



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:42 PM BST

PDB ID : 1Q55  
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)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

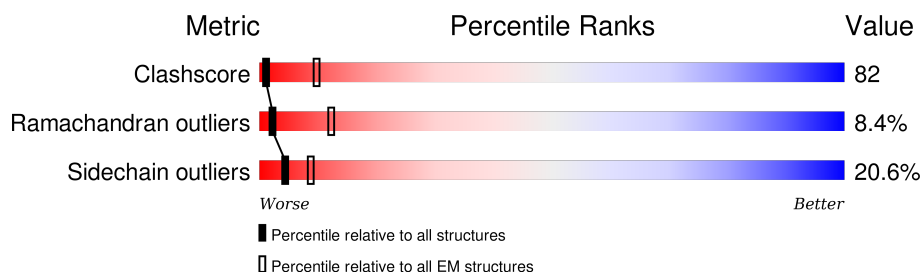
# 1 Overall quality at a glance

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)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	880	16% 30% 11% • 39%
1	B	880	16% 30% 11% • 39%
1	C	880	16% 30% 11% • 39%
1	D	880	17% 30% 11% • 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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-
2	NAG	A	904	-	-	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	904	-	-	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	904	-	-	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	904	-	-	X	-
3	NDG	A	902	-	-	X	-
3	NDG	B	902	-	-	X	-
3	NDG	C	902	-	-	X	-
3	NDG	D	902	-	-	X	-

## 2 Entry composition [i](#)

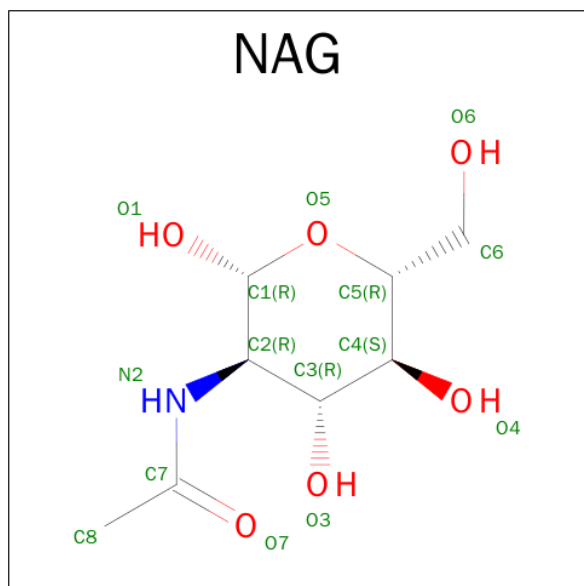
There are 4 unique types of molecules in this entry. The entry contains 17652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	

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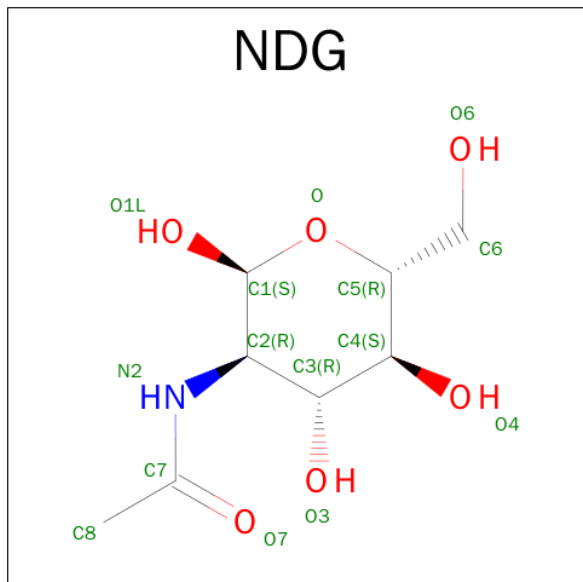
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	C	1	Total	C	N	O	0
			56	32	4	20	
3	C	1	Total	C	N	O	0
			56	32	4	20	
3	C	1	Total	C	N	O	0
			56	32	4	20	

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Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	1	Total	C	N	O	0
			56	32	4	20	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

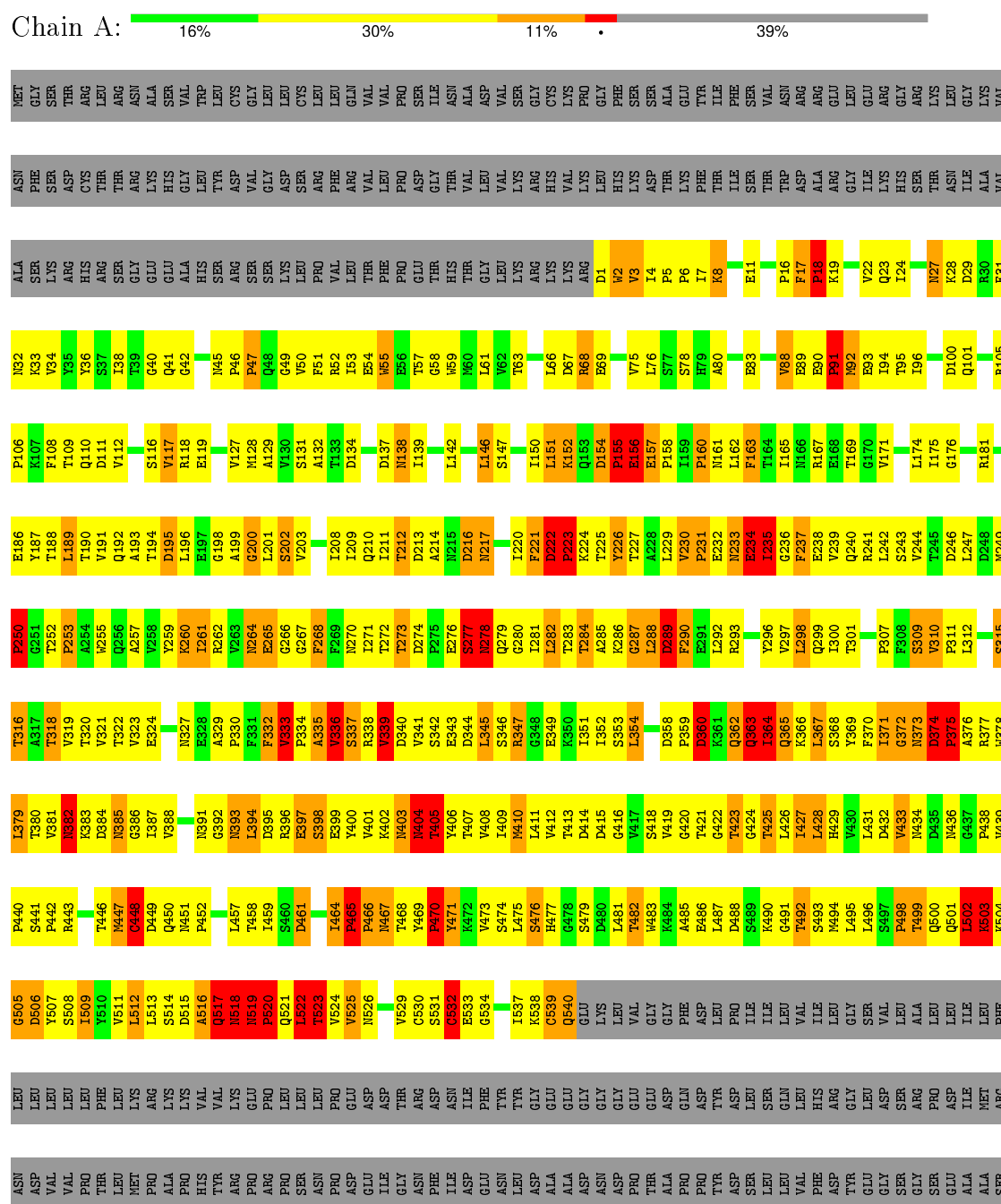
Mol	Chain	Residues	Atoms		AltConf
4	B	12	Total	Ca	0
			12	12	
4	A	12	Total	Ca	0
			12	12	
4	D	12	Total	Ca	0
			12	12	
4	C	12	Total	Ca	0
			12	12	



### 3 Residue-property plots

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



Chain B:  16% 30% 11% • 39%



ALA	ALA	ILE	L502	G437	A376	F311	D246	G176	F31	ALA	ASN	MET
SER	SER	LEU	K503	P438	W377	L312	D247	R181	R105	SER	GLY	GLY
LEU	LEU	PHE	K504	P439	W378	L313	D248	R181	P106	THR	PHE	THR
LEU	LEU	ASN	G505	P440	L379	S315	M249	E186	K107	ARG	ASP	ARG
SER	SER	LEU	D506	S441	L380	T316	P250	E187	F108	HIS	CYS	LEU
SER	SER	VAL	Y507	P442	W381	K317	T252	Y187	T109	ARG	THR	LEU
LEU	LEU	VAL	S508	R443	K382	T318	P253	L189	Q110	SER	THR	LEU
LEU	LEU	PRO	L509	L443	K383	T319	P254	T189	D111	GLY	ARG	ASN
THR	THR	PHE	Y510	T446	D384	T320	A254	T190	V112	LYS	LYS	ALA
SER	SER	LEU	W511	M447	D385	T321	A255	Y191	Q41	GLU	HIS	SER
LEU	LEU	LYS	L512	C448	K386	T322	Q256	Q192	S116	ALA	GLY	VAL
ASN	ASN	MET	L513	D449	L387	T323	A257	A193	V117	HIS	LEU	TRP
PRO	PRO	ARG	L514	D450	W388	E324	Z258	A193	R118	ASP	TYR	LEU
ASN	ASN	LYS	S514	Q450	L389	E325	Z259	D195	E119	ARG	ASP	CYS
ASP	ASP	PRO	D515	M451	L390	E326	Z260	L196	P47	SER	VAL	GLY
GLU	GLU	HIS	A516	P452	N391	N327	L261	E197	Q122	SER	GLY	LEU
VAL	VAL	TYR	Q517	G392	K393	P330	R262	G198	V127	LYS	ASP	LEU
ASP	ASP	ARG	W518	L457	L394	F331	P263	A199	M128	LEU	SER	CYS
TRP	TRP	PRO	N519	T458	D395	F332	M264	G200	F51	PRO	ARG	LEU
ASN	ASN	ARG	P520	L459	K396	F333	E265	L201	A129	PHE	VAL	LEU
ASN	ASN	LEU	Q521	S460	K397	P334	G266	E202	V130	ARG	GLN	LEU
LEU	LEU	SER	L522	D461	S398	P335	G267	Y203	S131	THR	VAL	VAL
SER	SER	ASN	T523	R462	K399	F336	P268		A132	PHE	LEU	VAL
ASP	ASP	PRO	W524	L464	E400	S337	F269	T208	T133	PRO	PRO	PRO
TRP	TRP	GLU	V525	P465	V401	R338	M270	L209	D134	GLU	ASP	ASN
GLY	GLY	ASP	N526	P466	K402	F339	L271	Q210	F57	THR	GLY	ILE
SER	SER	ILE	Q527	M467	N403	D340	T272	T211	D137	HIS	THR	ASN
GLY	GLY	THR	W529	T468	K404	D341	T273	T212	N138	THR	VAL	ALA
ASN	ASN	ARG	C530	Y469	N405	S342	D274	D213	L139	GLY	LEU	VAL
PHE	PHE	ASN	S531	P470	T406	E343	Z275	K214	V62	LEU	VAL	VAL
ASN	ASN	ILE	C532	Y471	L407	D344	E276	M215	L142	LYS	VAL	VAL
ILE	ILE	ASN	E533	K472	V408	L345	S277	D216		ARG	LYS	SER
ASP	ASP	ILE	G534	S474	I409	S346	N278	N217	L146	ARG	ARG	GLY
GLU	GLU	PHE	Q535	L475	M410	R347	Q279	N217	S147	HIS	VAL	CYS
ASN	ASN	TYR	W537	L475	L411	G348	G280		L147	LYS	HIS	LYS
GLY	GLY	GLY	K538	S476	V412	E349	L281	T220	D148	LYS	PRO	GLY
ALA	ALA	GLU	C539	H477	V413	F350	L282	F221	I150	ARG	LEU	PRO
ALA	ALA	GLU	Q540	G478	T413	K350	L282	F222	L151	W2	HIS	PHE
ASP	ASP	GLY	L541	S479	D414	T351	T283	P223	K152	V3	LYS	SER
ASP	ASP	GLY	L542	D480	D415	T352	T284	K224	Q153	I4	ASP	SER
ASP	ASP	GLY	L543	L481	K416	S353	A285	T225	L76	P5	THR	ALA
GLU	GLU	PRO	W544	T482	V417	L354	K286	Y226	S77	P6	LYS	GLU
GLU	GLU	GLU	VAL	P482	G417		G287	T227	E156	I7	PHE	TYR
GLY	GLY	GLU	L545	L483	S418		L288	K228	A157	K8	THR	ILE
ALA	ALA	ASP	GLY	K484	V419	D358	L288	K228	E157		ILE	PHE
PRO	PRO	GLN	PHE	L485	G420	P359	L229	L229	P158		THR	SER
PRO	PRO	GLN	ASP	E486	T421	D360	F290	V230	E159		THR	SER
PRO	PRO	TYR	LEU	L487	G422	K361	E291	P231	P160	E11	THR	VAL
ASP	ASP	ASP	PRO	D488	T423	Q362	L292	E232	N161		THR	ASN
ILE	ILE	LEU	ILE	S489	G424	Q363	R293	E233	L162	P16	TRP	ASN
SER	SER	LEU	LEU	K490	T425	K364		E234	F163	F17	ASP	ARG
LEU	LEU	SER	LEU	R491	L426	Q365	Y296	E236	E39	ALA	ASP	ARG
LEU	LEU	GLN	VAL	T492	L427	K366	V297	G236	T164	ARG	GLY	LEU
VAL	VAL	LEU	VAL	G493	L428	L367	G298	G237	E30	GLY	LEU	GLU
PHE	PHE	HIS	LEU	M494	L429	K368	Q299	E238	N166	V22	ILE	GLU
ASP	ASP	ASP	LEU	A494	H429	S368	Q299	E238	R167	Q23	LYS	ARG
GLY	GLY	TYR	GLY	L495	W430	V369	I300	V239	E168	I24	HIS	GLY
GLY	GLY	GLY	GLY	L496	L431	F370	I301	Q240	T169	K25	SER	ARG
GLU	GLU	LEU	VAL	S497	L432	T371		K241	G170	S26	THR	LYS
ASP	ASP	GLY	VAL	L497	D432	N372		L242	V171	N27	ASN	LEU
LEU	LEU	ASP	LEU	S498	V433	K373	P307	L243		K28	ILE	GLY
GLY	GLY	ARG	ALA	T499	N434	N374	F308	S243	L174	D29	VAL	VAL
PRO	PRO	PRO	GLY	Q500	W435	D374	S309	V244	D100	E30	ALA	GLY
GLY	GLY	GLU	LEU	L501	P436	E275	Q340	V245	G101		VAL	VAL

- Molecule 1: EP-cadherin

Chain D: 

ASN	PHE	SER	ASP	CYS	THR	THR	THR	ARG	LYS	HIS	GLY	LEU	GLY	SER	VAL	TRP	LEU	CYS	GLY	VAL	GLN	VAL	PRO	ASP	GLY	ILE	ASN	ALA	ASP	VAL	SER	GLY	CYS	LYS	PRO	GLY	PHE	SER	SER	ALA	GLU	TYR	ILE	PHE	SER	VAL	ASN	ARG	GLU	LEU	GLU	ARG	GLY	LYS	ASN	LEU	GLY	LYS	VAL
MET	GLY	SER	THR	ARG	LEU	ARG	ASN	ALA	SER	VAL	TRP	LEU	CYS	GLY	VAL	GLN	VAL	PRO	ASP	GLY	ILE	ASN	ALA	ASP	VAL	SER	GLY	CYS	LYS	PRO	GLY	PHE	SER	SER	ALA	GLU	TYR	ILE	PHE	SER	VAL	ASN	ARG	GLU	LEU	GLU	ARG	GLY	LYS	ASN	LEU	GLY	LYS	VAL					




## 4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
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 ( $e^-/\text{\AA}^2$ )	120000	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	50000	Depositor
Image detector	GATAN 794	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
1	B	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
1	C	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
1	D	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
All	All	0.70	32/17104 (0.2%)	1.39	312/23356 (1.3%)

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

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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	ALA	CA-CB	-8.36	1.34	1.52
1	C	335	ALA	CA-CB	-8.34	1.34	1.52
1	A	335	ALA	CA-CB	-8.33	1.34	1.52
1	D	335	ALA	CA-CB	-8.33	1.34	1.52
1	D	539	CYS	CB-SG	8.16	1.96	1.82
1	B	539	CYS	CB-SG	8.16	1.96	1.82
1	A	539	CYS	CB-SG	8.14	1.96	1.82
1	C	539	CYS	CB-SG	8.14	1.96	1.82
1	C	223	PRO	CG-CD	7.02	1.73	1.50
1	D	223	PRO	CG-CD	7.02	1.73	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	PRO	CG-CD	6.99	1.73	1.50
1	B	223	PRO	CG-CD	6.99	1.73	1.50
1	D	523	THR	N-CA	-6.25	1.33	1.46
1	C	523	THR	N-CA	-6.24	1.33	1.46
1	A	523	THR	N-CA	-6.23	1.33	1.46
1	B	523	THR	N-CA	-6.21	1.33	1.46
1	A	522	LEU	N-CA	-5.99	1.34	1.46
1	C	522	LEU	N-CA	-5.99	1.34	1.46
1	D	522	LEU	N-CA	-5.98	1.34	1.46
1	C	18	PRO	N-CD	5.97	1.56	1.47
1	B	522	LEU	N-CA	-5.96	1.34	1.46
1	D	18	PRO	N-CD	5.93	1.56	1.47
1	B	18	PRO	N-CD	5.91	1.56	1.47
1	A	18	PRO	N-CD	5.88	1.56	1.47
1	A	530	CYS	CB-SG	5.53	1.91	1.82
1	B	530	CYS	CB-SG	5.52	1.91	1.82
1	C	530	CYS	CB-SG	5.49	1.91	1.82
1	D	530	CYS	CB-SG	5.45	1.91	1.82
1	B	499	THR	CA-CB	5.05	1.66	1.53
1	A	499	THR	CA-CB	5.04	1.66	1.53
1	C	499	THR	CA-CB	5.03	1.66	1.53
1	D	499	THR	CA-CB	5.02	1.66	1.53

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	520	PRO	CA-C-N	-13.29	87.96	117.20
1	A	520	PRO	CA-C-N	-13.29	87.96	117.20
1	D	520	PRO	CA-C-N	-13.27	88.01	117.20
1	C	520	PRO	CA-C-N	-13.27	88.02	117.20
1	C	235	ILE	N-CA-C	12.74	145.40	111.00
1	C	290	PHE	N-CA-C	12.74	145.40	111.00
1	B	235	ILE	N-CA-C	12.74	145.39	111.00
1	A	290	PHE	N-CA-C	12.73	145.38	111.00
1	D	290	PHE	N-CA-C	12.73	145.38	111.00
1	A	235	ILE	N-CA-C	12.72	145.34	111.00
1	B	290	PHE	N-CA-C	12.72	145.35	111.00
1	D	235	ILE	N-CA-C	12.71	145.32	111.00
1	B	374	ASP	N-CA-C	11.62	142.38	111.00
1	D	374	ASP	N-CA-C	11.62	142.38	111.00
1	A	374	ASP	N-CA-C	11.60	142.32	111.00
1	C	374	ASP	N-CA-C	11.59	142.29	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	C	398	SER	N-CA-C	11.38	141.74	111.00
1	B	398	SER	N-CA-C	11.37	141.69	111.00
1	D	398	SER	N-CA-C	11.37	141.69	111.00
1	A	398	SER	N-CA-C	11.36	141.67	111.00
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	222	ASP	CB-CG-OD2	10.09	127.39	118.30
1	A	222	ASP	CB-CG-OD2	10.09	127.38	118.30
1	C	222	ASP	CB-CG-OD2	10.05	127.34	118.30
1	D	222	ASP	CB-CG-OD2	10.00	127.30	118.30
1	C	236	GLY	N-CA-C	-9.99	88.12	113.10
1	A	236	GLY	N-CA-C	-9.99	88.13	113.10
1	B	236	GLY	N-CA-C	-9.97	88.17	113.10
1	D	236	GLY	N-CA-C	-9.97	88.17	113.10
1	D	230	VAL	C-N-CD	-9.96	98.69	120.60
1	A	230	VAL	C-N-CD	-9.95	98.71	120.60
1	C	230	VAL	C-N-CD	-9.94	98.72	120.60
1	B	230	VAL	C-N-CD	-9.94	98.73	120.60
1	D	374	ASP	CB-CA-C	-9.68	91.05	110.40
1	C	376	ALA	N-CA-C	9.67	137.12	111.00
1	B	376	ALA	N-CA-C	9.67	137.11	111.00
1	B	374	ASP	CB-CA-C	-9.66	91.07	110.40
1	D	376	ALA	N-CA-C	9.66	137.09	111.00
1	C	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	A	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	A	376	ALA	N-CA-C	9.63	137.01	111.00
1	D	522	LEU	CA-CB-CG	-9.39	93.71	115.30
1	C	522	LEU	CA-CB-CG	-9.37	93.75	115.30
1	B	522	LEU	CA-CB-CG	-9.37	93.76	115.30
1	A	522	LEU	CA-CB-CG	-9.36	93.78	115.30
1	D	520	PRO	N-CA-C	9.31	136.32	112.10
1	B	223	PRO	N-CA-C	-9.30	87.91	112.10
1	D	223	PRO	N-CA-C	-9.30	87.91	112.10
1	A	221	PHE	C-N-CA	-9.30	98.44	121.70
1	B	221	PHE	C-N-CA	-9.30	98.45	121.70
1	C	223	PRO	N-CA-C	-9.30	87.91	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	PRO	N-CA-C	9.30	136.27	112.10
1	C	221	PHE	C-N-CA	-9.30	98.46	121.70
1	C	481	LEU	N-CA-C	-9.29	85.91	111.00
1	B	481	LEU	N-CA-C	-9.29	85.92	111.00
1	B	520	PRO	N-CA-C	9.29	136.25	112.10
1	D	481	LEU	N-CA-C	-9.29	85.92	111.00
1	A	223	PRO	N-CA-C	-9.28	87.96	112.10
1	A	481	LEU	N-CA-C	-9.28	85.94	111.00
1	C	520	PRO	N-CA-C	9.28	136.23	112.10
1	D	221	PHE	C-N-CA	-9.28	98.49	121.70
1	C	481	LEU	CA-CB-CG	-8.77	95.12	115.30
1	B	481	LEU	CA-CB-CG	-8.76	95.16	115.30
1	D	481	LEU	CA-CB-CG	-8.75	95.17	115.30
1	A	481	LEU	CA-CB-CG	-8.73	95.21	115.30
1	B	289	ASP	C-N-CA	-8.43	100.62	121.70
1	A	289	ASP	C-N-CA	-8.42	100.65	121.70
1	C	289	ASP	C-N-CA	-8.42	100.66	121.70
1	D	289	ASP	C-N-CA	-8.41	100.68	121.70
1	A	516	ALA	N-CA-C	-8.36	88.42	111.00
1	D	516	ALA	N-CA-C	-8.36	88.44	111.00
1	B	516	ALA	N-CA-C	-8.35	88.45	111.00
1	C	516	ALA	N-CA-C	-8.35	88.47	111.00
1	D	222	ASP	C-N-CD	-8.21	102.54	120.60
1	C	222	ASP	C-N-CD	-8.21	102.55	120.60
1	B	222	ASP	C-N-CD	-8.20	102.56	120.60
1	A	222	ASP	C-N-CD	-8.20	102.57	120.60
1	A	290	PHE	CA-C-N	-8.19	99.18	117.20
1	B	290	PHE	CA-C-N	-8.19	99.19	117.20
1	C	290	PHE	CA-C-N	-8.18	99.21	117.20
1	D	290	PHE	CA-C-N	-8.17	99.23	117.20
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
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	233	ASN	N-CA-C	7.87	132.26	111.00
1	D	233	ASN	N-CA-C	7.87	132.24	111.00
1	B	233	ASN	N-CA-C	7.86	132.23	111.00
1	C	233	ASN	N-CA-C	7.86	132.23	111.00
1	A	336	VAL	N-CA-C	7.82	132.12	111.00
1	B	336	VAL	N-CA-C	7.81	132.09	111.00
1	B	522	LEU	C-N-CA	-7.81	102.18	121.70
1	C	522	LEU	C-N-CA	-7.80	102.19	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	336	VAL	N-CA-C	7.80	132.07	111.00
1	A	522	LEU	C-N-CA	-7.80	102.19	121.70
1	D	522	LEU	C-N-CA	-7.80	102.19	121.70
1	C	336	VAL	N-CA-C	7.80	132.05	111.00
1	D	362	GLN	N-CA-C	-7.72	90.15	111.00
1	C	362	GLN	N-CA-C	-7.72	90.17	111.00
1	B	362	GLN	N-CA-C	-7.71	90.17	111.00
1	A	362	GLN	N-CA-C	-7.70	90.21	111.00
1	C	234	GLU	N-CA-C	-7.59	90.51	111.00
1	A	234	GLU	N-CA-C	-7.58	90.52	111.00
1	B	234	GLU	N-CA-C	-7.58	90.52	111.00
1	D	234	GLU	N-CA-C	-7.58	90.53	111.00
1	D	234	GLU	C-N-CA	7.43	140.27	121.70
1	A	234	GLU	C-N-CA	7.42	140.26	121.70
1	C	234	GLU	C-N-CA	7.42	140.25	121.70
1	B	234	GLU	C-N-CA	7.39	140.17	121.70
1	A	521	GLN	C-N-CA	-7.37	103.27	121.70
1	B	521	GLN	C-N-CA	-7.37	103.27	121.70
1	D	521	GLN	C-N-CA	-7.37	103.28	121.70
1	C	521	GLN	C-N-CA	-7.35	103.33	121.70
1	A	277	SER	N-CA-C	-7.21	91.54	111.00
1	B	277	SER	N-CA-C	-7.19	91.58	111.00
1	D	277	SER	N-CA-C	-7.19	91.58	111.00
1	C	277	SER	N-CA-C	-7.19	91.58	111.00
1	A	337	SER	N-CA-C	-7.17	91.64	111.00
1	C	337	SER	N-CA-C	-7.17	91.65	111.00
1	B	337	SER	N-CA-C	-7.16	91.66	111.00
1	D	337	SER	N-CA-C	-7.16	91.66	111.00
1	C	503	LYS	N-CA-C	7.02	129.94	111.00
1	A	503	LYS	N-CA-C	7.01	129.94	111.00
1	B	503	LYS	N-CA-C	7.01	129.93	111.00
1	D	503	LYS	N-CA-C	7.00	129.90	111.00
1	D	523	THR	N-CA-CB	-6.95	97.10	110.30
1	A	523	THR	N-CA-CB	-6.94	97.12	110.30
1	C	523	THR	N-CA-CB	-6.94	97.12	110.30
1	B	523	THR	N-CA-CB	-6.93	97.12	110.30
1	D	492	THR	N-CA-C	6.80	129.35	111.00
1	A	492	THR	N-CA-C	6.78	129.29	111.00
1	C	492	THR	N-CA-C	6.77	129.29	111.00
1	B	492	THR	N-CA-C	6.76	129.27	111.00
1	B	448	CYS	CA-CB-SG	-6.70	101.95	114.00
1	A	448	CYS	CA-CB-SG	-6.69	101.95	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	CYS	CA-CB-SG	-6.69	101.96	114.00
1	D	448	CYS	CA-CB-SG	-6.68	101.98	114.00
1	D	476	SER	N-CA-C	6.58	128.78	111.00
1	A	398	SER	C-N-CA	-6.58	105.25	121.70
1	C	476	SER	N-CA-C	6.58	128.76	111.00
1	B	476	SER	N-CA-C	6.57	128.74	111.00
1	C	398	SER	C-N-CA	-6.57	105.28	121.70
1	D	398	SER	C-N-CA	-6.57	105.28	121.70
1	A	476	SER	N-CA-C	6.56	128.72	111.00
1	B	398	SER	C-N-CA	-6.56	105.29	121.70
1	C	491	GLY	N-CA-C	6.54	129.45	113.10
1	B	491	GLY	N-CA-C	6.54	129.44	113.10
1	D	491	GLY	N-CA-C	6.53	129.42	113.10
1	A	491	GLY	N-CA-C	6.52	129.41	113.10
1	B	525	VAL	N-CA-C	-6.51	93.43	111.00
1	D	525	VAL	N-CA-C	-6.50	93.44	111.00
1	A	525	VAL	N-CA-C	-6.50	93.45	111.00
1	C	525	VAL	N-CA-C	-6.50	93.46	111.00
1	B	335	ALA	N-CA-C	-6.33	93.90	111.00
1	D	335	ALA	N-CA-C	-6.33	93.91	111.00
1	A	335	ALA	N-CA-C	-6.32	93.94	111.00
1	C	532	CYS	N-CA-C	6.32	128.05	111.00
1	A	532	CYS	N-CA-C	6.31	128.03	111.00
1	B	532	CYS	N-CA-C	6.31	128.03	111.00
1	C	335	ALA	N-CA-C	-6.31	93.97	111.00
1	D	532	CYS	N-CA-C	6.29	127.98	111.00
1	B	234	GLU	CA-C-N	-6.29	103.37	117.20
1	D	234	GLU	CA-C-N	-6.28	103.39	117.20
1	A	234	GLU	CA-C-N	-6.25	103.44	117.20
1	C	234	GLU	CA-C-N	-6.25	103.44	117.20
1	A	235	ILE	CA-C-N	-6.16	103.88	116.20
1	D	222	ASP	N-CA-C	6.16	127.63	111.00
1	B	222	ASP	N-CA-C	6.16	127.62	111.00
1	C	222	ASP	N-CA-C	6.15	127.61	111.00
1	A	222	ASP	N-CA-C	6.15	127.61	111.00
1	A	397	GLU	C-N-CA	-6.14	106.36	121.70
1	D	235	ILE	CA-C-N	-6.14	103.93	116.20
1	B	235	ILE	CA-C-N	-6.13	103.93	116.20
1	D	397	GLU	C-N-CA	-6.13	106.38	121.70
1	C	235	ILE	CA-C-N	-6.12	103.96	116.20
1	B	397	GLU	C-N-CA	-6.12	106.41	121.70
1	C	397	GLU	C-N-CA	-6.11	106.43	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	B	503	LYS	CB-CA-C	-6.10	98.20	110.40
1	A	503	LYS	CB-CA-C	-6.10	98.21	110.40
1	B	18	PRO	CA-N-CD	-6.09	102.98	111.50
1	C	503	LYS	CB-CA-C	-6.08	98.24	110.40
1	D	503	LYS	CB-CA-C	-6.08	98.24	110.40
1	D	18	PRO	CA-N-CD	-6.07	103.00	111.50
1	C	502	LEU	N-CA-C	6.05	127.35	111.00
1	D	502	LEU	N-CA-C	6.05	127.35	111.00
1	B	502	LEU	N-CA-C	6.05	127.33	111.00
1	A	502	LEU	N-CA-C	6.03	127.29	111.00
1	C	2	TRP	N-CA-C	-6.02	94.74	111.00
1	A	2	TRP	N-CA-C	-6.02	94.74	111.00
1	B	2	TRP	N-CA-C	-6.01	94.76	111.00
1	D	2	TRP	N-CA-C	-6.01	94.77	111.00
1	A	374	ASP	C-N-CD	5.98	140.95	128.40
1	B	374	ASP	C-N-CD	5.97	140.94	128.40
1	B	222	ASP	N-CA-CB	5.96	121.33	110.60
1	D	222	ASP	N-CA-CB	5.96	121.33	110.60
1	C	374	ASP	C-N-CD	5.96	140.91	128.40
1	D	374	ASP	C-N-CD	5.96	140.91	128.40
1	A	222	ASP	N-CA-CB	5.95	121.31	110.60
1	C	222	ASP	N-CA-CB	5.94	121.30	110.60
1	A	364	ILE	N-CA-C	-5.92	95.01	111.00
1	C	364	ILE	N-CA-C	-5.92	95.03	111.00
1	B	364	ILE	N-CA-C	-5.90	95.06	111.00
1	D	364	ILE	N-CA-C	-5.90	95.06	111.00
1	A	382	ASN	N-CA-C	-5.83	95.26	111.00
1	D	382	ASN	N-CA-C	-5.83	95.26	111.00
1	A	376	ALA	CA-C-N	-5.82	104.39	117.20
1	C	382	ASN	N-CA-C	-5.82	95.29	111.00
1	B	382	ASN	N-CA-C	-5.82	95.29	111.00
1	C	376	ALA	CA-C-N	-5.81	104.42	117.20
1	B	376	ALA	CA-C-N	-5.81	104.43	117.20
1	D	376	ALA	CA-C-N	-5.79	104.45	117.20
1	B	471	TYR	N-CA-C	5.74	126.50	111.00
1	C	471	TYR	N-CA-C	5.73	126.47	111.00
1	D	471	TYR	N-CA-C	5.72	126.45	111.00
1	A	471	TYR	N-CA-C	5.71	126.42	111.00
1	A	481	LEU	CA-C-N	-5.70	104.65	117.20
1	C	481	LEU	CA-C-N	-5.69	104.69	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	LEU	CA-C-N	-5.68	104.70	117.20
1	D	481	LEU	CA-C-N	-5.68	104.70	117.20
1	A	374	ASP	C-N-CA	-5.67	98.17	122.00
1	B	374	ASP	C-N-CA	-5.67	98.19	122.00
1	C	374	ASP	C-N-CA	-5.66	98.24	122.00
1	D	374	ASP	C-N-CA	-5.66	98.25	122.00
1	C	403	ASN	N-CA-C	-5.64	95.78	111.00
1	D	403	ASN	N-CA-C	-5.63	95.79	111.00
1	A	403	ASN	N-CA-C	-5.63	95.79	111.00
1	B	403	ASN	N-CA-C	-5.63	95.80	111.00
1	D	221	PHE	CA-C-N	5.58	129.48	117.20
1	C	221	PHE	CA-C-N	5.57	129.46	117.20
1	A	505	GLY	N-CA-C	5.57	127.01	113.10
1	B	221	PHE	CA-C-N	5.57	129.44	117.20
1	B	505	GLY	N-CA-C	5.57	127.01	113.10
1	D	505	GLY	N-CA-C	5.57	127.01	113.10
1	A	221	PHE	CA-C-N	5.55	129.41	117.20
1	C	505	GLY	N-CA-C	5.55	126.98	113.10
1	C	502	LEU	CB-CA-C	-5.54	99.68	110.20
1	D	502	LEU	CB-CA-C	-5.54	99.68	110.20
1	B	502	LEU	CB-CA-C	-5.53	99.70	110.20
1	A	502	LEU	CB-CA-C	-5.51	99.72	110.20
1	D	157	GLU	C-N-CD	-5.49	108.53	120.60
1	C	157	GLU	C-N-CD	-5.47	108.56	120.60
1	B	157	GLU	C-N-CD	-5.46	108.58	120.60
1	A	157	GLU	C-N-CD	-5.45	108.61	120.60
1	C	519	ASN	N-CA-C	5.35	125.44	111.00
1	B	519	ASN	N-CA-C	5.35	125.43	111.00
1	D	519	ASN	N-CA-C	5.35	125.44	111.00
1	A	519	ASN	N-CA-C	5.34	125.41	111.00
1	B	405	THR	N-CA-C	5.32	125.38	111.00
1	A	405	THR	N-CA-C	5.31	125.34	111.00
1	C	405	THR	N-CA-C	5.31	125.34	111.00
1	D	405	THR	N-CA-C	5.31	125.33	111.00
1	C	367	LEU	CA-CB-CG	-5.30	103.10	115.30
1	B	367	LEU	CA-CB-CG	-5.30	103.12	115.30
1	A	367	LEU	CA-CB-CG	-5.29	103.13	115.30
1	D	367	LEU	CA-CB-CG	-5.29	103.14	115.30
1	B	290	PHE	O-C-N	5.22	131.06	122.70
1	A	521	GLN	N-CA-C	-5.21	96.92	111.00
1	D	521	GLN	N-CA-C	-5.21	96.94	111.00
1	C	521	GLN	N-CA-C	-5.20	96.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	521	GLN	N-CA-C	-5.20	96.96	111.00
1	A	290	PHE	O-C-N	5.18	130.99	122.70
1	C	290	PHE	O-C-N	5.18	131.00	122.70
1	D	520	PRO	C-N-CA	5.17	134.63	121.70
1	D	290	PHE	O-C-N	5.17	130.97	122.70
1	C	520	PRO	C-N-CA	5.17	134.62	121.70
1	D	532	CYS	N-CA-CB	-5.17	101.30	110.60
1	B	532	CYS	N-CA-CB	-5.16	101.31	110.60
1	C	532	CYS	N-CA-CB	-5.16	101.32	110.60
1	A	520	PRO	C-N-CA	5.15	134.58	121.70
1	B	520	PRO	C-N-CA	5.14	134.55	121.70
1	A	532	CYS	N-CA-CB	-5.14	101.35	110.60
1	A	18	PRO	CA-CB-CG	-5.14	94.24	104.00
1	B	522	LEU	N-CA-C	-5.13	97.15	111.00
1	C	18	PRO	CA-CB-CG	-5.13	94.26	104.00
1	D	18	PRO	CA-CB-CG	-5.12	94.27	104.00
1	C	522	LEU	N-CA-C	-5.12	97.18	111.00
1	D	522	LEU	N-CA-C	-5.12	97.18	111.00
1	B	18	PRO	CA-CB-CG	-5.12	94.28	104.00
1	A	339	VAL	N-CA-C	5.11	124.80	111.00
1	B	339	VAL	N-CA-C	5.11	124.80	111.00
1	C	339	VAL	N-CA-C	5.11	124.79	111.00
1	A	522	LEU	N-CA-C	-5.10	97.24	111.00
1	D	339	VAL	N-CA-C	5.10	124.76	111.00
1	B	16	PRO	C-N-CA	-5.08	109.01	121.70
1	D	16	PRO	C-N-CA	-5.07	109.02	121.70
1	A	16	PRO	C-N-CA	-5.07	109.03	121.70
1	C	16	PRO	C-N-CA	-5.07	109.02	121.70
1	A	332	PHE	N-CA-C	-5.05	97.37	111.00
1	C	332	PHE	N-CA-C	-5.03	97.41	111.00
1	C	539	CYS	N-CA-C	5.03	124.59	111.00
1	D	332	PHE	N-CA-C	-5.03	97.42	111.00
1	D	470	PRO	N-CA-C	5.03	125.18	112.10
1	B	234	GLU	O-C-N	5.03	130.75	122.70
1	A	470	PRO	N-CA-C	5.02	125.16	112.10
1	B	332	PHE	N-CA-C	-5.02	97.44	111.00
1	B	470	PRO	N-CA-C	5.02	125.15	112.10
1	A	539	CYS	N-CA-C	5.01	124.54	111.00
1	C	221	PHE	N-CA-C	5.01	124.54	111.00
1	C	470	PRO	N-CA-C	5.01	125.12	112.10
1	D	221	PHE	N-CA-C	5.01	124.53	111.00
1	A	221	PHE	N-CA-C	5.01	124.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	PHE	N-CA-C	5.00	124.52	111.00
1	D	539	CYS	N-CA-C	5.00	124.51	111.00

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	757	0
1	B	4191	0	4089	752	0
1	C	4191	0	4087	717	0
1	D	4191	0	4086	711	0
2	A	154	0	143	84	0
2	B	154	0	143	83	0
2	C	154	0	143	84	0
2	D	154	0	143	84	0
3	A	56	0	52	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	56	0	52	16	0
3	C	56	0	52	16	0
3	D	56	0	52	15	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	17128	2836	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 82.

All (2836) 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:C:24:ILE:HG21	1:D:2:TRP:CA	1.42	1.48
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:A:1:ASP:O	1:B:94:ILE:CA	1.71	1.35
1:C:27:ASN:HD21	1:D:90:GLU:CB	1.39	1.32
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:C:92:MET:HE1	1:D:2:TRP:CB	1.67	1.24
1:C:24:ILE:CG2	1:D:2:TRP:CA	2.00	1.23
1:C:27:ASN:ND2	1:D:90:GLU:HB3	1.53	1.23
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:D:540:GLN:O	1:D:540:GLN:CD	1.79	1.21
1:A:540:GLN:CD	1:A:540:GLN:O	1.79	1.20
1:B:8:LYS:HD2	1:B:8:LYS:H	1.04	1.20
1:B:540:GLN:O	1:B:540:GLN:CD	1.79	1.20
1:A:93:GLU:C	1:B:2:TRP:HB3	1.61	1.20
1:C:92:MET:CE	1:D:2:TRP:HB2	1.70	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:GLN:CD	1:C:540:GLN:O	1.79	1.19
1:C:27:ASN:CG	1:D:90:GLU:HB3	1.61	1.19
1:A:2:TRP:HD1	1:B:93:GLU:CD	1.46	1.18
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:93:GLU:O	1:B:2:TRP:CB	1.94	1.16
1:A:5:PRO:CA	1:B:5:PRO:HG3	1.74	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:C:8:LYS:HD2	1:C:8:LYS:H	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:D:482:THR:HG23	1:D:499:THR:CG2	1.75	1.15
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.15
1:B:450:GLN:HG2	1:B:532:CYS:O	1.43	1.15
1:C:27:ASN:ND2	1:D:90:GLU:CG	2.10	1.15
1:C:423:THR:HB	2:C:810:NAG:C7	1.76	1.15
1:A:450:GLN:HG2	1:A:532:CYS:O	1.44	1.15
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:482:THR:HG23	1:B:499:THR:CG2	1.75	1.14
1:B:301:THR:HG21	2:B:805:NAG:H82	1.29	1.14
1:A:90:GLU:HB2	1:B:90:GLU:N	1.63	1.14
1:C:338:ARG:HD3	1:C:352:ILE:HG22	1.26	1.14
1:C:301:THR:HG21	2:C:805:NAG:H82	1.29	1.14
1:C:92:MET:HE3	1:D:2:TRP:HB2	1.27	1.12
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:154:ASP:C	2:D:801:NAG:H82	1.70	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:D:32:ASN:HD21	1:D:83:GLU:HB2	0.98	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:C:154:ASP:C	2:C:801:NAG:H82	1.70	1.10
1:B:154:ASP:C	2:B:801:NAG:H82	1.70	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:THR:HG21	2:D:807:NAG:C8	1.82	1.10
1:A:154:ASP:C	2:A:801:NAG:H82	1.70	1.10
1:A:338:ARG:HD3	1:A:352:ILE:HG22	1.25	1.10
1:A:227:THR:HG21	2:A:807:NAG:C8	1.82	1.10
1:D:301:THR:HG21	2:D:805:NAG:H82	1.29	1.09
1:B:32:ASN:HD21	1:B:83:GLU:HB2	0.98	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:O	1:C:222:ASP:OD1	1.69	1.09
1:A:301:THR:HG21	2:A:805:NAG:H82	1.29	1.08
1:B:227:THR:HG21	2:B:807:NAG:C8	1.82	1.08
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.08
1:C:32:ASN:HD21	1:C:83:GLU:HB2	0.98	1.08
1:D:234:GLU:H	1:D:235:ILE:HG23	1.08	1.08
1:C:290:PHE:HB2	1:C:292:LEU:N	1.69	1.08
1:A:32:ASN:HD21	1:A:83:GLU:HB2	0.98	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:C:27:ASN:OD1	1:D:90:GLU:HB3	1.53	1.07
1:D:485:ALA:O	1:D:486:GLU:HG2	1.54	1.07
1:B:485:ALA:O	1:B:486:GLU:HG2	1.54	1.07
1:D:222:ASP:OD1	1:D:222:ASP:O	1.69	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
1:B:482:THR:HG23	1:B:499:THR:HG22	1.09	1.07
1:A:485:ALA:O	1:A:486:GLU:HG2	1.55	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:A:482:THR:HG23	1:A:499:THR:HG22	1.09	1.07
1:B:474:SER:HB2	1:B:512:LEU:HG	1.25	1.07
1:A:8:LYS:HD2	1:A:8:LYS:H	1.04	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:D:450:GLN:CG	1:D:532:CYS:O	2.02	1.06
1:B:337:SER:HA	1:B:427:ILE:HG23	1.38	1.06
1:B:290:PHE:HB2	1:B:292:LEU:N	1.69	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:ILE:CD1	1:D:465:PRO:CD	2.20	1.06
1:D:290:PHE:HB2	1:D:292:LEU:N	1.69	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: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:D:482:THR:HG23	1:D:499:THR:HG22	1.09	1.05
1:C:469:TYR:CD1	1:C:470:PRO:HD2	1.91	1.05
1:A:469:TYR:CD1	1:A:470:PRO:HD2	1.91	1.05
1:A:450:GLN:CG	1:A:532:CYS:O	2.03	1.05
1:A:464:ILE:CD1	1:A:465:PRO:CD	2.20	1.05
1:C:27:ASN:ND2	1:D:90:GLU:HG2	1.69	1.05
1:B:522:LEU:HD22	1:B:523:THR:HB	1.39	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:C:482:THR:HG21	1:C:499:THR:H	1.23	1.04
1:C:92:MET:HE1	1:D:2:TRP:HB3	1.14	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
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:464:ILE:CD1	1:B:465:PRO:CD	2.20	1.02
1:B:403:ASN:HB2	3:B:902:NDG:C8	1.90	1.02
1:D:403:ASN:HB2	3:D:902:NDG:C8	1.90	1.02
1:C:403:ASN:HB2	3:C:902:NDG:C8	1.90	1.02
1:A:522:LEU:HD22	1:A:523:THR:HB	1.39	1.02
1:A:403:ASN:HB2	3:A:902:NDG:C8	1.90	1.02
1:A:337:SER:HA	1:A:427:ILE:HG23	1.38	1.02
1:D:482:THR:HG21	1:D:499:THR:H	1.23	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:GLN:HB2	1:A:533:GLU:HA	1.41	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:B:432:ASP:OD2	1:B:464:ILE:HG22	1.60	1.00
1:C:432:ASP:OD2	1:C:464:ILE:HG22	1.60	1.00
1:A:1:ASP:O	1:B:94:ILE:HA	0.89	1.00
1:B:290:PHE:HZ	1:B:296:TYR:HH	1.05	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:CD1	1:B:93:GLU:CD	2.34	1.00
1:A:2:TRP:HB2	1:B:93:GLU:OE1	1.58	1.00
1:C:464:ILE:CD1	1:C:465:PRO:CD	2.20	0.99
1:A:188:THR:HG23	1:A:208:ILE:HG12	1.43	0.99
1:A:274:ASP:O	1:A:278:ASN:HA	1.61	0.99
1:D:432:ASP:OD2	1:D:464:ILE:HG22	1.60	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:A:92:MET:SD	1:B:3:VAL:CG1	2.50	0.99
1:D:450:GLN:HB2	1:D:533:GLU:HA	1.41	0.99
1:C:188:THR:HG23	1:C:208:ILE:HG12	1.43	0.99
1:A:320:THR:HG21	2:A:807:NAG:N2	1.78	0.99
1:D:482:THR:CG2	1:D:499:THR:H	1.76	0.99
1:C:274:ASP:O	1:C:278:ASN:HA	1.61	0.99
1:C:2:TRP:HZ2	1:D:53:ILE:HD11	1.28	0.99
1:B:188:THR:HG23	1:B:208:ILE:HG12	1.43	0.98
1:A:290:PHE:HZ	1:A:296:TYR:HH	1.05	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:C:523:THR:HG23	1:C:524:VAL:H	1.26	0.98
1:B:274:ASP:O	1:B:278:ASN:HA	1.61	0.98
1:C:482:THR:CG2	1:C:499:THR:H	1.76	0.97
1:D:188:THR:HG23	1:D:208:ILE:HG12	1.43	0.97
1:C:320:THR:HG21	2:C:807:NAG:N2	1.78	0.97
1:A:3:VAL:C	1:B:3:VAL:HB	1.85	0.96
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:D:320:THR:HG21	2:D:807:NAG:HN2	1.31	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:HG21	2:A:807:NAG:H83	1.48	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:B:235:ILE:CG1	1:B:287:GLY:HA2	1.96	0.96
1:A:93:GLU:C	1:B:2:TRP:CB	2.31	0.95
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:235:ILE:CG1	1:C:287:GLY:HA2	1.96	0.95
1:C:227:THR:HG21	2:C:807:NAG:H83	1.48	0.95
1:A:235:ILE:CG1	1:A:287:GLY:HA2	1.96	0.95
1:D:32:ASN:HD21	1:D:83:GLU:CB	1.79	0.95
1:A:32:ASN:HD21	1:A:83:GLU:CB	1.79	0.95
1:A:523:THR:HG23	1:A:524:VAL:H	1.27	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:D:464:ILE:HD12	1:D:465:PRO:HD2	0.94	0.94
1:B:290:PHE:CB	1:B:292:LEU:H	1.79	0.94
1:A:396:ARG:HH22	1:A:464:ILE:HB	1.33	0.94
1:A:366:LYS:CG	1:A:367:LEU:H	1.80	0.94
1:C:366:LYS:CG	1:C:367:LEU:H	1.80	0.94
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:D:27:ASN:HD22	1:D:28:LYS:N	1.66	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:C:464:ILE:HD12	1:C:465:PRO:HD2	0.94	0.93
1:B:352:ILE:HG13	1:B:388:VAL:HB	1.51	0.93
1:D:227:THR:HG21	2:D:807:NAG:C7	1.99	0.93
1:B:32:ASN:ND2	1:B:83:GLU:HB2	1.84	0.93
1:C:32:ASN:ND2	1:C:83:GLU:HB2	1.84	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:D:32:ASN:ND2	1:D:83:GLU:HB2	1.84	0.93
1:A:352:ILE:HG13	1:A:388:VAL:HB	1.51	0.93
1:D:289:ASP:O	1:D:290:PHE:HB3	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:446:THR:HG23	1:C:539:CYS:SG	2.09	0.93
1:B:195:ASP:HB2	1:B:201:LEU:H	1.34	0.93
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:A:482:THR:HG21	1:A:499:THR:N	1.81	0.92
1:D:482:THR:HG21	1:D:499:THR:N	1.81	0.92
1:B:396:ARG:HH22	1:B:464:ILE:HB	1.33	0.92
1:A:32:ASN:ND2	1:A:83:GLU:HB2	1.84	0.92
1:D:352:ILE:HG13	1:D:388:VAL:HB	1.51	0.92
1:B:403:ASN:HB2	3:B:902:NDG:C7	2.00	0.92
1:D:396:ARG:HH22	1:D:464:ILE:HB	1.33	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:B:464:ILE:HD12	1:B:465:PRO:HD2	0.94	0.92
2:C:805:NAG:H62	2:C:806:NAG:C7	2.00	0.92
1:D:404:ASN:ND2	1:D:404:ASN:O	2.03	0.92
1:A:464:ILE:HD12	1:A:465:PRO:HD2	0.94	0.92
1:C:227:THR:HG21	2:C:807:NAG:C7	1.99	0.92
1:A:8:LYS:CD	1:A:8:LYS:H	1.74	0.92
2:B:805:NAG:H62	2:B:806:NAG:C7	2.00	0.92
1:A:404:ASN:ND2	1:A:404:ASN:O	2.03	0.92
1:B:446:THR:HG23	1:B:539:CYS:SG	2.10	0.92
1:D:403:ASN:HB2	3:D:902:NDG:C7	2.00	0.92
1:C:403:ASN:HB2	3:C:902:NDG: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:D:464:ILE:HD12	1:D:465:PRO:HD3	1.53	0.91
1:C:8:LYS:CD	1:C:8:LYS:H	1.74	0.91
1:B:227:THR:HG21	2:B:807:NAG:H83	1.48	0.91
1:C:335:ALA:CB	3:C:811:NDG:O6	2.18	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:C:24:ILE:HB	1:D:2:TRP:N	1.79	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:805:NAG:H62	2:A:806:NAG:C7	2.00	0.91
1:D:335:ALA:CB	3:D:811:NDG:O6	2.18	0.91
1:B:404:ASN:ND2	1:B:404:ASN:O	2.03	0.91
1:A:340:ASP:HA	1:A:429:HIS:HB3	1.53	0.91
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:A:335:ALA:CB	3:A:811:NDG:O6	2.18	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:D:8:LYS:H	1:D:8:LYS:CD	1.74	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:B:517:GLN:O	1:B:519:ASN:N	2.03	0.90
1:A:403:ASN:HB2	3:A:902:NDG:C7	2.00	0.90
1:B:464:ILE:HD12	1:B:465:PRO:HD3	1.53	0.90
1:A:234:GLU:N	1:A:235:ILE:HG23	1.86	0.90
1:C:338:ARG:HD3	1:C:352:ILE:CG2	2.02	0.90
2:C:805:NAG:O5	2:C:806:NAG:H83	1.71	0.90
1:C:340:ASP:HA	1:C:429:HIS:HB3	1.53	0.90
1:D:340:ASP:HA	1:D:429:HIS:HB3	1.53	0.90
1:C:378:TRP:HB2	1:C:379:LEU:HD23	1.53	0.90
1:C:449:ASP:H	1:C:532:CYS:HB3	1.37	0.90
1:B:234:GLU:N	1:B:235:ILE:HG23	1.86	0.90
1:C:27:ASN:HD21	1:D:90:GLU:CG	1.75	0.90
1:C:8:LYS:HD2	1:C:8:LYS:N	1.87	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: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:517:GLN:O	1:A:519:ASN:N	2.03	0.89
1:C:396:ARG:NH2	1:C:464:ILE:CG2	2.35	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:523:THR:HG23	1:C:524:VAL:CG2	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ILE:HD12	1:A:465:PRO:HD3	1.53	0.89
1:C:27:ASN:OD1	1:D:90:GLU:C	2.09	0.89
1:D:518:ASN:O	1:D:520:PRO:HD3	1.72	0.89
1:D:523:THR:HG23	1:D:524:VAL:CG2	2.03	0.89
1:A:523:THR:HG23	1:A:524:VAL:CG2	2.03	0.89
1:B:338:ARG:HD3	1:B:352:ILE:CG2	2.02	0.89
1:A:8:LYS:HD2	1:A:8:LYS:N	1.87	0.89
1:C:518:ASN:O	1:C:520:PRO:HD3	1.72	0.89
1:B:371:ILE:CD1	1:B:381:VAL:HG11	2.03	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:B:396:ARG:NH2	1:B:464:ILE:CG2	2.35	0.89
1:A:92:MET:SD	1:B:3:VAL:HG12	2.12	0.89
1:B:320:THR:HG21	2:B:807:NAG:HN2	1.31	0.89
1:A:371:ILE:CD1	1:A:381:VAL:HG11	2.03	0.89
1:D:343:GLU:HB3	1:D:433:VAL:HG21	1.55	0.89
2:B:805:NAG:O5	2:B:806:NAG:H83	1.71	0.89
1:B:374:ASP:O	1:B:375:PRO:C	2.06	0.89
1:C:371:ILE:CD1	1:C:381:VAL:HG11	2.03	0.89
1:D:378:TRP:HB2	1:D:379:LEU:HD23	1.53	0.88
1:D:396:ARG:NH2	1:D:464:ILE:CG2	2.35	0.88
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:D:318:THR:HG21	2:D:806:NAG:H5	1.56	0.88
1:D:464:ILE:HD11	1:D:465:PRO:HD2	1.53	0.88
1:A:2:TRP:CB	1:B:93:GLU:OE1	2.21	0.88
1:C:343:GLU:HB3	1:C:433:VAL:HG21	1.55	0.88
1:B:523:THR:HG23	1:B:524:VAL:CG2	2.03	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:C:154:ASP:HB3	1:C:155:PRO:HD2	1.54	0.88
1:D:221:PHE:HE1	1:D:315:SER:O	1.56	0.88
1:B:221:PHE:HE1	1:B:315:SER:O	1.56	0.88
1:A:486:GLU:HB2	1:A:495:LEU:HB2	1.56	0.88
1:B:333:VAL:HB	1:B:334:PRO:HD3	1.56	0.88
1:D:371:ILE:CD1	1:D:381:VAL:HG11	2.03	0.88
1:B:449:ASP:H	1:B:532:CYS:HB3	1.37	0.88
1:B:154:ASP:HB3	1:B:155:PRO:HD2	1.54	0.88
1:C:1:ASP:CG	1:D:26:SER:HA	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:154:ASP:HB3	1:D:155:PRO:HD2	1.54	0.87
1:B:486:GLU:HB2	1:B:495:LEU:HB2	1.56	0.87
1:A:374:ASP:O	1:A:375:PRO:C	2.06	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:D:483:TRP:CZ3	1:D:498:PRO:HG3	2.09	0.87
1:C:486:GLU:HB2	1:C:495:LEU:HB2	1.56	0.87
1:D:441:SER:OG	1:D:442:PRO:HD3	1.75	0.87
1:C:333:VAL:HB	1:C:334:PRO:HD3	1.56	0.87
1:A:257:ALA:O	1:A:273:THR:HG21	1.74	0.87
1:B:257:ALA:O	1:B:273:THR:HG21	1.74	0.87
1:B:343:GLU:HB3	1:B:433:VAL:HG21	1.55	0.87
1:C:318:THR:HG21	2:C:806:NAG:H5	1.56	0.87
1:A:441:SER:OG	1:A:442:PRO:HD3	1.75	0.87
1:D:374:ASP:O	1:D:375:PRO:C	2.06	0.87
1:D:523:THR:HG23	1:D:524:VAL:N	1.90	0.87
1:B:440:PRO:CD	1:B:522:LEU:HD12	2.05	0.87
1:B:523:THR:HG23	1:B:524:VAL:N	1.90	0.86
1:C:320:THR:HG21	2:C:807:NAG:C2	2.05	0.86
1:C:2:TRP:HZ2	1:D:53:ILE:CD1	1.88	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:440:PRO:CD	1:D:522:LEU:HD12	2.05	0.86
1:B:464:ILE:HD11	1:B:465:PRO:HD2	1.53	0.86
1:A:1:ASP:HB2	1:B:92:MET:C	1.92	0.86
1:C:440:PRO:CD	1:C:522:LEU:HD12	2.05	0.86
1:A:333:VAL:HB	1:A:334:PRO:HD3	1.56	0.86
1:A:320:THR:HG21	2:A:807:NAG:C2	2.05	0.86
1:B:441:SER:OG	1:B:442:PRO:HD3	1.75	0.86
1:A:523:THR:HG23	1:A:524:VAL:N	1.90	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:464:ILE:HD12	1:D:465:PRO:N	1.91	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:HE1	1.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:THR:HG21	2:D:807:NAG:C2	2.05	0.85
1:C:257:ALA:O	1:C:273:THR:HG21	1.74	0.85
1:B:423:THR:CB	2:B:810:NAG:C7	2.54	0.85
1:A:440:PRO:CD	1:A:522:LEU:HD12	2.05	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:D:235:ILE:HG13	1:D:287:GLY:HA2	1.58	0.85
1:C:523:THR:HG23	1:C:524:VAL:N	1.90	0.85
1:A:90:GLU:CB	1:B:90:GLU:N	2.26	0.85
1:B:451:ASN:N	1:B:533:GLU:O	2.10	0.85
1:A:343:GLU:HB3	1:A:433:VAL:HG21	1.55	0.85
1:C:483:TRP:HZ2	1:C:507:TYR:CE1	1.95	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:423:THR:CB	2:C:810:NAG:C7	2.54	0.85
1:A:451:ASN:N	1:A:533:GLU:O	2.10	0.85
1:D:451:ASN:N	1:D:533:GLU:O	2.10	0.85
1:D:440:PRO:HD2	1:D:522:LEU:HD12	1.59	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:C:464:ILE:HD12	1:C:465:PRO:HD3	1.53	0.84
1:B:483:TRP:HZ2	1:B:507:TYR:CE1	1.95	0.84
1:C:27:ASN:CG	1:D:90:GLU:CG	2.44	0.84
1:D:483:TRP:HZ2	1:D:507:TYR:CE1	1.95	0.84
1:B:464:ILE:HD12	1:B:465:PRO:N	1.91	0.84
1:B:440:PRO:HD2	1:B:522:LEU:HD12	1.59	0.84
1:C:27:ASN:CG	1:D:90:GLU:CB	2.33	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:C:451:ASN:N	1:C:533:GLU:O	2.10	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:464:ILE:HD12	1:C:465:PRO:N	1.91	0.84
1:A:375:PRO:HB3	1:A:400:TYR:CE2	2.12	0.84
1:C:375:PRO:HB3	1:C:400:TYR:CE2	2.12	0.84
1:C:230:VAL:O	1:C:324:GLU:N	2.11	0.84
1:C:438:PRO:HB3	1:C:471:TYR:HE2	1.41	0.83
1:D:396:ARG:NE	1:D:432:ASP:HB2	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:374:ASP:O	1:C:375:PRO:C	2.06	0.83
1:C:147:SER:OG	1:C:167:ARG:HD2	1.78	0.83
1:D:438:PRO:HB3	1:D:471:TYR:HE2	1.41	0.83
1:C:396:ARG:NE	1:C:432:ASP:HB2	1.93	0.83
1:C:235:ILE:HG13	1:C:287:GLY:HA2	1.58	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: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: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: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: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:423:THR:CB	2:A:810:NAG:N2	2.42	0.83
1:A:155:PRO:HB2	2:A:801:NAG:H81	1.59	0.83
1:A:147:SER:OG	1:A:167:ARG:HD2	1.78	0.83
1:A:446:THR:HG21	1:A:537:ILE:O	1.79	0.82
1:D:482:THR:HG21	1:D:500:GLN:N	1.94	0.82
1:C:155:PRO:HB2	2:C:801:NAG:H81	1.59	0.82
1:B:230:VAL:O	1:B:324:GLU:N	2.11	0.82
1:A:154:ASP:HB3	2:A:801:NAG:N2	1.95	0.82
1:B:446:THR:HG21	1:B:537:ILE:O	1.79	0.82
1:A:423:THR:HB	2:A:810:NAG:N2	1.93	0.82
1:A:230:VAL:O	1:A:324:GLU:N	2.11	0.82
1:A:1:ASP:O	1:B:95:THR:N	2.11	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:OD2	1:D:289:ASP:O	1.97	0.82
1:A:396:ARG:NE	1:A:432:ASP:HB2	1.93	0.82
1:C:423:THR:HB	2:C:810:NAG:N2	1.93	0.82
1:C:289:ASP:O	1:C:289:ASP:OD2	1.97	0.82
1:B:289:ASP:OD2	1:B:289:ASP:O	1.97	0.82
1:C:446:THR:HG21	1:C:537:ILE:O	1.79	0.82
1:A:92:MET:SD	1:B:3:VAL:HG13	2.19	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PHE:HD2	1:A:293:ARG:H	1.28	0.82
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:277:SER:C	1:D:278:ASN:HD22	1.83	0.82
1:A:92:MET:SD	1:B:3:VAL:CA	2.68	0.81
1:A:289:ASP:OD2	1:A:289:ASP:O	1.97	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:B:32:ASN:ND2	1:B:83:GLU:H	1.76	0.81
1:A:234:GLU:H	1:A:235:ILE:CG2	1.92	0.81
1:B:423:THR:CB	2:B:810:NAG:N2	2.42	0.81
1:D:423:THR:CB	2:D: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:155:PRO:HB2	2:D:801:NAG:H81	1.59	0.81
1:C:517:GLN:C	1:C:519:ASN:H	1.84	0.81
1:B:154:ASP:HB3	2:B:801:NAG:HN2	1.45	0.81
1:A:154:ASP:HB3	2:A:801:NAG:HN2	1.45	0.81
1:A:32:ASN:ND2	1:A:83:GLU:H	1.77	0.81
1:C:277:SER:C	1:C:278:ASN:HD22	1.84	0.81
1:D:446:THR:HG21	1:D:537:ILE:O	1.79	0.81
1:A:540:GLN:OE1	1:A:540:GLN:O	1.97	0.81
1:A:90:GLU:HB2	1:B:90:GLU:CB	2.10	0.81
1:A:517:GLN:C	1:A:519:ASN:H	1.84	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:D:517:GLN:C	1:D:519:ASN:H	1.84	0.81
1:C:28:LYS:HD3	1:C:88:VAL:HG12	1.61	0.81
1:C:469:TYR:CD2	1:C:470:PRO:HD2	2.16	0.81
1:C:154:ASP:HB3	2:C:801:NAG:N2	1.95	0.81
1:A:277:SER:C	1:A:278:ASN:HD22	1.84	0.81
1:B:234:GLU:H	1:B:235:ILE:CG2	1.92	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:D:28:LYS:HD3	1:D:88:VAL:HG12	1.61	0.81
1:C:482:THR:HG21	1:C:500:GLN:N	1.95	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:496:LEU:HD21	1:C:509:ILE:HD13	1.63	0.81
1:D:540:GLN:O	1:D:540:GLN:OE1	1.97	0.80
1:C:2:TRP:CZ2	1:D:53:ILE:HD11	2.15	0.80
1:A:127:VAL:HG13	1:A:128:MET:H	1.46	0.80
1:A:396:ARG:HH21	1:A:464:ILE:HG22	1.46	0.80
1:A:482:THR:HG21	1:A:500:GLN:N	1.95	0.80
1:A:469:TYR:CD2	1:A:470:PRO:HD2	2.16	0.80
1:A:299:GLN:HG2	1:A:318:THR:HG23	1.62	0.80
1:B:277:SER:C	1:B:278:ASN:HD22	1.83	0.80
1:C:540:GLN:O	1:C:540:GLN:OE1	1.97	0.80
1:B:396:ARG:HH21	1:B:464:ILE:HG22	1.46	0.80
1:A:290:PHE:CE2	1:A:293:ARG:HB2	2.16	0.80
1:A:27:ASN:HD22	1:A:27:ASN:C	1.85	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:A:432:ASP:OD2	1:A:464:ILE:CG2	2.30	0.80
1:B:540:GLN:OE1	1:B:540:GLN:O	1.97	0.80
1:C:423:THR:CB	2:C:810:NAG:N2	2.42	0.80
2:D:904:NAG:H3	2:D:904:NAG:O7	1.82	0.80
1:A:28:LYS:HD3	1:A:88:VAL:HG12	1.61	0.80
1:B:469:TYR:CD2	1:B:470:PRO:HD2	2.16	0.80
1:A:486:GLU:O	1:A:494:MET:HA	1.81	0.80
1:A:406:TYR:CD1	2:A:808:NAG:H83	2.17	0.80
1:C:154:ASP:HB3	2:C:801:NAG:HN2	1.45	0.80
1:B:290:PHE:CE2	1:B:293:ARG:HB2	2.16	0.80
1:D:469:TYR:CD2	1:D:470:PRO:HD2	2.16	0.80
1:C:523:THR:CG2	1:C:524:VAL:H	1.94	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:B:482:THR:OG1	1:B:500:GLN:HG2	1.82	0.80
1:C:222:ASP:C	1:C:222:ASP:OD1	2.20	0.80
1:D:290:PHE:HD2	1:D:293:ARG:H	1.28	0.80
1:D:485:ALA:O	1:D:486:GLU:CG	2.30	0.80
1:D:406:TYR:CD1	2:D:808:NAG:H83	2.17	0.80
1:C:396:ARG:HD3	1:C:431:LEU:C	2.03	0.80
1:C:27:ASN:HD22	1:C:27:ASN:C	1.85	0.80
1:A:371:ILE:HD11	1:A:381:VAL:HG11	1.64	0.80
1:C:22:VAL:HG21	1:D:5:PRO:HG3	1.61	0.79
1:B:299:GLN:HG2	1:B:318:THR:HG23	1.62	0.79
1:B:517:GLN:C	1:B:519:ASN:H	1.84	0.79
1:B:265:GLU:HB3	1:B:268:PHE:HE2	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:ARG:HH21	1:C:464:ILE:HG22	1.46	0.79
1:C:432:ASP:OD2	1:C:464:ILE:CG2	2.30	0.79
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:B:232:GLU:HG3	1:B:290:PHE:N	1.98	0.79
1:C:406:TYR:CD1	2:C:808:NAG:H83	2.17	0.79
1:D:496:LEU:HD21	1:D:509:ILE:HD13	1.63	0.79
1:D:396:ARG:HD3	1:D:431:LEU:C	2.03	0.79
1:D:432:ASP:OD2	1:D:464:ILE:CG2	2.30	0.79
1:C:449:ASP:HB3	1:C:532:CYS:H	1.47	0.79
1:C:155:PRO:C	1:C:157:GLU:H	1.86	0.79
1:A:155:PRO:C	1:A:157:GLU:H	1.86	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:B:432:ASP:OD2	1:B:464:ILE:CG2	2.30	0.79
1:A:232:GLU:HG3	1:A:290:PHE:N	1.98	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:C:540:GLN:CG	1:C:540:GLN:O	2.30	0.79
1:C:154:ASP:CB	1:C:155:PRO:HD2	2.13	0.79
1:A:222:ASP:OD1	1:A:222:ASP:C	2.20	0.79
1:A:485:ALA:O	1:A:486:GLU:CG	2.31	0.79
1:D:396:ARG:HH21	1:D:464:ILE:HG22	1.46	0.79
1:B:365:GLN:HG3	1:B:365:GLN:O	1.82	0.79
1:B:396:ARG:HD3	1:B:431:LEU:C	2.02	0.79
1:D:540:GLN:O	1:D:540:GLN:CG	2.31	0.79
1:D:482:THR:OG1	1:D:500:GLN:HG2	1.82	0.79
2:C:809:NAG:H61	2:C:810:NAG:H62	1.65	0.79
1:C:232:GLU:HG3	1:C:290:PHE:N	1.98	0.79
2:C:904:NAG:H3	2:C:904:NAG:O7	1.82	0.79
1:A:540:GLN:CG	1:A:540:GLN:O	2.30	0.78
1:D:155:PRO:C	1:D:157:GLU:H	1.86	0.78
2:B:904:NAG:H3	2:B:904:NAG:O7	1.82	0.78
1:C:238:GLU:HA	1:C:283:THR:HG22	1.66	0.78
1:C:127:VAL:HG13	1:C:128:MET:H	1.46	0.78
1:C:365:GLN:O	1:C:365:GLN:HG3	1.82	0.78
1:D:154:ASP:CB	1:D:155:PRO:HD2	2.13	0.78
1:B:406:TYR:CD1	2:B:808:NAG:H83	2.17	0.78
1:D:371:ILE:HD11	1:D:381:VAL:HG11	1.64	0.78
1:B:147:SER:OG	1:B:167:ARG:CG	2.32	0.78
1:D:449:ASP:HB3	1:D:532:CYS:H	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HG21	2:A:805:NAG:C8	2.12	0.78
1:D:486:GLU:O	1:D:494:MET:HA	1.81	0.78
1:B:155:PRO:C	1:B:157:GLU:H	1.86	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:B:222:ASP:C	1:B:222:ASP:OD1	2.20	0.78
1:C:234:GLU:H	1:C:235:ILE:CG2	1.92	0.78
1:C:501:GLN:O	1:C:501:GLN:HG2	1.84	0.78
2:B:809:NAG:H61	2:B:810:NAG:H62	1.65	0.78
2:A:904:NAG:O7	2:A:904:NAG:H3	1.82	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:C:147:SER:OG	1:C:167:ARG:CG	2.32	0.78
1:B:496:LEU:HD21	1:B:509:ILE:HD13	1.63	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
1:B:485:ALA:O	1:B:486:GLU:CG	2.30	0.78
1:A:156:GLU:HG3	1:A:160:PRO:HB3	1.66	0.78
1:A:396:ARG:HD3	1:A:431:LEU:C	2.03	0.78
1:D:222:ASP:OD1	1:D:222:ASP:C	2.20	0.78
1:A:365:GLN:HG3	1:A:365:GLN:O	1.82	0.78
2:D:809:NAG:H61	2:D:810:NAG:H62	1.65	0.77
1:C:485:ALA:O	1:C:486:GLU:CG	2.30	0.77
1:A:194:THR:HB	1:A:198:GLY:HA2	1.66	0.77
1:D:127:VAL:HG13	1:D:128:MET:H	1.46	0.77
1:C:156:GLU:HG3	1:C:160:PRO:HB3	1.66	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:D:223:PRO:HD2	1:D:226:TYR:OH	1.85	0.77
1:C:524:VAL:CG2	2:C:904:NAG:H81	2.14	0.77
1:C:371:ILE:HD11	1:C:381:VAL:HG11	1.64	0.77
1:B:501:GLN:HG2	1:B:501:GLN:O	1.84	0.77
1:C:301:THR:HG21	2:C:805:NAG:C8	2.12	0.77
1:D:290:PHE:HZ	1:D:296:TYR:HH	1.29	0.77
1:D:432:ASP:CG	1:D:464:ILE:HG22	2.05	0.77
1:C:223:PRO:HD2	1:C:226:TYR:OH	1.85	0.77
1:B:194:THR:HB	1:B:198:GLY:HA2	1.67	0.77
1:B:371:ILE:HD11	1:B:381:VAL:HG11	1.64	0.77
1:A:505:GLY:C	1:A:506:ASP:OD1	2.23	0.77
1:B:362:GLN:O	1:B:364:ILE:HG23	1.85	0.77
1:C:147:SER:OG	1:C:167:ARG:CD	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:GLY:C	1:C:506:ASP:OD1	2.23	0.77
1:A:501:GLN:O	1:A:501:GLN:HG2	1.84	0.77
1:D:238:GLU:HA	1:D:283:THR:HG22	1.66	0.77
1:A:1:ASP:O	1:B:94:ILE:C	2.23	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:505:GLY:C	1:D:506:ASP:OD1	2.23	0.77
1:D:501:GLN:HG2	1:D:501:GLN:O	1.84	0.77
1:A:238:GLU:HA	1:A:283:THR:HG22	1.66	0.77
1:A:147:SER:OG	1:A:167:ARG:CG	2.32	0.77
1:D:27:ASN:HD22	1:D:27:ASN:C	1.85	0.77
1:A:366:LYS:CG	1:A:367:LEU:N	2.48	0.77
1:B:196:LEU:HB2	1:B:199:ALA:HB3	1.67	0.77
1:B:147:SER:OG	1:B:167:ARG:CD	2.32	0.77
1:B:540:GLN:CG	1:B:540:GLN:O	2.31	0.77
1:D:301:THR:HG21	2:D:805:NAG:C8	2.13	0.77
1:D:366:LYS:CG	1:D:367:LEU:N	2.48	0.77
1:C:362:GLN:O	1:C:364:ILE:HG23	1.85	0.77
2:A:809:NAG:H61	2:A:810:NAG:H62	1.65	0.76
1:B:27:ASN:C	1:B:27:ASN:HD22	1.85	0.76
1:C:196:LEU:HB2	1:C:199:ALA:HB3	1.67	0.76
1:C:195:ASP:HB3	1:C:200:GLY:HA3	1.65	0.76
1:A:432:ASP:CG	1:A:464:ILE:HG22	2.05	0.76
1:C:27:ASN:HD21	1:D:90:GLU:HB2	1.46	0.76
1:D:524:VAL:CG2	2:D:904:NAG:H81	2.14	0.76
1:B:290:PHE:HD2	1:B:293:ARG:H	1.28	0.76
1:A:196:LEU:HB2	1:A:199:ALA:HB3	1.67	0.76
1:A:362:GLN:O	1:A:364:ILE:HG23	1.85	0.76
1:A:449:ASP:HB3	1:A:532:CYS:H	1.47	0.76
1:A:147:SER:OG	1:A:167:ARG:CD	2.32	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:482:THR:CG2	1:B:499:THR:CG2	2.62	0.76
1:B:272:THR:HG22	1:B:273:THR:H	1.51	0.76
1:B:505:GLY:C	1:B:506:ASP:OD1	2.23	0.76
1:B:368:SER:HG	1:B:370:PHE:HE1	1.31	0.76
1:B:432:ASP:CG	1:B:464:ILE:HG22	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HD2	1:A:226:TYR:OH	1.85	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:A:272:THR:HG22	1:A:273:THR:H	1.51	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:523:THR:HG23	1:C:524:VAL:HG22	1.67	0.76
1:C:371:ILE:HD12	1:C:410:MET:HB3	1.68	0.76
1:B:396:ARG:HH21	1:B:464:ILE:CG2	1.98	0.75
1:D:482:THR:CG2	1:D:499:THR:CG2	2.62	0.75
1:D:440:PRO:HB3	1:D:457:LEU:HD21	1.67	0.75
1:C:448:CYS:SG	1:C:537:ILE:HG22	2.26	0.75
1:A:523:THR:HG23	1:A:524:VAL:HG22	1.67	0.75
1:C:440:PRO:HB3	1:C:457:LEU:HD21	1.67	0.75
1:C:366:LYS:CG	1:C:367:LEU:N	2.48	0.75
1:D:272:THR:HG22	1:D:273:THR:H	1.51	0.75
1:C:432:ASP:CG	1:C:464:ILE:HG22	2.05	0.75
1:D:290:PHE:CD2	1:D:293:ARG:N	2.55	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: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:B:396:ARG:NH2	1:B:464:ILE:HB	2.02	0.75
1:A:449:ASP:HB3	1:A:532:CYS:N	2.02	0.75
1:C:449:ASP:HB3	1:C:532:CYS:N	2.02	0.75
1:B:448:CYS:SG	1:B:537:ILE:HG22	2.26	0.75
1:A:188:THR:HG23	1:A:208:ILE:CG1	2.16	0.75
1:D:194:THR:HB	1:D:198:GLY:HA2	1.67	0.75
1:A:371:ILE:HD12	1:A:410:MET:HB3	1.68	0.75
1:D:448:CYS:SG	1:D:537:ILE:HG22	2.27	0.74
1:B:449:ASP:HB3	1:B:532:CYS:N	2.02	0.74
1:D:449:ASP:HB3	1:D:532:CYS:N	2.02	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:C:396:ARG:HH21	1:C:464:ILE:CG2	1.99	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:A:396:ARG:NH2	1:A:464:ILE:HB	2.02	0.74
1:A:92:MET:HE1	1:B:3:VAL:HG13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:TRP:CE2	1:B:95:THR:OG1	2.32	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:C:241:ARG:HE	1:C:281:ILE:HD12	1.51	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:D:196:LEU:HB2	1:D:199:ALA:HB3	1.67	0.74
1:D:396:ARG:HH21	1:D:464:ILE:CG2	1.98	0.74
1:B:451:ASN:O	1:B:534:GLY:HA2	1.88	0.74
1:A:333:VAL:CB	1:A:334:PRO:HD3	2.18	0.74
1:D:371:ILE:HD12	1:D:410:MET:HB3	1.68	0.73
1:A:241:ARG:HE	1:A:281:ILE:HD12	1.51	0.73
1:D:320:THR:CG2	2:D:807:NAG:HN2	2.01	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: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:C:290:PHE:HZ	1:C:296:TYR:HH	1.35	0.73
1:B:371:ILE:HD12	1:B:410:MET:HB3	1.68	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:D:450:GLN:HG3	1:D:533:GLU:OE2	1.88	0.73
1:A:223:PRO:HB2	1:A:226:TYR:CE2	2.23	0.73
1:C:451:ASN:O	1:C:534:GLY:HA2	1.88	0.73
1:C:276:GLU:HG3	1:C:277:SER:H	1.54	0.73
1:B:366:LYS:CG	1:B:367:LEU:N	2.48	0.73
1:B:364:ILE:HG13	1:B:364:ILE:O	1.87	0.73
1:A:364:ILE:HG13	1:A:364:ILE:O	1.87	0.73
1:C:273:THR:O	2:C:803:NAG:H82	1.89	0.73
1:D:368:SER:HG	1:D:370:PHE:HE1	1.37	0.73
1:C:396:ARG:NH2	1:C:464:ILE:HB	2.02	0.73
1:D:373:ASN:ND2	1:D:374:ASP:H	1.87	0.73
1:A:364:ILE:CG1	1:A:364:ILE:O	2.37	0.73
1:C:298:LEU:N	1:C:298:LEU:HD23	2.03	0.73
1:D:342:SER:HA	1:D:431:LEU:HB2	1.71	0.73
1:C:188:THR:HG23	1:C:208:ILE:CG1	2.16	0.73
1:B:474:SER:CB	1:B:512:LEU:HG	2.14	0.73
1:D:333:VAL:CB	1:D:334:PRO:HD3	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ARG:HH21	1:A:464:ILE:CG2	1.98	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:373:ASN:ND2	1:A:374:ASP:H	1.87	0.73
1:B:298:LEU:HD23	1:B:298:LEU:N	2.03	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:364:ILE:O	1:D:364:ILE:CG1	2.37	0.72
1:A:298:LEU:HD23	1:A:298:LEU:N	2.03	0.72
1:C:368:SER:HG	1:C:370:PHE:HE1	1.35	0.72
1:D:396:ARG:NH2	1:D:464:ILE:HB	2.02	0.72
1:A:273:THR:O	2:A:803:NAG:H82	1.89	0.72
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:D:523:THR:CG2	1:D:524:VAL:N	2.46	0.72
1:B:276:GLU:HG3	1:B:277:SER:H	1.54	0.72
1:C:23:GLN:HG2	1:D:3:VAL:HG21	1.71	0.72
1:D:320:THR:CG2	2:D:807:NAG:N2	2.51	0.72
1:A:33:LYS:HB3	1:A:83:GLU:HG2	1.71	0.72
1:D:511:VAL:HG23	1:D:523:THR:O	1.89	0.72
1:C:373:ASN:ND2	1:C:374:ASP:H	1.87	0.72
1:D:273:THR:O	2:D:803:NAG:H82	1.89	0.72
1:B:364:ILE:CG1	1:B:364:ILE:O	2.37	0.72
1:C:364:ILE:O	1:C:364:ILE:CG1	2.37	0.72
1:B:273:THR:O	2:B:803:NAG:H82	1.89	0.72
1:D:394:LEU:N	1:D:394:LEU:HD12	2.05	0.72
1:B:320:THR:CG2	2:B:807:NAG:N2	2.52	0.72
1:B:511:VAL:HG23	1:B:523:THR:O	1.89	0.72
1:B:394:LEU:N	1:B:394:LEU:HD12	2.05	0.72
1:D:223:PRO:HB2	1:D:226:TYR:CE2	2.23	0.72
1:B:320:THR:CG2	2:B:807:NAG:HN2	2.01	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: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:366:LYS:HG3	1:A:367:LEU:N	2.04	0.71
1:A:320:THR:CG2	2:A:807:NAG:N2	2.52	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ASN:ND2	1:B:374:ASP:H	1.87	0.71
1:D:434:ASN:OD1	1:D:467:ASN:HB3	1.91	0.71
1:D:414:ASP:HB3	1:D:420:GLY:HA3	1.73	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:A:276:GLU:HG3	1:A:277:SER:H	1.54	0.71
1:C:394:LEU:HD12	1:C:394:LEU:N	2.05	0.71
1:B:434:ASN:OD1	1:B:467:ASN:HB3	1.91	0.71
1:A:4:ILE:HD13	1:B:3:VAL:N	2.06	0.71
1:C:414:ASP:HB3	1:C:420:GLY:HA3	1.73	0.71
1:C:320:THR:CG2	2:C:807:NAG:N2	2.52	0.71
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.71
1:A:394:LEU:N	1:A:394:LEU:HD12	2.05	0.71
1:A:187:TYR:HA	2:A:801:NAG:C7	2.21	0.71
1:C:320:THR:CG2	2:C:807:NAG:HN2	2.02	0.71
1:A:403:ASN:CB	3:A:902:NDG:N2	2.54	0.71
1:D:403:ASN:CB	3:D:902:NDG:N2	2.54	0.71
1:C:276:GLU:CG	1:C:277:SER:H	2.03	0.71
1:B:187:TYR:HA	2:B:801:NAG:C7	2.21	0.71
1:A:316:THR:O	2:A:806:NAG:H82	1.91	0.71
1:A:276:GLU:CG	1:A:277:SER:H	2.03	0.71
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:B:405:THR:OG1	1:B:406:TYR:N	2.22	0.70
1:C:434:ASN:OD1	1:C:467:ASN:HB3	1.91	0.70
1:D:289:ASP:O	1:D:289:ASP:CG	2.30	0.70
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.74	0.70
1:B:337:SER:CA	1:B:427:ILE:HG23	2.20	0.70
1:C:403:ASN:CB	3:C:902:NDG:N2	2.54	0.70
1:A:92:MET:CE	1:B:3:VAL:HG13	2.22	0.70
1:D:483:TRP:CZ2	1:D:507:TYR:HE1	2.09	0.70
1:D:474:SER:CB	1:D:512:LEU:HG	2.14	0.70
1:D:276:GLU:CG	1:D:277:SER:H	2.03	0.70
1:B:342:SER:HA	1:B:431:LEU:HB2	1.71	0.70
1:D:485:ALA:C	1:D:486:GLU:HG2	2.11	0.70
1:C:485:ALA:C	1:C:486:GLU:HG2	2.11	0.70
1:B:316:THR:O	2:B:806:NAG:H82	1.91	0.70
1:B:403:ASN:CB	3:B:902:NDG:N2	2.54	0.70
1:C:337:SER:CA	1:C:427:ILE:HG23	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:THR:OG1	1:D:406:TYR:N	2.22	0.70
1:C:483:TRP:CZ2	1:C:507:TYR:HE1	2.09	0.70
1:C:482:THR:CG2	1:C:499:THR:CG2	2.62	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
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:227:THR:O	2:C:812:NAG:O5	2.09	0.70
1:B:290:PHE:CD2	1:B:293:ARG:N	2.55	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:485:ALA:C	1:B:486:GLU:HG2	2.11	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:483:TRP:CZ2	1:A:507:TYR:HE1	2.09	0.70
1:A:90:GLU:H	1:B:90:GLU:HB3	1.55	0.70
1:D:523:THR:HG23	1:D:524:VAL:HG23	1.74	0.70
1:D:229:LEU:HD23	1:D:322:THR:HB	1.73	0.70
1:A:3:VAL:C	1:B:3:VAL:CB	2.60	0.69
1:A:485:ALA:C	1:A:486:GLU:HG2	2.11	0.69
1:A:434:ASN:OD1	1:A:467:ASN:HB3	1.91	0.69
1:A:227:THR:O	2:A:812:NAG:O5	2.09	0.69
1:C:289:ASP:CG	1:C:289:ASP:O	2.29	0.69
1:C:316:THR:O	2:C:806:NAG:H82	1.91	0.69
1:D:186:GLU:OE1	2:D:801:NAG:H62	1.93	0.69
1:C:474:SER:HB2	1:C:512:LEU:CG	2.15	0.69
1:A:221:PHE:CE1	1:A:315:SER:O	2.45	0.69
1:C:438:PRO:HB3	1:C:471:TYR:CE2	2.26	0.69
1:B:53:ILE:HG13	1:B:59:TRP:O	1.93	0.69
1:B:438:PRO:HB3	1:B:471:TYR:CE2	2.26	0.69
1:C:27:ASN:C	1:C:27:ASN:ND2	2.46	0.69
1:C:187:TYR:HA	2:C:801:NAG:C7	2.21	0.69
1:B:186:GLU:OE1	2:B:801:NAG:H62	1.93	0.69
1:A:186:GLU:OE1	2:A:801:NAG:H62	1.93	0.69
1:C:221:PHE:CE1	1:C:315:SER:O	2.45	0.69
1:C:405:THR:OG1	1:C:406:TYR:N	2.22	0.69
1:B:366:LYS:HG3	1:B:367:LEU:N	2.04	0.69
1:C:229:LEU:HD23	1:C:322:THR:HB	1.73	0.69
1:B:229:LEU:HD23	1:B:322:THR:HB	1.73	0.69
1:C:94:ILE:HG21	1:D:2:TRP:HH2	1.57	0.69
1:C:53:ILE:HG13	1:C:59:TRP:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:LEU:HD12	1:D:280:GLY:O	1.93	0.69
1:C:242:LEU:HD12	1:C:280:GLY:O	1.93	0.69
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.74	0.69
1:A:27:ASN:C	1:A:27:ASN:ND2	2.46	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:C:92:MET:HB3	1:D:2:TRP:CD1	2.28	0.68
1:B:482:THR:HG21	1:B:500:GLN:H	1.59	0.68
1:D:1:ASP:CG	1:D:2:TRP:H	1.96	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:229:LEU:HD23	1:A:322:THR:HB	1.73	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: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:A:53:ILE:HG13	1:A:59:TRP:O	1.93	0.68
1:D:396:ARG:HE	1:D:432:ASP:HB2	1.57	0.68
1:A:405:THR:OG1	1:A:406:TYR:N	2.22	0.68
1:A:272:THR:HG22	1:A:273:THR:N	2.09	0.68
1:A:289:ASP:CG	1:A:289:ASP:O	2.29	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:C:396:ARG:HE	1:C:432:ASP:HB2	1.57	0.68
1:B:155:PRO:HB2	2:B:801:NAG:C8	2.24	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:D:517:GLN:C	1:D:519:ASN:N	2.47	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:A:137:ASP:OD2	1:A:139:ILE:HG22	1.94	0.68
1:A:222:ASP:CG	1:A:222:ASP:O	2.32	0.68
1:D:440:PRO:HA	1:D:458:THR:O	1.94	0.68
1:B:517:GLN:C	1:B:519:ASN:N	2.46	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:A:242:LEU:HD12	1:A:280:GLY:O	1.93	0.68
1:D:290:PHE:HZ	1:D:296:TYR:OH	1.77	0.68
1:A:282:LEU:HD23	1:A:283:THR:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:HE	1:B:432:ASP:CB	2.07	0.67
1:D:396:ARG:HD3	1:D:431:LEU:O	1.94	0.67
1:C:155:PRO:HB2	2:C:801:NAG:C8	2.24	0.67
1:A:474:SER:HB2	1:A:512:LEU:CG	2.15	0.67
1:D:53:ILE:HG13	1:D:59:TRP:O	1.93	0.67
1:B:333:VAL:HB	1:B:334:PRO:CD	2.24	0.67
1:C:282:LEU:HD23	1:C:283:THR:H	1.58	0.67
1:A:1:ASP:CG	1:A:2:TRP:H	1.96	0.67
1:B:1:ASP:CG	1:B:2:TRP:H	1.96	0.67
1:A:423:THR:HB	2:A:810:NAG:C8	2.24	0.67
1:C:440:PRO:HA	1:C:458:THR:O	1.94	0.67
1:A:337:SER:CA	1:A:427:ILE:HG23	2.20	0.67
1:B:137:ASP:OD2	1:B:139:ILE:HG22	1.94	0.67
1:D:195:ASP:HB2	1:D:201:LEU:N	2.08	0.67
1:C:272:THR:HG22	1:C:273:THR:N	2.09	0.67
1:A:396:ARG:NH2	1:A:464:ILE:CB	2.58	0.67
1:D:482:THR:HG21	1:D:500:GLN:H	1.59	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:C:289:ASP:O	1:C:290:PHE:CB	2.25	0.67
1:A:373:ASN:ND2	1:A:374:ASP:N	2.43	0.67
3:B:902:NDG:H3	3:B:902:NDG:O7	1.95	0.67
1:B:440:PRO:HA	1:B:458:THR:O	1.94	0.67
1:B:373:ASN:ND2	1:B:374:ASP:N	2.43	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:D:396:ARG:HE	1:D:432:ASP:CB	2.07	0.67
1:D:27:ASN:C	1:D:27:ASN:ND2	2.46	0.67
1:D:423:THR:HB	2:D:810:NAG:C8	2.24	0.67
1:C:290:PHE:HZ	1:C:296:TYR:OH	1.77	0.67
1:D:337:SER:CA	1:D:427:ILE:HG23	2.20	0.67
1:B:401:VAL:HG13	1:B:405:THR:O	1.95	0.67
1:D:401:VAL:HG13	1:D:405:THR:O	1.95	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:D:347:ARG:CG	1:D:392:GLY:H	2.08	0.67
1:D:137:ASP:OD2	1:D:139:ILE:HG22	1.94	0.67
1:C:396:ARG:NH2	1:C:464:ILE:CB	2.58	0.67
1:D:474:SER:HB2	1:D:512:LEU:CG	2.15	0.67
1:A:474:SER:CB	1:A:512:LEU:HG	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:VAL:HG13	1:C:405:THR:O	1.95	0.67
1:C:195:ASP:HB2	1:C:201:LEU:N	2.08	0.67
1:A:396:ARG:HE	1:A:432:ASP:HB2	1.57	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:32:ASN:CG	1:D:33:LYS:H	1.99	0.67
1:B:403:ASN:HB2	3:B:902:NDG:N2	2.10	0.67
1:D:373:ASN:ND2	1:D:374:ASP:N	2.43	0.67
1:C:333:VAL:HB	1:C:334:PRO:CD	2.24	0.67
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:B:320:THR:HG21	2:B:807:NAG:H2	1.76	0.67
3:A:902:NDG:O7	3:A:902:NDG:H3	1.95	0.67
1:A:396:ARG:HD3	1:A:431:LEU:O	1.94	0.66
1:D:222:ASP:CG	1:D:222:ASP:O	2.32	0.66
1:A:440:PRO:HA	1:A:458:THR:O	1.94	0.66
1:A:403:ASN:HB2	3:A:902:NDG:N2	2.10	0.66
1:C:347:ARG:CD	1:C:392:GLY:H	2.07	0.66
1:D:446:THR:CG2	1:D:537:ILE:O	2.44	0.66
1:C:482:THR:HG21	1:C:500:GLN:H	1.59	0.66
1:C:423:THR:HB	2:C:810:NAG:C8	2.24	0.66
1:C:187:TYR:HA	2:C:801:NAG:C8	2.25	0.66
1:B:187:TYR:HA	2:B:801:NAG:C8	2.25	0.66
1:A:187:TYR:HA	2:A:801:NAG:C8	2.25	0.66
1:B:524:VAL:HG21	2:B:904:NAG:H81	1.77	0.66
1:B:464:ILE:O	1:B:467:ASN:HB2	1.96	0.66
1:A:396:ARG:HE	1:A:432:ASP:CB	2.07	0.66
1:A:290:PHE:HZ	1:A:296:TYR:OH	1.77	0.66
1:A:401:VAL:HG13	1:A:405:THR:O	1.95	0.66
1:C:464:ILE:O	1:C:467:ASN:HB2	1.96	0.66
1:B:524:VAL:HG23	2:B:904:NAG:H81	1.78	0.66
1:A:524:VAL:HG21	2:A:904:NAG:H81	1.76	0.66
1:C:366:LYS:HG3	1:C:367:LEU:HG	1.77	0.66
1:A:195:ASP:HB2	1:A:201:LEU:N	2.08	0.66
1:B:396:ARG:HD3	1:B:431:LEU:O	1.94	0.66
1:B:32:ASN:CG	1:B:33:LYS:H	1.98	0.66
1:C:320:THR:HG21	2:C:807:NAG:H2	1.76	0.66
1:C:222:ASP:O	1:C:222:ASP:CG	2.32	0.66
3:C:902:NDG:H3	3:C:902:NDG:O7	1.95	0.66
1:A:347:ARG:HD2	1:A:392:GLY:H	1.60	0.66
1:D:347:ARG:CD	1:D:392:GLY:H	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASP:OD2	1:C:139:ILE:HG22	1.94	0.66
1:D:396:ARG:NH2	1:D:464:ILE:CB	2.58	0.66
1:B:224:LYS:HE3	1:B:316:THR:O	1.95	0.66
1:C:524:VAL:HG21	2:C:904:NAG:H81	1.77	0.66
1:B:347:ARG:HD2	1:B:392:GLY:H	1.60	0.66
1:B:347:ARG:CD	1:B:392:GLY:H	2.07	0.66
1:D:440:PRO:HD2	1:D:522:LEU:CD1	2.26	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: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
1:A:224:LYS:HE3	1:A:316:THR:O	1.95	0.66
1:B:289:ASP:O	1:B:289:ASP:CG	2.29	0.66
1:A:366:LYS:HG3	1:A:367:LEU:HG	1.77	0.66
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:C:224:LYS:HE3	1:C:316:THR:O	1.95	0.66
1:D:224:LYS:HE3	1:D:316:THR:O	1.95	0.66
1:C:32:ASN:CG	1:C:33:LYS:H	1.99	0.66
1:A:32:ASN:CG	1:A:33:LYS:H	1.99	0.66
1:B:440:PRO:HD3	1:B:522:LEU:HD12	1.78	0.66
1:C:524:VAL:HG23	2:C:904:NAG:H81	1.78	0.66
1:C:347:ARG:CG	1:C:392:GLY:H	2.08	0.66
1:A:464:ILE:O	1:A:467:ASN:HB2	1.96	0.66
1:C:1:ASP:CA	1:D:26:SER:C	2.61	0.66
1:D:32:ASN:ND2	1:D:83:GLU:N	2.44	0.66
1:B:222:ASP:O	1:B:222:ASP:CG	2.32	0.66
1:C:1:ASP:CG	1:D:26:SER:CA	2.56	0.65
2:C:809:NAG:C6	2:C:810:NAG:H62	2.26	0.65
1:B:482:THR:OG1	1:B:500:GLN:CG	2.44	0.65
1:B:27:ASN:ND2	1:B:27:ASN:C	2.46	0.65
1:D:524:VAL:HG21	2:D:904:NAG:H81	1.76	0.65
1:D:282:LEU:HD23	1:D:283:THR:H	1.58	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: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: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:D:232:GLU:HG2	1:D:289:ASP:HA	1.77	0.65
1:C:403:ASN:HB2	3:C:902:NDG:N2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:VAL:HB	1:A:334:PRO:CD	2.24	0.65
1:C:1:ASP:CB	1:D:26:SER:CA	2.68	0.65
1:B:446:THR:CG2	1:B:537:ILE:O	2.44	0.65
2:A:809:NAG:C6	2:A:810:NAG:H62	2.26	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
2:D:904:NAG:O7	2:D:904:NAG:C3	2.45	0.65
1:C:488:ASP:HB2	1:C:493:SER:OG	1.97	0.65
1:D:403:ASN:HB2	3:D:902:NDG:N2	2.10	0.65
1:D:366:LYS:HG3	1:D:367:LEU:HG	1.77	0.65
1:D:464:ILE:O	1:D:467:ASN:HB2	1.96	0.65
1:C:482:THR:OG1	1:C:500:GLN:CG	2.44	0.65
1:C:517:GLN:C	1:C:519:ASN:N	2.47	0.65
1:C:232:GLU:HG2	1:C:289:ASP:HA	1.77	0.65
1:A:32:ASN:ND2	1:A:83:GLU:N	2.44	0.65
1:B:488:ASP:HB2	1:B:493:SER:OG	1.97	0.65
1:A:488:ASP:HB2	1:A:493:SER:OG	1.97	0.65
1:B:290:PHE:HZ	1:B:296:TYR:OH	1.76	0.65
3:D:902:NDG:O7	3:D:902:NDG:H3	1.95	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:C:265:GLU:HB3	1:C:268:PHE:CE2	2.31	0.65
1:B:341:VAL:HG21	1:B:345:LEU:HD12	1.79	0.65
2:D:809:NAG:C6	2:D:810:NAG:H62	2.26	0.65
1:C:232:GLU:HG3	1:C:290:PHE:H	1.61	0.65
1:B:366:LYS:HG3	1:B:367:LEU:HG	1.77	0.65
2:B:904:NAG:O7	2:B:904:NAG:C3	2.45	0.65
1:C:341:VAL:HG21	1:C:345:LEU:HD12	1.79	0.65
1:C:212:THR:HG22	1:C:213:ASP:H	1.62	0.65
2:D:805:NAG:C6	2:D:806:NAG:C7	2.74	0.65
1:A:440:PRO:HD3	1:A:522:LEU:HD12	1.78	0.65
1:C:440:PRO:HD3	1:C:522:LEU:HD12	1.78	0.65
1:B:364:ILE:HD12	1:B:364:ILE:O	1.97	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
1:C:327:ASN:HA	1:C:360:ASP:OD2	1.97	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:B:469:TYR:CD2	1:B:470:PRO:CD	2.80	0.64
2:A:904:NAG:O7	2:A:904:NAG:C3	2.45	0.64
1:B:289:ASP:O	1:B:290:PHE:CB	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:HG3	1:B:392:GLY:H	1.62	0.64
1:A:364:ILE:HD12	1:A:364:ILE:O	1.98	0.64
1:C:60:MET:SD	1:D:2:TRP:CH2	2.90	0.64
1:A:341:VAL:HG21	1:A:345:LEU:HD12	1.79	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:C:78:SER:N	1:D:2:TRP:HE1	1.96	0.64
1:A:343:GLU:HB3	1:A:433:VAL:CG2	2.28	0.64
1:B:343:GLU:HB3	1:B:433:VAL:CG2	2.28	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:B:212:THR:HG22	1:B:213:ASP:H	1.62	0.64
1:B:440:PRO:HD2	1:B:522:LEU:CD1	2.26	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: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:346:SER:OG	1:A:349:GLU:HG3	1.97	0.64
1:A:327:ASN:HA	1:A:360:ASP:OD2	1.97	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:406:TYR:CE1	2:C:808:NAG:H83	2.32	0.64
1:C:346:SER:OG	1:C:349:GLU:HG3	1.97	0.64
1:A:469:TYR:CD2	1:A:470:PRO:CD	2.81	0.64
1:D:221:PHE:CE1	1:D:315:SER:O	2.45	0.64
1:B:406:TYR:CE1	2:B:808:NAG:H83	2.32	0.64
1:D:375:PRO:HB3	1:D:400:TYR:CD2	2.33	0.64
1:B:327:ASN:HA	1:B:360:ASP:OD2	1.97	0.64
1:D:341:VAL:HG21	1:D:345:LEU:HD12	1.79	0.64
1:D:504:LYS:NZ	1:D:531:SER:OG	2.31	0.64
1:A:446:THR:CG2	1:A:539:CYS:SG	2.86	0.64
1:D:154:ASP:O	2:D:801:NAG:H82	1.98	0.64
1:D:227:THR:CG2	2:D:807:NAG:C7	2.76	0.64
1:A:375:PRO:HB3	1:A:400:TYR:CD2	2.33	0.64
1:D:409:ILE:HG12	1:D:425:THR:HG23	1.80	0.64
1:C:518:ASN:O	1:C:520:PRO:CD	2.46	0.64
1:D:440:PRO:HD3	1:D:522:LEU:HD12	1.78	0.64
1:A:524:VAL:HG23	2:A:904:NAG:H81	1.78	0.64
1:A:406:TYR:CE1	2:A:808:NAG:H83	2.32	0.64
1:C:343:GLU:HB3	1:C:433:VAL:CG2	2.28	0.63
1:D:232:GLU:HG3	1:D:290:PHE:H	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:PRO:HB3	1:C:400:TYR:CD2	2.33	0.63
1:C:403:ASN:HB2	3:C:902:NDG:H8C1	1.78	0.63
1:B:371:ILE:HG22	1:B:372:GLY:N	2.14	0.63
1:B:265:GLU:HB3	1:B:268:PHE:CE2	2.31	0.63
1:A:364:ILE:CD1	1:A:364:ILE:O	2.46	0.63
1:D:343:GLU:HB3	1:D:433:VAL:CG2	2.28	0.63
1:D:446:THR:CG2	1:D:539:CYS:SG	2.86	0.63
1:C:482:THR:HG21	1:C:499:THR:CA	2.27	0.63
1:A:419:VAL:HG13	2:A:809:NAG:O7	1.98	0.63
1:C:154:ASP:O	2:C:801:NAG:H82	1.98	0.63
1:B:403:ASN:CB	3:B:902:NDG:C7	2.76	0.63
1:D:364:ILE:O	1:D:364:ILE:HD12	1.97	0.63
1:C:364:ILE:O	1:C:364:ILE:CD1	2.46	0.63
1:A:368:SER:HG	1:A:370:PHE:HE1	1.45	0.63
1:C:22:VAL:HG22	1:C:23:GLN:N	2.14	0.63
1:A:409:ILE:HG12	1:A:425:THR:HG23	1.80	0.63
1:A:347:ARG:HG3	1:A:392:GLY:H	1.62	0.63
1:C:371:ILE:HG22	1:C:372:GLY:N	2.14	0.63
1:A:22:VAL:HG22	1:A:23:GLN:N	2.14	0.63
1:C:504:LYS:NZ	1:C:531:SER:OG	2.31	0.63
1:A:482:THR:HG22	1:A:499:THR:N	2.13	0.63
2:B:805:NAG:C6	2:B:806:NAG:C7	2.74	0.63
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:C:347:ARG:HG3	1:C:392:GLY:H	1.62	0.63
1:A:147:SER:OG	1:A:167:ARG:HG3	1.99	0.63
1:B:504:LYS:NZ	1:B:531:SER:OG	2.31	0.63
1:A:482:THR:HG21	1:A:499:THR:CA	2.27	0.63
1:B:469:TYR:CE1	1:B:470:PRO:HD2	2.34	0.63
1:C:469:TYR:CD2	1:C:470:PRO:CD	2.81	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: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:A:518:ASN:O	1:A:520:PRO:CD	2.46	0.63
1:D:347:ARG:HG3	1:D:392:GLY:H	1.62	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:B:154:ASP:CA	2:B:801:NAG:H82	2.29	0.63
1:B:486:GLU:O	1:B:495:LEU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:346:SER:OG	1:B:349:GLU:HG3	1.97	0.63
1:B:419:VAL:HG13	2:B:809:NAG:O7	1.98	0.63
1:A:504:LYS:NZ	1:A:531:SER:OG	2.32	0.63
1:C:486:GLU:O	1:C:494:MET:CA	2.46	0.63
2:C:904:NAG:C3	2:C:904:NAG:O7	2.45	0.63
1:D:482:THR:HG21	1:D:499:THR:CA	2.27	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:B:154:ASP:O	2:B:801:NAG:H82	1.98	0.63
1:B:127:VAL:HG22	1:B:128:MET:N	2.14	0.63
1:B:364:ILE:CD1	1:B:364:ILE:O	2.46	0.63
1:C:411:LEU:HD22	1:C:421:THR:HG23	1.81	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: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:B:374:ASP:O	1:B:375:PRO:O	2.17	0.62
1:A:265:GLU:HB3	1:A:268:PHE:CE2	2.31	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
1:D:486:GLU:O	1:D:494:MET:CA	2.46	0.62
1:C:403:ASN:CB	3:C:902:NDG:C7	2.76	0.62
1:D:364:ILE:O	1:D:364:ILE:CD1	2.46	0.62
1:A:469:TYR:CE1	1:A:470:PRO:HD2	2.34	0.62
1:A:154:ASP:CA	2:A:801:NAG:H82	2.29	0.62
1:D:371:ILE:HG22	1:D:372:GLY:N	2.14	0.62
1:A:127:VAL:HG22	1:A:128:MET:N	2.14	0.62
1:D:486:GLU:O	1:D:495:LEU:N	2.31	0.62
1:A:524:VAL:HG23	2:A:904:NAG:C8	2.29	0.62
1:C:374:ASP:O	1:C:375:PRO:O	2.17	0.62
1:B:518:ASN:O	1:B:520:PRO:CD	2.46	0.62
1:B:22:VAL:HG22	1:B:23:GLN:N	2.14	0.62
1:D:419:VAL:HG13	2:D:809:NAG:O7	1.98	0.62
1:D:154:ASP:CA	2:D:801:NAG:H82	2.29	0.62
1:C:227:THR:CG2	2:C:807:NAG:C7	2.76	0.62
2:A:805:NAG:C6	2:A:806:NAG:C7	2.74	0.62
1:C:32:ASN:ND2	1:C:83:GLU:N	2.45	0.62
1:B:524:VAL:HG23	2:B:904:NAG:C8	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:LYS:HG3	1:D:367:LEU:N	2.04	0.62
1:B:446:THR:CG2	1:B:539:CYS:SG	2.86	0.62
1:A:517:GLN:C	1:A:519:ASN:N	2.47	0.62
1:D:403:ASN:CB	3:D:902:NDG:C7	2.76	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:C:524:VAL:CG2	2:C:904:NAG:C8	2.78	0.62
1:B:142:LEU:HB3	1:B:196:LEU:HA	1.81	0.62
1:D:371:ILE:CG2	1:D:372:GLY:H	2.13	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:B:232:GLU:HG3	1:B:290:PHE:H	1.61	0.62
1:C:469:TYR:CE1	1:C:470:PRO:HD2	2.34	0.62
1:B:486:GLU:O	1:B:494:MET:CA	2.46	0.62
1:B:482:THR:HG22	1:B:499:THR:N	2.13	0.62
1:A:403:ASN:O	1:A:405:THR:N	2.33	0.62
1:A:2:TRP:CZ3	1:B:6:PRO:HG3	2.35	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:B:212:THR:HG22	1:B:213:ASP:N	2.15	0.61
1:D:68:ARG:HD3	1:D:100:ASP:HA	1.82	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:A:371:ILE:HG22	1:A:372:GLY:N	2.14	0.61
1:B:508:SER:HB3	1:B:526:ASN:OD1	2.00	0.61
1:A:411:LEU:HD22	1:A:421:THR:HG23	1.81	0.61
1:A:181:ARG:NE	1:A:213:ASP:OD1	2.34	0.61
1:C:403:ASN:O	1:C:405:THR:N	2.33	0.61
1:A:68:ARG:HD3	1:A:100:ASP:HA	1.82	0.61
1:A:449:ASP:H	1:A:532:CYS:CB	2.12	0.61
1:C:154:ASP:O	1:C:155:PRO:C	2.36	0.61
1:B:181:ARG:NE	1:B:213:ASP:OD1	2.34	0.61
1:A:212:THR:HG22	1:A:213:ASP:N	2.15	0.61
1:D:524:VAL:CG2	2:D:904:NAG:C8	2.78	0.61
1:B:371:ILE:CG2	1:B:372:GLY:H	2.13	0.61
1:B:524:VAL:CG2	2:B:904:NAG:C8	2.78	0.61
1:D:379:LEU:H	1:D:379:LEU:HD23	1.66	0.61
1:C:68:ARG:HD3	1:C:100:ASP:HA	1.82	0.61
1:A:374:ASP:O	1:A:375:PRO:O	2.17	0.61
1:D:403:ASN:O	1:D:405:THR:N	2.33	0.61
1:D:127:VAL:HG22	1:D:128:MET:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:SER:HB3	1:C:526:ASN:OD1	2.00	0.61
1:D:154:ASP:O	1:D:155:PRO:C	2.37	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:379:LEU:H	1:A:379:LEU:HD23	1.66	0.61
1:C:181:ARG:NE	1:C:213:ASP:OD1	2.34	0.61
1:A:475:LEU:O	1:A:479:SER:HB3	2.01	0.61
1:D:469:TYR:CE1	1:D:470:PRO:HD2	2.34	0.61
1:D:181:ARG:NE	1:D:213:ASP:OD1	2.34	0.61
1:C:212:THR:HG22	1:C:213:ASP:N	2.15	0.61
1:A:403:ASN:HB2	3:A:902:NDG:H8C1	1.78	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:B:154:ASP:O	1:B:155:PRO:C	2.36	0.60
1:D:232:GLU:CG	1:D:290:PHE:N	2.64	0.60
1:A:486:GLU:O	1:A:495:LEU:N	2.31	0.60
1:B:403:ASN:HB2	3:B:902:NDG:H8C1	1.78	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:C:27:ASN:OD1	1:D:90:GLU:CG	2.47	0.60
1:D:403:ASN:HB2	3:D:902:NDG:H8C1	1.78	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: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:154:ASP:O	1:A:155:PRO:C	2.36	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: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:116:SER:HA	1:C:210:GLN:O	2.02	0.60
1:D:482:THR:HG22	1:D:499:THR:N	2.13	0.60
1:B:155:PRO:C	1:B:157:GLU:N	2.56	0.60
1:D:189:LEU:HD23	1:D:189:LEU:N	2.17	0.60
1:A:24:ILE:CB	1:B:1:ASP:H2	2.15	0.60
1:B:449:ASP:H	1:B:532:CYS:CB	2.12	0.60
1:A:514:SER:HA	1:A:517:GLN:O	2.02	0.60
1:D:146:LEU:HA	1:D:194:THR:O	2.02	0.60
1:A:239:VAL:HG13	1:A:240:GLN:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:VAL:HG13	1:D:240:GLN:H	1.67	0.60
1:B:508:SER:HA	1:B:526:ASN:HA	1.84	0.60
1:A:450:GLN:HB2	1:A:533:GLU:CA	2.26	0.59
1:B:523:THR:CG2	1:B:524:VAL:H	1.94	0.59
1:C:443:ARG:HH11	1:C:443:ARG:HG3	1.67	0.59
1:C:24:ILE:HG21	1:D:2:TRP:HA	0.65	0.59
1:D:155:PRO:C	1:D:157:GLU:N	2.56	0.59
1:C:514:SER:HA	1:C:517:GLN:O	2.02	0.59
1:A:403:ASN:CB	3:A:902:NDG:C7	2.76	0.59
1:B:379:LEU:HD23	1:B:379:LEU:H	1.66	0.59
1:C:447:MET:HB2	1:C:529:VAL:HG22	1.84	0.59
1:D:508:SER:HA	1:D:526:ASN:HA	1.84	0.59
1:B:49:GLY:O	1:B:63:THR:HG21	2.02	0.59
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:A:508:SER:HA	1:A:526:ASN:HA	1.84	0.59
1:C:336:VAL:HB	1:C:426:LEU:HD23	1.84	0.59
1:B:268:PHE:HA	1:B:285:ALA:HB3	1.84	0.59
1:C:189:LEU:HD23	1:C:189:LEU:N	2.17	0.59
1:B:189:LEU:N	1:B:189:LEU:HD23	2.17	0.59
1:C:155:PRO:C	1:C:157:GLU:N	2.56	0.59
1:D:336:VAL:HB	1:D:426:LEU:HD23	1.84	0.59
1:A:447:MET:HB2	1:A:529:VAL:HG22	1.84	0.59
1:C:1:ASP:HB2	1:D:27:ASN:N	2.17	0.59
1:A:221:PHE:HA	1:A:244:VAL:HG12	1.85	0.59
1:D:367:LEU:CB	1:D:413:THR:O	2.51	0.59
1:A:146:LEU:HA	1:A:194:THR:O	2.02	0.59
1:B:475:LEU:O	1:B:479:SER:HB3	2.01	0.59
1:A:116:SER:HA	1:A:210:GLN:O	2.02	0.59
1:C:475:LEU:O	1:C:479:SER:HB3	2.01	0.59
1:D:475:LEU:O	1:D:479:SER:HB3	2.01	0.59
1:B:32:ASN:HD22	1:B:83:GLU:H	1.51	0.59
1:A:268:PHE:HA	1:A:285:ALA:HB3	1.85	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:D:415:ASP:OD1	1:D:416:GLY:N	2.26	0.59
1:C:309:SER:O	1:C:310:VAL:HG23	2.03	0.59
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.68	0.59
1:C:449:ASP:H	1:C:532:CYS:CB	2.12	0.59
1:B:286:LYS:O	1:B:287:GLY:O	2.21	0.59
1:B:232:GLU:HG2	1:B:289:ASP:CA	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:GLU:O	1:C:495:LEU:N	2.31	0.59
1:B:146:LEU:HA	1:B:194:THR:O	2.02	0.59
1:D:195:ASP:CB	1:D:200:GLY:HA3	2.33	0.59
1:B:473:VAL:HA	1:B:513:LEU:HD23	1.85	0.59
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.68	0.59
1:D:396:ARG:NH2	1:D:464:ILE:HG21	2.17	0.59
1:C:232:GLU:CG	1:C:290:PHE:N	2.64	0.59
1:C:232:GLU:HG2	1:C:289:ASP:CA	2.33	0.59
1:D:518:ASN:O	1:D:520:PRO:CD	2.46	0.59
1:A:189:LEU:N	1:A:189:LEU:HD23	2.17	0.59
1:A:49:GLY:O	1:A:63:THR:HG21	2.02	0.59
1:B:116:SER:HA	1:B:210:GLN:O	2.02	0.59
1:A:232:GLU:CG	1:A:290:PHE:N	2.64	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:C:406:TYR:HB3	1:C:428:LEU:CD2	2.33	0.58
1:C:146:LEU:HA	1:C:194:THR:O	2.02	0.58
1:B:447:MET:HB2	1:B:529:VAL:HG22	1.84	0.58
1:B:443:ARG:HA	1:B:525:VAL:HG13	1.85	0.58
1:A:309:SER:O	1:A:310:VAL:HG23	2.03	0.58
1:C:49:GLY:O	1:C:63:THR:HG21	2.02	0.58
1:A:537:ILE:HG12	1:A:538:LYS:N	2.19	0.58
1:D:299:GLN:C	1:D:300:ILE:HD12	2.24	0.58
1:D:406:TYR:HB3	1:D:428:LEU:CD2	2.33	0.58
1:C:367:LEU:CB	1:C:413:THR:O	2.51	0.58
1:B:239:VAL:HG13	1:B:240:GLN:H	1.67	0.58
1:A:38:ILE:HG22	1:A:53:ILE:HG22	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:443:ARG:HA	1:A:525:VAL:HG13	1.85	0.58
1:D:286:LYS:O	1:D:287:GLY:O	2.21	0.58
1:A:367:LEU:CB	1:A:413:THR:O	2.51	0.58
1:D:49:GLY:O	1:D:63:THR:HG21	2.02	0.58
1:D:443:ARG:HA	1:D:525:VAL:HG13	1.85	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:CA	2.51	0.58
1:C:235:ILE:HG12	1:C:287:GLY:HA2	1.82	0.58
1:B:335:ALA:HB1	3:B:811:NDG:C6	2.33	0.58
1:D:38:ILE:HG22	1:D:53:ILE:HG22	1.85	0.58
1:C:195:ASP:CB	1:C:200:GLY:HA3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:PHE:HA	1:D:285:ALA:HB3	1.85	0.58
1:B:396:ARG:NH2	1:B:464:ILE:HG21	2.17	0.58
1:C:366:LYS:HG3	1:C:367:LEU:N	2.04	0.58
1:A:336:VAL:HB	1:A:426:LEU:HD23	1.84	0.58
1:B:221:PHE:HA	1:B:244:VAL:HG12	1.85	0.58
1:D:232:GLU:HG2	1:D:289:ASP:CA	2.33	0.58
1:B:232:GLU:CG	1:B:290:PHE:N	2.64	0.58
1:C:268:PHE:HA	1:C:285:ALA:HB3	1.85	0.58
1:B:363:GLN:O	1:B:364:ILE:HG22	2.03	0.58
1:A:296:TYR:HB2	1:A:321:VAL:HB	1.86	0.58
1:B:299:GLN:C	1:B:300:ILE:HD12	2.24	0.58
1:D:154:ASP:CB	1:D:155:PRO:CD	2.82	0.58
1:C:226:TYR:CE2	1:C:242:LEU:HD23	2.39	0.58
1:A:232:GLU:HG2	1:A:289:ASP:CA	2.33	0.58
1:C:335:ALA:HB1	3:C:811:NDG:C6	2.33	0.58
1:B:195:ASP:CB	1:B:200:GLY:HA3	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: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:C:154:ASP:CB	1:C:155:PRO:CD	2.82	0.58
1:D:320:THR:CG2	2:D:807:NAG:C2	2.76	0.58
1:B:296:TYR:HB2	1:B:321:VAL:HB	1.86	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:B:332:PHE:CD2	1:B:424:GLY:HA3	2.39	0.58
1:D:309:SER:O	1:D:310:VAL:HG23	2.03	0.58
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:68:ARG:HG3	1:B:69:GLU:N	2.19	0.57
1:C:332:PHE:CD2	1:C:424:GLY:HA3	2.39	0.57
1:C:60:MET:SD	1:D:2:TRP:CZ3	2.97	0.57
1:D:450:GLN:HB2	1:D:533:GLU:CA	2.26	0.57
1:D:154:ASP:CB	2:D:801:NAG:HN2	2.16	0.57
1:A:299:GLN:C	1:A:300:ILE:HD12	2.24	0.57
1:B:406:TYR:HB3	1:B:428:LEU:HD21	1.87	0.57
1:C:406:TYR:HB3	1:C:428:LEU:HD21	1.87	0.57
1:D:332:PHE:CD2	1:D:424:GLY:HA3	2.39	0.57
1:D:537:ILE:HG12	1:D:538:LYS:N	2.19	0.57
1:C:299:GLN:C	1:C:300:ILE:HD12	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:PHE:HA	1:D:244:VAL:HG12	1.85	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: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:A:226:TYR:CE2	1:A:242:LEU:HD23	2.39	0.57
1:B:505:GLY:HA2	1:B:529:VAL:H	1.69	0.57
1:B:38:ILE:HG22	1:B:53:ILE:HG22	1.85	0.57
1:C:38:ILE:HG22	1:C:53:ILE:HG22	1.85	0.57
1:A:155:PRO:C	1:A:157:GLU:N	2.56	0.57
1:D:235:ILE:HG12	1:D:287:GLY:HA2	1.82	0.57
1:C:537:ILE:HG12	1:C:538:LYS:N	2.19	0.57
1:D:363:GLN:O	1:D:364:ILE:HG22	2.03	0.57
1:A:393:ASN:C	1:A:394:LEU:HD12	2.25	0.57
1:B:42:GLY:HA2	1:B:47:PRO:O	2.04	0.57
1:C:286:LYS:O	1:C:287:GLY:O	2.21	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:A:505:GLY:HA2	1:A:529:VAL:H	1.70	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:C:393:ASN:C	1:C:394:LEU:HD12	2.25	0.57
1:C:443:ARG:HA	1:C:525:VAL:HG13	1.85	0.57
1:C:189:LEU:HD21	1:C:209:ILE:HD12	1.87	0.57
1:B:108:PHE:CE1	1:B:203:VAL:HG23	2.40	0.57
1:B:154:ASP:CB	1:B:155:PRO:CD	2.82	0.57
1:A:473:VAL:HA	1:A:513:LEU:HD23	1.85	0.57
1:C:473:VAL:HA	1:C:513:LEU:HD23	1.85	0.57
1:A:68:ARG:HG3	1:A:69:GLU:N	2.19	0.57
1:A:259:TYR:O	1:A:260:LYS:HB3	2.05	0.57
1:A:108:PHE:CE1	1:A:203:VAL:HG23	2.40	0.57
1:D:393:ASN:C	1:D:394:LEU:HD12	2.25	0.56
1:C:259:TYR:O	1:C:260:LYS:HB3	2.05	0.56
1:D:378:TRP:O	1:D:391:ASN:HB2	2.06	0.56
1:A:332:PHE:CD2	1:A:424:GLY:HA3	2.39	0.56
1:A:396:ARG:NH2	1:A:464:ILE:HG21	2.17	0.56
1:C:396:ARG:NH2	1:C:464:ILE:HG21	2.17	0.56
1:C:330:PRO:HD3	1:C:414:ASP:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:VAL:HG12	1:C:338:ARG:HB2	1.87	0.56
1:A:222:ASP:N	1:A:243:SER:O	2.38	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:D:394:LEU:N	1:D:394:LEU:CD1	2.69	0.56
1:B:259:TYR:O	1:B:260:LYS:HB3	2.05	0.56
1:D:108:PHE:CE1	1:D:203:VAL:HG23	2.40	0.56
1:A:42:GLY:HA2	1:A:47:PRO:O	2.04	0.56
1:C:108:PHE:CE1	1:C:203:VAL:HG23	2.40	0.56
1:A:336:VAL:HG12	1:A:338:ARG:HB2	1.87	0.56
1:B:393:ASN:C	1:B:394:LEU:HD12	2.25	0.56
1:C:68:ARG:HG3	1:C:69:GLU:N	2.19	0.56
1:C:162:LEU:O	1:C:174:LEU:HD12	2.06	0.56
1:B:537:ILE:HG12	1:B:538:LYS:N	2.19	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: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: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: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:A:378:TRP:O	1:A:391:ASN:HB2	2.06	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:D:336:VAL:HG12	1:D:338:ARG:HB2	1.87	0.56
1:D:162:LEU:O	1:D:174:LEU:HD12	2.06	0.56
1:C:369:TYR:HD1	1:C:383:LYS:O	1.88	0.56
1:C:27:ASN:CG	1:D:90:GLU:HG3	2.24	0.56
1:D:330:PRO:HD3	1:D:414:ASP:HB2	1.86	0.56
1:D:296:TYR:HB2	1:D:321:VAL:HB	1.86	0.56
1:D:222:ASP:N	1:D:243:SER:O	2.38	0.56
1:A:522:LEU:CD2	1:A:523:THR:HB	2.26	0.56
1:A:406:TYR:HB3	1:A:428:LEU:HD21	1.86	0.56
1:A:365:GLN:O	1:A:365:GLN:CG	2.54	0.56
1:B:394:LEU:CD1	1:B:394:LEU:N	2.69	0.56
1:C:118:ARG:HA	1:C:212:THR:HB	1.87	0.56
1:A:118:ARG:HA	1:A:212:THR:HB	1.87	0.56
1:B:439:VAL:HG13	1:B:522:LEU:HD11	1.88	0.56
1:C:439:VAL:HG13	1:C:522:LEU:HD11	1.88	0.56
1:C:394:LEU:N	1:C:394:LEU:CD1	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:VAL:HG21	1:D:351:ILE:CG2	2.36	0.56
1:B:333:VAL:CG2	1:B:334:PRO:HD3	2.36	0.56
1:B:272:THR:CG2	1:B:273:THR:H	2.19	0.56
1:D:439:VAL:HG13	1:D:522:LEU:HD11	1.88	0.55
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:A:482:THR:HG21	1:A:499:THR:C	2.27	0.55
1:A:90:GLU:HB2	1:B:90:GLU:O	2.06	0.55
1:C:155:PRO:N	2:C:801:NAG:H82	2.20	0.55
1:A:154:ASP:CB	2:A:801:NAG:HN2	2.16	0.55
1:D:406:TYR:HB3	1:D:428:LEU:HD21	1.87	0.55
1:D:365:GLN:O	1:D:365:GLN:CG	2.54	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:D:118:ARG:HA	1:D:212:THR:HB	1.88	0.55
1:D:32:ASN:CG	1:D:33:LYS:N	2.59	0.55
1:B:336:VAL:HG12	1:B:338:ARG:HB2	1.87	0.55
1:C:32:ASN:CG	1:C:33:LYS:N	2.59	0.55
1:A:32:ASN:CG	1:A:33:LYS:N	2.59	0.55
1:A:439:VAL:HG13	1:A:522:LEU:HD11	1.88	0.55
1:C:339:VAL:HG21	1:C:351:ILE:CG2	2.36	0.55
1:B:155:PRO:N	2:B:801:NAG:H82	2.20	0.55
1:C:378:TRP:O	1:C:391:ASN:HB2	2.06	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:D:459:ILE:HG21	1:D:471:TYR:CE2	2.42	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:A:339:VAL:HG21	1:A:351:ILE:CG2	2.36	0.55
1:A:195:ASP:CB	1:A:200:GLY:HA3	2.33	0.55
1:C:333:VAL:CG2	1:C:334:PRO:HD3	2.36	0.55
1:C:268:PHE:CD2	1:C:268:PHE:N	2.75	0.55
1:B:415:ASP:OD1	1:B:416:GLY:N	2.27	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:D:155:PRO:N	2:D:801:NAG:H82	2.20	0.55
1:C:154:ASP:CG	1:C:155:PRO:CD	2.75	0.55
1:A:155:PRO:HG2	2:A:801:NAG:O7	2.07	0.55
1:D:335:ALA:HB1	3:D:811:NDG:C6	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ASN:N	1:D:278:ASN:HD22	2.05	0.55
1:D:369:TYR:HD1	1:D:383:LYS:O	1.88	0.55
1:C:1:ASP:N	1:D:26:SER:C	2.60	0.55
1:C:482:THR:HG22	1:C:499:THR:H	1.70	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:B:32:ASN:CG	1:B:33:LYS:N	2.59	0.55
1:A:459:ILE:HG21	1:A:471:TYR:CE2	2.42	0.55
1:D:333:VAL:CG2	1:D:334:PRO:HD3	2.36	0.55
1:C:92:MET:O	1:D:2:TRP:NE1	2.40	0.55
1:B:419:VAL:CG1	1:B:420:GLY:N	2.70	0.55
1:C:155:PRO:HG2	2:C:801:NAG:O7	2.07	0.55
1:B:155:PRO:HG2	2:B:801:NAG:O7	2.07	0.55
1:D:117:VAL:O	1:D:211:ILE:HA	2.07	0.55
1:D:154:ASP:CG	1:D:155:PRO:CD	2.75	0.55
1:C:320:THR:CG2	2:C:807:NAG:C2	2.76	0.55
1:A:438:PRO:HB2	1:A:513:LEU:HD12	1.89	0.55
1:D:75:VAL:O	1:D:76:LEU:HD23	2.07	0.55
1:A:432:ASP:CG	1:A:464:ILE:CG2	2.74	0.54
1:A:3:VAL:CG1	1:B:4:ILE:CD1	2.44	0.54
1:C:28:LYS:HB3	1:C:88:VAL:HG11	1.89	0.54
1:D:155:PRO:HG2	2:D:801:NAG:O7	2.07	0.54
1:B:117:VAL:O	1:B:211:ILE:HA	2.07	0.54
1:C:226:TYR:O	1:C:227:THR:CG2	2.55	0.54
1:B:226:TYR:O	1:B:227:THR:CG2	2.55	0.54
1:C:367:LEU:C	1:C:367:LEU:HD12	2.28	0.54
1:D:272:THR:CG2	1:D:273:THR:H	2.19	0.54
1:B:438:PRO:HB2	1:B:513:LEU:HD12	1.89	0.54
1:B:363:GLN:C	1:B:364:ILE:CG2	2.75	0.54
1:B:169:THR:OG1	1:B:171:VAL:HG23	2.07	0.54
1:C:92:MET:CB	1:D:2:TRP:CD1	2.90	0.54
1:A:75:VAL:O	1:A:76:LEU:HD23	2.08	0.54
1:D:419:VAL:CG1	1:D:420:GLY:N	2.70	0.54
1:A:154:ASP:CG	1:A:155:PRO:CD	2.75	0.54
1:C:226:TYR:HB2	1:C:319:VAL:HG22	1.90	0.54
1:B:459:ILE:HG21	1:B:471:TYR:CE2	2.42	0.54
1:A:268:PHE:CD2	1:A:268:PHE:N	2.75	0.54
1:C:75:VAL:O	1:C:76:LEU:HD23	2.08	0.54
1:D:466:PRO:O	1:D:468:THR:N	2.40	0.54
1:B:450:GLN:CB	1:B:532:CYS:O	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:THR:CG2	1:C:273:THR:H	2.19	0.54
1:D:490:LYS:O	1:D:490:LYS:HG2	2.08	0.54
1:C:432:ASP:CG	1:C:464:ILE:CG2	2.74	0.54
1:C:78:SER:H	1:D:2:TRP:HE1	1.55	0.54
1:B:75:VAL:O	1:B:76:LEU:HD23	2.08	0.54
1:C:450:GLN:CB	1:C:532:CYS:O	2.56	0.54
1:B:466:PRO:O	1:B:468:THR:N	2.40	0.54
1:C:466:PRO:O	1:C:468:THR:N	2.40	0.54
1:B:482:THR:HG21	1:B:499:THR:C	2.27	0.54
1:C:117:VAL:O	1:C:211:ILE:HA	2.07	0.54
1:B:154:ASP:CG	1:B:155:PRO:CD	2.75	0.54
1:A:32:ASN:HD22	1:A:83:GLU:H	1.51	0.54
1:B:367:LEU:HD12	1:B:367:LEU:C	2.28	0.54
1:A:363:GLN:C	1:A:364:ILE:CG2	2.75	0.54
1:C:169:THR:OG1	1:C:171:VAL:HG23	2.07	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:C:318:THR:CG2	2:C:806:NAG:H5	2.34	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:D:482:THR:HG21	1:D:499:THR:C	2.27	0.54
1:A:154:ASP:CB	1:A:155:PRO:CD	2.82	0.54
1:D:371:ILE:HG23	1:D:372:GLY:H	1.73	0.54
1:D:217:ASN:ND2	1:D:217:ASN:N	2.56	0.54
1:C:482:THR:HG21	1:C:499:THR:C	2.27	0.54
1:C:352:ILE:HG13	1:C:388:VAL:CB	2.33	0.54
1:A:320:THR:CG2	2:A:807:NAG:C2	2.76	0.54
1:D:367:LEU:C	1:D:367:LEU:HD12	2.28	0.54
1:C:363:GLN:C	1:C:364:ILE:CG2	2.75	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:D:450:GLN:CB	1:D:532:CYS:O	2.56	0.54
1:D:403:ASN:HB2	3:D:902:NDG:H8C2	1.87	0.54
1:A:278:ASN:N	1:A:278:ASN:HD22	2.05	0.54
1:C:252:THR:HG23	1:C:253:PRO:HD2	1.90	0.54
1:B:432:ASP:CG	1:B:464:ILE:CG2	2.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:ARG:NH1	1:D:443:ARG:HG3	2.23	0.54
1:A:169:THR:OG1	1:A:171:VAL:HG23	2.07	0.54
1:D:169:THR:OG1	1:D:171:VAL:HG23	2.07	0.54
1:D:28:LYS:HB3	1:D:88:VAL:HG11	1.89	0.53
1:A:450:GLN:CB	1:A:532:CYS:O	2.56	0.53
1:A:117:VAL:O	1:A:211:ILE:HA	2.07	0.53
1:D:276:GLU:CG	1:D:277:SER:N	2.71	0.53
1:D:363:GLN:C	1:D:364:ILE:CG2	2.75	0.53
1:C:443:ARG:NH1	1:C:443:ARG:HG3	2.23	0.53
1:C:217:ASN:N	1:C:217:ASN:ND2	2.56	0.53
1:D:252:THR:HG23	1:D:253:PRO:HD2	1.91	0.53
1:A:217:ASN:N	1:A:217:ASN:ND2	2.56	0.53
1:C:490:LYS:O	1:C:490:LYS:HG2	2.08	0.53
1:C:32:ASN:HD22	1:C:83:GLU:H	1.51	0.53
1:A:490:LYS:HG2	1:A:490:LYS:O	2.08	0.53
1:A:155:PRO:N	2:A:801:NAG:H82	2.20	0.53
1:D:352:ILE:CG1	1:D:388:VAL:HB	2.33	0.53
1:C:278:ASN:HD22	1:C:278:ASN:N	2.05	0.53
1:B:268:PHE:N	1:B:268:PHE:CD2	2.75	0.53
1:B:22:VAL:HG22	1:B:23:GLN:H	1.73	0.53
1:C:332:PHE:HD2	1:C:424:GLY:HA3	1.73	0.53
1:A:249:MET:O	1:A:252:THR:HB	2.09	0.53
1:B:533:GLU:HA	1:B:533:GLU:OE2	2.09	0.53
1:B:403:ASN:HB2	3:B:902:NDG:H8C2	1.87	0.53
1:C:276:GLU:CG	1:C:277:SER:N	2.71	0.53
1:A:28:LYS:HB3	1:A:88:VAL:HG11	1.89	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:A:533:GLU:OE2	1:A:533:GLU:HA	2.09	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: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:C:242:LEU:O	1:C:279:GLN:HB3	2.09	0.53
1:D:522:LEU:CD2	1:D:523:THR:HB	2.26	0.53
1:A:458:THR:HG22	1:A:493:SER:HB3	1.91	0.53
1:A:403:ASN:C	1:A:405:THR:H	2.12	0.53
1:D:403:ASN:C	1:D:405:THR:H	2.12	0.53
1:A:367:LEU:HD12	1:A:367:LEU:C	2.28	0.53
1:A:347:ARG:HG3	1:A:391:ASN:HA	1.91	0.53
1:D:241:ARG:NE	1:D:281:ILE:HD12	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:THR:HG23	1:B:253:PRO:HD2	1.90	0.53
1:A:482:THR:CG2	1:A:499:THR:CA	2.87	0.53
1:D:533:GLU:HA	1:D:533:GLU:OE2	2.09	0.53
1:C:371:ILE:HG23	1:C:372:GLY:H	1.73	0.53
1:C:365:GLN:O	1:C:365:GLN:CG	2.54	0.53
1:A:242:LEU:O	1:A:279:GLN:HB3	2.09	0.53
1:B:242:LEU:O	1:B:279:GLN:HB3	2.09	0.53
1:C:458:THR:HG22	1:C:493:SER:HB3	1.90	0.53
1:A:276:GLU:CG	1:A:277:SER:N	2.71	0.53
1:A:482:THR:HG22	1:A:499:THR:H	1.70	0.53
1:C:512:LEU:HD11	1:C:519:ASN:HD21	1.74	0.53
1:A:226:TYR:HB2	1:A:319:VAL:HG22	1.90	0.53
1:A:31:PHE:CD2	1:A:32:ASN:HB2	2.44	0.53
1:D:367:LEU:HD13	1:D:412:VAL:HG23	1.91	0.53
1:C:347:ARG:HG3	1:C:391:ASN:HA	1.91	0.53
1:A:371:ILE:HG23	1:A:372:GLY:H	1.73	0.53
1:C:438:PRO:HB2	1:C:513:LEU:HD12	1.89	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:C:1:ASP:CB	1:D:26:SER:C	2.77	0.53
1:C:450:GLN:HB2	1:C:533:GLU:CA	2.26	0.53
1:A:482:THR:HG22	1:A:482:THR:O	2.08	0.53
1:A:330:PRO:HB3	1:A:358:ASP:HB2	1.89	0.53
1:B:512:LEU:HD11	1:B:519:ASN:HD21	1.74	0.53
1:C:373:ASN:HB3	1:C:409:ILE:H	1.74	0.53
1:C:2:TRP:CZ2	1:D:53:ILE:CD1	2.80	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:D:138:ASN:HD22	1:D:138:ASN:C	2.13	0.52
1:C:1:ASP:H1	1:D:26:SER:C	2.07	0.52
1:C:31:PHE:CD2	1:C:32:ASN:HB2	2.44	0.52
1:D:458:THR:HG22	1:D:493:SER:HB3	1.90	0.52
1:D:426:LEU:O	1:D:426:LEU:HD13	2.10	0.52
1:A:373:ASN:HB3	1:A:409:ILE:H	1.73	0.52
1:B:369:TYR:O	1:B:383:LYS:HG2	2.09	0.52
1:C:426:LEU:HD13	1:C:426:LEU:O	2.10	0.52
1:A:318:THR:CG2	2:A:806:NAG:H5	2.34	0.52
1:B:403:ASN:C	1:B:405:THR:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LEU:O	3:C:804:NDG:C8	2.57	0.52
1:C:249:MET:O	1:C:252:THR:HB	2.08	0.52
1:D:105:ARG:HG3	1:D:106:PRO:HD2	1.91	0.52
1:A:2:TRP:CZ2	1:B:95:THR:CG2	2.89	0.52
2:D:809:NAG:H61	2:D:810:NAG:C6	2.39	0.52
1:B:426:LEU:HD13	1:B:426:LEU:O	2.09	0.52
1:D:194:THR:HG22	1:D:195:ASP:N	2.25	0.52
1:A:312:LEU:O	3:A:804:NDG:C8	2.57	0.52
1:C:369:TYR:O	1:C:383:LYS:HG2	2.09	0.52
1:B:217:ASN:N	1:B:217:ASN:ND2	2.56	0.52
1:B:105:ARG:HG3	1:B:106:PRO:HD2	1.91	0.52
1:C:1:ASP:OD1	1:D:26:SER:N	2.27	0.52
1:C:22:VAL:HG22	1:C:23:GLN:H	1.73	0.52
1:A:154:ASP:C	2:A:801:NAG:C8	2.62	0.52
1:B:226:TYR:HB2	1:B:319:VAL:HG22	1.89	0.52
1:B:458:THR:HG22	1:B:493:SER:HB3	1.91	0.52
1:B:373:ASN:HB3	1:B:409:ILE:H	1.74	0.52
1:D:369:TYR:O	1:D:383:LYS:HG2	2.09	0.52
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.91	0.52
1:C:138:ASN:HD22	1:C:138:ASN:C	2.13	0.52
1:D:242:LEU:O	1:D:279:GLN:HB3	2.09	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:A:272:THR:CG2	2:A:803:NAG:HN2	2.23	0.52
1:B:482:THR:CG2	1:B:499:THR:CA	2.87	0.52
1:B:318:THR:CG2	2:B:806:NAG:H5	2.34	0.52
1:D:512:LEU:HD11	1:D:519:ASN:HD21	1.74	0.52
1:B:336:VAL:O	1:B:426:LEU:HD22	2.10	0.52
1:D:221:PHE:HB3	1:D:223:PRO:O	2.10	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:A:512:LEU:HD11	1:A:519:ASN:HD21	1.75	0.52
1:A:347:ARG:HD2	1:A:392:GLY:N	2.25	0.52
1:C:505:GLY:O	1:C:506:ASP:OD1	2.28	0.52
1:A:332:PHE:HD2	1:A:424:GLY:HA3	1.73	0.52
1:A:155:PRO:CD	2:A:801:NAG:H82	2.40	0.52
1:A:402:LYS:C	1:A:403:ASN:O	2.46	0.52
1:B:367:LEU:HD13	1:B:412:VAL:HG23	1.91	0.52
1:A:22:VAL:HG22	1:A:23:GLN:H	1.73	0.52
1:B:312:LEU:O	3:B:804:NDG:C8	2.57	0.52
1:C:94:ILE:CG2	1:D:2:TRP:CH2	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:TRP:HZ3	1:B:6:PRO:HG3	1.74	0.52
1:C:272:THR:CG2	2:C:803:NAG:HN2	2.23	0.52
1:C:268:PHE:C	1:C:285:ALA:HB3	2.30	0.52
1:B:268:PHE:C	1:B:285:ALA:HB3	2.30	0.52
1:D:268:PHE:CD2	1:D:268:PHE:N	2.75	0.52
1:B:138:ASN:C	1:B:138:ASN:HD22	2.13	0.52
1:C:450:GLN:CG	1:C:533:GLU:OE2	2.58	0.52
1:B:450:GLN:CG	1:B:533:GLU:OE2	2.58	0.52
1:D:155:PRO:CD	2:D:801:NAG:H82	2.40	0.52
1:B:194:THR:HG22	1:B:195:ASP:N	2.25	0.52
1:B:347:ARG:HD2	1:B:392:GLY:N	2.25	0.52
1:D:312:LEU:O	3:D:804:NDG:C8	2.57	0.52
1:A:252:THR:HG23	1:A:253:PRO:HD2	1.91	0.52
1:C:27:ASN:OD1	1:D:90:GLU:HG3	2.10	0.51
1:A:426:LEU:HD13	1:A:426:LEU:O	2.09	0.51
1:A:221:PHE:HB3	1:A:223:PRO:O	2.10	0.51
1:D:523:THR:CG2	1:D:524:VAL:H	1.94	0.51
1:B:514:SER:HB3	1:B:517:GLN:O	2.10	0.51
1:A:369:TYR:O	1:A:383:LYS:HG2	2.09	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:C:221:PHE:HB3	1:C:223:PRO:O	2.10	0.51
1:D:234:GLU:HB2	1:D:235:ILE:HG22	1.93	0.51
1:C:458:THR:HA	1:C:493:SER:HA	1.93	0.51
1:A:266:GLY:N	1:A:268:PHE:CE2	2.76	0.51
1:B:266:GLY:N	1:B:268:PHE:CE2	2.76	0.51
1:D:268:PHE:C	1:D:285:ALA:HB3	2.30	0.51
1:A:505:GLY:O	1:A:506:ASP:OD1	2.28	0.51
1:B:505:GLY:O	1:B:506:ASP:OD1	2.28	0.51
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.24	0.51
1:B:234:GLU:HB2	1:B:235:ILE:HG22	1.93	0.51
1:C:338:ARG:HB3	1:C:339:VAL:HG22	1.92	0.51
1:B:352:ILE:HG13	1:B:388:VAL:CB	2.33	0.51
1:C:403:ASN:C	1:C:405:THR:H	2.12	0.51
1:B:278:ASN:N	1:B:278:ASN:HD22	2.05	0.51
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:D:31:PHE:CD2	1:D:32:ASN:HB2	2.44	0.51
1:D:428:LEU:O	1:D:428:LEU:HD23	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ARG:HG3	1:C:106:PRO:HD2	1.91	0.51
1:C:533:GLU:OE2	1:C:533:GLU:HA	2.09	0.51
1:A:450:GLN:CG	1:A:533:GLU:OE2	2.58	0.51
1:C:297:VAL:CG2	2:C:807:NAG:H62	2.41	0.51
1:D:336:VAL:O	1:D:426:LEU:HD22	2.10	0.51
1:B:428:LEU:HD23	1:B:428:LEU:O	2.11	0.51
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.23	0.51
1:D:432:ASP:CG	1:D:464:ILE:CG2	2.74	0.51
1:A:234:GLU:HB2	1:A:235:ILE:HG22	1.93	0.51
1:C:290:PHE:CE2	1:C:293:ARG:CB	2.92	0.51
1:A:428:LEU:O	1:A:428:LEU:HD23	2.11	0.51
1:C:428:LEU:HD23	1:C:428:LEU:O	2.11	0.51
1:D:22:VAL:HG22	1:D:23:GLN:H	1.73	0.51
1:B:142:LEU:O	1:B:196:LEU:HD23	2.11	0.51
1:A:194:THR:HG22	1:A:195:ASP:N	2.25	0.51
1:D:272:THR:CG2	2:D:803:NAG:HN2	2.23	0.51
1:A:268:PHE:C	1:A:285:ALA:HB3	2.30	0.51
1:A:514:SER:HB3	1:A:517:GLN:O	2.10	0.51
1:D:505:GLY:O	1:D:506:ASP:OD1	2.28	0.51
1:D:80:ALA:O	1:D:88:VAL:HG23	2.11	0.51
1:A:91:PRO:HD2	1:B:89:GLU:OE1	2.10	0.51
1:C:336:VAL:O	1:C:426:LEU:HD22	2.10	0.51
1:D:338:ARG:HB3	1:D:339:VAL:HG22	1.92	0.51
1:A:403:ASN:HB2	3:A:902:NDG:H8C2	1.87	0.51
1:B:290:PHE:CE2	1:B:293:ARG:CB	2.92	0.51
1:B:155:PRO:CD	2:B:801:NAG:H82	2.40	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:368:SER:OG	1:A:370:PHE:HE1	1.94	0.51
1:D:76:LEU:O	1:D:94:ILE:N	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: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:A:33:LYS:HB3	1:A:83:GLU:CG	2.40	0.51
1:B:397:GLU:OE1	1:B:397:GLU:N	2.44	0.51
1:A:290:PHE:CE2	1:A:293:ARG:CB	2.92	0.50
1:A:450:GLN:CB	1:A:533:GLU:HA	2.29	0.50
1:D:423:THR:HB	2:D:810:NAG:H83	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:LYS:C	1:B:403:ASN:O	2.46	0.50
1:A:382:ASN:OD1	1:A:385:ASN:N	2.45	0.50
1:C:397:GLU:N	1:C:397:GLU:OE1	2.45	0.50
1:C:1:ASP:HB2	1:D:26:SER:C	2.31	0.50
1:A:227:THR:CG2	2:A:807:NAG:H83	2.32	0.50
1:A:471:TYR:N	1:A:471:TYR:CD1	2.79	0.50
1:A:458:THR:HG22	1:A:493:SER:CB	2.42	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:B:151:LEU:HD12	1:B:190:THR:O	2.11	0.50
1:C:217:ASN:N	1:C:217:ASN:HD22	2.09	0.50
1:D:482:THR:CG2	1:D:499:THR:CA	2.87	0.50
1:C:419:VAL:HG22	2:C:809:NAG:H81	1.93	0.50
1:B:338:ARG:HB3	1:B:339:VAL:HG22	1.92	0.50
1:C:347:ARG:HD2	1:C:392:GLY:N	2.25	0.50
1:B:471:TYR:CD1	1:B:471:TYR:N	2.79	0.50
1:C:368:SER:OG	1:C:370:PHE:HE1	1.94	0.50
1:A:217:ASN:N	1:A:217:ASN:HD22	2.09	0.50
1:D:382:ASN:OD1	1:D:385:ASN:N	2.45	0.50
1:A:432:ASP:CB	1:A:464:ILE:CG2	2.89	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:D:450:GLN:CG	1:D:533:GLU:OE2	2.58	0.50
1:D:154:ASP:O	2:D:801:NAG:C8	2.60	0.50
1:B:186:GLU:OE1	2:B:801:NAG:C6	2.59	0.50
1:C:458:THR:HG22	1:C:493:SER:CB	2.41	0.50
1:D:327:ASN:OD1	1:D:360:ASP:OD1	2.30	0.50
1:B:327:ASN:OD1	1:B:360:ASP:OD1	2.30	0.50
1:B:109:THR:HG22	1:B:110:GLN:HG3	1.94	0.50
1:A:138:ASN:C	1:A:138:ASN:HD22	2.13	0.50
2:C:809:NAG:H61	2:C:810:NAG:C6	2.39	0.50
1:D:419:VAL:HG22	2:D:809:NAG:H81	1.94	0.50
1:C:514:SER:HB3	1:C:517:GLN:O	2.10	0.50
1:B:155:PRO:HG2	2:B:801:NAG:C7	2.42	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
2:A:807:NAG:H3	2:A:807:NAG:O7	2.11	0.50
1:B:522:LEU:CD2	1:B:523:THR:HB	2.26	0.50
1:C:471:TYR:CD1	1:C:471:TYR:N	2.79	0.50
1:B:217:ASN:HD22	1:B:217:ASN:N	2.10	0.50
1:C:109:THR:HG22	1:C:110:GLN:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:ASP:CB	1:C:532:CYS:N	2.74	0.50
1:C:154:ASP:O	2:C:801:NAG:C8	2.60	0.50
2:D:812:NAG:C1	2:D:812:NAG:O7	2.60	0.50
1:A:154:ASP:O	2:A:801:NAG:C8	2.60	0.50
2:B:807:NAG:H3	2:B:807:NAG:O7	2.11	0.50
1:B:458:THR:HG22	1:B:493:SER:CB	2.42	0.50
1:B:335:ALA:CB	3:B:811:NDG:C6	2.90	0.50
1:D:142:LEU:O	1:D:196:LEU:HD23	2.11	0.50
1:D:471:TYR:CD1	1:D:471:TYR:N	2.79	0.50
1:A:327:ASN:OD1	1:A:360:ASP:OD1	2.30	0.50
1:C:11:GLU:OE2	1:C:69:GLU:OE1	2.30	0.50
1:D:151:LEU:HD12	1:D:190:THR:O	2.11	0.50
1:D:217:ASN:HD22	1:D:217:ASN:N	2.09	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:432:ASP:CB	1:B:464:ILE:CG2	2.89	0.50
1:C:450:GLN:CB	1:C:533:GLU:HA	2.29	0.50
1:C:155:PRO:HG2	2:C:801:NAG:C7	2.42	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:C:227:THR:CG2	2:C:807:NAG:H83	2.32	0.50
1:D:458:THR:HA	1:D:493:SER:HA	1.93	0.50
1:B:457:LEU:HD23	1:B:494:MET:SD	2.52	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:D:363:GLN:C	1:D:364:ILE:HG23	2.32	0.50
1:A:93:GLU:C	1:B:2:TRP:HB2	2.28	0.50
1:D:186:GLU:OE1	2:D:801:NAG:C6	2.59	0.50
1:B:154:ASP:O	2:B:801:NAG:C8	2.60	0.50
1:D:290:PHE:CE2	1:D:293:ARG:CB	2.92	0.50
1:B:373:ASN:ND2	1:B:374:ASP:OD1	2.45	0.50
1:C:522:LEU:CD2	1:C:523:THR:HB	2.26	0.50
1:A:80:ALA:O	1:A:88:VAL:HG23	2.11	0.50
1:C:142:LEU:O	1:C:196:LEU:HD23	2.11	0.50
1:A:363:GLN:C	1:A:364:ILE:HG23	2.32	0.50
1:D:11:GLU:OE2	1:D:69:GLU:OE1	2.30	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:D:297:VAL:CG2	2:D:807:NAG:H62	2.41	0.50
1:A:155:PRO:O	1:A:157:GLU:N	2.43	0.50
1:B:227:THR:CG2	2:B:807:NAG:H83	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:H	1:B:151:LEU:HD12	1.77	0.50
1:A:216:ASP:HB2	1:A:217:ASN:ND2	2.27	0.50
1:C:382:ASN:OD1	1:C:385:ASN:N	2.45	0.50
1:C:449:ASP:CB	1:C:532:CYS:H	2.22	0.49
1:A:449:ASP:CB	1:A:532:CYS:N	2.74	0.49
1:C:155:PRO:CD	2:C:801:NAG:H82	2.40	0.49
2:D:807:NAG:O7	2:D:807:NAG:H3	2.11	0.49
1:B:458:THR:HA	1:B:493:SER:HA	1.93	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:D:216:ASP:HB2	1:D:217:ASN:ND2	2.27	0.49
1:A:261:ILE:HD11	1:A:264:ASN:HD22	1.77	0.49
1:C:482:THR:CG2	1:C:499:THR:CA	2.87	0.49
1:D:482:THR:HG22	1:D:499:THR:H	1.70	0.49
1:A:419:VAL:HG22	2:A:809:NAG:H81	1.94	0.49
1:B:27:ASN:C	1:B:29:ASP:H	2.15	0.49
1:A:458:THR:HA	1:A:493:SER:HA	1.93	0.49
1:A:335:ALA:CB	3:A:811:NDG:C6	2.90	0.49
1:D:402:LYS:C	1:D:403:ASN:O	2.46	0.49
1:D:367:LEU:HB2	1:D:413:THR:O	2.12	0.49
1:B:109:THR:HG22	1:B:110:GLN:CG	2.42	0.49
1:B:382:ASN:OD1	1:B:385:ASN:N	2.45	0.49
1:A:92:MET:HB3	1:B:2:TRP:H	1.77	0.49
1:C:154:ASP:C	2:C:801:NAG:C8	2.62	0.49
1:B:155:PRO:O	1:B:157:GLU:N	2.43	0.49
1:D:457:LEU:HD23	1:D:494:MET:SD	2.52	0.49
1:D:335:ALA:CB	3:D:811:NDG:C6	2.90	0.49
1:C:367:LEU:HB2	1:C:413:THR:O	2.12	0.49
1:A:27:ASN:C	1:A:29:ASP:H	2.15	0.49
1:A:151:LEU:HD12	1:A:190:THR:O	2.11	0.49
1:C:109:THR:HG22	1:C:110:GLN:CG	2.42	0.49
1:A:109:THR:HG22	1:A:110:GLN:HG3	1.93	0.49
1:C:432:ASP:CB	1:C:464:ILE:CG2	2.89	0.49
1:C:28:LYS:CD	1:C:88:VAL:HG12	2.38	0.49
1:D:27:ASN:C	1:D:29:ASP:H	2.15	0.49
1:B:336:VAL:CG1	1:B:338:ARG:HB2	2.43	0.49
1:A:457:LEU:HD23	1:A:494:MET:SD	2.52	0.49
1:C:457:LEU:HD23	1:C:494:MET:SD	2.52	0.49
1:C:403:ASN:HB2	3:C:902:NDG:H8C2	1.87	0.49
1:C:151:LEU:HD12	1:C:151:LEU:H	1.78	0.49
1:D:109:THR:HG22	1:D:110:GLN:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:THR:HG22	1:D:110:GLN:HG3	1.94	0.49
1:B:396:ARG:CZ	1:B:432:ASP:HB2	2.41	0.49
1:A:4:ILE:HD13	1:B:2:TRP:CA	2.42	0.49
2:A:809:NAG:H62	2:A:810:NAG:O6	2.13	0.49
1:B:482:THR:O	1:B:482:THR:HG22	2.09	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:282:LEU:CD2	1:A:283:THR:N	2.76	0.49
1:A:109:THR:HG22	1:A:110:GLN:CG	2.42	0.49
1:D:432:ASP:CB	1:D:464:ILE:HG21	2.43	0.49
1:A:4:ILE:HD13	1:B:1:ASP:O	2.13	0.49
1:C:482:THR:O	1:C:482:THR:HG22	2.09	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:A:226:TYR:C	1:A:227:THR:HG23	2.33	0.49
1:C:226:TYR:C	1:C:227:THR:HG23	2.33	0.49
2:C:812:NAG:C1	2:C:812:NAG:O7	2.60	0.49
1:A:224:LYS:HE3	2:A:806:NAG:H82	1.95	0.49
1:C:363:GLN:C	1:C:364:ILE:HG23	2.32	0.49
1:D:261:ILE:HD11	1:D:264:ASN:HD22	1.77	0.49
1:A:396:ARG:CZ	1:A:432:ASP:HB2	2.41	0.49
2:B:809:NAG:H62	2:B:810:NAG:O6	2.13	0.49
1:B:451:ASN:O	1:B:534:GLY:CA	2.60	0.49
2:D:809:NAG:H62	2:D:810:NAG:O6	2.13	0.49
1:A:90:GLU:CB	1:B:90:GLU:O	2.60	0.49
1:B:80:ALA:O	1:B:88:VAL:HG23	2.11	0.49
1:C:336:VAL:CG1	1:C:338:ARG:HB2	2.43	0.49
1:D:449:ASP:CB	1:D:532:CYS:N	2.74	0.49
1:D:155:PRO:HG2	2:D:801:NAG:C7	2.42	0.49
1:D:512:LEU:HD11	1:D:519:ASN:ND2	2.28	0.49
1:D:8:LYS:CD	1:D:8:LYS:N	2.51	0.49
1:A:186:GLU:OE1	2:A:801:NAG:C6	2.59	0.49
1:B:226:TYR:C	1:B:227:THR:HG23	2.33	0.49
1:D:273:THR:H	2:D:803:NAG:HN2	1.60	0.49
1:C:282:LEU:CD2	1:C:283:THR:N	2.76	0.49
1:B:68:ARG:HD3	1:B:100:ASP:CA	2.43	0.49
1:D:151:LEU:H	1:D:151:LEU:HD12	1.78	0.49
1:D:151:LEU:O	1:D:152:LYS:HB2	2.13	0.49
1:D:432:ASP:CB	1:D:464:ILE:CG2	2.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLN:HA	1:A:203:VAL:O	2.13	0.49
1:C:252:THR:CG2	1:C:253:PRO:HD2	2.43	0.49
1:C:216:ASP:HB2	1:C:217:ASN:ND2	2.27	0.49
1:A:252:THR:CG2	1:A:253:PRO:HD2	2.43	0.49
1:C:396:ARG:CZ	1:C:432:ASP:HB2	2.41	0.49
1:D:154:ASP:CG	1:D:155:PRO:HD2	2.33	0.49
1:A:367:LEU:HB2	1:A:413:THR:O	2.12	0.49
1:A:281:ILE:O	1:A:281:ILE:HG23	2.13	0.49
1:C:327:ASN:OD1	1:C:360:ASP:OD1	2.30	0.49
1:C:261:ILE:HD11	1:C:264:ASN:HD22	1.77	0.49
1:A:76:LEU:O	1:A:94:ILE:N	2.44	0.49
1:C:352:ILE:CG1	1:C:388:VAL:HB	2.33	0.49
1:C:224:LYS:HE3	2:C:806:NAG:H82	1.95	0.49
1:D:451:ASN:O	1:D:534:GLY:CA	2.60	0.49
1:B:352:ILE:CG1	1:B:388:VAL:HB	2.33	0.49
1:D:224:LYS:CE	2:D:806:NAG:C8	2.91	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:B:365:GLN:HA	1:B:416:GLY:HA3	1.95	0.49
1:D:241:ARG:HE	1:D:281:ILE:CD1	2.24	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:27:ASN:OD1	1:D:91:PRO:O	2.31	0.48
1:C:402:LYS:C	1:C:403:ASN:O	2.46	0.48
1:D:276:GLU:HG3	1:D:277:SER:N	2.25	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:D:67:ASP:OD2	1:D:69:GLU:HB2	2.13	0.48
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: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:154:ASP:CG	1:A:155:PRO:HD2	2.33	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:B:363:GLN:C	1:B:364:ILE:HG23	2.32	0.48
1:C:27:ASN:C	1:C:29:ASP:H	2.16	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
2:C:807:NAG:H3	2:C:807:NAG:O7	2.11	0.48
1:D:496:LEU:HD21	1:D:509:ILE:CD1	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LEU:N	1:C:298:LEU:CD2	2.75	0.48
1:A:11:GLU:OE2	1:A:69:GLU:OE1	2.30	0.48
1:B:151:LEU:O	1:B:152:LYS:HB2	2.13	0.48
1:A:150:ILE:HD11	1:A:165:ILE:HB	1.96	0.48
1:B:432:ASP:CB	1:B:464:ILE:HG21	2.43	0.48
1:A:432:ASP:CB	1:A:464:ILE:HG21	2.43	0.48
1:B:449:ASP:CB	1:B:532:CYS:N	2.74	0.48
2:C:809:NAG:C6	2:C:810:NAG:C6	2.92	0.48
1:A:336:VAL:CG1	1:A:338:ARG:HB2	2.43	0.48
1:D:367:LEU:HD13	1:D:412:VAL:CG2	2.43	0.48
1:C:281:ILE:HG23	1:C:281:ILE:O	2.13	0.48
1:A:67:ASP:OD2	1:A:69:GLU:HB2	2.14	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:A:151:LEU:HD12	1:A:151:LEU:H	1.78	0.48
1:D:119:GLU:OE2	1:D:216:ASP:OD1	2.32	0.48
1:B:252:THR:CG2	1:B:253:PRO:HD2	2.43	0.48
1:B:119:GLU:OE2	1:B:216:ASP:OD1	2.32	0.48
2:D:809:NAG:C6	2:D:810:NAG:C6	2.92	0.48
1:A:512:LEU:HD11	1:A:519:ASN:ND2	2.28	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
1:C:250:PRO:O	1:C:255:TRP:CE3	2.66	0.48
1:A:2:TRP:HZ3	1:B:6:PRO:CG	2.27	0.48
1:C:155:PRO:O	1:C:157:GLU:N	2.43	0.48
1:B:512:LEU:HD11	1:B:519:ASN:ND2	2.28	0.48
1:A:241:ARG:HE	1:A:281:ILE:CD1	2.24	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
1:D:310:VAL:HG12	1:D:312:LEU:HG	1.95	0.48
1:B:4:ILE:HA	1:B:5:PRO:HD3	1.72	0.48
2:A:809:NAG:C6	2:A:810:NAG:C6	2.92	0.48
1:C:224:LYS:CE	2:C:806:NAG:C8	2.91	0.48
1:D:155:PRO:O	1:D:157:GLU:N	2.43	0.48
1:C:276:GLU:HG3	1:C:277:SER:N	2.25	0.48
1:A:367:LEU:HD13	1:A:412:VAL:CG2	2.43	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:D:397:GLU:OE1	1:D:397:GLU:N	2.45	0.48
1:A:397:GLU:OE1	1:A:397:GLU:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:423:THR:HB	2:A:810:NAG:H83	1.93	0.48
1:D:225:THR:HA	1:D:318:THR:O	2.14	0.48
1:A:28:LYS:CD	1:A:88:VAL:HG12	2.38	0.48
1:A:333:VAL:CB	1:A:334:PRO:CD	2.88	0.48
1:C:273:THR:H	2:C:803:NAG:HN2	1.60	0.48
1:D:537:ILE:CG1	1:D:538:LYS:N	2.77	0.48
1:A:537:ILE:CG1	1:A:538:LYS:N	2.77	0.48
1:D:482:THR:HG22	1:D:482:THR:O	2.09	0.48
1:C:33:LYS:HB3	1:C:83:GLU:CG	2.40	0.48
1:D:352:ILE:HG13	1:D:388:VAL:CB	2.33	0.48
1:C:367:LEU:HG	1:C:367:LEU:H	1.41	0.48
1:B:273:THR:H	2:B:803:NAG:HN2	1.60	0.48
1:D:266:GLY:N	1:D:268:PHE:CE2	2.76	0.48
1:D:250:PRO:O	1:D:255:TRP:CE3	2.67	0.48
1:D:41:GLN:HA	1:D:45:ASN:HB2	1.95	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:D:226:TYR:C	1:D:227:THR:HG23	2.33	0.48
2:A:812:NAG:C1	2:A:812:NAG:O7	2.60	0.48
1:A:225:THR:HA	1:A:318:THR:O	2.14	0.48
1:C:266:GLY:N	1:C:268:PHE:CE2	2.76	0.48
1:A:365:GLN:HA	1:A:416:GLY:HA3	1.95	0.48
1:D:68:ARG:HD3	1:D:100:ASP:CA	2.43	0.48
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.95	0.48
1:A:250:PRO:O	1:A:255:TRP:CE3	2.66	0.48
1:B:250:PRO:O	1:B:255:TRP:CE3	2.67	0.48
1:D:261:ILE:CD1	1:D:264:ASN:ND2	2.77	0.48
1:B:224:LYS:CE	2:B:806:NAG:C8	2.91	0.47
1:C:300:ILE:N	1:C:300:ILE:HD12	2.29	0.47
1:C:537:ILE:CG1	1:C:538:LYS:N	2.77	0.47
1:A:241:ARG:NE	1:A:281:ILE:HD12	2.22	0.47
1:B:365:GLN:CG	1:B:365:GLN:O	2.54	0.47
1:A:68:ARG:HD3	1:A:100:ASP:CA	2.43	0.47
1:B:418:SER:O	1:B:419:VAL:HG23	2.14	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:41:GLN:HA	1:A:45:ASN:HB2	1.95	0.47
1:C:150:ILE:HD11	1:C:165:ILE:HB	1.96	0.47
1:A:3:VAL:C	1:B:3:VAL:CG2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:SER:O	1:A:419:VAL:HG23	2.14	0.47
1:D:514:SER:CA	1:D:517:GLN:O	2.62	0.47
1:C:154:ASP:CG	1:C:155:PRO:HD2	2.33	0.47
1:A:224:LYS:CE	2:A:806:NAG:C8	2.91	0.47
1:A:514:SER:CA	1:A:517:GLN:O	2.62	0.47
1:C:365:GLN:HA	1:C:416:GLY:HA3	1.95	0.47
1:B:150:ILE:HD11	1:B:165:ILE:HB	1.96	0.47
1:B:36:TYR:O	1:B:55:TRP:HA	2.15	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:D:301:THR:CG2	1:D:316:THR:HG23	2.45	0.47
1:B:514:SER:CA	1:B:517:GLN:O	2.62	0.47
1:A:379:LEU:CD2	1:A:379:LEU:H	2.22	0.47
1:D:371:ILE:HD12	1:D:371:ILE:HA	1.65	0.47
1:A:50:VAL:HB	1:A:51:PHE:CD1	2.50	0.47
1:D:246:ASP:C	1:D:247:LEU:HD12	2.35	0.47
1:A:4:ILE:HA	1:A:5:PRO:HD3	1.72	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:C:514:SER:CA	1:C:517:GLN:O	2.62	0.47
1:D:300:ILE:HD12	1:D:300:ILE:N	2.30	0.47
1:C:320:THR:CB	2:C:807:NAG:N2	2.78	0.47
1:B:333:VAL:CB	1:B:334:PRO:CD	2.88	0.47
1:D:281:ILE:HG23	1:D:281:ILE:O	2.13	0.47
1:A:151:LEU:O	1:A:152:LYS:HB2	2.13	0.47
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.32	0.47
1:A:4:ILE:CD1	1:B:1:ASP:O	2.62	0.47
1:B:225:THR:HA	1:B:318:THR:O	2.14	0.47
1:A:89:GLU:OE1	1:B:90:GLU:HG2	2.14	0.47
1:D:379:LEU:H	1:D:379:LEU:CD2	2.22	0.47
1:A:273:THR:H	2:A:803:NAG:HN2	1.60	0.47
1:B:368:SER:OG	1:B:370:PHE:HE1	1.94	0.47
1:A:261:ILE:CD1	1:A:264:ASN:ND2	2.77	0.47
1:A:246:ASP:C	1:A:247:LEU:HD12	2.35	0.47
1:A:36:TYR:O	1:A:55:TRP:HA	2.15	0.47
1:C:23:GLN:HB2	1:C:59:TRP:CE3	2.50	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:A:451:ASN:O	1:A:534:GLY:CA	2.60	0.47
2:B:812:NAG:O7	2:B:812:NAG:C1	2.60	0.47
1:C:119:GLU:OE2	1:C:216:ASP:OD1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:CD1	1:B:264:ASN:ND2	2.77	0.47
1:D:150:ILE:HD11	1:D:165:ILE:HB	1.96	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:B:33:LYS:HB3	1:B:83:GLU:CG	2.40	0.47
1:A:300:ILE:HD12	1:A:300:ILE:N	2.29	0.47
1:C:268:PHE:CA	1:C:285:ALA:HB3	2.45	0.47
1:C:261:ILE:CD1	1:C:264:ASN:ND2	2.77	0.47
1:A:6:PRO:HD3	1:B:5:PRO:HG2	1.97	0.47
1:D:418:SER:O	1:D:419:VAL:HG23	2.14	0.47
1:D:272:THR:HG23	2:D:803:NAG:HN2	1.80	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:A:3:VAL:O	1:B:3:VAL:CG2	2.63	0.47
1:C:451:ASN:O	1:C:534:GLY:CA	2.60	0.47
1:B:320:THR:CB	2:B:807:NAG:N2	2.78	0.47
1:C:373:ASN:CG	1:C:374:ASP:H	2.18	0.47
1:D:374:ASP:OD1	1:D:374:ASP:N	2.49	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:D:268:PHE:CA	1:D:285:ALA:HB3	2.45	0.47
1:C:108:PHE:HE1	1:C:203:VAL:HG23	1.80	0.47
1:C:246:ASP:C	1:C:247:LEU:HD12	2.35	0.47
1:D:36:TYR:O	1:D:55:TRP:HA	2.15	0.47
1:A:93:GLU:O	1:B:2:TRP:C	2.53	0.46
1:C:226:TYR:O	1:C:227:THR:HG23	2.15	0.46
1:B:272:THR:HG23	2:B:803:NAG:HN2	1.80	0.46
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
1:D:108:PHE:HE1	1:D:203:VAL:HG23	1.80	0.46
1:A:2:TRP:N	1:B:93:GLU:C	2.47	0.46
1:B:408:VAL:O	1:B:426:LEU:N	2.48	0.46
1:B:154:ASP:CG	1:B:155:PRO:HD2	2.33	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:A:8:LYS:CD	1:A:8:LYS:N	2.51	0.46
1:B:374:ASP:OD1	1:B:374:ASP:N	2.49	0.46
1:C:440:PRO:HB3	1:C:457:LEU:CD2	2.43	0.46
1:D:506:ASP:N	1:D:506:ASP:OD1	2.49	0.46
1:C:363:GLN:O	1:C:364:ILE:CG2	2.63	0.46
1:B:41:GLN:HA	1:B:45:ASN:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ASN:OD1	1:C:271:ILE:N	2.49	0.46
1:D:448:CYS:SG	1:D:537:ILE:CG2	3.01	0.46
1:B:448:CYS:SG	1:B:537:ILE:CG2	3.01	0.46
1:C:418:SER:O	1:C:419:VAL:HG23	2.14	0.46
1:A:320:THR:CB	2:A:807:NAG:N2	2.78	0.46
1:A:301:THR:CG2	1:A:316:THR:HG23	2.45	0.46
1:A:522:LEU:HB3	1:A:523:THR:H	1.57	0.46
1:D:374:ASP:C	1:D:375:PRO:O	2.54	0.46
1:D:415:ASP:CG	1:D:416:GLY:H	2.16	0.46
1:D:271:ILE:HG23	1:D:271:ILE:O	2.15	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:A:373:ASN:CG	1:A:374:ASP:H	2.18	0.46
1:B:373:ASN:CG	1:B:374:ASP:H	2.18	0.46
1:C:374:ASP:C	1:C:375:PRO:O	2.54	0.46
1:B:268:PHE:CA	1:B:285:ALA:HB3	2.45	0.46
1:C:100:ASP:OD1	1:C:101:GLN:N	2.49	0.46
1:A:270:ASN:OD1	1:A:271:ILE:N	2.49	0.46
1:C:36:TYR:O	1:C:55:TRP:HA	2.15	0.46
1:D:50:VAL:HB	1:D:51:PHE:CD1	2.50	0.46
1:A:90:GLU:HB2	1:B:90:GLU:C	2.35	0.46
1:D:450:GLN:CB	1:D:533:GLU:HA	2.29	0.46
1:A:408:VAL:O	1:A:426:LEU:N	2.49	0.46
1:C:374:ASP:OD1	1:C:374:ASP:N	2.49	0.46
1:B:241:ARG:HE	1:B:281:ILE:CD1	2.24	0.46
1:A:496:LEU:HD21	1:A:509:ILE:CD1	2.38	0.46
1:D:363:GLN:O	1:D:364:ILE:CG2	2.64	0.46
1:D:310:VAL:HG12	1:D:311:PRO:O	2.15	0.46
1:D:252:THR:HA	1:D:253:PRO:HD3	1.81	0.46
1:C:271:ILE:HG23	1:C:271:ILE:O	2.15	0.46
1:D:270:ASN:OD1	1:D:271:ILE:N	2.49	0.46
1:B:481:LEU:HA	1:B:481:LEU:HD12	1.50	0.46
1:A:374:ASP:OD1	1:A:374:ASP:N	2.49	0.46
1:B:363:GLN:O	1:B:364:ILE:CG2	2.63	0.46
1:A:298:LEU:CD2	1:A:298:LEU:N	2.75	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: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:B:449:ASP:CB	1:B:532:CYS:H	2.22	0.46
1:D:187:TYR:HE1	1:D:211:ILE:HD11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:CB	2:A:801:NAG:C8	2.94	0.46
1:B:524:VAL:HG21	2:B:904:NAG:C8	2.44	0.46
1:A:511:VAL:N	1:A:523:THR:O	2.46	0.46
1:D:23:GLN:HB2	1:D:59:TRP:CE3	2.50	0.46
1:C:448:CYS:SG	1:C:537:ILE:CG2	3.01	0.46
1:B:459:ILE:HD12	1:B:459:ILE:N	2.31	0.46
1:D:282:LEU:CD2	1:D:283:THR:N	2.76	0.46
1:A:100:ASP:OD1	1:A:101:GLN:N	2.49	0.46
1:A:271:ILE:O	1:A:271:ILE:HG23	2.15	0.46
1:B:270:ASN:OD1	1:B:271:ILE:N	2.49	0.46
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.16	0.46
1:B:50:VAL:HB	1:B:51:PHE:CD1	2.50	0.46
1:A:449:ASP:CB	1:A:532:CYS:H	2.22	0.46
1:B:300:ILE:N	1:B:300:ILE:HD12	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:A:109:THR:CB	1:A:131:SER:HB2	2.46	0.46
1:D:109:THR:CB	1:D:131:SER:HB2	2.46	0.46
1:B:246:ASP:C	1:B:247:LEU:HD12	2.35	0.46
1:C:421:THR:HG21	2:C:809:NAG:H61	1.98	0.46
1:B:262:ARG:HG3	1:B:299:GLN:HB2	1.98	0.46
1:D:449:ASP:CB	1:D:532:CYS:H	2.22	0.46
1:C:117:VAL:O	1:C:212:THR:N	2.46	0.46
1:A:226:TYR:O	1:A:227:THR:HG23	2.15	0.46
1:C:272:THR:HG23	2:C:803:NAG:HN2	1.80	0.46
1:D:459:ILE:HD12	1:D:459:ILE:N	2.31	0.46
1:D:298:LEU:N	1:D:298:LEU:CD2	2.75	0.46
1:A:252:THR:HA	1:A:253:PRO:HD3	1.81	0.46
1:C:450:GLN:CB	1:C:533:GLU:OE2	2.64	0.46
1:A:117:VAL:O	1:A:212:THR:N	2.46	0.46
1:D:262:ARG:HG3	1:D:299:GLN:HB2	1.98	0.46
1:B:227:THR:N	2:B:812:NAG:H2	2.31	0.46
1:B:440:PRO:HB3	1:B:457:LEU:CD2	2.43	0.46
1:D:100:ASP:OD1	1:D:101:GLN:N	2.49	0.46
1:A:483:TRP:CZ2	1:A:507:TYR:CE1	2.87	0.45
1:D:461:ASP:HB3	1:D:468:THR:CG2	2.46	0.45
2:B:809:NAG:H61	2:B:810:NAG:C6	2.39	0.45
2:C:805:NAG:C5	2:C:806:NAG:H83	2.46	0.45
1:D:450:GLN:CB	1:D:533:GLU:OE2	2.64	0.45
1:A:339:VAL:HG11	1:A:351:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:THR:CG2	1:D:381:VAL:N	2.79	0.45
1:C:459:ILE:HD12	1:C:459:ILE:N	2.31	0.45
1:B:128:MET:HB3	1:B:129:ALA:H	1.62	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:B:54:GLU:HB2	1:B:57:THR:OG1	2.16	0.45
1:B:8:LYS:N	1:B:8:LYS:CD	2.51	0.45
1:B:450:GLN:CB	1:B:533:GLU:OE2	2.64	0.45
1:B:339:VAL:HG11	1:B:351:ILE:HG23	1.98	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:D:373:ASN:CG	1:D:374:ASP:H	2.18	0.45
1:B:506:ASP:N	1:B:506:ASP:OD1	2.49	0.45
1:B:23:GLN:HB2	1:B:59:TRP:CE3	2.50	0.45
1:B:310:VAL:HG12	1:B:311:PRO:O	2.15	0.45
1:D:468:THR:C	1:D:469:TYR:O	2.54	0.45
1:A:450:GLN:CB	1:A:533:GLU:OE2	2.64	0.45
1:C:408:VAL:O	1:C:426:LEU:N	2.49	0.45
1:A:473:VAL:CG2	1:A:487:LEU:HD21	2.46	0.45
1:C:473:VAL:CG2	1:C:487:LEU:HD21	2.46	0.45
1:A:152:LYS:O	1:A:189:LEU:HA	2.17	0.45
1:D:312:LEU:O	3:D:804:NDG:H8C1	2.17	0.45
1:B:461:ASP:HB3	1:B:468:THR:CG2	2.46	0.45
1:C:339:VAL:HG11	1:C:351:ILE:HG23	1.98	0.45
1:D:227:THR:N	2:D:812:NAG:H2	2.31	0.45
1:A:187:TYR:HE1	1:A:211:ILE:HD11	1.81	0.45
1:C:380:THR:HG22	1:C:381:VAL:N	2.32	0.45
1:C:380:THR:CG2	1:C:381:VAL:N	2.79	0.45
1:A:95:THR:N	1:B:2:TRP:CZ3	2.85	0.45
1:B:286:LYS:C	1:B:287:GLY:O	2.55	0.45
1:A:468:THR:C	1:A:469:TYR:O	2.54	0.45
1:C:461:ASP:HB3	1:C:468:THR:CG2	2.46	0.45
1:A:227:THR:N	2:A:812:NAG:H2	2.31	0.45
1:A:519:ASN:CG	1:A:519:ASN:O	2.55	0.45
1:B:271:ILE:HG23	1:B:271:ILE:O	2.15	0.45
1:C:482:THR:O	1:C:483:TRP:CD2	2.70	0.45
1:A:286:LYS:C	1:A:287:GLY:O	2.55	0.45
1:B:469:TYR:CD2	1:B:470:PRO:N	2.85	0.45
1:A:421:THR:HG21	2:A:809:NAG:H61	1.98	0.45
1:C:227:THR:N	2:C:812:NAG:H2	2.31	0.45
2:A:805:NAG:C5	2:A:806:NAG:H83	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:N	1:A:459:ILE:HD12	2.31	0.45
1:D:339:VAL:HG11	1:D:351:ILE:HG23	1.98	0.45
1:A:276:GLU:HG3	1:A:277:SER:N	2.25	0.45
1:C:194:THR:CG2	1:C:195:ASP:N	2.79	0.45
1:D:194:THR:CG2	1:D:195:ASP:N	2.79	0.45
1:D:380:THR:HG22	1:D:381:VAL:N	2.32	0.45
1:C:109:THR:HB	1:C:131:SER:HB2	1.99	0.45
1:B:468:THR:C	1:B:469:TYR:O	2.54	0.45
2:C:805:NAG:H62	2:C:806:NAG:N2	2.31	0.45
1:C:286:LYS:C	1:C:287:GLY:O	2.55	0.45
1:A:262:ARG:HG3	1:A:299:GLN:HB2	1.98	0.45
1:A:485:ALA:O	1:A:486:GLU:OE1	2.35	0.45
1:B:381:VAL:HA	1:B:387:ILE:O	2.16	0.45
1:A:381:VAL:HA	1:A:387:ILE:O	2.16	0.45
1:B:152:LYS:O	1:B:189:LEU:HA	2.17	0.45
1:C:261:ILE:HD11	1:C:264:ASN:ND2	2.32	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
2:B:805:NAG:H62	2:B:806:NAG:N2	2.31	0.45
1:C:227:THR:HG22	1:C:320:THR:HB	1.98	0.45
1:B:374:ASP:C	1:B:375:PRO:O	2.54	0.45
1:A:134:ASP:HB2	1:A:146:LEU:HD11	1.99	0.45
1:D:368:SER:OG	1:D:370:PHE:HE1	1.94	0.45
1:C:162:LEU:HB2	1:C:163:PHE:CE1	2.52	0.45
1:B:162:LEU:HB2	1:B:163:PHE:CE1	2.52	0.45
1:C:54:GLU:HB2	1:C:57:THR:OG1	2.16	0.45
1:C:262:ARG:HG3	1:C:299:GLN:HB2	1.98	0.45
1:A:227:THR:HG22	1:A:320:THR:HB	1.98	0.45
1:B:522:LEU:HD23	1:B:522:LEU:HA	1.36	0.45
1:B:194:THR:CG2	1:B:195:ASP:N	2.79	0.45
1:A:194:THR:CG2	1:A:195:ASP:N	2.79	0.45
1:B:312:LEU:O	3:B:804:NDG:H8C1	2.17	0.45
1:D:396:ARG:NH2	1:D:464:ILE:HG22	2.12	0.45
1:A:24:ILE:HG21	1:B:1:ASP:H2	1.82	0.45
1:C:25:LYS:HB2	1:D:3:VAL:HG11	1.62	0.45
1:D:449:ASP:N	1:D:532:CYS:HB3	2.19	0.45
1:D:32:ASN:ND2	1:D:83:GLU:CB	2.62	0.45
1:C:519:ASN:O	1:C:519:ASN:CG	2.55	0.45
1:D:286:LYS:C	1:D:287:GLY:O	2.55	0.45
1:D:381:VAL:HA	1:D:387:ILE:O	2.17	0.45
1:B:473:VAL:CG2	1:B:487:LEU:HD21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:473:VAL:CG2	1:D:487:LEU:HD21	2.47	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:C:92:MET:CB	1:D:2:TRP:HD1	2.29	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:D:408:VAL:O	1:D:426:LEU:N	2.49	0.44
1:B:519:ASN:O	1:B:519:ASN:CG	2.55	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:A:380:THR:CG2	1:A:381:VAL:N	2.79	0.44
1:C:371:ILE:HD13	1:C:381:VAL:HG11	1.95	0.44
1:D:152:LYS:O	1:D:189:LEU:HA	2.17	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:A:426:LEU:HD13	1:A:426:LEU:C	2.37	0.44
1:B:367:LEU:HG	1:B:367:LEU:H	1.41	0.44
1:C:109:THR:CB	1:C:131:SER:HB2	2.46	0.44
1:A:261:ILE:HD11	1:A:264:ASN:ND2	2.32	0.44
1:C:3:VAL:HB	1:C:4:ILE:H	1.51	0.44
1:A:2:TRP:CE3	1:B:6:PRO:HG3	2.52	0.44
1:A:482:THR:O	1:A:483:TRP:CD2	2.70	0.44
1:B:336:VAL:HG11	1:B:338:ARG:HD2	1.99	0.44
1:C:187:TYR:CE1	1:C:211:ILE:HD11	2.52	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:B:380:THR:CG2	1:B:381:VAL:N	2.79	0.44
1:C:381:VAL:HA	1:C:387:ILE:O	2.16	0.44
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.44
1:D:469:TYR:CE2	1:D:470:PRO:HB2	2.52	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:469:TYR:CD2	1:C:470:PRO:N	2.85	0.44
1:C:134:ASP:HB2	1:C:146:LEU:HD11	1.99	0.44
1:A:380:THR:HG22	1:A:381:VAL:N	2.32	0.44
1:A:272:THR:HG23	2:A:803:NAG:HN2	1.81	0.44
1:A:162:LEU:HB2	1:A:163:PHE:CE1	2.52	0.44
1:A:540:GLN:O	1:A:540:GLN:NE2	2.47	0.44
1:D:421:THR:CG2	1:D:422:GLY:N	2.81	0.44
1:C:461:ASP:HB3	1:C:468:THR:HG22	2.00	0.44
1:B:187:TYR:CE1	1:B:211:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:805:NAG:H62	2:D:806:NAG:N2	2.31	0.44
1:C:524:VAL:HG21	2:C:904:NAG:C8	2.44	0.44
1:C:333:VAL:CB	1:C:334:PRO:CD	2.88	0.44
1:D:261:ILE:HD11	1:D:264:ASN:ND2	2.32	0.44
1:C:86:SER:HA	1:C:87:PRO:HD3	1.83	0.44
1:B:435:ASP:HB2	1:B:436:ASN:H	1.59	0.44
1:C:336:VAL:HG11	1:C:338:ARG:HD2	1.99	0.44
1:D:442:PRO:HD2	1:D:457:LEU:HD12	2.00	0.44
1:A:442:PRO:HD2	1:A:457:LEU:HD12	2.00	0.44
1:A:374:ASP:C	1:A:375:PRO:O	2.54	0.44
1:C:481:LEU:HD12	1:C:481:LEU:HA	1.50	0.44
1:A:92:MET:SD	1:B:3:VAL:N	2.90	0.44
1:A:3:VAL:O	1:B:3:VAL:HB	2.16	0.44
1:D:461:ASP:HB3	1:D:468:THR:HG22	2.00	0.44
1:B:421:THR:HG21	2:B:809:NAG:H61	1.98	0.44
1:B:482:THR:O	1:B:483:TRP:CD2	2.70	0.44
1:A:187:TYR:CE1	1:A:211:ILE:HD11	2.52	0.44
1:B:442:PRO:HD2	1:B:457:LEU:HD12	2.00	0.44
1:B:485:ALA:O	1:B:486:GLU:OE1	2.35	0.44
1:A:194:THR:HG23	1:A:201:LEU:O	2.18	0.44
1:A:127:VAL:HG13	1:A:128:MET:N	2.25	0.44
1:B:127:VAL:HG13	1:B:128:MET:N	2.25	0.44
1:A:108:PHE:HE1	1:A:203:VAL:HG23	1.80	0.44
1:D:162:LEU:HB2	1:D:163:PHE:CE1	2.52	0.44
1:B:261:ILE:HD11	1:B:264:ASN:ND2	2.32	0.44
1:A:461:ASP:HB3	1:A:468:THR:CG2	2.46	0.44
1:C:469:TYR:CE2	1:C:470:PRO:HB2	2.52	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:C:232:GLU:HA	1:C:288:LEU:HD12	1.99	0.44
1:D:336:VAL:HG11	1:D:338:ARG:HD2	1.99	0.44
1:B:290:PHE:CD2	1:B:293:ARG:O	2.71	0.44
1:A:27:ASN:ND2	1:A:28:LYS:N	2.50	0.44
1:A:128:MET:HB3	1:A:129:ALA:H	1.62	0.44
1:C:415:ASP:CG	1:C:416:GLY:H	2.17	0.44
1:D:151:LEU:N	1:D:151:LEU:HD12	2.33	0.44
1:A:109:THR:HB	1:A:131:SER:HB2	1.99	0.44
1:D:220:ILE:O	1:D:220:ILE:HG22	2.18	0.44
1:A:95:THR:N	1:B:2:TRP:CE3	2.86	0.44
1:A:232:GLU:HA	1:A:288:LEU:HD12	1.99	0.44
1:A:450:GLN:HG3	1:A:532:CYS:O	2.10	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:LEU:C	1:C:426:LEU:HD13	2.37	0.44
1:C:514:SER:HG	1:C:519:ASN:HA	1.82	0.44
1:B:220:ILE:O	1:B:220:ILE:HG22	2.18	0.44
1:A:24:ILE:HG21	1:B:1:ASP:N	2.33	0.43
1:C:22:VAL:CG2	1:C:23:GLN:N	2.81	0.43
1:A:290:PHE:CD2	1:A:293:ARG:O	2.71	0.43
1:A:419:VAL:HG13	1:A:420:GLY:N	2.33	0.43
1:B:426:LEU:HD13	1:B:426:LEU:C	2.37	0.43
1:D:232:GLU:HA	1:D:288:LEU:HD12	2.00	0.43
1:C:290:PHE:CD2	1:C:293:ARG:O	2.71	0.43
1:A:239:VAL:HG13	1:A:240:GLN:N	2.33	0.43
1:A:368:SER:CB	1:A:370:PHE:HE1	2.31	0.43
1:A:247:LEU:HD12	1:A:247:LEU:N	2.33	0.43
1:B:354:LEU:HD12	1:B:386:GLY:O	2.18	0.43
1:D:27:ASN:ND2	1:D:28:LYS:N	2.50	0.43
1:A:469:TYR:CE2	1:A:470:PRO:HB2	2.52	0.43
1:B:224:LYS:HE3	2:B:806:NAG:C8	2.48	0.43
2:A:805:NAG:H62	2:A:806:NAG:N2	2.31	0.43
1:B:297:VAL:HG21	2:B:807:NAG:H62	2.01	0.43
1:D:524:VAL:HG21	2:D:904:NAG:C8	2.44	0.43
1:A:441:SER:CB	1:A:442:PRO:HD3	2.47	0.43
1:A:312:LEU:O	3:A:804:NDG:H8C1	2.17	0.43
1:A:260:LYS:HB3	1:A:260:LYS:HE3	1.81	0.43
1:B:247:LEU:HD12	1:B:247:LEU:N	2.33	0.43
1:C:354:LEU:HD12	1:C:386:GLY:O	2.18	0.43
1:A:3:VAL:HG11	1:B:4:ILE:HD12	1.83	0.43
1:B:1:ASP:CG	1:B:2:TRP:N	2.70	0.43
1:A:24:ILE:CG2	1:B:1:ASP:H2	2.31	0.43
1:B:90:GLU:O	1:B:91:PRO:O	2.37	0.43
1:D:187:TYR:CE1	1:D:211:ILE:HD11	2.52	0.43
1:D:155:PRO:CB	2:D:801:NAG:C8	2.94	0.43
1:D:224:LYS:HE3	2:D:806:NAG:C8	2.48	0.43
1:A:32:ASN:HD22	1:A:83:GLU:N	2.13	0.43
1:D:426:LEU:C	1:D:426:LEU:HD13	2.37	0.43
1:D:194:THR:HG23	1:D:201:LEU:O	2.18	0.43
1:A:272:THR:CG2	1:A:273:THR:N	2.76	0.43
1:C:368:SER:CB	1:C:370:PHE:HE1	2.31	0.43
1:C:90:GLU:O	1:C:91:PRO:O	2.37	0.43
1:D:539:CYS:HB3	1:D:540:GLN:H	1.46	0.43
1:A:539:CYS:HB3	1:A:540:GLN:H	1.45	0.43
1:A:421:THR:CG2	1:A:422:GLY:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:805:NAG:C5	2:B:806:NAG:H83	2.46	0.43
1:A:90:GLU:HG3	1:B:89:GLU:CD	2.30	0.43
1:C:32:ASN:ND2	1:C:83:GLU:CB	2.62	0.43
1:D:290:PHE:CD2	1:D:293:ARG:O	2.71	0.43
1:C:442:PRO:HD2	1:C:457:LEU:HD12	2.00	0.43
1:C:194:THR:HG23	1:C:201:LEU:O	2.18	0.43
1:D:134:ASP:HB2	1:D:146:LEU:HD11	1.99	0.43
1:D:128:MET:HB3	1:D:129:ALA:H	1.62	0.43
1:C:312:LEU:O	3:C:804:NDG:H8C1	2.17	0.43
1:A:354:LEU:HD12	1:A:386:GLY:O	2.18	0.43
1:D:354:LEU:HD12	1:D:386:GLY:O	2.18	0.43
1:A:92:MET:SD	1:B:2:TRP:C	2.97	0.43
1:C:421:THR:CG2	1:C:422:GLY:N	2.81	0.43
1:B:482:THR:HG22	1:B:499:THR:H	1.70	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:B:67:ASP:OD1	1:B:69:GLU:HB2	2.18	0.43
1:B:461:ASP:HB3	1:B:468:THR:HG22	2.00	0.43
1:B:154:ASP:HB3	2:B:801:NAG:C7	2.48	0.43
1:A:224:LYS:HE3	2:A:806:NAG:C8	2.48	0.43
1:C:32:ASN:HD22	1:C:83:GLU:N	2.13	0.43
1:D:441:SER:CB	1:D:442:PRO:HD3	2.47	0.43
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.81	0.43
1:B:232:GLU:HA	1:B:288:LEU:HD12	1.99	0.43
1:D:22:VAL:CG2	1:D:23:GLN:N	2.81	0.43
1:D:272:THR:CG2	1:D:273:THR:N	2.76	0.43
1:C:67:ASP:OD1	1:C:69:GLU:HB2	2.18	0.43
1:A:151:LEU:HD12	1:A:151:LEU:N	2.33	0.43
2:B:810:NAG:O7	2:B:810:NAG:C1	2.67	0.43
1:B:155:PRO:CB	2:B:801:NAG:C8	2.94	0.43
1:A:524:VAL:HG21	2:A:904:NAG:C8	2.44	0.43
1:A:367:LEU:HG	1:A:367:LEU:H	1.41	0.43
1:B:194:THR:HG23	1:B:201:LEU:O	2.18	0.43
1:A:518:ASN:C	1:A:520:PRO:CD	2.87	0.43
1:B:333:VAL:HG23	1:B:334:PRO:HD3	2.01	0.43
1:B:415:ASP:CG	1:B:416:GLY:H	2.16	0.43
1:B:22:VAL:CG2	1:B:23:GLN:N	2.81	0.43
1:D:67:ASP:OD1	1:D:69:GLU:HB2	2.18	0.43
1:B:371:ILE:HG13	1:B:410:MET:SD	2.59	0.43
1:B:371:ILE:HD13	1:B:381:VAL:HG11	1.95	0.43
1:D:378:TRP:HB2	1:D:379:LEU:H	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:60:MET:SD	1:D:2:TRP:HH2	2.41	0.43
1:A:1:ASP:OD2	1:B:93:GLU:HB3	1.79	0.43
1:A:469:TYR:CE2	1:A:470:PRO:HD2	2.54	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:B:441:SER:CB	1:B:442:PRO:HD3	2.47	0.43
1:C:366:LYS:HG2	1:C:367:LEU:H	1.75	0.43
1:B:378:TRP:HB2	1:B:379:LEU:H	1.64	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:90:GLU:O	1:A:91:PRO:O	2.37	0.43
1:C:224:LYS:HE3	2:C:806:NAG:C8	2.48	0.43
1:D:519:ASN:CG	1:D:519:ASN:O	2.55	0.43
1:A:339:VAL:HG21	1:A:351:ILE:HG22	2.01	0.43
1:C:518:ASN:C	1:C:520:PRO:CD	2.87	0.43
1:A:371:ILE:HD13	1:A:381:VAL:HG11	1.95	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:D:247:LEU:N	1:D:247:LEU:HD12	2.33	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:HG22	1:C:220:ILE:O	2.18	0.43
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
2:A:810:NAG:C1	2:A:810:NAG:O7	2.67	0.42
1:C:419:VAL:HG13	1:C:420:GLY:N	2.33	0.42
1:C:188:THR:H	2:C:801:NAG:H83	1.84	0.42
1:D:297:VAL:HG21	2:D:807:NAG:H62	2.01	0.42
1:C:297:VAL:HG21	2:C:807:NAG:H62	2.01	0.42
1:C:409:ILE:HD13	3:C:811:NDG:H8C3	2.01	0.42
1:D:518:ASN:C	1:D:520:PRO:CD	2.87	0.42
1:D:371:ILE:HG13	1:D:410:MET:SD	2.59	0.42
1:A:333:VAL:HG23	1:A:334:PRO:HD3	2.01	0.42
1:C:128:MET:HB3	1:C:129:ALA:H	1.62	0.42
1:A:250:PRO:HA	1:A:255:TRP:CG	2.54	0.42
1:C:40:GLY:O	1:C:45:ASN:HB2	2.19	0.42
1:C:247:LEU:N	1:C:247:LEU:HD12	2.33	0.42
1:C:5:PRO:HA	1:C:6:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:ASP:CG	1:D:344:ASP:O	2.57	0.42
1:C:27:ASN:ND2	1:C:28:LYS:N	2.50	0.42
1:A:195:ASP:HB3	1:A:196:LEU:HG	2.01	0.42
1:B:518:ASN:C	1:B:520:PRO:CD	2.87	0.42
1:D:347:ARG:HG3	1:D:392:GLY:N	2.33	0.42
1:D:333:VAL:HG23	1:D:334:PRO:HD3	2.01	0.42
1:D:239:VAL:HG13	1:D:240:GLN:N	2.34	0.42
1:B:151:LEU:N	1:B:151:LEU:HD12	2.33	0.42
1:C:250:PRO:HA	1:C:255:TRP:CG	2.55	0.42
1:B:490:LYS:O	1:B:490:LYS:CG	2.67	0.42
1:D:109:THR:HB	1:D:131:SER:HB2	1.99	0.42
1:A:175:ILE:CG2	1:A:176:GLY:N	2.82	0.42
1:D:86:SER:HA	1:D:87:PRO:HD3	1.83	0.42
1:A:344:ASP:O	1:A:344:ASP:CG	2.57	0.42
1:A:3:VAL:HA	1:B:3:VAL:HB	2.00	0.42
1:D:469:TYR:CE2	1:D:470:PRO:HD2	2.54	0.42
1:A:461:ASP:HB3	1:A:468:THR:HG22	2.00	0.42
1:D:188:THR:H	2:D:801:NAG:H83	1.84	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:D:522:LEU:HB3	1:D:523:THR:H	1.57	0.42
1:B:371:ILE:HD12	1:B:371:ILE:HA	1.65	0.42
1:C:333:VAL:HG23	1:C:334:PRO:HD3	2.01	0.42
1:C:241:ARG:HE	1:C:281:ILE:CD1	2.24	0.42
1:C:490:LYS:CG	1:C:490:LYS:O	2.67	0.42
1:A:515:ASP:OD1	1:A:516:ALA:N	2.53	0.42
1:A:220:ILE:O	1:A:220:ILE:HG22	2.18	0.42
1:C:396:ARG:NH2	1:C:464:ILE:HG22	2.12	0.42
1:B:5:PRO:HA	1:B:6:PRO:HD3	1.85	0.42
1:D:90:GLU:O	1:D:91:PRO:O	2.37	0.42
1:D:540:GLN:NE2	1:D:540:GLN:O	2.47	0.42
1:B:421:THR:CG2	1:B:422:GLY:N	2.81	0.42
1:B:339:VAL:HG21	1:B:351:ILE:HG22	2.01	0.42
2:D:805:NAG:C5	2:D:806:NAG:H83	2.46	0.42
1:B:33:LYS:NZ	1:B:56:GLU:OE1	2.42	0.42
1:B:511:VAL:N	1:B:523:THR:O	2.46	0.42
1:D:195:ASP:HB3	1:D:196:LEU:HG	2.01	0.42
1:A:371:ILE:HA	1:A:410:MET:HB3	2.02	0.42
1:A:371:ILE:HG13	1:A:410:MET:SD	2.59	0.42
1:D:347:ARG:HD2	1:D:392:GLY:CA	2.50	0.42
1:D:371:ILE:HD13	1:D:381:VAL:HG11	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ILE:CG2	1:C:176:GLY:N	2.82	0.42
1:A:449:ASP:N	1:A:532:CYS:HB3	2.19	0.42
2:D:810:NAG:C1	2:D:810:NAG:O7	2.67	0.42
1:B:371:ILE:HA	1:B:410:MET:HB3	2.02	0.42
1:B:250:PRO:HA	1:B:255:TRP:CG	2.54	0.42
1:A:138:ASN:C	1:A:138:ASN:ND2	2.73	0.42
1:B:264:ASN:HB3	1:B:267:GLY:HA2	2.01	0.42
1:A:264:ASN:HB3	1:A:267:GLY:HA2	2.01	0.42
1:C:468:THR:C	1:C:469:TYR:O	2.54	0.42
1:B:299:GLN:CG	1:B:318:THR:HG23	2.42	0.42
1:C:154:ASP:HB3	2:C:801:NAG:C7	2.48	0.42
1:A:513:LEU:C	1:A:514:SER:HG	2.23	0.42
1:B:439:VAL:HA	1:B:440:PRO:HD3	1.81	0.42
1:D:230:VAL:O	1:D:323:VAL:HA	2.20	0.42
1:A:261:ILE:H	1:A:261:ILE:HD13	1.84	0.42
1:C:264:ASN:HB3	1:C:267:GLY:HA2	2.01	0.42
1:B:515:ASP:OD1	1:B:516:ALA:N	2.53	0.42
1:A:3:VAL:C	1:B:4:ILE:O	2.19	0.42
1:C:339:VAL:HG21	1:C:351:ILE:HG22	2.01	0.42
1:D:409:ILE:HD13	3:D:811:NDG:H8C3	2.01	0.42
1:C:371:ILE:HA	1:C:371:ILE:HD12	1.65	0.42
1:C:371:ILE:HG13	1:C:410:MET:SD	2.59	0.42
1:C:239:VAL:HG13	1:C:240:GLN:N	2.34	0.42
1:C:230:VAL:O	1:C:323:VAL:HA	2.20	0.42
1:D:261:ILE:HD13	1:D:261:ILE:H	1.85	0.42
1:B:7:ILE:O	1:B:96:ILE:HG23	2.20	0.42
1:C:502:LEU:HD23	1:C:502:LEU:HA	1.82	0.42
1:B:344:ASP:CG	1:B:344:ASP:O	2.57	0.42
1:A:409:ILE:HD13	3:A:811:NDG:H8C3	2.01	0.42
1:B:195:ASP:HB3	1:B:196:LEU:HG	2.01	0.42
1:C:195:ASP:HB3	1:C:196:LEU:HG	2.01	0.42
1:A:505:GLY:H	1:A:529:VAL:HB	1.85	0.42
1:B:505:GLY:H	1:B:529:VAL:HB	1.85	0.42
1:C:483:TRP:CZ2	1:C:507:TYR:CE1	2.87	0.42
1:D:117:VAL:O	1:D:212:THR:N	2.46	0.42
1:A:297:VAL:HG21	2:A:807:NAG:H62	2.01	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:A:239:VAL:HG11	1:A:282:LEU:HD22	2.02	0.42
1:B:230:VAL:O	1:B:323:VAL:HA	2.20	0.42
1:B:67:ASP:CG	1:B:69:GLU:HB2	2.40	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:B:175:ILE:CG2	1:B:176:GLY:N	2.82	0.42
1:C:449:ASP:N	1:C:532:CYS:HB3	2.19	0.42
1:A:231:PRO:O	1:A:288:LEU:HD12	2.20	0.42
1:B:27:ASN:ND2	1:B:28:LYS:N	2.50	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:C:347:ARG:HD2	1:C:392:GLY:CA	2.50	0.42
1:A:230:VAL:O	1:A:323:VAL:HA	2.20	0.42
1:C:151:LEU:HD12	1:C:151:LEU:N	2.33	0.42
1:A:490:LYS:CG	1:A:490:LYS:O	2.67	0.42
1:B:138:ASN:C	1:B:138:ASN:ND2	2.73	0.42
1:B:261:ILE:HD13	1:B:261:ILE:H	1.85	0.42
1:C:261:ILE:HD13	1:C:261:ILE:H	1.85	0.42
1:C:515:ASP:OD1	1:C:516:ALA:N	2.52	0.42
1:B:469:TYR:CE2	1:B:470:PRO:HD2	2.54	0.41
1:D:419:VAL:HG13	1:D:420:GLY:N	2.33	0.41
1:C:474:SER:N	1:C:512:LEU:O	2.53	0.41
1:B:409:ILE:HD13	3:B:811:NDG:H8C3	2.01	0.41
1:C:371:ILE:HA	1:C:410:MET:HB3	2.02	0.41
1:C:505:GLY:H	1:C:529:VAL:HB	1.85	0.41
1:D:368:SER:CB	1:D:370:PHE:HE1	2.31	0.41
1:B:23:GLN:HB2	1:B:59:TRP:CD2	2.55	0.41
1:D:67:ASP:CG	1:D:69:GLU:HB2	2.40	0.41
1:B:108:PHE:HA	1:B:132:ALA:CB	2.50	0.41
1:A:108:PHE:HA	1:A:132:ALA:CB	2.50	0.41
1:C:138:ASN:C	1:C:138:ASN:ND2	2.73	0.41
2:C:810:NAG:C1	2:C:810:NAG:O7	2.67	0.41
1:A:90:GLU:N	1:B:90:GLU:CB	2.57	0.41
1:D:474:SER:N	1:D:512:LEU:O	2.53	0.41
1:C:118:ARG:CA	1:C:212:THR:HB	2.51	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:D:339:VAL:HG21	1:D:351:ILE:HG22	2.01	0.41
1:A:67:ASP:CG	1:A:69:GLU:HB2	2.40	0.41
1:C:108:PHE:HA	1:C:132:ALA:CB	2.50	0.41
1:D:264:ASN:HB3	1:D:267:GLY:HA2	2.02	0.41
1:D:250:PRO:HA	1:D:255:TRP:CG	2.54	0.41
1:D:515:ASP:OD1	1:D:516:ALA:N	2.53	0.41
1:D:154:ASP:HB3	2:D:801:NAG:C7	2.48	0.41
1:B:239:VAL:HG11	1:B:282:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLN:HA	1:A:58:GLY:O	2.21	0.41
1:C:235:ILE:HG21	1:C:235:ILE:HD13	1.84	0.41
1:B:335:ALA:HB3	3:B:811:NDG:O6	2.15	0.41
1:A:111:ASP:O	1:A:112:VAL:HG13	2.21	0.41
1:A:4:ILE:HD13	1:B:2:TRP:HA	2.03	0.41
1:A:235:ILE:CD1	1:A:287:GLY:HA2	2.50	0.41
1:D:329:ALA:HA	1:D:330:PRO:HD3	1.87	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:367:LEU:H	1:D:367:LEU:HG	1.41	0.41
1:B:347:ARG:HD2	1:B:392:GLY:CA	2.50	0.41
1:C:239:VAL:HG11	1:C:282:LEU:HD22	2.02	0.41
1:C:230:VAL:HG23	1:C:323:VAL:HA	2.03	0.41
1:B:127:VAL:HG22	1:B:128:MET:HG3	2.03	0.41
1:C:67:ASP:CG	1:C:69:GLU:HB2	2.40	0.41
1:D:490:LYS:O	1:D:490:LYS:CG	2.67	0.41
1:D:502:LEU:HD23	1:D:502:LEU:HA	1.82	0.41
1:C:344:ASP:CG	1:C:344:ASP:O	2.57	0.41
1:A:7:ILE:O	1:A:96:ILE:HG23	2.20	0.41
1:B:423:THR:CG2	2:B:810:NAG:N2	2.84	0.41
1:A:400:TYR:O	1:A:401:VAL:C	2.59	0.41
1:A:366:LYS:HG2	1:A:367:LEU:H	1.74	0.41
1:C:127:VAL:HG22	1:C:128:MET:HG3	2.03	0.41
1:D:127:VAL:HG22	1:D:128:MET:HG3	2.03	0.41
1:C:237:PHE:N	1:C:284:THR:OG1	2.42	0.41
1:C:7:ILE:O	1:C:96:ILE:HG23	2.20	0.41
1:D:7:ILE:O	1:D:96:ILE:HG23	2.20	0.41
1:A:423:THR:CG2	2:A:810:NAG:N2	2.84	0.41
1:A:297:VAL:HG22	2:A:807:NAG:H62	2.03	0.41
1:B:514:SER:HG	1:B:519:ASN:HA	1.85	0.41
1:D:230:VAL:HG23	1:D:323:VAL:HA	2.03	0.41
1:B:230:VAL:HG23	1:B:323:VAL:HA	2.03	0.41
1:A:127:VAL:HG22	1:A:128:MET:HG3	2.03	0.41
1:D:505:GLY:H	1:D:529:VAL:HB	1.85	0.41
1:D:68:ARG:HD3	1:D:100:ASP:CB	2.51	0.41
1:A:108:PHE:CZ	1:A:191:VAL:HG23	2.56	0.41
1:D:25:LYS:NZ	1:D:29:ASP:OD2	2.39	0.41
1:D:439:VAL:HA	1:D:440:PRO:HD3	1.81	0.41
1:B:400:TYR:O	1:B:401:VAL:C	2.59	0.41
1:D:371:ILE:HA	1:D:410:MET:HB3	2.02	0.41
1:D:108:PHE:CZ	1:D:191:VAL:HG23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:PHE:CZ	1:C:191:VAL:HG23	2.56	0.41
1:B:237:PHE:N	1:B:284:THR:OG1	2.42	0.41
1:C:432:ASP:CG	1:C:433:VAL:N	2.74	0.41
1:C:23:GLN:HB2	1:C:59:TRP:CD2	2.55	0.41
1:D:448:CYS:C	1:D:452:PRO:HG3	2.40	0.41
1:A:231:PRO:O	1:A:235:ILE:HD13	2.21	0.41
1:C:423:THR:CG2	2:C:810:NAG:N2	2.84	0.41
1:A:90:GLU:HG3	1:B:89:GLU:CG	2.46	0.41
1:D:212:THR:CG2	1:D:213:ASP:H	2.32	0.41
1:B:297:VAL:HG22	2:B:807:NAG:H62	2.03	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: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:A:440:PRO:HB3	1:A:457:LEU:CD2	2.43	0.41
1:C:127:VAL:HG13	1:C:128:MET:N	2.25	0.41
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.51	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:C:119:GLU:CG	1:C:214:ALA:HB3	2.51	0.41
1:A:252:THR:O	1:A:255:TRP:N	2.54	0.41
1:B:249:MET:O	1:B:252:THR:CB	2.69	0.41
1:D:481:LEU:HA	1:D:481:LEU:HD12	1.50	0.41
1:B:62:VAL:HG13	1:B:62:VAL:O	2.21	0.41
1:C:62:VAL:O	1:C:62:VAL:HG13	2.21	0.41
1:C:122:GLN:HE21	1:C:122:GLN:HB3	1.58	0.41
1:C:193:ALA:O	1:C:202:SER:HA	2.21	0.41
1:A:329:ALA:HA	1:A:330:PRO:HD3	1.87	0.41
1:D:423:THR:CG2	2:D:810:NAG:N2	2.84	0.41
1:A:223:PRO:HB2	1:A:226:TYR:CZ	2.56	0.41
1:C:319:VAL:CG1	1:C:320:THR:N	2.84	0.41
1:C:409:ILE:HD13	3:C:811:NDG:C8	2.52	0.41
1:C:347:ARG:HG3	1:C:392:GLY:N	2.33	0.41
1:C:272:THR:O	1:C:281:ILE:HG22	2.21	0.41
1:D:239:VAL:HG11	1:D:282:LEU:HD22	2.02	0.41
1:A:108:PHE:HA	1:A:132:ALA:HB2	2.03	0.41
1:A:42:GLY:CA	1:A:47:PRO:O	2.69	0.41
1:C:249:MET:O	1:C:252:THR:CB	2.69	0.41
1:D:193:ALA:O	1:D:202:SER:HA	2.21	0.41
1:D:111:ASP:O	1:D:112:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ALA:O	1:A:202:SER:HA	2.21	0.41
1:B:111:ASP:O	1:B:112:VAL:HG13	2.21	0.41
1:B:86:SER:HA	1:B:87:PRO:HD3	1.83	0.41
1:B:432:ASP:CG	1:B:433:VAL:N	2.74	0.40
1:A:449:ASP:HB2	1:A:531:SER:HA	2.03	0.40
1:C:226:TYR:HB2	1:C:319:VAL:CG2	2.52	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:D:373:ASN:CG	1:D:374:ASP:N	2.75	0.40
1:A:272:THR:O	1:A:281:ILE:HG22	2.21	0.40
1:A:23:GLN:HB2	1:A:59:TRP:CD2	2.55	0.40
1:C:68:ARG:HD3	1:C:100:ASP:CB	2.51	0.40
1:D:119:GLU:CG	1:D:214:ALA:HB3	2.51	0.40
1:D:138:ASN:ND2	1:D:138:ASN:C	2.73	0.40
1:B:119:GLU:CG	1:B:214:ALA:HB3	2.51	0.40
1:B:19:LYS:HB3	1:B:62:VAL:CG1	2.52	0.40
1:D:464:ILE:CD1	1:D:465:PRO:N	2.73	0.40
1:A:3:VAL:HG21	1:B:4:ILE:HG13	1.18	0.40
1:D:154:ASP:C	2:D:801:NAG:C8	2.62	0.40
1:A:319:VAL:CG1	1:A:320:THR:N	2.84	0.40
1:A:32:ASN:ND2	1:A:83:GLU:CB	2.62	0.40
1:B:272:THR:O	1:B:281:ILE:HG22	2.22	0.40
1:B:438:PRO:HB2	1:B:513:LEU:CD1	2.51	0.40
1:C:438:PRO:HB2	1:C:513:LEU:CD1	2.51	0.40
1:D:127:VAL:HG13	1:D:128:MET:N	2.25	0.40
1:C:252:THR:O	1:C:255:TRP:N	2.54	0.40
1:D:502:LEU:HD22	1:D:503:LYS:H	1.85	0.40
1:D:62:VAL:O	1:D:62:VAL:HG13	2.21	0.40
1:D:396:ARG:HH21	1:D:432:ASP:CG	2.25	0.40
1:D:432:ASP:CG	1:D:433:VAL:N	2.74	0.40
1:A:373:ASN:CG	1:A:374:ASP:N	2.75	0.40
1:D:23:GLN:HB2	1:D:59:TRP:CD2	2.55	0.40
1:C:42:GLY:CA	1:C:47:PRO:O	2.69	0.40
1:A:259:TYR:O	1:A:260:LYS:CB	2.69	0.40
1:D:19:LYS:HB3	1:D:62:VAL:HG12	2.03	0.40
1:B:502:LEU:HD22	1:B:503:LYS:H	1.85	0.40
1:A:502:LEU:HD22	1:A:503:LYS:H	1.86	0.40
1:C:111:ASP:O	1:C:112:VAL:HG13	2.21	0.40
1:C:316:THR:OG1	2:C:806:NAG:H83	2.21	0.40
1:D:223:PRO:HB2	1:D:226:TYR:CZ	2.56	0.40
1:A:226:TYR:HB2	1:A:319:VAL:CG2	2.52	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:A:34:VAL:CG1	1:A:80:ALA:HB1	2.52	0.40
1:A:415:ASP:CG	1:A:416:GLY:H	2.16	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:C:108:PHE:HA	1:C:132:ALA:HB2	2.03	0.40
1:B:162:LEU:HD13	1:B:179:LEU:HD21	2.04	0.40
1:A:119:GLU:CG	1:A:214:ALA:HB3	2.51	0.40
1:D:385:ASN:ND2	1:D:385:ASN:O	2.55	0.40
1:A:237:PHE:N	1:A:284:THR:OG1	2.42	0.40
1:A:24:ILE:CG2	1:B:1:ASP:N	2.84	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:A:409:ILE:HD13	3:A:811:NDG:C8	2.51	0.40
1:C:439:VAL:HA	1:C:440:PRO:HD3	1.81	0.40
1:D:438:PRO:HB2	1:D:513:LEU:CD1	2.51	0.40
1:B:68:ARG:HD3	1:B:100:ASP:CB	2.51	0.40
1:C:138:ASN:HD22	1:C:138:ASN:N	2.19	0.40
1:C:385:ASN:ND2	1:C:385:ASN:O	2.55	0.40
1:C:435:ASP:HB2	1:C:436:ASN:H	1.58	0.40
1:D:435:ASP:HB2	1:D:436:ASN:H	1.58	0.40
1:B:193:ALA:O	1:B:202:SER:HA	2.21	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%)	1	18
1	B	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	18
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	18
All	All	2152/3520 (61%)	1604 (74%)	368 (17%)	180 (8%)	2	18

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

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

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

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Mol	Chain	Res	Type
1	C	152	LYS
1	C	223	PRO
1	C	359	PRO
1	C	375	PRO
1	D	152	LYS
1	D	223	PRO
1	D	359	PRO
1	D	375	PRO
1	A	160	PRO
1	A	265	GLU
1	A	278	ASN
1	A	289	ASP
1	A	482	THR
1	B	160	PRO
1	B	265	GLU
1	B	278	ASN
1	B	289	ASP
1	B	482	THR
1	C	160	PRO
1	C	265	GLU
1	C	278	ASN
1	C	289	ASP
1	C	482	THR
1	D	160	PRO
1	D	265	GLU
1	D	278	ASN
1	D	289	ASP
1	D	482	THR
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

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Mol	Chain	Res	Type
1	D	154	ASP
1	D	307	PRO
1	A	222	ASP
1	B	222	ASP
1	C	222	ASP
1	D	222	ASP
1	A	200	GLY
1	B	200	GLY
1	C	200	GLY
1	D	200	GLY
1	A	47	PRO
1	A	158	PRO
1	B	47	PRO
1	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%)	381 (79%)	99 (21%)	1	10
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	10
1	C	480/779 (62%)	381 (79%)	99 (21%)	1	10
1	D	480/779 (62%)	381 (79%)	99 (21%)	1	10
All	All	1920/3116 (62%)	1524 (79%)	396 (21%)	4	10

All (396) 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

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Mol	Chain	Res	Type
1	A	27	ASN
1	A	52	ARG
1	A	61	LEU
1	A	66	LEU
1	A	68	ARG
1	A	88	VAL
1	A	91	PRO
1	A	92	MET
1	A	117	VAL
1	A	138	ASN
1	A	146	LEU
1	A	151	LEU
1	A	155	PRO
1	A	156	GLU
1	A	161	ASN
1	A	163	PHE
1	A	189	LEU
1	A	195	ASP
1	A	202	SER
1	A	216	ASP
1	A	217	ASN
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	250	PRO
1	A	253	PRO
1	A	261	ILE
1	A	264	ASN
1	A	268	PHE
1	A	273	THR
1	A	277	SER
1	A	278	ASN
1	A	282	LEU
1	A	284	THR
1	A	288	LEU
1	A	298	LEU
1	A	309	SER
1	A	310	VAL

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Mol	Chain	Res	Type
1	A	315	SER
1	A	316	THR
1	A	318	THR
1	A	333	VAL
1	A	336	VAL
1	A	339	VAL
1	A	345	LEU
1	A	353	SER
1	A	354	LEU
1	A	360	ASP
1	A	363	GLN
1	A	364	ILE
1	A	365	GLN
1	A	371	ILE
1	A	373	ASN
1	A	375	PRO
1	A	379	LEU
1	A	382	ASN
1	A	384	ASP
1	A	385	ASN
1	A	393	ASN
1	A	394	LEU
1	A	395	ASP
1	A	398	SER
1	A	399	GLU
1	A	404	ASN
1	A	405	THR
1	A	407	THR
1	A	410	MET
1	A	423	THR
1	A	425	THR
1	A	427	ILE
1	A	428	LEU
1	A	433	VAL
1	A	436	ASN
1	A	447	MET
1	A	448	CYS
1	A	461	ASP
1	A	464	ILE
1	A	465	PRO
1	A	466	PRO
1	A	470	PRO

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Mol	Chain	Res	Type
1	A	477	HIS
1	A	492	THR
1	A	509	ILE
1	A	512	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	A	520	PRO
1	A	522	LEU
1	A	523	THR
1	A	532	CYS
1	A	540	GLN
1	B	8	LYS
1	B	18	PRO
1	B	19	LYS
1	B	27	ASN
1	B	52	ARG
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	117	VAL
1	B	138	ASN
1	B	146	LEU
1	B	151	LEU
1	B	155	PRO
1	B	156	GLU
1	B	161	ASN
1	B	163	PHE
1	B	189	LEU
1	B	195	ASP
1	B	202	SER
1	B	216	ASP
1	B	217	ASN
1	B	223	PRO
1	B	226	TYR
1	B	231	PRO
1	B	233	ASN
1	B	234	GLU
1	B	235	ILE

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Mol	Chain	Res	Type
1	B	237	PHE
1	B	250	PRO
1	B	253	PRO
1	B	261	ILE
1	B	264	ASN
1	B	268	PHE
1	B	273	THR
1	B	277	SER
1	B	278	ASN
1	B	282	LEU
1	B	284	THR
1	B	288	LEU
1	B	298	LEU
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	345	LEU
1	B	353	SER
1	B	354	LEU
1	B	360	ASP
1	B	363	GLN
1	B	364	ILE
1	B	365	GLN
1	B	371	ILE
1	B	373	ASN
1	B	375	PRO
1	B	379	LEU
1	B	382	ASN
1	B	384	ASP
1	B	385	ASN
1	B	393	ASN
1	B	394	LEU
1	B	395	ASP
1	B	398	SER
1	B	399	GLU
1	B	404	ASN
1	B	405	THR

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Mol	Chain	Res	Type
1	B	407	THR
1	B	410	MET
1	B	423	THR
1	B	425	THR
1	B	427	ILE
1	B	428	LEU
1	B	433	VAL
1	B	436	ASN
1	B	447	MET
1	B	448	CYS
1	B	461	ASP
1	B	464	ILE
1	B	465	PRO
1	B	466	PRO
1	B	470	PRO
1	B	477	HIS
1	B	492	THR
1	B	509	ILE
1	B	512	LEU
1	B	517	GLN
1	B	518	ASN
1	B	519	ASN
1	B	520	PRO
1	B	522	LEU
1	B	523	THR
1	B	532	CYS
1	B	540	GLN
1	C	8	LYS
1	C	18	PRO
1	C	19	LYS
1	C	27	ASN
1	C	52	ARG
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	117	VAL
1	C	138	ASN
1	C	146	LEU
1	C	151	LEU

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Mol	Chain	Res	Type
1	C	155	PRO
1	C	156	GLU
1	C	161	ASN
1	C	163	PHE
1	C	189	LEU
1	C	195	ASP
1	C	202	SER
1	C	216	ASP
1	C	217	ASN
1	C	223	PRO
1	C	226	TYR
1	C	231	PRO
1	C	233	ASN
1	C	234	GLU
1	C	235	ILE
1	C	237	PHE
1	C	250	PRO
1	C	253	PRO
1	C	261	ILE
1	C	264	ASN
1	C	268	PHE
1	C	273	THR
1	C	277	SER
1	C	278	ASN
1	C	282	LEU
1	C	284	THR
1	C	288	LEU
1	C	298	LEU
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	345	LEU
1	C	353	SER
1	C	354	LEU
1	C	360	ASP
1	C	363	GLN
1	C	364	ILE

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Mol	Chain	Res	Type
1	C	365	GLN
1	C	371	ILE
1	C	373	ASN
1	C	375	PRO
1	C	379	LEU
1	C	382	ASN
1	C	384	ASP
1	C	385	ASN
1	C	393	ASN
1	C	394	LEU
1	C	395	ASP
1	C	398	SER
1	C	399	GLU
1	C	404	ASN
1	C	405	THR
1	C	407	THR
1	C	410	MET
1	C	423	THR
1	C	425	THR
1	C	427	ILE
1	C	428	LEU
1	C	433	VAL
1	C	436	ASN
1	C	447	MET
1	C	448	CYS
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	512	LEU
1	C	517	GLN
1	C	518	ASN
1	C	519	ASN
1	C	520	PRO
1	C	522	LEU
1	C	523	THR
1	C	532	CYS
1	C	540	GLN

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Mol	Chain	Res	Type
1	D	8	LYS
1	D	18	PRO
1	D	19	LYS
1	D	27	ASN
1	D	52	ARG
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	117	VAL
1	D	138	ASN
1	D	146	LEU
1	D	151	LEU
1	D	155	PRO
1	D	156	GLU
1	D	161	ASN
1	D	163	PHE
1	D	189	LEU
1	D	195	ASP
1	D	202	SER
1	D	216	ASP
1	D	217	ASN
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	250	PRO
1	D	253	PRO
1	D	261	ILE
1	D	264	ASN
1	D	268	PHE
1	D	273	THR
1	D	277	SER
1	D	278	ASN
1	D	282	LEU
1	D	284	THR
1	D	288	LEU

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Mol	Chain	Res	Type
1	D	298	LEU
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	345	LEU
1	D	353	SER
1	D	354	LEU
1	D	360	ASP
1	D	363	GLN
1	D	364	ILE
1	D	365	GLN
1	D	371	ILE
1	D	373	ASN
1	D	375	PRO
1	D	379	LEU
1	D	382	ASN
1	D	384	ASP
1	D	385	ASN
1	D	393	ASN
1	D	394	LEU
1	D	395	ASP
1	D	398	SER
1	D	399	GLU
1	D	404	ASN
1	D	405	THR
1	D	407	THR
1	D	410	MET
1	D	423	THR
1	D	425	THR
1	D	427	ILE
1	D	428	LEU
1	D	433	VAL
1	D	436	ASN
1	D	447	MET
1	D	448	CYS
1	D	461	ASP
1	D	464	ILE

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Mol	Chain	Res	Type
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	512	LEU
1	D	517	GLN
1	D	518	ASN
1	D	519	ASN
1	D	520	PRO
1	D	522	LEU
1	D	523	THR
1	D	532	CYS
1	D	540	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) 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	104	ASN
1	A	110	GLN
1	A	122	GLN
1	A	138	ASN
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	455	GLN
1	A	467	ASN
1	A	517	GLN
1	A	519	ASN
1	B	12	ASN

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Mol	Chain	Res	Type
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	233	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	393	ASN
1	B	404	ASN
1	B	455	GLN
1	B	467	ASN
1	B	517	GLN
1	B	519	ASN
1	C	12	ASN
1	C	27	ASN
1	C	32	ASN
1	C	45	ASN
1	C	104	ASN
1	C	110	GLN
1	C	122	GLN
1	C	138	ASN
1	C	217	ASN
1	C	233	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	393	ASN
1	C	404	ASN
1	C	455	GLN

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

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	801	1	14,14,15	0.64	0	15,19,21	0.89	0
2	NAG	A	802	1	14,14,15	0.73	0	15,19,21	0.82	1 (6%)
2	NAG	A	803	1	14,14,15	0.91	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	A	804	1	14,14,15	0.62	0	15,19,21	0.82	0
2	NAG	A	805	1	14,14,15	0.69	0	15,19,21	1.17	1 (6%)
2	NAG	A	806	1	14,14,15	0.55	0	15,19,21	1.40	2 (13%)
2	NAG	A	807	1	14,14,15	0.64	0	15,19,21	1.13	1 (6%)
2	NAG	A	808	1	14,14,15	0.66	0	15,19,21	0.70	0
2	NAG	A	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.96	1 (6%)
2	NAG	A	810	1	14,14,15	0.64	0	15,19,21	1.09	1 (6%)
3	NDG	A	811	1	14,14,15	0.82	0	15,19,21	2.17	1 (6%)
2	NAG	A	812	1	14,14,15	0.83	1 (7%)	15,19,21	0.75	1 (6%)
3	NDG	A	902	1	14,14,15	1.08	1 (7%)	15,19,21	0.96	0
3	NDG	A	903	1	14,14,15	0.51	0	15,19,21	0.64	0
2	NAG	A	904	1	14,14,15	0.76	1 (7%)	15,19,21	0.79	1 (6%)
2	NAG	B	801	1	14,14,15	0.63	0	15,19,21	0.88	0
2	NAG	B	802	1	14,14,15	0.72	0	15,19,21	0.82	1 (6%)
2	NAG	B	803	1	14,14,15	0.92	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	B	804	1	14,14,15	0.63	0	15,19,21	0.81	0
2	NAG	B	805	1	14,14,15	0.69	0	15,19,21	1.16	1 (6%)
2	NAG	B	806	1	14,14,15	0.55	0	15,19,21	1.41	2 (13%)
2	NAG	B	807	1	14,14,15	0.63	0	15,19,21	1.13	1 (6%)
2	NAG	B	808	1	14,14,15	0.67	0	15,19,21	0.69	0
2	NAG	B	809	1	14,14,15	0.77	1 (7%)	15,19,21	0.97	1 (6%)
2	NAG	B	810	1	14,14,15	0.63	0	15,19,21	1.09	2 (13%)
3	NDG	B	811	1	14,14,15	0.82	0	15,19,21	2.17	1 (6%)
2	NAG	B	812	1	14,14,15	0.82	1 (7%)	15,19,21	0.76	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NDG	B	902	1	14,14,15	1.07	1 (7%)	15,19,21	0.95	0
3	NDG	B	903	1	14,14,15	0.51	0	15,19,21	0.64	0
2	NAG	B	904	1	14,14,15	0.76	1 (7%)	15,19,21	0.78	1 (6%)
2	NAG	C	801	1	14,14,15	0.65	0	15,19,21	0.88	0
2	NAG	C	802	1	14,14,15	0.72	0	15,19,21	0.82	1 (6%)
2	NAG	C	803	1	14,14,15	0.92	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	C	804	1	14,14,15	0.62	0	15,19,21	0.82	0
2	NAG	C	805	1	14,14,15	0.68	0	15,19,21	1.16	1 (6%)
2	NAG	C	806	1	14,14,15	0.56	0	15,19,21	1.41	2 (13%)
2	NAG	C	807	1	14,14,15	0.63	0	15,19,21	1.14	1 (6%)
2	NAG	C	808	1	14,14,15	0.66	0	15,19,21	0.70	0
2	NAG	C	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.97	1 (6%)
2	NAG	C	810	1	14,14,15	0.62	0	15,19,21	1.09	2 (13%)
3	NDG	C	811	1	14,14,15	0.82	0	15,19,21	2.16	1 (6%)
2	NAG	C	812	1	14,14,15	0.82	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	C	902	1	14,14,15	1.08	1 (7%)	15,19,21	0.96	0
3	NDG	C	903	1	14,14,15	0.51	0	15,19,21	0.64	0
2	NAG	C	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.79	1 (6%)
2	NAG	D	801	1	14,14,15	0.66	0	15,19,21	0.88	0
2	NAG	D	802	1	14,14,15	0.71	0	15,19,21	0.83	1 (6%)
2	NAG	D	803	1	14,14,15	0.92	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	D	804	1	14,14,15	0.63	0	15,19,21	0.82	0
2	NAG	D	805	1	14,14,15	0.68	0	15,19,21	1.16	1 (6%)
2	NAG	D	806	1	14,14,15	0.54	0	15,19,21	1.41	2 (13%)
2	NAG	D	807	1	14,14,15	0.63	0	15,19,21	1.14	1 (6%)
2	NAG	D	808	1	14,14,15	0.66	0	15,19,21	0.69	0
2	NAG	D	809	1	14,14,15	0.75	1 (7%)	15,19,21	0.97	1 (6%)
2	NAG	D	810	1	14,14,15	0.62	0	15,19,21	1.09	2 (13%)
3	NDG	D	811	1	14,14,15	0.82	0	15,19,21	2.17	1 (6%)
2	NAG	D	812	1	14,14,15	0.83	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	D	902	1	14,14,15	1.08	1 (7%)	15,19,21	0.96	0
3	NDG	D	903	1	14,14,15	0.51	0	15,19,21	0.64	0
2	NAG	D	904	1	14,14,15	0.76	1 (7%)	15,19,21	0.79	1 (6%)

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	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	807	1	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1	-	0/6/23/26	0/1/1/1
2	NAG	A	809	1	-	0/6/23/26	0/1/1/1
2	NAG	A	810	1	-	0/6/23/26	0/1/1/1
3	NDG	A	811	1	-	0/6/23/26	0/1/1/1
2	NAG	A	812	1	-	0/6/23/26	0/1/1/1
3	NDG	A	902	1	-	0/6/23/26	0/1/1/1
3	NDG	A	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	904	1	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1	-	0/6/23/26	0/1/1/1
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1
2	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NDG	B	804	1	-	0/6/23/26	0/1/1/1
2	NAG	B	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	807	1	-	0/6/23/26	0/1/1/1
2	NAG	B	808	1	-	0/6/23/26	0/1/1/1
2	NAG	B	809	1	-	0/6/23/26	0/1/1/1
2	NAG	B	810	1	-	0/6/23/26	0/1/1/1
3	NDG	B	811	1	-	0/6/23/26	0/1/1/1
2	NAG	B	812	1	-	0/6/23/26	0/1/1/1
3	NDG	B	902	1	-	0/6/23/26	0/1/1/1
3	NDG	B	903	1	-	0/6/23/26	0/1/1/1
2	NAG	B	904	1	-	0/6/23/26	0/1/1/1
2	NAG	C	801	1	-	0/6/23/26	0/1/1/1
2	NAG	C	802	1	-	0/6/23/26	0/1/1/1
2	NAG	C	803	1	-	0/6/23/26	0/1/1/1
3	NDG	C	804	1	-	0/6/23/26	0/1/1/1
2	NAG	C	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	807	1	-	0/6/23/26	0/1/1/1
2	NAG	C	808	1	-	0/6/23/26	0/1/1/1
2	NAG	C	809	1	-	0/6/23/26	0/1/1/1
2	NAG	C	810	1	-	0/6/23/26	0/1/1/1
3	NDG	C	811	1	-	0/6/23/26	0/1/1/1
2	NAG	C	812	1	-	0/6/23/26	0/1/1/1

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	904	NAG	C1-C2	-2.45	1.49	1.52
2	D	904	NAG	C1-C2	-2.39	1.49	1.52
2	B	904	NAG	C1-C2	-2.39	1.49	1.52
2	A	904	NAG	C1-C2	-2.38	1.49	1.52
2	C	812	NAG	C1-C2	-2.32	1.49	1.52
2	D	812	NAG	C1-C2	-2.31	1.49	1.52
2	B	812	NAG	C1-C2	-2.30	1.49	1.52
2	A	812	NAG	C1-C2	-2.29	1.49	1.52
2	B	809	NAG	C1-C2	-2.05	1.49	1.52
2	C	809	NAG	C1-C2	-2.05	1.49	1.52
2	D	809	NAG	C1-C2	-2.03	1.49	1.52
2	A	809	NAG	C1-C2	-2.03	1.49	1.52
2	D	803	NAG	O5-C5	2.34	1.48	1.43
2	B	803	NAG	O5-C5	2.35	1.48	1.43
2	A	803	NAG	O5-C5	2.36	1.48	1.43
2	C	803	NAG	O5-C5	2.37	1.48	1.43
3	B	902	NDG	C1-C2	3.13	1.56	1.52
3	D	902	NDG	C1-C2	3.18	1.57	1.52
3	C	902	NDG	C1-C2	3.19	1.57	1.52
3	A	902	NDG	C1-C2	3.20	1.57	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-7.84	112.91	123.11
3	D	811	NDG	C2-N2-C7	-7.82	112.94	123.11
3	A	811	NDG	C2-N2-C7	-7.80	112.96	123.11
3	C	811	NDG	C2-N2-C7	-7.78	112.98	123.11
2	C	806	NAG	C2-N2-C7	-3.90	118.03	123.11
2	D	806	NAG	C2-N2-C7	-3.89	118.05	123.11
2	B	806	NAG	C2-N2-C7	-3.88	118.05	123.11
2	A	806	NAG	C2-N2-C7	-3.86	118.08	123.11
2	A	805	NAG	C2-N2-C7	-3.42	118.65	123.11
2	B	805	NAG	C2-N2-C7	-3.40	118.68	123.11
2	D	805	NAG	C2-N2-C7	-3.39	118.69	123.11
2	C	805	NAG	C2-N2-C7	-3.38	118.71	123.11
2	D	807	NAG	C2-N2-C7	-3.32	118.79	123.11
2	C	807	NAG	C2-N2-C7	-3.31	118.80	123.11
2	A	807	NAG	C2-N2-C7	-3.30	118.81	123.11
2	B	807	NAG	C2-N2-C7	-3.28	118.84	123.11
2	B	803	NAG	C2-N2-C7	-3.27	118.85	123.11
2	C	803	NAG	C2-N2-C7	-3.26	118.86	123.11
2	A	803	NAG	C2-N2-C7	-3.26	118.87	123.11
2	D	803	NAG	C2-N2-C7	-3.25	118.88	123.11
2	B	810	NAG	C4-C3-C2	-2.55	107.39	111.34
2	D	810	NAG	C4-C3-C2	-2.54	107.40	111.34
2	A	810	NAG	C4-C3-C2	-2.53	107.41	111.34
2	C	810	NAG	C4-C3-C2	-2.53	107.41	111.34
2	C	806	NAG	C4-C3-C2	-2.53	107.42	111.34
2	B	806	NAG	C4-C3-C2	-2.52	107.43	111.34
2	D	806	NAG	C4-C3-C2	-2.50	107.47	111.34
2	A	806	NAG	C4-C3-C2	-2.49	107.47	111.34
2	C	812	NAG	C2-N2-C7	-2.40	119.99	123.11
2	D	812	NAG	C2-N2-C7	-2.39	120.00	123.11
2	B	812	NAG	C2-N2-C7	-2.38	120.00	123.11
2	A	812	NAG	C2-N2-C7	-2.34	120.06	123.11
2	C	904	NAG	C2-N2-C7	-2.27	120.15	123.11
2	A	809	NAG	O5-C5-C4	-2.27	106.38	110.13
2	B	809	NAG	O5-C5-C4	-2.26	106.39	110.13
2	A	904	NAG	C2-N2-C7	-2.25	120.17	123.11
2	B	904	NAG	C2-N2-C7	-2.25	120.17	123.11
2	D	809	NAG	O5-C5-C4	-2.25	106.40	110.13
2	D	904	NAG	C2-N2-C7	-2.25	120.17	123.11
2	C	809	NAG	O5-C5-C4	-2.24	106.42	110.13
2	A	802	NAG	C2-N2-C7	-2.17	120.28	123.11
2	D	802	NAG	C2-N2-C7	-2.17	120.28	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	NAG	C2-N2-C7	-2.17	120.29	123.11
2	C	802	NAG	C2-N2-C7	-2.16	120.30	123.11
2	C	810	NAG	C1-O5-C5	-2.02	109.17	112.14
2	D	810	NAG	C1-O5-C5	-2.00	109.20	112.14
2	B	810	NAG	C1-O5-C5	-2.00	109.20	112.14
2	B	803	NAG	C1-O5-C5	2.24	115.44	112.14
2	A	803	NAG	C1-O5-C5	2.25	115.44	112.14
2	C	803	NAG	C1-O5-C5	2.26	115.46	112.14
2	D	803	NAG	C1-O5-C5	2.28	115.49	112.14

All (8) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

52 monomers are involved in 398 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	21	0
2	A	803	NAG	4	0
3	A	804	NDG	2	0
2	A	805	NAG	7	0
2	A	806	NAG	11	0
2	A	807	NAG	17	0
2	A	808	NAG	2	0
2	A	809	NAG	8	0
2	A	810	NAG	13	0
3	A	811	NDG	6	0
2	A	812	NAG	3	0
3	A	902	NDG	8	0
2	A	904	NAG	8	0
2	B	801	NAG	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	803	NAG	4	0
3	B	804	NDG	2	0
2	B	805	NAG	7	0
2	B	806	NAG	11	0
2	B	807	NAG	17	0
2	B	808	NAG	2	0
2	B	809	NAG	8	0
2	B	810	NAG	13	0
3	B	811	NDG	6	0
2	B	812	NAG	3	0
3	B	902	NDG	8	0
2	B	904	NAG	8	0
2	C	801	NAG	21	0
2	C	803	NAG	4	0
3	C	804	NDG	2	0
2	C	805	NAG	7	0
2	C	806	NAG	12	0
2	C	807	NAG	16	0
2	C	808	NAG	2	0
2	C	809	NAG	8	0
2	C	810	NAG	13	0
3	C	811	NDG	6	0
2	C	812	NAG	3	0
3	C	902	NDG	8	0
2	C	904	NAG	8	0
2	D	801	NAG	21	0
2	D	803	NAG	4	0
3	D	804	NDG	2	0
2	D	805	NAG	7	0
2	D	806	NAG	12	0
2	D	807	NAG	16	0
2	D	808	NAG	2	0
2	D	809	NAG	8	0
2	D	810	NAG	13	0
3	D	811	NDG	5	0
2	D	812	NAG	3	0
3	D	902	NDG	8	0
2	D	904	NAG	8	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.