10.04	132.38	119.84
1	B	230	VAL	C-N-CA	10.04	132.38	119.84
1	A	332	PHE	N-CA-C	-9.97	97.37	110.53
1	C	332	PHE	N-CA-C	-9.94	97.41	110.53
1	D	332	PHE	N-CA-C	-9.93	97.42	110.53
1	B	332	PHE	N-CA-C	-9.91	97.44	110.53
1	C	221	PHE	N-CA-C	9.78	124.54	109.96
1	D	221	PHE	N-CA-C	9.78	124.53	109.96
1	A	221	PHE	N-CA-C	9.77	124.52	109.96
1	B	221	PHE	N-CA-C	9.77	124.52	109.96
1	D	374	ASP	CB-CA-C	-9.71	91.05	110.17
1	B	374	ASP	CB-CA-C	-9.70	91.07	110.17
1	D	362	GLN	N-CA-C	-9.69	90.15	110.80
1	C	374	ASP	CB-CA-C	-9.69	91.08	110.17
1	A	374	ASP	CB-CA-C	-9.69	91.08	110.17
1	C	362	GLN	N-CA-C	-9.69	90.17	110.80
1	B	405	THR	N-CA-C	9.69	125.38	110.36
1	B	362	GLN	N-CA-C	-9.69	90.17	110.80
1	A	362	GLN	N-CA-C	-9.67	90.21	110.80
1	A	405	THR	N-CA-C	9.67	125.34	110.36
1	C	405	THR	N-CA-C	9.67	125.34	110.36
1	D	405	THR	N-CA-C	9.66	125.33	110.36
1	B	249	MET	CA-C-N	9.59	131.83	119.84
1	B	249	MET	C-N-CA	9.59	131.83	119.84
1	A	221	PHE	CA-C-N	-9.57	98.44	121.80
1	A	221	PHE	C-N-CA	-9.57	98.44	121.80
1	B	221	PHE	CA-C-N	-9.57	98.45	121.80
1	B	221	PHE	C-N-CA	-9.57	98.45	121.80
1	C	221	PHE	CA-C-N	-9.57	98.46	121.80
1	C	221	PHE	C-N-CA	-9.57	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	MET	CA-C-N	9.56	131.79	119.84
1	C	249	MET	C-N-CA	9.56	131.79	119.84
1	A	249	MET	CA-C-N	9.56	131.79	119.84
1	A	249	MET	C-N-CA	9.56	131.79	119.84
1	D	221	PHE	CA-C-N	-9.55	98.49	121.80
1	D	221	PHE	C-N-CA	-9.55	98.49	121.80
1	C	398	SER	CA-C-N	-9.54	105.28	122.46
1	C	398	SER	C-N-CA	-9.54	105.28	122.46
1	D	398	SER	CA-C-N	-9.54	105.28	122.46
1	D	398	SER	C-N-CA	-9.54	105.28	122.46
1	B	398	SER	CA-C-N	-9.54	105.29	122.46
1	B	398	SER	C-N-CA	-9.54	105.29	122.46
1	C	234	GLU	N-CA-C	-9.53	90.51	110.80
1	A	234	GLU	N-CA-C	-9.52	90.52	110.80
1	B	234	GLU	N-CA-C	-9.52	90.52	110.80
1	D	234	GLU	N-CA-C	-9.52	90.53	110.80
1	D	249	MET	CA-C-N	9.50	131.72	119.84
1	D	249	MET	C-N-CA	9.50	131.72	119.84
1	A	319	VAL	N-CA-C	9.43	122.51	108.46
1	B	319	VAL	N-CA-C	9.43	122.50	108.46
1	D	319	VAL	N-CA-C	9.41	122.48	108.46
1	C	319	VAL	N-CA-C	9.40	122.47	108.46
1	C	479	SER	N-CA-C	-9.23	101.72	113.16
1	A	479	SER	N-CA-C	-9.21	101.73	113.16
1	B	479	SER	N-CA-C	-9.20	101.75	113.16
1	A	337	SER	N-CA-C	-9.17	91.64	108.24
1	D	479	SER	N-CA-C	-9.17	101.79	113.16
1	C	337	SER	N-CA-C	-9.16	91.65	108.24
1	B	337	SER	N-CA-C	-9.16	91.66	108.24
1	D	337	SER	N-CA-C	-9.16	91.66	108.24
1	C	503	LYS	N-CA-C	8.99	129.94	110.80
1	A	503	LYS	N-CA-C	8.98	129.94	110.80
1	B	503	LYS	N-CA-C	8.98	129.93	110.80
1	C	403	ASN	N-CA-C	-8.98	95.78	109.79
1	D	403	ASN	N-CA-C	-8.97	95.79	109.79
1	A	403	ASN	N-CA-C	-8.97	95.79	109.79
1	B	403	ASN	N-CA-C	-8.97	95.80	109.79
1	D	503	LYS	N-CA-C	8.97	129.90	110.80
1	A	382	ASN	N-CA-C	-8.62	95.26	108.96
1	D	382	ASN	N-CA-C	-8.62	95.26	108.96
1	C	382	ASN	N-CA-C	-8.60	95.29	108.96
1	B	382	ASN	N-CA-C	-8.60	95.29	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	GLN	N-CA-C	-8.49	96.92	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	B	521	GLN	N-CA-C	-8.46	96.96	109.15
1	D	476	SER	N-CA-C	8.44	128.78	110.80
1	C	476	SER	N-CA-C	8.43	128.76	110.80
1	B	476	SER	N-CA-C	8.42	128.74	110.80
1	A	476	SER	N-CA-C	8.41	128.72	110.80
1	D	397	GLU	N-CA-C	8.41	123.27	112.34
1	C	397	GLU	N-CA-C	8.39	123.24	112.34
1	B	397	GLU	N-CA-C	8.38	123.23	112.34
1	A	397	GLU	N-CA-C	8.35	123.20	112.34
1	D	520	PRO	CA-C-N	8.32	134.63	121.66
1	D	520	PRO	C-N-CA	8.32	134.63	121.66
1	C	520	PRO	CA-C-N	8.31	134.62	121.66
1	C	520	PRO	C-N-CA	8.31	134.62	121.66
1	A	520	PRO	CA-C-N	8.28	134.58	121.66
1	A	520	PRO	C-N-CA	8.28	134.58	121.66
1	B	520	PRO	CA-C-N	8.27	134.55	121.66
1	B	520	PRO	C-N-CA	8.27	134.55	121.66
1	C	291	GLU	N-CA-C	-8.26	101.29	112.94
1	B	291	GLU	N-CA-C	-8.25	101.30	112.94
1	A	291	GLU	N-CA-C	-8.24	101.31	112.94
1	D	291	GLU	N-CA-C	-8.23	101.33	112.94
1	C	532	CYS	N-CA-C	8.10	128.05	110.80
1	A	254	ALA	N-CA-C	-8.10	102.43	112.88
1	A	532	CYS	N-CA-C	8.09	128.03	110.80
1	B	532	CYS	N-CA-C	8.09	128.03	110.80
1	D	254	ALA	N-CA-C	-8.07	102.47	112.88
1	B	31	PHE	N-CA-C	8.07	121.25	111.40
1	B	254	ALA	N-CA-C	-8.07	102.47	112.88
1	D	31	PHE	N-CA-C	8.07	121.24	111.40
1	D	532	CYS	N-CA-C	8.07	127.98	110.80
1	B	222	ASP	N-CA-C	8.06	127.62	109.81
1	C	254	ALA	N-CA-C	-8.06	102.48	112.88
1	D	222	ASP	N-CA-C	8.06	127.63	109.81
1	A	31	PHE	N-CA-C	8.06	121.23	111.40
1	C	222	ASP	N-CA-C	8.06	127.61	109.81
1	A	222	ASP	N-CA-C	8.05	127.61	109.81
1	C	31	PHE	N-CA-C	8.04	121.21	111.40
1	A	46	PRO	C-N-CD	-8.03	102.93	120.60
1	C	46	PRO	C-N-CD	-8.03	102.94	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	46	PRO	C-N-CD	-8.03	102.94	120.60
1	B	46	PRO	C-N-CD	-8.01	102.97	120.60
1	A	290	PHE	CA-C-O	7.96	129.82	121.38
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	D	397	GLU	CA-C-N	-7.94	106.38	121.54
1	D	397	GLU	C-N-CA	-7.94	106.38	121.54
1	D	290	PHE	CA-C-O	7.93	129.78	121.38
1	C	290	PHE	CA-C-O	7.93	129.78	121.38
1	B	397	GLU	CA-C-N	-7.92	106.41	121.54
1	B	397	GLU	C-N-CA	-7.92	106.41	121.54
1	D	523	THR	N-CA-CB	-7.92	97.10	110.49
1	A	523	THR	N-CA-CB	-7.91	97.12	110.49
1	C	397	GLU	CA-C-N	-7.91	106.43	121.54
1	C	397	GLU	C-N-CA	-7.91	106.43	121.54
1	C	523	THR	N-CA-CB	-7.91	97.12	110.49
1	B	523	THR	N-CA-CB	-7.91	97.12	110.49
1	B	290	PHE	CA-C-O	7.89	129.75	121.38
1	A	222	ASP	CA-CB-CG	-7.86	104.74	112.60
1	D	222	ASP	CA-CB-CG	-7.85	104.75	112.60
1	C	222	ASP	CA-CB-CG	-7.84	104.76	112.60
1	B	222	ASP	CA-CB-CG	-7.82	104.78	112.60
1	B	381	VAL	N-CA-C	7.81	119.86	108.53
1	A	381	VAL	N-CA-C	7.81	119.86	108.53
1	D	381	VAL	N-CA-C	7.80	119.84	108.53
1	C	381	VAL	N-CA-C	7.79	119.83	108.53
1	C	502	LEU	N-CA-C	7.77	127.35	110.80
1	D	502	LEU	N-CA-C	7.77	127.35	110.80
1	B	502	LEU	N-CA-C	7.76	127.33	110.80
1	A	502	LEU	N-CA-C	7.74	127.29	110.80
1	A	246	ASP	N-CA-C	-7.72	99.10	110.52
1	B	432	ASP	N-CA-C	7.72	122.42	109.76
1	A	432	ASP	N-CA-C	7.72	122.42	109.76
1	D	432	ASP	N-CA-C	7.70	122.39	109.76
1	D	246	ASP	N-CA-C	-7.70	99.13	110.52
1	B	246	ASP	N-CA-C	-7.69	99.13	110.52
1	C	432	ASP	N-CA-C	7.69	122.38	109.76
1	C	246	ASP	N-CA-C	-7.68	99.15	110.52
1	A	315	SER	N-CA-C	7.67	120.91	108.41
1	C	315	SER	N-CA-C	7.67	120.91	108.41
1	C	17	PHE	CA-C-O	-7.65	113.71	120.60
1	B	525	VAL	N-CA-C	-7.65	93.43	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	525	VAL	N-CA-C	-7.65	93.44	109.34
1	D	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	113.73	120.60
1	C	525	VAL	N-CA-C	-7.63	93.46	109.34
1	B	315	SER	N-CA-C	7.63	120.85	108.41
1	D	17	PHE	CA-C-O	-7.62	113.75	120.60
1	B	17	PHE	CA-C-O	-7.61	113.75	120.60
1	B	522	LEU	N-CA-C	-7.61	97.15	108.34
1	D	522	LEU	N-CA-C	-7.59	97.18	108.34
1	C	522	LEU	N-CA-C	-7.59	97.18	108.34
1	C	320	THR	N-CA-C	7.58	120.88	108.52
1	D	290	PHE	CA-C-N	7.58	134.04	122.37
1	D	290	PHE	C-N-CA	7.58	134.04	122.37
1	C	290	PHE	CA-C-N	7.58	134.04	122.37
1	C	290	PHE	C-N-CA	7.58	134.04	122.37
1	B	320	THR	N-CA-C	7.56	120.84	108.52
1	A	522	LEU	N-CA-C	-7.55	97.24	108.34
1	A	320	THR	N-CA-C	7.55	120.82	108.52
1	A	290	PHE	CA-C-N	7.54	133.98	122.37
1	A	290	PHE	C-N-CA	7.54	133.98	122.37
1	D	320	THR	N-CA-C	7.54	120.80	108.52
1	B	290	PHE	CA-C-N	7.52	133.96	122.37
1	B	290	PHE	C-N-CA	7.52	133.96	122.37
1	C	522	LEU	N-CA-CB	7.48	118.54	111.59
1	B	522	LEU	N-CA-CB	7.47	118.54	111.59
1	A	339	VAL	N-CA-C	7.43	124.80	109.34
1	B	339	VAL	N-CA-C	7.43	124.80	109.34
1	B	290	PHE	O-C-N	7.43	131.06	123.26
1	C	339	VAL	N-CA-C	7.43	124.79	109.34
1	D	522	LEU	N-CA-CB	7.42	118.49	111.59
1	D	339	VAL	N-CA-C	7.42	124.76	109.34
1	A	522	LEU	N-CA-CB	7.41	118.48	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	D	217	ASN	N-CA-C	7.39	121.71	109.95
1	C	217	ASN	N-CA-C	7.39	121.69	109.95
1	B	217	ASN	N-CA-C	7.38	121.68	109.95
1	D	252	THR	CA-C-N	7.38	129.06	119.84
1	D	252	THR	C-N-CA	7.38	129.06	119.84
1	A	217	ASN	N-CA-C	7.37	121.67	109.95
1	C	62	VAL	N-CA-C	-7.37	97.81	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	THR	CA-C-N	7.37	129.06	119.84
1	B	252	THR	C-N-CA	7.37	129.06	119.84
1	C	290	PHE	O-C-N	7.37	131.00	123.26
1	A	290	PHE	O-C-N	7.37	130.99	123.26
1	B	62	VAL	N-CA-C	-7.36	97.83	108.36
1	A	62	VAL	N-CA-C	-7.35	97.85	108.36
1	D	62	VAL	N-CA-C	-7.35	97.86	108.36
1	D	290	PHE	O-C-N	7.35	130.97	123.26
1	A	252	THR	CA-C-N	7.33	129.01	119.84
1	A	252	THR	C-N-CA	7.33	129.01	119.84
1	C	379	LEU	N-CA-C	7.19	119.59	110.24
1	B	379	LEU	N-CA-C	7.18	119.57	110.24
1	A	266	GLY	N-CA-C	-7.17	103.32	115.80
1	C	266	GLY	N-CA-C	-7.17	103.32	115.80
1	B	266	GLY	N-CA-C	-7.17	103.32	115.80
1	D	379	LEU	N-CA-C	7.17	119.56	110.24
1	D	266	GLY	N-CA-C	-7.16	103.34	115.80
1	A	379	LEU	N-CA-C	7.15	119.54	110.24
1	B	90	GLU	N-CA-C	-7.14	99.19	109.48
1	D	90	GLU	N-CA-C	-7.13	99.20	109.48
1	A	90	GLU	N-CA-C	-7.11	99.25	109.48
1	D	358	ASP	CA-C-N	7.10	128.71	119.84
1	D	358	ASP	C-N-CA	7.10	128.71	119.84
1	C	90	GLU	N-CA-C	-7.09	99.27	109.48
1	A	358	ASP	CA-C-N	7.08	128.69	119.84
1	A	358	ASP	C-N-CA	7.08	128.69	119.84
1	C	358	ASP	CA-C-N	7.08	128.69	119.84
1	C	358	ASP	C-N-CA	7.08	128.69	119.84
1	C	519	ASN	N-CA-C	7.07	125.44	109.81
1	D	519	ASN	N-CA-C	7.07	125.44	109.81
1	B	519	ASN	N-CA-C	7.07	125.43	109.81
1	A	519	ASN	N-CA-C	7.06	125.41	109.81
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	A	485	ALA	N-CA-C	7.04	120.43	110.50
1	D	485	ALA	N-CA-C	7.03	120.42	110.50
1	B	485	ALA	N-CA-C	7.03	120.41	110.50
1	A	399	GLU	N-CA-C	7.03	121.71	112.72
1	C	485	ALA	N-CA-C	7.02	120.40	110.50
1	B	194	THR	N-CA-C	7.02	120.59	109.50
1	D	399	GLU	N-CA-C	7.01	121.69	112.72
1	C	399	GLU	N-CA-C	7.01	121.69	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	THR	N-CA-C	7.00	120.57	109.50
1	B	399	GLU	N-CA-C	7.00	121.68	112.72
1	A	194	THR	N-CA-C	7.00	120.56	109.50
1	C	194	THR	N-CA-C	7.00	120.55	109.50
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	B	439	VAL	CA-C-N	6.96	126.72	119.76
1	B	439	VAL	C-N-CA	6.96	126.72	119.76
1	A	104	ASN	N-CA-C	6.95	120.26	109.07
1	C	439	VAL	CA-C-N	6.95	126.71	119.76
1	C	439	VAL	C-N-CA	6.95	126.71	119.76
1	B	104	ASN	N-CA-C	6.94	120.24	109.07
1	D	104	ASN	N-CA-C	6.93	120.22	109.07
1	C	104	ASN	N-CA-C	6.92	120.22	109.07
1	A	439	VAL	CA-C-N	6.91	126.67	119.76
1	A	439	VAL	C-N-CA	6.91	126.67	119.76
1	A	481	LEU	CA-C-O	6.90	126.03	118.65
1	D	252	THR	N-CA-C	6.89	119.35	110.39
1	A	364	ILE	N-CA-C	-6.89	95.01	109.34
1	D	481	LEU	CA-C-O	6.89	126.02	118.65
1	C	364	ILE	N-CA-C	-6.88	95.03	109.34
1	B	364	ILE	N-CA-C	-6.87	95.06	109.34
1	C	252	THR	N-CA-C	6.87	119.32	110.39
1	C	491	GLY	N-CA-C	6.87	129.45	113.18
1	D	364	ILE	N-CA-C	-6.87	95.06	109.34
1	B	221	PHE	CA-C-O	-6.86	112.81	120.70
1	C	481	LEU	CA-C-O	6.86	125.99	118.65
1	B	491	GLY	N-CA-C	6.86	129.44	113.18
1	A	252	THR	N-CA-C	6.86	119.31	110.39
1	D	491	GLY	N-CA-C	6.85	129.42	113.18
1	A	491	GLY	N-CA-C	6.85	129.41	113.18
1	B	481	LEU	CA-C-O	6.85	125.98	118.65
1	A	520	PRO	CA-C-O	6.84	129.09	121.36
1	A	221	PHE	CA-C-O	-6.84	112.84	120.70
1	C	221	PHE	CA-C-O	-6.83	112.84	120.70
1	B	252	THR	N-CA-C	6.83	119.27	110.39
1	D	221	PHE	CA-C-O	-6.83	112.84	120.70
1	D	520	PRO	CA-C-O	6.83	129.08	121.36
1	C	119	GLU	N-CA-C	6.82	118.72	111.28
1	B	520	PRO	CA-C-O	6.82	129.06	121.36
1	C	520	PRO	CA-C-O	6.81	129.06	121.36
1	D	119	GLU	N-CA-C	6.79	118.68	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	GLU	N-CA-C	6.78	118.67	111.28
1	B	119	GLU	N-CA-C	6.77	118.66	111.28
1	A	484	LYS	CA-C-N	6.71	131.48	120.94
1	A	484	LYS	C-N-CA	6.71	131.48	120.94
1	B	484	LYS	CA-C-N	6.69	131.44	120.94
1	B	484	LYS	C-N-CA	6.69	131.44	120.94
1	C	484	LYS	CA-C-N	6.69	131.44	120.94
1	C	484	LYS	C-N-CA	6.69	131.44	120.94
1	D	484	LYS	CA-C-N	6.68	131.43	120.94
1	D	484	LYS	C-N-CA	6.68	131.43	120.94
1	A	2	TRP	N-CA-C	-6.62	94.74	107.57
1	C	2	TRP	N-CA-C	-6.62	94.74	107.57
1	B	2	TRP	N-CA-C	-6.60	94.76	107.57
1	D	2	TRP	N-CA-C	-6.60	94.77	107.57
1	B	46	PRO	CA-C-N	6.56	142.74	127.00
1	B	46	PRO	C-N-CA	6.56	142.74	127.00
1	A	46	PRO	CA-C-N	6.56	142.74	127.00
1	A	46	PRO	C-N-CA	6.56	142.74	127.00
1	C	46	PRO	CA-C-N	6.55	142.72	127.00
1	C	46	PRO	C-N-CA	6.55	142.72	127.00
1	C	486	GLU	N-CA-C	6.55	118.47	108.52
1	D	46	PRO	CA-C-N	6.55	142.71	127.00
1	D	46	PRO	C-N-CA	6.55	142.71	127.00
1	A	486	GLU	N-CA-C	6.54	118.46	108.52
1	B	232	GLU	N-CA-C	6.53	118.99	111.02
1	D	486	GLU	N-CA-C	6.53	118.45	108.52
1	B	437	GLY	CA-C-N	6.53	128.00	119.84
1	B	437	GLY	C-N-CA	6.53	128.00	119.84
1	A	232	GLU	N-CA-C	6.52	118.98	111.02
1	A	437	GLY	CA-C-N	6.52	127.99	119.84
1	A	437	GLY	C-N-CA	6.52	127.99	119.84
1	C	232	GLU	N-CA-C	6.51	118.97	111.02
1	D	437	GLY	CA-C-N	6.51	127.98	119.84
1	D	437	GLY	C-N-CA	6.51	127.98	119.84
1	B	335	ALA	N-CA-C	-6.51	93.90	107.37
1	D	335	ALA	N-CA-C	-6.50	93.91	107.37
1	B	486	GLU	N-CA-C	6.50	118.40	108.52
1	C	437	GLY	CA-C-N	6.49	127.95	119.84
1	C	437	GLY	C-N-CA	6.49	127.95	119.84
1	D	232	GLU	N-CA-C	6.49	118.94	111.02
1	A	335	ALA	N-CA-C	-6.49	93.94	107.37
1	C	539	CYS	N-CA-C	6.48	124.59	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	335	ALA	N-CA-C	-6.47	93.97	107.37
1	D	522	LEU	CA-CB-CG	-6.45	93.71	116.30
1	A	539	CYS	N-CA-C	6.45	124.54	110.80
1	C	522	LEU	CA-CB-CG	-6.44	93.75	116.30
1	B	522	LEU	CA-CB-CG	-6.44	93.76	116.30
1	D	539	CYS	N-CA-C	6.44	124.51	110.80
1	A	522	LEU	CA-CB-CG	-6.43	93.78	116.30
1	B	121	VAL	N-CA-C	6.43	117.48	110.21
1	B	539	CYS	N-CA-C	6.43	124.50	110.80
1	D	230	VAL	C-N-CD	-6.42	98.69	125.00
1	C	400	TYR	N-CA-C	-6.42	103.57	111.40
1	A	230	VAL	C-N-CD	-6.41	98.71	125.00
1	C	230	VAL	C-N-CD	-6.41	98.72	125.00
1	D	121	VAL	N-CA-C	6.41	117.45	110.21
1	B	230	VAL	C-N-CD	-6.41	98.73	125.00
1	B	400	TYR	N-CA-C	-6.41	103.59	111.40
1	C	121	VAL	N-CA-C	6.40	117.44	110.21
1	A	121	VAL	N-CA-C	6.40	117.44	110.21
1	D	400	TYR	N-CA-C	-6.39	103.60	111.40
1	C	531	SER	N-CA-C	6.39	124.41	110.80
1	A	400	TYR	N-CA-C	-6.38	103.61	111.40
1	B	531	SER	N-CA-C	6.37	124.38	110.80
1	A	531	SER	N-CA-C	6.36	124.36	110.80
1	D	531	SER	N-CA-C	6.35	124.33	110.80
1	A	328	GLU	N-CA-C	6.35	120.27	110.42
1	B	42	GLY	N-CA-C	-6.34	107.54	115.08
1	D	42	GLY	N-CA-C	-6.33	107.54	115.08
1	C	42	GLY	N-CA-C	-6.33	107.55	115.08
1	D	328	GLU	N-CA-C	6.33	120.23	110.42
1	A	42	GLY	N-CA-C	-6.33	107.55	115.08
1	B	328	GLU	N-CA-C	6.32	120.22	110.42
1	C	26	SER	N-CA-C	-6.32	99.39	109.76
1	A	26	SER	N-CA-C	-6.32	99.40	109.76
1	A	431	LEU	N-CA-C	6.32	119.01	109.41
1	C	328	GLU	N-CA-C	6.31	120.21	110.42
1	D	26	SER	N-CA-C	-6.31	99.41	109.76
1	D	431	LEU	N-CA-C	6.31	119.00	109.41
1	B	26	SER	N-CA-C	-6.31	99.42	109.76
1	C	431	LEU	N-CA-C	6.29	118.97	109.41
1	B	431	LEU	N-CA-C	6.27	118.94	109.41
1	C	380	THR	N-CA-C	6.27	118.70	108.55
1	A	380	THR	N-CA-C	6.26	118.69	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	GLN	N-CA-C	6.25	118.91	110.29
1	D	380	THR	N-CA-C	6.25	118.67	108.55
1	C	304	ASN	N-CA-C	-6.24	100.97	110.14
1	A	122	GLN	N-CA-C	6.24	118.89	110.29
1	B	304	ASN	N-CA-C	-6.23	100.98	110.14
1	D	122	GLN	N-CA-C	6.23	118.89	110.29
1	A	304	ASN	N-CA-C	-6.23	100.98	110.14
1	B	380	THR	N-CA-C	6.23	118.64	108.55
1	C	122	GLN	N-CA-C	6.21	118.86	110.29
1	D	304	ASN	N-CA-C	-6.21	101.01	110.14
1	A	186	GLU	N-CA-C	6.21	118.41	107.61
1	A	413	THR	N-CA-C	6.21	119.02	108.90
1	A	233	ASN	CB-CA-C	-6.21	103.26	111.82
1	C	233	ASN	CB-CA-C	-6.19	103.28	111.82
1	B	413	THR	N-CA-C	6.19	118.98	108.90
1	B	233	ASN	CB-CA-C	-6.18	103.29	111.82
1	D	413	THR	N-CA-C	6.18	118.98	108.90
1	D	233	ASN	CB-CA-C	-6.18	103.29	111.82
1	C	413	THR	N-CA-C	6.17	118.96	108.90
1	D	470	PRO	N-CA-C	6.17	125.18	112.47
1	A	163	PHE	N-CA-C	6.17	118.33	109.14
1	D	186	GLU	N-CA-C	6.16	118.33	107.61
1	A	470	PRO	N-CA-C	6.16	125.16	112.47
1	B	222	ASP	N-CA-CB	6.16	121.33	110.37
1	D	222	ASP	N-CA-CB	6.16	121.33	110.37
1	B	186	GLU	N-CA-C	6.16	118.32	107.61
1	B	470	PRO	N-CA-C	6.16	125.15	112.47
1	C	163	PHE	N-CA-C	6.15	118.31	109.14
1	B	163	PHE	N-CA-C	6.15	118.31	109.14
1	A	222	ASP	N-CA-CB	6.15	121.31	110.37
1	D	163	PHE	N-CA-C	6.15	118.30	109.14
1	D	39	THR	N-CA-C	6.15	119.05	109.52
1	C	470	PRO	N-CA-C	6.14	125.12	112.47
1	B	503	LYS	CB-CA-C	-6.14	98.20	110.42
1	C	222	ASP	N-CA-CB	6.14	121.30	110.37
1	A	503	LYS	CB-CA-C	-6.14	98.21	110.42
1	C	39	THR	N-CA-C	6.14	119.03	109.52
1	B	234	GLU	O-C-N	6.13	130.75	122.59
1	C	503	LYS	CB-CA-C	-6.12	98.24	110.42
1	B	39	THR	N-CA-C	6.12	119.01	109.52
1	D	503	LYS	CB-CA-C	-6.12	98.24	110.42
1	C	186	GLU	N-CA-C	6.12	118.38	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	THR	N-CA-C	6.11	118.98	109.52
1	C	18	PRO	CA-N-CD	-6.10	102.96	111.50
1	A	18	PRO	CA-N-CD	-6.10	102.96	111.50
1	D	234	GLU	O-C-N	6.09	130.69	122.59
1	B	18	PRO	CA-N-CD	-6.09	102.98	111.50
1	D	18	PRO	CA-N-CD	-6.07	103.00	111.50
1	A	234	GLU	O-C-N	6.07	130.66	122.59
1	A	376	ALA	CA-C-N	6.05	133.10	121.54
1	A	376	ALA	C-N-CA	6.05	133.10	121.54
1	C	481	LEU	CA-CB-CG	-6.05	95.12	116.30
1	C	234	GLU	O-C-N	6.05	130.64	122.59
1	D	376	ALA	CA-C-N	6.05	133.09	121.54
1	D	376	ALA	C-N-CA	6.05	133.09	121.54
1	C	157	GLU	CA-C-N	6.05	141.51	127.00
1	C	157	GLU	C-N-CA	6.05	141.51	127.00
1	D	157	GLU	CA-C-N	6.04	141.50	127.00
1	D	157	GLU	C-N-CA	6.04	141.50	127.00
1	B	481	LEU	CA-CB-CG	-6.04	95.16	116.30
1	B	157	GLU	CA-C-N	6.04	141.49	127.00
1	B	157	GLU	C-N-CA	6.04	141.49	127.00
1	D	481	LEU	CA-CB-CG	-6.04	95.17	116.30
1	B	488	ASP	N-CA-C	-6.03	102.00	110.50
1	A	481	LEU	CA-CB-CG	-6.03	95.21	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	D	488	ASP	N-CA-C	-6.03	102.00	110.50
1	C	376	ALA	CA-C-N	6.02	133.04	121.54
1	C	376	ALA	C-N-CA	6.02	133.04	121.54
1	A	488	ASP	N-CA-C	-6.02	102.02	110.50
1	A	157	GLU	CA-C-N	6.02	141.44	127.00
1	A	157	GLU	C-N-CA	6.02	141.44	127.00
1	C	488	ASP	N-CA-C	-6.00	102.03	110.50
1	C	504	LYS	N-CA-C	5.92	119.35	108.58
1	D	504	LYS	N-CA-C	5.91	119.34	108.58
1	B	504	LYS	N-CA-C	5.91	119.33	108.58
1	A	504	LYS	N-CA-C	5.89	119.30	108.58
1	B	245	THR	N-CA-C	5.89	117.07	107.23
1	C	245	THR	N-CA-C	5.88	117.06	107.23
1	D	245	THR	N-CA-C	5.87	117.04	107.23
1	A	245	THR	N-CA-C	5.87	117.03	107.23
1	D	314	THR	CA-C-N	-5.84	114.77	123.00
1	D	314	THR	C-N-CA	-5.84	114.77	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	GLY	N-CA-C	5.84	127.01	113.18
1	B	505	GLY	N-CA-C	5.84	127.01	113.18
1	D	505	GLY	N-CA-C	5.84	127.01	113.18
1	A	314	THR	CA-C-N	-5.82	114.79	123.00
1	A	314	THR	C-N-CA	-5.82	114.79	123.00
1	C	505	GLY	N-CA-C	5.82	126.98	113.18
1	C	314	THR	CA-C-N	-5.81	114.81	123.00
1	C	314	THR	C-N-CA	-5.81	114.81	123.00
1	B	314	THR	CA-C-N	-5.80	114.81	123.00
1	B	314	THR	C-N-CA	-5.80	114.81	123.00
1	B	481	LEU	O-C-N	5.78	128.66	121.84
1	C	481	LEU	O-C-N	5.78	128.66	121.84
1	A	481	LEU	O-C-N	5.76	128.64	121.84
1	A	326	VAL	N-CA-C	-5.76	99.98	108.85
1	A	465	PRO	CA-C-N	5.76	140.82	127.00
1	A	465	PRO	C-N-CA	5.76	140.82	127.00
1	B	469	TYR	CA-C-N	5.75	127.03	119.84
1	B	469	TYR	C-N-CA	5.75	127.03	119.84
1	C	469	TYR	CA-C-N	5.74	127.02	119.84
1	C	469	TYR	C-N-CA	5.74	127.02	119.84
1	B	465	PRO	CA-C-N	5.74	140.77	127.00
1	B	465	PRO	C-N-CA	5.74	140.77	127.00
1	D	469	TYR	CA-C-N	5.74	127.01	119.84
1	D	469	TYR	C-N-CA	5.74	127.01	119.84
1	D	481	LEU	O-C-N	5.73	128.60	121.84
1	D	326	VAL	N-CA-C	-5.73	100.03	108.85
1	B	326	VAL	N-CA-C	-5.72	100.04	108.85
1	C	326	VAL	N-CA-C	-5.72	100.05	108.85
1	C	465	PRO	CA-C-N	5.72	140.72	127.00
1	C	465	PRO	C-N-CA	5.72	140.72	127.00
1	A	469	TYR	CA-C-N	5.71	126.98	119.84
1	A	469	TYR	C-N-CA	5.71	126.98	119.84
1	D	465	PRO	CA-C-N	5.71	140.72	127.00
1	D	465	PRO	C-N-CA	5.71	140.72	127.00
1	B	520	PRO	O-C-N	5.70	130.12	122.89
1	D	520	PRO	O-C-N	5.68	130.11	122.89
1	A	353	SER	N-CA-C	-5.68	99.86	108.67
1	C	520	PRO	O-C-N	5.67	130.10	122.89
1	A	376	ALA	CA-C-O	5.67	127.39	121.15
1	B	353	SER	N-CA-C	-5.67	99.88	108.67
1	A	520	PRO	O-C-N	5.66	130.08	122.89
1	D	353	SER	N-CA-C	-5.66	99.89	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	353	SER	N-CA-C	-5.65	99.91	108.67
1	A	235	ILE	N-CA-CB	-5.63	101.93	111.23
1	B	235	ILE	N-CA-CB	-5.63	101.93	111.23
1	C	235	ILE	N-CA-CB	-5.63	101.94	111.23
1	A	365	GLN	CA-C-N	-5.62	112.86	123.27
1	A	365	GLN	C-N-CA	-5.62	112.86	123.27
1	D	235	ILE	N-CA-CB	-5.60	101.98	111.23
1	B	376	ALA	CA-C-O	5.60	127.31	121.15
1	D	376	ALA	CA-C-O	5.60	127.31	121.15
1	C	376	ALA	CA-C-O	5.59	127.30	121.15
1	C	365	GLN	CA-C-N	-5.59	112.93	123.27
1	C	365	GLN	C-N-CA	-5.59	112.93	123.27
1	C	418	SER	N-CA-C	5.58	122.69	110.80
1	B	365	GLN	CA-C-N	-5.58	112.95	123.27
1	B	365	GLN	C-N-CA	-5.58	112.95	123.27
1	B	133	THR	N-CA-C	5.57	117.54	109.07
1	C	133	THR	N-CA-C	5.57	117.54	109.07
1	D	237	PHE	N-CA-C	5.57	117.56	108.76
1	D	418	SER	N-CA-C	5.57	122.67	110.80
1	B	237	PHE	N-CA-C	5.57	117.56	108.76
1	A	133	THR	N-CA-C	5.56	117.53	109.07
1	B	418	SER	N-CA-C	5.56	122.65	110.80
1	C	237	PHE	N-CA-C	5.56	117.55	108.76
1	D	365	GLN	CA-C-N	-5.56	112.98	123.27
1	D	365	GLN	C-N-CA	-5.56	112.98	123.27
1	A	237	PHE	N-CA-C	5.56	117.54	108.76
1	D	133	THR	N-CA-C	5.56	117.52	109.07
1	A	418	SER	N-CA-C	5.54	122.61	110.80
1	A	538	LYS	N-CA-C	-5.50	102.14	110.28
1	C	224	LYS	N-CA-C	-5.50	107.12	113.88
1	C	538	LYS	N-CA-C	-5.50	102.15	110.28
1	D	157	GLU	C-N-CD	-5.49	108.53	120.60
1	B	538	LYS	N-CA-C	-5.48	102.16	110.28
1	D	222	ASP	C-N-CD	-5.48	102.54	125.00
1	C	222	ASP	C-N-CD	-5.48	102.55	125.00
1	C	157	GLU	C-N-CD	-5.47	108.56	120.60
1	B	222	ASP	C-N-CD	-5.47	102.56	125.00
1	A	222	ASP	C-N-CD	-5.47	102.57	125.00
1	D	538	LYS	N-CA-C	-5.47	102.19	110.28
1	A	224	LYS	N-CA-C	-5.47	107.16	113.88
1	B	157	GLU	C-N-CD	-5.46	108.58	120.60
1	B	224	LYS	N-CA-C	-5.46	107.16	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ILE	CA-C-N	5.45	125.99	120.38
1	A	4	ILE	C-N-CA	5.45	125.99	120.38
1	B	480	ASP	CA-C-N	5.45	128.56	120.17
1	B	480	ASP	C-N-CA	5.45	128.56	120.17
1	A	157	GLU	C-N-CD	-5.45	108.61	120.60
1	D	224	LYS	N-CA-C	-5.44	107.19	113.88
1	D	235	ILE	CA-C-N	5.44	132.07	121.41
1	D	235	ILE	C-N-CA	5.44	132.07	121.41
1	D	532	CYS	N-CA-CB	-5.44	101.30	110.49
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	B	532	CYS	N-CA-CB	-5.43	101.31	110.49
1	B	235	ILE	CA-C-N	5.43	132.05	121.41
1	B	235	ILE	C-N-CA	5.43	132.05	121.41
1	D	392	GLY	N-CA-C	5.43	122.06	112.83
1	C	532	CYS	N-CA-CB	-5.43	101.32	110.49
1	B	392	GLY	N-CA-C	5.42	122.05	112.83
1	B	4	ILE	CA-C-N	5.42	125.97	120.38
1	B	4	ILE	C-N-CA	5.42	125.97	120.38
1	D	4	ILE	CA-C-N	5.42	125.96	120.38
1	D	4	ILE	C-N-CA	5.42	125.96	120.38
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	448	CYS	CA-CB-SG	-5.42	101.95	114.40
1	A	448	CYS	CA-CB-SG	-5.41	101.95	114.40
1	C	392	GLY	N-CA-C	5.41	122.03	112.83
1	C	448	CYS	CA-CB-SG	-5.41	101.96	114.40
1	A	392	GLY	N-CA-C	5.41	122.02	112.83
1	A	532	CYS	N-CA-CB	-5.41	101.35	110.49
1	A	235	ILE	CA-C-N	5.41	132.01	121.41
1	A	235	ILE	C-N-CA	5.41	132.01	121.41
1	D	448	CYS	CA-CB-SG	-5.40	101.98	114.40
1	A	480	ASP	CA-C-N	5.40	128.48	120.17
1	A	480	ASP	C-N-CA	5.40	128.48	120.17
1	C	480	ASP	CA-C-N	5.40	128.48	120.17
1	C	480	ASP	C-N-CA	5.40	128.48	120.17
1	C	502	LEU	CB-CA-C	-5.40	99.68	110.42
1	D	502	LEU	CB-CA-C	-5.40	99.68	110.42
1	C	4	ILE	CA-C-N	5.39	125.94	120.38
1	C	4	ILE	C-N-CA	5.39	125.94	120.38
1	B	502	LEU	CB-CA-C	-5.39	99.70	110.42
1	C	209	ILE	N-CA-C	5.38	115.71	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	LEU	CB-CA-C	-5.38	99.72	110.42
1	A	209	ILE	N-CA-C	5.37	115.69	108.17
1	D	209	ILE	N-CA-C	5.37	115.68	108.17
1	B	209	ILE	N-CA-C	5.35	115.66	108.17
1	D	527	ALA	N-CA-C	5.34	117.04	107.80
1	A	527	ALA	N-CA-C	5.33	117.02	107.80
1	C	527	ALA	N-CA-C	5.32	117.01	107.80
1	B	527	ALA	N-CA-C	5.32	117.00	107.80
1	C	142	LEU	N-CA-C	-5.32	106.02	112.88
1	D	250	PRO	N-CA-C	5.30	123.39	112.47
1	A	142	LEU	N-CA-C	-5.30	106.05	112.88
1	B	295	GLN	N-CA-C	5.29	118.43	109.76
1	C	465	PRO	N-CA-C	5.29	115.55	110.47
1	B	142	LEU	N-CA-C	-5.28	106.06	112.88
1	C	295	GLN	N-CA-C	5.28	118.42	109.76
1	D	295	GLN	N-CA-C	5.28	118.42	109.76
1	B	250	PRO	N-CA-C	5.28	123.35	112.47
1	A	423	THR	N-CA-C	5.28	116.91	108.41
1	D	142	LEU	N-CA-C	-5.28	106.07	112.88
1	D	465	PRO	N-CA-C	5.28	115.54	110.47
1	A	465	PRO	N-CA-C	5.28	115.53	110.47
1	A	250	PRO	N-CA-C	5.27	123.33	112.47
1	A	295	GLN	N-CA-C	5.27	118.40	109.76
1	B	465	PRO	N-CA-C	5.26	115.52	110.47
1	C	250	PRO	N-CA-C	5.26	123.30	112.47
1	B	520	PRO	CA-CB-CG	-5.25	94.52	104.50
1	C	316	THR	N-CA-C	5.25	117.63	110.55
1	C	423	THR	N-CA-C	5.25	116.86	108.41
1	A	520	PRO	CA-CB-CG	-5.24	94.54	104.50
1	D	520	PRO	CA-CB-CG	-5.24	94.54	104.50
1	B	506	ASP	N-CA-C	5.24	121.96	110.80
1	C	520	PRO	CA-CB-CG	-5.24	94.55	104.50
1	A	316	THR	N-CA-C	5.24	117.62	110.55
1	B	537	ILE	N-CA-C	5.24	117.31	109.20
1	D	316	THR	N-CA-C	5.24	117.62	110.55
1	B	423	THR	N-CA-C	5.22	116.82	108.41
1	C	506	ASP	N-CA-C	5.22	121.93	110.80
1	D	235	ILE	CA-C-O	5.22	127.31	120.78
1	A	506	ASP	N-CA-C	5.22	121.92	110.80
1	D	423	THR	N-CA-C	5.22	116.82	108.41
1	A	221	PHE	CB-CA-C	-5.22	102.64	110.16
1	D	467	ASN	N-CA-C	5.22	121.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	537	ILE	N-CA-C	5.21	117.28	109.20
1	B	235	ILE	CA-C-O	5.21	127.29	120.78
1	C	537	ILE	N-CA-C	5.21	117.28	109.20
1	D	506	ASP	N-CA-C	5.21	121.89	110.80
1	A	235	ILE	CA-C-O	5.21	127.29	120.78
1	A	537	ILE	N-CA-C	5.21	117.27	109.20
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	502	LEU	CA-C-N	5.20	131.48	121.54
1	D	502	LEU	C-N-CA	5.20	131.48	121.54
1	A	467	ASN	N-CA-C	5.20	121.87	110.80
1	B	467	ASN	N-CA-C	5.20	121.87	110.80
1	C	467	ASN	N-CA-C	5.20	121.87	110.80
1	A	336	VAL	N-CA-CB	-5.19	105.13	110.95
1	C	465	PRO	CA-C-O	5.19	124.64	120.90
1	B	316	THR	N-CA-C	5.19	117.56	110.55
1	A	502	LEU	CA-C-N	5.19	131.45	121.54
1	A	502	LEU	C-N-CA	5.19	131.45	121.54
1	B	502	LEU	CA-C-N	5.19	131.44	121.54
1	B	502	LEU	C-N-CA	5.19	131.44	121.54
1	B	221	PHE	CB-CA-C	-5.18	102.69	110.16
1	C	221	PHE	CB-CA-C	-5.18	102.70	110.16
1	C	235	ILE	CA-C-O	5.18	127.26	120.78
1	C	294	LYS	N-CA-C	-5.17	107.62	114.04
1	D	221	PHE	CB-CA-C	-5.17	102.72	110.16
1	A	465	PRO	CA-C-O	5.17	124.62	120.90
1	A	294	LYS	N-CA-C	-5.16	107.64	114.04
1	B	465	PRO	CA-C-O	5.16	124.61	120.90
1	B	336	VAL	N-CA-CB	-5.15	105.18	110.95
1	C	336	VAL	N-CA-CB	-5.15	105.18	110.95
1	D	249	MET	N-CA-C	5.15	121.20	109.81
1	A	18	PRO	CA-CB-CG	-5.14	94.24	104.00
1	A	394	LEU	N-CA-C	-5.13	102.56	109.95
1	D	294	LYS	N-CA-C	-5.13	107.68	114.04
1	D	336	VAL	N-CA-CB	-5.13	105.20	110.95
1	B	154	ASP	CA-C-N	-5.13	113.43	119.84
1	B	154	ASP	C-N-CA	-5.13	113.43	119.84
1	C	18	PRO	CA-CB-CG	-5.13	94.26	104.00
1	C	249	MET	N-CA-C	5.12	121.14	109.81
1	B	249	MET	N-CA-C	5.12	121.13	109.81
1	D	18	PRO	CA-CB-CG	-5.12	94.27	104.00
1	B	394	LEU	N-CA-C	-5.12	102.58	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	PRO	CA-CB-CG	-5.12	94.28	104.00
1	A	249	MET	N-CA-C	5.11	121.11	109.81
1	C	154	ASP	CA-C-N	-5.11	113.46	119.84
1	C	154	ASP	C-N-CA	-5.11	113.46	119.84
1	D	465	PRO	CA-C-O	5.10	124.57	120.90
1	B	294	LYS	N-CA-C	-5.10	107.72	114.04
1	D	154	ASP	CA-C-N	-5.10	113.47	119.84
1	D	154	ASP	C-N-CA	-5.10	113.47	119.84
1	A	154	ASP	CA-C-N	-5.08	113.49	119.84
1	A	154	ASP	C-N-CA	-5.08	113.49	119.84
1	D	508	SER	N-CA-C	5.07	118.21	110.36
1	C	419	VAL	N-CA-C	5.05	114.93	107.75
1	B	508	SER	N-CA-C	5.05	118.19	110.36
1	C	508	SER	N-CA-C	5.05	118.19	110.36
1	A	508	SER	N-CA-C	5.04	118.18	110.36
1	A	419	VAL	N-CA-C	5.02	114.88	107.75
1	D	419	VAL	N-CA-C	5.01	114.87	107.75
1	B	5	PRO	N-CA-C	5.01	116.81	110.70
1	B	419	VAL	N-CA-C	5.01	114.86	107.75

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	4086	777	0
1	B	4191	0	4089	770	0
1	C	4191	0	4087	743	0
1	D	4191	0	4086	733	0
2	A	182	0	169	87	0
2	B	182	0	169	88	0
2	C	182	0	169	87	0
2	D	182	0	169	88	0
3	A	28	0	24	9	0
3	B	28	0	24	9	0
3	C	28	0	24	9	0
3	D	28	0	24	8	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	17120	2897	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 83.

All (2897) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.61
1:D:464:ILE:HD12	1:D:465:PRO:CD	1.30	1.59
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.56
1:C:464:ILE:HD12	1:C:465:PRO:CD	1.30	1.56
1:D:464:ILE:CD1	1:D:465:PRO:HD2	1.50	1.42
1:C:464:ILE:CD1	1:C:465:PRO:HD2	1.50	1.42
1:A:464:ILE:CD1	1:A:465:PRO:HD2	1.50	1.40
1:B:464:ILE:CD1	1:B:465:PRO:HD2	1.50	1.39
1:C:92:MET:HE3	1:D:2:TRP:CB	1.55	1.36
1:C:24:ILE:HG21	1:D:2:TRP:CA	1.42	1.35
1:C:27:ASN:HD21	1:D:90:GLU:CB	1.39	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ASP:OD1	1:D:26:SER:CA	1.80	1.30
1:A:93:GLU:O	1:B:2:TRP:HB3	1.12	1.29
1:C:24:ILE:CG2	1:D:2:TRP:HA	1.54	1.28
1:C:22:VAL:CG2	1:D:5:PRO:HG3	1.63	1.27
1:D:540:GLN:O	1:D:540:GLN:CD	1.79	1.26
1:A:540:GLN:O	1:A:540:GLN:CD	1.79	1.25
1:A:93:GLU:C	1:B:2:TRP:HB3	1.61	1.25
1:B:540:GLN:O	1:B:540:GLN:CD	1.79	1.25
1:C:540:GLN:O	1:C:540:GLN:CD	1.79	1.24
1:C:24:ILE:CG2	1:D:2:TRP:CA	2.00	1.23
1:C:27:ASN:CG	1:D:90:GLU:HB3	1.61	1.23
1:A:2:TRP:HD1	1:B:93:GLU:CD	1.46	1.23
1:C:27:ASN:ND2	1:D:90:GLU:HB3	1.53	1.23
1:A:1:ASP:O	1:B:94:ILE:CA	1.71	1.22
1:C:27:ASN:ND2	1:D:90:GLU:CB	2.02	1.22
1:C:1:ASP:OD1	1:D:26:SER:HA	1.04	1.21
1:B:8:LYS:H	1:B:8:LYS:HD2	1.04	1.20
1:C:92:MET:CE	1:D:2:TRP:HB2	1.70	1.19
1:C:450:GLN:HG2	1:C:532:CYS:O	1.43	1.18
1:A:2:TRP:CD1	1:B:93:GLU:OE1	1.97	1.18
1:C:482:THR:HG23	1:C:499:THR:CG2	1.75	1.17
1:B:234:GLU:H	1:B:235:ILE:HG23	1.08	1.17
1:A:5:PRO:CA	1:B:5:PRO:HG3	1.74	1.16
1:A:93:GLU:O	1:B:2:TRP:CB	1.94	1.16
1:A:234:GLU:H	1:A:235:ILE:HG23	1.08	1.16
1:A:482:THR:HG23	1:A:499:THR:CG2	1.75	1.16
1:D:154:ASP:C	2:D:801:NAG:H82	1.70	1.16
1:C:8:LYS:H	1:C:8:LYS:HD2	1.04	1.16
1:D:469:TYR:CG	1:D:470:PRO:HD2	1.81	1.16
1:A:469:TYR:CG	1:A:470:PRO:HD2	1.81	1.15
1:B:423:THR:HB	2:B:810:NAG:C7	1.76	1.15
1:B:469:TYR:CG	1:B:470:PRO:HD2	1.80	1.15
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.15
1:D:482:THR:HG23	1:D:499:THR:CG2	1.75	1.15
1:B:154:ASP:C	2:B:801:NAG:H82	1.70	1.15
1:B:450:GLN:HG2	1:B:532:CYS:O	1.43	1.15
1:A:450:GLN:HG2	1:A:532:CYS:O	1.44	1.15
1:C:27:ASN:ND2	1:D:90:GLU:CG	2.10	1.15
1:C:154:ASP:C	2:C:801:NAG:H82	1.70	1.15
1:C:423:THR:HB	2:C:810:NAG:C7	1.76	1.15
1:A:154:ASP:C	2:A:801:NAG:H82	1.70	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:THR:HB	2:D:810:NAG:C7	1.76	1.15
1:C:469:TYR:CG	1:C:470:PRO:HD2	1.81	1.14
1:B:301:THR:HG21	2:B:805:NAG:H82	1.29	1.14
1:B:482:THR:HG23	1:B:499:THR:CG2	1.75	1.14
1:A:90:GLU:HB2	1:B:90:GLU:N	1.63	1.14
1:A:403:ASN:HB2	2:A:902:NAG:H83	1.30	1.14
1:C:301:THR:HG21	2:C:805:NAG:H82	1.29	1.14
1:C:338:ARG:HD3	1:C:352:ILE:HG22	1.26	1.14
1:D:450:GLN:HG2	1:D:532:CYS:O	1.43	1.12
1:C:92:MET:CE	1:D:2:TRP:CB	2.27	1.12
1:C:234:GLU:H	1:C:235:ILE:HG23	1.08	1.12
1:D:474:SER:HB2	1:D:512:LEU:HG	1.25	1.11
1:D:8:LYS:H	1:D:8:LYS:HD2	1.04	1.11
1:B:338:ARG:HD3	1:B:352:ILE:HG22	1.26	1.11
1:C:474:SER:HB2	1:C:512:LEU:HG	1.25	1.11
1:D:32:ASN:HD21	1:D:83:GLU:HB2	0.98	1.11
1:D:227:THR:HG21	2:D:807:NAG:C8	1.82	1.10
1:A:227:THR:HG21	2:A:807:NAG:C8	1.82	1.10
1:A:338:ARG:HD3	1:A:352:ILE:HG22	1.25	1.10
1:D:403:ASN:HB2	2:D:902:NAG:H83	1.30	1.09
1:B:32:ASN:HD21	1:B:83:GLU:HB2	0.98	1.09
1:D:301:THR:HG21	2:D:805:NAG:H82	1.29	1.09
1:A:222:ASP:OD1	1:A:222:ASP:O	1.69	1.09
1:C:227:THR:HG21	2:C:807:NAG:C8	1.82	1.09
1:A:3:VAL:N	1:B:4:ILE:O	1.58	1.09
1:C:222:ASP:OD1	1:C:222:ASP:O	1.69	1.09
1:A:301:THR:HG21	2:A:805:NAG:H82	1.29	1.08
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.08
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
1:A:32:ASN:HD21	1:A:83:GLU:HB2	0.98	1.08
1:C:290:PHE:HB2	1:C:292:LEU:N	1.69	1.08
1:D:234:GLU:H	1:D:235:ILE:HG23	1.08	1.08
1:A:2:TRP:CH2	1:B:95:THR:HG21	1.88	1.08
1:B:222:ASP:O	1:B:222:ASP:OD1	1.69	1.08
1:B:485:ALA:O	1:B:486:GLU:HG2	1.54	1.07
1:C:27:ASN:OD1	1:D:90:GLU:HB3	1.53	1.07
1:D:222:ASP:OD1	1:D:222:ASP:O	1.69	1.07
1:D:485:ALA:O	1:D:486:GLU:HG2	1.54	1.07
1:C:450:GLN:CG	1:C:532:CYS:O	2.03	1.07
1:C:482:THR:HG23	1:C:499:THR:HG22	1.09	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ALA:O	1:A:486:GLU:HG2	1.55	1.07
1:B:482:THR:HG23	1:B:499:THR:HG22	1.09	1.07
1:D:338:ARG:HD3	1:D:352:ILE:HG22	1.26	1.07
1:A:5:PRO:HA	1:B:5:PRO:HG3	1.08	1.07
1:C:403:ASN:HB2	2:C:902:NAG:H83	1.30	1.07
1:A:8:LYS:H	1:A:8:LYS:HD2	1.04	1.07
1:A:482:THR:HG23	1:A:499:THR:HG22	1.09	1.07
1:B:403:ASN:HB2	2:B:902:NAG:H83	1.30	1.07
1:B:474:SER:HB2	1:B:512:LEU:HG	1.25	1.07
1:A:290:PHE:HB2	1:A:292:LEU:N	1.69	1.06
1:D:337:SER:HA	1:D:427:ILE:HG23	1.38	1.06
1:A:335:ALA:HB1	3:A:811:NDG:O6	1.54	1.06
1:A:92:MET:SD	1:B:3:VAL:HA	1.94	1.06
1:B:450:GLN:CG	1:B:532:CYS:O	2.02	1.06
1:A:2:TRP:CD2	1:B:95:THR:OG1	2.07	1.06
1:B:290:PHE:HB2	1:B:292:LEU:N	1.69	1.06
1:B:337:SER:HA	1:B:427:ILE:HG23	1.38	1.06
1:D:450:GLN:CG	1:D:532:CYS:O	2.02	1.06
1:B:335:ALA:HB1	3:B:811:NDG:O6	1.54	1.06
1:C:485:ALA:O	1:C:486:GLU:HG2	1.54	1.06
1:D:290:PHE:HB2	1:D:292:LEU:N	1.69	1.06
1:D:464:ILE:CD1	1:D:465:PRO:CD	2.20	1.06
1:B:469:TYR:CD1	1:B:470:PRO:HD2	1.91	1.05
1:C:335:ALA:HB1	3:C:811:NDG:O6	1.54	1.05
1:C:22:VAL:HG23	1:D:5:PRO:HG3	1.06	1.05
1:C:469:TYR:CD1	1:C:470:PRO:HD2	1.91	1.05
1:D:482:THR:HG23	1:D:499:THR:HG22	1.09	1.05
1:A:450:GLN:CG	1:A:532:CYS:O	2.03	1.05
1:A:469:TYR:CD1	1:A:470:PRO:HD2	1.91	1.05
1:A:464:ILE:CD1	1:A:465:PRO:CD	2.20	1.05
1:B:522:LEU:HD22	1:B:523:THR:HB	1.39	1.05
1:C:27:ASN:ND2	1:D:90:GLU:HG2	1.69	1.05
1:D:335:ALA:HB1	3:D:811:NDG:O6	1.54	1.05
1:D:469:TYR:CD1	1:D:470:PRO:HD2	1.92	1.05
1:B:290:PHE:HB2	1:B:292:LEU:H	0.88	1.04
1:A:2:TRP:CD1	1:B:93:GLU:CD	2.34	1.04
1:C:482:THR:HG21	1:C:499:THR:H	1.23	1.04
1:C:290:PHE:HB2	1:C:292:LEU:H	0.88	1.04
1:A:290:PHE:HB2	1:A:292:LEU:H	0.88	1.03
1:D:522:LEU:HD22	1:D:523:THR:HB	1.39	1.03
1:A:5:PRO:HA	1:B:5:PRO:CG	1.89	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:THR:CG2	1:A:499:THR:N	2.22	1.03
1:C:337:SER:HA	1:C:427:ILE:HG23	1.38	1.03
1:A:482:THR:HG21	1:A:499:THR:H	1.23	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	1.03
1:B:482:THR:CG2	1:B:499:THR:N	2.22	1.02
1:C:522:LEU:HD22	1:C:523:THR:HB	1.39	1.02
1:B:450:GLN:HB2	1:B:533:GLU:HA	1.41	1.02
1:B:482:THR:HG21	1:B:499:THR:H	1.23	1.02
1:D:290:PHE:HB2	1:D:292:LEU:H	0.89	1.02
1:B:403:ASN:HB2	2:B:902:NAG:C8	1.90	1.02
1:B:464:ILE:CD1	1:B:465:PRO:CD	2.20	1.02
1:D:403:ASN:HB2	2:D:902:NAG:C8	1.90	1.02
1:C:403:ASN:HB2	2:C:902:NAG:C8	1.90	1.02
1:A:337:SER:HA	1:A:427:ILE:HG23	1.38	1.02
1:A:403:ASN:HB2	2:A:902:NAG:C8	1.90	1.02
1:A:522:LEU:HD22	1:A:523:THR:HB	1.39	1.02
1:A:450:GLN:HB2	1:A:533:GLU:HA	1.41	1.01
1:D:482:THR:HG21	1:D:499:THR:H	1.23	1.01
1:A:432:ASP:OD2	1:A:464:ILE:HG22	1.60	1.01
1:D:274:ASP:O	1:D:278:ASN:HA	1.61	1.01
1:A:93:GLU:C	1:B:2:TRP:CB	2.31	1.01
1:A:3:VAL:C	1:B:3:VAL:HB	1.85	1.01
1:B:432:ASP:OD2	1:B:464:ILE:HG22	1.60	1.00
1:C:27:ASN:CG	1:D:90:GLU:CB	2.33	1.00
1:C:432:ASP:OD2	1:C:464:ILE:HG22	1.60	1.00
1:C:27:ASN:OD1	1:D:90:GLU:CB	2.08	1.00
1:C:450:GLN:HB2	1:C:533:GLU:HA	1.41	1.00
1:A:2:TRP:HB2	1:B:93:GLU:OE1	1.58	1.00
1:A:188:THR:HG23	1:A:208:ILE:HG12	1.43	0.99
1:C:464:ILE:CD1	1:C:465:PRO:CD	2.20	0.99
1:A:274:ASP:O	1:A:278:ASN:HA	1.61	0.99
1:A:482:THR:CG2	1:A:499:THR:H	1.76	0.99
1:B:482:THR:CG2	1:B:499:THR:H	1.76	0.99
1:D:432:ASP:OD2	1:D:464:ILE:HG22	1.60	0.99
1:A:92:MET:SD	1:B:3:VAL:CG1	2.50	0.99
1:A:320:THR:HG21	2:A:807:NAG:N2	1.78	0.99
1:C:188:THR:HG23	1:C:208:ILE:HG12	1.43	0.99
1:D:450:GLN:HB2	1:D:533:GLU:HA	1.41	0.99
1:C:2:TRP:HZ2	1:D:53:ILE:HD11	1.28	0.99
1:C:274:ASP:O	1:C:278:ASN:HA	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:THR:CG2	1:D:499:THR:H	1.76	0.99
1:B:188:THR:HG23	1:B:208:ILE:HG12	1.43	0.98
1:A:366:LYS:HG3	1:A:367:LEU:H	1.28	0.98
1:B:320:THR:HG21	2:B:807:NAG:N2	1.78	0.98
1:D:320:THR:HG21	2:D:807:NAG:N2	1.78	0.98
1:B:274:ASP:O	1:B:278:ASN:HA	1.61	0.98
1:C:523:THR:HG23	1:C:524:VAL:H	1.26	0.98
1:C:482:THR:CG2	1:C:499:THR:H	1.76	0.97
1:C:320:THR:HG21	2:C:807:NAG:N2	1.78	0.97
1:D:188:THR:HG23	1:D:208:ILE:HG12	1.43	0.97
1:D:366:LYS:HG3	1:D:367:LEU:H	1.28	0.96
1:B:366:LYS:HG3	1:B:367:LEU:H	1.28	0.96
1:C:482:THR:HG21	1:C:499:THR:N	1.81	0.96
1:D:235:ILE:CG1	1:D:287:GLY:HA2	1.96	0.96
1:D:523:THR:HG23	1:D:524:VAL:H	1.27	0.96
1:A:227:THR:HG21	2:A:807:NAG:H83	1.48	0.96
1:D:320:THR:HG21	2:D:807:NAG:HN2	1.31	0.96
1:C:320:THR:HG21	2:C:807:NAG:HN2	1.31	0.96
1:A:290:PHE:CB	1:A:292:LEU:H	1.79	0.96
1:C:92:MET:HE3	1:D:2:TRP:HB2	0.96	0.96
1:B:235:ILE:CG1	1:B:287:GLY:HA2	1.96	0.96
1:D:290:PHE:CB	1:D:292:LEU:H	1.79	0.95
1:C:366:LYS:HG3	1:C:367:LEU:H	1.28	0.95
1:B:482:THR:HG21	1:B:499:THR:N	1.81	0.95
1:C:32:ASN:HD21	1:C:83:GLU:CB	1.79	0.95
1:A:76:LEU:HB2	1:B:2:TRP:HE1	1.31	0.95
1:C:227:THR:HG21	2:C:807:NAG:H83	1.48	0.95
1:C:235:ILE:CG1	1:C:287:GLY:HA2	1.96	0.95
1:A:32:ASN:HD21	1:A:83:GLU:CB	1.79	0.95
1:A:235:ILE:CG1	1:A:287:GLY:HA2	1.96	0.95
1:A:523:THR:HG23	1:A:524:VAL:H	1.27	0.95
1:D:32:ASN:HD21	1:D:83:GLU:CB	1.79	0.95
1:B:32:ASN:HD21	1:B:83:GLU:CB	1.79	0.95
1:B:523:THR:HG23	1:B:524:VAL:H	1.26	0.95
1:C:94:ILE:HG21	1:D:2:TRP:CH2	2.01	0.94
1:A:289:ASP:O	1:A:290:PHE:HB3	1.67	0.94
1:C:289:ASP:O	1:C:290:PHE:HB3	1.67	0.94
1:B:290:PHE:CB	1:B:292:LEU:H	1.79	0.94
1:D:464:ILE:HD12	1:D:465:PRO:HD2	0.94	0.94
1:A:366:LYS:CG	1:A:367:LEU:H	1.80	0.94
1:A:396:ARG:HH22	1:A:464:ILE:HB	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ASN:OD1	1:D:90:GLU:C	2.09	0.94
1:C:366:LYS:CG	1:C:367:LEU:H	1.80	0.94
1:A:1:ASP:HB2	1:B:92:MET:C	1.92	0.93
1:D:227:THR:HG21	2:D:807:NAG:H83	1.48	0.93
1:D:366:LYS:CG	1:D:367:LEU:H	1.80	0.93
1:A:227:THR:HG21	2:A:807:NAG:C7	1.99	0.93
1:B:227:THR:HG21	2:B:807:NAG:C7	1.99	0.93
1:B:374:ASP:O	1:B:375:PRO:C	2.06	0.93
1:D:27:ASN:HD22	1:D:28:LYS:N	1.66	0.93
1:B:32:ASN:ND2	1:B:83:GLU:HB2	1.84	0.93
1:B:352:ILE:HG13	1:B:388:VAL:HB	1.51	0.93
1:C:32:ASN:ND2	1:C:83:GLU:HB2	1.84	0.93
1:C:464:ILE:HD12	1:C:465:PRO:HD2	0.94	0.93
1:D:227:THR:HG21	2:D:807:NAG:C7	1.99	0.93
1:A:320:THR:HG21	2:A:807:NAG:HN2	1.31	0.93
1:B:366:LYS:CG	1:B:367:LEU:H	1.80	0.93
1:A:352:ILE:HG13	1:A:388:VAL:HB	1.51	0.93
1:D:32:ASN:ND2	1:D:83:GLU:HB2	1.84	0.93
1:D:289:ASP:O	1:D:290:PHE:HB3	1.67	0.93
1:A:27:ASN:HD22	1:A:28:LYS:N	1.66	0.93
1:A:90:GLU:H	1:B:90:GLU:CB	1.81	0.93
1:C:352:ILE:HG13	1:C:388:VAL:HB	1.51	0.93
1:B:27:ASN:HD22	1:B:28:LYS:N	1.66	0.93
1:C:290:PHE:CB	1:C:292:LEU:H	1.79	0.93
1:B:8:LYS:H	1:B:8:LYS:CD	1.74	0.93
1:B:195:ASP:HB2	1:B:201:LEU:H	1.34	0.93
1:C:446:THR:HG23	1:C:539:CYS:SG	2.09	0.93
1:A:482:THR:HG21	1:A:499:THR:N	1.81	0.92
1:C:1:ASP:CG	1:D:26:SER:HA	1.92	0.92
1:C:22:VAL:HG23	1:D:5:PRO:CG	1.96	0.92
1:D:446:THR:HG23	1:D:539:CYS:SG	2.09	0.92
1:D:482:THR:HG21	1:D:499:THR:N	1.81	0.92
1:A:32:ASN:ND2	1:A:83:GLU:HB2	1.84	0.92
1:A:374:ASP:O	1:A:375:PRO:C	2.06	0.92
1:B:396:ARG:HH22	1:B:464:ILE:HB	1.33	0.92
1:B:403:ASN:HB2	2:B:902:NAG:C7	2.00	0.92
1:D:352:ILE:HG13	1:D:388:VAL:HB	1.51	0.92
1:A:446:THR:HG23	1:A:539:CYS:SG	2.09	0.92
1:C:195:ASP:HB2	1:C:201:LEU:H	1.34	0.92
1:D:396:ARG:HH22	1:D:464:ILE:HB	1.33	0.92
1:B:464:ILE:HD12	1:B:465:PRO:HD2	0.94	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:805:NAG:H62	2:C:806:NAG:C7	2.00	0.92
1:D:404:ASN:O	1:D:404:ASN:ND2	2.03	0.92
1:A:464:ILE:HD12	1:A:465:PRO:HD2	0.94	0.92
1:A:8:LYS:H	1:A:8:LYS:CD	1.74	0.92
1:C:227:THR:HG21	2:C:807:NAG:C7	1.99	0.92
1:A:404:ASN:O	1:A:404:ASN:ND2	2.03	0.92
2:B:805:NAG:H62	2:B:806:NAG:C7	2.00	0.92
1:B:446:THR:HG23	1:B:539:CYS:SG	2.10	0.92
1:C:403:ASN:HB2	2:C:902:NAG:C7	2.00	0.92
1:D:374:ASP:O	1:D:375:PRO:C	2.06	0.92
1:D:403:ASN:HB2	2:D:902:NAG:C7	2.00	0.92
1:A:195:ASP:HB2	1:A:201:LEU:H	1.34	0.91
1:D:195:ASP:HB2	1:D:201:LEU:H	1.34	0.91
1:B:289:ASP:O	1:B:290:PHE:HB3	1.67	0.91
1:B:335:ALA:CB	3:B:811:NDG:O6	2.18	0.91
1:B:227:THR:HG21	2:B:807:NAG:H83	1.48	0.91
1:C:8:LYS:H	1:C:8:LYS:CD	1.74	0.91
1:C:335:ALA:CB	3:C:811:NDG:O6	2.18	0.91
1:D:464:ILE:HD12	1:D:465:PRO:HD3	1.53	0.91
1:C:396:ARG:HH22	1:C:464:ILE:HB	1.33	0.91
2:D:805:NAG:H62	2:D:806:NAG:C7	2.00	0.91
1:D:234:GLU:N	1:D:235:ILE:HG23	1.86	0.91
2:A:805:NAG:O5	2:A:806:NAG:H83	1.71	0.91
2:A:805:NAG:H62	2:A:806:NAG:C7	2.00	0.91
1:B:404:ASN:ND2	1:B:404:ASN:O	2.03	0.91
1:C:27:ASN:HD22	1:C:28:LYS:N	1.66	0.91
1:C:234:GLU:N	1:C:235:ILE:HG23	1.86	0.91
1:D:335:ALA:CB	3:D:811:NDG:O6	2.18	0.91
1:A:340:ASP:HA	1:A:429:HIS:HB3	1.53	0.91
1:A:335:ALA:CB	3:A:811:NDG:O6	2.18	0.90
1:C:464:ILE:HD11	1:C:465:PRO:HD2	1.53	0.90
1:C:517:GLN:O	1:C:519:ASN:N	2.03	0.90
1:C:404:ASN:O	1:C:404:ASN:ND2	2.03	0.90
1:A:154:ASP:HB3	1:A:155:PRO:HD2	1.54	0.90
2:D:805:NAG:O5	2:D:806:NAG:H83	1.71	0.90
1:B:518:ASN:O	1:B:520:PRO:HD3	1.72	0.90
1:A:338:ARG:HD3	1:A:352:ILE:CG2	2.02	0.90
1:A:378:TRP:HB2	1:A:379:LEU:HD23	1.53	0.90
1:D:8:LYS:H	1:D:8:LYS:CD	1.74	0.90
1:A:403:ASN:HB2	2:A:902:NAG:C7	2.00	0.90
1:B:517:GLN:O	1:B:519:ASN:N	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLU:N	1:A:235:ILE:HG23	1.86	0.90
1:B:464:ILE:HD12	1:B:465:PRO:HD3	1.53	0.90
1:C:338:ARG:HD3	1:C:352:ILE:CG2	2.02	0.90
1:C:340:ASP:HA	1:C:429:HIS:HB3	1.53	0.90
1:C:378:TRP:HB2	1:C:379:LEU:HD23	1.53	0.90
2:C:805:NAG:O5	2:C:806:NAG:H83	1.71	0.90
1:D:340:ASP:HA	1:D:429:HIS:HB3	1.53	0.90
1:B:234:GLU:N	1:B:235:ILE:HG23	1.86	0.90
1:C:449:ASP:H	1:C:532:CYS:HB3	1.37	0.90
1:C:8:LYS:HD2	1:C:8:LYS:N	1.87	0.90
1:C:27:ASN:HD21	1:D:90:GLU:CG	1.75	0.90
1:D:8:LYS:HD2	1:D:8:LYS:N	1.87	0.90
1:D:338:ARG:HD3	1:D:352:ILE:CG2	2.02	0.90
1:A:517:GLN:O	1:A:519:ASN:N	2.03	0.89
1:B:8:LYS:HD2	1:B:8:LYS:N	1.87	0.89
1:D:517:GLN:O	1:D:519:ASN:N	2.03	0.89
1:A:76:LEU:HB2	1:B:2:TRP:NE1	1.87	0.89
1:A:90:GLU:H	1:B:90:GLU:HB2	1.37	0.89
1:A:518:ASN:O	1:A:520:PRO:HD3	1.72	0.89
1:C:396:ARG:NH2	1:C:464:ILE:CG2	2.35	0.89
1:C:27:ASN:CG	1:D:90:GLU:CG	2.44	0.89
1:C:523:THR:HG23	1:C:524:VAL:CG2	2.03	0.89
1:A:464:ILE:HD12	1:A:465:PRO:HD3	1.53	0.89
1:D:518:ASN:O	1:D:520:PRO:HD3	1.72	0.89
1:A:523:THR:HG23	1:A:524:VAL:CG2	2.03	0.89
1:D:523:THR:HG23	1:D:524:VAL:CG2	2.03	0.89
1:A:8:LYS:HD2	1:A:8:LYS:N	1.87	0.89
1:B:338:ARG:HD3	1:B:352:ILE:CG2	2.02	0.89
1:B:371:ILE:CD1	1:B:381:VAL:HG11	2.03	0.89
1:C:518:ASN:O	1:C:520:PRO:HD3	1.72	0.89
1:B:340:ASP:HA	1:B:429:HIS:HB3	1.53	0.89
1:B:378:TRP:HB2	1:B:379:LEU:HD23	1.53	0.89
1:A:92:MET:SD	1:B:3:VAL:HG12	2.12	0.89
1:A:371:ILE:CD1	1:A:381:VAL:HG11	2.03	0.89
1:B:320:THR:HG21	2:B:807:NAG:HN2	1.31	0.89
1:B:396:ARG:NH2	1:B:464:ILE:CG2	2.35	0.89
1:C:92:MET:CE	1:D:2:TRP:HB3	2.03	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:D:343:GLU:HB3	1:D:433:VAL:HG21	1.55	0.89
1:D:378:TRP:HB2	1:D:379:LEU:HD23	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ARG:NH2	1:A:464:ILE:CG2	2.35	0.88
1:A:464:ILE:HD11	1:A:465:PRO:HD2	1.53	0.88
1:C:24:ILE:HB	1:D:2:TRP:N	1.79	0.88
1:D:318:THR:HG21	2:D:806:NAG:H5	1.56	0.88
1:D:396:ARG:NH2	1:D:464:ILE:CG2	2.35	0.88
1:A:2:TRP:CB	1:B:93:GLU:OE1	2.21	0.88
1:D:464:ILE:HD11	1:D:465:PRO:HD2	1.53	0.88
1:B:523:THR:HG23	1:B:524:VAL:CG2	2.03	0.88
1:C:343:GLU:HB3	1:C:433:VAL:HG21	1.55	0.88
1:D:486:GLU:HB2	1:D:495:LEU:HB2	1.56	0.88
1:A:221:PHE:HE1	1:A:315:SER:O	1.56	0.88
1:A:486:GLU:HB2	1:A:495:LEU:HB2	1.56	0.88
1:B:221:PHE:HE1	1:B:315:SER:O	1.56	0.88
1:B:333:VAL:HB	1:B:334:PRO:HD3	1.56	0.88
1:C:154:ASP:HB3	1:C:155:PRO:HD2	1.54	0.88
1:C:374:ASP:O	1:C:375:PRO:C	2.06	0.88
1:D:221:PHE:HE1	1:D:315:SER:O	1.56	0.88
1:D:371:ILE:CD1	1:D:381:VAL:HG11	2.03	0.88
1:B:154:ASP:HB3	1:B:155:PRO:HD2	1.54	0.88
1:B:449:ASP:H	1:B:532:CYS:HB3	1.37	0.88
1:A:483:TRP:CZ3	1:A:498:PRO:HG3	2.09	0.88
1:D:333:VAL:HB	1:D:334:PRO:HD3	1.56	0.88
1:A:449:ASP:H	1:A:532:CYS:HB3	1.37	0.88
1:C:221:PHE:HE1	1:C:315:SER:O	1.56	0.88
1:A:2:TRP:CZ2	1:B:95:THR:HG21	2.09	0.87
1:B:486:GLU:HB2	1:B:495:LEU:HB2	1.56	0.87
1:D:154:ASP:HB3	1:D:155:PRO:HD2	1.54	0.87
1:A:90:GLU:HB2	1:B:90:GLU:CA	2.04	0.87
1:B:318:THR:HG21	2:B:806:NAG:H5	1.56	0.87
1:D:449:ASP:H	1:D:532:CYS:HB3	1.37	0.87
1:A:2:TRP:CG	1:B:93:GLU:OE1	2.27	0.87
1:A:3:VAL:HG11	1:B:4:ILE:CD1	1.65	0.87
1:C:483:TRP:CZ3	1:C:498:PRO:HG3	2.09	0.87
1:C:486:GLU:HB2	1:C:495:LEU:HB2	1.56	0.87
1:D:483:TRP:CZ3	1:D:498:PRO:HG3	2.09	0.87
1:A:257:ALA:O	1:A:273:THR:HG21	1.74	0.87
1:C:333:VAL:HB	1:C:334:PRO:HD3	1.56	0.87
1:D:441:SER:OG	1:D:442:PRO:HD3	1.75	0.87
1:B:257:ALA:O	1:B:273:THR:HG21	1.74	0.87
1:A:441:SER:OG	1:A:442:PRO:HD3	1.75	0.87
1:B:343:GLU:HB3	1:B:433:VAL:HG21	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:THR:HG21	2:C:806:NAG:H5	1.56	0.87
1:B:440:PRO:CD	1:B:522:LEU:HD12	2.05	0.87
1:D:523:THR:HG23	1:D:524:VAL:N	1.90	0.87
1:B:523:THR:HG23	1:B:524:VAL:N	1.90	0.86
1:C:2:TRP:HZ2	1:D:53:ILE:CD1	1.88	0.86
1:C:320:THR:HG21	2:C:807:NAG:C2	2.05	0.86
1:D:257:ALA:O	1:D:273:THR:HG21	1.74	0.86
1:B:483:TRP:CZ3	1:B:498:PRO:HG3	2.09	0.86
1:D:277:SER:C	1:D:278:ASN:HD22	1.83	0.86
1:D:440:PRO:CD	1:D:522:LEU:HD12	2.05	0.86
1:A:333:VAL:HB	1:A:334:PRO:HD3	1.56	0.86
1:B:464:ILE:HD11	1:B:465:PRO:HD2	1.53	0.86
1:C:440:PRO:CD	1:C:522:LEU:HD12	2.05	0.86
1:A:320:THR:HG21	2:A:807:NAG:C2	2.05	0.86
1:A:523:THR:HG23	1:A:524:VAL:N	1.90	0.86
1:B:441:SER:OG	1:B:442:PRO:HD3	1.75	0.86
1:C:277:SER:C	1:C:278:ASN:HD22	1.84	0.86
1:C:517:GLN:C	1:C:519:ASN:H	1.84	0.86
1:A:517:GLN:C	1:A:519:ASN:H	1.84	0.86
1:A:318:THR:HG21	2:A:806:NAG:H5	1.56	0.86
1:A:423:THR:CB	2:A:810:NAG:C7	2.54	0.86
1:D:517:GLN:C	1:D:519:ASN:H	1.84	0.86
1:A:277:SER:C	1:A:278:ASN:HD22	1.84	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:HE1	1.24	0.85
1:D:320:THR:HG21	2:D:807:NAG:C2	2.05	0.85
1:D:464:ILE:HD12	1:D:465:PRO:N	1.91	0.85
1:C:257:ALA:O	1:C:273:THR:HG21	1.74	0.85
1:A:440:PRO:CD	1:A:522:LEU:HD12	2.05	0.85
1:B:423:THR:CB	2:B:810:NAG:C7	2.54	0.85
1:C:441:SER:OG	1:C:442:PRO:HD3	1.75	0.85
1:B:320:THR:HG21	2:B:807:NAG:C2	2.05	0.85
1:C:523:THR:HG23	1:C:524:VAL:N	1.90	0.85
1:D:235:ILE:HG13	1:D:287:GLY:HA2	1.58	0.85
1:A:90:GLU:CB	1:B:90:GLU:N	2.26	0.85
1:A:343:GLU:HB3	1:A:433:VAL:HG21	1.55	0.85
1:B:277:SER:C	1:B:278:ASN:HD22	1.83	0.85
1:B:451:ASN:N	1:B:533:GLU:O	2.10	0.85
1:A:90:GLU:N	1:B:90:GLU:HB2	1.91	0.85
1:A:438:PRO:HB3	1:A:471:TYR:HE2	1.41	0.85
1:C:483:TRP:HZ2	1:C:507:TYR:CE1	1.95	0.85
1:A:27:ASN:HD22	1:A:27:ASN:C	1.85	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ASN:N	1:A:533:GLU:O	2.10	0.85
1:C:423:THR:CB	2:C:810:NAG:C7	2.54	0.85
1:D:440:PRO:HD2	1:D:522:LEU:HD12	1.59	0.85
1:D:451:ASN:N	1:D:533:GLU:O	2.10	0.85
1:A:1:ASP:O	1:B:94:ILE:HA	0.89	0.85
1:A:483:TRP:HZ2	1:A:507:TYR:CE1	1.95	0.85
1:D:423:THR:CB	2:D:810:NAG:C7	2.54	0.85
1:A:464:ILE:HD12	1:A:465:PRO:N	1.91	0.85
1:B:438:PRO:HB3	1:B:471:TYR:HE2	1.41	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:CE1	1.95	0.84
1:C:464:ILE:HD12	1:C:465:PRO:HD3	1.53	0.84
1:D:483:TRP:HZ2	1:D:507:TYR:CE1	1.95	0.84
1:C:222:ASP:OD1	1:C:222:ASP:C	2.20	0.84
1:B:440:PRO:HD2	1:B:522:LEU:HD12	1.59	0.84
1:B:464:ILE:HD12	1:B:465:PRO:N	1.91	0.84
1:C:27:ASN:HD22	1:C:27:ASN:C	1.85	0.84
1:C:396:ARG:HD3	1:C:431:LEU:C	2.03	0.84
1:B:517:GLN:C	1:B:519:ASN:H	1.84	0.84
1:A:235:ILE:HG13	1:A:287:GLY:HA2	1.57	0.84
1:D:483:TRP:HZ2	1:D:507:TYR:HE1	1.24	0.84
1:C:440:PRO:HD2	1:C:522:LEU:HD12	1.59	0.84
1:D:396:ARG:HD3	1:D:431:LEU:C	2.03	0.84
1:B:235:ILE:HG13	1:B:287:GLY:HA2	1.57	0.84
1:B:375:PRO:HB3	1:B:400:TYR:CE2	2.12	0.84
1:C:451:ASN:N	1:C:533:GLU:O	2.10	0.84
1:A:222:ASP:OD1	1:A:222:ASP:C	2.20	0.84
1:A:375:PRO:HB3	1:A:400:TYR:CE2	2.12	0.84
1:C:230:VAL:O	1:C:324:GLU:N	2.11	0.84
1:C:375:PRO:HB3	1:C:400:TYR:CE2	2.12	0.84
1:C:464:ILE:HD12	1:C:465:PRO:N	1.91	0.84
1:C:438:PRO:HB3	1:C:471:TYR:HE2	1.41	0.83
1:B:423:THR:HB	2:B:810:NAG:N2	1.93	0.83
1:B:469:TYR:CG	1:B:470:PRO:CD	2.61	0.83
1:D:396:ARG:NE	1:D:432:ASP:HB2	1.93	0.83
1:D:375:PRO:HB3	1:D:400:TYR:CE2	2.12	0.83
1:D:423:THR:HB	2:D:810:NAG:N2	1.93	0.83
1:B:396:ARG:HD3	1:B:431:LEU:C	2.02	0.83
1:C:147:SER:OG	1:C:167:ARG:HD2	1.78	0.83
1:D:155:PRO:C	1:D:157:GLU:H	1.86	0.83
1:D:438:PRO:HB3	1:D:471:TYR:HE2	1.41	0.83
1:C:235:ILE:HG13	1:C:287:GLY:HA2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:ARG:NE	1:C:432:ASP:HB2	1.93	0.83
1:D:32:ASN:ND2	1:D:83:GLU:H	1.77	0.83
1:C:448:CYS:O	1:C:452:PRO:HG3	1.78	0.83
1:D:230:VAL:O	1:D:324:GLU:N	2.11	0.83
1:B:155:PRO:C	1:B:157:GLU:H	1.86	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:C:483:TRP:HZ2	1:C:507:TYR:HE1	1.24	0.83
1:A:440:PRO:HD2	1:A:522:LEU:HD12	1.59	0.83
1:B:147:SER:OG	1:B:167:ARG:HD2	1.78	0.83
1:C:32:ASN:ND2	1:C:83:GLU:H	1.77	0.83
1:D:234:GLU:H	1:D:235:ILE:CG2	1.92	0.83
1:A:147:SER:OG	1:A:167:ARG:HD2	1.78	0.83
1:A:155:PRO:HB2	2:A:801:NAG:H81	1.59	0.83
1:A:423:THR:CB	2:A:810:NAG:N2	2.42	0.83
1:D:448:CYS:O	1:D:452:PRO:HG3	1.79	0.83
1:D:469:TYR:CG	1:D:470:PRO:CD	2.61	0.83
1:A:446:THR:HG21	1:A:537:ILE:O	1.79	0.82
1:B:230:VAL:O	1:B:324:GLU:N	2.11	0.82
1:C:155:PRO:HB2	2:C:801:NAG:H81	1.59	0.82
1:D:482:THR:HG21	1:D:500:GLN:N	1.94	0.82
1:A:154:ASP:HB3	2:A:801:NAG:N2	1.95	0.82
1:A:155:PRO:C	1:A:157:GLU:H	1.86	0.82
1:A:230:VAL:O	1:A:324:GLU:N	2.11	0.82
1:A:396:ARG:HD3	1:A:431:LEU:C	2.03	0.82
1:A:423:THR:HB	2:A:810:NAG:N2	1.93	0.82
1:B:446:THR:HG21	1:B:537:ILE:O	1.79	0.82
1:D:222:ASP:OD1	1:D:222:ASP:C	2.20	0.82
1:A:1:ASP:O	1:B:95:THR:N	2.11	0.82
1:C:155:PRO:C	1:C:157:GLU:H	1.86	0.82
1:C:469:TYR:CG	1:C:470:PRO:CD	2.61	0.82
1:D:154:ASP:HB3	2:D:801:NAG:HN2	1.45	0.82
1:D:289:ASP:O	1:D:289:ASP:OD2	1.97	0.82
1:A:396:ARG:NE	1:A:432:ASP:HB2	1.93	0.82
1:B:289:ASP:O	1:B:289:ASP:OD2	1.97	0.82
1:C:289:ASP:O	1:C:289:ASP:OD2	1.97	0.82
1:C:423:THR:HB	2:C:810:NAG:N2	1.93	0.82
1:C:446:THR:HG21	1:C:537:ILE:O	1.79	0.82
1:A:505:GLY:C	1:A:506:ASP:OD1	2.23	0.82
1:A:92:MET:SD	1:B:3:VAL:HG13	2.19	0.82
1:A:290:PHE:HD2	1:A:293:ARG:H	1.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TRP:HZ2	1:A:507:TYR:HE1	1.24	0.82
1:B:154:ASP:HB3	2:B:801:NAG:N2	1.95	0.82
1:B:155:PRO:HB2	2:B:801:NAG:H81	1.60	0.82
1:D:432:ASP:CG	1:D:464:ILE:HG22	2.05	0.82
1:A:1:ASP:O	1:B:94:ILE:C	2.23	0.81
1:A:92:MET:SD	1:B:3:VAL:CA	2.68	0.81
1:C:505:GLY:C	1:C:506:ASP:OD1	2.23	0.81
1:D:505:GLY:C	1:D:506:ASP:OD1	2.23	0.81
1:A:289:ASP:O	1:A:289:ASP:OD2	1.97	0.81
1:B:32:ASN:ND2	1:B:83:GLU:H	1.76	0.81
1:D:154:ASP:HB3	2:D:801:NAG:N2	1.95	0.81
1:D:299:GLN:HG2	1:D:318:THR:HG23	1.62	0.81
1:A:32:ASN:ND2	1:A:83:GLU:H	1.77	0.81
1:A:154:ASP:HB3	2:A:801:NAG:HN2	1.45	0.81
1:A:234:GLU:H	1:A:235:ILE:CG2	1.92	0.81
1:B:154:ASP:HB3	2:B:801:NAG:HN2	1.45	0.81
1:B:423:THR:CB	2:B:810:NAG:N2	2.42	0.81
1:B:482:THR:HG21	1:B:500:GLN:N	1.95	0.81
1:C:299:GLN:HG2	1:C:318:THR:HG23	1.62	0.81
1:D:27:ASN:HD22	1:D:27:ASN:C	1.85	0.81
1:D:155:PRO:HB2	2:D:801:NAG:H81	1.59	0.81
1:D:423:THR:CB	2:D:810:NAG:N2	2.42	0.81
1:A:90:GLU:HB2	1:B:90:GLU:CB	2.10	0.81
1:A:540:GLN:O	1:A:540:GLN:OE1	1.97	0.81
1:B:27:ASN:HD22	1:B:27:ASN:C	1.85	0.81
1:D:446:THR:HG21	1:D:537:ILE:O	1.79	0.81
1:A:432:ASP:CG	1:A:464:ILE:HG22	2.05	0.81
1:A:448:CYS:O	1:A:452:PRO:HG3	1.79	0.81
1:B:486:GLU:O	1:B:494:MET:HA	1.81	0.81
1:B:448:CYS:O	1:B:452:PRO:HG3	1.79	0.81
1:C:28:LYS:HD3	1:C:88:VAL:HG12	1.61	0.81
1:C:154:ASP:HB3	2:C:801:NAG:N2	1.95	0.81
1:C:469:TYR:CD2	1:C:470:PRO:HD2	2.16	0.81
1:B:234:GLU:H	1:B:235:ILE:CG2	1.92	0.81
1:B:432:ASP:CG	1:B:464:ILE:HG22	2.05	0.81
1:B:505:GLY:C	1:B:506:ASP:OD1	2.23	0.81
1:C:290:PHE:HD2	1:C:293:ARG:H	1.28	0.81
1:C:486:GLU:O	1:C:494:MET:HA	1.81	0.81
1:A:469:TYR:CG	1:A:470:PRO:CD	2.61	0.81
1:B:28:LYS:HD3	1:B:88:VAL:HG12	1.61	0.81
1:C:290:PHE:CE2	1:C:293:ARG:HB2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:THR:HG21	1:C:500:GLN:N	1.95	0.81
1:C:496:LEU:HD21	1:C:509:ILE:HD13	1.63	0.81
1:D:28:LYS:HD3	1:D:88:VAL:HG12	1.61	0.81
1:A:127:VAL:HG13	1:A:128:MET:H	1.46	0.80
1:C:2:TRP:CZ2	1:D:53:ILE:HD11	2.15	0.80
1:D:540:GLN:O	1:D:540:GLN:OE1	1.97	0.80
1:A:299:GLN:HG2	1:A:318:THR:HG23	1.62	0.80
1:A:396:ARG:HH21	1:A:464:ILE:HG22	1.46	0.80
1:A:469:TYR:CD2	1:A:470:PRO:HD2	2.16	0.80
1:A:482:THR:HG21	1:A:500:GLN:N	1.95	0.80
1:C:540:GLN:O	1:C:540:GLN:OE1	1.97	0.80
1:A:290:PHE:CE2	1:A:293:ARG:HB2	2.16	0.80
1:A:496:LEU:HD21	1:A:509:ILE:HD13	1.63	0.80
1:B:127:VAL:HG13	1:B:128:MET:H	1.46	0.80
1:B:396:ARG:HH21	1:B:464:ILE:HG22	1.46	0.80
1:A:28:LYS:HD3	1:A:88:VAL:HG12	1.61	0.80
1:A:432:ASP:OD2	1:A:464:ILE:CG2	2.30	0.80
1:B:540:GLN:O	1:B:540:GLN:OE1	1.97	0.80
1:C:423:THR:CB	2:C:810:NAG:N2	2.42	0.80
1:A:406:TYR:CD1	2:A:808:NAG:H83	2.17	0.80
1:A:486:GLU:O	1:A:494:MET:HA	1.81	0.80
1:B:469:TYR:CD2	1:B:470:PRO:HD2	2.16	0.80
1:C:432:ASP:CG	1:C:464:ILE:HG22	2.05	0.80
1:B:290:PHE:CE2	1:B:293:ARG:HB2	2.16	0.80
1:C:154:ASP:HB3	2:C:801:NAG:HN2	1.45	0.80
1:A:265:GLU:HB3	1:A:268:PHE:HE2	1.46	0.80
1:C:265:GLU:HB3	1:C:268:PHE:HE2	1.46	0.80
1:C:523:THR:CG2	1:C:524:VAL:H	1.94	0.80
1:D:469:TYR:CD2	1:D:470:PRO:HD2	2.16	0.80
1:B:482:THR:OG1	1:B:500:GLN:HG2	1.82	0.80
1:D:290:PHE:HD2	1:D:293:ARG:H	1.28	0.80
1:D:406:TYR:CD1	2:D:808:NAG:H83	2.17	0.80
1:D:485:ALA:O	1:D:486:GLU:CG	2.30	0.80
1:A:371:ILE:HD11	1:A:381:VAL:HG11	1.64	0.80
1:B:265:GLU:HB3	1:B:268:PHE:HE2	1.46	0.79
1:B:299:GLN:HG2	1:B:318:THR:HG23	1.62	0.79
1:C:22:VAL:HG21	1:D:5:PRO:HG3	1.61	0.79
1:B:232:GLU:HG3	1:B:290:PHE:N	1.98	0.79
1:C:396:ARG:HH21	1:C:464:ILE:HG22	1.46	0.79
1:C:406:TYR:CD1	2:C:808:NAG:H83	2.17	0.79
1:C:432:ASP:OD2	1:C:464:ILE:CG2	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:THR:OG1	1:C:500:GLN:HG2	1.82	0.79
1:D:290:PHE:CE2	1:D:293:ARG:HB2	2.16	0.79
1:D:496:LEU:HD21	1:D:509:ILE:HD13	1.63	0.79
1:C:449:ASP:HB3	1:C:532:CYS:H	1.47	0.79
1:D:432:ASP:OD2	1:D:464:ILE:CG2	2.30	0.79
1:A:482:THR:OG1	1:A:500:GLN:HG2	1.82	0.79
1:B:195:ASP:HB3	1:B:200:GLY:HA3	1.65	0.79
1:A:232:GLU:HG3	1:A:290:PHE:N	1.98	0.79
1:B:432:ASP:OD2	1:B:464:ILE:CG2	2.30	0.79
1:D:265:GLU:HB3	1:D:268:PHE:HE2	1.46	0.79
1:A:154:ASP:CB	1:A:155:PRO:HD2	2.13	0.79
1:A:485:ALA:O	1:A:486:GLU:CG	2.31	0.79
1:C:154:ASP:CB	1:C:155:PRO:HD2	2.13	0.79
1:C:540:GLN:O	1:C:540:GLN:CG	2.30	0.79
1:B:365:GLN:O	1:B:365:GLN:HG3	1.82	0.79
1:D:396:ARG:HH21	1:D:464:ILE:HG22	1.46	0.79
2:C:809:NAG:H61	2:C:810:NAG:H62	1.65	0.79
1:D:482:THR:OG1	1:D:500:GLN:HG2	1.82	0.79
1:C:232:GLU:HG3	1:C:290:PHE:N	1.98	0.79
1:A:540:GLN:O	1:A:540:GLN:CG	2.30	0.78
1:C:127:VAL:HG13	1:C:128:MET:H	1.46	0.78
1:C:238:GLU:HA	1:C:283:THR:HG22	1.66	0.78
1:C:365:GLN:HG3	1:C:365:GLN:O	1.82	0.78
1:B:147:SER:OG	1:B:167:ARG:CG	2.32	0.78
1:B:406:TYR:CD1	2:B:808:NAG:H83	2.17	0.78
1:D:154:ASP:CB	1:D:155:PRO:HD2	2.13	0.78
1:D:371:ILE:HD11	1:D:381:VAL:HG11	1.64	0.78
1:A:301:THR:HG21	2:A:805:NAG:C8	2.12	0.78
1:D:449:ASP:HB3	1:D:532:CYS:H	1.47	0.78
1:D:486:GLU:O	1:D:494:MET:HA	1.81	0.78
1:B:154:ASP:CB	1:B:155:PRO:HD2	2.13	0.78
1:D:232:GLU:HG3	1:D:290:PHE:N	1.98	0.78
1:C:234:GLU:H	1:C:235:ILE:CG2	1.92	0.78
1:C:501:GLN:HG2	1:C:501:GLN:O	1.84	0.78
1:A:524:VAL:CG2	2:A:904:NAG:H81	2.14	0.78
1:B:238:GLU:HA	1:B:283:THR:HG22	1.66	0.78
1:B:496:LEU:HD21	1:B:509:ILE:HD13	1.63	0.78
2:B:809:NAG:H61	2:B:810:NAG:H62	1.65	0.78
1:C:147:SER:OG	1:C:167:ARG:CG	2.32	0.78
1:A:195:ASP:HB3	1:A:200:GLY:HA3	1.65	0.78
1:B:156:GLU:HG3	1:B:160:PRO:HB3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLU:HG3	1:A:160:PRO:HB3	1.66	0.78
1:B:485:ALA:O	1:B:486:GLU:CG	2.30	0.78
1:A:365:GLN:HG3	1:A:365:GLN:O	1.82	0.78
1:A:194:THR:HB	1:A:198:GLY:HA2	1.66	0.77
1:C:156:GLU:HG3	1:C:160:PRO:HB3	1.66	0.77
1:C:485:ALA:O	1:C:486:GLU:CG	2.30	0.77
1:D:127:VAL:HG13	1:D:128:MET:H	1.46	0.77
2:D:809:NAG:H61	2:D:810:NAG:H62	1.65	0.77
1:A:93:GLU:O	1:B:2:TRP:O	2.01	0.77
1:B:449:ASP:HB3	1:B:532:CYS:H	1.47	0.77
1:B:501:GLN:O	1:B:501:GLN:HG2	1.84	0.77
1:C:371:ILE:HD11	1:C:381:VAL:HG11	1.64	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:C:301:THR:HG21	2:C:805:NAG:C8	2.12	0.77
1:B:194:THR:HB	1:B:198:GLY:HA2	1.67	0.77
1:B:362:GLN:O	1:B:364:ILE:HG23	1.85	0.77
1:B:371:ILE:HD11	1:B:381:VAL:HG11	1.64	0.77
1:C:223:PRO:HD2	1:C:226:TYR:OH	1.85	0.77
1:A:501:GLN:HG2	1:A:501:GLN:O	1.84	0.77
1:C:147:SER:OG	1:C:167:ARG:CD	2.32	0.77
1:D:238:GLU:HA	1:D:283:THR:HG22	1.66	0.77
1:B:223:PRO:HD2	1:B:226:TYR:OH	1.85	0.77
1:B:524:VAL:CG2	2:B:904:NAG:H81	2.14	0.77
1:D:195:ASP:HB3	1:D:200:GLY:HA3	1.65	0.77
1:D:362:GLN:O	1:D:364:ILE:HG23	1.85	0.77
1:D:501:GLN:O	1:D:501:GLN:HG2	1.84	0.77
1:A:147:SER:OG	1:A:167:ARG:CG	2.32	0.77
1:A:238:GLU:HA	1:A:283:THR:HG22	1.66	0.77
1:A:366:LYS:CG	1:A:367:LEU:N	2.48	0.77
1:B:147:SER:OG	1:B:167:ARG:CD	2.32	0.77
1:B:196:LEU:HB2	1:B:199:ALA:HB3	1.67	0.77
1:B:540:GLN:O	1:B:540:GLN:CG	2.31	0.77
1:C:362:GLN:O	1:C:364:ILE:HG23	1.85	0.77
1:D:301:THR:HG21	2:D:805:NAG:C8	2.13	0.77
2:A:809:NAG:H61	2:A:810:NAG:H62	1.65	0.76
1:C:195:ASP:HB3	1:C:200:GLY:HA3	1.65	0.76
1:C:196:LEU:HB2	1:C:199:ALA:HB3	1.67	0.76
1:C:27:ASN:HD21	1:D:90:GLU:HB2	1.46	0.76
1:D:540:GLN:O	1:D:540:GLN:CG	2.31	0.76
1:A:196:LEU:HB2	1:A:199:ALA:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:GLN:O	1:A:364:ILE:HG23	1.85	0.76
1:B:290:PHE:HD2	1:B:293:ARG:H	1.28	0.76
1:D:524:VAL:CG2	2:D:904:NAG:H81	2.14	0.76
1:A:147:SER:OG	1:A:167:ARG:CD	2.32	0.76
1:A:449:ASP:HB3	1:A:532:CYS:H	1.47	0.76
1:C:186:GLU:O	2:C:801:NAG:O7	2.03	0.76
1:D:241:ARG:HE	1:D:281:ILE:HD12	1.51	0.76
1:D:365:GLN:HG3	1:D:365:GLN:O	1.82	0.76
1:B:272:THR:HG22	1:B:273:THR:H	1.51	0.76
1:B:482:THR:CG2	1:B:499:THR:CG2	2.62	0.76
1:A:482:THR:CG2	1:A:499:THR:CG2	2.62	0.76
1:C:194:THR:HB	1:C:198:GLY:HA2	1.67	0.76
1:A:186:GLU:O	2:A:801:NAG:O7	2.03	0.76
1:A:223:PRO:HD2	1:A:226:TYR:OH	1.85	0.76
1:A:272:THR:HG22	1:A:273:THR:H	1.51	0.76
1:B:440:PRO:HB3	1:B:457:LEU:HD21	1.67	0.76
1:B:523:THR:HG23	1:B:524:VAL:HG22	1.67	0.76
1:C:272:THR:HG22	1:C:273:THR:H	1.51	0.76
1:D:156:GLU:HG3	1:D:160:PRO:HB3	1.66	0.76
1:C:1:ASP:N	1:D:26:SER:O	2.19	0.76
1:B:188:THR:HG23	1:B:208:ILE:CG1	2.16	0.76
1:C:371:ILE:HD12	1:C:410:MET:HB3	1.68	0.76
1:C:523:THR:HG23	1:C:524:VAL:HG22	1.67	0.76
1:B:396:ARG:HH21	1:B:464:ILE:CG2	1.98	0.75
1:C:448:CYS:SG	1:C:537:ILE:HG22	2.26	0.75
1:D:440:PRO:HB3	1:D:457:LEU:HD21	1.67	0.75
1:D:482:THR:CG2	1:D:499:THR:CG2	2.62	0.75
1:A:523:THR:HG23	1:A:524:VAL:HG22	1.67	0.75
1:C:366:LYS:CG	1:C:367:LEU:N	2.48	0.75
1:C:440:PRO:HB3	1:C:457:LEU:HD21	1.67	0.75
1:D:272:THR:HG22	1:D:273:THR:H	1.51	0.75
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.75
1:C:364:ILE:O	1:C:364:ILE:HG13	1.87	0.75
1:D:186:GLU:O	2:D:801:NAG:O7	2.03	0.75
1:D:289:ASP:O	1:D:289:ASP:CG	2.30	0.75
1:D:290:PHE:CD2	1:D:293:ARG:N	2.55	0.75
1:A:448:CYS:SG	1:A:537:ILE:HG22	2.27	0.75
1:D:523:THR:HG23	1:D:524:VAL:HG22	1.67	0.75
1:A:449:ASP:HB3	1:A:532:CYS:N	2.02	0.75
1:B:396:ARG:NH2	1:B:464:ILE:HB	2.02	0.75
1:C:485:ALA:C	1:C:486:GLU:HG2	2.11	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:ALA:C	1:D:486:GLU:HG2	2.11	0.75
1:C:449:ASP:HB3	1:C:532:CYS:N	2.02	0.75
1:A:188:THR:HG23	1:A:208:ILE:CG1	2.16	0.75
1:A:371:ILE:HD12	1:A:410:MET:HB3	1.68	0.75
1:B:448:CYS:SG	1:B:537:ILE:HG22	2.26	0.75
1:D:194:THR:HB	1:D:198:GLY:HA2	1.67	0.75
1:B:449:ASP:HB3	1:B:532:CYS:N	2.02	0.74
1:B:485:ALA:C	1:B:486:GLU:HG2	2.11	0.74
1:D:448:CYS:SG	1:D:537:ILE:HG22	2.27	0.74
1:D:449:ASP:HB3	1:D:532:CYS:N	2.02	0.74
1:B:186:GLU:O	2:B:801:NAG:O7	2.03	0.74
1:B:301:THR:HG21	2:B:805:NAG:C8	2.12	0.74
1:D:188:THR:HG23	1:D:208:ILE:CG1	2.16	0.74
1:A:440:PRO:HB3	1:A:457:LEU:HD21	1.67	0.74
1:B:241:ARG:HE	1:B:281:ILE:HD12	1.51	0.74
1:C:396:ARG:HH21	1:C:464:ILE:CG2	1.99	0.74
1:A:2:TRP:CE2	1:B:95:THR:OG1	2.32	0.74
1:A:396:ARG:NH2	1:A:464:ILE:HB	2.02	0.74
1:A:485:ALA:C	1:A:486:GLU:HG2	2.11	0.74
1:C:241:ARG:HE	1:C:281:ILE:HD12	1.51	0.74
1:C:450:GLN:HG3	1:C:533:GLU:OE2	1.88	0.74
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.74
1:A:3:VAL:C	1:B:3:VAL:CB	2.60	0.74
1:A:289:ASP:O	1:A:290:PHE:CB	2.25	0.74
1:B:450:GLN:HG3	1:B:533:GLU:OE2	1.88	0.74
1:A:450:GLN:HG3	1:A:533:GLU:OE2	1.88	0.74
1:D:451:ASN:O	1:D:534:GLY:HA2	1.88	0.74
1:C:289:ASP:O	1:C:289:ASP:CG	2.29	0.74
1:D:196:LEU:HB2	1:D:199:ALA:HB3	1.67	0.74
1:B:451:ASN:O	1:B:534:GLY:HA2	1.88	0.74
1:D:396:ARG:HH21	1:D:464:ILE:CG2	1.98	0.74
1:A:333:VAL:CB	1:A:334:PRO:HD3	2.18	0.74
1:A:241:ARG:HE	1:A:281:ILE:HD12	1.51	0.73
1:D:371:ILE:HD12	1:D:410:MET:HB3	1.68	0.73
1:B:333:VAL:CB	1:B:334:PRO:HD3	2.18	0.73
1:D:298:LEU:N	1:D:298:LEU:HD23	2.03	0.73
1:D:320:THR:CG2	2:D:807:NAG:HN2	2.01	0.73
1:A:290:PHE:HE2	1:A:293:ARG:HB2	1.52	0.73
1:A:290:PHE:CD2	1:A:293:ARG:N	2.55	0.73
1:A:320:THR:CG2	2:A:807:NAG:HN2	2.02	0.73
1:B:371:ILE:HD12	1:B:410:MET:HB3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:PHE:HZ	1:C:296:TYR:HH	1.35	0.73
1:D:364:ILE:O	1:D:364:ILE:HG13	1.87	0.73
1:A:5:PRO:N	1:B:5:PRO:HG3	2.02	0.73
1:A:223:PRO:HB2	1:A:226:TYR:CE2	2.23	0.73
1:D:450:GLN:HG3	1:D:533:GLU:OE2	1.88	0.73
1:A:27:ASN:C	1:A:27:ASN:ND2	2.46	0.73
1:A:290:PHE:HZ	1:A:296:TYR:HH	1.35	0.73
1:A:364:ILE:O	1:A:364:ILE:HG13	1.87	0.73
1:B:364:ILE:HG13	1:B:364:ILE:O	1.87	0.73
1:B:366:LYS:CG	1:B:367:LEU:N	2.48	0.73
1:C:276:GLU:HG3	1:C:277:SER:H	1.54	0.73
1:C:451:ASN:O	1:C:534:GLY:HA2	1.88	0.73
1:D:1:ASP:CG	1:D:2:TRP:H	1.96	0.73
1:C:273:THR:O	2:C:803:NAG:H82	1.89	0.73
1:A:92:MET:HE1	1:B:3:VAL:HG13	1.70	0.73
1:A:364:ILE:O	1:A:364:ILE:CG1	2.37	0.73
1:C:298:LEU:HD23	1:C:298:LEU:N	2.03	0.73
1:C:396:ARG:NH2	1:C:464:ILE:HB	2.02	0.73
1:D:335:ALA:HB1	3:D:811:NDG:H6	1.54	0.73
1:D:373:ASN:ND2	1:D:374:ASP:H	1.87	0.73
1:A:289:ASP:O	1:A:289:ASP:CG	2.29	0.73
1:B:474:SER:CB	1:B:512:LEU:HG	2.14	0.73
1:C:188:THR:HG23	1:C:208:ILE:CG1	2.16	0.73
1:D:333:VAL:CB	1:D:334:PRO:HD3	2.18	0.73
1:D:342:SER:HA	1:D:431:LEU:HB2	1.71	0.73
1:A:373:ASN:ND2	1:A:374:ASP:H	1.87	0.73
1:A:396:ARG:HH21	1:A:464:ILE:CG2	1.98	0.73
1:B:298:LEU:N	1:B:298:LEU:HD23	2.03	0.73
1:C:223:PRO:HB2	1:C:226:TYR:CE2	2.23	0.73
1:C:290:PHE:CD2	1:C:293:ARG:N	2.55	0.73
1:A:451:ASN:O	1:A:534:GLY:HA2	1.88	0.72
1:B:223:PRO:HB2	1:B:226:TYR:CE2	2.24	0.72
1:C:333:VAL:CB	1:C:334:PRO:HD3	2.18	0.72
1:C:511:VAL:HG23	1:C:523:THR:O	1.89	0.72
1:D:290:PHE:HZ	1:D:296:TYR:HH	1.35	0.72
1:A:222:ASP:O	1:A:222:ASP:CG	2.32	0.72
1:A:298:LEU:N	1:A:298:LEU:HD23	2.03	0.72
1:D:364:ILE:O	1:D:364:ILE:CG1	2.37	0.72
1:A:273:THR:O	2:A:803:NAG:H82	1.89	0.72
1:C:27:ASN:ND2	1:C:27:ASN:C	2.46	0.72
1:D:396:ARG:NH2	1:D:464:ILE:HB	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:CD1	1:B:1:ASP:H2	2.02	0.72
1:C:290:PHE:HE2	1:C:293:ARG:HB2	1.52	0.72
1:A:342:SER:HA	1:A:431:LEU:HB2	1.71	0.72
1:B:1:ASP:CG	1:B:2:TRP:H	1.96	0.72
1:B:276:GLU:HG3	1:B:277:SER:H	1.54	0.72
1:D:523:THR:CG2	1:D:524:VAL:N	2.46	0.72
1:A:33:LYS:HB3	1:A:83:GLU:HG2	1.71	0.72
1:B:364:ILE:O	1:B:364:ILE:CG1	2.37	0.72
1:C:23:GLN:HG2	1:D:3:VAL:HG21	1.71	0.72
1:C:364:ILE:O	1:C:364:ILE:CG1	2.37	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:320:THR:CG2	2:D:807:NAG:N2	2.51	0.72
1:D:511:VAL:HG23	1:D:523:THR:O	1.89	0.72
1:B:273:THR:O	2:B:803:NAG:H82	1.89	0.72
1:D:394:LEU:HD12	1:D:394:LEU:N	2.05	0.72
1:A:1:ASP:CG	1:A:2:TRP:H	1.96	0.72
1:B:320:THR:CG2	2:B:807:NAG:N2	2.52	0.72
1:B:394:LEU:N	1:B:394:LEU:HD12	2.05	0.72
1:B:511:VAL:HG23	1:B:523:THR:O	1.89	0.72
1:A:511:VAL:HG23	1:A:523:THR:O	1.89	0.72
1:B:276:GLU:CG	1:B:277:SER:H	2.03	0.72
1:B:320:THR:CG2	2:B:807:NAG:HN2	2.01	0.72
1:D:27:ASN:C	1:D:27:ASN:ND2	2.46	0.72
1:D:223:PRO:HB2	1:D:226:TYR:CE2	2.23	0.72
1:D:290:PHE:HE2	1:D:293:ARG:HB2	1.52	0.71
1:D:33:LYS:HB3	1:D:83:GLU:HG2	1.71	0.71
1:D:276:GLU:HG3	1:D:277:SER:H	1.54	0.71
1:A:320:THR:CG2	2:A:807:NAG:N2	2.52	0.71
1:B:373:ASN:ND2	1:B:374:ASP:H	1.87	0.71
1:D:32:ASN:CG	1:D:33:LYS:H	1.99	0.71
1:A:90:GLU:OE2	1:B:88:VAL:O	2.09	0.71
1:B:33:LYS:HB3	1:B:83:GLU:HG2	1.71	0.71
1:B:290:PHE:HE2	1:B:293:ARG:HB2	1.52	0.71
1:D:414:ASP:HB3	1:D:420:GLY:HA3	1.73	0.71
1:D:434:ASN:OD1	1:D:467:ASN:HB3	1.91	0.71
1:A:276:GLU:HG3	1:A:277:SER:H	1.54	0.71
1:B:290:PHE:HZ	1:B:296:TYR:HH	1.35	0.71
1:C:394:LEU:HD12	1:C:394:LEU:N	2.05	0.71
1:D:222:ASP:O	1:D:222:ASP:CG	2.32	0.71
1:B:434:ASN:OD1	1:B:467:ASN:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HD13	1:B:3:VAL:N	2.06	0.71
1:A:394:LEU:HD12	1:A:394:LEU:N	2.05	0.71
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.71
1:C:320:THR:CG2	2:C:807:NAG:N2	2.52	0.71
1:C:414:ASP:HB3	1:C:420:GLY:HA3	1.73	0.71
1:A:187:TYR:HA	2:A:801:NAG:C7	2.21	0.71
1:A:403:ASN:CB	2:A:902:NAG:N2	2.54	0.71
1:C:222:ASP:O	1:C:222:ASP:CG	2.32	0.71
1:C:276:GLU:CG	1:C:277:SER:H	2.03	0.71
1:C:320:THR:CG2	2:C:807:NAG:HN2	2.02	0.71
1:D:403:ASN:CB	2:D:902:NAG:N2	2.54	0.71
1:A:276:GLU:CG	1:A:277:SER:H	2.03	0.71
1:A:316:THR:O	2:A:806:NAG:H82	1.91	0.71
1:B:187:TYR:HA	2:B:801:NAG:C7	2.21	0.71
1:B:405:THR:OG1	1:B:406:TYR:N	2.22	0.70
1:B:414:ASP:HB3	1:B:420:GLY:HA3	1.73	0.70
1:B:483:TRP:CZ2	1:B:507:TYR:HE1	2.09	0.70
1:C:33:LYS:HB3	1:C:83:GLU:HG2	1.71	0.70
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.74	0.70
1:B:289:ASP:O	1:B:289:ASP:CG	2.29	0.70
1:B:337:SER:CA	1:B:427:ILE:HG23	2.20	0.70
1:C:32:ASN:CG	1:C:33:LYS:H	1.99	0.70
1:C:403:ASN:CB	2:C:902:NAG:N2	2.54	0.70
1:C:434:ASN:OD1	1:C:467:ASN:HB3	1.91	0.70
1:A:32:ASN:CG	1:A:33:LYS:H	1.99	0.70
1:A:92:MET:CE	1:B:3:VAL:HG13	2.22	0.70
1:D:276:GLU:CG	1:D:277:SER:H	2.03	0.70
1:D:474:SER:CB	1:D:512:LEU:HG	2.14	0.70
1:D:483:TRP:CZ2	1:D:507:TYR:HE1	2.09	0.70
1:B:222:ASP:O	1:B:222:ASP:CG	2.32	0.70
1:B:342:SER:HA	1:B:431:LEU:HB2	1.71	0.70
1:B:316:THR:O	2:B:806:NAG:H82	1.91	0.70
1:B:403:ASN:CB	2:B:902:NAG:N2	2.54	0.70
1:C:1:ASP:CG	1:D:26:SER:CA	2.56	0.70
1:C:1:ASP:CA	1:D:26:SER:C	2.61	0.70
1:C:337:SER:CA	1:C:427:ILE:HG23	2.20	0.70
1:D:405:THR:OG1	1:D:406:TYR:N	2.22	0.70
1:C:482:THR:CG2	1:C:499:THR:CG2	2.62	0.70
1:C:483:TRP:CZ2	1:C:507:TYR:HE1	2.09	0.70
1:D:227:THR:O	2:D:812:NAG:O5	2.09	0.70
1:A:414:ASP:HB3	1:A:420:GLY:HA3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:PHE:CD2	1:B:293:ARG:N	2.55	0.70
1:C:227:THR:O	2:C:812:NAG:O5	2.09	0.70
1:D:187:TYR:HA	2:D:801:NAG:C7	2.21	0.70
1:D:316:THR:O	2:D:806:NAG:H82	1.91	0.70
1:C:342:SER:HA	1:C:431:LEU:HB2	1.71	0.70
1:C:474:SER:CB	1:C:512:LEU:HG	2.14	0.70
1:B:32:ASN:CG	1:B:33:LYS:H	1.98	0.70
1:B:128:MET:HE1	1:B:207:ALA:HB1	1.74	0.70
1:B:227:THR:O	2:B:812:NAG:O5	2.09	0.70
1:C:523:THR:HG23	1:C:524:VAL:HG23	1.74	0.70
1:A:90:GLU:H	1:B:90:GLU:HB3	1.55	0.70
1:A:483:TRP:CZ2	1:A:507:TYR:HE1	2.09	0.70
1:D:229:LEU:HD23	1:D:322:THR:HB	1.73	0.70
1:D:523:THR:HG23	1:D:524:VAL:HG23	1.74	0.70
1:A:434:ASN:OD1	1:A:467:ASN:HB3	1.91	0.69
1:C:517:GLN:C	1:C:519:ASN:N	2.47	0.69
1:A:227:THR:O	2:A:812:NAG:O5	2.09	0.69
1:B:27:ASN:C	1:B:27:ASN:ND2	2.46	0.69
1:C:316:THR:O	2:C:806:NAG:H82	1.91	0.69
1:C:474:SER:HB2	1:C:512:LEU:CG	2.15	0.69
1:D:128:MET:HE1	1:D:207:ALA:HB1	1.74	0.69
1:D:186:GLU:OE1	2:D:801:NAG:H62	1.93	0.69
1:A:221:PHE:CE1	1:A:315:SER:O	2.45	0.69
1:B:53:ILE:HG13	1:B:59:TRP:O	1.93	0.69
1:C:438:PRO:HB3	1:C:471:TYR:CE2	2.26	0.69
1:B:438:PRO:HB3	1:B:471:TYR:CE2	2.26	0.69
1:A:2:TRP:CG	1:B:95:THR:HG1	2.04	0.69
1:A:186:GLU:OE1	2:A:801:NAG:H62	1.93	0.69
1:B:186:GLU:OE1	2:B:801:NAG:H62	1.93	0.69
1:B:229:LEU:HD23	1:B:322:THR:HB	1.73	0.69
1:B:366:LYS:HG3	1:B:367:LEU:N	2.04	0.69
1:C:187:TYR:HA	2:C:801:NAG:C7	2.21	0.69
1:C:221:PHE:CE1	1:C:315:SER:O	2.45	0.69
1:C:229:LEU:HD23	1:C:322:THR:HB	1.73	0.69
1:C:53:ILE:HG13	1:C:59:TRP:O	1.93	0.69
1:C:94:ILE:HG21	1:D:2:TRP:HH2	1.57	0.69
1:D:242:LEU:HD12	1:D:280:GLY:O	1.93	0.69
1:A:282:LEU:HD23	1:A:283:THR:H	1.58	0.69
1:B:282:LEU:HD23	1:B:283:THR:H	1.58	0.69
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.74	0.69
1:C:242:LEU:HD12	1:C:280:GLY:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:THR:HG21	1:B:500:GLN:H	1.59	0.68
1:C:92:MET:HB3	1:D:2:TRP:CD1	2.28	0.68
1:A:229:LEU:HD23	1:A:322:THR:HB	1.73	0.68
1:A:482:THR:HG21	1:A:500:GLN:H	1.58	0.68
1:C:186:GLU:OE1	2:C:801:NAG:H62	1.93	0.68
1:A:53:ILE:HG13	1:A:59:TRP:O	1.93	0.68
1:A:128:MET:HE1	1:A:207:ALA:HB1	1.74	0.68
1:B:272:THR:HG22	1:B:273:THR:N	2.09	0.68
1:C:282:LEU:HD23	1:C:283:THR:N	2.08	0.68
1:C:396:ARG:HD3	1:C:431:LEU:O	1.94	0.68
1:D:320:THR:HG21	2:D:807:NAG:H2	1.76	0.68
1:A:272:THR:HG22	1:A:273:THR:N	2.09	0.68
1:C:405:THR:OG1	1:C:406:TYR:N	2.22	0.68
1:D:366:LYS:CG	1:D:367:LEU:N	2.48	0.68
1:D:396:ARG:HE	1:D:432:ASP:HB2	1.57	0.68
1:A:438:PRO:HB3	1:A:471:TYR:CE2	2.26	0.68
1:B:282:LEU:HD23	1:B:283:THR:N	2.08	0.68
1:B:155:PRO:HB2	2:B:801:NAG:C8	2.24	0.68
1:C:396:ARG:HE	1:C:432:ASP:HB2	1.57	0.68
1:A:155:PRO:HB2	2:A:801:NAG:C8	2.24	0.68
1:B:242:LEU:HD12	1:B:280:GLY:O	1.93	0.68
1:D:371:ILE:CG2	1:D:372:GLY:N	2.57	0.68
1:A:137:ASP:OD2	1:A:139:ILE:HG22	1.94	0.68
1:A:320:THR:HG21	2:A:807:NAG:H2	1.76	0.68
1:B:221:PHE:CE1	1:B:315:SER:O	2.45	0.68
1:D:438:PRO:HB3	1:D:471:TYR:CE2	2.26	0.68
1:B:371:ILE:CG2	1:B:372:GLY:N	2.57	0.68
1:C:371:ILE:CG2	1:C:372:GLY:N	2.57	0.68
1:D:440:PRO:HA	1:D:458:THR:O	1.94	0.68
1:A:242:LEU:HD12	1:A:280:GLY:O	1.93	0.68
1:A:282:LEU:HD23	1:A:283:THR:N	2.08	0.68
1:D:290:PHE:HZ	1:D:296:TYR:OH	1.77	0.68
1:A:405:THR:OG1	1:A:406:TYR:N	2.22	0.67
1:A:474:SER:HB2	1:A:512:LEU:CG	2.15	0.67
1:B:333:VAL:HB	1:B:334:PRO:CD	2.24	0.67
1:B:396:ARG:HE	1:B:432:ASP:CB	2.07	0.67
1:C:128:MET:HE1	1:C:207:ALA:HB1	1.74	0.67
1:C:155:PRO:HB2	2:C:801:NAG:C8	2.24	0.67
1:C:282:LEU:HD23	1:C:283:THR:H	1.58	0.67
1:D:53:ILE:HG13	1:D:59:TRP:O	1.93	0.67
1:D:396:ARG:HD3	1:D:431:LEU:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:SER:CA	1:A:427:ILE:HG23	2.20	0.67
1:A:423:THR:HB	2:A:810:NAG:C8	2.24	0.67
1:B:137:ASP:OD2	1:B:139:ILE:HG22	1.94	0.67
1:C:92:MET:HE1	1:D:2:TRP:HB3	1.76	0.67
1:C:440:PRO:HA	1:C:458:THR:O	1.94	0.67
1:C:92:MET:HE1	1:D:2:TRP:O	1.94	0.67
1:C:272:THR:HG22	1:C:273:THR:N	2.09	0.67
1:D:195:ASP:HB2	1:D:201:LEU:N	2.08	0.67
1:A:396:ARG:NH2	1:A:464:ILE:CB	2.58	0.67
1:D:155:PRO:HB2	2:D:801:NAG:C8	2.24	0.67
1:D:272:THR:HG22	1:D:273:THR:N	2.09	0.67
1:D:282:LEU:HD23	1:D:283:THR:N	2.08	0.67
1:D:482:THR:HG21	1:D:500:GLN:H	1.59	0.67
1:A:373:ASN:ND2	1:A:374:ASP:N	2.43	0.67
1:C:289:ASP:O	1:C:290:PHE:CB	2.25	0.67
1:A:347:ARG:CD	1:A:392:GLY:H	2.07	0.67
1:B:347:ARG:CG	1:B:392:GLY:H	2.08	0.67
1:B:373:ASN:ND2	1:B:374:ASP:N	2.43	0.67
1:B:440:PRO:HA	1:B:458:THR:O	1.94	0.67
1:A:347:ARG:CG	1:A:392:GLY:H	2.08	0.67
1:A:371:ILE:CG2	1:A:372:GLY:N	2.57	0.67
1:B:401:VAL:HG13	1:B:405:THR:O	1.95	0.67
1:C:290:PHE:HZ	1:C:296:TYR:OH	1.77	0.67
1:D:137:ASP:OD2	1:D:139:ILE:HG22	1.94	0.67
1:D:337:SER:CA	1:D:427:ILE:HG23	2.20	0.67
1:D:347:ARG:CG	1:D:392:GLY:H	2.08	0.67
1:D:396:ARG:HE	1:D:432:ASP:CB	2.07	0.67
1:D:401:VAL:HG13	1:D:405:THR:O	1.95	0.67
1:D:423:THR:HB	2:D:810:NAG:C8	2.24	0.67
1:A:474:SER:CB	1:A:512:LEU:HG	2.14	0.67
1:C:195:ASP:HB2	1:C:201:LEU:N	2.08	0.67
1:C:396:ARG:NH2	1:C:464:ILE:CB	2.58	0.67
1:C:401:VAL:HG13	1:C:405:THR:O	1.95	0.67
1:D:474:SER:HB2	1:D:512:LEU:CG	2.15	0.67
1:A:396:ARG:HE	1:A:432:ASP:HB2	1.57	0.67
1:B:403:ASN:HB2	2:B:902:NAG:N2	2.10	0.67
1:C:333:VAL:HB	1:C:334:PRO:CD	2.24	0.67
1:C:396:ARG:HE	1:C:432:ASP:CB	2.07	0.67
1:D:187:TYR:HA	2:D:801:NAG:C8	2.25	0.67
1:D:373:ASN:ND2	1:D:374:ASP:N	2.43	0.67
1:B:320:THR:HG21	2:B:807:NAG:H2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:HE	1:B:432:ASP:HB2	1.57	0.67
1:B:423:THR:HB	2:B:810:NAG:C8	2.24	0.67
1:A:396:ARG:HD3	1:A:431:LEU:O	1.94	0.66
1:A:403:ASN:HB2	2:A:902:NAG:N2	2.10	0.66
1:A:440:PRO:HA	1:A:458:THR:O	1.94	0.66
1:C:347:ARG:CD	1:C:392:GLY:H	2.07	0.66
1:A:187:TYR:HA	2:A:801:NAG:C8	2.25	0.66
1:B:187:TYR:HA	2:B:801:NAG:C8	2.25	0.66
1:B:524:VAL:HG21	2:B:904:NAG:H81	1.77	0.66
1:C:187:TYR:HA	2:C:801:NAG:C8	2.25	0.66
1:C:423:THR:HB	2:C:810:NAG:C8	2.24	0.66
1:C:482:THR:HG21	1:C:500:GLN:H	1.59	0.66
1:D:446:THR:CG2	1:D:537:ILE:O	2.44	0.66
1:A:290:PHE:HZ	1:A:296:TYR:OH	1.77	0.66
1:A:396:ARG:HE	1:A:432:ASP:CB	2.07	0.66
1:A:401:VAL:HG13	1:A:405:THR:O	1.95	0.66
1:B:464:ILE:O	1:B:467:ASN:HB2	1.96	0.66
1:A:195:ASP:HB2	1:A:201:LEU:N	2.08	0.66
1:A:524:VAL:HG21	2:A:904:NAG:H81	1.76	0.66
1:B:290:PHE:HZ	1:B:296:TYR:OH	1.76	0.66
1:B:524:VAL:HG23	2:B:904:NAG:H81	1.78	0.66
1:C:366:LYS:HG3	1:C:367:LEU:HG	1.77	0.66
1:C:464:ILE:O	1:C:467:ASN:HB2	1.96	0.66
1:A:347:ARG:HD2	1:A:392:GLY:H	1.60	0.66
1:B:396:ARG:HD3	1:B:431:LEU:O	1.94	0.66
1:C:137:ASP:OD2	1:C:139:ILE:HG22	1.94	0.66
1:C:320:THR:HG21	2:C:807:NAG:H2	1.76	0.66
1:D:347:ARG:CD	1:D:392:GLY:H	2.07	0.66
1:B:224:LYS:HE3	1:B:316:THR:O	1.95	0.66
1:B:347:ARG:CD	1:B:392:GLY:H	2.07	0.66
1:B:347:ARG:HD2	1:B:392:GLY:H	1.60	0.66
1:C:154:ASP:O	1:C:155:PRO:C	2.36	0.66
1:C:524:VAL:HG21	2:C:904:NAG:H81	1.77	0.66
1:D:396:ARG:NH2	1:D:464:ILE:CB	2.58	0.66
1:B:232:GLU:HG2	1:B:289:ASP:HA	1.77	0.66
1:C:373:ASN:ND2	1:C:374:ASP:N	2.43	0.66
1:D:440:PRO:HD2	1:D:522:LEU:CD1	2.26	0.66
1:A:224:LYS:HE3	1:A:316:THR:O	1.95	0.66
1:A:366:LYS:HG3	1:A:367:LEU:HG	1.77	0.66
1:A:446:THR:CG2	1:A:537:ILE:O	2.44	0.66
2:B:809:NAG:C6	2:B:810:NAG:H62	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:THR:CG2	1:C:537:ILE:O	2.44	0.66
1:A:482:THR:OG1	1:A:500:GLN:CG	2.44	0.66
1:B:440:PRO:HD3	1:B:522:LEU:HD12	1.78	0.66
1:C:224:LYS:HE3	1:C:316:THR:O	1.95	0.66
1:C:347:ARG:CG	1:C:392:GLY:H	2.08	0.66
1:C:524:VAL:HG23	2:C:904:NAG:H81	1.78	0.66
1:D:154:ASP:O	1:D:155:PRO:C	2.37	0.66
1:D:224:LYS:HE3	1:D:316:THR:O	1.95	0.66
1:A:464:ILE:O	1:A:467:ASN:HB2	1.96	0.66
1:D:32:ASN:ND2	1:D:83:GLU:N	2.44	0.66
1:B:482:THR:OG1	1:B:500:GLN:CG	2.44	0.65
2:C:809:NAG:C6	2:C:810:NAG:H62	2.26	0.65
1:D:282:LEU:HD23	1:D:283:THR:H	1.58	0.65
1:D:524:VAL:HG21	2:D:904:NAG:H81	1.76	0.65
1:A:440:PRO:HD2	1:A:522:LEU:CD1	2.26	0.65
1:B:195:ASP:HB2	1:B:201:LEU:N	2.08	0.65
1:B:396:ARG:NH2	1:B:464:ILE:CB	2.58	0.65
2:C:805:NAG:C6	2:C:806:NAG:C7	2.74	0.65
1:D:540:GLN:CD	1:D:540:GLN:C	2.60	0.65
1:A:24:ILE:HD12	1:B:1:ASP:H2	1.61	0.65
1:A:232:GLU:HG2	1:A:289:ASP:HA	1.77	0.65
1:A:333:VAL:HB	1:A:334:PRO:CD	2.24	0.65
1:C:403:ASN:HB2	2:C:902:NAG:N2	2.10	0.65
1:D:232:GLU:HG2	1:D:289:ASP:HA	1.77	0.65
2:A:809:NAG:C6	2:A:810:NAG:H62	2.26	0.65
1:B:154:ASP:O	1:B:155:PRO:C	2.36	0.65
1:B:446:THR:CG2	1:B:537:ILE:O	2.44	0.65
1:B:517:GLN:C	1:B:519:ASN:N	2.46	0.65
1:C:1:ASP:CB	1:D:26:SER:CA	2.68	0.65
1:C:488:ASP:HB2	1:C:493:SER:OG	1.97	0.65
1:D:366:LYS:HG3	1:D:367:LEU:HG	1.77	0.65
1:D:403:ASN:HB2	2:D:902:NAG:N2	2.10	0.65
1:D:488:ASP:HB2	1:D:493:SER:OG	1.97	0.65
1:D:524:VAL:HG23	2:D:904:NAG:H81	1.78	0.65
1:A:32:ASN:ND2	1:A:83:GLU:N	2.44	0.65
1:A:488:ASP:HB2	1:A:493:SER:OG	1.97	0.65
1:B:488:ASP:HB2	1:B:493:SER:OG	1.97	0.65
1:C:232:GLU:HG2	1:C:289:ASP:HA	1.77	0.65
1:C:482:THR:OG1	1:C:500:GLN:CG	2.44	0.65
1:D:464:ILE:O	1:D:467:ASN:HB2	1.96	0.65
1:B:341:VAL:HG21	1:B:345:LEU:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:GLU:HB3	1:C:268:PHE:CE2	2.31	0.65
1:C:347:ARG:HD2	1:C:392:GLY:H	1.60	0.65
1:D:333:VAL:HB	1:D:334:PRO:CD	2.24	0.65
1:B:366:LYS:HG3	1:B:367:LEU:HG	1.77	0.65
1:C:232:GLU:HG3	1:C:290:PHE:H	1.61	0.65
2:D:809:NAG:C6	2:D:810:NAG:H62	2.26	0.65
1:C:341:VAL:HG21	1:C:345:LEU:HD12	1.79	0.65
1:A:440:PRO:HD3	1:A:522:LEU:HD12	1.78	0.65
1:B:364:ILE:O	1:B:364:ILE:HD12	1.97	0.65
1:C:212:THR:HG22	1:C:213:ASP:H	1.62	0.65
1:C:327:ASN:HA	1:C:360:ASP:OD2	1.97	0.65
1:C:440:PRO:HD3	1:C:522:LEU:HD12	1.78	0.65
1:D:327:ASN:HA	1:D:360:ASP:OD2	1.97	0.65
1:D:346:SER:OG	1:D:349:GLU:HG3	1.97	0.65
2:D:805:NAG:C6	2:D:806:NAG:C7	2.74	0.65
1:A:232:GLU:HG3	1:A:290:PHE:H	1.61	0.65
1:D:265:GLU:HB3	1:D:268:PHE:CE2	2.31	0.65
1:A:364:ILE:O	1:A:364:ILE:HD12	1.98	0.64
1:B:347:ARG:HG3	1:B:392:GLY:H	1.62	0.64
1:B:469:TYR:CD2	1:B:470:PRO:CD	2.80	0.64
1:A:341:VAL:HG21	1:A:345:LEU:HD12	1.79	0.64
1:C:60:MET:SD	1:D:2:TRP:CH2	2.90	0.64
1:A:155:PRO:C	1:A:157:GLU:N	2.56	0.64
1:C:440:PRO:HD2	1:C:522:LEU:CD1	2.26	0.64
1:D:347:ARG:HD2	1:D:392:GLY:H	1.60	0.64
1:A:343:GLU:HB3	1:A:433:VAL:CG2	2.28	0.64
1:C:78:SER:N	1:D:2:TRP:HE1	1.96	0.64
1:B:212:THR:HG22	1:B:213:ASP:H	1.62	0.64
1:B:343:GLU:HB3	1:B:433:VAL:CG2	2.28	0.64
1:B:440:PRO:HD2	1:B:522:LEU:CD1	2.26	0.64
1:B:482:THR:HG21	1:B:499:THR:CA	2.27	0.64
1:D:212:THR:HG22	1:D:213:ASP:H	1.62	0.64
1:D:406:TYR:CE1	2:D:808:NAG:H83	2.32	0.64
1:A:2:TRP:CG	1:B:95:THR:OG1	2.50	0.64
1:A:327:ASN:HA	1:A:360:ASP:OD2	1.97	0.64
1:A:346:SER:OG	1:A:349:GLU:HG3	1.97	0.64
1:D:469:TYR:CD2	1:D:470:PRO:CD	2.80	0.64
1:D:482:THR:OG1	1:D:500:GLN:CG	2.44	0.64
1:A:212:THR:HG22	1:A:213:ASP:H	1.62	0.64
1:B:32:ASN:ND2	1:B:83:GLU:N	2.44	0.64
1:C:346:SER:OG	1:C:349:GLU:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:TYR:CE1	2:C:808:NAG:H83	2.32	0.64
1:A:469:TYR:CD2	1:A:470:PRO:CD	2.81	0.64
1:B:327:ASN:HA	1:B:360:ASP:OD2	1.97	0.64
1:B:406:TYR:CE1	2:B:808:NAG:H83	2.32	0.64
1:D:221:PHE:CE1	1:D:315:SER:O	2.45	0.64
1:D:341:VAL:HG21	1:D:345:LEU:HD12	1.79	0.64
1:D:375:PRO:HB3	1:D:400:TYR:CD2	2.33	0.64
1:D:504:LYS:NZ	1:D:531:SER:OG	2.31	0.64
1:A:375:PRO:HB3	1:A:400:TYR:CD2	2.33	0.64
1:A:446:THR:CG2	1:A:539:CYS:SG	2.86	0.64
1:C:518:ASN:O	1:C:520:PRO:CD	2.46	0.64
1:D:227:THR:CG2	2:D:807:NAG:C7	2.76	0.64
1:D:409:ILE:HG12	1:D:425:THR:HG23	1.80	0.64
1:A:406:TYR:CE1	2:A:808:NAG:H83	2.32	0.64
1:A:524:VAL:HG23	2:A:904:NAG:H81	1.78	0.64
1:D:440:PRO:HD3	1:D:522:LEU:HD12	1.78	0.64
1:A:364:ILE:O	1:A:364:ILE:CD1	2.46	0.63
1:B:265:GLU:HB3	1:B:268:PHE:CE2	2.31	0.63
1:C:343:GLU:HB3	1:C:433:VAL:CG2	2.28	0.63
1:C:375:PRO:HB3	1:C:400:TYR:CD2	2.33	0.63
1:D:232:GLU:HG3	1:D:290:PHE:H	1.61	0.63
1:A:419:VAL:HG13	2:A:809:NAG:O7	1.98	0.63
1:B:403:ASN:CB	2:B:902:NAG:C7	2.76	0.63
1:C:154:ASP:O	2:C:801:NAG:H82	1.98	0.63
1:C:364:ILE:O	1:C:364:ILE:CD1	2.46	0.63
1:C:482:THR:HG21	1:C:499:THR:CA	2.27	0.63
1:D:343:GLU:HB3	1:D:433:VAL:CG2	2.28	0.63
1:D:364:ILE:O	1:D:364:ILE:HD12	1.97	0.63
1:D:446:THR:CG2	1:D:539:CYS:SG	2.86	0.63
1:A:22:VAL:HG22	1:A:23:GLN:N	2.14	0.63
1:A:347:ARG:HG3	1:A:392:GLY:H	1.62	0.63
1:A:409:ILE:HG12	1:A:425:THR:HG23	1.80	0.63
1:C:22:VAL:HG22	1:C:23:GLN:N	2.14	0.63
1:C:371:ILE:HG22	1:C:372:GLY:N	2.14	0.63
1:C:504:LYS:NZ	1:C:531:SER:OG	2.31	0.63
1:A:147:SER:OG	1:A:167:ARG:HG3	1.99	0.63
1:A:482:THR:HG22	1:A:499:THR:N	2.13	0.63
1:B:504:LYS:NZ	1:B:531:SER:OG	2.31	0.63
2:B:805:NAG:C6	2:B:806:NAG:C7	2.74	0.63
1:C:1:ASP:H1	1:D:26:SER:C	2.07	0.63
1:C:347:ARG:HG3	1:C:392:GLY:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:ILE:HG12	1:C:425:THR:HG23	1.80	0.63
1:C:446:THR:CG2	1:C:539:CYS:SG	2.86	0.63
1:D:299:GLN:C	1:D:300:ILE:HD12	2.24	0.63
1:A:154:ASP:O	1:A:155:PRO:C	2.36	0.63
1:A:482:THR:HG21	1:A:499:THR:CA	2.27	0.63
1:A:518:ASN:O	1:A:520:PRO:CD	2.46	0.63
1:A:523:THR:CG2	1:A:524:VAL:H	1.94	0.63
1:B:375:PRO:HB3	1:B:400:TYR:CD2	2.33	0.63
1:B:409:ILE:HG12	1:B:425:THR:HG23	1.80	0.63
1:B:469:TYR:CE1	1:B:470:PRO:HD2	2.34	0.63
1:C:147:SER:OG	1:C:167:ARG:HG3	1.99	0.63
1:C:364:ILE:O	1:C:364:ILE:HD12	1.97	0.63
1:C:469:TYR:CD2	1:C:470:PRO:CD	2.81	0.63
1:D:22:VAL:HG22	1:D:23:GLN:N	2.14	0.63
1:D:142:LEU:HB3	1:D:196:LEU:HA	1.81	0.63
1:D:347:ARG:HG3	1:D:392:GLY:H	1.62	0.63
1:A:142:LEU:HB3	1:A:196:LEU:HA	1.81	0.63
1:B:147:SER:OG	1:B:167:ARG:HG3	1.99	0.63
1:B:154:ASP:CA	2:B:801:NAG:H82	2.29	0.63
1:B:346:SER:OG	1:B:349:GLU:HG3	1.97	0.63
1:B:486:GLU:O	1:B:495:LEU:N	2.31	0.63
1:A:504:LYS:NZ	1:A:531:SER:OG	2.32	0.63
1:B:371:ILE:HG22	1:B:372:GLY:N	2.14	0.63
1:B:419:VAL:HG13	2:B:809:NAG:O7	1.98	0.63
1:C:486:GLU:O	1:C:494:MET:CA	2.46	0.63
1:B:127:VAL:HG22	1:B:128:MET:N	2.14	0.63
1:B:154:ASP:O	2:B:801:NAG:H82	1.98	0.63
1:B:364:ILE:O	1:B:364:ILE:CD1	2.46	0.63
1:C:419:VAL:HG13	2:C:809:NAG:O7	1.98	0.63
1:D:411:LEU:HD22	1:D:421:THR:HG23	1.81	0.63
1:D:482:THR:HG21	1:D:499:THR:CA	2.27	0.63
1:A:154:ASP:O	2:A:801:NAG:H82	1.98	0.63
1:C:142:LEU:HB3	1:C:196:LEU:HA	1.81	0.63
1:C:411:LEU:HD22	1:C:421:THR:HG23	1.81	0.63
1:A:265:GLU:HB3	1:A:268:PHE:CE2	2.31	0.62
1:B:374:ASP:O	1:B:375:PRO:O	2.17	0.62
1:B:411:LEU:HD22	1:B:421:THR:HG23	1.81	0.62
1:B:474:SER:HB2	1:B:512:LEU:CG	2.15	0.62
1:C:415:ASP:OD1	1:C:416:GLY:N	2.27	0.62
1:A:3:VAL:CG1	1:B:4:ILE:HD13	2.28	0.62
1:A:227:THR:CG2	2:A:807:NAG:C7	2.76	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ASN:CB	2:C:902:NAG:C7	2.76	0.62
1:D:364:ILE:O	1:D:364:ILE:CD1	2.46	0.62
1:D:486:GLU:O	1:D:494:MET:CA	2.46	0.62
1:A:127:VAL:HG22	1:A:128:MET:N	2.14	0.62
1:A:154:ASP:CA	2:A:801:NAG:H82	2.29	0.62
1:A:469:TYR:CE1	1:A:470:PRO:HD2	2.34	0.62
1:D:371:ILE:HG22	1:D:372:GLY:N	2.14	0.62
1:A:299:GLN:C	1:A:300:ILE:HD12	2.24	0.62
1:A:524:VAL:HG23	2:A:904:NAG:C8	2.29	0.62
1:B:22:VAL:HG22	1:B:23:GLN:N	2.14	0.62
1:B:299:GLN:C	1:B:300:ILE:HD12	2.24	0.62
1:B:518:ASN:O	1:B:520:PRO:CD	2.46	0.62
1:C:374:ASP:O	1:C:375:PRO:O	2.17	0.62
1:D:486:GLU:O	1:D:495:LEU:N	2.31	0.62
2:A:805:NAG:C6	2:A:806:NAG:C7	2.74	0.62
1:B:524:VAL:HG23	2:B:904:NAG:C8	2.29	0.62
1:C:32:ASN:ND2	1:C:83:GLU:N	2.45	0.62
1:C:227:THR:CG2	2:C:807:NAG:C7	2.76	0.62
1:C:299:GLN:C	1:C:300:ILE:HD12	2.24	0.62
1:D:154:ASP:CA	2:D:801:NAG:H82	2.29	0.62
1:D:366:LYS:HG3	1:D:367:LEU:N	2.04	0.62
1:D:419:VAL:HG13	2:D:809:NAG:O7	1.98	0.62
1:A:371:ILE:CG2	1:A:372:GLY:H	2.13	0.62
1:A:508:SER:HB3	1:A:526:ASN:OD1	2.00	0.62
1:B:446:THR:CG2	1:B:539:CYS:SG	2.86	0.62
1:D:154:ASP:C	2:D:801:NAG:C8	2.62	0.62
1:D:403:ASN:CB	2:D:902:NAG:C7	2.76	0.62
1:B:142:LEU:HB3	1:B:196:LEU:HA	1.81	0.62
1:C:524:VAL:CG2	2:C:904:NAG:C8	2.78	0.62
1:D:371:ILE:CG2	1:D:372:GLY:H	2.13	0.62
1:B:232:GLU:HG3	1:B:290:PHE:H	1.61	0.62
1:D:449:ASP:H	1:D:532:CYS:CB	2.12	0.62
1:D:524:VAL:HG23	2:D:904:NAG:C8	2.29	0.62
1:A:393:ASN:C	1:A:394:LEU:HD12	2.25	0.62
1:B:486:GLU:O	1:B:494:MET:CA	2.46	0.62
1:C:469:TYR:CE1	1:C:470:PRO:HD2	2.34	0.62
1:D:393:ASN:C	1:D:394:LEU:HD12	2.25	0.62
1:A:403:ASN:O	1:A:405:THR:N	2.33	0.62
1:B:482:THR:HG22	1:B:499:THR:N	2.13	0.62
1:D:517:GLN:C	1:D:519:ASN:N	2.47	0.62
1:A:2:TRP:CZ3	1:B:6:PRO:HG3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:THR:HG22	1:B:213:ASP:N	2.15	0.61
1:B:235:ILE:HG12	1:B:287:GLY:HA2	1.82	0.61
1:C:154:ASP:CA	2:C:801:NAG:H82	2.29	0.61
1:D:68:ARG:HD3	1:D:100:ASP:HA	1.82	0.61
1:A:371:ILE:HG22	1:A:372:GLY:N	2.14	0.61
1:A:486:GLU:O	1:A:494:MET:CA	2.46	0.61
1:A:524:VAL:CG2	2:A:904:NAG:C8	2.78	0.61
1:B:508:SER:HB3	1:B:526:ASN:OD1	2.00	0.61
1:C:393:ASN:C	1:C:394:LEU:HD12	2.25	0.61
1:A:68:ARG:HD3	1:A:100:ASP:HA	1.82	0.61
1:A:181:ARG:NE	1:A:213:ASP:OD1	2.34	0.61
1:A:411:LEU:HD22	1:A:421:THR:HG23	1.81	0.61
1:C:403:ASN:O	1:C:405:THR:N	2.33	0.61
1:A:212:THR:HG22	1:A:213:ASP:N	2.15	0.61
1:A:449:ASP:H	1:A:532:CYS:CB	2.12	0.61
1:B:181:ARG:NE	1:B:213:ASP:OD1	2.34	0.61
1:B:371:ILE:CG2	1:B:372:GLY:H	2.13	0.61
1:D:524:VAL:CG2	2:D:904:NAG:C8	2.78	0.61
1:B:524:VAL:CG2	2:B:904:NAG:C8	2.78	0.61
1:C:68:ARG:HD3	1:C:100:ASP:HA	1.82	0.61
1:D:155:PRO:C	1:D:157:GLU:N	2.56	0.61
1:D:379:LEU:HD23	1:D:379:LEU:H	1.66	0.61
1:A:374:ASP:O	1:A:375:PRO:O	2.17	0.61
1:C:508:SER:HB3	1:C:526:ASN:OD1	2.00	0.61
1:D:127:VAL:HG22	1:D:128:MET:N	2.14	0.61
1:D:403:ASN:O	1:D:405:THR:N	2.33	0.61
1:A:379:LEU:HD23	1:A:379:LEU:H	1.66	0.61
1:C:524:VAL:HG23	2:C:904:NAG:C8	2.29	0.61
1:D:374:ASP:O	1:D:375:PRO:O	2.17	0.61
1:A:475:LEU:O	1:A:479:SER:HB3	2.01	0.61
1:B:393:ASN:C	1:B:394:LEU:HD12	2.25	0.61
1:C:181:ARG:NE	1:C:213:ASP:OD1	2.34	0.61
1:B:403:ASN:CB	2:B:902:NAG:H83	2.21	0.61
1:D:432:ASP:CG	1:D:464:ILE:CG2	2.74	0.61
1:A:32:ASN:CG	1:A:33:LYS:N	2.59	0.61
1:C:212:THR:HG22	1:C:213:ASP:N	2.15	0.61
1:D:181:ARG:NE	1:D:213:ASP:OD1	2.34	0.61
1:D:469:TYR:CE1	1:D:470:PRO:HD2	2.34	0.61
1:C:371:ILE:CG2	1:C:372:GLY:H	2.13	0.60
1:D:508:SER:HB3	1:D:526:ASN:OD1	1.99	0.60
1:A:486:GLU:O	1:A:495:LEU:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:GLU:CG	1:D:290:PHE:N	2.64	0.60
1:C:127:VAL:HG22	1:C:128:MET:N	2.14	0.60
1:A:94:ILE:N	1:B:2:TRP:CB	2.55	0.60
1:B:68:ARG:HD3	1:B:100:ASP:HA	1.82	0.60
1:C:239:VAL:HG13	1:C:240:GLN:H	1.67	0.60
1:A:24:ILE:HB	1:B:1:ASP:N	2.17	0.60
1:A:482:THR:HG21	1:A:499:THR:C	2.27	0.60
1:B:227:THR:CG2	2:B:807:NAG:C7	2.76	0.60
1:B:403:ASN:O	1:B:405:THR:N	2.33	0.60
1:D:212:THR:HG22	1:D:213:ASP:N	2.15	0.60
1:D:514:SER:HA	1:D:517:GLN:O	2.02	0.60
1:A:415:ASP:OD1	1:A:416:GLY:N	2.27	0.60
1:C:508:SER:HA	1:C:526:ASN:HA	1.84	0.60
1:B:336:VAL:HB	1:B:426:LEU:HD23	1.84	0.60
1:C:27:ASN:CG	1:D:90:GLU:HG3	2.24	0.60
1:C:116:SER:HA	1:C:210:GLN:O	2.02	0.60
1:A:154:ASP:CG	1:A:155:PRO:CD	2.75	0.60
1:D:189:LEU:N	1:D:189:LEU:HD23	2.17	0.60
1:D:482:THR:HG22	1:D:499:THR:N	2.13	0.60
1:A:24:ILE:CB	1:B:1:ASP:H2	2.15	0.60
1:A:239:VAL:HG13	1:A:240:GLN:H	1.67	0.60
1:A:514:SER:HA	1:A:517:GLN:O	2.02	0.60
1:B:449:ASP:H	1:B:532:CYS:CB	2.12	0.60
1:B:508:SER:HA	1:B:526:ASN:HA	1.84	0.60
1:D:146:LEU:HA	1:D:194:THR:O	2.02	0.60
1:D:239:VAL:HG13	1:D:240:GLN:H	1.67	0.60
1:A:450:GLN:HB2	1:A:533:GLU:CA	2.26	0.59
1:B:363:GLN:C	1:B:364:ILE:CG2	2.75	0.59
1:B:523:THR:CG2	1:B:524:VAL:H	1.94	0.59
1:C:154:ASP:CG	1:C:155:PRO:CD	2.75	0.59
1:C:443:ARG:HG3	1:C:443:ARG:HH11	1.67	0.59
1:A:403:ASN:CB	2:A:902:NAG:C7	2.76	0.59
1:B:32:ASN:CG	1:B:33:LYS:N	2.59	0.59
1:B:49:GLY:O	1:B:63:THR:HG21	2.02	0.59
1:B:379:LEU:HD23	1:B:379:LEU:H	1.66	0.59
1:C:1:ASP:N	1:D:26:SER:C	2.60	0.59
1:C:24:ILE:HG21	1:D:2:TRP:HA	0.65	0.59
1:C:447:MET:HB2	1:C:529:VAL:HG22	1.84	0.59
1:C:514:SER:HA	1:C:517:GLN:O	2.02	0.59
1:D:508:SER:HA	1:D:526:ASN:HA	1.84	0.59
1:A:508:SER:HA	1:A:526:ASN:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:LEU:HD23	1:C:379:LEU:H	1.66	0.59
1:D:447:MET:HB2	1:D:529:VAL:HG22	1.84	0.59
1:B:189:LEU:N	1:B:189:LEU:HD23	2.17	0.59
1:B:268:PHE:HA	1:B:285:ALA:HB3	1.84	0.59
1:C:189:LEU:N	1:C:189:LEU:HD23	2.17	0.59
1:C:336:VAL:HB	1:C:426:LEU:HD23	1.84	0.59
1:C:367:LEU:C	1:C:367:LEU:HD12	2.28	0.59
1:D:363:GLN:C	1:D:364:ILE:CG2	2.75	0.59
1:A:447:MET:HB2	1:A:529:VAL:HG22	1.84	0.59
1:B:154:ASP:CG	1:B:155:PRO:CD	2.75	0.59
1:D:336:VAL:HB	1:D:426:LEU:HD23	1.84	0.59
1:A:116:SER:HA	1:A:210:GLN:O	2.02	0.59
1:A:146:LEU:HA	1:A:194:THR:O	2.02	0.59
1:A:221:PHE:HA	1:A:244:VAL:HG12	1.85	0.59
1:A:432:ASP:CG	1:A:464:ILE:CG2	2.74	0.59
1:B:475:LEU:O	1:B:479:SER:HB3	2.01	0.59
1:C:1:ASP:HB2	1:D:27:ASN:N	2.17	0.59
1:C:475:LEU:O	1:C:479:SER:HB3	2.01	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:D:475:LEU:O	1:D:479:SER:HB3	2.01	0.59
1:A:268:PHE:HA	1:A:285:ALA:HB3	1.85	0.59
1:A:367:LEU:HD12	1:A:367:LEU:C	2.28	0.59
1:B:32:ASN:HD22	1:B:83:GLU:H	1.51	0.59
1:D:116:SER:HA	1:D:210:GLN:O	2.02	0.59
1:B:367:LEU:CB	1:B:413:THR:O	2.51	0.59
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.68	0.59
1:C:309:SER:O	1:C:310:VAL:HG23	2.03	0.59
1:D:415:ASP:OD1	1:D:416:GLY:N	2.26	0.59
1:A:443:ARG:HH11	1:A:443:ARG:HG3	1.68	0.59
1:B:146:LEU:HA	1:B:194:THR:O	2.02	0.59
1:B:232:GLU:HG2	1:B:289:ASP:CA	2.33	0.59
1:B:286:LYS:O	1:B:287:GLY:O	2.21	0.59
1:B:367:LEU:C	1:B:367:LEU:HD12	2.28	0.59
1:B:473:VAL:HA	1:B:513:LEU:HD23	1.85	0.59
1:B:482:THR:HG21	1:B:499:THR:C	2.27	0.59
1:C:449:ASP:H	1:C:532:CYS:CB	2.12	0.59
1:C:486:GLU:O	1:C:495:LEU:N	2.31	0.59
1:D:195:ASP:CB	1:D:200:GLY:HA3	2.33	0.59
1:A:49:GLY:O	1:A:63:THR:HG21	2.02	0.59
1:A:189:LEU:HD23	1:A:189:LEU:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLN:C	1:A:364:ILE:CG2	2.75	0.59
1:B:116:SER:HA	1:B:210:GLN:O	2.02	0.59
1:C:232:GLU:HG2	1:C:289:ASP:CA	2.33	0.59
1:C:232:GLU:CG	1:C:290:PHE:N	2.64	0.59
1:C:432:ASP:CG	1:C:464:ILE:CG2	2.74	0.59
1:D:396:ARG:NH2	1:D:464:ILE:HG21	2.17	0.59
1:D:482:THR:HG21	1:D:499:THR:C	2.27	0.59
1:D:518:ASN:O	1:D:520:PRO:CD	2.46	0.59
1:A:232:GLU:CG	1:A:290:PHE:N	2.64	0.58
1:A:309:SER:O	1:A:310:VAL:HG23	2.03	0.58
1:A:335:ALA:HB1	3:A:811:NDG:C6	2.33	0.58
1:A:406:TYR:HB3	1:A:428:LEU:CD2	2.33	0.58
1:B:406:TYR:HB3	1:B:428:LEU:CD2	2.33	0.58
1:B:443:ARG:HA	1:B:525:VAL:HG13	1.85	0.58
1:B:447:MET:HB2	1:B:529:VAL:HG22	1.84	0.58
1:C:49:GLY:O	1:C:63:THR:HG21	2.02	0.58
1:C:146:LEU:HA	1:C:194:THR:O	2.02	0.58
1:C:406:TYR:HB3	1:C:428:LEU:CD2	2.33	0.58
1:A:38:ILE:HG22	1:A:53:ILE:HG22	1.85	0.58
1:A:537:ILE:HG12	1:A:538:LYS:N	2.19	0.58
1:B:239:VAL:HG13	1:B:240:GLN:H	1.67	0.58
1:C:367:LEU:CB	1:C:413:THR:O	2.51	0.58
1:C:482:THR:HG21	1:C:499:THR:C	2.27	0.58
1:D:406:TYR:HB3	1:D:428:LEU:CD2	2.33	0.58
1:A:443:ARG:HA	1:A:525:VAL:HG13	1.85	0.58
1:B:514:SER:HA	1:B:517:GLN:O	2.02	0.58
1:D:473:VAL:HA	1:D:513:LEU:HD23	1.85	0.58
1:A:367:LEU:CB	1:A:413:THR:O	2.51	0.58
1:B:309:SER:O	1:B:310:VAL:HG23	2.03	0.58
1:C:27:ASN:OD1	1:D:90:GLU:CG	2.47	0.58
1:D:49:GLY:O	1:D:63:THR:HG21	2.02	0.58
1:D:286:LYS:O	1:D:287:GLY:O	2.21	0.58
1:D:443:ARG:HA	1:D:525:VAL:HG13	1.85	0.58
1:B:335:ALA:HB1	3:B:811:NDG:C6	2.33	0.58
1:C:27:ASN:OD1	1:D:90:GLU:CA	2.51	0.58
1:C:195:ASP:CB	1:C:200:GLY:HA3	2.33	0.58
1:C:235:ILE:HG12	1:C:287:GLY:HA2	1.82	0.58
1:C:363:GLN:C	1:C:364:ILE:CG2	2.75	0.58
1:D:38:ILE:HG22	1:D:53:ILE:HG22	1.85	0.58
1:D:154:ASP:O	2:D:801:NAG:H82	1.98	0.58
1:D:268:PHE:HA	1:D:285:ALA:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ASN:C	1:A:405:THR:H	2.12	0.58
1:B:396:ARG:NH2	1:B:464:ILE:HG21	2.17	0.58
1:B:432:ASP:CG	1:B: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:221:PHE:HA	1:B:244:VAL:HG12	1.85	0.58
1:B:232:GLU:CG	1:B:290:PHE:N	2.64	0.58
1:B:363:GLN:O	1:B:364:ILE:HG22	2.03	0.58
1:C:268:PHE:HA	1:C:285:ALA:HB3	1.85	0.58
1:C:366:LYS:HG3	1:C:367:LEU:N	2.04	0.58
1:D:232:GLU:HG2	1:D:289:ASP:CA	2.33	0.58
1:D:367:LEU:C	1:D:367:LEU:HD12	2.28	0.58
1:A:296:TYR:HB2	1:A:321:VAL:HB	1.86	0.58
1:C:226:TYR:CE2	1:C:242:LEU:HD23	2.39	0.58
1:D:154:ASP:CB	1:D:155:PRO:CD	2.82	0.58
1:A:232:GLU:HG2	1:A:289:ASP:CA	2.33	0.58
1:A:240:GLN:HG3	1:A:241:ARG:N	2.19	0.58
1:A:363:GLN:O	1:A:364:ILE:HG22	2.03	0.58
1:B:195:ASP:CB	1:B:200:GLY:HA3	2.33	0.58
1:C:335:ALA:HB1	3:C:811:NDG:C6	2.33	0.58
1:D:443:ARG:HH11	1:D:443:ARG:HG3	1.67	0.58
1:A:286:LYS:O	1:A:287:GLY:O	2.21	0.58
1:A:330:PRO:HD3	1:A:414:ASP:HB2	1.86	0.58
1:B:296:TYR:HB2	1:B:321:VAL:HB	1.86	0.58
1:B:332:PHE:CD2	1:B:424:GLY:HA3	2.39	0.58
1:C:154:ASP:CB	1:C:155:PRO:CD	2.82	0.58
1:C:240:GLN:HG3	1:C:241:ARG:N	2.19	0.58
1:C:363:GLN:O	1:C:364:ILE:HG22	2.03	0.58
1:D:309:SER:O	1:D:310:VAL:HG23	2.03	0.58
1:D:320:THR:CG2	2:D:807:NAG:C2	2.76	0.58
1:D:403:ASN:C	1:D:405:THR:H	2.12	0.58
1:B:68:ARG:HG3	1:B:69:GLU:N	2.19	0.57
1:B:154:ASP:C	2:B:801:NAG:C8	2.62	0.57
1:C:332:PHE:CD2	1:C:424:GLY:HA3	2.39	0.57
1:D:32:ASN:HD22	1:D:83:GLU:H	1.51	0.57
1:D:226:TYR:CE2	1:D:242:LEU:HD23	2.39	0.57
1:B:406:TYR:HB3	1:B:428:LEU:HD21	1.87	0.57
1:C:60:MET:SD	1:D:2:TRP:CZ3	2.97	0.57
1:C:406:TYR:HB3	1:C:428:LEU:HD21	1.87	0.57
1:D:154:ASP:CB	2:D:801:NAG:HN2	2.16	0.57
1:D:332:PHE:CD2	1:D:424:GLY:HA3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:GLN:HB2	1:D:533:GLU:CA	2.26	0.57
1:B:226:TYR:CE2	1:B:242:LEU:HD23	2.39	0.57
1:B:240:GLN:HG3	1:B:241:ARG:N	2.19	0.57
1:C:42:GLY:HA2	1:C:47:PRO:O	2.04	0.57
1:D:42:GLY:HA2	1:D:47:PRO:O	2.04	0.57
1:D:221:PHE:HA	1:D:244:VAL:HG12	1.85	0.57
1:D:537:ILE:HG12	1:D:538:LYS:N	2.19	0.57
1:A:226:TYR:CE2	1:A:242:LEU:HD23	2.39	0.57
1:B:38:ILE:HG22	1:B:53:ILE:HG22	1.85	0.57
1:B:505:GLY:HA2	1:B:529:VAL:H	1.69	0.57
1:C:1:ASP:CB	1:D:26:SER:C	2.77	0.57
1:C:22:VAL:CG2	1:D:5:PRO:CG	2.59	0.57
1:C:482:THR:HG22	1:C:499:THR:N	2.13	0.57
1:C:38:ILE:HG22	1:C:53:ILE:HG22	1.85	0.57
1:C:537:ILE:HG12	1:C:538:LYS:N	2.19	0.57
1:D:32:ASN:CG	1:D:33:LYS:N	2.59	0.57
1:D:235:ILE:HG12	1:D:287:GLY:HA2	1.82	0.57
1:D:363:GLN:O	1:D:364:ILE:HG22	2.03	0.57
1:B:42:GLY:HA2	1:B:47:PRO:O	2.04	0.57
1:C:32:ASN:CG	1:C:33:LYS:N	2.59	0.57
1:D:138:ASN:C	1:D:138:ASN:HD22	2.13	0.57
1:B:403:ASN:C	1:B:405:THR:H	2.12	0.57
1:C:138:ASN:HD22	1:C:138:ASN:C	2.13	0.57
1:C:286:LYS:O	1:C:287:GLY:O	2.21	0.57
1:C:403:ASN:CB	2:C:902:NAG:H83	2.21	0.57
1:A:505:GLY:HA2	1:A:529:VAL:H	1.70	0.57
1:B:450:GLN:HB2	1:B:533:GLU:CA	2.26	0.57
1:C:221:PHE:HA	1:C:244:VAL:HG12	1.85	0.57
1:D:240:GLN:HG3	1:D:241:ARG:N	2.19	0.57
1:D:505:GLY:HA2	1:D:529:VAL:H	1.69	0.57
1:A:235:ILE:HG12	1:A:287:GLY:HA2	1.82	0.57
1:B:108:PHE:CE1	1:B:203:VAL:HG23	2.40	0.57
1:C:189:LEU:HD21	1:C:209:ILE:HD12	1.87	0.57
1:C:443:ARG:HA	1:C:525:VAL:HG13	1.85	0.57
1:A:68:ARG:HG3	1:A:69:GLU:N	2.19	0.57
1:A:108:PHE:CE1	1:A:203:VAL:HG23	2.40	0.57
1:A:259:TYR:O	1:A:260:LYS:HB3	2.05	0.57
1:A:473:VAL:HA	1:A:513:LEU:HD23	1.85	0.57
1:B:138:ASN:C	1:B:138:ASN:HD22	2.13	0.57
1:B:154:ASP:CB	1:B:155:PRO:CD	2.82	0.57
1:C:473:VAL:HA	1:C:513:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:TYR:O	1:C:260:LYS:HB3	2.05	0.56
1:A:332:PHE:CD2	1:A:424:GLY:HA3	2.39	0.56
1:C:92:MET:HE3	1:D:2:TRP:CG	2.33	0.56
1:D:378:TRP:O	1:D:391:ASN:HB2	2.06	0.56
1:A:42:GLY:HA2	1:A:47:PRO:O	2.04	0.56
1:A:222:ASP:N	1:A:243:SER:O	2.38	0.56
1:A:396:ARG:NH2	1:A:464:ILE:HG21	2.17	0.56
1:B:259:TYR:O	1:B:260:LYS:HB3	2.05	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:222:ASP:N	1:C:243:SER:O	2.38	0.56
1:C:296:TYR:HB2	1:C:321:VAL:HB	1.86	0.56
1:C:330:PRO:HD3	1:C:414:ASP:HB2	1.86	0.56
1:C:336:VAL:HG12	1:C:338:ARG:HB2	1.87	0.56
1:C:396:ARG:NH2	1:C:464:ILE:HG21	2.17	0.56
1:D:108:PHE:CE1	1:D:203:VAL:HG23	2.40	0.56
1:D:394:LEU:N	1:D:394:LEU:CD1	2.69	0.56
1:A:336:VAL:HG12	1:A:338:ARG:HB2	1.87	0.56
1:C:68:ARG:HG3	1:C:69:GLU:N	2.19	0.56
1:C:92:MET:HE1	1:D:2:TRP:CB	2.26	0.56
1:C:162:LEU:O	1:C:174:LEU:HD12	2.06	0.56
1:A:162:LEU:O	1:A:174:LEU:HD12	2.06	0.56
1:A:369:TYR:HD1	1:A:383:LYS:O	1.88	0.56
1:B:222:ASP:N	1:B:243:SER:O	2.38	0.56
1:B:378:TRP:O	1:B:391:ASN:HB2	2.06	0.56
1:B:537:ILE:HG12	1:B:538:LYS:N	2.19	0.56
1:C:505:GLY:HA2	1:C:529:VAL:H	1.69	0.56
1:D:189:LEU:HD21	1:D:209:ILE:HD12	1.87	0.56
1:D:268:PHE:C	1:D:285:ALA:HB3	2.30	0.56
1:A:378:TRP:O	1:A:391:ASN:HB2	2.06	0.56
1:B:330:PRO:HD3	1:B:414:ASP:HB2	1.86	0.56
1:C:154:ASP:CB	2:C:801:NAG:HN2	2.16	0.56
1:C:403:ASN:C	1:C:405:THR:H	2.12	0.56
1:D:68:ARG:HG3	1:D:69:GLU:N	2.19	0.56
1:D:259:TYR:O	1:D:260:LYS:HB3	2.05	0.56
1:C:369:TYR:HD1	1:C:383:LYS:O	1.88	0.56
1:D:162:LEU:O	1:D:174:LEU:HD12	2.06	0.56
1:D:336:VAL:HG12	1:D:338:ARG:HB2	1.87	0.56
1:A:268:PHE:C	1:A:285:ALA:HB3	2.30	0.56
1:A:365:GLN:O	1:A:365:GLN:CG	2.54	0.56
1:A:406:TYR:HB3	1:A:428:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LEU:CD2	1:A:523:THR:HB	2.26	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:D:296:TYR:HB2	1:D:321:VAL:HB	1.86	0.56
1:D:330:PRO:HD3	1:D:414:ASP:HB2	1.86	0.56
1:A:118:ARG:HA	1:A:212:THR:HB	1.87	0.56
1:A:154:ASP:C	2:A:801:NAG:C8	2.62	0.56
1:B:439:VAL:HG13	1:B:522:LEU:HD11	1.88	0.56
1:C:118:ARG:HA	1:C:212:THR:HB	1.87	0.56
1:C:268:PHE:C	1:C:285:ALA:HB3	2.30	0.56
1:C:394:LEU:N	1:C:394:LEU:CD1	2.69	0.56
1:C:439:VAL:HG13	1:C:522:LEU:HD11	1.88	0.56
1:B:272:THR:CG2	1:B:273:THR:H	2.19	0.56
1:B:333:VAL:CG2	1:B:334:PRO:HD3	2.36	0.56
1:D:339:VAL:HG21	1:D:351:ILE:CG2	2.36	0.56
1:A:189:LEU:HD21	1:A:209:ILE:HD12	1.87	0.55
1:B:162:LEU:O	1:B:174:LEU:HD12	2.06	0.55
1:B:369:TYR:HD1	1:B:383:LYS:O	1.88	0.55
1:D:439:VAL:HG13	1:D:522:LEU:HD11	1.88	0.55
1:A:90:GLU:HB2	1:B:90:GLU:O	2.06	0.55
1:A:154:ASP:CB	2:A:801:NAG:HN2	2.16	0.55
1:A:394:LEU:N	1:A:394:LEU:CD1	2.69	0.55
1:B:189:LEU:HD21	1:B:209:ILE:HD12	1.87	0.55
1:C:155:PRO:N	2:C:801:NAG:H82	2.20	0.55
1:D:365:GLN:O	1:D:365:GLN:CG	2.54	0.55
1:D:406:TYR:HB3	1:D:428:LEU:HD21	1.87	0.55
1:A:439:VAL:HG13	1:A:522:LEU:HD11	1.88	0.55
1:B:336:VAL:HG12	1:B:338:ARG:HB2	1.87	0.55
1:D:118:ARG:HA	1:D:212:THR:HB	1.88	0.55
1:A:272:THR:CG2	1:A:273:THR:H	2.19	0.55
1:A:333:VAL:CG2	1:A:334:PRO:HD3	2.36	0.55
1:B:155:PRO:N	2:B:801:NAG:H82	2.20	0.55
1:C:339:VAL:HG21	1:C:351:ILE:CG2	2.36	0.55
1:C:378:TRP:O	1:C:391:ASN:HB2	2.06	0.55
1:D:459:ILE:HG21	1:D:471:TYR:CE2	2.42	0.55
1:A:195:ASP:CB	1:A:200:GLY:HA3	2.33	0.55
1:A:339:VAL:HG21	1:A:351:ILE:CG2	2.36	0.55
1:A:419:VAL:CG1	1:A:420:GLY:N	2.70	0.55
1:B:339:VAL:HG21	1:B:351:ILE:CG2	2.36	0.55
1:B:415:ASP:OD1	1:B:416:GLY:N	2.27	0.55
1:C:268:PHE:CD2	1:C:268:PHE:N	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:VAL:CG2	1:C:334:PRO:HD3	2.36	0.55
1:A:4:ILE:CD1	1:B:3:VAL:N	2.69	0.55
1:C:419:VAL:CG1	1:C:420:GLY:N	2.70	0.55
1:C:459:ILE:HG21	1:C:471:TYR:CE2	2.42	0.55
1:A:138:ASN:HD22	1:A:138:ASN:C	2.13	0.55
1:A:155:PRO:HG2	2:A:801:NAG:O7	2.07	0.55
1:B:289:ASP:O	1:B:290:PHE:CB	2.25	0.55
1:D:155:PRO:N	2:D:801:NAG:H82	2.20	0.55
1:D:278:ASN:HD22	1:D:278:ASN:N	2.05	0.55
1:D:335:ALA:HB1	3:D:811:NDG:C6	2.33	0.55
1:D:369:TYR:HD1	1:D:383:LYS:O	1.88	0.55
1:A:459:ILE:HG21	1:A:471:TYR:CE2	2.42	0.55
1:B:28:LYS:HB3	1:B:88:VAL:HG11	1.89	0.55
1:B:118:ARG:HA	1:B:212:THR:HB	1.87	0.55
1:B:154:ASP:CB	2:B:801:NAG:HN2	2.16	0.55
1:C:482:THR:HG22	1:C:499:THR:H	1.70	0.55
1:D:333:VAL:CG2	1:D:334:PRO:HD3	2.36	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:B:419:VAL:CG1	1:B:420:GLY:N	2.70	0.55
1:C:92:MET:O	1:D:2:TRP:NE1	2.40	0.55
1:C:155:PRO:HG2	2:C:801:NAG:O7	2.07	0.55
1:A:438:PRO:HB2	1:A:513:LEU:HD12	1.89	0.55
1:A:513:LEU:C	1:A:514:SER:HG	2.15	0.55
1:C:320:THR:CG2	2:C:807:NAG:C2	2.76	0.55
1:D:75:VAL:O	1:D:76:LEU:HD23	2.07	0.55
1:D:117:VAL:O	1:D:211:ILE:HA	2.07	0.55
1:D:363:GLN:C	1:D:364:ILE:HG23	2.32	0.55
1:A:3:VAL:CG1	1:B:4:ILE:CD1	2.44	0.54
1:B:117:VAL:O	1:B:211:ILE:HA	2.07	0.54
1:B:226:TYR:O	1:B:227:THR:CG2	2.55	0.54
1:B:402:LYS:C	1:B:403:ASN:O	2.46	0.54
1:C:28:LYS:HB3	1:C:88:VAL:HG11	1.89	0.54
1:C:226:TYR:O	1:C:227:THR:CG2	2.55	0.54
1:D:27:ASN:C	1:D:29:ASP:H	2.15	0.54
1:D:155:PRO:HG2	2:D:801:NAG:O7	2.07	0.54
1:A:363:GLN:C	1:A:364:ILE:HG23	2.32	0.54
1:B:169:THR:OG1	1:B:171:VAL:HG23	2.07	0.54
1:B:438:PRO:HB2	1:B:513:LEU:HD12	1.89	0.54
1:C:1:ASP:HB2	1:D:26:SER:C	2.31	0.54
1:D:272:THR:CG2	1:D:273:THR:H	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:O	1:A:76:LEU:HD23	2.08	0.54
1:A:268:PHE:CD2	1:A:268:PHE:N	2.75	0.54
1:B:459:ILE:HG21	1:B:471:TYR:CE2	2.42	0.54
1:C:92:MET:CB	1:D:2:TRP:CD1	2.90	0.54
1:C:226:TYR:HB2	1:C:319:VAL:HG22	1.90	0.54
1:D:419:VAL:CG1	1:D:420:GLY:N	2.70	0.54
1:B:450:GLN:CB	1:B:532:CYS:O	2.56	0.54
1:C:75:VAL:O	1:C:76:LEU:HD23	2.08	0.54
1:C:272:THR:CG2	1:C:273:THR:H	2.19	0.54
1:D:466:PRO:O	1:D:468:THR:N	2.40	0.54
1:D:490:LYS:O	1:D:490:LYS:HG2	2.08	0.54
1:A:27:ASN:C	1:A:29:ASP:H	2.15	0.54
1:A:32:ASN:HD22	1:A:83:GLU:H	1.51	0.54
1:A:402:LYS:C	1:A:403:ASN:O	2.46	0.54
1:B:27:ASN:C	1:B:29:ASP:H	2.15	0.54
1:B:75:VAL:O	1:B:76:LEU:HD23	2.08	0.54
1:B:466:PRO:O	1:B:468:THR:N	2.40	0.54
1:C:78:SER:H	1:D:2:TRP:HE1	1.55	0.54
1:C:117:VAL:O	1:C:211:ILE:HA	2.07	0.54
1:C:169:THR:OG1	1:C:171:VAL:HG23	2.07	0.54
1:C:450:GLN:CB	1:C:532:CYS:O	2.56	0.54
1:C:466:PRO:O	1:C:468:THR:N	2.40	0.54
1:A:226:TYR:O	1:A:227:THR:CG2	2.55	0.54
1:B:332:PHE:HD2	1:B:424:GLY:HA3	1.73	0.54
1:C:154:ASP:C	2:C:801:NAG:C8	2.62	0.54
1:C:318:THR:CG2	2:C:806:NAG:H5	2.34	0.54
1:C:330:PRO:HB3	1:C:358:ASP:HB2	1.89	0.54
1:D:330:PRO:HB3	1:D:358:ASP:HB2	1.89	0.54
1:D:402:LYS:C	1:D:403:ASN:O	2.46	0.54
1:D:403:ASN:CB	2:D:902:NAG:H83	2.21	0.54
1:A:154:ASP:CB	1:A:155:PRO:CD	2.82	0.54
1:A:226:TYR:C	1:A:227:THR:HG23	2.33	0.54
1:D:217:ASN:N	1:D:217:ASN:ND2	2.56	0.54
1:D:371:ILE:HG23	1:D:372:GLY:H	1.73	0.54
1:A:320:THR:CG2	2:A:807:NAG:C2	2.76	0.54
1:B:226:TYR:C	1:B:227:THR:HG23	2.33	0.54
1:C:352:ILE:HG13	1:C:388:VAL:CB	2.33	0.54
1:D:332:PHE:HD2	1:D:424:GLY:HA3	1.73	0.54
1:A:3:VAL:CA	1:B:3:VAL:HB	2.37	0.54
1:A:78:SER:OG	1:B:1:ASP:HA	2.08	0.54
1:A:278:ASN:HD22	1:A:278:ASN:N	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:THR:HG23	1:C:253:PRO:HD2	1.90	0.54
1:D:450:GLN:CB	1:D:532:CYS:O	2.56	0.54
1:A:93:GLU:C	1:B:2:TRP:HB2	2.28	0.54
1:A:169:THR:OG1	1:A:171:VAL:HG23	2.07	0.54
1:B:276:GLU:CG	1:B:277:SER:N	2.71	0.54
1:B:371:ILE:HG23	1:B:372:GLY:H	1.73	0.54
1:C:335:ALA:HB1	3:C:811:NDG:H6	1.69	0.54
1:D:154:ASP:CG	1:D:155:PRO:HD2	2.33	0.54
1:D:169:THR:OG1	1:D:171:VAL:HG23	2.07	0.54
1:D:226:TYR:HB2	1:D:319:VAL:HG22	1.89	0.54
1:D:226:TYR:O	1:D:227:THR:CG2	2.55	0.54
1:D:443:ARG:HG3	1:D:443:ARG:NH1	2.23	0.54
1:A:117:VAL:O	1:A:211:ILE:HA	2.07	0.53
1:A:217:ASN:N	1:A:217:ASN:ND2	2.56	0.53
1:A:450:GLN:CB	1:A:532:CYS:O	2.56	0.53
1:C:217:ASN:N	1:C:217:ASN:ND2	2.56	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:490:LYS:HG2	1:C:490:LYS:O	2.08	0.53
1:D:28:LYS:HB3	1:D:88:VAL:HG11	1.89	0.53
1:D:252:THR:HG23	1:D:253:PRO:HD2	1.91	0.53
1:D:276:GLU:CG	1:D:277:SER:N	2.71	0.53
1:A:490:LYS:O	1:A:490:LYS:HG2	2.08	0.53
1:A:517:GLN:C	1:A:519:ASN:N	2.47	0.53
1:C:27:ASN:C	1:C:29:ASP:H	2.16	0.53
1:C:32:ASN:HD22	1:C:83:GLU:H	1.51	0.53
1:A:155:PRO:N	2:A:801:NAG:H82	2.20	0.53
1:A:249:MET:O	1:A:252:THR:HB	2.09	0.53
1:A:415:ASP:CG	1:A:416:GLY:H	2.16	0.53
1:B:22:VAL:HG22	1:B:23:GLN:H	1.73	0.53
1:B:268:PHE:CD2	1:B:268:PHE:N	2.75	0.53
1:C:278:ASN:HD22	1:C:278:ASN:N	2.05	0.53
1:C:332:PHE:HD2	1:C:424:GLY:HA3	1.73	0.53
1:D:352:ILE:CG1	1:D:388:VAL:HB	2.33	0.53
1:A:28:LYS:HB3	1:A:88:VAL:HG11	1.89	0.53
1:A:154:ASP:CG	1:A:155:PRO:HD2	2.33	0.53
1:B:249:MET:O	1:B:252:THR:HB	2.09	0.53
1:B:490:LYS:O	1:B:490:LYS:HG2	2.08	0.53
1:B:533:GLU:HA	1:B:533:GLU:OE2	2.09	0.53
1:C:276:GLU:CG	1:C:277:SER:N	2.71	0.53
1:A:533:GLU:HA	1:A:533:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:LEU:HD13	1:C:412:VAL:HG23	1.91	0.53
1:D:249:MET:O	1:D:252:THR:HB	2.08	0.53
1:D:318:THR:CG2	2:D:806:NAG:H5	2.34	0.53
1:D:373:ASN:HB3	1:D:409:ILE:H	1.74	0.53
1:A:347:ARG:HG3	1:A:391:ASN:HA	1.91	0.53
1:A:458:THR:HG22	1:A:493:SER:HB3	1.91	0.53
1:B:252:THR:HG23	1:B:253:PRO:HD2	1.90	0.53
1:C:242:LEU:O	1:C:279:GLN:HB3	2.09	0.53
1:D:241:ARG:NE	1:D:281:ILE:HD12	2.22	0.53
1:D:522:LEU:CD2	1:D:523:THR:HB	2.26	0.53
1:A:482:THR:CG2	1:A:499:THR:CA	2.87	0.53
1:C:365:GLN:O	1:C:365:GLN:CG	2.54	0.53
1:C:371:ILE:HG23	1:C:372:GLY:H	1.73	0.53
1:D:533:GLU:HA	1:D:533:GLU:OE2	2.09	0.53
1:A:242:LEU:O	1:A:279:GLN:HB3	2.09	0.53
1:A:276:GLU:CG	1:A:277:SER:N	2.71	0.53
1:B:242:LEU:O	1:B:279:GLN:HB3	2.09	0.53
1:C:402:LYS:C	1:C:403:ASN:O	2.46	0.53
1:C:458:THR:HG22	1:C:493:SER:HB3	1.90	0.53
1:C:513:LEU:C	1:C:514:SER:HG	2.17	0.53
1:A:31:PHE:CD2	1:A:32:ASN:HB2	2.44	0.53
1:A:226:TYR:HB2	1:A:319:VAL:HG22	1.90	0.53
1:A:371:ILE:HG23	1:A:372:GLY:H	1.73	0.53
1:A:482:THR:HG22	1:A:499:THR:H	1.70	0.53
1:C:226:TYR:C	1:C:227:THR:HG23	2.33	0.53
1:C:347:ARG:HG3	1:C:391:ASN:HA	1.91	0.53
1:C:438:PRO:HB2	1:C:513:LEU:HD12	1.89	0.53
1:C:512:LEU:HD11	1:C:519:ASN:HD21	1.74	0.53
1:D:367:LEU:HD13	1:D:412:VAL:HG23	1.91	0.53
1:D:438:PRO:HB2	1:D:513:LEU:HD12	1.89	0.53
1:A:92:MET:O	1:B:2:TRP:HB2	2.08	0.53
1:A:330:PRO:HB3	1:A:358:ASP:HB2	1.89	0.53
1:A:482:THR:HG22	1:A:482:THR:O	2.08	0.53
1:B:512:LEU:HD11	1:B:519:ASN:HD21	1.74	0.53
1:C:2:TRP:CZ2	1:D:53:ILE:CD1	2.80	0.53
1:C:373:ASN:HB3	1:C:409:ILE:H	1.74	0.53
1:C:450:GLN:HB2	1:C:533:GLU:CA	2.26	0.53
1:A:466:PRO:O	1:A:468:THR:N	2.40	0.52
1:B:330:PRO:HB3	1:B:358:ASP:HB2	1.89	0.52
1:B:450:GLN:CB	1:B:533:GLU:HA	2.29	0.52
1:A:373:ASN:HB3	1:A:409:ILE:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:TYR:O	1:B:383:LYS:HG2	2.09	0.52
1:C:31:PHE:CD2	1:C:32:ASN:HB2	2.44	0.52
1:D:426:LEU:O	1:D:426:LEU:HD13	2.10	0.52
1:D:458:THR:HG22	1:D:493:SER:HB3	1.90	0.52
1:D:513:LEU:C	1:D:514:SER:HG	2.17	0.52
1:A:318:THR:CG2	2:A:806:NAG:H5	2.34	0.52
1:A:403:ASN:CB	2:A:902:NAG:H83	2.21	0.52
1:B:347:ARG:HG3	1:B:391:ASN:HA	1.91	0.52
1:C:241:ARG:NE	1:C:281:ILE:HD12	2.22	0.52
1:C:249:MET:O	1:C:252:THR:HB	2.08	0.52
1:C:312:LEU:O	3:C:804:NDG:C8	2.57	0.52
1:C:426:LEU:O	1:C:426:LEU:HD13	2.10	0.52
1:D:105:ARG:HG3	1:D:106:PRO:HD2	1.91	0.52
1:D:226:TYR:C	1:D:227:THR:HG23	2.33	0.52
1:A:2:TRP:CZ2	1:B:95:THR:CG2	2.89	0.52
1:A:312:LEU:O	3:A:804:NDG:C8	2.57	0.52
1:B:105:ARG:HG3	1:B:106:PRO:HD2	1.91	0.52
1:B:217:ASN:N	1:B:217:ASN:ND2	2.56	0.52
1:B:426:LEU:O	1:B:426:LEU:HD13	2.09	0.52
1:C:369:TYR:O	1:C:383:LYS:HG2	2.09	0.52
2:D:809:NAG:H61	2:D:810:NAG:C6	2.39	0.52
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.91	0.52
1:B:226:TYR:HB2	1:B:319:VAL:HG22	1.89	0.52
1:B:373:ASN:HB3	1:B:409:ILE:H	1.74	0.52
1:B:458:THR:HG22	1:B:493:SER:HB3	1.91	0.52
1:C:22:VAL:HG22	1:C:23:GLN:H	1.73	0.52
1:C:154:ASP:CG	1:C:155:PRO:HD2	2.33	0.52
1:D:369:TYR:O	1:D:383:LYS:HG2	2.09	0.52
1:A:272:THR:CG2	2:A:803:NAG:HN2	2.23	0.52
1:A:367:LEU:HD13	1:A:412:VAL:HG23	1.91	0.52
1:C:194:THR:HG22	1:C:195:ASP:N	2.25	0.52
1:D:242:LEU:O	1:D:279:GLN:HB3	2.09	0.52
1:A:3:VAL:C	1:B:3:VAL:CG2	2.82	0.52
1:A:332:PHE:HD2	1:A:424:GLY:HA3	1.73	0.52
1:A:347:ARG:HD2	1:A:392:GLY:N	2.25	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:B:221:PHE:HB3	1:B:223:PRO:O	2.10	0.52
1:B:318:THR:CG2	2:B:806:NAG:H5	2.34	0.52
1:B:336:VAL:O	1:B:426:LEU:HD22	2.10	0.52
1:B:482:THR:CG2	1:B:499:THR:CA	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:GLY:O	1:C:506:ASP:OD1	2.28	0.52
1:D:221:PHE:HB3	1:D:223:PRO:O	2.10	0.52
1:D:512:LEU:HD11	1:D:519:ASN:HD21	1.74	0.52
1:A:22:VAL:HG22	1:A:23:GLN:H	1.73	0.52
1:A:155:PRO:CD	2:A:801:NAG:H82	2.40	0.52
1:A:246:ASP:C	1:A:247:LEU:HD12	2.35	0.52
1:B:312:LEU:O	3:B:804:NDG:C8	2.57	0.52
1:B:367:LEU:HD13	1:B:412:VAL:HG23	1.91	0.52
1:C:155:PRO:C	1:C:157:GLU:N	2.56	0.52
1:A:2:TRP:HZ3	1:B:6:PRO:HG3	1.74	0.52
1:C:94:ILE:CG2	1:D:2:TRP:CH2	2.72	0.52
1:C:246:ASP:C	1:C:247:LEU:HD12	2.35	0.52
1:C:272:THR:CG2	2:C:803:NAG:HN2	2.23	0.52
1:D:268:PHE:CD2	1:D:268:PHE:N	2.75	0.52
1:A:252:THR:HG23	1:A:253:PRO:HD2	1.91	0.52
1:B:347:ARG:HD2	1:B:392:GLY:N	2.25	0.52
1:B:450:GLN:CG	1:B:533:GLU:OE2	2.58	0.52
1:C:450:GLN:CG	1:C:533:GLU:OE2	2.58	0.52
1:D:312:LEU:O	3:D:804:NDG:C8	2.57	0.52
1:A:221:PHE:HB3	1:A:223:PRO:O	2.10	0.51
1:A:369:TYR:O	1:A:383:LYS:HG2	2.09	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:27:ASN:OD1	1:D:90:GLU:HG3	2.10	0.51
1:D:523:THR:CG2	1:D:524:VAL:H	1.94	0.51
1:A:266:GLY:N	1:A:268:PHE:CE2	2.76	0.51
1:A:505:GLY:O	1:A:506:ASP:OD1	2.28	0.51
1:B:266:GLY:N	1:B:268:PHE:CE2	2.76	0.51
1:B:415:ASP:CG	1:B:416:GLY:H	2.16	0.51
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.24	0.51
1:C:221:PHE:HB3	1:C:223:PRO:O	2.10	0.51
1:C:458:THR:HA	1:C:493:SER:HA	1.93	0.51
1:D:234:GLU:HB2	1:D:235:ILE:HG22	1.93	0.51
1:D:396:ARG:CZ	1:D:432:ASP:HB2	2.41	0.51
1:D:514:SER:HB3	1:D:517:GLN:O	2.10	0.51
1:B:234:GLU:HB2	1:B:235:ILE:HG22	1.93	0.51
1:B:278:ASN:HD22	1:B:278:ASN:N	2.05	0.51
1:B:352:ILE:HG13	1:B:388:VAL:CB	2.33	0.51
1:B:505:GLY:O	1:B:506:ASP:OD1	2.28	0.51
1:C:338:ARG:HB3	1:C:339:VAL:HG22	1.92	0.51
1:C:373:ASN:CG	1:C:374:ASP:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ARG:HG3	1:D:391:ASN:HA	1.91	0.51
1:A:24:ILE:HB	1:B:1:ASP:H2	1.76	0.51
1:A:93:GLU:O	1:B:2:TRP:C	2.53	0.51
1:A:142:LEU:O	1:A:196:LEU:HD23	2.11	0.51
1:B:272:THR:CG2	2:B:803:NAG:HN2	2.23	0.51
1:C:105:ARG:HG3	1:C:106:PRO:HD2	1.91	0.51
1:D:31:PHE:CD2	1:D:32:ASN:HB2	2.44	0.51
1:D:155:PRO:CD	2:D:801:NAG:H82	2.40	0.51
1:D:428:LEU:O	1:D:428:LEU:HD23	2.11	0.51
1:A:443:ARG:HG3	1:A:443:ARG:NH1	2.23	0.51
1:A:450:GLN:CG	1:A:533:GLU:OE2	2.58	0.51
1:B:154:ASP:CG	1:B:155:PRO:HD2	2.33	0.51
1:B:428:LEU:HD23	1:B:428:LEU:O	2.11	0.51
1:C:297:VAL:CG2	2:C:807:NAG:H62	2.41	0.51
1:C:533:GLU:HA	1:C:533:GLU:OE2	2.09	0.51
1:D:336:VAL:O	1:D:426:LEU:HD22	2.10	0.51
1:A:194:THR:HG22	1:A:195:ASP:N	2.25	0.51
1:A:234:GLU:HB2	1:A:235:ILE:HG22	1.93	0.51
1:A:428:LEU:O	1:A:428:LEU:HD23	2.11	0.51
1:B:142:LEU:O	1:B:196:LEU:HD23	2.11	0.51
1:C:290:PHE:CE2	1:C:293:ARG:CB	2.92	0.51
1:C:428:LEU:O	1:C:428:LEU:HD23	2.11	0.51
1:D:22:VAL:HG22	1:D:23:GLN:H	1.73	0.51
1:D:246:ASP:C	1:D:247:LEU:HD12	2.35	0.51
1:D:272:THR:CG2	2:D:803:NAG:HN2	2.23	0.51
1:D:374:ASP:C	1:D:375:PRO:O	2.54	0.51
1:D:415:ASP:CG	1:D:416:GLY:H	2.16	0.51
1:A:373:ASN:CG	1:A:374:ASP:H	2.18	0.51
1:A:514:SER:HB3	1:A:517:GLN:O	2.10	0.51
1:B:373:ASN:CG	1:B:374:ASP:H	2.18	0.51
1:C:374:ASP:C	1:C:375:PRO:O	2.54	0.51
1:D:194:THR:HG22	1:D:195:ASP:N	2.25	0.51
1:D:505:GLY:O	1:D:506:ASP:OD1	2.28	0.51
1:A:90:GLU:HB2	1:B:90:GLU:C	2.35	0.51
1:A:91:PRO:HD2	1:B:89:GLU:OE1	2.10	0.51
1:B:194:THR:HG22	1:B:195:ASP:N	2.25	0.51
1:B:246:ASP:C	1:B:247:LEU:HD12	2.35	0.51
1:B:290:PHE:CE2	1:B:293:ARG:CB	2.92	0.51
1:C:336:VAL:O	1:C:426:LEU:HD22	2.10	0.51
1:D:80:ALA:O	1:D:88:VAL:HG23	2.11	0.51
1:D:338:ARG:HB3	1:D:339:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:SER:OG	1:A:370:PHE:HE1	1.94	0.51
1:B:155:PRO:CD	2:B:801:NAG:H82	2.40	0.51
1:D:76:LEU:O	1:D:94:ILE:N	2.44	0.51
1:D:227:THR:CG2	2:D:807:NAG:H83	2.32	0.51
1:D:347:ARG:HD2	1:D:392:GLY:N	2.25	0.51
1:A:33:LYS:HB3	1:A:83:GLU:CG	2.40	0.51
1:A:336:VAL:O	1:A:426:LEU:HD22	2.10	0.51
1:A:338:ARG:HB3	1:A:339:VAL:HG22	1.92	0.51
1:B:397:GLU:N	1:B:397:GLU:OE1	2.44	0.51
1:C:80:ALA:O	1:C:88:VAL:HG23	2.11	0.51
1:C:234:GLU:HB2	1:C:235:ILE:HG22	1.93	0.51
1:A:290:PHE:CE2	1:A:293:ARG:CB	2.92	0.50
1:A:382:ASN:OD1	1:A:385:ASN:N	2.45	0.50
1:A:450:GLN:CB	1:A:533:GLU:HA	2.29	0.50
1:B:28:LYS:CD	1:B:88:VAL:HG12	2.38	0.50
1:B:297:VAL:CG2	2:B:807:NAG:H62	2.41	0.50
1:C:397:GLU:OE1	1:C:397:GLU:N	2.45	0.50
1:D:368:SER:OG	1:D:370:PHE:HE1	1.94	0.50
1:D:423:THR:HB	2:D:810:NAG:H83	1.93	0.50
1:A:227:THR:CG2	2:A:807:NAG:H83	2.32	0.50
1:A:458:THR:HG22	1:A:493:SER:CB	2.42	0.50
1:A:471:TYR:CD1	1:A:471:TYR:N	2.79	0.50
1:B:151:LEU:HD12	1:B:190:THR:O	2.11	0.50
1:B:241:ARG:NE	1:B:281:ILE:HD12	2.22	0.50
1:C:151:LEU:HD12	1:C:190:THR:O	2.11	0.50
1:C:217:ASN:N	1:C:217:ASN:HD22	2.09	0.50
1:A:217:ASN:N	1:A:217:ASN:HD22	2.09	0.50
1:B:338:ARG:HB3	1:B:339:VAL:HG22	1.92	0.50
1:B:471:TYR:N	1:B:471:TYR:CD1	2.79	0.50
1:C:347:ARG:HD2	1:C:392:GLY:N	2.25	0.50
1:C:368:SER:OG	1:C:370:PHE:HE1	1.94	0.50
1:C:419:VAL:HG22	2:C:809:NAG:H81	1.93	0.50
1:D:382:ASN:OD1	1:D:385:ASN:N	2.45	0.50
1:D:482:THR:CG2	1:D:499:THR:CA	2.87	0.50
1:A:432:ASP:CB	1:A:464:ILE:CG2	2.89	0.50
1:B:109:THR:HG22	1:B:110:GLN:HG3	1.94	0.50
1:B:186:GLU:OE1	2:B:801:NAG:C6	2.59	0.50
1:B:327:ASN:OD1	1:B:360:ASP:OD1	2.30	0.50
1:C:76:LEU:O	1:C:94:ILE:N	2.44	0.50
1:C:423:THR:HB	2:C:810:NAG:H83	1.93	0.50
1:C:458:THR:HG22	1:C:493:SER:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:ASP:O	2:D:801:NAG:C8	2.60	0.50
1:D:327:ASN:OD1	1:D:360:ASP:OD1	2.30	0.50
1:D:450:GLN:CG	1:D:533:GLU:OE2	2.58	0.50
1:A:155:PRO:HG2	2:A:801:NAG:C7	2.42	0.50
1:A:297:VAL:CG2	2:A:807:NAG:H62	2.41	0.50
1:B:155:PRO:HG2	2:B:801:NAG:C7	2.42	0.50
1:B:217:ASN:N	1:B:217:ASN:HD22	2.10	0.50
1:B:522:LEU:CD2	1:B:523:THR:HB	2.26	0.50
1:C:109:THR:HG22	1:C:110:GLN:HG3	1.94	0.50
1:C:471:TYR:N	1:C:471:TYR:CD1	2.79	0.50
1:C:514:SER:HB3	1:C:517:GLN:O	2.10	0.50
2:C:809:NAG:H61	2:C:810:NAG:C6	2.39	0.50
1:D:373:ASN:CG	1:D:374:ASP:H	2.18	0.50
1:D:419:VAL:HG22	2:D:809:NAG:H81	1.94	0.50
1:A:327:ASN:OD1	1:A:360:ASP:OD1	2.30	0.50
1:B:216:ASP:HB2	1:B:217:ASN:ND2	2.27	0.50
1:B:261:ILE:HD11	1:B:264:ASN:HD22	1.77	0.50
1:B:335:ALA:CB	3:B:811:NDG:C6	2.90	0.50
1:B:458:THR:HG22	1:B:493:SER:CB	2.42	0.50
1:C:11:GLU:OE2	1:C:69:GLU:OE1	2.30	0.50
1:C:154:ASP:O	2:C:801:NAG:C8	2.60	0.50
1:C:449:ASP:CB	1:C:532:CYS:N	2.74	0.50
1:D:142:LEU:O	1:D:196:LEU:HD23	2.11	0.50
1:D:151:LEU:HD12	1:D:190:THR:O	2.11	0.50
1:D:217:ASN:N	1:D:217:ASN:HD22	2.09	0.50
1:D:468:THR:C	1:D:469:TYR:O	2.54	0.50
1:D:471:TYR:CD1	1:D:471:TYR:N	2.79	0.50
1:A:352:ILE:HG13	1:A:388:VAL:CB	2.33	0.50
1:A:352:ILE:CG1	1:A:388:VAL:HB	2.33	0.50
1:B:368:SER:OG	1:B:370:PHE:HE1	1.94	0.50
1:B:432:ASP:CB	1:B:464:ILE:CG2	2.89	0.50
1:B:457:LEU:HD23	1:B:494:MET:SD	2.52	0.50
1:C:155:PRO:HG2	2:C:801:NAG:C7	2.42	0.50
1:C:227:THR:CG2	2:C:807:NAG:H83	2.32	0.50
1:C:335:ALA:CB	3:C:811:NDG:C6	2.90	0.50
1:C:373:ASN:ND2	1:C:374:ASP:OD1	2.45	0.50
1:C:450:GLN:CB	1:C:533:GLU:HA	2.29	0.50
1:D:458:THR:HA	1:D:493:SER:HA	1.93	0.50
1:A:80:ALA:O	1:A:88:VAL:HG23	2.11	0.50
1:A:468:THR:C	1:A:469:TYR:O	2.54	0.50
1:B:154:ASP:O	2:B:801:NAG:C8	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LYS:C	1:B:287:GLY:O	2.55	0.50
1:B:373:ASN:ND2	1:B:374:ASP:OD1	2.45	0.50
1:C:142:LEU:O	1:C:196:LEU:HD23	2.11	0.50
1:C:522:LEU:CD2	1:C:523:THR:HB	2.26	0.50
1:D:11:GLU:OE2	1:D:69:GLU:OE1	2.30	0.50
1:D:186:GLU:OE1	2:D:801:NAG:C6	2.59	0.50
1:D:290:PHE:CE2	1:D:293:ARG:CB	2.92	0.50
1:A:155:PRO:O	1:A:157:GLU:N	2.43	0.50
1:A:216:ASP:HB2	1:A:217:ASN:ND2	2.27	0.50
1:A:286:LYS:C	1:A:287:GLY:O	2.55	0.50
1:B:151:LEU:HD12	1:B:151:LEU:H	1.77	0.50
1:B:227:THR:CG2	2:B:807:NAG:H83	2.32	0.50
1:B:419:VAL:HG22	2:B:809:NAG:H81	1.94	0.50
1:C:186:GLU:OE1	2:C:801:NAG:C6	2.59	0.50
1:C:382:ASN:OD1	1:C:385:ASN:N	2.45	0.50
1:D:297:VAL:CG2	2:D:807:NAG:H62	2.41	0.50
1:A:261:ILE:HD11	1:A:264:ASN:HD22	1.77	0.49
1:A:449:ASP:CB	1:A:532:CYS:N	2.74	0.49
1:B:276:GLU:HG3	1:B:277:SER:N	2.25	0.49
1:B:367:LEU:HB2	1:B:413:THR:O	2.12	0.49
1:B:458:THR:HA	1:B:493:SER:HA	1.93	0.49
1:B:468:THR:C	1:B:469:TYR:O	2.54	0.49
1:B:513:LEU:C	1:B:514:SER:HG	2.18	0.49
1:C:155:PRO:CD	2:C:801:NAG:H82	2.40	0.49
1:C:286:LYS:C	1:C:287:GLY:O	2.55	0.49
1:C:449:ASP:CB	1:C:532:CYS:H	2.22	0.49
1:D:216:ASP:HB2	1:D:217:ASN:ND2	2.27	0.49
1:A:335:ALA:CB	3:A:811:NDG:C6	2.90	0.49
1:A:419:VAL:HG22	2:A:809:NAG:H81	1.94	0.49
1:A:458:THR:HA	1:A:493:SER:HA	1.93	0.49
1:B:109:THR:HG22	1:B:110:GLN:CG	2.42	0.49
1:B:374:ASP:C	1:B:375:PRO:O	2.54	0.49
1:B:382:ASN:OD1	1:B:385:ASN:N	2.45	0.49
1:C:482:THR:CG2	1:C:499:THR:CA	2.87	0.49
1:D:367:LEU:HB2	1:D:413:THR:O	2.12	0.49
1:D:482:THR:HG22	1:D:499:THR:H	1.70	0.49
1:A:92:MET:HB3	1:B:2:TRP:H	1.77	0.49
1:A:109:THR:HG22	1:A:110:GLN:HG3	1.93	0.49
1:A:151:LEU:HD12	1:A:190:THR:O	2.11	0.49
1:B:155:PRO:O	1:B:157:GLU:N	2.43	0.49
1:C:109:THR:HG22	1:C:110:GLN:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:LEU:HB2	1:C:413:THR:O	2.12	0.49
1:D:335:ALA:CB	3:D:811:NDG:C6	2.90	0.49
1:D:457:LEU:HD23	1:D:494:MET:SD	2.52	0.49
1:A:457:LEU:HD23	1:A:494:MET:SD	2.52	0.49
1:B:336:VAL:CG1	1:B:338:ARG:HB2	2.43	0.49
1:C:28:LYS:CD	1:C:88:VAL:HG12	2.38	0.49
1:C:151:LEU:HD12	1:C:151:LEU:H	1.78	0.49
1:C:432:ASP:CB	1:C:464:ILE:CG2	2.89	0.49
1:C:457:LEU:HD23	1:C:494:MET:SD	2.52	0.49
1:C:519:ASN:CG	1:C:519:ASN:O	2.55	0.49
1:D:109:THR:HG22	1:D:110:GLN:CG	2.42	0.49
1:D:109:THR:HG22	1:D:110:GLN:HG3	1.94	0.49
1:D:286:LYS:C	1:D:287:GLY:O	2.55	0.49
1:A:4:ILE:HD13	1:B:2:TRP:CA	2.42	0.49
1:A:109:THR:HG22	1:A:110:GLN:CG	2.42	0.49
1:A:282:LEU:CD2	1:A:283:THR:N	2.76	0.49
2:A:809:NAG:H62	2:A:810:NAG:O6	2.13	0.49
1:B:396:ARG:CZ	1:B:432:ASP:HB2	2.41	0.49
1:B:482:THR:HG22	1:B:482:THR:O	2.09	0.49
1:B:519:ASN:O	1:B:519:ASN:CG	2.55	0.49
1:C:426:LEU:HD13	1:C:426:LEU:C	2.37	0.49
1:C:512:LEU:HD11	1:C:519:ASN:ND2	2.28	0.49
1:D:458:THR:HG22	1:D:493:SER:CB	2.42	0.49
1:A:4:ILE:HD13	1:B:1:ASP:O	2.13	0.49
1:A:224:LYS:HE3	2:A:806:NAG:H82	1.95	0.49
1:A:426:LEU:HD13	1:A:426:LEU:C	2.37	0.49
1:B:423:THR:HB	2:B:810:NAG:H83	1.94	0.49
1:D:33:LYS:HB3	1:D:83:GLU:CG	2.40	0.49
1:D:261:ILE:HD11	1:D:264:ASN:HD22	1.77	0.49
1:D:432:ASP:CB	1:D:464:ILE:HG21	2.43	0.49
1:A:90:GLU:CB	1:B:90:GLU:O	2.60	0.49
1:A:186:GLU:OE1	2:A:801:NAG:C6	2.59	0.49
1:A:396:ARG:CZ	1:A:432:ASP:HB2	2.41	0.49
1:B:68:ARG:HD3	1:B:100:ASP:CA	2.43	0.49
1:B:80:ALA:O	1:B:88:VAL:HG23	2.11	0.49
1:B:451:ASN:O	1:B:534:GLY:CA	2.60	0.49
2:B:809:NAG:H62	2:B:810:NAG:O6	2.13	0.49
1:C:282:LEU:CD2	1:C:283:THR:N	2.76	0.49
1:C:336:VAL:CG1	1:C:338:ARG:HB2	2.43	0.49
1:C:482:THR:HG22	1:C:482:THR:O	2.09	0.49
1:D:8:LYS:CD	1:D:8:LYS:N	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:LEU:HD12	1:D:151:LEU:H	1.78	0.49
1:D:151:LEU:O	1:D:152:LYS:HB2	2.13	0.49
1:D:155:PRO:HG2	2:D:801:NAG:C7	2.42	0.49
1:D:273:THR:H	2:D:803:NAG:HN2	1.60	0.49
1:D:426:LEU:HD13	1:D:426:LEU:C	2.37	0.49
1:D:449:ASP:CB	1:D:532:CYS:N	2.74	0.49
1:D:512:LEU:HD11	1:D:519:ASN:ND2	2.28	0.49
2:D:809:NAG:H62	2:D:810:NAG:O6	2.13	0.49
1:A:192:GLN:HA	1:A:203:VAL:O	2.13	0.49
1:A:252:THR:CG2	1:A:253:PRO:HD2	2.43	0.49
1:B:11:GLU:OE2	1:B:69:GLU:OE1	2.30	0.49
1:B:192:GLN:HA	1:B:203:VAL:O	2.13	0.49
1:C:216:ASP:HB2	1:C:217:ASN:ND2	2.27	0.49
1:C:252:THR:CG2	1:C:253:PRO:HD2	2.43	0.49
1:D:432:ASP:CB	1:D:464:ILE:CG2	2.89	0.49
1:A:1:ASP:CG	1:A:2:TRP:N	2.70	0.49
1:A:33:LYS:NZ	1:A:56:GLU:OE1	2.42	0.49
1:A:281:ILE:HG23	1:A:281:ILE:O	2.13	0.49
1:A:367:LEU:HB2	1:A:413:THR:O	2.12	0.49
1:C:261:ILE:HD11	1:C:264:ASN:HD22	1.77	0.49
1:C:327:ASN:OD1	1:C:360:ASP:OD1	2.30	0.49
1:C:396:ARG:CZ	1:C:432:ASP:HB2	2.41	0.49
1:A:76:LEU:O	1:A:94:ILE:N	2.44	0.49
1:A:374:ASP:C	1:A:375:PRO:O	2.54	0.49
1:B:352:ILE:CG1	1:B:388:VAL:HB	2.33	0.49
1:B:365:GLN:HA	1:B:416:GLY:HA3	1.95	0.49
1:C:68:ARG:HD3	1:C:100:ASP:CA	2.43	0.49
1:C:192:GLN:HA	1:C:203:VAL:O	2.13	0.49
1:C:224:LYS:HE3	2:C:806:NAG:H82	1.95	0.49
1:C:352:ILE:CG1	1:C:388:VAL:HB	2.33	0.49
1:D:224:LYS:CE	2:D:806:NAG:C8	2.91	0.49
1:D:241:ARG:HE	1:D:281:ILE:CD1	2.24	0.49
1:D:336:VAL:CG1	1:D:338:ARG:HB2	2.43	0.49
1:D:373:ASN:ND2	1:D:374:ASP:OD1	2.45	0.49
1:D:451:ASN:O	1:D:534:GLY:CA	2.60	0.49
1:A:519:ASN:CG	1:A:519:ASN:O	2.55	0.48
1:B:282:LEU:CD2	1:B:283:THR:N	2.76	0.48
1:B:496:LEU:HD21	1:B:509:ILE:CD1	2.38	0.48
1:C:27:ASN:OD1	1:D:91:PRO:O	2.31	0.48
1:C:415:ASP:CG	1:C:416:GLY:H	2.17	0.48
1:D:67:ASP:OD2	1:D:69:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:GLN:HA	1:D:203:VAL:O	2.13	0.48
1:D:252:THR:CG2	1:D:253:PRO:HD2	2.43	0.48
1:D:276:GLU:HG3	1:D:277:SER:N	2.25	0.48
1:A:373:ASN:ND2	1:A:374:ASP:OD1	2.45	0.48
1:B:281:ILE:HG23	1:B:281:ILE:O	2.13	0.48
1:C:432:ASP:CB	1:C:464:ILE:HG21	2.43	0.48
2:C:809:NAG:H62	2:C:810:NAG:O6	2.13	0.48
1:A:11:GLU:OE2	1:A:69:GLU:OE1	2.30	0.48
1:A:150:ILE:HD11	1:A:165:ILE:HB	1.96	0.48
1:B:151:LEU:O	1:B:152:LYS:HB2	2.13	0.48
1:C:298:LEU:N	1:C:298:LEU:CD2	2.75	0.48
1:D:28:LYS:CD	1:D:88:VAL:HG12	2.38	0.48
1:D:224:LYS:HE3	2:D:806:NAG:H82	1.95	0.48
1:D:496:LEU:HD21	1:D:509:ILE:CD1	2.38	0.48
1:A:67:ASP:OD2	1:A:69:GLU:HB2	2.14	0.48
1:A:151:LEU:HD12	1:A:151:LEU:H	1.78	0.48
1:A:336:VAL:CG1	1:A:338:ARG:HB2	2.43	0.48
1:A:432:ASP:CB	1:A:464:ILE:HG21	2.43	0.48
1:B:119:GLU:OE2	1:B:216:ASP:OD1	2.32	0.48
1:B:252:THR:CG2	1:B:253:PRO:HD2	2.43	0.48
1:B:426:LEU:HD13	1:B:426:LEU:C	2.37	0.48
1:B:432:ASP:CB	1:B:464:ILE:HG21	2.43	0.48
1:B:449:ASP:CB	1:B:532:CYS:N	2.74	0.48
1:C:67:ASP:OD2	1:C:69:GLU:HB2	2.14	0.48
1:C:151:LEU:O	1:C:152:LYS:HB2	2.13	0.48
1:C:281:ILE:HG23	1:C:281:ILE:O	2.13	0.48
2:C:809:NAG:C6	2:C:810:NAG:C6	2.92	0.48
1:D:119:GLU:OE2	1:D:216:ASP:OD1	2.32	0.48
1:D:367:LEU:HD13	1:D:412:VAL:CG2	2.43	0.48
1:A:512:LEU:HD11	1:A:519:ASN:ND2	2.28	0.48
1:C:33:LYS:NZ	1:C:56:GLU:OE1	2.43	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:365:GLN:HA	1:D:416:GLY:HA3	1.95	0.48
2:D:809:NAG:C6	2:D:810:NAG:C6	2.92	0.48
1:A:2:TRP:HZ3	1:B:6:PRO:CG	2.27	0.48
1:A:241:ARG:HE	1:A:281:ILE:CD1	2.24	0.48
1:B:512:LEU:HD11	1:B:519:ASN:ND2	2.28	0.48
1:C:155:PRO:O	1:C:157:GLU:N	2.43	0.48
1:C:272:THR:CG2	1:C:273:THR:N	2.76	0.48
1:C:310:VAL:HG12	1:C:312:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:VAL:HG12	1:D:312:LEU:HG	1.95	0.48
1:A:367:LEU:HD13	1:A:412:VAL:CG2	2.43	0.48
1:A:397:GLU:OE1	1:A:397:GLU:N	2.44	0.48
2:A:809:NAG:C6	2:A:810:NAG:C6	2.92	0.48
1:B:4:ILE:HA	1:B:5:PRO:HD3	1.72	0.48
1:B:67:ASP:OD2	1:B:69:GLU:HB2	2.13	0.48
1:B:310:VAL:HG12	1:B:312:LEU:HG	1.95	0.48
1:C:41:GLN:HA	1:C:45:ASN:HB2	1.95	0.48
1:C:224:LYS:CE	2:C:806:NAG:C8	2.91	0.48
1:C:276:GLU:HG3	1:C:277:SER:N	2.25	0.48
1:D:155:PRO:O	1:D:157:GLU:N	2.43	0.48
1:D:397:GLU:OE1	1:D:397:GLU:N	2.45	0.48
1:A:28:LYS:CD	1:A:88:VAL:HG12	2.38	0.48
1:A:92:MET:SD	1:B:2:TRP:C	2.97	0.48
1:A:333:VAL:CB	1:A:334:PRO:CD	2.88	0.48
1:A:423:THR:HB	2:A:810:NAG:H83	1.93	0.48
1:B:76:LEU:O	1:B:94:ILE:N	2.44	0.48
2:B:809:NAG:C6	2:B:810:NAG:C6	2.92	0.48
1:C:273:THR:H	2:C:803:NAG:HN2	1.60	0.48
1:D:225:THR:HA	1:D:318:THR:O	2.14	0.48
1:A:2:TRP:H	1:B:93:GLU:C	2.22	0.48
1:A:537:ILE:CG1	1:A:538:LYS:N	2.77	0.48
1:B:273:THR:H	2:B:803:NAG:HN2	1.60	0.48
1:C:33:LYS:HB3	1:C:83:GLU:CG	2.40	0.48
1:C:367:LEU:H	1:C:367:LEU:HG	1.41	0.48
1:D:41:GLN:HA	1:D:45:ASN:HB2	1.95	0.48
1:D:250:PRO:O	1:D:255:TRP:CE3	2.67	0.48
1:D:266:GLY:N	1:D:268:PHE:CE2	2.76	0.48
1:D:352:ILE:HG13	1:D:388:VAL:CB	2.33	0.48
1:D:482:THR:HG22	1:D:482:THR:O	2.09	0.48
1:D:537:ILE:CG1	1:D:538:LYS:N	2.77	0.48
1:A:24:ILE:HD12	1:B:1:ASP:N	2.28	0.48
1:A:90:GLU:HB2	1:B:90:GLU:HB3	1.92	0.48
1:A:225:THR:HA	1:A:318:THR:O	2.14	0.48
1:A:250:PRO:O	1:A:255:TRP:CE3	2.66	0.48
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.95	0.48
1:A:365:GLN:HA	1:A:416:GLY:HA3	1.95	0.48
1:A:518:ASN:C	1:A:520:PRO:CD	2.87	0.48
1:B:250:PRO:O	1:B:255:TRP:CE3	2.67	0.48
1:C:266:GLY:N	1:C:268:PHE:CE2	2.76	0.48
1:D:68:ARG:HD3	1:D:100:ASP:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ILE:CD1	1:D:264:ASN:ND2	2.77	0.48
1:A:68:ARG:HD3	1:A:100:ASP:CA	2.43	0.47
1:A:241:ARG:NE	1:A:281:ILE:HD12	2.22	0.47
1:B:224:LYS:CE	2:B:806:NAG:C8	2.91	0.47
1:B:365:GLN:O	1:B:365:GLN:CG	2.54	0.47
1:C:300:ILE:HD12	1:C:300:ILE:N	2.29	0.47
1:A:41:GLN:HA	1:A:45:ASN:HB2	1.95	0.47
1:B:418:SER:O	1:B:419:VAL:HG23	2.14	0.47
1:C:150:ILE:HD11	1:C:165:ILE:HB	1.96	0.47
1:C:225:THR:HA	1:C:318:THR:O	2.14	0.47
1:C:496:LEU:HD21	1:C:509:ILE:CD1	2.38	0.47
1:A:154:ASP:O	2:A:801:NAG:C8	2.60	0.47
1:A:224:LYS:CE	2:A:806:NAG:C8	2.91	0.47
1:A:418:SER:O	1:A:419:VAL:HG23	2.14	0.47
1:A:514:SER:CA	1:A:517:GLN:O	2.62	0.47
1:B:36:TYR:O	1:B:55:TRP:HA	2.15	0.47
1:B:150:ILE:HD11	1:B:165:ILE:HB	1.96	0.47
1:C:365:GLN:HA	1:C:416:GLY:HA3	1.95	0.47
1:C:518:ASN:C	1:C:520:PRO:CD	2.87	0.47
1:D:514:SER:CA	1:D:517:GLN:O	2.62	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:379:LEU:H	1:A:379:LEU:CD2	2.22	0.47
2:A:809:NAG:H61	2:A:810:NAG:C6	2.39	0.47
1:B:117:VAL:O	1:B:212:THR:N	2.46	0.47
1:B:514:SER:CA	1:B:517:GLN:O	2.62	0.47
1:D:301:THR:CG2	1:D:316:THR:HG23	2.45	0.47
1:D:344:ASP:O	1:D:344:ASP:CG	2.57	0.47
1:D:371:ILE:HD12	1:D:371:ILE:HA	1.65	0.47
1:A:4:ILE:HA	1:A:5:PRO:HD3	1.72	0.47
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.32	0.47
1:A:151:LEU:O	1:A:152:LYS:HB2	2.13	0.47
1:B:224:LYS:HE3	2:B:806:NAG:H82	1.95	0.47
1:B:301:THR:CG2	1:B:316:THR:HG23	2.45	0.47
1:B:333:VAL:CB	1:B:334:PRO:CD	2.88	0.47
1:B:518:ASN:C	1:B:520:PRO:CD	2.87	0.47
1:C:320:THR:CB	2:C:807:NAG:N2	2.78	0.47
1:C:514:SER:CA	1:C:517:GLN:O	2.62	0.47
1:C:537:ILE:CG1	1:C:538:LYS:N	2.77	0.47
1:D:281:ILE:O	1:D:281:ILE:HG23	2.13	0.47
1:D:300:ILE:HD12	1:D:300:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:519:ASN:CG	1:D:519:ASN:O	2.55	0.47
1:A:4:ILE:CD1	1:B:1:ASP:O	2.62	0.47
1:A:36:TYR:O	1:A:55:TRP:HA	2.15	0.47
1:A:89:GLU:OE1	1:B:90:GLU:HG2	2.14	0.47
1:A:90:GLU:HG3	1:B:89:GLU:CD	2.30	0.47
1:A:261:ILE:CD1	1:A:264:ASN:ND2	2.77	0.47
1:A:273:THR:H	2:A:803:NAG:HN2	1.60	0.47
1:B:225:THR:HA	1:B:318:THR:O	2.14	0.47
1:D:379:LEU:H	1:D:379:LEU:CD2	2.22	0.47
1:A:138:ASN:C	1:A:138:ASN:ND2	2.73	0.47
1:A:451:ASN:O	1:A:534:GLY:CA	2.60	0.47
1:B:261:ILE:CD1	1:B:264:ASN:ND2	2.77	0.47
1:B:537:ILE:CG1	1:B:538:LYS:N	2.77	0.47
1:B:539:CYS:HB3	1:B:540:GLN:H	1.45	0.47
1:C:23:GLN:HB2	1:C:59:TRP:CE3	2.50	0.47
1:C:119:GLU:OE2	1:C:216:ASP:OD1	2.32	0.47
1:D:150:ILE:HD11	1:D:165:ILE:HB	1.96	0.47
1:A:344:ASP:O	1:A:344:ASP:CG	2.57	0.47
1:B:33:LYS:HB3	1:B:83:GLU:CG	2.40	0.47
1:C:261:ILE:CD1	1:C:264:ASN:ND2	2.77	0.47
1:C:268:PHE:CA	1:C:285:ALA:HB3	2.45	0.47
1:C:301:THR:CG2	1:C:316:THR:HG23	2.45	0.47
1:D:226:TYR:O	1:D:227:THR:HG23	2.15	0.47
1:A:6:PRO:HD3	1:B:5:PRO:HG2	1.97	0.47
1:A:23:GLN:HB2	1:A:59:TRP:CE3	2.50	0.47
1:A:310:VAL:HG12	1:A:311:PRO:O	2.15	0.47
1:B:344:ASP:CG	1:B:344:ASP:O	2.57	0.47
1:D:272:THR:HG23	2:D:803:NAG:HN2	1.80	0.47
1:D:418:SER:O	1:D:419:VAL:HG23	2.14	0.47
1:A:3:VAL:O	1:B:3:VAL:CG2	2.63	0.47
1:A:300:ILE:HD12	1:A:300:ILE:N	2.29	0.47
1:B:320:THR:CB	2:B:807:NAG:N2	2.78	0.47
1:B:366:LYS:HG2	1:B:367:LEU:H	1.75	0.47
1:B:367:LEU:HD13	1:B:412:VAL:CG2	2.43	0.47
1:C:108:PHE:HE1	1:C:203:VAL:HG23	1.80	0.47
1:C:451:ASN:O	1:C:534:GLY:CA	2.60	0.47
1:D:36:TYR:O	1:D:55:TRP:HA	2.15	0.47
1:D:268:PHE:CA	1:D:285:ALA:HB3	2.45	0.47
1:D:374:ASP:N	1:D:374:ASP:OD1	2.49	0.47
1:A:268:PHE:CA	1:A:285:ALA:HB3	2.45	0.46
1:A:363:GLN:O	1:A:364:ILE:CG2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:CG	1:B:69:GLU:HB2	2.40	0.46
1:B:272:THR:HG23	2:B:803:NAG:HN2	1.80	0.46
1:C:226:TYR:O	1:C:227:THR:HG23	2.15	0.46
1:D:33:LYS:NZ	1:D:56:GLU:OE1	2.42	0.46
1:D:108:PHE:HE1	1:D:203:VAL:HG23	1.80	0.46
1:A:8:LYS:CD	1:A:8:LYS:N	2.51	0.46
1:B:41:GLN:HA	1:B:45:ASN:HB2	1.95	0.46
1:B:374:ASP:N	1:B:374:ASP:OD1	2.49	0.46
1:B:408:VAL:O	1:B:426:LEU:N	2.48	0.46
1:C:270:ASN:OD1	1:C:271:ILE:N	2.49	0.46
1:C:363:GLN:O	1:C:364:ILE:CG2	2.63	0.46
1:C:440:PRO:HB3	1:C:457:LEU:CD2	2.43	0.46
1:C:448:CYS:C	1:C:452:PRO:HG3	2.40	0.46
1:D:320:THR:CB	2:D:807:NAG:N2	2.78	0.46
1:D:440:PRO:HB3	1:D:457:LEU:CD2	2.43	0.46
1:D:506:ASP:OD1	1:D:506:ASP:N	2.49	0.46
1:A:301:THR:CG2	1:A:316:THR:HG23	2.45	0.46
1:A:320:THR:CB	2:A:807:NAG:N2	2.78	0.46
1:A:522:LEU:HB3	1:A:523:THR:H	1.57	0.46
1:B:448:CYS:SG	1:B:537:ILE:CG2	3.01	0.46
1:C:67:ASP:CG	1:C:69:GLU:HB2	2.40	0.46
1:C:418:SER:O	1:C:419:VAL:HG23	2.14	0.46
1:D:67:ASP:CG	1:D:69:GLU:HB2	2.40	0.46
1:D:271:ILE:HG23	1:D:271:ILE:O	2.15	0.46
1:D:448:CYS:SG	1:D:537:ILE:CG2	3.01	0.46
1:A:67:ASP:CG	1:A:69:GLU:HB2	2.40	0.46
1:A:270:ASN:OD1	1:A:271:ILE:N	2.49	0.46
1:A:448:CYS:SG	1:A:537:ILE:CG2	3.01	0.46
1:B:226:TYR:O	1:B:227:THR:HG23	2.15	0.46
1:B:268:PHE:CA	1:B:285:ALA:HB3	2.45	0.46
1:C:36:TYR:O	1:C:55:TRP:HA	2.15	0.46
1:C:100:ASP:OD1	1:C:101:GLN:N	2.49	0.46
1:C:138:ASN:C	1:C:138:ASN:ND2	2.73	0.46
1:D:50:VAL:HB	1:D:51:PHE:CD1	2.50	0.46
1:A:408:VAL:O	1:A:426:LEU:N	2.49	0.46
1:A:496:LEU:HD21	1:A:509:ILE:CD1	2.38	0.46
1:B:241:ARG:HE	1:B:281:ILE:CD1	2.24	0.46
1:B:481:LEU:HA	1:B:481:LEU:HD12	1.50	0.46
1:C:271:ILE:HG23	1:C:271:ILE:O	2.15	0.46
1:C:374:ASP:N	1:C:374:ASP:OD1	2.49	0.46
1:D:252:THR:HA	1:D:253:PRO:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ASN:OD1	1:D:271:ILE:N	2.49	0.46
1:D:310:VAL:HG12	1:D:311:PRO:O	2.15	0.46
1:D:363:GLN:O	1:D:364:ILE:CG2	2.64	0.46
1:D:450:GLN:CB	1:D:533:GLU:HA	2.29	0.46
1:A:298:LEU:N	1:A:298:LEU:CD2	2.75	0.46
1:A:374:ASP:N	1:A:374:ASP:OD1	2.49	0.46
1:B:100:ASP:OD1	1:B:101:GLN:N	2.49	0.46
1:B:108:PHE:HE1	1:B:203:VAL:HG23	1.80	0.46
1:B:363:GLN:O	1:B:364:ILE:CG2	2.63	0.46
1:C:50:VAL:HB	1:C:51:PHE:CD1	2.50	0.46
1:D:54:GLU:HB2	1:D:57:THR:OG1	2.16	0.46
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.16	0.46
1:A:100:ASP:OD1	1:A:101:GLN:N	2.49	0.46
1:A:155:PRO:CB	2:A:801:NAG:C8	2.94	0.46
1:A:271:ILE:HG23	1:A:271:ILE:O	2.15	0.46
1:A:511:VAL:N	1:A:523:THR:O	2.46	0.46
1:B:50:VAL:HB	1:B:51:PHE:CD1	2.50	0.46
1:B:138:ASN:C	1:B:138:ASN:ND2	2.73	0.46
1:B:270:ASN:OD1	1:B:271:ILE:N	2.49	0.46
1:B:449:ASP:CB	1:B:532:CYS:H	2.22	0.46
1:B:459:ILE:HD12	1:B:459:ILE:N	2.31	0.46
1:B:524:VAL:HG21	2:B:904:NAG:C8	2.44	0.46
1:C:344:ASP:O	1:C:344:ASP:CG	2.57	0.46
1:C:448:CYS:SG	1:C:537:ILE:CG2	3.01	0.46
1:D:23:GLN:HB2	1:D:59:TRP:CE3	2.50	0.46
1:D:187:TYR:HE1	1:D:211:ILE:HD11	1.81	0.46
1:D:282:LEU:CD2	1:D:283:THR:N	2.76	0.46
1:A:109:THR:CB	1:A:131:SER:HB2	2.46	0.46
1:A:400:TYR:O	1:A:401:VAL:C	2.59	0.46
1:A:449:ASP:CB	1:A:532:CYS:H	2.22	0.46
1:B:300:ILE:HD12	1:B:300:ILE:N	2.29	0.46
1:C:155:PRO:CB	2:C:801:NAG:C8	2.94	0.46
1:C:187:TYR:HE1	1:C:211:ILE:HD11	1.81	0.46
1:C:506:ASP:OD1	1:C:506:ASP:N	2.49	0.46
1:D:109:THR:CB	1:D:131:SER:HB2	2.46	0.46
1:A:226:TYR:O	1:A:227:THR:HG23	2.15	0.46
1:A:252:THR:HA	1:A:253:PRO:HD3	1.81	0.46
1:B:262:ARG:HG3	1:B:299:GLN:HB2	1.98	0.46
1:C:117:VAL:O	1:C:212:THR:N	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:LEU:N	1:D:298:LEU:CD2	2.75	0.46
1:D:449:ASP:CB	1:D:532:CYS:H	2.22	0.46
1:D:459:ILE:N	1:D:459:ILE:HD12	2.31	0.46
1:A:117:VAL:O	1:A:212:THR:N	2.46	0.46
1:B:227:THR:N	2:B:812:NAG:H2	2.31	0.46
1:B:400:TYR:O	1:B:401:VAL:C	2.59	0.46
1:B:440:PRO:HB3	1:B:457:LEU:CD2	2.43	0.46
1:C:450:GLN:CB	1:C:533:GLU:OE2	2.64	0.46
1:D:100:ASP:OD1	1:D:101:GLN:N	2.49	0.46
1:D:262:ARG:HG3	1:D:299:GLN:HB2	1.98	0.46
1:A:339:VAL:HG11	1:A:351:ILE:HG23	1.98	0.45
1:A:373:ASN:CG	1:A:374:ASP:N	2.75	0.45
1:A:483:TRP:CZ2	1:A:507:TYR:CE1	2.87	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
2:B:809:NAG:H61	2:B:810:NAG:C6	2.39	0.45
1:C:152:LYS:O	1:C:189:LEU:HA	2.17	0.45
1:C:310:VAL:HG12	1:C:311:PRO:O	2.15	0.45
1:C:432:ASP:CG	1:C:433:VAL:N	2.74	0.45
1:C:459:ILE:HD12	1:C:459:ILE:N	2.31	0.45
2:C:805:NAG:C5	2:C:806:NAG:H83	2.46	0.45
1:D:380:THR:CG2	1:D:381:VAL:N	2.79	0.45
1:D:448:CYS:C	1:D:452:PRO:HG3	2.40	0.45
1:D:450:GLN:CB	1:D:533:GLU:OE2	2.64	0.45
1:D:461:ASP:HB3	1:D:468:THR:CG2	2.46	0.45
1:B:8:LYS:CD	1:B:8:LYS:N	2.51	0.45
1:B:23:GLN:HB2	1:B:59:TRP:CE3	2.50	0.45
1:B:187:TYR:HE1	1:B:211:ILE:HD11	1.81	0.45
1:B:227:THR:HG22	1:B:320:THR:HB	1.98	0.45
1:B:310:VAL:HG12	1:B:311:PRO:O	2.15	0.45
1:B:339:VAL:HG11	1:B:351:ILE:HG23	1.98	0.45
1:B:450:GLN:CB	1:B:533:GLU:OE2	2.64	0.45
1:B:506:ASP:OD1	1:B:506:ASP:N	2.49	0.45
1:A:152:LYS:O	1:A:189:LEU:HA	2.17	0.45
1:A:450:GLN:CB	1:A:533:GLU:OE2	2.64	0.45
1:A:473:VAL:CG2	1:A:487:LEU:HD21	2.46	0.45
1:C:408:VAL:O	1:C:426:LEU:N	2.49	0.45
1:C:473:VAL:CG2	1:C:487:LEU:HD21	2.46	0.45
1:D:312:LEU:O	3:D:804:NDG:H8C1	2.17	0.45
1:A:187:TYR:HE1	1:A:211:ILE:HD11	1.81	0.45
1:B:461:ASP:HB3	1:B:468:THR:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:VAL:HG11	1:C:351:ILE:HG23	1.98	0.45
1:C:373:ASN:CG	1:C:374:ASP:N	2.75	0.45
1:C:380:THR:CG2	1:C:381:VAL:N	2.79	0.45
1:C:380:THR:HG22	1:C:381:VAL:N	2.32	0.45
1:D:227:THR:N	2:D:812:NAG:H2	2.31	0.45
1:D:373:ASN:CG	1:D:374:ASP:N	2.75	0.45
1:A:95:THR:N	1:B:2:TRP:CZ3	2.85	0.45
1:A:227:THR:N	2:A:812:NAG:H2	2.31	0.45
1:B:271:ILE:O	1:B:271:ILE:HG23	2.15	0.45
1:C:461:ASP:HB3	1:C:468:THR:CG2	2.46	0.45
1:D:138:ASN:C	1:D:138:ASN:ND2	2.73	0.45
1:D:432:ASP:CG	1:D:433:VAL:N	2.74	0.45
1:A:276:GLU:HG3	1:A:277:SER:N	2.25	0.45
1:A:421:THR:HG21	2:A:809:NAG:H61	1.98	0.45
1:A:459:ILE:N	1:A:459:ILE:HD12	2.31	0.45
2:A:805:NAG:C5	2:A:806:NAG:H83	2.46	0.45
1:B:469:TYR:CD2	1:B:470:PRO:N	2.85	0.45
1:C:109:THR:HB	1:C:131:SER:HB2	1.99	0.45
1:C:194:THR:CG2	1:C:195:ASP:N	2.79	0.45
1:C:227:THR:N	2:C:812:NAG:H2	2.31	0.45
1:C:482:THR:O	1:C:483:TRP:CD2	2.70	0.45
1:D:194:THR:CG2	1:D:195:ASP:N	2.79	0.45
1:D:339:VAL:HG11	1:D:351:ILE:HG23	1.98	0.45
1:D:380:THR:HG22	1:D:381:VAL:N	2.32	0.45
1:D:396:ARG:HH21	1:D:432:ASP:CG	2.25	0.45
1:A:262:ARG:HG3	1:A:299:GLN:HB2	1.98	0.45
1:A:381:VAL:HA	1:A:387:ILE:O	2.16	0.45
1:A:485:ALA:O	1:A:486:GLU:OE1	2.35	0.45
1:B:152:LYS:O	1:B:189:LEU:HA	2.17	0.45
1:B:381:VAL:HA	1:B:387:ILE:O	2.16	0.45
1:C:261:ILE:HD11	1:C:264:ASN:ND2	2.32	0.45
2:C:805:NAG:H62	2:C:806:NAG:N2	2.31	0.45
1:A:134:ASP:HB2	1:A:146:LEU:HD11	1.99	0.45
1:B:162:LEU:HB2	1:B:163:PHE:CE1	2.52	0.45
2:B:805:NAG:H62	2:B:806:NAG:N2	2.31	0.45
1:C:54:GLU:HB2	1:C:57:THR:OG1	2.16	0.45
1:C:162:LEU:HB2	1:C:163:PHE:CE1	2.52	0.45
1:C:227:THR:HG22	1:C:320:THR:HB	1.98	0.45
1:D:469:TYR:CD2	1:D:470:PRO:N	2.85	0.45
1:D:482:THR:O	1:D:483:TRP:CD2	2.70	0.45
1:A:194:THR:CG2	1:A:195:ASP:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:HG22	1:A:320:THR:HB	1.98	0.45
1:A:432:ASP:CG	1:A:433:VAL:N	2.74	0.45
1:B:194:THR:CG2	1:B:195:ASP:N	2.79	0.45
1:B:312:LEU:O	3:B:804:NDG:H8C1	2.17	0.45
1:B:522:LEU:HA	1:B:522:LEU:HD23	1.36	0.45
1:C:262:ARG:HG3	1:C:299:GLN:HB2	1.98	0.45
1:A:24:ILE:HG21	1:B:1:ASP:H2	1.82	0.45
1:A:506:ASP:OD1	1:A:506:ASP:N	2.49	0.45
1:B:249:MET:HA	1:B:250:PRO:HD3	1.85	0.45
1:B:473:VAL:CG2	1:B:487:LEU:HD21	2.47	0.45
1:C:25:LYS:HB2	1:D:3:VAL:HG11	1.62	0.45
1:C:396:ARG:HH21	1:C:432:ASP:CG	2.25	0.45
1:C:403:ASN:C	1:C:405:THR:N	2.75	0.45
1:C:468:THR:C	1:C:469:TYR:O	2.54	0.45
1:D:32:ASN:ND2	1:D:83:GLU:CB	2.62	0.45
1:D:381:VAL:HA	1:D:387:ILE:O	2.17	0.45
1:D:396:ARG:NH2	1:D:464:ILE:HG22	2.12	0.45
1:D:449:ASP:N	1:D:532:CYS:HB3	2.19	0.45
1:D:473:VAL:CG2	1:D:487:LEU:HD21	2.47	0.45
1:A:380:THR:CG2	1:A:381:VAL:N	2.79	0.44
1:A:396:ARG:HH21	1:A:432:ASP:CG	2.25	0.44
1:B:109:THR:CB	1:B:131:SER:HB2	2.46	0.44
1:B:109:THR:HB	1:B:131:SER:HB2	1.99	0.44
1:B:134:ASP:HB2	1:B:146:LEU:HD11	1.99	0.44
1:B:380:THR:HG22	1:B:381:VAL:N	2.32	0.44
1:C:92:MET:CB	1:D:2:TRP:HD1	2.29	0.44
1:C:371:ILE:HD13	1:C:381:VAL:HG11	1.95	0.44
1:D:31:PHE:CD2	1:D:31:PHE:C	2.95	0.44
1:D:152:LYS:O	1:D:189:LEU:HA	2.17	0.44
1:D:408:VAL:O	1:D:426:LEU:N	2.49	0.44
1:D:421:THR:HG21	2:D:809:NAG:H61	1.98	0.44
1:D:485:ALA:O	1:D:486:GLU:OE1	2.35	0.44
1:A:261:ILE:HD11	1:A:264:ASN:ND2	2.32	0.44
1:A:448:CYS:C	1:A:452:PRO:HG3	2.40	0.44
1:B:367:LEU:H	1:B:367:LEU:HG	1.41	0.44
1:B:448:CYS:C	1:B:452:PRO:HG3	2.40	0.44
1:C:3:VAL:HB	1:C:4:ILE:H	1.51	0.44
1:C:109:THR:CB	1:C:131:SER:HB2	2.46	0.44
1:A:2:TRP:CE3	1:B:6:PRO:HG3	2.52	0.44
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.44
1:A:482:THR:O	1:A:483:TRP:CD2	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:VAL:HG11	1:B:338:ARG:HD2	1.99	0.44
1:B:380:THR:CG2	1:B:381:VAL:N	2.79	0.44
1:C:92:MET:HE2	1:D:1:ASP:OD2	2.17	0.44
1:C:187:TYR:CE1	1:C:211:ILE:HD11	2.52	0.44
1:C:381:VAL:HA	1:C:387:ILE:O	2.16	0.44
1:D:227:THR:HG22	1:D:320:THR:HB	1.98	0.44
1:D:366:LYS:HG2	1:D:367:LEU:H	1.75	0.44
1:A:162:LEU:HB2	1:A:163:PHE:CE1	2.52	0.44
1:A:272:THR:HG23	2:A:803:NAG:HN2	1.81	0.44
1:A:380:THR:HG22	1:A:381:VAL:N	2.32	0.44
1:A:469:TYR:CD2	1:A:470:PRO:N	2.85	0.44
1:B:469:TYR:CE2	1:B:470:PRO:HB2	2.52	0.44
1:C:134:ASP:HB2	1:C:146:LEU:HD11	1.99	0.44
1:C:469:TYR:CD2	1:C:470:PRO:N	2.85	0.44
1:D:469:TYR:CE2	1:D:470:PRO:HB2	2.52	0.44
1:B:187:TYR:CE1	1:B:211:ILE:HD11	2.52	0.44
1:B:335:ALA:HB1	3:B:811:NDG:H6	1.76	0.44
1:B:396:ARG:HH21	1:B:432:ASP:CG	2.25	0.44
1:B:435:ASP:HB2	1:B:436:ASN:H	1.59	0.44
1:C:86:SER:HA	1:C:87:PRO:HD3	1.83	0.44
1:C:333:VAL:CB	1:C:334:PRO:CD	2.88	0.44
1:C:461:ASP:HB3	1:C:468:THR:HG22	2.00	0.44
1:C:524:VAL:HG21	2:C:904:NAG:C8	2.44	0.44
1:D:261:ILE:HD11	1:D:264:ASN:ND2	2.32	0.44
1:D:421:THR:CG2	1:D:422:GLY:N	2.81	0.44
2:D:805:NAG:H62	2:D:806:NAG:N2	2.31	0.44
1:A:250:PRO:C	1:A:252:THR:H	2.26	0.44
1:A:442:PRO:HD2	1:A:457:LEU:HD12	2.00	0.44
1:B:373:ASN:CG	1:B:374:ASP:N	2.75	0.44
1:C:336:VAL:HG11	1:C:338:ARG:HD2	1.99	0.44
1:C:481:LEU:HD12	1:C:481:LEU:HA	1.50	0.44
1:D:442:PRO:HD2	1:D:457:LEU:HD12	2.00	0.44
1:A:92:MET:SD	1:B:3:VAL:N	2.90	0.44
1:A:108:PHE:HE1	1:A:203:VAL:HG23	1.80	0.44
1:A:127:VAL:HG13	1:A:128:MET:N	2.25	0.44
1:A:187:TYR:CE1	1:A:211:ILE:HD11	2.52	0.44
1:A:194:THR:HG23	1:A:201:LEU:O	2.18	0.44
1:B:127:VAL:HG13	1:B:128:MET:N	2.25	0.44
1:B:261:ILE:HD11	1:B:264:ASN:ND2	2.32	0.44
1:B:421:THR:HG21	2:B:809:NAG:H61	1.98	0.44
1:B:442:PRO:HD2	1:B:457:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:THR:O	1:B:483:TRP:CD2	2.70	0.44
1:B:485:ALA:O	1:B:486:GLU:OE1	2.35	0.44
1:B:489:SER:C	1:B:491:GLY:H	2.26	0.44
1:D:162:LEU:HB2	1:D:163:PHE:CE1	2.52	0.44
1:D:250:PRO:C	1:D:252:THR:H	2.26	0.44
1:D:461:ASP:HB3	1:D:468:THR:HG22	2.00	0.44
1:A:27:ASN:ND2	1:A:28:LYS:N	2.50	0.44
1:A:109:THR:HB	1:A:131:SER:HB2	1.99	0.44
1:A:128:MET:HB3	1:A:129:ALA:H	1.62	0.44
1:A:154:ASP:HB3	2:A:801:NAG:C7	2.48	0.44
1:A:299:GLN:CG	1:A:318:THR:HG23	2.42	0.44
1:A:461:ASP:HB3	1:A:468:THR:CG2	2.46	0.44
1:A:489:SER:C	1:A:491:GLY:H	2.26	0.44
1:B:290:PHE:CD2	1:B:293:ARG:O	2.71	0.44
1:C:181:ARG:NH1	1:C:249:MET:HE3	2.33	0.44
1:C:232:GLU:HA	1:C:288:LEU:HD12	1.99	0.44
1:C:469:TYR:CE2	1:C:470:PRO:HB2	2.52	0.44
1:D:151:LEU:HD12	1:D:151:LEU:N	2.33	0.44
1:D:336:VAL:HG11	1:D:338:ARG:HD2	1.99	0.44
1:A:95:THR:N	1:B:2:TRP:CE3	2.86	0.44
1:A:181:ARG:NH1	1:A:249:MET:HE3	2.33	0.44
1:A:232:GLU:HA	1:A:288:LEU:HD12	1.99	0.44
1:A:335:ALA:HB1	3:A:811:NDG:H6	1.71	0.44
1:A:450:GLN:HG3	1:A:532:CYS:O	2.10	0.44
1:B:220:ILE:O	1:B:220:ILE:HG22	2.18	0.44
1:B:250:PRO:C	1:B:252:THR:H	2.26	0.44
1:A:24:ILE:HG21	1:B:1:ASP:N	2.33	0.43
1:A:239:VAL:HG13	1:A:240:GLN:N	2.33	0.43
1:A:247:LEU:HD12	1:A:247:LEU:N	2.33	0.43
1:A:290:PHE:CD2	1:A:293:ARG:O	2.71	0.43
1:A:368:SER:CB	1:A:370:PHE:HE1	2.31	0.43
1:A:419:VAL:HG13	1:A:420:GLY:N	2.33	0.43
1:B:155:PRO:C	1:B:157:GLU:N	2.56	0.43
1:B:354:LEU:HD12	1:B:386:GLY:O	2.18	0.43
1:B:432:ASP:CG	1:B:433:VAL:N	2.74	0.43
1:C:22:VAL:CG2	1:C:23:GLN:N	2.81	0.43
1:C:290:PHE:CD2	1:C:293:ARG:O	2.71	0.43
1:D:232:GLU:HA	1:D:288:LEU:HD12	2.00	0.43
1:A:260:LYS:HB3	1:A:260:LYS:HE3	1.81	0.43
1:A:312:LEU:O	3:A:804:NDG:H8C1	2.17	0.43
1:A:441:SER:CB	1:A:442:PRO:HD3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:TYR:CE2	1:A:470:PRO:HB2	2.52	0.43
2:A:805:NAG:H62	2:A:806:NAG:N2	2.31	0.43
1:B:1:ASP:CG	1:B:2:TRP:N	2.70	0.43
1:B:224:LYS:HE3	2:B:806:NAG:C8	2.48	0.43
1:B:247:LEU:HD12	1:B:247:LEU:N	2.33	0.43
1:B:297:VAL:HG21	2:B:807:NAG:H62	2.01	0.43
1:C:354:LEU:HD12	1:C:386:GLY:O	2.18	0.43
1:C:482:THR:C	1:C:483:TRP:CG	2.96	0.43
1:D:385:ASN:O	1:D:386:GLY:C	2.62	0.43
1:D:524:VAL:HG21	2:D:904:NAG:C8	2.44	0.43
1:A:3:VAL:HG11	1:B:4:ILE:HD12	1.83	0.43
1:A:24:ILE:CG2	1:B:1:ASP:H2	2.31	0.43
1:A:32:ASN:HD22	1:A:83:GLU:N	2.13	0.43
1:A:272:THR:CG2	1:A:273:THR:N	2.76	0.43
1:B:90:GLU:O	1:B:91:PRO:O	2.37	0.43
1:C:90:GLU:O	1:C:91:PRO:O	2.37	0.43
1:C:289:ASP:C	1:C:290:PHE:CD1	2.97	0.43
1:C:368:SER:CB	1:C:370:PHE:HE1	2.31	0.43
1:D:155:PRO:CB	2:D:801:NAG:C8	2.94	0.43
1:D:187:TYR:CE1	1:D:211:ILE:HD11	2.52	0.43
1:D:194:THR:HG23	1:D:201:LEU:O	2.18	0.43
1:D:224:LYS:HE3	2:D:806:NAG:C8	2.48	0.43
1:A:289:ASP:C	1:A:290:PHE:CD1	2.97	0.43
1:A:354:LEU:HD12	1:A:386:GLY:O	2.18	0.43
1:A:539:CYS:HB3	1:A:540:GLN:H	1.45	0.43
2:B:805:NAG:C5	2:B:806:NAG:H83	2.46	0.43
1:C:32:ASN:ND2	1:C:83:GLU:CB	2.62	0.43
1:C:194:THR:HG23	1:C:201:LEU:O	2.18	0.43
1:C:312:LEU:O	3:C:804:NDG:H8C1	2.17	0.43
1:C:442:PRO:HD2	1:C:457:LEU:HD12	2.00	0.43
1:C:489:SER:C	1:C:491:GLY:H	2.26	0.43
1:D:128:MET:HB3	1:D:129:ALA:H	1.62	0.43
1:D:134:ASP:HB2	1:D:146:LEU:HD11	1.99	0.43
1:D:290:PHE:CD2	1:D:293:ARG:O	2.71	0.43
1:D:354:LEU:HD12	1:D:386:GLY:O	2.18	0.43
1:D:400:TYR:O	1:D:401:VAL:C	2.59	0.43
1:D:539:CYS:HB3	1:D:540:GLN:H	1.46	0.43
1:A:482:THR:C	1:A:483:TRP:CG	2.96	0.43
1:B:67:ASP:OD1	1:B:69:GLU:HB2	2.18	0.43
1:B:289:ASP:C	1:B:290:PHE:CD1	2.97	0.43
1:B:385:ASN:O	1:B:386:GLY:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:THR:HG22	1:B:499:THR:H	1.70	0.43
1:B:482:THR:C	1:B:483:TRP:CG	2.96	0.43
1:C:400:TYR:O	1:C:401:VAL:C	2.59	0.43
1:C:421:THR:CG2	1:C:422:GLY:N	2.81	0.43
1:C:441:SER:CB	1:C:442:PRO:HD3	2.47	0.43
1:C:485:ALA:O	1:C:486:GLU:OE1	2.35	0.43
1:D:458:THR:C	1:D:459:ILE:HD12	2.44	0.43
1:A:151:LEU:HD12	1:A:151:LEU:N	2.33	0.43
1:A:224:LYS:HE3	2:A:806:NAG:C8	2.48	0.43
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.81	0.43
1:B:154:ASP:HB3	2:B:801:NAG:C7	2.48	0.43
1:B:232:GLU:HA	1:B:288:LEU:HD12	1.99	0.43
1:B:458:THR:C	1:B:459:ILE:HD12	2.44	0.43
1:B:461:ASP:HB3	1:B:468:THR:HG22	2.00	0.43
1:C:32:ASN:HD22	1:C:83:GLU:N	2.13	0.43
1:C:67:ASP:OD1	1:C:69:GLU:HB2	2.18	0.43
1:D:22:VAL:CG2	1:D:23:GLN:N	2.81	0.43
1:D:181:ARG:NH1	1:D:249:MET:HE3	2.33	0.43
1:D:272:THR:CG2	1:D:273:THR:N	2.76	0.43
1:D:441:SER:CB	1:D:442:PRO:HD3	2.47	0.43
1:A:343:GLU:CD	1:A:395:ASP:HA	2.44	0.43
1:A:367:LEU:H	1:A:367:LEU:HG	1.41	0.43
1:A:385:ASN:O	1:A:386:GLY:C	2.62	0.43
1:A:524:VAL:HG21	2:A:904:NAG:C8	2.44	0.43
1:B:22:VAL:CG2	1:B:23:GLN:N	2.81	0.43
1:B:155:PRO:CB	2:B:801:NAG:C8	2.94	0.43
1:B:181:ARG:NH1	1:B:249:MET:HE3	2.33	0.43
1:B:194:THR:HG23	1:B:201:LEU:O	2.18	0.43
1:B:333:VAL:HG23	1:B:334:PRO:HD3	2.01	0.43
1:D:67:ASP:OD1	1:D:69:GLU:HB2	2.18	0.43
1:B:33:LYS:NZ	1:B:56:GLU:OE1	2.42	0.43
1:B:239:VAL:HG13	1:B:240:GLN:N	2.33	0.43
1:B:368:SER:CB	1:B:370:PHE:HE1	2.31	0.43
1:B:371:ILE:HD13	1:B:381:VAL:HG11	1.95	0.43
1:B:371:ILE:HG13	1:B:410:MET:SD	2.59	0.43
1:C:250:PRO:C	1:C:252:THR:H	2.26	0.43
1:D:378:TRP:HB2	1:D:379:LEU:H	1.64	0.43
1:A:188:THR:H	2:A:801:NAG:H83	1.84	0.43
1:A:336:VAL:HG11	1:A:338:ARG:HD2	1.99	0.43
1:A:469:TYR:CE2	1:A:470:PRO:HD2	2.54	0.43
1:B:378:TRP:HB2	1:B:379:LEU:H	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ASN:C	1:B:405:THR:N	2.76	0.43
1:B:441:SER:CB	1:B:442:PRO:HD3	2.47	0.43
1:C:60:MET:SD	1:D:2:TRP:HH2	2.41	0.43
1:C:366:LYS:HG2	1:C:367:LEU:H	1.75	0.43
1:D:40:GLY:O	1:D:45:ASN:HB2	2.19	0.43
1:D:175:ILE:CG2	1:D:176:GLY:N	2.82	0.43
1:A:2:TRP:CE3	1:B:95:THR:CB	3.02	0.43
1:A:22:VAL:CG2	1:A:23:GLN:N	2.80	0.43
1:A:40:GLY:O	1:A:45:ASN:HB2	2.19	0.43
1:A:90:GLU:O	1:A:91:PRO:O	2.37	0.43
1:A:232:GLU:CG	1:A:289:ASP:C	2.92	0.43
1:A:339:VAL:HG21	1:A:351:ILE:HG22	2.01	0.43
1:A:371:ILE:HD13	1:A:381:VAL:HG11	1.95	0.43
1:A:458:THR:C	1:A:459:ILE:HD12	2.44	0.43
1:B:40:GLY:O	1:B:45:ASN:HB2	2.19	0.43
1:C:4:ILE:HA	1:C:5:PRO:HD3	1.72	0.43
1:C:220:ILE:O	1:C:220:ILE:HG22	2.18	0.43
1:C:224:LYS:HE3	2:C:806:NAG:C8	2.48	0.43
1:C:232:GLU:CG	1:C:289:ASP:C	2.92	0.43
1:D:232:GLU:CG	1:D:289:ASP:C	2.92	0.43
1:D:247:LEU:HD12	1:D:247:LEU:N	2.33	0.43
1:A:250:PRO:HA	1:A:255:TRP:CG	2.54	0.42
1:A:277:SER:O	1:A:278:ASN:C	2.62	0.42
1:A:333:VAL:HG23	1:A:334:PRO:HD3	2.01	0.42
1:B:31:PHE:CD2	1:B:31:PHE:C	2.95	0.42
1:B:396:ARG:NH2	1:B:464:ILE:HG22	2.12	0.42
1:B:419:VAL:HG13	1:B:420:GLY:N	2.33	0.42
1:C:5:PRO:HA	1:C:6:PRO:HD3	1.86	0.42
1:C:40:GLY:O	1:C:45:ASN:HB2	2.19	0.42
1:C:128:MET:HB3	1:C:129:ALA:H	1.62	0.42
1:C:188:THR:H	2:C:801:NAG:H83	1.84	0.42
1:C:247:LEU:HD12	1:C:247:LEU:N	2.33	0.42
1:C:297:VAL:HG21	2:C:807:NAG:H62	2.01	0.42
1:C:343:GLU:CD	1:C:395:ASP:HA	2.44	0.42
1:C:409:ILE:HD13	3:C:811:NDG:H8C3	2.01	0.42
1:C:419:VAL:HG13	1:C:420:GLY:N	2.33	0.42
1:D:297:VAL:HG21	2:D:807:NAG:H62	2.01	0.42
1:D:343:GLU:CD	1:D:395:ASP:HA	2.44	0.42
1:D:371:ILE:HG13	1:D:410:MET:SD	2.59	0.42
1:A:175:ILE:CG2	1:A:176:GLY:N	2.82	0.42
1:A:195:ASP:HB3	1:A:196:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:HD12	1:B:151:LEU:N	2.33	0.42
1:B:490:LYS:O	1:B:490:LYS:CG	2.67	0.42
1:C:27:ASN:ND2	1:C:28:LYS:N	2.50	0.42
1:C:250:PRO:HA	1:C:255:TRP:CG	2.55	0.42
1:D:86:SER:HA	1:D:87:PRO:HD3	1.83	0.42
1:D:109:THR:HB	1:D:131:SER:HB2	1.99	0.42
1:D:239:VAL:HG13	1:D:240:GLN:N	2.34	0.42
1:D:277:SER:O	1:D:278:ASN:C	2.62	0.42
1:D:333:VAL:HG23	1:D:334:PRO:HD3	2.01	0.42
1:D:347:ARG:HG3	1:D:392:GLY:N	2.33	0.42
1:D:482:THR:C	1:D:483:TRP:CG	2.96	0.42
1:A:3:VAL:HA	1:B:3:VAL:HB	2.00	0.42
1:A:461:ASP:HB3	1:A:468:THR:HG22	2.00	0.42
1:A:515:ASP:OD1	1:A:516:ALA:N	2.53	0.42
1:B:188:THR:H	2:B:801:NAG:H83	1.84	0.42
1:B:320:THR:CG2	2:B:807:NAG:C2	2.76	0.42
1:B:371:ILE:HD12	1:B:371:ILE:HA	1.65	0.42
1:C:241:ARG:HE	1:C:281:ILE:CD1	2.24	0.42
1:C:333:VAL:HG23	1:C:334:PRO:HD3	2.01	0.42
1:C:490:LYS:O	1:C:490:LYS:CG	2.67	0.42
1:D:188:THR:H	2:D:801:NAG:H83	1.84	0.42
1:D:289:ASP:C	1:D:290:PHE:CD1	2.97	0.42
1:D:469:TYR:CE2	1:D:470:PRO:HD2	2.54	0.42
1:D:522:LEU:HB3	1:D:523:THR:H	1.57	0.42
1:A:371:ILE:HG13	1:A:410:MET:SD	2.59	0.42
1:A:371:ILE:HA	1:A:410:MET:HB3	2.02	0.42
1:A:519:ASN:O	1:A:520:PRO:C	2.59	0.42
1:B:5:PRO:HA	1:B:6:PRO:HD3	1.85	0.42
1:B:339:VAL:HG21	1:B:351:ILE:HG22	2.01	0.42
1:B:421:THR:CG2	1:B:422:GLY:N	2.81	0.42
1:B:511:VAL:N	1:B:523:THR:O	2.46	0.42
1:C:175:ILE:CG2	1:C:176:GLY:N	2.82	0.42
1:C:396:ARG:NH2	1:C:464:ILE:HG22	2.12	0.42
1:D:90:GLU:O	1:D:91:PRO:O	2.37	0.42
1:D:195:ASP:HB3	1:D:196:LEU:HG	2.01	0.42
1:D:347:ARG:HD2	1:D:392:GLY:CA	2.50	0.42
1:D:368:SER:CB	1:D:370:PHE:HE1	2.31	0.42
1:D:371:ILE:HD13	1:D:381:VAL:HG11	1.95	0.42
2:D:805:NAG:C5	2:D:806:NAG:H83	2.46	0.42
1:A:264:ASN:HB3	1:A:267:GLY:HA2	2.01	0.42
1:A:449:ASP:N	1:A:532:CYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:CG	1:B:289:ASP:C	2.92	0.42
1:B:250:PRO:HA	1:B:255:TRP:CG	2.54	0.42
1:B:264:ASN:HB3	1:B:267:GLY:HA2	2.01	0.42
1:B:371:ILE:HA	1:B:410:MET:HB3	2.02	0.42
1:D:226:TYR:C	1:D:227:THR:CG2	2.92	0.42
1:A:261:ILE:HD13	1:A:261:ILE:H	1.84	0.42
1:B:277:SER:O	1:B:278:ASN:C	2.62	0.42
1:B:299:GLN:CG	1:B:318:THR:HG23	2.42	0.42
1:B:439:VAL:HA	1:B:440:PRO:HD3	1.81	0.42
1:B:515:ASP:OD1	1:B:516:ALA:N	2.53	0.42
1:C:154:ASP:HB3	2:C:801:NAG:C7	2.48	0.42
1:C:264:ASN:HB3	1:C:267:GLY:HA2	2.01	0.42
1:C:277:SER:O	1:C:278:ASN:C	2.62	0.42
1:D:230:VAL:O	1:D:323:VAL:HA	2.20	0.42
1:B:7:ILE:O	1:B:96:ILE:HG23	2.20	0.42
1:C:226:TYR:C	1:C:227:THR:CG2	2.92	0.42
1:C:230:VAL:O	1:C:323:VAL:HA	2.20	0.42
1:C:239:VAL:HG13	1:C:240:GLN:N	2.34	0.42
1:C:252:THR:C	1:C:254:ALA:H	2.28	0.42
1:C:339:VAL:HG21	1:C:351:ILE:HG22	2.01	0.42
1:C:371:ILE:HD12	1:C:371:ILE:HA	1.65	0.42
1:C:371:ILE:HG13	1:C:410:MET:SD	2.59	0.42
1:C:458:THR:C	1:C:459:ILE:HD12	2.44	0.42
1:C:502:LEU:HA	1:C:502:LEU:HD23	1.82	0.42
1:D:261:ILE:HD13	1:D:261:ILE:H	1.85	0.42
1:D:409:ILE:HD13	3:D:811:NDG:H8C3	2.01	0.42
1:D:489:SER:C	1:D:491:GLY:H	2.26	0.42
1:A:409:ILE:HD13	3:A:811:NDG:H8C3	2.01	0.42
1:A:421:THR:CG2	1:A:422:GLY:N	2.81	0.42
1:A:505:GLY:H	1:A:529:VAL:HB	1.85	0.42
1:B:195:ASP:HB3	1:B:196:LEU:HG	2.01	0.42
1:B:505:GLY:H	1:B:529:VAL:HB	1.85	0.42
1:C:195:ASP:HB3	1:C:196:LEU:HG	2.01	0.42
1:A:239:VAL:HG11	1:A:282:LEU:HD22	2.02	0.42
1:A:297:VAL:HG21	2:A:807:NAG:H62	2.01	0.42
1:B:175:ILE:CG2	1:B:176:GLY:N	2.82	0.42
1:B:226:TYR:C	1:B:227:THR:CG2	2.93	0.42
1:B:230:VAL:O	1:B:323:VAL:HA	2.20	0.42
1:B:231:PRO:O	1:B:288:LEU:HD12	2.20	0.42
1:C:378:TRP:HB2	1:C:379:LEU:H	1.64	0.42
1:C:483:TRP:CZ2	1:C:507:TYR:CE1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:PHE:HA	1:D:132:ALA:CB	2.50	0.42
1:D:117:VAL:O	1:D:212:THR:N	2.46	0.42
1:A:230:VAL:O	1:A:323:VAL:HA	2.20	0.42
1:A:231:PRO:O	1:A:288:LEU:HD12	2.20	0.42
1:A:347:ARG:HD2	1:A:392:GLY:CA	2.49	0.42
1:A:347:ARG:HG3	1:A:392:GLY:N	2.33	0.42
1:A:490:LYS:O	1:A:490:LYS:CG	2.67	0.42
1:B:261:ILE:HD13	1:B:261:ILE:H	1.85	0.42
1:C:151:LEU:HD12	1:C:151:LEU:N	2.33	0.42
1:C:261:ILE:H	1:C:261:ILE:HD13	1.85	0.42
1:C:347:ARG:HD2	1:C:392:GLY:CA	2.50	0.42
1:C:449:ASP:N	1:C:532:CYS:HB3	2.19	0.42
1:C:515:ASP:OD1	1:C:516:ALA:N	2.52	0.42
1:A:108:PHE:HA	1:A:132:ALA:CB	2.50	0.41
1:B:23:GLN:HB2	1:B:59:TRP:CD2	2.55	0.41
1:B:108:PHE:HA	1:B:132:ALA:CB	2.50	0.41
1:B:409:ILE:HD13	3:B:811:NDG:H8C3	2.01	0.41
1:B:469:TYR:CE2	1:B:470:PRO:HD2	2.54	0.41
1:C:371:ILE:HA	1:C:410:MET:HB3	2.02	0.41
1:C:474:SER:N	1:C:512:LEU:O	2.53	0.41
1:C:505:GLY:H	1:C:529:VAL:HB	1.85	0.41
1:D:419:VAL:HG13	1:D:420:GLY:N	2.33	0.41
1:A:90:GLU:N	1:B:90:GLU:CB	2.57	0.41
1:A:403:ASN:C	1:A:405:THR:N	2.76	0.41
1:A:474:SER:N	1:A:512:LEU:O	2.53	0.41
1:A:522:LEU:HA	1:A:522:LEU:HD23	1.36	0.41
1:B:343:GLU:CD	1:B:395:ASP:HA	2.44	0.41
1:C:108:PHE:HA	1:C:132:ALA:CB	2.50	0.41
1:C:118:ARG:CA	1:C:212:THR:HB	2.51	0.41
1:D:250:PRO:HA	1:D:255:TRP:CG	2.54	0.41
1:D:264:ASN:HB3	1:D:267:GLY:HA2	2.02	0.41
1:D:339:VAL:HG21	1:D:351:ILE:HG22	2.01	0.41
1:D:474:SER:N	1:D:512:LEU:O	2.53	0.41
1:D:515:ASP:OD1	1:D:516:ALA:N	2.53	0.41
1:D:519:ASN:O	1:D:520:PRO:C	2.59	0.41
1:A:23:GLN:HA	1:A:58:GLY:O	2.21	0.41
1:A:220:ILE:O	1:A:220:ILE:HG22	2.18	0.41
1:A:226:TYR:C	1:A:227:THR:CG2	2.92	0.41
1:B:239:VAL:HG11	1:B:282:LEU:HD22	2.02	0.41
1:D:154:ASP:HB3	2:D:801:NAG:C7	2.48	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:111:ASP:O	1:A:112:VAL:HG13	2.21	0.41
1:B:335:ALA:HB3	3:B:811:NDG:O6	2.15	0.41
1:C:235:ILE:HG21	1:C:235:ILE:HD13	1.84	0.41
1:A:4:ILE:HD13	1:B:2:TRP:HA	2.03	0.41
1:A:7:ILE:O	1:A:96:ILE:HG23	2.20	0.41
1:A:235:ILE:CD1	1:A:287:GLY:HA2	2.50	0.41
1:B:127:VAL:HG22	1:B:128:MET:HG3	2.03	0.41
1:B:347:ARG:HD2	1:B:392:GLY:CA	2.50	0.41
1:C:230:VAL:HG23	1:C:323:VAL:HA	2.03	0.41
1:C:239:VAL:HG11	1:C:282:LEU:HD22	2.02	0.41
1:C:469:TYR:CE2	1:C:470:PRO:HD2	2.54	0.41
1:D:118:ARG:CA	1:D:212:THR:HB	2.51	0.41
1:D:329:ALA:HA	1:D:330:PRO:HD3	1.87	0.41
1:D:367:LEU:H	1:D:367:LEU:HG	1.41	0.41
1:D:490:LYS:O	1:D:490:LYS:CG	2.67	0.41
1:D:502:LEU:HA	1:D:502:LEU:HD23	1.82	0.41
1:A:366:LYS:HG2	1:A:367:LEU:H	1.74	0.41
1:B:252:THR:C	1:B:254:ALA:H	2.28	0.41
1:B:423:THR:CG2	2:B:810:NAG:N2	2.84	0.41
1:C:7:ILE:O	1:C:96:ILE:HG23	2.20	0.41
1:C:127:VAL:HG22	1:C:128:MET:HG3	2.03	0.41
1:C:237:PHE:N	1:C:284:THR:OG1	2.42	0.41
1:C:385:ASN:O	1:C:386:GLY:C	2.62	0.41
1:D:7:ILE:O	1:D:96:ILE:HG23	2.20	0.41
1:D:127:VAL:HG22	1:D:128:MET:HG3	2.03	0.41
1:A:108:PHE:CZ	1:A:191:VAL:HG23	2.56	0.41
1:A:127:VAL:HG22	1:A:128:MET:HG3	2.03	0.41
1:A:297:VAL:HG22	2:A:807:NAG:H62	2.03	0.41
1:A:423:THR:CG2	2:A:810:NAG:N2	2.84	0.41
1:B:230:VAL:HG23	1:B:323:VAL:HA	2.03	0.41
1:D:68:ARG:HD3	1:D:100:ASP:CB	2.51	0.41
1:D:230:VAL:HG23	1:D:323:VAL:HA	2.03	0.41
1:D:505:GLY:H	1:D:529:VAL:HB	1.85	0.41
1:A:252:THR:C	1:A:254:ALA:H	2.28	0.41
1:B:237:PHE:N	1:B:284:THR:OG1	2.42	0.41
1:C:108:PHE:CZ	1:C:191:VAL:HG23	2.56	0.41
1:D:108:PHE:CZ	1:D:191:VAL:HG23	2.56	0.41
1:D:252:THR:C	1:D:254:ALA:H	2.28	0.41
1:D:371:ILE:HA	1:D:410:MET:HB3	2.02	0.41
1:D:439:VAL:HA	1:D:440:PRO:HD3	1.81	0.41
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PRO:O	1:A:235:ILE:HD13	2.21	0.41
1:A:252:THR:O	1:A:255:TRP:N	2.54	0.41
1:A:440:PRO:HB3	1:A:457:LEU:CD2	2.43	0.41
1:B:62:VAL:HG13	1:B:62:VAL:O	2.21	0.41
1:B:108:PHE:HA	1:B:132:ALA:HB2	2.03	0.41
1:B:108:PHE:CZ	1:B:191:VAL:HG23	2.56	0.41
1:B:249:MET:O	1:B:252:THR:CB	2.69	0.41
1:B:297:VAL:HG22	2:B:807:NAG:H62	2.03	0.41
1:C:23:GLN:HB2	1:C:59:TRP:CD2	2.55	0.41
1:C:119:GLU:CG	1:C:214:ALA:HB3	2.51	0.41
1:C:122:GLN:HE21	1:C:122:GLN:HB3	1.58	0.41
1:C:127:VAL:HG13	1:C:128:MET:N	2.25	0.41
1:C:193:ALA:O	1:C:202:SER:HA	2.21	0.41
1:C:231:PRO:O	1:C:288:LEU:HD12	2.20	0.41
1:C:290:PHE:CG	1:C:292:LEU:HB2	2.56	0.41
1:C:423:THR:CG2	2:C:810:NAG:N2	2.84	0.41
1:D:212:THR:CG2	1:D:213:ASP:H	2.32	0.41
1:D:231:PRO:O	1:D:288:LEU:HD12	2.20	0.41
1:D:231:PRO:O	1:D:235:ILE:HD13	2.21	0.41
1:D:290:PHE:CG	1:D:292:LEU:HB2	2.56	0.41
1:D:481:LEU:HA	1:D:481:LEU:HD12	1.50	0.41
1:A:42:GLY:CA	1:A:47:PRO:O	2.69	0.41
1:A:108:PHE:HA	1:A:132:ALA:HB2	2.03	0.41
1:A:193:ALA:O	1:A:202:SER:HA	2.21	0.41
1:A:223:PRO:HB2	1:A:226:TYR:CZ	2.56	0.41
1:A:329:ALA:HA	1:A:330:PRO:HD3	1.87	0.41
1:A:409:ILE:C	1:A:410:MET:HG2	2.46	0.41
1:B:86:SER:HA	1:B:87:PRO:HD3	1.83	0.41
1:B:111:ASP:O	1:B:112:VAL:HG13	2.21	0.41
1:C:249:MET:O	1:C:252:THR:CB	2.69	0.41
1:C:272:THR:O	1:C:281:ILE:HG22	2.21	0.41
1:C:347:ARG:HG3	1:C:392:GLY:N	2.33	0.41
1:C:409:ILE:HD13	3:C:811:NDG:C8	2.52	0.41
1:D:111:ASP:O	1:D:112:VAL:HG13	2.21	0.41
1:D:193:ALA:O	1:D:202:SER:HA	2.21	0.41
1:D:227:THR:C	2:D:812:NAG:O5	2.64	0.41
1:D:239:VAL:HG11	1:D:282:LEU:HD22	2.02	0.41
1:D:423:THR:CG2	2:D:810:NAG:N2	2.84	0.41
1:A:23:GLN:HB2	1:A:59:TRP:CD2	2.55	0.40
1:A:272:THR:O	1:A:281:ILE:HG22	2.21	0.40
1:A:449:ASP:HB2	1:A:531:SER:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LYS:HB3	1:B:62:VAL:CG1	2.52	0.40
1:B:119:GLU:CG	1:B:214:ALA:HB3	2.51	0.40
1:B:226:TYR:HB2	1:B:319:VAL:CG2	2.52	0.40
1:B:474:SER:N	1:B:512:LEU:O	2.54	0.40
1:C:68:ARG:HD3	1:C:100:ASP:CB	2.51	0.40
1:C:226:TYR:HB2	1:C:319:VAL:CG2	2.52	0.40
1:D:119:GLU:CG	1:D:214:ALA:HB3	2.51	0.40
1:A:3:VAL:HG21	1:B:4:ILE:HG13	1.18	0.40
1:A:32:ASN:ND2	1:A:83:GLU:CB	2.62	0.40
1:A:319:VAL:CG1	1:A:320:THR:N	2.84	0.40
1:B:227:THR:C	2:B:812:NAG:O5	2.64	0.40
1:B:272:THR:O	1:B:281:ILE:HG22	2.22	0.40
1:B:409:ILE:C	1:B:410:MET:HG2	2.46	0.40
1:B:438:PRO:HB2	1:B:513:LEU:CD1	2.51	0.40
1:C:252:THR:O	1:C:255:TRP:N	2.54	0.40
1:C:438:PRO:HB2	1:C:513:LEU:CD1	2.51	0.40
1:C:519:ASN:O	1:C:520:PRO:C	2.59	0.40
1:D:62:VAL:O	1:D:62:VAL:HG13	2.21	0.40
1:D:127:VAL:HG13	1:D:128:MET:N	2.25	0.40
1:D:464:ILE:CD1	1:D:465:PRO:N	2.73	0.40
1:D:502:LEU:HD22	1:D:503:LYS:H	1.85	0.40
1:A:259:TYR:O	1:A:260:LYS:CB	2.69	0.40
1:A:502:LEU:HD22	1:A:503:LYS:H	1.86	0.40
1:B:502:LEU:HD22	1:B:503:LYS:H	1.85	0.40
1:C:42:GLY:CA	1:C:47:PRO:O	2.69	0.40
1:C:111:ASP:O	1:C:112:VAL:HG13	2.21	0.40
1:C:222:ASP:H	1:C:243:SER:C	2.30	0.40
1:D:19:LYS:HB3	1:D:62:VAL:HG12	2.03	0.40
1:D:23:GLN:HB2	1:D:59:TRP:CD2	2.55	0.40
1:A:34:VAL:CG1	1:A:80:ALA:HB1	2.52	0.40
1:A:119:GLU:CG	1:A:214:ALA:HB3	2.51	0.40
1:A:226:TYR:HB2	1:A:319:VAL:CG2	2.52	0.40
1:A:237:PHE:N	1:A:284:THR:OG1	2.42	0.40
1:A:451:ASN:C	1:A:534:GLY:HA2	2.46	0.40
1:B:23:GLN:HA	1:B:58:GLY:O	2.21	0.40
1:B:42:GLY:CA	1:B:47:PRO:O	2.69	0.40
1:B:162:LEU:HD13	1:B:179:LEU:HD21	2.04	0.40
1:C:108:PHE:HA	1:C:132:ALA:HB2	2.03	0.40
1:C:316:THR:OG1	2:C:806:NAG:H83	2.21	0.40
1:C:409:ILE:C	1:C:410:MET:HG2	2.46	0.40
1:D:223:PRO:HB2	1:D:226:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:THR:OG1	2:D:806:NAG:H83	2.21	0.40
1:D:385:ASN:O	1:D:385:ASN:ND2	2.55	0.40
1:A:24:ILE:CG2	1:B:1:ASP:N	2.84	0.40
1:A:409:ILE:HD13	3:A:811:NDG:C8	2.51	0.40
1:B:68:ARG:HD3	1:B:100:ASP:CB	2.51	0.40
1:B:193:ALA:O	1:B:202:SER:HA	2.21	0.40
1:B:450:GLN:HG3	1:B:532:CYS:O	2.10	0.40
1:B:483:TRP:CZ2	1:B:507:TYR:CE1	2.87	0.40
1:C:138:ASN:HD22	1:C:138:ASN:N	2.19	0.40
1:C:292:LEU:C	1:C:293:ARG:HG2	2.47	0.40
1:C:385:ASN:O	1:C:385:ASN:ND2	2.55	0.40
1:C:435:ASP:HB2	1:C:436:ASN:H	1.58	0.40
1:C:439:VAL:HA	1:C:440:PRO:HD3	1.81	0.40
1:D:243:SER:C	1:D:244:VAL:HG13	2.47	0.40
1:D:435:ASP:HB2	1:D:436:ASN:H	1.58	0.40
1:D:438:PRO:HB2	1:D:513:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	0	9
1	B	538/880 (61%)	401 (74%)	92 (17%)	45 (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%)	1604 (74%)	368 (17%)	180 (8%)	1	9

All (180) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	B	158	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.

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	192	GLN
1	A	217	ASN
1	A	233	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
1	A	467	ASN
1	A	517	GLN
1	A	519	ASN
1	B	12	ASN
1	B	27	ASN
1	B	32	ASN
1	B	45	ASN
1	B	104	ASN
1	B	110	GLN
1	B	122	GLN
1	B	138	ASN
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

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Mol	Chain	Res	Type
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
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	97	ASN
1	D	104	ASN
1	D	110	GLN
1	D	122	GLN
1	D	138	ASN
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

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Mol	Chain	Res	Type
1	D	385	ASN
1	D	391	ASN
1	D	393	ASN
1	D	404	ASN
1	D	455	GLN
1	D	467	ASN
1	D	517	GLN
1	D	519	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	810	1	14,14,15	0.65	0	17,19,21	1.33	4 (23%)
2	NAG	A	805	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
2	NAG	C	802	1	14,14,15	0.77	1 (7%)	17,19,21	0.85	0
2	NAG	C	902	1	14,14,15	1.14	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	D	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	808	1	14,14,15	0.66	0	17,19,21	0.70	0
2	NAG	A	810	1	14,14,15	0.67	0	17,19,21	1.34	4 (23%)
2	NAG	C	903	1	14,14,15	0.55	0	17,19,21	0.78	0
2	NAG	D	801	1	14,14,15	0.72	0	17,19,21	0.98	1 (5%)
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	B	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.69	1 (5%)
2	NAG	B	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	C	808	1	14,14,15	0.66	0	17,19,21	0.69	0
2	NAG	B	903	1	14,14,15	0.55	0	17,19,21	0.79	0
3	NDG	D	804	1	14,14,15	0.66	0	17,19,21	0.78	0
2	NAG	A	802	1	14,14,15	0.78	1 (7%)	17,19,21	0.85	0
2	NAG	C	904	1	14,14,15	0.79	1 (7%)	17,19,21	0.70	1 (5%)
3	NDG	C	811	1	14,14,15	0.87	0	17,19,21	1.95	1 (5%)
2	NAG	A	902	1	14,14,15	1.14	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	D	812	1	14,14,15	0.84	1 (7%)	17,19,21	0.76	1 (5%)
3	NDG	A	804	1	14,14,15	0.65	0	17,19,21	0.78	0
2	NAG	A	803	1	14,14,15	0.99	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	A	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.93	0
2	NAG	A	806	1	14,14,15	0.56	0	17,19,21	1.38	3 (17%)
2	NAG	B	809	1	14,14,15	0.78	1 (7%)	17,19,21	0.94	0
2	NAG	B	806	1	14,14,15	0.57	0	17,19,21	1.39	3 (17%)
2	NAG	A	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
3	NDG	A	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	B	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
2	NAG	D	808	1	14,14,15	0.66	0	17,19,21	0.69	0
2	NAG	D	810	1	14,14,15	0.66	0	17,19,21	1.33	4 (23%)
2	NAG	D	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	B	801	1	14,14,15	0.69	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	B	902	1	14,14,15	1.13	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	D	802	1	14,14,15	0.77	1 (7%)	17,19,21	0.85	0
2	NAG	B	810	1	14,14,15	0.66	0	17,19,21	1.33	4 (23%)
2	NAG	C	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	D	902	1	14,14,15	1.14	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	A	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	C	807	1	14,14,15	0.64	0	17,19,21	1.20	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	D	903	1	14,14,15	0.55	0	17,19,21	0.78	0
2	NAG	C	801	1	14,14,15	0.71	0	17,19,21	0.98	1 (5%)
3	NDG	C	804	1	14,14,15	0.64	0	17,19,21	0.78	0
3	NDG	D	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	D	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	C	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	C	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	D	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
3	NDG	B	804	1	14,14,15	0.65	0	17,19,21	0.77	0
2	NAG	A	903	1	14,14,15	0.55	0	17,19,21	0.79	0
2	NAG	B	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
3	NDG	B	811	1	14,14,15	0.87	0	17,19,21	1.97	1 (5%)
2	NAG	C	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
2	NAG	A	812	1	14,14,15	0.84	1 (7%)	17,19,21	0.74	1 (5%)
2	NAG	D	806	1	14,14,15	0.56	0	17,19,21	1.39	3 (17%)
2	NAG	D	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	B	808	1	14,14,15	0.67	0	17,19,21	0.69	0
2	NAG	B	805	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)

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

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

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

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NAG	C1-C2	3.42	1.57	1.52
2	C	902	NAG	C1-C2	3.41	1.57	1.52
2	D	902	NAG	C1-C2	3.40	1.57	1.52
2	B	902	NAG	C1-C2	3.35	1.56	1.52
2	C	803	NAG	O5-C5	2.68	1.48	1.43
2	A	803	NAG	O5-C5	2.67	1.48	1.43
2	B	803	NAG	O5-C5	2.66	1.48	1.43
2	D	803	NAG	O5-C5	2.65	1.48	1.43
2	C	904	NAG	C1-C2	-2.48	1.49	1.52
2	D	904	NAG	C1-C2	-2.42	1.49	1.52
2	B	904	NAG	C1-C2	-2.41	1.49	1.52
2	A	904	NAG	C1-C2	-2.40	1.49	1.52
2	C	812	NAG	C1-C2	-2.34	1.49	1.52
2	D	812	NAG	C1-C2	-2.33	1.49	1.52
2	B	812	NAG	C1-C2	-2.31	1.49	1.52
2	A	812	NAG	C1-C2	-2.30	1.49	1.52
2	A	802	NAG	C1-C2	2.13	1.55	1.52
2	B	802	NAG	C1-C2	2.11	1.55	1.52
2	C	802	NAG	C1-C2	2.11	1.55	1.52
2	C	809	NAG	C1-C2	-2.06	1.49	1.52
2	B	809	NAG	C1-C2	-2.06	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	809	NAG	C1-C2	-2.04	1.49	1.52
2	D	809	NAG	C1-C2	-2.03	1.49	1.52
2	D	802	NAG	C1-C2	2.01	1.55	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-7.46	112.91	122.90
3	D	811	NDG	C2-N2-C7	-7.43	112.94	122.90
3	A	811	NDG	C2-N2-C7	-7.43	112.95	122.90
3	C	811	NDG	C2-N2-C7	-7.40	112.99	122.90
2	C	806	NAG	C2-N2-C7	-3.63	118.03	122.90
2	D	806	NAG	C2-N2-C7	-3.63	118.04	122.90
2	B	806	NAG	C2-N2-C7	-3.62	118.05	122.90
2	A	806	NAG	C2-N2-C7	-3.60	118.08	122.90
2	A	805	NAG	C2-N2-C7	-3.16	118.67	122.90
2	B	805	NAG	C2-N2-C7	-3.15	118.68	122.90
2	D	805	NAG	C2-N2-C7	-3.15	118.68	122.90
2	C	805	NAG	C2-N2-C7	-3.13	118.70	122.90
2	D	807	NAG	C2-N2-C7	-3.07	118.79	122.90
2	C	807	NAG	C2-N2-C7	-3.06	118.80	122.90
2	A	807	NAG	C2-N2-C7	-3.05	118.81	122.90
2	B	807	NAG	C2-N2-C7	-3.03	118.84	122.90
2	B	803	NAG	C2-N2-C7	-3.02	118.86	122.90
2	C	803	NAG	C2-N2-C7	-3.02	118.86	122.90
2	A	803	NAG	C2-N2-C7	-3.01	118.86	122.90
2	D	803	NAG	C2-N2-C7	-3.00	118.88	122.90
2	C	810	NAG	C1-C2-N2	2.55	114.45	110.43
2	A	810	NAG	C1-C2-N2	2.54	114.44	110.43
2	B	810	NAG	C1-C2-N2	2.52	114.40	110.43
2	D	810	NAG	C1-C2-N2	2.51	114.39	110.43
2	B	810	NAG	C4-C3-C2	-2.48	107.38	111.02
2	D	810	NAG	C4-C3-C2	-2.47	107.40	111.02
2	A	810	NAG	C4-C3-C2	-2.46	107.41	111.02
2	C	806	NAG	C4-C3-C2	-2.46	107.41	111.02
2	C	810	NAG	C4-C3-C2	-2.46	107.41	111.02
2	D	803	NAG	C1-O5-C5	2.46	115.48	112.19
2	B	806	NAG	C4-C3-C2	-2.45	107.43	111.02
2	C	803	NAG	C1-O5-C5	2.45	115.46	112.19
2	A	803	NAG	C1-O5-C5	2.43	115.45	112.19
2	B	803	NAG	C1-O5-C5	2.43	115.44	112.19
2	D	806	NAG	C4-C3-C2	-2.42	107.47	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	806	NAG	C4-C3-C2	-2.42	107.48	111.02
2	B	810	NAG	O5-C1-C2	-2.37	107.63	111.29
2	D	810	NAG	O5-C1-C2	-2.36	107.63	111.29
2	A	810	NAG	O5-C1-C2	-2.35	107.66	111.29
2	C	810	NAG	O5-C1-C2	-2.33	107.69	111.29
2	C	810	NAG	C1-O5-C5	-2.26	109.16	112.19
2	D	810	NAG	C1-O5-C5	-2.23	109.20	112.19
2	B	810	NAG	C1-O5-C5	-2.23	109.20	112.19
2	A	810	NAG	C1-O5-C5	-2.21	109.22	112.19
2	C	812	NAG	C2-N2-C7	-2.17	119.99	122.90
2	D	812	NAG	C2-N2-C7	-2.17	119.99	122.90
2	B	902	NAG	O5-C1-C2	2.17	114.65	111.29
2	B	812	NAG	C2-N2-C7	-2.16	120.01	122.90
2	B	801	NAG	C1-C2-N2	-2.16	107.03	110.43
2	A	801	NAG	C1-C2-N2	-2.15	107.05	110.43
2	C	801	NAG	C1-C2-N2	-2.15	107.05	110.43
2	A	902	NAG	O5-C1-C2	2.13	114.59	111.29
2	D	801	NAG	C1-C2-N2	-2.13	107.07	110.43
2	C	902	NAG	O5-C1-C2	2.13	114.59	111.29
2	A	812	NAG	C2-N2-C7	-2.12	120.06	122.90
2	D	902	NAG	O5-C1-C2	2.11	114.55	111.29
2	C	807	NAG	O5-C1-C2	-2.09	108.06	111.29
2	B	807	NAG	O5-C1-C2	-2.07	108.08	111.29
2	A	807	NAG	O5-C1-C2	-2.07	108.09	111.29
2	C	904	NAG	C2-N2-C7	-2.05	120.15	122.90
2	D	807	NAG	O5-C1-C2	-2.05	108.12	111.29
2	A	904	NAG	C2-N2-C7	-2.04	120.17	122.90
2	B	904	NAG	C2-N2-C7	-2.03	120.18	122.90
2	D	904	NAG	C2-N2-C7	-2.03	120.18	122.90
2	A	806	NAG	O5-C1-C2	-2.03	108.15	111.29
2	D	902	NAG	C1-O5-C5	2.03	114.91	112.19
2	C	902	NAG	C1-O5-C5	2.03	114.90	112.19
2	D	806	NAG	O5-C1-C2	-2.02	108.16	111.29
2	C	806	NAG	O5-C1-C2	-2.02	108.17	111.29
2	B	806	NAG	O5-C1-C2	-2.01	108.17	111.29

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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atoms
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	807	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	A	802	NAG	C4-C5-C6-O6
2	B	802	NAG	C4-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
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	D	802	NAG	O5-C5-C6-O6
2	A	802	NAG	O5-C5-C6-O6
2	C	802	NAG	O5-C5-C6-O6
2	B	802	NAG	O5-C5-C6-O6
2	A	904	NAG	C4-C5-C6-O6
2	B	904	NAG	C4-C5-C6-O6
2	C	904	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	904	NAG	C4-C5-C6-O6
2	C	805	NAG	C4-C5-C6-O6
2	A	805	NAG	C4-C5-C6-O6
2	B	805	NAG	C4-C5-C6-O6
2	D	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	A	904	NAG	O5-C5-C6-O6
2	B	904	NAG	O5-C5-C6-O6
2	D	904	NAG	O5-C5-C6-O6
2	C	904	NAG	O5-C5-C6-O6
2	C	801	NAG	C4-C5-C6-O6
2	A	801	NAG	C4-C5-C6-O6
2	B	801	NAG	C4-C5-C6-O6
2	D	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	D	903	NAG	C4-C5-C6-O6
2	A	903	NAG	C4-C5-C6-O6
2	B	903	NAG	C4-C5-C6-O6
2	C	903	NAG	C4-C5-C6-O6
2	D	808	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	806	NAG	C4-C5-C6-O6
2	A	808	NAG	C4-C5-C6-O6
2	C	806	NAG	C4-C5-C6-O6
2	B	808	NAG	C4-C5-C6-O6
2	C	808	NAG	C4-C5-C6-O6
2	A	806	NAG	C4-C5-C6-O6
2	D	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	A	801	NAG	O5-C5-C6-O6
2	B	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
2	D	902	NAG	C1-C2-N2-C7
2	B	806	NAG	O5-C5-C6-O6
2	C	806	NAG	O5-C5-C6-O6
2	A	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	D	806	NAG	O5-C5-C6-O6
2	D	812	NAG	C4-C5-C6-O6
2	A	812	NAG	C4-C5-C6-O6
2	C	812	NAG	C4-C5-C6-O6

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

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

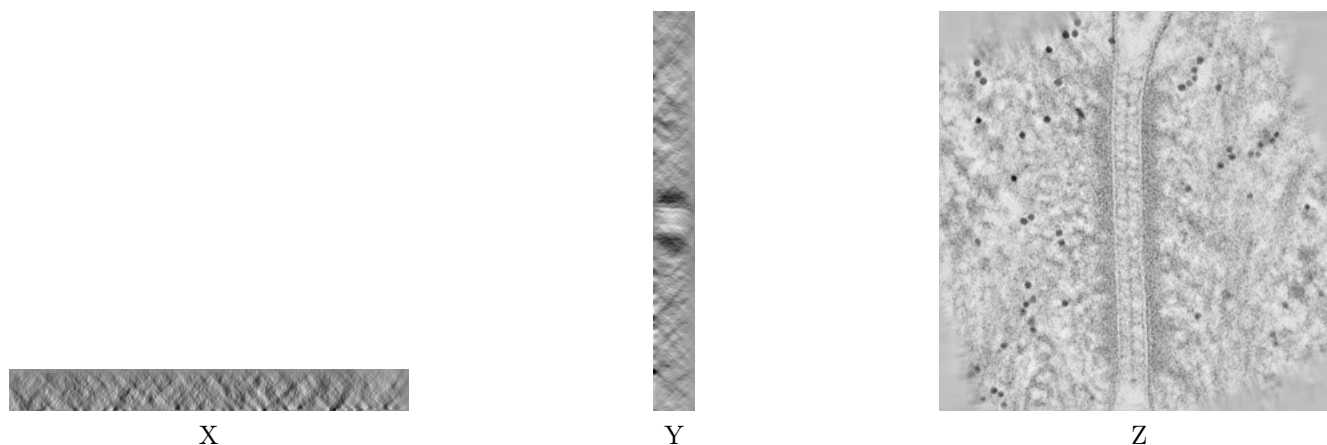
5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Tomogram visualisation [i](#)

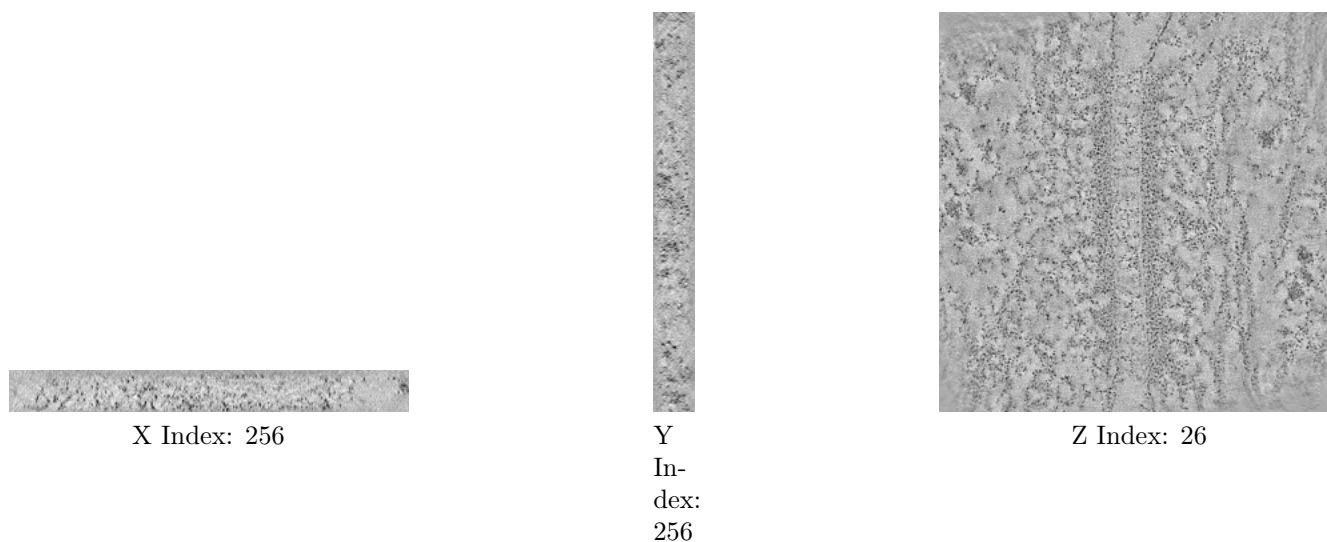
This section contains visualisations of the EMDB entry EMD-1052. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



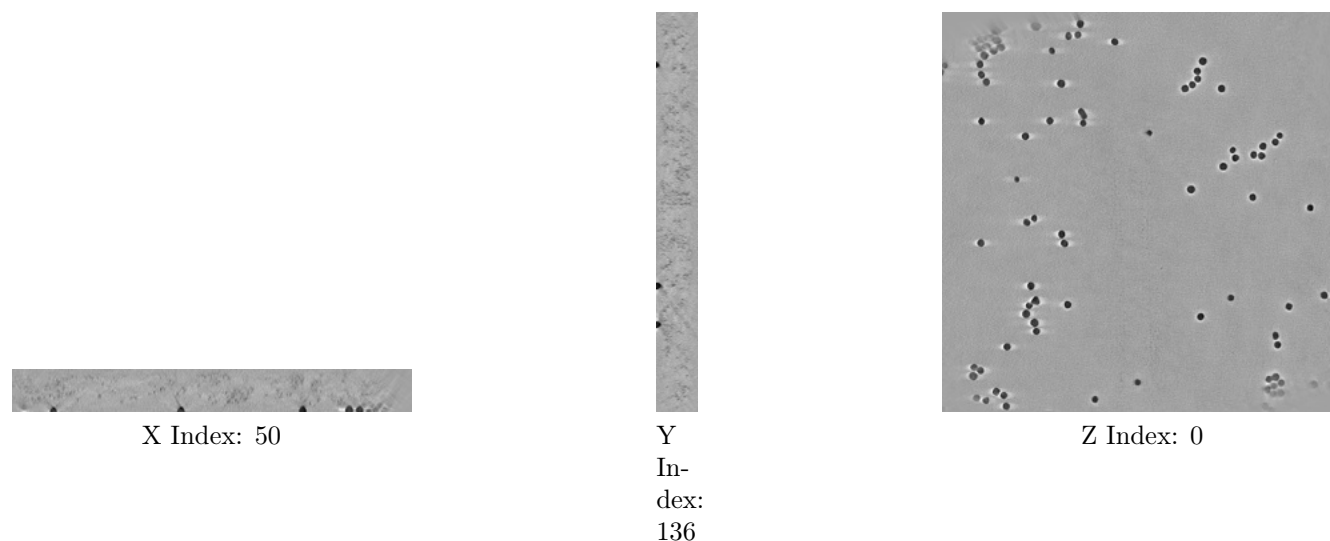
The images above show the tomogram projected in three orthogonal directions.

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.

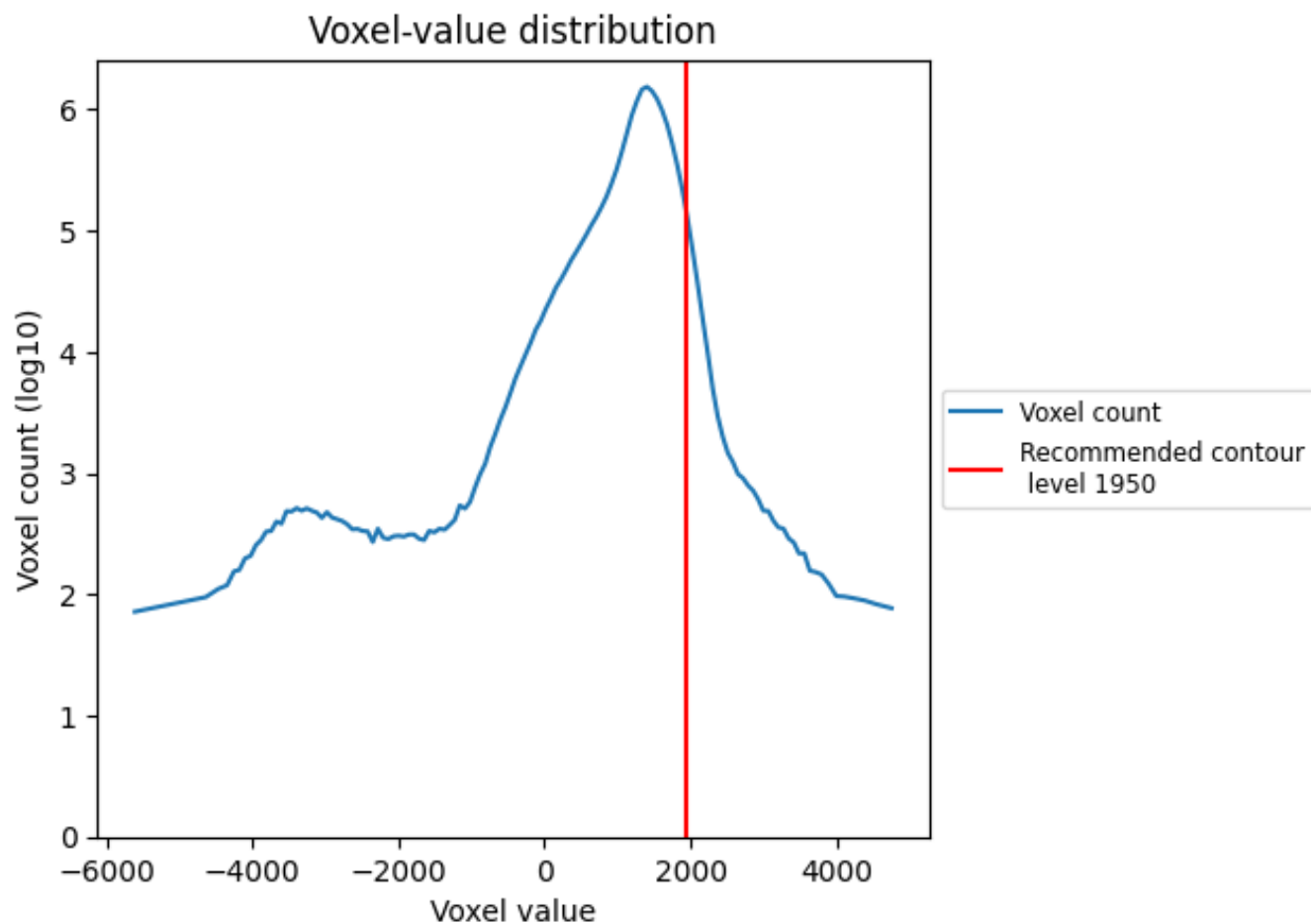
6.5 Mask visualisation [i](#)

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.

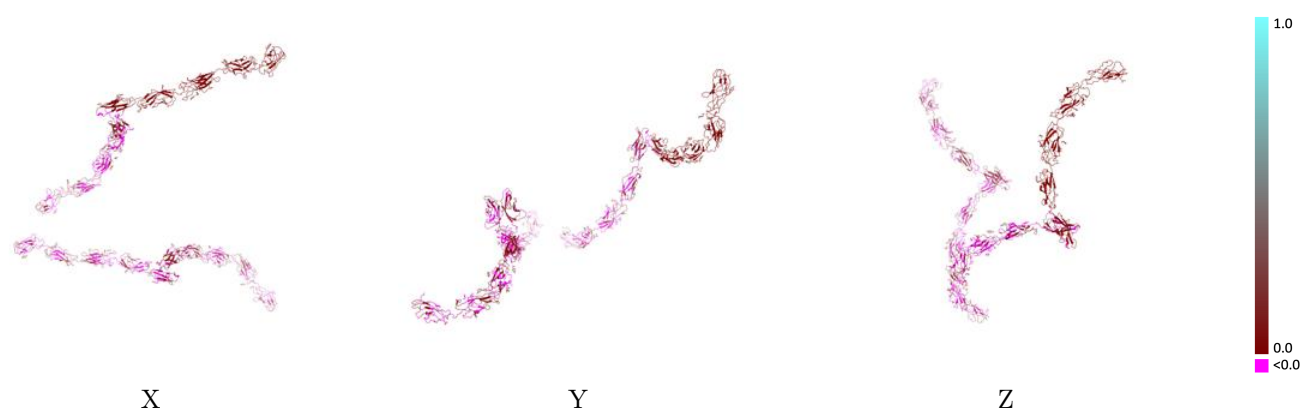
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1052 and PDB model 1Q55. 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](#)

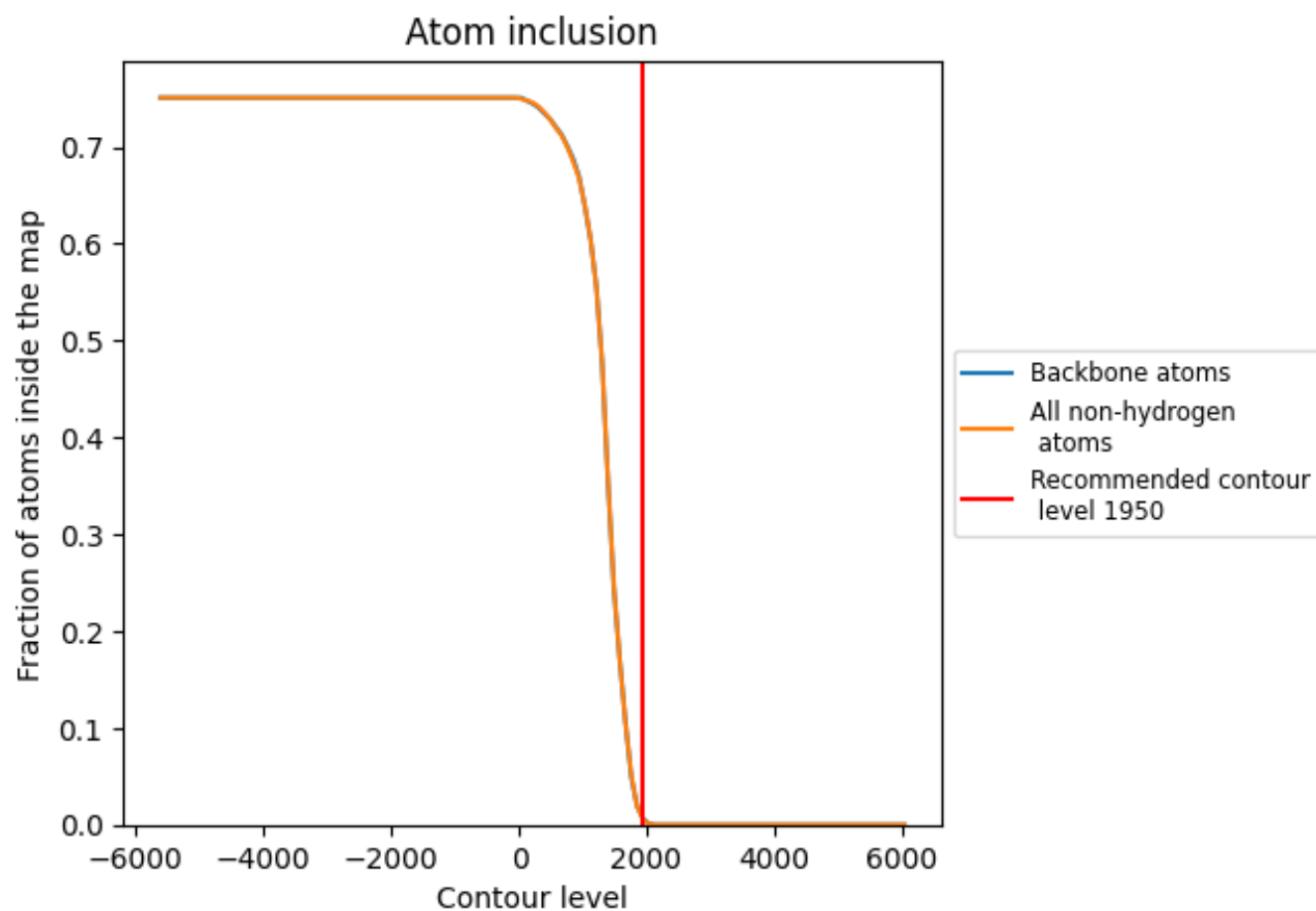


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



At the recommended contour level, 1% of all backbone atoms, 0% 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	0.0050	0.0050
A	0.0130	0.0190
B	0.0010	-0.0010
C	0.0040	0.0010
D	0.0000	-0.0010

