



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:05 am GMT

PDB ID : 1Q5B
EMDB ID: : EMD-1052
Title : lambda-shaped TRANS and CIS interactions of cadherins model based on fitting C-cadherin (1L3W) to 3D map of desmosomes obtained by electron tomography
Authors : He, W.; Cowin, P.; Stokes, D.L.
Deposited on : 2003-08-06
Resolution : 30.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

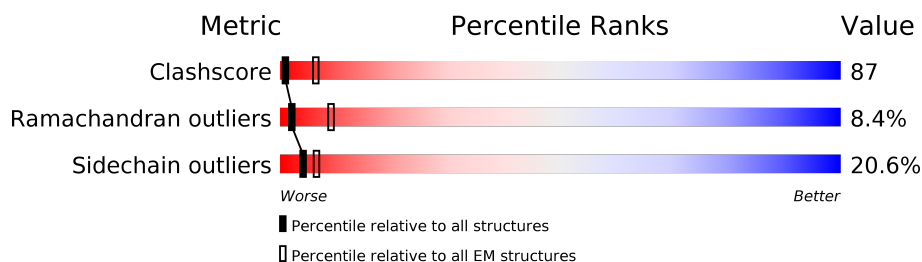
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 ≥ 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	
1	B	880	
1	C	880	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	801	-	-	X	-
2	NAG	A	805	X	-	X	-
2	NAG	A	806	X	-	X	-
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-
3	NDG	A	902	-	-	X	-
3	NDG	B	811	-	-	X	-
3	NDG	B	902	-	-	X	-
3	NDG	C	902	-	-	X	-

2 Entry composition [i](#)

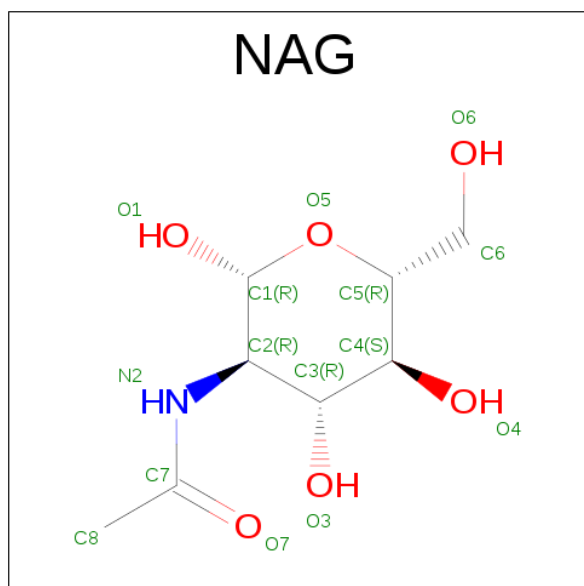
There are 4 unique types of molecules in this entry. The entry contains 13239 atoms, of which 0 are hydrogens and 0 are deuteriums.

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		

- 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	
2	A	1	Total	C	N	O	0
			154	88	11	55	

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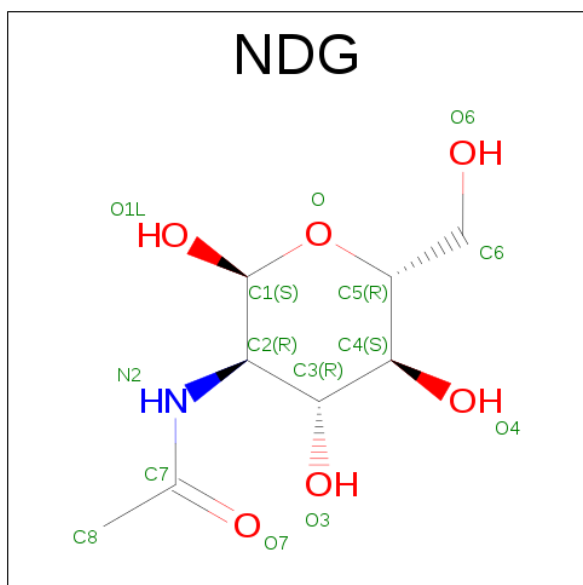
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	B	1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

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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	

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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	

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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	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	

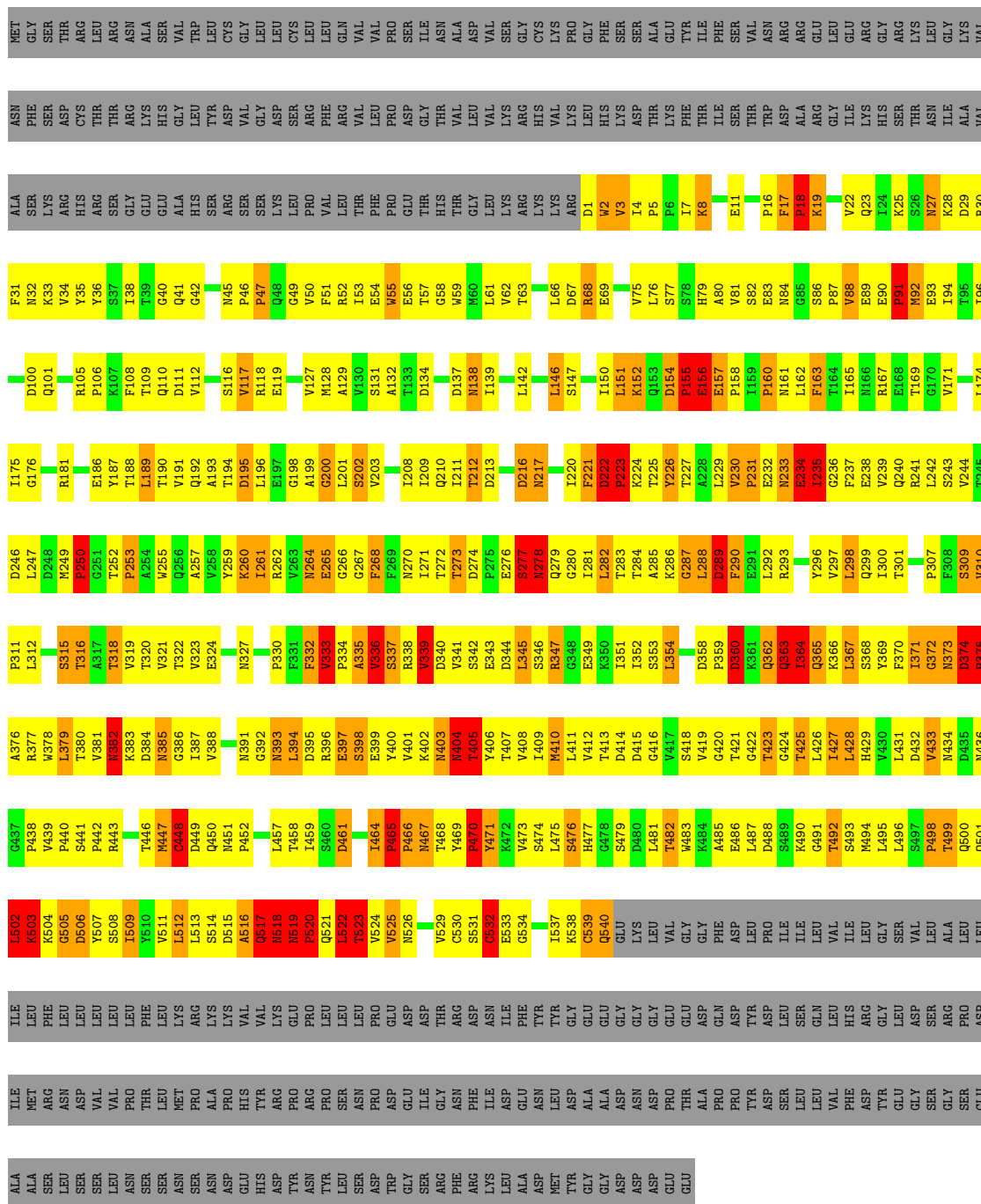
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

LEU
SER
SER
LEU
ASN
SER
SER
ASN
SER
ASN
ASP
GLU
HIS
ASP
TYR
ASN
TYR
LEU
SER
ASP
TRP
GLY
SER
ARG
PHE
ARG
LYS
LEU
ALA
ASP
MET
TYR
GLY
GLY
ASP
ASP
ASP
GLU
GLU

- Molecule 1: EP-cadherin

Chain B: 16% 31% 11% . 39%



- Molecule 1: EP-cadherin

Chain C:

GLU	ASP	LEU	Q501	G437	A376	P311	D246	G176	F31	ALA	ASN	MET
ALA	ILE	ILE	L502	P433	W378	L312	L247	R181	N32	SER	PHE	GLY
ALA	MET	PHE	K503	W439	W378	L312	D248	R181	K33	LYS	SER	THR
SER	ARG	ASP	G504	P440	L379	S315	M249	E186	N34	ARG	ASP	ARG
LEU	ASN	LEU	G505	S441	T380	T316	P250	E187	Y35	HIS	THR	LEU
SER	ASP	LEU	D506	P442	W381	A317	G251	T188	Y36	ARG	THR	ARG
SER	VAL	LEU	Y507	R443	N382	T318	T252	T189	S37	SER	THR	ASN
LEU	VAL	LEU	S508	V444	K383	T319	P253	L189	F108	GLY	ARG	ASN
ASN	VAL	LEU	L509	T445	D384	T320	A254	T190	T39	GLU	GLU	ALA
SER	THR	PHE	Y510	T446	N385	V321	W255	V191	Q110	GLU	HIS	SER
SER	THR	LEU	G511	M447	G386	T322	G256	Q192	D111	ALA	GLY	VAL
ASN	MET	LYS	L512	G448	L387	V323	A257	A193	G42	HIS	LEU	TRP
SER	PRO	LEU	L513	D449	V388	E324	V258	T194	A43	SER	TYR	LEU
ASN	ALA	LYS	S514	A450	N391	N327	W259	D195	D44	ARG	ASP	CYS
ASP	PRO	LYS	D515	N451	G392	N327	K260	L196	W117	VAL	VAL	GLY
GLU	HIS	VAL	A516	P452	G392	N327	D261	E197	R118	SER	GLY	LEU
HIS	TYR	VAL	G517	L394	N393	P330	K262	G198	E119	LYS	ASP	LEU
ASP	ARG	LYS	N518	L457	L394	F331	V263	A199	Q48	LEU	SER	CYS
TYR	PRO	GLU	N519	T458	D395	F332	K264	G200	G49	PRO	ARG	LEU
ASN	ARG	PRO	P520	T459	K396	V332	E265	L201	V50	VAL	PHE	LEU
TYR	PRO	LEU	Q521	S460	P334	P334	G266	S202	F51	LEU	ARG	GLN
LEU	SER	LEU	L522	D461	S398	A335	G267	V203	R52	THR	VAL	VAL
SER	ASN	LEU	T523	P523	K399	V336	F268	T208	E53	PHE	LEU	VAL
ASP	PRO	PRO	V524	T464	Y400	S337	P269	T208	T53	PRO	PRO	PRO
TRP	ASP	GLU	V525	P465	Y401	R338	N270	L209	W85	GLU	ASP	SER
GLY	ILE	ASP	N526	P466	K402	V339	T271	Q210	E56	THR	GLY	ILE
SER	GLU	ASP	N467	T471	N403	D340	T272	T211	T57	HIS	THR	ASN
ARG	ASN	THR	V529	T468	N404	V341	D273	T212	G58	THR	VAL	ALA
PHE	ASN	ARG	C530	Y469	T405	S242	D274	D213	W59	GLY	LEU	ASP
ARG	PHE	ASP	S531	P470	Y406	E343	P275	A214	M60	VAL	VAL	VAL
LYS	ILE	ASN	G532	Y471	T407	D344	E276	N215	L61	LYS	LYS	SER
LEU	ASP	ILE	E533	T472	Y408	L345	S277	G216	V62	ARG	ARG	GLY
ALA	GLU	PHE	G534	S473	I409	S346	N278	N217	T63	LYS	HIS	CYS
ASP	ASN	TYR	S474	S474	M410	R347	Q279	N217	S147	VAL	VAL	LYS
MET	LEU	TYR	T537	L475	L411	G348	G280	L220	L66	ARG	LYS	PRO
TYR	ASP	GLY	K538	S476	V412	E349	L281	F221	D87	LEU	LEU	GLY
GLY	ALA	GLU	C539	H477	T413	K350	L282	Q222	R68	HIS	HIS	PHE
ALA	GLU	ALA	Q540	G478	D414	T351	T283	P223	E69	W2	LYS	THR
ASP	ASP	GLY	GLU	S479	D415	L352	T284	K224	Q153	V3	ASP	SER
ASP	ASN	GLY	L540	A480	G416	S353	K285	T225	D154	I4	THR	ALA
ASP	ASP	GLY	LEU	L481	W417	L354	K286	Y226	P155	P6	LYS	GLU
GLU	PRO	GLU	VAL	T482	S418	L354	G287	T227	S77	I7	PHE	TYR
GLU	THR	GLU	GLY	W483	V419	D358	L288	A228	E157	K8	THR	ILE
ALA	ALA	ASP	GLY	K484	G420	P359	D289	L229	H79	ILE	THR	PHE
PRO	PRO	GLN	PHE	A485	T421	D360	F290	V230	I159	E11	THR	SER
PRO	PRO	ASP	ASP	E486	G422	K361	E291	V231	K160	P16	TRP	ASN
TYR	TYR	TYR	LEU	L487	T423	G362	L282	E232	N161	F17	ASP	ARG
ASP	ASP	ASP	PRO	D483	G424	Q363	R293	N233	L162	ALA	ASP	ARG
SER	SER	LEU	ILE	S489	T425	L364	E234	E234	F163	ARG	ASP	ARG
LEU	LEU	LEU	ILE	K490	L426	Q365	Y296	L235	T164	GLY	ARG	GLU
LEU	LEU	GLN	LEU	G491	T427	Q366	V297	G236	I165	GLY	GLY	LEU
VAL	VAL	VAL	VAL	T492	L428	L367	L298	F237	N166	ILE	ILE	GLU
PHE	PHE	HIS	ILE	H429	H429	S368	Q299	E238	R167	LYS	LYS	ARG
ASP	ASP	ARG	LEU	M494	V430	Y369	I300	V239	E188	HIS	HIS	GLY
GLY	GLY	GLY	GLY	L495	L431	F370	T301	Q240	T169	K25	ARG	ARG
TYR	TYR	GLY	TYR	L496	L431	F370	T301	Q240	T169	S26	THR	LYS
GLU	GLU	GLY	VAL	L496	L431	F370	T301	Q240	T169	N27	ASN	LEU
GLY	GLY	GLY	VAL	S497	D432	G372	F307	L242	V171	K28	ILE	GLY
SER	SER	ARG	VAL	P498	N434	N373	F308	S243	V171	D29	ALA	VAL
GLY	GLY	ARG	ALA	T499	D435	D374	S309	V244	L174	E50	VAL	VAL
SER	SER	ARG	LEU	D500	N436	P375	P340	W245	L175	VAL	VAL	VAL

4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of tilted images used	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	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	120000	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	68276	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%)	1.44	81/5839 (1.4%)
1	B	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
1	C	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
All	All	0.70	24/12828 (0.2%)	1.41	239/17517 (1.4%)

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	1	4
1	B	0	4
1	C	0	4
All	All	1	12

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ALA	CA-CB	-8.37	1.34	1.52
1	C	335	ALA	CA-CB	-8.35	1.34	1.52
1	B	335	ALA	CA-CB	-8.33	1.34	1.52
1	C	539	CYS	CB-SG	8.18	1.96	1.82
1	A	539	CYS	CB-SG	8.17	1.96	1.82
1	B	539	CYS	CB-SG	8.15	1.96	1.82
1	B	223	PRO	CG-CD	7.02	1.73	1.50
1	A	223	PRO	CG-CD	7.00	1.73	1.50
1	C	223	PRO	CG-CD	7.00	1.73	1.50
1	A	523	THR	N-CA	-6.26	1.33	1.46
1	C	523	THR	N-CA	-6.25	1.33	1.46
1	B	523	THR	N-CA	-6.24	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	LEU	N-CA	-5.98	1.34	1.46
1	A	18	PRO	N-CD	5.97	1.56	1.47
1	C	18	PRO	N-CD	5.97	1.56	1.47
1	B	522	LEU	N-CA	-5.97	1.34	1.46
1	C	522	LEU	N-CA	-5.96	1.34	1.46
1	B	18	PRO	N-CD	5.91	1.56	1.47
1	A	530	CYS	CB-SG	5.53	1.91	1.82
1	C	530	CYS	CB-SG	5.49	1.91	1.82
1	B	530	CYS	CB-SG	5.46	1.91	1.82
1	A	499	THR	CA-CB	5.05	1.66	1.53
1	C	499	THR	CA-CB	5.04	1.66	1.53
1	B	499	THR	CA-CB	5.02	1.66	1.53

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	LYS	N-CA-CB	-28.44	59.41	110.60
1	A	520	PRO	CA-C-N	-13.30	87.95	117.20
1	C	520	PRO	CA-C-N	-13.29	87.97	117.20
1	B	520	PRO	CA-C-N	-13.28	87.99	117.20
1	C	290	PHE	N-CA-C	12.74	145.39	111.00
1	B	290	PHE	N-CA-C	12.73	145.38	111.00
1	C	235	ILE	N-CA-C	12.72	145.35	111.00
1	A	235	ILE	N-CA-C	12.72	145.34	111.00
1	B	235	ILE	N-CA-C	12.72	145.34	111.00
1	A	290	PHE	N-CA-C	12.71	145.32	111.00
1	C	374	ASP	N-CA-C	11.61	142.36	111.00
1	B	374	ASP	N-CA-C	11.61	142.35	111.00
1	A	374	ASP	N-CA-C	11.61	142.34	111.00
1	A	17	PHE	C-N-CD	-11.55	95.19	120.60
1	C	17	PHE	C-N-CD	-11.54	95.20	120.60
1	B	17	PHE	C-N-CD	-11.54	95.22	120.60
1	C	398	SER	N-CA-C	11.38	141.74	111.00
1	B	398	SER	N-CA-C	11.37	141.70	111.00
1	A	398	SER	N-CA-C	11.36	141.68	111.00
1	B	465	PRO	C-N-CD	-11.04	96.31	120.60
1	A	465	PRO	C-N-CD	-11.03	96.33	120.60
1	C	465	PRO	C-N-CD	-11.03	96.33	120.60
1	C	222	ASP	CB-CG-OD2	10.07	127.36	118.30
1	B	222	ASP	CB-CG-OD2	10.06	127.35	118.30
1	A	222	ASP	CB-CG-OD2	10.03	127.33	118.30
1	A	236	GLY	N-CA-C	-9.99	88.11	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	GLY	N-CA-C	-9.98	88.15	113.10
1	C	236	GLY	N-CA-C	-9.97	88.16	113.10
1	C	230	VAL	C-N-CD	-9.94	98.72	120.60
1	A	230	VAL	C-N-CD	-9.94	98.73	120.60
1	B	230	VAL	C-N-CD	-9.92	98.77	120.60
1	A	374	ASP	CB-CA-C	-9.67	91.05	110.40
1	C	374	ASP	CB-CA-C	-9.67	91.06	110.40
1	B	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	C	376	ALA	N-CA-C	9.66	137.08	111.00
1	B	376	ALA	N-CA-C	9.65	137.04	111.00
1	A	376	ALA	N-CA-C	9.64	137.04	111.00
1	C	522	LEU	CA-CB-CG	-9.39	93.71	115.30
1	B	522	LEU	CA-CB-CG	-9.38	93.74	115.30
1	A	522	LEU	CA-CB-CG	-9.36	93.77	115.30
1	C	223	PRO	N-CA-C	-9.31	87.89	112.10
1	B	223	PRO	N-CA-C	-9.30	87.91	112.10
1	B	520	PRO	N-CA-C	9.30	136.28	112.10
1	A	221	PHE	C-N-CA	-9.30	98.46	121.70
1	B	221	PHE	C-N-CA	-9.29	98.46	121.70
1	A	223	PRO	N-CA-C	-9.29	87.94	112.10
1	A	520	PRO	N-CA-C	9.29	136.25	112.10
1	B	481	LEU	N-CA-C	-9.29	85.92	111.00
1	C	221	PHE	C-N-CA	-9.28	98.50	121.70
1	C	481	LEU	N-CA-C	-9.28	85.94	111.00
1	A	481	LEU	N-CA-C	-9.27	85.97	111.00
1	C	520	PRO	N-CA-C	9.27	136.19	112.10
1	C	481	LEU	CA-CB-CG	-8.76	95.16	115.30
1	B	481	LEU	CA-CB-CG	-8.76	95.16	115.30
1	A	481	LEU	CA-CB-CG	-8.75	95.17	115.30
1	A	289	ASP	C-N-CA	-8.43	100.62	121.70
1	B	289	ASP	C-N-CA	-8.42	100.66	121.70
1	C	289	ASP	C-N-CA	-8.41	100.67	121.70
1	A	516	ALA	N-CA-C	-8.35	88.47	111.00
1	B	516	ALA	N-CA-C	-8.35	88.46	111.00
1	C	516	ALA	N-CA-C	-8.35	88.46	111.00
1	C	222	ASP	C-N-CD	-8.22	102.51	120.60
1	B	222	ASP	C-N-CD	-8.21	102.54	120.60
1	A	290	PHE	CA-C-N	-8.20	99.16	117.20
1	B	290	PHE	CA-C-N	-8.19	99.18	117.20
1	A	222	ASP	C-N-CD	-8.19	102.59	120.60
1	C	290	PHE	CA-C-N	-8.17	99.22	117.20
1	A	46	PRO	C-N-CD	-8.05	102.89	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	PRO	C-N-CD	-8.03	102.92	120.60
1	B	46	PRO	C-N-CD	-8.03	102.93	120.60
1	B	233	ASN	N-CA-C	7.88	132.28	111.00
1	C	233	ASN	N-CA-C	7.87	132.26	111.00
1	A	233	ASN	N-CA-C	7.86	132.22	111.00
1	A	336	VAL	N-CA-C	7.82	132.10	111.00
1	B	336	VAL	N-CA-C	7.81	132.09	111.00
1	C	336	VAL	N-CA-C	7.80	132.05	111.00
1	B	522	LEU	C-N-CA	-7.79	102.21	121.70
1	C	522	LEU	C-N-CA	-7.78	102.25	121.70
1	A	522	LEU	C-N-CA	-7.78	102.25	121.70
1	B	362	GLN	N-CA-C	-7.71	90.18	111.00
1	C	362	GLN	N-CA-C	-7.71	90.19	111.00
1	A	362	GLN	N-CA-C	-7.71	90.20	111.00
1	A	234	GLU	N-CA-C	-7.59	90.51	111.00
1	B	234	GLU	N-CA-C	-7.58	90.52	111.00
1	C	234	GLU	N-CA-C	-7.58	90.53	111.00
1	A	234	GLU	C-N-CA	7.42	140.24	121.70
1	C	234	GLU	C-N-CA	7.41	140.22	121.70
1	B	234	GLU	C-N-CA	7.41	140.22	121.70
1	C	521	GLN	C-N-CA	-7.38	103.24	121.70
1	A	521	GLN	C-N-CA	-7.38	103.25	121.70
1	B	521	GLN	C-N-CA	-7.38	103.26	121.70
1	A	490	LYS	CB-CA-C	7.32	125.04	110.40
1	C	277	SER	N-CA-C	-7.21	91.53	111.00
1	B	277	SER	N-CA-C	-7.21	91.54	111.00
1	A	277	SER	N-CA-C	-7.20	91.56	111.00
1	A	337	SER	N-CA-C	-7.19	91.59	111.00
1	C	337	SER	N-CA-C	-7.18	91.62	111.00
1	B	337	SER	N-CA-C	-7.16	91.67	111.00
1	B	503	LYS	N-CA-C	7.01	129.94	111.00
1	A	503	LYS	N-CA-C	7.00	129.91	111.00
1	C	503	LYS	N-CA-C	7.00	129.89	111.00
1	C	523	THR	N-CA-CB	-6.95	97.09	110.30
1	B	523	THR	N-CA-CB	-6.95	97.10	110.30
1	A	523	THR	N-CA-CB	-6.93	97.13	110.30
1	C	492	THR	N-CA-C	6.78	129.31	111.00
1	A	492	THR	N-CA-C	6.78	129.30	111.00
1	B	492	THR	N-CA-C	6.75	129.23	111.00
1	B	448	CYS	CA-CB-SG	-6.70	101.95	114.00
1	C	448	CYS	CA-CB-SG	-6.70	101.95	114.00
1	A	448	CYS	CA-CB-SG	-6.68	101.98	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	398	SER	C-N-CA	-6.57	105.27	121.70
1	A	398	SER	C-N-CA	-6.57	105.29	121.70
1	B	476	SER	N-CA-C	6.57	128.72	111.00
1	A	476	SER	N-CA-C	6.56	128.72	111.00
1	C	476	SER	N-CA-C	6.56	128.70	111.00
1	B	491	GLY	N-CA-C	6.55	129.47	113.10
1	B	398	SER	C-N-CA	-6.55	105.33	121.70
1	A	491	GLY	N-CA-C	6.53	129.43	113.10
1	C	491	GLY	N-CA-C	6.51	129.38	113.10
1	C	525	VAL	N-CA-C	-6.51	93.42	111.00
1	B	525	VAL	N-CA-C	-6.50	93.46	111.00
1	A	525	VAL	N-CA-C	-6.48	93.50	111.00
1	C	335	ALA	N-CA-C	-6.32	93.92	111.00
1	A	335	ALA	N-CA-C	-6.32	93.95	111.00
1	B	335	ALA	N-CA-C	-6.31	93.96	111.00
1	B	532	CYS	N-CA-C	6.30	128.01	111.00
1	A	532	CYS	N-CA-C	6.30	128.00	111.00
1	C	532	CYS	N-CA-C	6.29	128.00	111.00
1	B	234	GLU	CA-C-N	-6.28	103.38	117.20
1	A	234	GLU	CA-C-N	-6.28	103.39	117.20
1	C	234	GLU	CA-C-N	-6.27	103.40	117.20
1	A	222	ASP	N-CA-C	6.17	127.64	111.00
1	C	222	ASP	N-CA-C	6.17	127.65	111.00
1	B	222	ASP	N-CA-C	6.15	127.61	111.00
1	A	235	ILE	CA-C-N	-6.14	103.91	116.20
1	A	397	GLU	C-N-CA	-6.14	106.35	121.70
1	C	235	ILE	CA-C-N	-6.14	103.93	116.20
1	B	235	ILE	CA-C-N	-6.13	103.94	116.20
1	B	397	GLU	C-N-CA	-6.12	106.40	121.70
1	C	397	GLU	C-N-CA	-6.11	106.42	121.70
1	A	18	PRO	CA-N-CD	-6.11	102.94	111.50
1	C	18	PRO	CA-N-CD	-6.10	102.97	111.50
1	B	503	LYS	CB-CA-C	-6.09	98.21	110.40
1	A	503	LYS	CB-CA-C	-6.07	98.25	110.40
1	B	18	PRO	CA-N-CD	-6.07	103.00	111.50
1	B	502	LEU	N-CA-C	6.07	127.40	111.00
1	C	503	LYS	CB-CA-C	-6.07	98.25	110.40
1	A	502	LEU	N-CA-C	6.04	127.31	111.00
1	C	502	LEU	N-CA-C	6.03	127.29	111.00
1	A	2	TRP	N-CA-C	-6.03	94.72	111.00
1	C	2	TRP	N-CA-C	-6.02	94.75	111.00
1	B	2	TRP	N-CA-C	-6.01	94.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	ASP	C-N-CD	5.97	140.95	128.40
1	C	374	ASP	C-N-CD	5.97	140.94	128.40
1	B	222	ASP	N-CA-CB	5.96	121.32	110.60
1	C	222	ASP	N-CA-CB	5.96	121.32	110.60
1	A	374	ASP	C-N-CD	5.95	140.90	128.40
1	A	222	ASP	N-CA-CB	5.95	121.31	110.60
1	C	364	ILE	N-CA-C	-5.93	94.99	111.00
1	A	364	ILE	N-CA-C	-5.93	95.00	111.00
1	B	364	ILE	N-CA-C	-5.93	95.00	111.00
1	B	376	ALA	CA-C-N	-5.85	104.33	117.20
1	A	376	ALA	CA-C-N	-5.83	104.36	117.20
1	C	376	ALA	CA-C-N	-5.83	104.36	117.20
1	A	382	ASN	N-CA-C	-5.83	95.27	111.00
1	C	382	ASN	N-CA-C	-5.82	95.28	111.00
1	B	382	ASN	N-CA-C	-5.81	95.31	111.00
1	B	471	TYR	N-CA-C	5.74	126.51	111.00
1	C	471	TYR	N-CA-C	5.74	126.49	111.00
1	A	471	TYR	N-CA-C	5.73	126.46	111.00
1	C	481	LEU	CA-C-N	-5.70	104.66	117.20
1	A	481	LEU	CA-C-N	-5.67	104.72	117.20
1	B	481	LEU	CA-C-N	-5.67	104.72	117.20
1	A	374	ASP	C-N-CA	-5.67	98.20	122.00
1	B	374	ASP	C-N-CA	-5.67	98.20	122.00
1	C	374	ASP	C-N-CA	-5.66	98.24	122.00
1	B	403	ASN	N-CA-C	-5.63	95.81	111.00
1	C	403	ASN	N-CA-C	-5.62	95.81	111.00
1	A	403	ASN	N-CA-C	-5.62	95.83	111.00
1	C	221	PHE	CA-C-N	5.58	129.49	117.20
1	B	221	PHE	CA-C-N	5.58	129.48	117.20
1	A	221	PHE	CA-C-N	5.57	129.46	117.20
1	A	505	GLY	N-CA-C	5.57	127.02	113.10
1	B	505	GLY	N-CA-C	5.54	126.96	113.10
1	B	502	LEU	CB-CA-C	-5.54	99.67	110.20
1	C	505	GLY	N-CA-C	5.54	126.94	113.10
1	A	502	LEU	CB-CA-C	-5.52	99.71	110.20
1	C	502	LEU	CB-CA-C	-5.51	99.72	110.20
1	A	157	GLU	C-N-CD	-5.48	108.54	120.60
1	B	157	GLU	C-N-CD	-5.47	108.57	120.60
1	C	157	GLU	C-N-CD	-5.46	108.58	120.60
1	B	519	ASN	N-CA-C	5.35	125.45	111.00
1	C	519	ASN	N-CA-C	5.35	125.44	111.00
1	A	519	ASN	N-CA-C	5.35	125.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	THR	N-CA-C	5.33	125.40	111.00
1	C	405	THR	N-CA-C	5.33	125.39	111.00
1	B	405	THR	N-CA-C	5.32	125.35	111.00
1	A	367	LEU	CA-CB-CG	-5.31	103.08	115.30
1	C	367	LEU	CA-CB-CG	-5.30	103.11	115.30
1	B	367	LEU	CA-CB-CG	-5.29	103.12	115.30
1	A	521	GLN	N-CA-C	-5.21	96.93	111.00
1	C	521	GLN	N-CA-C	-5.21	96.93	111.00
1	B	521	GLN	N-CA-C	-5.21	96.94	111.00
1	A	290	PHE	O-C-N	5.19	131.01	122.70
1	C	290	PHE	O-C-N	5.18	130.99	122.70
1	C	532	CYS	N-CA-CB	-5.18	101.28	110.60
1	C	520	PRO	C-N-CA	5.17	134.63	121.70
1	A	532	CYS	N-CA-CB	-5.16	101.31	110.60
1	B	290	PHE	O-C-N	5.16	130.96	122.70
1	B	520	PRO	C-N-CA	5.15	134.58	121.70
1	B	532	CYS	N-CA-CB	-5.14	101.35	110.60
1	A	520	PRO	C-N-CA	5.13	134.54	121.70
1	A	18	PRO	CA-CB-CG	-5.13	94.25	104.00
1	B	522	LEU	N-CA-C	-5.12	97.17	111.00
1	A	522	LEU	N-CA-C	-5.11	97.19	111.00
1	B	18	PRO	CA-CB-CG	-5.11	94.28	104.00
1	A	339	VAL	N-CA-C	5.11	124.80	111.00
1	C	18	PRO	CA-CB-CG	-5.11	94.29	104.00
1	B	339	VAL	N-CA-C	5.10	124.77	111.00
1	C	339	VAL	N-CA-C	5.10	124.77	111.00
1	C	522	LEU	N-CA-C	-5.10	97.23	111.00
1	B	16	PRO	C-N-CA	-5.09	108.98	121.70
1	C	16	PRO	C-N-CA	-5.08	109.00	121.70
1	A	16	PRO	C-N-CA	-5.07	109.02	121.70
1	A	332	PHE	N-CA-C	-5.04	97.39	111.00
1	C	332	PHE	N-CA-C	-5.04	97.40	111.00
1	B	234	GLU	O-C-N	5.03	130.75	122.70
1	B	332	PHE	N-CA-C	-5.03	97.43	111.00
1	A	470	PRO	N-CA-C	5.02	125.16	112.10
1	B	221	PHE	N-CA-C	5.02	124.56	111.00
1	C	234	GLU	O-C-N	5.01	130.72	122.70
1	C	539	CYS	N-CA-C	5.01	124.53	111.00
1	A	539	CYS	N-CA-C	5.01	124.53	111.00
1	B	470	PRO	N-CA-C	5.01	125.13	112.10
1	B	539	CYS	N-CA-C	5.01	124.53	111.00
1	C	221	PHE	N-CA-C	5.01	124.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	PHE	N-CA-C	5.01	124.52	111.00
1	A	234	GLU	O-C-N	5.00	130.71	122.70
1	C	470	PRO	N-CA-C	5.00	125.11	112.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	490	LYS	CA

All (12) 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

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	4081	822	0
1	B	4191	0	4087	811	0
1	C	4191	0	4085	858	0
2	A	154	0	143	85	0
2	B	154	0	143	84	0
2	C	154	0	143	83	0
3	A	56	0	52	16	0
3	B	56	0	52	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	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
All	All	13239	0	12838	2266	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 87.

All (2266) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PRO:HB2	1:C:35:TYR:CE2	1.24	1.62
1:B:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.58
1:C:464:ILE:HD12	1:C:465:PRO:CD	1.30	1.56
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.55
1:A:87:PRO:CG	1:B:89:GLU:HB3	1.16	1.54
1:B:81:VAL:O	1:C:2:TRP:CD2	1.68	1.44
1:A:43:ALA:HB1	1:C:79:HIS:CE1	1.32	1.44
1:C:464:ILE:CD1	1:C:465:PRO:HD2	1.50	1.41
1:B:464:ILE:CD1	1:B:465:PRO:HD2	1.50	1.41
1:A:464:ILE:CD1	1:A:465:PRO:HD2	1.50	1.37
1:B:86:SER:CB	1:C:4:ILE:N	1.87	1.36
1:A:87:PRO:CG	1:B:89:GLU:CB	2.03	1.36
1:B:82:SER:N	1:C:2:TRP:CA	1.86	1.36
1:A:46:PRO:CB	1:C:35:TYR:CE2	2.10	1.34
1:A:40:GLY:O	1:C:79:HIS:CB	1.74	1.33
1:A:82:SER:O	1:B:91:PRO:HD2	1.18	1.32
1:B:82:SER:N	1:C:2:TRP:HA	1.03	1.32
1:A:75:VAL:O	1:C:87:PRO:CG	1.80	1.29
1:B:81:VAL:C	1:C:2:TRP:HA	1.48	1.29
1:A:40:GLY:O	1:C:79:HIS:HB3	1.21	1.29
1:B:86:SER:HB2	1:C:3:VAL:C	1.50	1.29
1:A:82:SER:OG	1:B:91:PRO:CB	1.79	1.28
1:A:43:ALA:CB	1:C:79:HIS:CE1	1.82	1.28
1:A:43:ALA:HB3	1:C:79:HIS:ND1	1.45	1.27
1:A:43:ALA:O	1:C:39:THR:HG23	1.30	1.25
1:A:31:PHE:HB2	1:B:93:GLU:OE2	1.08	1.25
1:A:82:SER:OG	1:B:91:PRO:HB2	1.12	1.23
1:C:540:GLN:CD	1:C:540:GLN:O	1.79	1.21
1:B:540:GLN:O	1:B:540:GLN:CD	1.79	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PRO:HG3	1:B:89:GLU:CB	1.66	1.19
1:A:540:GLN:CD	1:A:540:GLN:O	1.79	1.19
1:A:31:PHE:CB	1:B:93:GLU:OE2	1.90	1.18
1:A:43:ALA:CB	1:C:79:HIS:ND1	2.00	1.18
1:B:450:GLN:HG2	1:B:532:CYS:O	1.43	1.18
1:B:81:VAL:O	1:C:2:TRP:CG	1.96	1.18
1:B:86:SER:HB3	1:C:4:ILE:N	1.54	1.18
1:C:474:SER:HB2	1:C:512:LEU:HG	1.25	1.18
1:A:84:ASN:HB2	1:B:79:HIS:CE1	1.77	1.17
1:A:46:PRO:HB2	1:C:35:TYR:CD2	1.79	1.17
1:C:482:THR:HG23	1:C:499:THR:CG2	1.75	1.17
1:C:8:LYS:HD2	1:C:8:LYS:H	1.04	1.17
1:A:49:GLY:C	1:C:44:ASP:OD1	1.83	1.16
1:A:43:ALA:O	1:C:39:THR:CG2	1.91	1.16
1:A:75:VAL:O	1:C:87:PRO:HG2	1.35	1.16
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.16
1:B:482:THR:HG23	1:B:499:THR:CG2	1.74	1.16
1:B:469:TYR:CG	1:B:470:PRO:HD2	1.81	1.16
1:C:450:GLN:HG2	1:C:532:CYS:O	1.44	1.16
1:B:86:SER:CB	1:C:3:VAL:C	2.12	1.15
1:A:482:THR:HG23	1:A:499:THR:CG2	1.75	1.15
1:B:234:GLU:H	1:B:235:ILE:HG23	1.08	1.15
1:A:450:GLN:HG2	1:A:532:CYS:O	1.44	1.15
1:C:469:TYR:CG	1:C:470:PRO:HD2	1.81	1.15
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.15
1:A:8:LYS:HD2	1:A:8:LYS:H	1.04	1.15
1:A:469:TYR:CG	1:A:470:PRO:HD2	1.81	1.14
1:B:423:THR:HB	2:B:810:NAG:C7	1.76	1.13
1:C:423:THR:HB	2:C:810:NAG:C7	1.76	1.13
1:B:8:LYS:HD2	1:B:8:LYS:H	1.04	1.13
1:B:81:VAL:CA	1:C:1:ASP:O	1.94	1.13
1:B:301:THR:HG21	2:B:805:NAG:H82	1.29	1.12
1:A:38:ILE:O	1:C:91:PRO:HB2	1.46	1.12
1:B:154:ASP:C	2:B:801:NAG:H82	1.70	1.12
1:C:154:ASP:C	2:C:801:NAG:H82	1.70	1.12
1:B:30:ARG:HH12	1:C:25:LYS:C	1.30	1.12
1:A:89:GLU:OE1	1:B:1:ASP:C	1.88	1.11
1:B:338:ARG:HD3	1:B:352:ILE:HG22	1.26	1.11
1:A:38:ILE:O	1:C:91:PRO:CB	1.73	1.11
1:A:75:VAL:CG1	1:C:87:PRO:HD2	1.81	1.11
1:A:154:ASP:C	2:A:801:NAG:H82	1.70	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ASP:O	1:C:222:ASP:OD1	1.69	1.10
1:A:46:PRO:CB	1:C:35:TYR:HE2	1.53	1.10
1:A:41:GLN:HB2	1:C:81:VAL:HG11	1.22	1.10
1:B:222:ASP:O	1:B:222:ASP:OD1	1.69	1.10
1:A:75:VAL:HG12	1:C:87:PRO:HD2	1.30	1.10
1:B:227:THR:HG21	2:B:807:NAG:C8	1.82	1.10
1:C:32:ASN:HD21	1:C:83:GLU:HB2	0.98	1.10
1:C:227:THR:HG21	2:C:807:NAG:C8	1.82	1.10
1:A:32:ASN:HD21	1:A:83:GLU:HB2	0.98	1.10
1:A:234:GLU:H	1:A:235:ILE:HG23	1.08	1.09
1:A:227:THR:HG21	2:A:807:NAG:C8	1.82	1.09
1:A:301:THR:HG21	2:A:805:NAG:H82	1.29	1.09
1:A:75:VAL:HB	1:C:87:PRO:HD3	1.31	1.09
1:C:338:ARG:HD3	1:C:352:ILE:HG22	1.26	1.09
1:A:222:ASP:OD1	1:A:222:ASP:O	1.69	1.09
1:C:234:GLU:H	1:C:235:ILE:HG23	1.08	1.09
1:A:90:GLU:O	1:B:1:ASP:OD1	1.70	1.08
1:A:338:ARG:HD3	1:A:352:ILE:HG22	1.26	1.07
1:A:482:THR:HG23	1:A:499:THR:HG22	1.09	1.07
1:A:485:ALA:O	1:A:486:GLU:HG2	1.54	1.07
1:B:32:ASN:HD21	1:B:83:GLU:HB2	0.98	1.07
1:C:450:GLN:CG	1:C:532:CYS:O	2.02	1.07
1:B:83:GLU:OE2	1:C:2:TRP:CZ2	2.07	1.07
1:B:450:GLN:CG	1:B:532:CYS:O	2.02	1.07
1:A:450:GLN:CG	1:A:532:CYS:O	2.03	1.07
1:B:82:SER:HB3	1:C:2:TRP:HB3	1.36	1.07
1:C:301:THR:HG21	2:C:805:NAG:H82	1.29	1.07
1:B:485:ALA:O	1:B:486:GLU:HG2	1.54	1.07
1:B:464:ILE:CD1	1:B:465:PRO:CD	2.20	1.06
1:C:485:ALA:O	1:C:486:GLU:HG2	1.54	1.06
1:A:335:ALA:HB1	3:A:811:NDG:O6	1.54	1.06
1:C:464:ILE:CD1	1:C:465:PRO:CD	2.20	1.06
1:B:474:SER:HB2	1:B:512:LEU:HG	1.25	1.06
1:A:290:PHE:HB2	1:A:292:LEU:N	1.69	1.06
1:B:335:ALA:HB1	3:B:811:NDG:O6	1.55	1.06
1:A:44:ASP:C	1:C:79:HIS:N	1.86	1.06
1:B:482:THR:HG23	1:B:499:THR:HG22	1.09	1.06
1:C:290:PHE:HB2	1:C:292:LEU:N	1.69	1.06
1:B:290:PHE:HB2	1:B:292:LEU:N	1.69	1.06
1:C:335:ALA:HB1	3:C:811:NDG:O6	1.54	1.05
1:A:90:GLU:HB2	1:B:2:TRP:HB2	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:SER:HA	1:B:427:ILE:HG23	1.38	1.05
1:C:337:SER:HA	1:C:427:ILE:HG23	1.38	1.05
1:B:290:PHE:HB2	1:B:292:LEU:H	0.89	1.05
1:A:87:PRO:CD	1:B:89:GLU:HB3	1.86	1.05
1:B:81:VAL:O	1:C:2:TRP:CE2	2.08	1.05
1:C:482:THR:HG23	1:C:499:THR:HG22	1.09	1.05
1:C:290:PHE:HB2	1:C:292:LEU:H	0.88	1.04
1:A:75:VAL:C	1:C:87:PRO:HG2	1.78	1.04
1:A:84:ASN:CB	1:B:79:HIS:HE1	1.70	1.04
1:B:86:SER:OG	1:C:5:PRO:N	1.90	1.04
1:A:469:TYR:CD1	1:A:470:PRO:HD2	1.92	1.04
1:B:469:TYR:CD1	1:B:470:PRO:HD2	1.91	1.03
1:C:469:TYR:CD1	1:C:470:PRO:HD2	1.91	1.03
1:A:522:LEU:HD22	1:A:523:THR:HB	1.39	1.03
1:A:77:SER:C	1:C:90:GLU:OE2	1.95	1.03
1:A:464:ILE:CD1	1:A:465:PRO:CD	2.20	1.03
1:B:522:LEU:HD22	1:B:523:THR:HB	1.39	1.03
1:B:482:THR:CG2	1:B:499:THR:N	2.22	1.03
1:C:482:THR:CG2	1:C:499:THR:N	2.22	1.03
1:A:84:ASN:HB2	1:B:79:HIS:HE1	0.91	1.03
1:A:39:THR:OG1	1:C:90:GLU:CA	2.00	1.02
1:A:482:THR:CG2	1:A:499:THR:N	2.22	1.02
1:C:403:ASN:HB2	3:C:902:NDG:C8	1.90	1.02
1:A:432:ASP:OD2	1:A:464:ILE:HG22	1.60	1.02
1:A:482:THR:HG21	1:A:499:THR:H	1.23	1.02
1:B:403:ASN:HB2	3:B:902:NDG:C8	1.90	1.02
1:B:432:ASP:OD2	1:B:464:ILE:HG22	1.60	1.02
1:A:49:GLY:CA	1:C:44:ASP:OD1	2.08	1.01
1:A:49:GLY:O	1:C:44:ASP:OD1	1.77	1.01
1:A:403:ASN:HB2	3:A:902:NDG:C8	1.90	1.01
1:B:450:GLN:HB2	1:B:533:GLU:HA	1.41	1.01
1:A:337:SER:HA	1:A:427:ILE:HG23	1.38	1.01
1:B:274:ASP:O	1:B:278:ASN:HA	1.61	1.01
1:C:274:ASP:O	1:C:278:ASN:HA	1.61	1.01
1:A:450:GLN:HB2	1:A:533:GLU:HA	1.41	1.01
1:B:188:THR:HG23	1:B:208:ILE:HG12	1.43	1.00
1:A:82:SER:HG	1:B:91:PRO:CB	1.61	1.00
1:A:290:PHE:HB2	1:A:292:LEU:H	0.88	1.00
1:B:81:VAL:HA	1:C:1:ASP:O	1.22	1.00
1:A:40:GLY:O	1:C:79:HIS:CG	2.13	1.00
1:A:274:ASP:O	1:A:278:ASN:HA	1.61	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:H	1:C:81:VAL:CG1	1.75	1.00
1:A:188:THR:HG23	1:A:208:ILE:HG12	1.43	0.99
1:A:482:THR:CG2	1:A:499:THR:H	1.76	0.99
1:A:523:THR:HG23	1:A:524:VAL:H	1.26	0.99
1:B:523:THR:HG23	1:B:524:VAL:H	1.26	0.99
1:B:366:LYS:HG3	1:B:367:LEU:H	1.28	0.99
1:B:482:THR:HG21	1:B:499:THR:H	1.23	0.99
1:C:432:ASP:OD2	1:C:464:ILE:HG22	1.60	0.99
1:C:320:THR:HG21	2:C:807:NAG:N2	1.78	0.99
1:C:482:THR:HG21	1:C:499:THR:H	1.23	0.99
1:B:320:THR:HG21	2:B:807:NAG:N2	1.78	0.98
1:C:188:THR:HG23	1:C:208:ILE:HG12	1.43	0.98
1:A:40:GLY:C	1:C:79:HIS:HB3	1.82	0.98
1:A:78:SER:N	1:C:90:GLU:OE2	1.97	0.98
1:A:320:THR:HG21	2:A:807:NAG:N2	1.78	0.98
1:B:83:GLU:HA	1:C:2:TRP:CH2	1.99	0.98
1:C:522:LEU:HD22	1:C:523:THR:HB	1.39	0.98
1:C:450:GLN:HB2	1:C:533:GLU:HA	1.41	0.98
1:A:35:TYR:OH	1:C:93:GLU:OE2	1.80	0.98
1:B:33:LYS:O	1:C:2:TRP:CE2	2.17	0.98
1:A:41:GLN:N	1:C:81:VAL:HG13	1.78	0.98
1:A:82:SER:O	1:B:91:PRO:CD	2.12	0.97
1:B:482:THR:CG2	1:B:499:THR:H	1.76	0.97
1:C:366:LYS:HG3	1:C:367:LEU:H	1.28	0.97
1:C:523:THR:HG23	1:C:524:VAL:H	1.26	0.97
1:B:86:SER:HB2	1:C:4:ILE:N	1.59	0.97
1:A:8:LYS:CD	1:A:8:LYS:H	1.74	0.97
1:C:482:THR:CG2	1:C:499:THR:H	1.76	0.96
1:A:39:THR:OG1	1:C:89:GLU:O	1.82	0.96
1:B:89:GLU:H	1:C:1:ASP:N	1.62	0.96
1:A:366:LYS:HG3	1:A:367:LEU:H	1.28	0.96
1:C:8:LYS:CD	1:C:8:LYS:H	1.74	0.96
1:A:235:ILE:CG1	1:A:287:GLY:HA2	1.96	0.96
1:A:32:ASN:HD21	1:A:83:GLU:CB	1.79	0.96
1:A:75:VAL:O	1:C:87:PRO:HG3	1.65	0.96
1:B:8:LYS:H	1:B:8:LYS:CD	1.74	0.96
1:B:82:SER:CB	1:C:2:TRP:HB3	1.90	0.96
1:A:41:GLN:CB	1:C:81:VAL:HG11	1.88	0.96
1:B:235:ILE:CG1	1:B:287:GLY:HA2	1.96	0.96
1:B:32:ASN:HD21	1:B:83:GLU:CB	1.79	0.96
1:A:48:GLN:NE2	1:C:53:ILE:HG21	1.81	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:THR:HG21	2:B:807:NAG:H83	1.48	0.96
1:B:89:GLU:N	1:C:1:ASP:HB2	1.80	0.95
1:A:39:THR:OG1	1:C:90:GLU:HA	1.66	0.95
1:A:78:SER:CA	1:C:90:GLU:OE2	2.15	0.95
1:A:290:PHE:CB	1:A:292:LEU:H	1.79	0.95
1:B:81:VAL:C	1:C:2:TRP:CA	2.22	0.95
1:C:235:ILE:CG1	1:C:287:GLY:HA2	1.96	0.95
1:A:366:LYS:CG	1:A:367:LEU:H	1.80	0.94
1:A:82:SER:OG	1:B:91:PRO:CA	2.14	0.94
1:A:91:PRO:HB3	1:C:90:GLU:OE1	1.66	0.94
1:C:290:PHE:CB	1:C:292:LEU:H	1.79	0.94
1:C:366:LYS:CG	1:C:367:LEU:H	1.80	0.94
1:A:44:ASP:C	1:C:79:HIS:H	1.51	0.94
1:A:227:THR:HG21	2:A:807:NAG:H83	1.48	0.94
1:B:81:VAL:C	1:C:2:TRP:CG	2.31	0.94
1:A:49:GLY:HA3	1:C:44:ASP:OD1	1.67	0.94
1:B:366:LYS:CG	1:B:367:LEU:H	1.80	0.94
1:C:32:ASN:HD21	1:C:83:GLU:CB	1.79	0.94
1:C:227:THR:HG21	2:C:807:NAG:H83	1.48	0.94
1:B:290:PHE:CB	1:B:292:LEU:H	1.79	0.93
1:A:289:ASP:O	1:A:290:PHE:HB3	1.67	0.93
1:C:396:ARG:HH22	1:C:464:ILE:HB	1.33	0.93
1:C:320:THR:HG21	2:C:807:NAG:HN2	1.31	0.93
1:C:482:THR:HG21	1:C:499:THR:N	1.81	0.93
1:A:41:GLN:CB	1:C:81:VAL:CG1	2.46	0.93
1:A:482:THR:HG21	1:A:499:THR:N	1.81	0.93
1:A:32:ASN:ND2	1:A:83:GLU:HB2	1.84	0.93
1:A:396:ARG:HH22	1:A:464:ILE:HB	1.33	0.93
1:B:464:ILE:HD12	1:B:465:PRO:HD2	0.94	0.93
1:B:289:ASP:O	1:B:290:PHE:HB3	1.67	0.93
1:B:86:SER:HB3	1:C:3:VAL:CB	1.98	0.93
1:A:195:ASP:HB2	1:A:201:LEU:H	1.34	0.92
2:A:805:NAG:H62	2:A:806:NAG:C7	2.00	0.92
1:A:87:PRO:HG2	1:B:89:GLU:CB	2.00	0.92
1:B:27:ASN:HD22	1:B:28:LYS:N	1.66	0.92
1:A:87:PRO:HG2	1:B:89:GLU:HB3	1.49	0.92
1:A:446:THR:HG23	1:A:539:CYS:SG	2.09	0.92
1:B:320:THR:HG21	2:B:807:NAG:HN2	1.31	0.92
2:C:805:NAG:H62	2:C:806:NAG:C7	2.00	0.92
1:C:446:THR:HG23	1:C:539:CYS:SG	2.09	0.92
1:A:335:ALA:CB	3:A:811:NDG:O6	2.18	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:THR:HG23	1:B:539:CYS:SG	2.09	0.92
1:A:27:ASN:HD22	1:A:28:LYS:N	1.66	0.92
1:C:403:ASN:HB2	3:C:902:NDG:C7	2.00	0.92
1:A:352:ILE:HG13	1:A:388:VAL:HB	1.51	0.92
1:A:43:ALA:HB1	1:C:79:HIS:HE1	1.18	0.92
1:B:403:ASN:HB2	3:B:902:NDG:C7	2.00	0.92
1:C:404:ASN:O	1:C:404:ASN:ND2	2.03	0.92
1:A:227:THR:HG21	2:A:807:NAG:C7	1.99	0.92
1:C:289:ASP:O	1:C:290:PHE:HB3	1.67	0.92
1:C:335:ALA:CB	3:C:811:NDG:O6	2.18	0.92
1:A:517:GLN:O	1:A:519:ASN:N	2.03	0.91
1:C:195:ASP:HB2	1:C:201:LEU:H	1.34	0.91
1:C:227:THR:HG21	2:C:807:NAG:C7	1.99	0.91
1:B:227:THR:HG21	2:B:807:NAG:C7	1.99	0.91
1:C:27:ASN:HD22	1:C:28:LYS:N	1.66	0.91
1:C:352:ILE:HG13	1:C:388:VAL:HB	1.51	0.91
1:B:32:ASN:ND2	1:B:83:GLU:HB2	1.84	0.91
1:B:195:ASP:HB2	1:B:201:LEU:H	1.34	0.91
1:B:464:ILE:HD12	1:B:465:PRO:HD3	1.53	0.91
1:C:32:ASN:ND2	1:C:83:GLU:HB2	1.84	0.91
1:A:404:ASN:ND2	1:A:404:ASN:O	2.03	0.91
1:A:403:ASN:HB2	3:A:902:NDG:C7	2.00	0.91
2:B:805:NAG:H62	2:B:806:NAG:C7	1.99	0.91
1:C:340:ASP:HA	1:C:429:HIS:HB3	1.53	0.91
1:B:396:ARG:HH22	1:B:464:ILE:HB	1.33	0.91
1:B:335:ALA:CB	3:B:811:NDG:O6	2.18	0.91
1:C:464:ILE:HD11	1:C:465:PRO:HD2	1.53	0.91
2:A:805:NAG:O5	2:A:806:NAG:H83	1.71	0.91
1:A:320:THR:HG21	2:A:807:NAG:HN2	1.31	0.91
1:B:352:ILE:HG13	1:B:388:VAL:HB	1.51	0.91
2:C:805:NAG:O5	2:C:806:NAG:H83	1.71	0.91
1:A:90:GLU:HB2	1:B:2:TRP:CB	2.00	0.90
1:B:404:ASN:ND2	1:B:404:ASN:O	2.03	0.90
1:A:464:ILE:HD12	1:A:465:PRO:HD2	0.94	0.90
1:B:86:SER:OG	1:C:4:ILE:C	2.08	0.90
1:B:518:ASN:O	1:B:520:PRO:HD3	1.72	0.90
1:B:30:ARG:NH1	1:C:25:LYS:C	2.00	0.90
1:B:82:SER:H	1:C:2:TRP:HA	1.12	0.90
1:A:340:ASP:HA	1:A:429:HIS:HB3	1.53	0.90
1:A:45:ASN:HA	1:C:37:SER:N	1.87	0.90
1:A:378:TRP:HB2	1:A:379:LEU:HD23	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:ASN:O	1:C:520:PRO:HD3	1.72	0.90
1:B:89:GLU:H	1:C:1:ASP:H3	1.16	0.90
1:C:464:ILE:HD12	1:C:465:PRO:HD2	0.94	0.90
1:A:234:GLU:N	1:A:235:ILE:HG23	1.86	0.90
1:B:482:THR:HG21	1:B:499:THR:N	1.81	0.90
2:B:805:NAG:O5	2:B:806:NAG:H83	1.71	0.90
1:A:518:ASN:O	1:A:520:PRO:HD3	1.72	0.90
1:B:396:ARG:NH2	1:B:464:ILE:CG2	2.35	0.90
1:B:517:GLN:O	1:B:519:ASN:N	2.03	0.90
1:C:517:GLN:O	1:C:519:ASN:N	2.03	0.90
1:A:374:ASP:O	1:A:375:PRO:C	2.06	0.89
1:A:396:ARG:NH2	1:A:464:ILE:CG2	2.35	0.89
1:A:464:ILE:HD11	1:A:465:PRO:HD2	1.53	0.89
1:B:374:ASP:O	1:B:375:PRO:C	2.06	0.89
1:C:464:ILE:HD12	1:C:465:PRO:HD3	1.53	0.89
1:B:234:GLU:N	1:B:235:ILE:HG23	1.86	0.89
1:A:523:THR:HG23	1:A:524:VAL:CG2	2.03	0.89
1:C:234:GLU:N	1:C:235:ILE:HG23	1.86	0.89
1:C:523:THR:HG23	1:C:524:VAL:CG2	2.03	0.89
1:C:378:TRP:HB2	1:C:379:LEU:HD23	1.53	0.89
1:A:371:ILE:CD1	1:A:381:VAL:HG11	2.03	0.89
1:A:449:ASP:H	1:A:532:CYS:HB3	1.37	0.89
1:B:338:ARG:HD3	1:B:352:ILE:CG2	2.02	0.89
1:B:464:ILE:HD11	1:B:465:PRO:HD2	1.53	0.89
1:C:371:ILE:CD1	1:C:381:VAL:HG11	2.03	0.89
1:B:154:ASP:HB3	1:B:155:PRO:HD2	1.54	0.89
1:C:221:PHE:HE1	1:C:315:SER:O	1.56	0.89
1:C:396:ARG:NH2	1:C:464:ILE:CG2	2.35	0.89
1:B:523:THR:HG23	1:B:524:VAL:CG2	2.03	0.89
1:A:8:LYS:HD2	1:A:8:LYS:N	1.87	0.89
1:C:154:ASP:HB3	1:C:155:PRO:HD2	1.54	0.89
1:B:8:LYS:HD2	1:B:8:LYS:N	1.87	0.88
1:B:371:ILE:CD1	1:B:381:VAL:HG11	2.03	0.88
1:C:343:GLU:HB3	1:C:433:VAL:HG21	1.55	0.88
1:C:338:ARG:HD3	1:C:352:ILE:CG2	2.02	0.88
1:A:338:ARG:HD3	1:A:352:ILE:CG2	2.02	0.88
1:B:340:ASP:HA	1:B:429:HIS:HB3	1.53	0.88
1:B:449:ASP:H	1:B:532:CYS:HB3	1.37	0.88
1:C:449:ASP:H	1:C:532:CYS:HB3	1.37	0.88
1:A:343:GLU:HB3	1:A:433:VAL:HG21	1.55	0.88
1:B:257:ALA:O	1:B:273:THR:HG21	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:TRP:HB2	1:B:379:LEU:HD23	1.53	0.88
1:A:221:PHE:HE1	1:A:315:SER:O	1.56	0.87
1:A:87:PRO:CD	1:B:89:GLU:CB	2.46	0.87
1:C:8:LYS:HD2	1:C:8:LYS:N	1.87	0.87
1:B:483:TRP:CZ3	1:B:498:PRO:HG3	2.09	0.87
1:C:257:ALA:O	1:C:273:THR:HG21	1.74	0.87
1:C:483:TRP:CZ3	1:C:498:PRO:HG3	2.09	0.87
1:B:86:SER:HB3	1:C:4:ILE:H	1.35	0.87
1:A:154:ASP:HB3	1:A:155:PRO:HD2	1.54	0.87
1:A:75:VAL:CG1	1:C:87:PRO:CD	2.53	0.87
1:C:320:THR:HG21	2:C:807:NAG:C2	2.05	0.87
1:A:318:THR:HG21	2:A:806:NAG:H5	1.56	0.87
1:A:333:VAL:HB	1:A:334:PRO:HD3	1.56	0.87
1:A:464:ILE:HD12	1:A:465:PRO:HD3	1.53	0.87
1:C:486:GLU:HB2	1:C:495:LEU:HB2	1.56	0.87
1:A:441:SER:OG	1:A:442:PRO:HD3	1.75	0.87
1:B:441:SER:OG	1:B:442:PRO:HD3	1.75	0.87
1:A:49:GLY:HA3	1:C:44:ASP:CG	1.95	0.87
1:B:320:THR:HG21	2:B:807:NAG:C2	2.05	0.87
1:A:257:ALA:O	1:A:273:THR:HG21	1.74	0.86
1:A:440:PRO:CD	1:A:522:LEU:HD12	2.05	0.86
1:A:75:VAL:HG12	1:C:87:PRO:CD	2.05	0.86
1:A:320:THR:HG21	2:A:807:NAG:C2	2.05	0.86
1:B:318:THR:HG21	2:B:806:NAG:H5	1.56	0.86
1:A:483:TRP:CZ3	1:A:498:PRO:HG3	2.09	0.86
1:A:523:THR:HG23	1:A:524:VAL:N	1.90	0.86
1:B:486:GLU:HB2	1:B:495:LEU:HB2	1.56	0.86
1:A:82:SER:HG	1:B:91:PRO:HB2	0.90	0.86
1:C:235:ILE:HG13	1:C:287:GLY:HA2	1.58	0.86
1:B:343:GLU:HB3	1:B:433:VAL:HG21	1.55	0.86
1:A:486:GLU:HB2	1:A:495:LEU:HB2	1.56	0.86
1:B:423:THR:CB	2:B:810:NAG:C7	2.54	0.86
1:C:441:SER:OG	1:C:442:PRO:HD3	1.75	0.86
1:A:90:GLU:CB	1:B:2:TRP:HB2	2.06	0.86
1:B:221:PHE:HE1	1:B:315:SER:O	1.56	0.86
1:C:523:THR:HG23	1:C:524:VAL:N	1.90	0.86
1:B:333:VAL:HB	1:B:334:PRO:HD3	1.56	0.86
1:C:318:THR:HG21	2:C:806:NAG:H5	1.55	0.86
1:A:235:ILE:HG13	1:A:287:GLY:HA2	1.58	0.85
1:B:438:PRO:HB3	1:B:471:TYR:HE2	1.41	0.85
1:B:440:PRO:CD	1:B:522:LEU:HD12	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:PRO:HB3	1:C:471:TYR:HE2	1.41	0.85
1:C:440:PRO:CD	1:C:522:LEU:HD12	2.05	0.85
1:A:423:THR:CB	2:A:810:NAG:C7	2.54	0.85
1:B:451:ASN:N	1:B:533:GLU:O	2.10	0.85
1:A:464:ILE:HD12	1:A:465:PRO:N	1.91	0.85
1:A:483:TRP:HZ2	1:A:507:TYR:CE1	1.95	0.85
1:B:464:ILE:HD12	1:B:465:PRO:N	1.91	0.85
1:C:333:VAL:HB	1:C:334:PRO:HD3	1.56	0.85
1:C:374:ASP:O	1:C:375:PRO:C	2.06	0.85
1:A:375:PRO:HB3	1:A:400:TYR:CE2	2.12	0.85
1:C:483:TRP:HZ2	1:C:507:TYR:CE1	1.95	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:CE1	1.95	0.85
1:C:423:THR:CB	2:C:810:NAG:C7	2.54	0.84
1:A:87:PRO:HG2	1:B:89:GLU:CG	2.06	0.84
1:C:375:PRO:HB3	1:C:400:TYR:CE2	2.12	0.84
1:C:440:PRO:HD2	1:C:522:LEU:HD12	1.59	0.84
1:B:483:TRP:HZ2	1:B:507:TYR:HE1	1.24	0.84
1:A:440:PRO:HD2	1:A:522:LEU:HD12	1.59	0.84
1:B:523:THR:HG23	1:B:524:VAL:N	1.90	0.84
1:B:84:ASN:ND2	1:C:5:PRO:HD3	1.92	0.84
1:A:483:TRP:HZ2	1:A:507:TYR:HE1	1.24	0.84
1:A:89:GLU:OE2	1:B:3:VAL:HG13	1.76	0.84
1:B:235:ILE:HG13	1:B:287:GLY:HA2	1.58	0.84
1:C:155:PRO:HB2	2:C:801:NAG:H81	1.59	0.84
1:C:464:ILE:HD12	1:C:465:PRO:N	1.91	0.84
1:A:230:VAL:O	1:A:324:GLU:N	2.11	0.84
1:C:396:ARG:NE	1:C:432:ASP:HB2	1.93	0.84
1:A:44:ASP:OD2	1:C:79:HIS:ND1	1.98	0.83
1:B:86:SER:CB	1:C:4:ILE:CA	2.56	0.83
1:A:48:GLN:NE2	1:C:53:ILE:CG2	2.39	0.83
1:A:396:ARG:NE	1:A:432:ASP:HB2	1.93	0.83
1:A:451:ASN:N	1:A:533:GLU:O	2.10	0.83
1:A:469:TYR:CG	1:A:470:PRO:CD	2.61	0.83
1:B:375:PRO:HB3	1:B:400:TYR:CE2	2.12	0.83
1:C:448:CYS:O	1:C:452:PRO:HG3	1.79	0.83
1:A:423:THR:HB	2:A:810:NAG:N2	1.93	0.83
1:B:147:SER:OG	1:B:167:ARG:HD2	1.78	0.83
1:C:32:ASN:ND2	1:C:83:GLU:H	1.76	0.83
1:C:451:ASN:N	1:C:533:GLU:O	2.10	0.83
1:C:28:LYS:HD3	1:C:88:VAL:HG12	1.61	0.83
1:A:155:PRO:HB2	2:A:801:NAG:H81	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASN:ND2	1:A:83:GLU:H	1.77	0.83
1:B:230:VAL:O	1:B:324:GLU:N	2.11	0.83
1:B:440:PRO:HD2	1:B:522:LEU:HD12	1.59	0.83
1:B:81:VAL:HA	1:C:1:ASP:C	1.98	0.83
1:C:147:SER:OG	1:C:167:ARG:HD2	1.78	0.83
1:A:423:THR:CB	2:A:810:NAG:N2	2.42	0.83
1:A:43:ALA:HB3	1:C:79:HIS:CG	2.09	0.83
1:A:234:GLU:H	1:A:235:ILE:CG2	1.92	0.83
1:A:289:ASP:OD2	1:A:289:ASP:O	1.97	0.83
1:A:89:GLU:OE1	1:B:1:ASP:CA	2.09	0.83
1:B:289:ASP:OD2	1:B:289:ASP:O	1.97	0.83
1:B:396:ARG:NE	1:B:432:ASP:HB2	1.93	0.83
1:A:87:PRO:HD3	1:B:89:GLU:HB2	1.61	0.83
1:B:423:THR:HB	2:B:810:NAG:N2	1.93	0.83
1:B:448:CYS:O	1:B:452:PRO:HG3	1.79	0.83
1:A:448:CYS:O	1:A:452:PRO:HG3	1.79	0.82
1:A:438:PRO:HB3	1:A:471:TYR:HE2	1.41	0.82
1:B:28:LYS:HD3	1:B:88:VAL:HG12	1.61	0.82
1:B:32:ASN:ND2	1:B:83:GLU:H	1.77	0.82
1:C:469:TYR:CG	1:C:470:PRO:CD	2.61	0.82
1:B:423:THR:CB	2:B:810:NAG:N2	2.42	0.82
1:B:83:GLU:OE2	1:C:2:TRP:HZ2	1.59	0.82
1:B:88:VAL:H	1:C:1:ASP:CA	1.92	0.82
1:C:446:THR:HG21	1:C:537:ILE:O	1.79	0.82
1:A:540:GLN:OE1	1:A:540:GLN:O	1.97	0.82
1:B:154:ASP:HB3	2:B:801:NAG:HN2	1.45	0.82
1:A:87:PRO:HD3	1:B:89:GLU:CB	2.10	0.82
1:C:230:VAL:O	1:C:324:GLU:N	2.11	0.82
1:A:154:ASP:HB3	2:A:801:NAG:N2	1.95	0.82
1:B:155:PRO:HB2	2:B:801:NAG:H81	1.59	0.82
1:A:44:ASP:HA	1:C:77:SER:O	1.79	0.82
1:C:423:THR:CB	2:C:810:NAG:N2	2.42	0.82
1:A:154:ASP:HB3	2:A:801:NAG:HN2	1.44	0.82
1:B:482:THR:HG21	1:B:500:GLN:N	1.94	0.82
1:A:75:VAL:HB	1:C:87:PRO:CD	2.10	0.81
1:B:154:ASP:HB3	2:B:801:NAG:N2	1.95	0.81
1:C:423:THR:HB	2:C:810:NAG:N2	1.93	0.81
1:C:482:THR:HG21	1:C:500:GLN:N	1.94	0.81
1:A:446:THR:HG21	1:A:537:ILE:O	1.79	0.81
1:C:154:ASP:HB3	2:C:801:NAG:N2	1.95	0.81
1:B:469:TYR:CG	1:B:470:PRO:CD	2.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLN:HG2	1:B:318:THR:HG23	1.63	0.81
1:C:277:SER:C	1:C:278:ASN:HD22	1.84	0.81
1:C:540:GLN:O	1:C:540:GLN:OE1	1.97	0.81
1:B:290:PHE:CE2	1:B:293:ARG:HB2	2.16	0.81
1:C:289:ASP:O	1:C:289:ASP:OD2	1.97	0.81
1:A:469:TYR:CD2	1:A:470:PRO:HD2	2.16	0.81
1:A:482:THR:HG21	1:A:500:GLN:N	1.94	0.81
1:B:446:THR:HG21	1:B:537:ILE:O	1.79	0.81
1:C:290:PHE:CE2	1:C:293:ARG:HB2	2.16	0.81
1:A:265:GLU:HB3	1:A:268:PHE:HE2	1.46	0.81
1:A:486:GLU:O	1:A:494:MET:HA	1.81	0.81
1:B:265:GLU:HB3	1:B:268:PHE:HE2	1.46	0.81
1:C:154:ASP:HB3	2:C:801:NAG:HN2	1.45	0.81
1:C:396:ARG:HH21	1:C:464:ILE:HG22	1.46	0.81
1:A:290:PHE:CE2	1:A:293:ARG:HB2	2.16	0.81
1:A:517:GLN:C	1:A:519:ASN:H	1.84	0.81
1:B:277:SER:C	1:B:278:ASN:HD22	1.83	0.81
1:A:396:ARG:HH21	1:A:464:ILE:HG22	1.46	0.80
1:B:290:PHE:HD2	1:B:293:ARG:H	1.28	0.80
1:A:299:GLN:HG2	1:A:318:THR:HG23	1.62	0.80
1:C:517:GLN:C	1:C:519:ASN:H	1.84	0.80
1:B:30:ARG:NH1	1:C:25:LYS:HG2	1.95	0.80
1:B:540:GLN:OE1	1:B:540:GLN:O	1.97	0.80
1:B:81:VAL:CA	1:C:2:TRP:HA	2.10	0.80
1:C:299:GLN:HG2	1:C:318:THR:HG23	1.62	0.80
1:A:432:ASP:OD2	1:A:464:ILE:CG2	2.30	0.80
1:A:28:LYS:HD3	1:A:88:VAL:HG12	1.61	0.80
1:B:432:ASP:OD2	1:B:464:ILE:CG2	2.30	0.80
1:B:517:GLN:C	1:B:519:ASN:H	1.84	0.80
1:A:84:ASN:CG	1:B:77:SER:OG	2.19	0.80
1:C:234:GLU:H	1:C:235:ILE:CG2	1.92	0.80
1:C:265:GLU:HB3	1:C:268:PHE:HE2	1.46	0.80
1:A:77:SER:O	1:C:90:GLU:OE2	1.97	0.80
1:C:127:VAL:HG13	1:C:128:MET:H	1.46	0.80
1:C:486:GLU:O	1:C:494:MET:HA	1.81	0.80
2:C:904:NAG:H3	2:C:904:NAG:O7	1.82	0.80
1:B:30:ARG:NH2	1:C:25:LYS:O	2.01	0.80
1:B:486:GLU:O	1:B:494:MET:HA	1.81	0.80
1:C:469:TYR:CD2	1:C:470:PRO:HD2	2.16	0.80
1:A:365:GLN:HG3	1:A:365:GLN:O	1.82	0.80
1:C:290:PHE:HZ	1:C:296:TYR:HH	1.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:TYR:CD2	1:B:470:PRO:HD2	2.16	0.80
1:B:396:ARG:HD3	1:B:431:LEU:C	2.02	0.79
1:A:82:SER:C	1:B:91:PRO:HD2	2.01	0.79
1:A:127:VAL:HG13	1:A:128:MET:H	1.46	0.79
1:A:27:ASN:HD22	1:A:27:ASN:C	1.85	0.79
1:A:290:PHE:HD2	1:A:293:ARG:H	1.28	0.79
1:B:540:GLN:CG	1:B:540:GLN:O	2.31	0.79
1:B:195:ASP:HB3	1:B:200:GLY:HA3	1.65	0.79
1:B:482:THR:OG1	1:B:500:GLN:HG2	1.82	0.79
1:C:290:PHE:HD2	1:C:293:ARG:H	1.28	0.79
1:C:406:TYR:CD1	2:C:808:NAG:H83	2.17	0.79
1:C:449:ASP:HB3	1:C:532:CYS:H	1.47	0.79
1:B:232:GLU:HG3	1:B:290:PHE:N	1.98	0.79
1:B:523:THR:CG2	1:B:524:VAL:H	1.94	0.79
1:B:86:SER:HB2	1:C:3:VAL:O	1.82	0.79
1:A:44:ASP:O	1:C:38:ILE:HA	1.83	0.79
1:A:496:LEU:HD21	1:A:509:ILE:HD13	1.63	0.79
1:B:27:ASN:HD22	1:B:27:ASN:C	1.85	0.79
1:B:496:LEU:HD21	1:B:509:ILE:HD13	1.63	0.79
2:B:904:NAG:H3	2:B:904:NAG:O7	1.82	0.79
1:C:155:PRO:C	1:C:157:GLU:H	1.86	0.79
1:C:432:ASP:OD2	1:C:464:ILE:CG2	2.30	0.79
1:C:496:LEU:HD21	1:C:509:ILE:HD13	1.63	0.79
1:A:195:ASP:HB3	1:A:200:GLY:HA3	1.65	0.79
1:A:485:ALA:O	1:A:486:GLU:CG	2.30	0.79
1:C:483:TRP:HZ2	1:C:507:TYR:HE1	1.24	0.79
1:A:449:ASP:HB3	1:A:532:CYS:H	1.47	0.79
1:B:127:VAL:HG13	1:B:128:MET:H	1.46	0.79
2:C:809:NAG:H61	2:C:810:NAG:H62	1.65	0.79
1:A:406:TYR:CD1	2:A:808:NAG:H83	2.17	0.79
1:B:234:GLU:H	1:B:235:ILE:CG2	1.92	0.79
1:B:365:GLN:O	1:B:365:GLN:HG3	1.82	0.79
1:C:232:GLU:HG3	1:C:290:PHE:N	1.98	0.79
1:A:222:ASP:C	1:A:222:ASP:OD1	2.20	0.79
1:A:277:SER:C	1:A:278:ASN:HD22	1.84	0.79
1:C:396:ARG:HD3	1:C:431:LEU:C	2.03	0.79
1:C:482:THR:OG1	1:C:500:GLN:HG2	1.82	0.79
1:A:155:PRO:C	1:A:157:GLU:H	1.86	0.78
1:A:78:SER:C	1:C:90:GLU:OE2	2.21	0.78
1:B:30:ARG:CZ	1:C:25:LYS:O	2.30	0.78
1:C:238:GLU:HA	1:C:283:THR:HG22	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLU:HG3	1:A:160:PRO:HB3	1.66	0.78
1:A:396:ARG:HD3	1:A:431:LEU:C	2.03	0.78
1:B:396:ARG:HH21	1:B:464:ILE:HG22	1.46	0.78
1:C:156:GLU:HG3	1:C:160:PRO:HB3	1.66	0.78
1:C:154:ASP:CB	1:C:155:PRO:HD2	2.13	0.78
1:C:485:ALA:O	1:C:486:GLU:CG	2.30	0.78
1:A:482:THR:OG1	1:A:500:GLN:HG2	1.82	0.78
1:B:155:PRO:C	1:B:157:GLU:H	1.86	0.78
1:B:30:ARG:HA	1:C:27:ASN:OD1	1.82	0.78
1:C:222:ASP:C	1:C:222:ASP:OD1	2.20	0.78
1:B:86:SER:HB2	1:C:4:ILE:CA	2.14	0.78
1:B:147:SER:OG	1:B:167:ARG:CG	2.32	0.78
1:B:485:ALA:O	1:B:486:GLU:CG	2.30	0.78
1:C:147:SER:OG	1:C:167:ARG:CD	2.32	0.78
1:B:406:TYR:CD1	2:B:808:NAG:H83	2.17	0.78
2:B:809:NAG:H61	2:B:810:NAG:H62	1.65	0.78
1:C:147:SER:OG	1:C:167:ARG:CG	2.32	0.78
2:A:904:NAG:O7	2:A:904:NAG:H3	1.82	0.78
1:B:147:SER:OG	1:B:167:ARG:CD	2.32	0.78
1:A:75:VAL:CB	1:C:87:PRO:HD3	2.10	0.78
1:A:154:ASP:CB	1:A:155:PRO:HD2	2.13	0.78
1:A:371:ILE:HD11	1:A:381:VAL:HG11	1.64	0.78
1:B:371:ILE:HD11	1:B:381:VAL:HG11	1.64	0.78
1:B:89:GLU:N	1:C:1:ASP:CB	2.47	0.78
1:A:89:GLU:OE1	1:B:2:TRP:N	2.18	0.77
1:A:290:PHE:HZ	1:A:296:TYR:HH	1.31	0.77
1:A:432:ASP:CG	1:A:464:ILE:HG22	2.05	0.77
1:B:154:ASP:CB	1:B:155:PRO:HD2	2.13	0.77
1:B:30:ARG:NH1	1:C:25:LYS:O	2.15	0.77
1:B:524:VAL:CG2	2:B:904:NAG:H81	2.14	0.77
1:A:232:GLU:HG3	1:A:290:PHE:N	1.98	0.77
1:A:540:GLN:CG	1:A:540:GLN:O	2.30	0.77
1:B:33:LYS:O	1:C:2:TRP:NE1	2.09	0.77
1:B:501:GLN:HG2	1:B:501:GLN:O	1.84	0.77
1:C:289:ASP:O	1:C:290:PHE:CB	2.25	0.77
1:C:371:ILE:HD11	1:C:381:VAL:HG11	1.64	0.77
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.77
1:A:89:GLU:CD	1:B:1:ASP:H3	1.86	0.77
1:B:82:SER:N	1:C:2:TRP:CB	2.35	0.77
1:B:301:THR:HG21	2:B:805:NAG:C8	2.12	0.77
1:B:523:THR:HG23	1:B:524:VAL:HG22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:GLN:HG3	1:C:365:GLN:O	1.82	0.77
1:A:41:GLN:N	1:C:81:VAL:CG1	2.41	0.77
1:A:301:THR:HG21	2:A:805:NAG:C8	2.12	0.77
1:A:505:GLY:C	1:A:506:ASP:OD1	2.23	0.77
2:A:809:NAG:H61	2:A:810:NAG:H62	1.65	0.77
1:B:222:ASP:OD1	1:B:222:ASP:C	2.20	0.77
1:B:505:GLY:C	1:B:506:ASP:OD1	2.23	0.77
1:C:27:ASN:HD22	1:C:27:ASN:C	1.85	0.77
1:C:540:GLN:CG	1:C:540:GLN:O	2.30	0.77
1:B:362:GLN:O	1:B:364:ILE:HG23	1.85	0.77
1:B:194:THR:HB	1:B:198:GLY:HA2	1.66	0.77
1:B:449:ASP:HB3	1:B:532:CYS:H	1.47	0.77
1:C:505:GLY:C	1:C:506:ASP:OD1	2.23	0.77
1:C:524:VAL:CG2	2:C:904:NAG:H81	2.14	0.77
1:C:195:ASP:HB3	1:C:200:GLY:HA3	1.65	0.77
1:A:238:GLU:HA	1:A:283:THR:HG22	1.66	0.76
1:B:223:PRO:HD2	1:B:226:TYR:OH	1.85	0.76
1:C:440:PRO:HB3	1:C:457:LEU:HD21	1.67	0.76
1:C:523:THR:HG23	1:C:524:VAL:HG22	1.67	0.76
1:B:238:GLU:HA	1:B:283:THR:HG22	1.66	0.76
1:B:432:ASP:CG	1:B:464:ILE:HG22	2.05	0.76
1:C:196:LEU:HB2	1:C:199:ALA:HB3	1.67	0.76
1:C:194:THR:HB	1:C:198:GLY:HA2	1.67	0.76
1:C:362:GLN:O	1:C:364:ILE:HG23	1.85	0.76
1:A:524:VAL:CG2	2:A:904:NAG:H81	2.14	0.76
1:B:82:SER:HB3	1:C:2:TRP:CB	2.14	0.76
1:C:501:GLN:O	1:C:501:GLN:HG2	1.84	0.76
1:A:272:THR:HG22	1:A:273:THR:H	1.51	0.76
1:A:366:LYS:CG	1:A:367:LEU:N	2.48	0.76
1:B:156:GLU:HG3	1:B:160:PRO:HB3	1.66	0.76
1:A:194:THR:HB	1:A:198:GLY:HA2	1.66	0.76
1:A:501:GLN:O	1:A:501:GLN:HG2	1.84	0.76
1:B:188:THR:HG23	1:B:208:ILE:CG1	2.16	0.76
1:A:362:GLN:O	1:A:364:ILE:HG23	1.85	0.76
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.76
1:B:82:SER:CA	1:C:2:TRP:CA	2.62	0.76
1:C:432:ASP:CG	1:C:464:ILE:HG22	2.05	0.76
1:A:188:THR:HG23	1:A:208:ILE:CG1	2.16	0.75
1:A:371:ILE:HD12	1:A:410:MET:HB3	1.68	0.75
1:C:223:PRO:HD2	1:C:226:TYR:OH	1.85	0.75
1:C:241:ARG:HE	1:C:281:ILE:HD12	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:LYS:CG	1:C:367:LEU:N	2.48	0.75
1:A:241:ARG:HE	1:A:281:ILE:HD12	1.51	0.75
1:A:289:ASP:O	1:A:290:PHE:CB	2.25	0.75
1:A:448:CYS:SG	1:A:537:ILE:HG22	2.27	0.75
1:A:523:THR:HG23	1:A:524:VAL:HG22	1.67	0.75
1:B:290:PHE:CD2	1:B:293:ARG:N	2.55	0.75
1:B:440:PRO:HB3	1:B:457:LEU:HD21	1.68	0.75
1:A:440:PRO:HB3	1:A:457:LEU:HD21	1.67	0.75
1:B:80:ALA:CB	1:C:1:ASP:HA	2.17	0.75
1:A:196:LEU:HB2	1:A:199:ALA:HB3	1.67	0.75
1:B:196:LEU:HB2	1:B:199:ALA:HB3	1.67	0.75
1:A:90:GLU:HB3	1:B:2:TRP:HD1	1.52	0.75
1:C:482:THR:CG2	1:C:499:THR:CG2	2.62	0.75
1:A:223:PRO:HD2	1:A:226:TYR:OH	1.85	0.75
1:B:272:THR:HG22	1:B:273:THR:H	1.51	0.75
1:B:290:PHE:HZ	1:B:296:TYR:HH	1.33	0.75
1:C:272:THR:HG22	1:C:273:THR:H	1.51	0.75
1:A:87:PRO:HG3	1:B:89:GLU:HB3	0.75	0.75
1:C:396:ARG:HH21	1:C:464:ILE:CG2	1.99	0.75
1:B:396:ARG:NH2	1:B:464:ILE:HB	2.02	0.75
1:C:301:THR:HG21	2:C:805:NAG:C8	2.12	0.75
1:A:396:ARG:NH2	1:A:464:ILE:HB	2.02	0.75
1:A:84:ASN:HD22	1:B:79:HIS:CE1	2.04	0.75
1:A:90:GLU:C	1:B:1:ASP:OD1	2.26	0.75
1:B:449:ASP:HB3	1:B:532:CYS:N	2.02	0.75
1:B:450:GLN:HG3	1:B:533:GLU:OE2	1.87	0.74
1:A:449:ASP:HB3	1:A:532:CYS:N	2.02	0.74
1:C:448:CYS:SG	1:C:537:ILE:HG22	2.27	0.74
1:C:449:ASP:HB3	1:C:532:CYS:N	2.02	0.74
1:B:241:ARG:HE	1:B:281:ILE:HD12	1.51	0.74
1:B:448:CYS:SG	1:B:537:ILE:HG22	2.27	0.74
1:A:450:GLN:HG3	1:A:533:GLU:OE2	1.88	0.74
1:C:188:THR:HG23	1:C:208:ILE:CG1	2.16	0.74
1:B:364:ILE:HG13	1:B:364:ILE:O	1.87	0.74
1:A:396:ARG:HH21	1:A:464:ILE:CG2	1.99	0.74
1:C:451:ASN:O	1:C:534:GLY:HA2	1.88	0.74
1:A:364:ILE:HG13	1:A:364:ILE:O	1.86	0.74
1:B:366:LYS:CG	1:B:367:LEU:N	2.48	0.74
1:B:223:PRO:HB2	1:B:226:TYR:CE2	2.23	0.74
1:B:298:LEU:HD23	1:B:298:LEU:N	2.03	0.74
1:C:290:PHE:CD2	1:C:293:ARG:N	2.55	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:GLN:HG3	1:C:533:GLU:OE2	1.88	0.74
1:B:451:ASN:O	1:B:534:GLY:HA2	1.88	0.73
1:A:87:PRO:HG2	1:B:89:GLU:HG3	1.67	0.73
1:A:290:PHE:HE2	1:A:293:ARG:HB2	1.52	0.73
1:B:371:ILE:HD12	1:B:410:MET:HB3	1.68	0.73
1:C:298:LEU:N	1:C:298:LEU:HD23	2.03	0.73
1:C:371:ILE:HD12	1:C:410:MET:HB3	1.68	0.73
1:A:223:PRO:HB2	1:A:226:TYR:CE2	2.23	0.73
1:C:223:PRO:HB2	1:C:226:TYR:CE2	2.23	0.73
1:B:81:VAL:O	1:C:2:TRP:CD1	2.42	0.73
1:C:320:THR:CG2	2:C:807:NAG:HN2	2.01	0.73
1:C:373:ASN:ND2	1:C:374:ASP:H	1.87	0.73
1:A:333:VAL:CB	1:A:334:PRO:HD3	2.18	0.73
1:A:373:ASN:ND2	1:A:374:ASP:H	1.87	0.73
1:C:33:LYS:HB3	1:C:83:GLU:HG2	1.71	0.73
1:B:373:ASN:ND2	1:B:374:ASP:H	1.87	0.73
1:A:276:GLU:HG3	1:A:277:SER:H	1.54	0.73
1:A:474:SER:CB	1:A:512:LEU:HG	2.14	0.73
1:A:273:THR:O	2:A:803:NAG:H82	1.89	0.73
1:B:333:VAL:CB	1:B:334:PRO:HD3	2.18	0.73
1:B:33:LYS:HB3	1:B:83:GLU:HG2	1.71	0.73
1:C:364:ILE:O	1:C:364:ILE:CG1	2.37	0.73
1:B:86:SER:HB3	1:C:3:VAL:HB	1.71	0.73
1:C:511:VAL:HG23	1:C:523:THR:O	1.89	0.73
1:A:75:VAL:CB	1:C:87:PRO:CD	2.67	0.73
1:C:320:THR:CG2	2:C:807:NAG:N2	2.52	0.72
1:C:396:ARG:NH2	1:C:464:ILE:HB	2.02	0.72
1:A:320:THR:CG2	2:A:807:NAG:N2	2.52	0.72
1:C:368:SER:HG	1:C:370:PHE:HE1	1.37	0.72
1:B:273:THR:O	2:B:803:NAG:H82	1.89	0.72
1:B:396:ARG:HH21	1:B:464:ILE:CG2	1.98	0.72
1:C:333:VAL:CB	1:C:334:PRO:HD3	2.18	0.72
1:A:35:TYR:HB3	1:B:90:GLU:OE1	1.89	0.72
1:B:320:THR:CG2	2:B:807:NAG:N2	2.52	0.72
1:A:298:LEU:HD23	1:A:298:LEU:N	2.03	0.72
1:C:290:PHE:HE2	1:C:293:ARG:HB2	1.52	0.72
1:C:342:SER:HA	1:C:431:LEU:HB2	1.71	0.72
1:A:451:ASN:O	1:A:534:GLY:HA2	1.88	0.72
1:A:511:VAL:HG23	1:A:523:THR:O	1.89	0.72
1:A:342:SER:HA	1:A:431:LEU:HB2	1.71	0.72
1:B:342:SER:HA	1:B:431:LEU:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PRO:CG	1:B:89:GLU:CG	2.67	0.72
1:B:276:GLU:CG	1:B:277:SER:H	2.03	0.72
1:B:276:GLU:HG3	1:B:277:SER:H	1.54	0.72
1:B:366:LYS:HG3	1:B:367:LEU:N	2.04	0.72
1:B:394:LEU:N	1:B:394:LEU:HD12	2.05	0.72
1:C:366:LYS:HG3	1:C:367:LEU:N	2.04	0.72
1:C:474:SER:CB	1:C:512:LEU:HG	2.14	0.72
1:C:364:ILE:O	1:C:364:ILE:HG13	1.87	0.72
1:A:33:LYS:HB3	1:A:83:GLU:HG2	1.71	0.72
1:B:474:SER:CB	1:B:512:LEU:HG	2.14	0.72
1:C:273:THR:O	2:C:803:NAG:H82	1.89	0.72
1:A:405:THR:OG1	1:A:406:TYR:N	2.22	0.71
1:A:90:GLU:HB3	1:B:2:TRP:CD1	2.25	0.71
1:A:28:LYS:NZ	1:B:4:ILE:H	1.87	0.71
1:B:80:ALA:HB3	1:C:1:ASP:HA	1.71	0.71
1:C:276:GLU:HG3	1:C:277:SER:H	1.54	0.71
1:A:364:ILE:O	1:A:364:ILE:CG1	2.37	0.71
1:C:474:SER:HB2	1:C:512:LEU:CG	2.15	0.71
1:A:482:THR:CG2	1:A:499:THR:CG2	2.62	0.71
1:A:227:THR:O	2:A:812:NAG:O5	2.09	0.71
1:B:511:VAL:HG23	1:B:523:THR:O	1.89	0.71
1:A:276:GLU:CG	1:A:277:SER:H	2.03	0.71
1:A:320:THR:CG2	2:A:807:NAG:HN2	2.02	0.71
1:A:394:LEU:N	1:A:394:LEU:HD12	2.05	0.71
1:C:276:GLU:CG	1:C:277:SER:H	2.03	0.71
1:C:229:LEU:HD23	1:C:322:THR:HB	1.73	0.71
1:C:227:THR:O	2:C:812:NAG:O5	2.09	0.71
1:B:364:ILE:CG1	1:B:364:ILE:O	2.37	0.71
1:C:394:LEU:HD12	1:C:394:LEU:N	2.05	0.71
1:A:434:ASN:OD1	1:A:467:ASN:HB3	1.91	0.71
1:B:414:ASP:HB3	1:B:420:GLY:HA3	1.73	0.71
1:B:227:THR:O	2:B:812:NAG:O5	2.09	0.71
1:C:316:THR:O	2:C:806:NAG:H82	1.91	0.71
1:A:48:GLN:HE22	1:C:53:ILE:HG21	1.54	0.71
1:B:229:LEU:HD23	1:B:322:THR:HB	1.73	0.71
1:B:35:TYR:N	1:C:2:TRP:CE2	2.56	0.71
1:C:337:SER:CA	1:C:427:ILE:HG23	2.20	0.71
1:C:434:ASN:OD1	1:C:467:ASN:HB3	1.91	0.71
1:A:48:GLN:HE22	1:C:53:ILE:CG2	2.03	0.71
1:A:290:PHE:CD2	1:A:293:ARG:N	2.55	0.71
1:A:474:SER:HB2	1:A:512:LEU:CG	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:THR:O	2:B:806:NAG:H82	1.91	0.71
1:A:368:SER:HG	1:A:370:PHE:HE1	1.39	0.71
1:A:438:PRO:HB3	1:A:471:TYR:CE2	2.26	0.71
1:A:187:TYR:HA	2:A:801:NAG:C7	2.21	0.71
1:C:187:TYR:HA	2:C:801:NAG:C7	2.21	0.71
1:A:366:LYS:HG3	1:A:367:LEU:N	2.04	0.70
1:A:414:ASP:HB3	1:A:420:GLY:HA3	1.73	0.70
1:C:403:ASN:CB	3:C:902:NDG:N2	2.54	0.70
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.70
1:B:290:PHE:HE2	1:B:293:ARG:HB2	1.52	0.70
1:B:403:ASN:CB	3:B:902:NDG:N2	2.54	0.70
1:B:434:ASN:OD1	1:B:467:ASN:HB3	1.90	0.70
1:B:482:THR:CG2	1:B:499:THR:CG2	2.62	0.70
1:B:83:GLU:OE2	1:C:2:TRP:CH2	2.44	0.70
1:B:438:PRO:HB3	1:B:471:TYR:CE2	2.26	0.70
1:C:485:ALA:C	1:C:486:GLU:HG2	2.11	0.70
1:A:316:THR:O	2:A:806:NAG:H82	1.91	0.70
1:B:187:TYR:HA	2:B:801:NAG:C7	2.21	0.70
1:A:403:ASN:CB	3:A:902:NDG:N2	2.54	0.70
1:B:320:THR:CG2	2:B:807:NAG:HN2	2.02	0.70
1:C:396:ARG:HE	1:C:432:ASP:HB2	1.57	0.70
1:B:337:SER:CA	1:B:427:ILE:HG23	2.20	0.70
1:C:483:TRP:CZ2	1:C:507:TYR:HE1	2.09	0.70
1:B:485:ALA:C	1:B:486:GLU:HG2	2.11	0.70
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.74	0.70
1:A:289:ASP:CG	1:A:289:ASP:O	2.29	0.69
1:A:46:PRO:HB2	1:C:35:TYR:HE2	0.91	0.69
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.74	0.69
1:A:229:LEU:HD23	1:A:322:THR:HB	1.73	0.69
1:A:485:ALA:C	1:A:486:GLU:HG2	2.11	0.69
1:A:53:ILE:HG13	1:A:59:TRP:O	1.93	0.69
1:B:27:ASN:ND2	1:B:27:ASN:C	2.46	0.69
1:B:186:GLU:OE1	2:B:801:NAG:H62	1.93	0.69
1:B:289:ASP:O	1:B:289:ASP:CG	2.30	0.69
1:B:483:TRP:CZ2	1:B:507:TYR:HE1	2.09	0.69
1:C:289:ASP:O	1:C:289:ASP:CG	2.30	0.69
1:B:396:ARG:HE	1:B:432:ASP:HB2	1.57	0.69
1:C:414:ASP:HB3	1:C:420:GLY:HA3	1.73	0.69
1:A:27:ASN:C	1:A:27:ASN:ND2	2.46	0.69
1:C:405:THR:OG1	1:C:406:TYR:N	2.22	0.69
1:B:289:ASP:O	1:B:290:PHE:CB	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ILE:HG13	1:B:59:TRP:O	1.93	0.69
1:C:438:PRO:HB3	1:C:471:TYR:CE2	2.26	0.69
1:C:186:GLU:OE1	2:C:801:NAG:H62	1.93	0.69
1:A:396:ARG:HE	1:A:432:ASP:HB2	1.57	0.69
1:A:186:GLU:OE1	2:A:801:NAG:H62	1.93	0.69
1:B:242:LEU:HD12	1:B:280:GLY:O	1.93	0.69
1:B:396:ARG:HD3	1:B:431:LEU:O	1.93	0.69
1:A:337:SER:CA	1:A:427:ILE:HG23	2.20	0.68
1:B:1:ASP:CG	1:B:2:TRP:H	1.96	0.68
1:C:195:ASP:HB2	1:C:201:LEU:N	2.08	0.68
1:C:242:LEU:HD12	1:C:280:GLY:O	1.93	0.68
1:B:282:LEU:HD23	1:B:283:THR:N	2.08	0.68
1:B:88:VAL:H	1:C:1:ASP:C	1.97	0.68
1:A:48:GLN:HG3	1:C:37:SER:HB2	1.76	0.68
1:A:242:LEU:HD12	1:A:280:GLY:O	1.93	0.68
1:C:53:ILE:HG13	1:C:59:TRP:O	1.93	0.68
1:C:482:THR:HG21	1:C:500:GLN:H	1.58	0.68
1:C:371:ILE:CG2	1:C:372:GLY:N	2.57	0.68
1:B:272:THR:HG22	1:B:273:THR:N	2.09	0.68
1:C:347:ARG:CD	1:C:392:GLY:H	2.07	0.68
1:B:290:PHE:HZ	1:B:296:TYR:OH	1.77	0.68
1:B:396:ARG:HE	1:B:432:ASP:CB	2.07	0.68
1:B:87:PRO:HA	1:C:1:ASP:O	1.94	0.68
1:C:155:PRO:HB2	2:C:801:NAG:C8	2.24	0.68
1:A:282:LEU:HD23	1:A:283:THR:H	1.59	0.68
1:A:347:ARG:CD	1:A:392:GLY:H	2.07	0.68
1:B:347:ARG:CD	1:B:392:GLY:H	2.07	0.68
1:B:155:PRO:HB2	2:B:801:NAG:C8	2.24	0.68
1:A:282:LEU:HD23	1:A:283:THR:N	2.08	0.68
1:B:440:PRO:HA	1:B:458:THR:O	1.94	0.68
1:C:282:LEU:HD23	1:C:283:THR:N	2.08	0.68
1:C:396:ARG:HD3	1:C:431:LEU:O	1.94	0.68
1:A:137:ASP:OD2	1:A:139:ILE:HG22	1.94	0.67
1:C:232:GLU:HG2	1:C:289:ASP:HA	1.76	0.67
1:A:272:THR:HG22	1:A:273:THR:N	2.09	0.67
1:A:155:PRO:HB2	2:A:801:NAG:C8	2.24	0.67
1:C:401:VAL:HG13	1:C:405:THR:O	1.95	0.67
1:A:482:THR:HG21	1:A:500:GLN:H	1.58	0.67
1:B:396:ARG:NH2	1:B:464:ILE:CB	2.58	0.67
1:C:137:ASP:OD2	1:C:139:ILE:HG22	1.94	0.67
1:C:221:PHE:CE1	1:C:315:SER:O	2.45	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLU:HG2	1:A:289:ASP:HA	1.77	0.67
1:A:371:ILE:CG2	1:A:372:GLY:N	2.57	0.67
1:B:232:GLU:HG2	1:B:289:ASP:HA	1.77	0.67
1:B:371:ILE:CG2	1:B:372:GLY:N	2.57	0.67
1:B:401:VAL:HG13	1:B:405:THR:O	1.95	0.67
1:C:396:ARG:NH2	1:C:464:ILE:CB	2.58	0.67
1:C:423:THR:HB	2:C:810:NAG:C8	2.24	0.67
1:C:523:THR:HG23	1:C:524:VAL:HG23	1.74	0.67
1:A:1:ASP:CG	1:A:2:TRP:H	1.96	0.67
3:A:902:NDG:O7	3:A:902:NDG:H3	1.95	0.67
1:B:333:VAL:HB	1:B:334:PRO:CD	2.24	0.67
1:B:347:ARG:CG	1:B:392:GLY:H	2.08	0.67
1:C:440:PRO:HA	1:C:458:THR:O	1.94	0.67
1:A:347:ARG:CG	1:A:392:GLY:H	2.08	0.67
1:A:195:ASP:HB2	1:A:201:LEU:N	2.08	0.67
1:A:290:PHE:HZ	1:A:296:TYR:OH	1.77	0.67
1:A:423:THR:HB	2:A:810:NAG:C8	2.24	0.67
1:A:403:ASN:HB2	3:A:902:NDG:N2	2.10	0.67
1:C:272:THR:HG22	1:C:273:THR:N	2.09	0.67
1:C:224:LYS:HE3	1:C:316:THR:O	1.95	0.67
1:B:187:TYR:HA	2:B:801:NAG:C8	2.25	0.67
1:B:224:LYS:HE3	1:B:316:THR:O	1.95	0.67
1:C:282:LEU:HD23	1:C:283:THR:H	1.58	0.67
1:C:320:THR:HG21	2:C:807:NAG:H2	1.76	0.67
1:A:224:LYS:HE3	1:A:316:THR:O	1.95	0.67
1:B:221:PHE:CE1	1:B:315:SER:O	2.45	0.67
1:B:403:ASN:HB2	3:B:902:NDG:N2	2.10	0.67
1:A:396:ARG:HD3	1:A:431:LEU:O	1.94	0.67
1:A:187:TYR:HA	2:A:801:NAG:C8	2.25	0.67
1:C:347:ARG:HD2	1:C:392:GLY:H	1.60	0.67
1:C:524:VAL:HG21	2:C:904:NAG:H81	1.76	0.67
1:A:366:LYS:HG3	1:A:367:LEU:HG	1.77	0.66
1:B:423:THR:HB	2:B:810:NAG:C8	2.24	0.66
1:B:87:PRO:C	1:C:3:VAL:N	2.48	0.66
1:C:464:ILE:O	1:C:467:ASN:HB2	1.96	0.66
1:A:222:ASP:CG	1:A:222:ASP:O	2.32	0.66
1:A:347:ARG:HD2	1:A:392:GLY:H	1.60	0.66
1:A:396:ARG:NH2	1:A:464:ILE:CB	2.58	0.66
1:B:482:THR:HG21	1:B:500:GLN:H	1.58	0.66
1:C:187:TYR:HA	2:C:801:NAG:C8	2.25	0.66
1:C:290:PHE:HZ	1:C:296:TYR:OH	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PRO:HA	1:A:458:THR:O	1.94	0.66
3:B:902:NDG:O7	3:B:902:NDG:H3	1.95	0.66
1:C:396:ARG:HE	1:C:432:ASP:CB	2.07	0.66
1:C:403:ASN:HB2	3:C:902:NDG:N2	2.10	0.66
1:A:396:ARG:HE	1:A:432:ASP:CB	2.07	0.66
1:B:282:LEU:HD23	1:B:283:THR:H	1.58	0.66
1:B:373:ASN:ND2	1:B:374:ASP:N	2.43	0.66
1:B:464:ILE:O	1:B:467:ASN:HB2	1.96	0.66
1:A:46:PRO:HB3	1:C:35:TYR:CE2	2.26	0.66
1:C:373:ASN:ND2	1:C:374:ASP:N	2.43	0.66
1:A:320:THR:HG21	2:A:807:NAG:H2	1.76	0.66
1:B:137:ASP:OD2	1:B:139:ILE:HG22	1.94	0.66
1:A:88:VAL:HA	1:B:92:MET:HG2	1.76	0.66
3:C:902:NDG:O7	3:C:902:NDG:H3	1.95	0.66
1:B:482:THR:OG1	1:B:500:GLN:CG	2.44	0.66
1:B:440:PRO:HD2	1:B:522:LEU:CD1	2.26	0.66
1:C:440:PRO:HD2	1:C:522:LEU:CD1	2.26	0.66
1:C:524:VAL:HG23	2:C:904:NAG:H81	1.78	0.66
1:A:401:VAL:HG13	1:A:405:THR:O	1.95	0.66
1:B:347:ARG:HD2	1:B:392:GLY:H	1.60	0.66
1:B:88:VAL:N	1:C:1:ASP:CA	2.58	0.66
1:C:366:LYS:HG3	1:C:367:LEU:HG	1.77	0.66
2:C:809:NAG:C6	2:C:810:NAG:H62	2.26	0.66
1:A:32:ASN:CG	1:A:33:LYS:H	1.98	0.66
1:A:373:ASN:ND2	1:A:374:ASP:N	2.43	0.66
1:A:446:THR:CG2	1:A:537:ILE:O	2.44	0.66
1:B:32:ASN:CG	1:B:33:LYS:H	1.98	0.66
1:B:366:LYS:HG3	1:B:367:LEU:HG	1.77	0.66
1:A:82:SER:OG	1:B:91:PRO:C	2.33	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:B:320:THR:HG21	2:B:807:NAG:H2	1.76	0.66
1:C:232:GLU:HG3	1:C:290:PHE:H	1.61	0.66
1:A:483:TRP:CZ2	1:A:507:TYR:HE1	2.09	0.66
1:A:488:ASP:HB2	1:A:493:SER:OG	1.97	0.65
2:A:805:NAG:C6	2:A:806:NAG:C7	2.74	0.65
1:B:524:VAL:HG21	2:B:904:NAG:H81	1.77	0.65
1:C:265:GLU:HB3	1:C:268:PHE:CE2	2.31	0.65
1:A:524:VAL:HG21	2:A:904:NAG:H81	1.77	0.65
1:B:405:THR:OG1	1:B:406:TYR:N	2.22	0.65
1:B:440:PRO:HD3	1:B:522:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:NZ	1:B:4:ILE:N	2.38	0.65
1:C:212:THR:HG22	1:C:213:ASP:H	1.62	0.65
1:C:32:ASN:CG	1:C:33:LYS:H	1.99	0.65
1:B:341:VAL:HG21	1:B:345:LEU:HD12	1.79	0.65
1:B:86:SER:HB3	1:C:3:VAL:C	1.99	0.65
1:C:488:ASP:HB2	1:C:493:SER:OG	1.97	0.65
1:C:32:ASN:ND2	1:C:83:GLU:N	2.44	0.65
1:C:341:VAL:HG21	1:C:345:LEU:HD12	1.79	0.65
1:C:403:ASN:HB2	3:C:902:NDG:H8C1	1.78	0.65
1:A:327:ASN:HA	1:A:360:ASP:OD2	1.97	0.65
1:A:464:ILE:O	1:A:467:ASN:HB2	1.96	0.65
1:A:32:ASN:ND2	1:A:83:GLU:N	2.44	0.65
1:B:195:ASP:HB2	1:B:201:LEU:N	2.08	0.65
1:C:222:ASP:O	1:C:222:ASP:CG	2.32	0.65
1:C:347:ARG:CG	1:C:392:GLY:H	2.08	0.65
2:B:809:NAG:C6	2:B:810:NAG:H62	2.26	0.65
1:C:327:ASN:HA	1:C:360:ASP:OD2	1.97	0.65
1:B:474:SER:HB2	1:B:512:LEU:CG	2.15	0.65
1:B:482:THR:HG21	1:B:499:THR:CA	2.27	0.65
1:C:333:VAL:HB	1:C:334:PRO:CD	2.24	0.65
2:A:809:NAG:C6	2:A:810:NAG:H62	2.26	0.65
1:B:88:VAL:N	1:C:1:ASP:C	2.50	0.65
1:C:440:PRO:HD3	1:C:522:LEU:HD12	1.78	0.65
1:A:364:ILE:O	1:A:364:ILE:HD12	1.97	0.64
1:B:524:VAL:HG23	2:B:904:NAG:H81	1.78	0.64
1:C:364:ILE:O	1:C:364:ILE:HD12	1.97	0.64
2:C:805:NAG:C6	2:C:806:NAG:C7	2.74	0.64
1:A:524:VAL:HG23	2:A:904:NAG:H81	1.78	0.64
1:C:347:ARG:HG3	1:C:392:GLY:H	1.62	0.64
1:C:482:THR:OG1	1:C:500:GLN:CG	2.44	0.64
1:B:364:ILE:HD12	1:B:364:ILE:O	1.98	0.64
1:B:403:ASN:HB2	3:B:902:NDG:H8C1	1.78	0.64
1:A:469:TYR:CD2	1:A:470:PRO:CD	2.81	0.64
1:A:440:PRO:HD2	1:A:522:LEU:CD1	2.26	0.64
1:B:232:GLU:HG3	1:B:290:PHE:H	1.61	0.64
1:B:446:THR:CG2	1:B:537:ILE:O	2.44	0.64
1:C:346:SER:OG	1:C:349:GLU:HG3	1.97	0.64
1:C:469:TYR:CD2	1:C:470:PRO:CD	2.81	0.64
1:A:333:VAL:HB	1:A:334:PRO:CD	2.24	0.64
1:A:375:PRO:HB3	1:A:400:TYR:CD2	2.33	0.64
1:B:504:LYS:NZ	1:B:531:SER:OG	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:904:NAG:O7	2:B:904:NAG:C3	2.45	0.64
1:B:33:LYS:O	1:C:2:TRP:CD1	2.46	0.64
1:A:212:THR:HG22	1:A:213:ASP:H	1.62	0.64
1:B:347:ARG:HG3	1:B:392:GLY:H	1.62	0.64
1:B:409:ILE:HG12	1:B:425:THR:HG23	1.80	0.64
1:B:406:TYR:CE1	2:B:808:NAG:H83	2.32	0.64
1:A:346:SER:OG	1:A:349:GLU:HG3	1.97	0.64
1:B:227:THR:CG2	2:B:807:NAG:C7	2.76	0.64
1:B:35:TYR:HB2	1:C:2:TRP:CZ2	2.33	0.64
1:B:488:ASP:HB2	1:B:493:SER:OG	1.97	0.64
1:C:415:ASP:OD1	1:C:416:GLY:N	2.27	0.64
1:C:406:TYR:CE1	2:C:808:NAG:H83	2.32	0.64
1:A:486:GLU:O	1:A:494:MET:CA	2.46	0.64
1:B:32:ASN:ND2	1:B:83:GLU:N	2.44	0.64
1:A:486:GLU:O	1:A:495:LEU:N	2.31	0.64
1:A:406:TYR:CE1	2:A:808:NAG:H83	2.32	0.64
1:C:364:ILE:O	1:C:364:ILE:CD1	2.46	0.64
1:C:375:PRO:HB3	1:C:400:TYR:CD2	2.33	0.64
1:A:403:ASN:HB2	3:A:902:NDG:H8C1	1.78	0.64
1:A:232:GLU:HG3	1:A:290:PHE:H	1.61	0.63
1:A:40:GLY:N	1:C:79:HIS:HD1	1.96	0.63
1:A:419:VAL:HG13	2:A:809:NAG:O7	1.98	0.63
1:B:364:ILE:CD1	1:B:364:ILE:O	2.46	0.63
1:B:371:ILE:HG22	1:B:372:GLY:N	2.14	0.63
1:A:482:THR:HG22	1:A:499:THR:N	2.13	0.63
1:A:154:ASP:O	2:A:801:NAG:H82	1.98	0.63
1:B:346:SER:OG	1:B:349:GLU:HG3	1.97	0.63
1:C:371:ILE:HG22	1:C:372:GLY:N	2.14	0.63
1:A:347:ARG:HG3	1:A:392:GLY:H	1.62	0.63
1:A:43:ALA:O	1:C:39:THR:HG21	1.92	0.63
1:A:518:ASN:O	1:A:520:PRO:CD	2.46	0.63
1:B:22:VAL:HG22	1:B:23:GLN:N	2.14	0.63
1:B:486:GLU:O	1:B:494:MET:CA	2.46	0.63
1:C:409:ILE:HG12	1:C:425:THR:HG23	1.80	0.63
1:C:419:VAL:HG13	2:C:809:NAG:O7	1.98	0.63
1:A:40:GLY:O	1:C:79:HIS:HB2	1.94	0.63
1:A:446:THR:CG2	1:A:539:CYS:SG	2.86	0.63
1:C:154:ASP:O	2:C:801:NAG:H82	1.98	0.63
2:C:904:NAG:C3	2:C:904:NAG:O7	2.45	0.63
1:A:341:VAL:HG21	1:A:345:LEU:HD12	1.79	0.63
1:B:154:ASP:O	2:B:801:NAG:H82	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:VAL:HG13	2:B:809:NAG:O7	1.98	0.63
1:C:504:LYS:NZ	1:C:531:SER:OG	2.31	0.63
1:A:127:VAL:HG22	1:A:128:MET:N	2.14	0.63
1:A:343:GLU:HB3	1:A:433:VAL:CG2	2.28	0.63
1:A:482:THR:HG21	1:A:499:THR:CA	2.27	0.63
1:B:212:THR:HG22	1:B:213:ASP:H	1.62	0.63
1:B:327:ASN:HA	1:B:360:ASP:OD2	1.97	0.63
1:C:142:LEU:HB3	1:C:196:LEU:HA	1.81	0.63
1:C:411:LEU:HD22	1:C:421:THR:HG23	1.81	0.63
1:A:142:LEU:HB3	1:A:196:LEU:HA	1.81	0.63
1:B:375:PRO:HB3	1:B:400:TYR:CD2	2.33	0.63
1:B:446:THR:CG2	1:B:539:CYS:SG	2.86	0.63
1:B:154:ASP:CA	2:B:801:NAG:H82	2.29	0.63
1:C:482:THR:HG21	1:C:499:THR:CA	2.27	0.63
1:B:403:ASN:CB	3:B:902:NDG:C7	2.76	0.63
1:C:154:ASP:CA	2:C:801:NAG:H82	2.29	0.63
1:A:364:ILE:O	1:A:364:ILE:CD1	2.46	0.63
1:A:87:PRO:CD	1:B:89:GLU:HB2	2.22	0.63
1:B:524:VAL:HG23	2:B:904:NAG:C8	2.29	0.63
1:C:22:VAL:HG22	1:C:23:GLN:N	2.14	0.63
1:C:469:TYR:CE1	1:C:470:PRO:HD2	2.34	0.63
1:A:40:GLY:H	1:C:79:HIS:HD1	1.47	0.62
1:A:504:LYS:NZ	1:A:531:SER:OG	2.31	0.62
1:A:154:ASP:CA	2:A:801:NAG:H82	2.29	0.62
2:A:904:NAG:O7	2:A:904:NAG:C3	2.45	0.62
1:B:142:LEU:HB3	1:B:196:LEU:HA	1.80	0.62
1:B:469:TYR:CD2	1:B:470:PRO:CD	2.81	0.62
1:C:127:VAL:HG22	1:C:128:MET:N	2.14	0.62
1:A:22:VAL:HG22	1:A:23:GLN:N	2.14	0.62
1:A:39:THR:CB	1:C:89:GLU:O	2.46	0.62
1:C:147:SER:OG	1:C:167:ARG:HG3	1.99	0.62
1:C:486:GLU:O	1:C:494:MET:CA	2.46	0.62
1:B:482:THR:HG22	1:B:499:THR:N	2.13	0.62
1:C:446:THR:CG2	1:C:539:CYS:SG	2.86	0.62
1:A:371:ILE:HG22	1:A:372:GLY:N	2.14	0.62
1:A:524:VAL:HG23	2:A:904:NAG:C8	2.29	0.62
1:A:31:PHE:CG	1:B:93:GLU:OE2	2.52	0.62
1:A:374:ASP:O	1:A:375:PRO:O	2.17	0.62
1:B:343:GLU:HB3	1:B:433:VAL:CG2	2.28	0.62
1:B:368:SER:HG	1:B:370:PHE:HE1	1.47	0.62
1:B:81:VAL:CA	1:C:1:ASP:C	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ILE:HG12	1:A:425:THR:HG23	1.80	0.62
1:A:440:PRO:HD3	1:A:522:LEU:HD12	1.78	0.62
1:C:374:ASP:O	1:C:375:PRO:O	2.17	0.62
1:A:44:ASP:O	1:C:38:ILE:CA	2.44	0.62
1:A:411:LEU:HD22	1:A:421:THR:HG23	1.81	0.62
1:B:147:SER:OG	1:B:167:ARG:HG3	1.99	0.62
1:B:265:GLU:HB3	1:B:268:PHE:CE2	2.31	0.62
1:B:517:GLN:C	1:B:519:ASN:N	2.47	0.62
1:C:486:GLU:O	1:C:495:LEU:N	2.31	0.62
1:B:222:ASP:O	1:B:222:ASP:CG	2.32	0.62
1:B:486:GLU:O	1:B:495:LEU:N	2.32	0.62
1:B:508:SER:HB3	1:B:526:ASN:OD1	2.00	0.62
1:C:343:GLU:HB3	1:C:433:VAL:CG2	2.28	0.62
1:A:508:SER:HB3	1:A:526:ASN:OD1	2.00	0.62
1:A:227:THR:CG2	2:A:807:NAG:C7	2.76	0.62
1:B:518:ASN:O	1:B:520:PRO:CD	2.46	0.62
1:C:524:VAL:HG23	2:C:904:NAG:C8	2.29	0.62
1:A:524:VAL:CG2	2:A:904:NAG:C8	2.78	0.61
1:B:411:LEU:HD22	1:B:421:THR:HG23	1.81	0.61
1:C:403:ASN:O	1:C:405:THR:N	2.33	0.61
1:B:449:ASP:H	1:B:532:CYS:CB	2.12	0.61
1:B:81:VAL:CA	1:C:2:TRP:CA	2.76	0.61
1:C:524:VAL:CG2	2:C:904:NAG:C8	2.78	0.61
1:A:221:PHE:CE1	1:A:315:SER:O	2.45	0.61
1:B:212:THR:HG22	1:B:213:ASP:N	2.15	0.61
1:A:181:ARG:NE	1:A:213:ASP:OD1	2.34	0.61
1:A:403:ASN:O	1:A:405:THR:N	2.33	0.61
1:B:181:ARG:NE	1:B:213:ASP:OD1	2.34	0.61
1:B:83:GLU:CA	1:C:2:TRP:CH2	2.65	0.61
1:B:524:VAL:CG2	2:B:904:NAG:C8	2.78	0.61
1:C:154:ASP:O	1:C:155:PRO:C	2.36	0.61
1:C:181:ARG:NE	1:C:213:ASP:OD1	2.34	0.61
1:C:235:ILE:HG12	1:C:287:GLY:HA2	1.82	0.61
1:B:68:ARG:HD3	1:B:100:ASP:HA	1.82	0.61
1:B:379:LEU:HD23	1:B:379:LEU:H	1.66	0.61
1:B:127:VAL:HG22	1:B:128:MET:N	2.14	0.61
1:B:469:TYR:CE1	1:B:470:PRO:HD2	2.34	0.61
1:B:374:ASP:O	1:B:375:PRO:O	2.17	0.61
1:A:89:GLU:CD	1:B:3:VAL:HG13	2.20	0.61
1:A:469:TYR:CE1	1:A:470:PRO:HD2	2.34	0.61
1:B:154:ASP:O	1:B:155:PRO:C	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LEU:O	1:B:479:SER:HB3	2.01	0.61
1:C:27:ASN:C	1:C:27:ASN:ND2	2.46	0.61
1:A:415:ASP:OD1	1:A:416:GLY:N	2.27	0.61
2:B:805:NAG:C6	2:B:806:NAG:C7	2.74	0.61
1:C:482:THR:HG22	1:C:499:THR:N	2.13	0.61
1:C:212:THR:HG22	1:C:213:ASP:N	2.15	0.61
1:C:68:ARG:HD3	1:C:100:ASP:HA	1.82	0.61
1:A:265:GLU:HB3	1:A:268:PHE:CE2	2.31	0.60
1:C:189:LEU:HD23	1:C:189:LEU:N	2.16	0.60
1:C:508:SER:HB3	1:C:526:ASN:OD1	2.00	0.60
1:A:379:LEU:H	1:A:379:LEU:HD23	1.66	0.60
1:B:403:ASN:O	1:B:405:THR:N	2.33	0.60
1:C:517:GLN:C	1:C:519:ASN:N	2.46	0.60
1:A:68:ARG:HD3	1:A:100:ASP:HA	1.82	0.60
1:A:371:ILE:CG2	1:A:372:GLY:H	2.13	0.60
1:B:371:ILE:CG2	1:B:372:GLY:H	2.13	0.60
1:B:30:ARG:HH12	1:C:25:LYS:HG2	1.59	0.60
1:C:379:LEU:HD23	1:C:379:LEU:H	1.66	0.60
1:A:403:ASN:CB	3:A:902:NDG:C7	2.76	0.60
1:B:239:VAL:HG13	1:B:240:GLN:H	1.67	0.60
1:B:415:ASP:OD1	1:B:416:GLY:N	2.27	0.60
1:B:396:ARG:NH2	1:B:464:ILE:HG21	2.17	0.60
1:A:232:GLU:CG	1:A:290:PHE:N	2.64	0.60
1:C:475:LEU:O	1:C:479:SER:HB3	2.01	0.60
1:A:212:THR:HG22	1:A:213:ASP:N	2.15	0.60
1:C:371:ILE:CG2	1:C:372:GLY:H	2.13	0.60
1:A:336:VAL:HB	1:A:426:LEU:HD23	1.84	0.60
1:B:86:SER:CB	1:C:3:VAL:CA	2.79	0.60
1:C:227:THR:CG2	2:C:807:NAG:C7	2.76	0.60
1:A:154:ASP:O	1:A:155:PRO:C	2.36	0.60
1:A:475:LEU:O	1:A:479:SER:HB3	2.01	0.60
1:C:146:LEU:HA	1:C:194:THR:O	2.02	0.60
1:B:116:SER:HA	1:B:210:GLN:O	2.02	0.60
1:A:514:SER:HA	1:A:517:GLN:O	2.02	0.60
1:C:116:SER:HA	1:C:210:GLN:O	2.02	0.60
1:A:155:PRO:C	1:A:157:GLU:N	2.56	0.59
1:B:81:VAL:C	1:C:2:TRP:CB	2.70	0.59
1:A:116:SER:HA	1:A:210:GLN:O	2.02	0.59
1:B:447:MET:HB2	1:B:529:VAL:HG22	1.84	0.59
1:B:189:LEU:N	1:B:189:LEU:HD23	2.17	0.59
1:A:189:LEU:HD23	1:A:189:LEU:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ARG:HH11	1:C:443:ARG:HG3	1.68	0.59
1:C:514:SER:HA	1:C:517:GLN:O	2.02	0.59
1:A:146:LEU:HA	1:A:194:THR:O	2.02	0.59
1:A:49:GLY:O	1:A:63:THR:HG21	2.02	0.59
1:B:232:GLU:CG	1:B:290:PHE:N	2.64	0.59
1:C:268:PHE:HA	1:C:285:ALA:HB3	1.85	0.59
1:A:239:VAL:HG13	1:A:240:GLN:H	1.67	0.59
1:B:367:LEU:CB	1:B:413:THR:O	2.51	0.59
1:C:518:ASN:O	1:C:520:PRO:CD	2.46	0.59
1:C:508:SER:HA	1:C:526:ASN:HA	1.84	0.59
1:B:221:PHE:HA	1:B:244:VAL:HG12	1.85	0.59
1:B:268:PHE:HA	1:B:285:ALA:HB3	1.85	0.59
1:B:38:ILE:HG22	1:B:53:ILE:HG22	1.85	0.59
1:C:309:SER:O	1:C:310:VAL:HG23	2.03	0.59
1:A:363:GLN:O	1:A:364:ILE:HG22	2.03	0.59
1:A:268:PHE:HA	1:A:285:ALA:HB3	1.85	0.59
1:A:286:LYS:O	1:A:287:GLY:O	2.21	0.59
1:A:38:ILE:HG22	1:A:53:ILE:HG22	1.85	0.59
1:A:154:ASP:CB	2:A:801:NAG:HN2	2.16	0.59
1:B:232:GLU:HG2	1:B:289:ASP:CA	2.33	0.59
1:B:299:GLN:C	1:B:300:ILE:HD12	2.24	0.59
1:A:473:VAL:HA	1:A:513:LEU:HD23	1.85	0.58
1:B:33:LYS:O	1:C:2:TRP:CD2	2.56	0.58
1:B:514:SER:HA	1:B:517:GLN:O	2.02	0.58
1:C:335:ALA:HB1	3:C:811:NDG:C6	2.33	0.58
1:B:473:VAL:HA	1:B:513:LEU:HD23	1.85	0.58
1:C:367:LEU:CB	1:C:413:THR:O	2.51	0.58
1:C:38:ILE:HG22	1:C:53:ILE:HG22	1.85	0.58
1:C:32:ASN:HD22	1:C:83:GLU:H	1.51	0.58
1:C:403:ASN:CB	3:C:902:NDG:C7	2.76	0.58
1:A:335:ALA:HB1	3:A:811:NDG:C6	2.33	0.58
1:B:195:ASP:CB	1:B:200:GLY:HA3	2.33	0.58
1:B:309:SER:O	1:B:310:VAL:HG23	2.03	0.58
1:B:443:ARG:HA	1:B:525:VAL:HG13	1.85	0.58
1:C:363:GLN:O	1:C:364:ILE:HG22	2.03	0.58
1:C:406:TYR:HB3	1:C:428:LEU:CD2	2.33	0.58
1:C:449:ASP:H	1:C:532:CYS:CB	2.12	0.58
1:C:447:MET:HB2	1:C:529:VAL:HG22	1.84	0.58
1:A:154:ASP:CB	1:A:155:PRO:CD	2.82	0.58
1:A:367:LEU:CB	1:A:413:THR:O	2.51	0.58
1:A:48:GLN:HG3	1:C:37:SER:CA	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:SER:HA	1:A:526:ASN:HA	1.84	0.58
1:B:146:LEU:HA	1:B:194:THR:O	2.02	0.58
1:C:473:VAL:HA	1:C:513:LEU:HD23	1.85	0.58
1:A:537:ILE:HG12	1:A:538:LYS:N	2.19	0.58
1:B:363:GLN:O	1:B:364:ILE:HG22	2.03	0.58
1:B:336:VAL:HB	1:B:426:LEU:HD23	1.84	0.58
1:C:232:GLU:HG2	1:C:289:ASP:CA	2.33	0.58
1:C:42:GLY:HA2	1:C:47:PRO:O	2.04	0.58
1:A:235:ILE:HG12	1:A:287:GLY:HA2	1.82	0.58
1:C:221:PHE:HA	1:C:244:VAL:HG12	1.85	0.58
1:C:232:GLU:CG	1:C:290:PHE:N	2.64	0.58
1:C:332:PHE:CD2	1:C:424:GLY:HA3	2.39	0.58
1:A:299:GLN:C	1:A:300:ILE:HD12	2.24	0.58
1:A:443:ARG:HA	1:A:525:VAL:HG13	1.85	0.58
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.67	0.58
1:C:195:ASP:CB	1:C:200:GLY:HA3	2.33	0.58
1:C:226:TYR:CE2	1:C:242:LEU:HD23	2.39	0.58
1:C:299:GLN:C	1:C:300:ILE:HD12	2.24	0.58
1:C:49:GLY:O	1:C:63:THR:HG21	2.02	0.58
1:A:221:PHE:HA	1:A:244:VAL:HG12	1.85	0.58
1:A:232:GLU:HG2	1:A:289:ASP:CA	2.33	0.58
1:B:332:PHE:CD2	1:B:424:GLY:HA3	2.39	0.58
1:B:154:ASP:CB	1:B:155:PRO:CD	2.82	0.58
1:B:406:TYR:HB3	1:B:428:LEU:CD2	2.33	0.58
1:B:42:GLY:HA2	1:B:47:PRO:O	2.04	0.58
1:B:49:GLY:O	1:B:63:THR:HG21	2.02	0.58
1:B:508:SER:HA	1:B:526:ASN:HA	1.84	0.58
1:C:239:VAL:HG13	1:C:240:GLN:H	1.67	0.58
1:C:240:GLN:HG3	1:C:241:ARG:N	2.19	0.58
1:C:537:ILE:HG12	1:C:538:LYS:N	2.19	0.58
1:A:309:SER:O	1:A:310:VAL:HG23	2.03	0.58
1:A:406:TYR:HB3	1:A:428:LEU:CD2	2.33	0.58
1:C:443:ARG:HA	1:C:525:VAL:HG13	1.85	0.58
1:C:154:ASP:CB	1:C:155:PRO:CD	2.82	0.57
1:C:286:LYS:O	1:C:287:GLY:O	2.21	0.57
1:A:48:GLN:NE2	1:C:37:SER:O	2.24	0.57
1:C:336:VAL:HB	1:C:426:LEU:HD23	1.84	0.57
1:A:447:MET:HB2	1:A:529:VAL:HG22	1.84	0.57
1:A:320:THR:CG2	2:A:807:NAG:C2	2.76	0.57
1:B:450:GLN:HB2	1:B:533:GLU:CA	2.26	0.57
1:A:45:ASN:CA	1:C:37:SER:N	2.56	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:TYR:HB3	1:C:428:LEU:HD21	1.86	0.57
1:A:332:PHE:CD2	1:A:424:GLY:HA3	2.39	0.57
1:B:286:LYS:O	1:B:287:GLY:O	2.21	0.57
1:A:330:PRO:HD3	1:A:414:ASP:HB2	1.86	0.57
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.67	0.57
1:A:505:GLY:HA2	1:A:529:VAL:H	1.69	0.57
1:B:226:TYR:CE2	1:B:242:LEU:HD23	2.39	0.57
1:A:222:ASP:N	1:A:243:SER:O	2.38	0.57
1:A:42:GLY:HA2	1:A:47:PRO:O	2.04	0.57
1:B:330:PRO:HD3	1:B:414:ASP:HB2	1.86	0.57
1:B:537:ILE:HG12	1:B:538:LYS:N	2.19	0.57
1:A:68:ARG:HG3	1:A:69:GLU:N	2.19	0.57
1:C:396:ARG:NH2	1:C:464:ILE:HG21	2.17	0.57
1:A:240:GLN:HG3	1:A:241:ARG:N	2.19	0.57
1:B:505:GLY:HA2	1:B:529:VAL:H	1.70	0.57
1:A:517:GLN:C	1:A:519:ASN:N	2.47	0.57
1:C:189:LEU:HD21	1:C:209:ILE:HD12	1.87	0.57
1:C:330:PRO:HD3	1:C:414:ASP:HB2	1.86	0.57
1:C:68:ARG:HG3	1:C:69:GLU:N	2.19	0.57
1:A:189:LEU:HD21	1:A:209:ILE:HD12	1.87	0.57
1:A:195:ASP:CB	1:A:200:GLY:HA3	2.33	0.57
1:C:108:PHE:CE1	1:C:203:VAL:HG23	2.40	0.57
1:A:369:TYR:HD1	1:A:383:LYS:O	1.88	0.57
1:B:222:ASP:N	1:B:243:SER:O	2.38	0.57
1:C:320:THR:CG2	2:C:807:NAG:C2	2.76	0.57
1:B:240:GLN:HG3	1:B:241:ARG:N	2.19	0.56
1:B:296:TYR:HB2	1:B:321:VAL:HB	1.86	0.56
1:B:336:VAL:HG12	1:B:338:ARG:HB2	1.87	0.56
1:B:82:SER:HB3	1:C:2:TRP:C	2.25	0.56
1:A:296:TYR:HB2	1:A:321:VAL:HB	1.86	0.56
1:A:449:ASP:H	1:A:532:CYS:CB	2.12	0.56
1:C:296:TYR:HB2	1:C:321:VAL:HB	1.86	0.56
1:C:369:TYR:HD1	1:C:383:LYS:O	1.88	0.56
1:C:393:ASN:C	1:C:394:LEU:HD12	2.25	0.56
1:C:505:GLY:HA2	1:C:529:VAL:H	1.70	0.56
1:C:155:PRO:N	2:C:801:NAG:H82	2.20	0.56
1:A:226:TYR:CE2	1:A:242:LEU:HD23	2.39	0.56
1:B:155:PRO:C	1:B:157:GLU:N	2.56	0.56
1:B:32:ASN:CG	1:B:33:LYS:N	2.59	0.56
1:B:378:TRP:O	1:B:391:ASN:HB2	2.06	0.56
1:C:222:ASP:N	1:C:243:SER:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:CE1	1:A:203:VAL:HG23	2.40	0.56
1:A:396:ARG:NH2	1:A:464:ILE:HG21	2.17	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:336:VAL:HG12	1:A:338:ARG:HB2	1.87	0.56
1:A:155:PRO:N	2:A:801:NAG:H82	2.20	0.56
1:B:108:PHE:CE1	1:B:203:VAL:HG23	2.40	0.56
1:B:118:ARG:HA	1:B:212:THR:HB	1.87	0.56
1:B:335:ALA:HB1	3:B:811:NDG:C6	2.33	0.56
1:A:48:GLN:NE2	1:C:53:ILE:HG22	2.20	0.56
1:B:154:ASP:CB	2:B:801:NAG:HN2	2.16	0.56
1:B:32:ASN:HD22	1:B:83:GLU:H	1.51	0.56
1:A:76:LEU:HA	1:C:87:PRO:HG2	1.88	0.56
1:B:189:LEU:HD21	1:B:209:ILE:HD12	1.87	0.56
1:B:393:ASN:C	1:B:394:LEU:HD12	2.25	0.56
1:B:86:SER:HB3	1:C:3:VAL:CA	2.36	0.56
1:C:32:ASN:CG	1:C:33:LYS:N	2.59	0.56
1:B:86:SER:CB	1:C:3:VAL:CB	2.79	0.56
1:B:259:TYR:O	1:B:260:LYS:HB3	2.05	0.56
1:B:30:ARG:CA	1:C:27:ASN:OD1	2.36	0.56
1:B:333:VAL:CG2	1:B:334:PRO:HD3	2.36	0.56
1:B:369:TYR:HD1	1:B:383:LYS:O	1.88	0.56
1:C:333:VAL:CG2	1:C:334:PRO:HD3	2.36	0.56
1:C:336:VAL:HG12	1:C:338:ARG:HB2	1.87	0.56
1:C:378:TRP:O	1:C:391:ASN:HB2	2.06	0.56
1:A:162:LEU:O	1:A:174:LEU:HD12	2.06	0.56
1:A:394:LEU:N	1:A:394:LEU:CD1	2.69	0.55
1:B:365:GLN:CG	1:B:365:GLN:O	2.54	0.55
1:B:155:PRO:N	2:B:801:NAG:H82	2.20	0.55
1:C:439:VAL:HG13	1:C:522:LEU:HD11	1.88	0.55
1:A:259:TYR:O	1:A:260:LYS:HB3	2.05	0.55
1:B:68:ARG:HG3	1:B:69:GLU:N	2.19	0.55
1:C:339:VAL:HG21	1:C:351:ILE:CG2	2.37	0.55
1:B:339:VAL:HG21	1:B:351:ILE:CG2	2.37	0.55
1:A:118:ARG:HA	1:A:212:THR:HB	1.87	0.55
1:A:393:ASN:C	1:A:394:LEU:HD12	2.25	0.55
1:A:459:ILE:HG21	1:A:471:TYR:CE2	2.42	0.55
1:A:32:ASN:HD22	1:A:83:GLU:H	1.51	0.55
1:B:272:THR:CG2	1:B:273:THR:H	2.19	0.55
1:A:339:VAL:HG21	1:A:351:ILE:CG2	2.36	0.55
1:A:406:TYR:HB3	1:A:428:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:TYR:HB3	1:B:428:LEU:HD21	1.87	0.55
1:C:155:PRO:HG2	2:C:801:NAG:O7	2.07	0.55
1:C:394:LEU:CD1	1:C:394:LEU:N	2.69	0.55
1:A:154:ASP:CG	1:A:155:PRO:CD	2.75	0.55
1:A:241:ARG:NE	1:A:281:ILE:HD12	2.22	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:B:278:ASN:HD22	1:B:278:ASN:N	2.05	0.55
1:C:117:VAL:O	1:C:211:ILE:HA	2.07	0.55
1:C:459:ILE:HG21	1:C:471:TYR:CE2	2.42	0.55
1:C:432:ASP:CG	1:C:464:ILE:CG2	2.74	0.55
1:C:403:ASN:HB2	3:C:902:NDG:H8C2	1.87	0.55
1:C:482:THR:HG21	1:C:499:THR:C	2.27	0.55
1:A:272:THR:CG2	1:A:273:THR:H	2.19	0.55
1:A:378:TRP:O	1:A:391:ASN:HB2	2.06	0.55
1:B:482:THR:HG21	1:B:499:THR:C	2.27	0.55
1:B:28:LYS:HB3	1:B:88:VAL:HG11	1.89	0.55
1:C:162:LEU:O	1:C:174:LEU:HD12	2.06	0.55
1:C:28:LYS:HB3	1:C:88:VAL:HG11	1.89	0.55
1:A:466:PRO:O	1:A:468:THR:N	2.40	0.55
1:A:155:PRO:HG2	2:A:801:NAG:O7	2.07	0.55
1:B:162:LEU:O	1:B:174:LEU:HD12	2.06	0.55
1:B:117:VAL:O	1:B:211:ILE:HA	2.07	0.55
1:C:226:TYR:O	1:C:227:THR:CG2	2.55	0.55
1:A:169:THR:OG1	1:A:171:VAL:HG23	2.07	0.55
1:A:41:GLN:CB	1:C:81:VAL:HG13	2.35	0.55
1:A:45:ASN:ND2	1:C:79:HIS:CA	2.40	0.55
1:B:226:TYR:O	1:B:227:THR:CG2	2.55	0.55
1:B:330:PRO:HB3	1:B:358:ASP:HB2	1.89	0.55
1:B:466:PRO:O	1:B:468:THR:N	2.40	0.55
1:B:75:VAL:O	1:B:76:LEU:HD23	2.07	0.55
1:C:154:ASP:CG	1:C:155:PRO:CD	2.75	0.55
1:C:259:TYR:O	1:C:260:LYS:HB3	2.05	0.55
1:C:363:GLN:C	1:C:364:ILE:CG2	2.75	0.55
1:A:333:VAL:CG2	1:A:334:PRO:HD3	2.36	0.54
1:B:419:VAL:CG1	1:B:420:GLY:N	2.70	0.54
1:A:226:TYR:HB2	1:A:319:VAL:HG22	1.90	0.54
1:B:438:PRO:HB2	1:B:513:LEU:HD12	1.89	0.54
1:C:268:PHE:N	1:C:268:PHE:CD2	2.75	0.54
1:A:226:TYR:O	1:A:227:THR:CG2	2.55	0.54
1:A:367:LEU:C	1:A:367:LEU:HD12	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:VAL:CG1	1:A:420:GLY:N	2.70	0.54
1:B:403:ASN:HB2	3:B:902:NDG:H8C2	1.87	0.54
1:A:49:GLY:HA3	1:C:44:ASP:OD2	2.05	0.54
1:A:84:ASN:ND2	1:B:77:SER:OG	2.41	0.54
1:B:363:GLN:C	1:B:364:ILE:CG2	2.75	0.54
1:B:155:PRO:HG2	2:B:801:NAG:O7	2.07	0.54
1:C:75:VAL:O	1:C:76:LEU:HD23	2.08	0.54
1:A:482:THR:HG21	1:A:499:THR:C	2.27	0.54
1:A:75:VAL:O	1:A:76:LEU:HD23	2.08	0.54
1:B:235:ILE:HG12	1:B:287:GLY:HA2	1.82	0.54
1:C:419:VAL:CG1	1:C:420:GLY:N	2.70	0.54
1:B:154:ASP:CG	1:B:155:PRO:CD	2.75	0.54
1:B:367:LEU:HD12	1:B:367:LEU:C	2.28	0.54
1:B:88:VAL:H	1:C:1:ASP:N	2.05	0.54
1:C:241:ARG:NE	1:C:281:ILE:HD12	2.22	0.54
1:C:154:ASP:CB	2:C:801:NAG:HN2	2.16	0.54
1:A:363:GLN:C	1:A:364:ILE:CG2	2.76	0.54
1:A:438:PRO:HB2	1:A:513:LEU:HD12	1.89	0.54
1:C:226:TYR:HB2	1:C:319:VAL:HG22	1.89	0.54
1:C:466:PRO:O	1:C:468:THR:N	2.40	0.54
1:A:371:ILE:HG23	1:A:372:GLY:H	1.73	0.54
1:B:439:VAL:HG13	1:B:522:LEU:HD11	1.88	0.54
1:B:432:ASP:CG	1:B:464:ILE:CG2	2.74	0.54
1:A:82:SER:OG	1:B:91:PRO:N	2.40	0.54
1:C:169:THR:OG1	1:C:171:VAL:HG23	2.07	0.54
1:C:490:LYS:O	1:C:490:LYS:HG2	2.08	0.54
1:A:154:ASP:C	2:A:801:NAG:C8	2.62	0.54
1:A:22:VAL:HG22	1:A:23:GLN:H	1.73	0.54
1:A:318:THR:CG2	2:A:806:NAG:H5	2.34	0.54
1:B:332:PHE:HD2	1:B:424:GLY:HA3	1.73	0.54
1:B:490:LYS:O	1:B:490:LYS:HG2	2.08	0.54
1:C:276:GLU:CG	1:C:277:SER:N	2.71	0.54
1:A:117:VAL:O	1:A:211:ILE:HA	2.07	0.54
1:B:459:ILE:HG21	1:B:471:TYR:CE2	2.42	0.54
1:C:332:PHE:HD2	1:C:424:GLY:HA3	1.73	0.54
1:C:438:PRO:HB2	1:C:513:LEU:HD12	1.89	0.54
1:B:84:ASN:HD22	1:C:5:PRO:HD3	1.73	0.54
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.23	0.53
1:A:84:ASN:ND2	1:B:79:HIS:CE1	2.76	0.53
1:A:373:ASN:HB3	1:A:409:ILE:H	1.74	0.53
1:A:28:LYS:HB3	1:A:88:VAL:HG11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:GLN:CB	1:B:532:CYS:O	2.56	0.53
1:C:272:THR:CG2	1:C:273:THR:H	2.19	0.53
1:C:371:ILE:HG23	1:C:372:GLY:H	1.73	0.53
1:C:458:THR:HG22	1:C:493:SER:HB3	1.90	0.53
1:A:330:PRO:HB3	1:A:358:ASP:HB2	1.89	0.53
1:B:249:MET:O	1:B:252:THR:HB	2.08	0.53
1:B:268:PHE:N	1:B:268:PHE:CD2	2.75	0.53
1:B:403:ASN:C	1:B:405:THR:H	2.12	0.53
1:B:458:THR:HG22	1:B:493:SER:HB3	1.90	0.53
1:A:48:GLN:HG3	1:C:37:SER:CB	2.37	0.53
1:B:252:THR:HG23	1:B:253:PRO:HD2	1.90	0.53
1:B:276:GLU:CG	1:B:277:SER:N	2.71	0.53
1:C:330:PRO:HB3	1:C:358:ASP:HB2	1.89	0.53
1:C:365:GLN:CG	1:C:365:GLN:O	2.54	0.53
1:C:318:THR:CG2	2:C:806:NAG:H5	2.34	0.53
1:A:369:TYR:O	1:A:383:LYS:HG2	2.09	0.53
1:A:450:GLN:CB	1:A:532:CYS:O	2.56	0.53
1:B:105:ARG:HG3	1:B:106:PRO:HD2	1.91	0.53
1:B:217:ASN:N	1:B:217:ASN:ND2	2.56	0.53
1:A:75:VAL:HG11	1:C:87:PRO:HD2	1.84	0.53
1:A:249:MET:O	1:A:252:THR:HB	2.09	0.53
1:A:522:LEU:CD2	1:A:523:THR:HB	2.26	0.53
1:A:533:GLU:OE2	1:A:533:GLU:HA	2.09	0.53
1:B:533:GLU:HA	1:B:533:GLU:OE2	2.09	0.53
1:C:105:ARG:HG3	1:C:106:PRO:HD2	1.91	0.53
1:C:249:MET:O	1:C:252:THR:HB	2.09	0.53
1:C:367:LEU:C	1:C:367:LEU:HD12	2.28	0.53
1:C:217:ASN:N	1:C:217:ASN:ND2	2.56	0.53
1:C:312:LEU:O	3:C:804:NDG:C8	2.57	0.53
1:C:31:PHE:CD2	1:C:32:ASN:HB2	2.44	0.53
1:C:482:THR:CG2	1:C:499:THR:CA	2.87	0.53
1:A:44:ASP:CB	1:C:77:SER:C	2.68	0.53
1:A:347:ARG:HG3	1:A:391:ASN:HA	1.91	0.53
1:A:88:VAL:HA	1:B:92:MET:CG	2.39	0.53
1:B:312:LEU:O	3:B:804:NDG:C8	2.57	0.53
1:C:252:THR:HG23	1:C:253:PRO:HD2	1.90	0.53
1:A:45:ASN:ND2	1:C:79:HIS:CB	2.69	0.53
1:A:276:GLU:CG	1:A:277:SER:N	2.71	0.53
1:A:242:LEU:O	1:A:279:GLN:HB3	2.09	0.53
1:A:458:THR:HG22	1:A:493:SER:HB3	1.91	0.53
1:B:169:THR:OG1	1:B:171:VAL:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:VAL:HG22	1:B:23:GLN:H	1.73	0.53
1:B:450:GLN:CB	1:B:533:GLU:HA	2.29	0.53
1:B:318:THR:CG2	2:B:806:NAG:H5	2.34	0.53
1:C:373:ASN:HB3	1:C:409:ILE:H	1.74	0.53
1:C:443:ARG:NH1	1:C:443:ARG:HG3	2.23	0.53
1:C:450:GLN:CB	1:C:532:CYS:O	2.56	0.53
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.91	0.53
1:A:367:LEU:HD13	1:A:412:VAL:HG23	1.91	0.53
1:A:512:LEU:HD11	1:A:519:ASN:HD21	1.74	0.53
1:B:367:LEU:HD13	1:B:412:VAL:HG23	1.91	0.53
1:B:352:ILE:CG1	1:B:388:VAL:HB	2.33	0.53
1:B:482:THR:O	1:B:482:THR:HG22	2.09	0.53
1:B:512:LEU:HD11	1:B:519:ASN:HD21	1.74	0.53
1:A:84:ASN:CG	1:B:77:SER:HG	2.12	0.53
1:C:512:LEU:HD11	1:C:519:ASN:HD21	1.74	0.53
1:B:226:TYR:HB2	1:B:319:VAL:HG22	1.89	0.52
1:B:242:LEU:O	1:B:279:GLN:HB3	2.09	0.52
1:B:426:LEU:HD13	1:B:426:LEU:O	2.10	0.52
1:C:242:LEU:O	1:C:279:GLN:HB3	2.09	0.52
1:C:268:PHE:C	1:C:285:ALA:HB3	2.30	0.52
1:C:403:ASN:C	1:C:405:THR:H	2.12	0.52
1:A:217:ASN:N	1:A:217:ASN:ND2	2.56	0.52
1:A:268:PHE:C	1:A:285:ALA:HB3	2.30	0.52
1:A:523:THR:CG2	1:A:524:VAL:H	1.94	0.52
1:A:312:LEU:O	3:A:804:NDG:C8	2.57	0.52
1:C:155:PRO:C	1:C:157:GLU:N	2.56	0.52
1:A:194:THR:HG22	1:A:195:ASP:N	2.25	0.52
1:B:194:THR:HG22	1:B:195:ASP:N	2.25	0.52
1:B:268:PHE:C	1:B:285:ALA:HB3	2.30	0.52
1:B:347:ARG:HG3	1:B:391:ASN:HA	1.91	0.52
1:C:22:VAL:HG22	1:C:23:GLN:H	1.73	0.52
1:A:403:ASN:C	1:A:405:THR:H	2.12	0.52
1:A:82:SER:O	1:B:90:GLU:OE2	2.25	0.52
1:C:227:THR:CG2	2:C:807:NAG:H83	2.32	0.52
1:B:227:THR:CG2	2:B:807:NAG:H83	2.32	0.52
1:C:369:TYR:O	1:C:383:LYS:HG2	2.09	0.52
1:B:86:SER:OG	1:C:4:ILE:CA	2.57	0.52
1:A:432:ASP:CG	1:A:464:ILE:CG2	2.74	0.52
1:B:373:ASN:HB3	1:B:409:ILE:H	1.74	0.52
1:B:89:GLU:N	1:C:1:ASP:H3	1.98	0.52
1:C:221:PHE:HB3	1:C:223:PRO:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ASN:N	1:C:278:ASN:HD22	2.05	0.52
1:C:28:LYS:CD	1:C:88:VAL:HG12	2.38	0.52
1:C:290:PHE:CE2	1:C:293:ARG:CB	2.92	0.52
1:C:347:ARG:HD2	1:C:392:GLY:N	2.25	0.52
1:C:367:LEU:HD13	1:C:412:VAL:HG23	1.91	0.52
1:C:533:GLU:OE2	1:C:533:GLU:HA	2.09	0.52
1:C:272:THR:CG2	2:C:803:NAG:HN2	2.23	0.52
1:A:252:THR:HG23	1:A:253:PRO:HD2	1.91	0.52
1:A:379:LEU:CD2	1:A:379:LEU:H	2.22	0.52
1:A:90:GLU:CB	1:B:2:TRP:CD1	2.92	0.52
1:B:369:TYR:O	1:B:383:LYS:HG2	2.09	0.52
1:B:396:ARG:CZ	1:B:432:ASP:HB2	2.40	0.52
1:C:138:ASN:HD22	1:C:138:ASN:C	2.13	0.52
1:A:31:PHE:CD2	1:A:32:ASN:HB2	2.44	0.52
1:A:33:LYS:HB3	1:A:83:GLU:CG	2.40	0.52
1:A:332:PHE:HD2	1:A:424:GLY:HA3	1.73	0.52
1:A:450:GLN:HB2	1:A:533:GLU:CA	2.26	0.52
1:B:155:PRO:CD	2:B:801:NAG:H82	2.40	0.52
1:B:88:VAL:CG2	1:C:2:TRP:O	2.47	0.52
1:A:403:ASN:HB2	3:A:902:NDG:H8C2	1.87	0.51
1:B:221:PHE:HB3	1:B:223:PRO:O	2.10	0.51
1:B:31:PHE:CD2	1:B:32:ASN:HB2	2.44	0.51
1:C:347:ARG:HG3	1:C:391:ASN:HA	1.91	0.51
1:C:505:GLY:O	1:C:506:ASP:OD1	2.28	0.51
1:A:45:ASN:ND2	1:C:79:HIS:HB3	2.25	0.51
1:A:41:GLN:CA	1:C:81:VAL:HG13	2.38	0.51
1:A:458:THR:HA	1:A:493:SER:HA	1.93	0.51
1:A:45:ASN:CG	1:C:79:HIS:CB	2.49	0.51
1:B:371:ILE:HG23	1:B:372:GLY:H	1.73	0.51
1:B:482:THR:CG2	1:B:499:THR:CA	2.87	0.51
1:C:450:GLN:CG	1:C:533:GLU:OE2	2.58	0.51
1:B:272:THR:CG2	2:B:803:NAG:HN2	2.23	0.51
1:B:8:LYS:N	1:B:8:LYS:CD	2.51	0.51
1:C:426:LEU:O	1:C:426:LEU:HD13	2.09	0.51
1:C:155:PRO:CD	2:C:801:NAG:H82	2.40	0.51
1:A:471:TYR:N	1:A:471:TYR:CD1	2.79	0.51
1:C:194:THR:HG22	1:C:195:ASP:N	2.25	0.51
1:C:336:VAL:O	1:C:426:LEU:HD22	2.10	0.51
1:A:428:LEU:O	1:A:428:LEU:HD23	2.11	0.51
1:B:333:VAL:CB	1:B:334:PRO:CD	2.88	0.51
1:B:514:SER:HB3	1:B:517:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:GLN:HB2	1:C:533:GLU:CA	2.26	0.51
1:A:426:LEU:HD13	1:A:426:LEU:O	2.10	0.51
1:A:482:THR:CG2	1:A:499:THR:CA	2.87	0.51
1:A:505:GLY:O	1:A:506:ASP:OD1	2.28	0.51
1:A:75:VAL:C	1:C:87:PRO:CG	2.53	0.51
1:C:151:LEU:HD12	1:C:190:THR:O	2.11	0.51
1:C:352:ILE:HG13	1:C:388:VAL:CB	2.33	0.51
1:C:396:ARG:CZ	1:C:432:ASP:HB2	2.41	0.51
1:C:514:SER:HB3	1:C:517:GLN:O	2.10	0.51
1:A:155:PRO:CD	2:A:801:NAG:H82	2.40	0.51
1:A:151:LEU:HD12	1:A:190:THR:O	2.11	0.51
1:A:336:VAL:O	1:A:426:LEU:HD22	2.10	0.51
1:A:38:ILE:O	1:C:91:PRO:HB3	1.94	0.51
1:A:514:SER:HB3	1:A:517:GLN:O	2.10	0.51
1:B:450:GLN:CG	1:B:533:GLU:OE2	2.58	0.51
1:B:471:TYR:CD1	1:B:471:TYR:N	2.79	0.51
1:B:505:GLY:O	1:B:506:ASP:OD1	2.28	0.51
1:B:522:LEU:CD2	1:B:523:THR:HB	2.26	0.51
2:B:809:NAG:H61	2:B:810:NAG:C6	2.39	0.51
1:C:297:VAL:CG2	2:C:807:NAG:H62	2.41	0.51
1:A:365:GLN:CG	1:A:365:GLN:O	2.54	0.51
1:B:154:ASP:C	2:B:801:NAG:C8	2.62	0.51
1:B:81:VAL:HA	1:C:2:TRP:CA	2.41	0.51
1:A:272:THR:CG2	2:A:803:NAG:HN2	2.23	0.51
1:B:142:LEU:O	1:B:196:LEU:HD23	2.11	0.51
1:B:458:THR:HG22	1:B:493:SER:CB	2.41	0.51
1:C:33:LYS:HB3	1:C:83:GLU:CG	2.40	0.51
1:C:80:ALA:O	1:C:88:VAL:HG23	2.11	0.51
1:A:142:LEU:O	1:A:196:LEU:HD23	2.11	0.51
1:A:297:VAL:CG2	2:A:807:NAG:H62	2.41	0.51
1:C:142:LEU:O	1:C:196:LEU:HD23	2.11	0.51
1:C:217:ASN:N	1:C:217:ASN:HD22	2.09	0.51
1:B:138:ASN:C	1:B:138:ASN:HD22	2.13	0.50
1:B:382:ASN:OD1	1:B:385:ASN:N	2.45	0.50
1:B:397:GLU:OE1	1:B:397:GLU:N	2.44	0.50
1:B:336:VAL:O	1:B:426:LEU:HD22	2.10	0.50
1:C:458:THR:HG22	1:C:493:SER:CB	2.42	0.50
1:A:138:ASN:C	1:A:138:ASN:HD22	2.13	0.50
1:A:221:PHE:HB3	1:A:223:PRO:O	2.10	0.50
1:A:347:ARG:HD2	1:A:392:GLY:N	2.25	0.50
1:A:450:GLN:CG	1:A:533:GLU:OE2	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LEU:HD21	1:A:509:ILE:CD1	2.38	0.50
1:A:449:ASP:CB	1:A:532:CYS:H	2.22	0.50
1:B:217:ASN:N	1:B:217:ASN:HD22	2.09	0.50
1:B:428:LEU:HD23	1:B:428:LEU:O	2.11	0.50
1:B:154:ASP:O	2:B:801:NAG:C8	2.60	0.50
1:B:88:VAL:HG22	1:C:2:TRP:O	1.63	0.50
1:C:154:ASP:O	2:C:801:NAG:C8	2.60	0.50
1:A:396:ARG:CZ	1:A:432:ASP:HB2	2.41	0.50
1:A:155:PRO:HG2	2:A:801:NAG:C7	2.42	0.50
1:B:261:ILE:HD11	1:B:264:ASN:HD22	1.77	0.50
1:B:82:SER:CB	1:C:2:TRP:CA	2.89	0.50
1:A:154:ASP:O	2:A:801:NAG:C8	2.60	0.50
1:B:368:SER:OG	1:B:370:PHE:HE1	1.94	0.50
1:B:28:LYS:CD	1:B:88:VAL:HG12	2.38	0.50
1:C:338:ARG:HB3	1:C:339:VAL:HG22	1.92	0.50
1:A:234:GLU:HB2	1:A:235:ILE:HG22	1.93	0.50
1:A:278:ASN:N	1:A:278:ASN:HD22	2.05	0.50
1:B:347:ARG:HD2	1:B:392:GLY:N	2.25	0.50
1:C:458:THR:HA	1:C:493:SER:HA	1.93	0.50
1:C:471:TYR:N	1:C:471:TYR:CD1	2.79	0.50
1:A:457:LEU:HD23	1:A:494:MET:SD	2.52	0.50
1:A:449:ASP:CB	1:A:532:CYS:N	2.74	0.50
1:B:423:THR:HB	2:B:810:NAG:H83	1.94	0.50
1:B:419:VAL:HG22	2:B:809:NAG:H81	1.93	0.50
1:C:155:PRO:O	1:C:157:GLU:N	2.43	0.50
1:C:276:GLU:HG3	1:C:277:SER:N	2.25	0.50
1:C:522:LEU:CD2	1:C:523:THR:HB	2.26	0.50
1:C:419:VAL:HG22	2:C:809:NAG:H81	1.93	0.50
1:A:216:ASP:HB2	1:A:217:ASN:ND2	2.27	0.50
1:A:84:ASN:CB	1:B:79:HIS:CE1	2.62	0.50
1:B:151:LEU:HD12	1:B:190:THR:O	2.11	0.50
1:B:276:GLU:HG3	1:B:277:SER:N	2.25	0.50
1:B:338:ARG:HB3	1:B:339:VAL:HG22	1.92	0.50
1:B:457:LEU:HD23	1:B:494:MET:SD	2.52	0.50
1:B:297:VAL:CG2	2:B:807:NAG:H62	2.41	0.50
1:C:109:THR:HG22	1:C:110:GLN:HG3	1.94	0.50
1:C:234:GLU:HB2	1:C:235:ILE:HG22	1.93	0.50
1:C:333:VAL:CB	1:C:334:PRO:CD	2.88	0.50
1:C:363:GLN:C	1:C:364:ILE:HG23	2.32	0.50
1:C:373:ASN:ND2	1:C:374:ASP:OD1	2.45	0.50
1:C:382:ASN:OD1	1:C:385:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:ASP:CB	1:C:464:ILE:CG2	2.89	0.50
1:A:186:GLU:OE1	2:A:801:NAG:C6	2.59	0.50
1:A:39:THR:OG1	1:C:89:GLU:C	2.47	0.50
1:A:458:THR:HG22	1:A:493:SER:CB	2.42	0.50
1:A:11:GLU:OE2	1:A:69:GLU:OE1	2.30	0.50
1:B:241:ARG:NE	1:B:281:ILE:HD12	2.22	0.50
1:B:363:GLN:C	1:B:364:ILE:HG23	2.32	0.50
1:B:432:ASP:CB	1:B:464:ILE:CG2	2.89	0.50
1:B:458:THR:HA	1:B:493:SER:HA	1.93	0.50
2:B:807:NAG:H3	2:B:807:NAG:O7	2.11	0.50
1:C:241:ARG:HE	1:C:281:ILE:CD1	2.24	0.50
1:C:428:LEU:HD23	1:C:428:LEU:O	2.11	0.50
1:C:449:ASP:CB	1:C:532:CYS:H	2.22	0.50
1:A:217:ASN:HD22	1:A:217:ASN:N	2.10	0.50
1:A:266:GLY:N	1:A:268:PHE:CE2	2.76	0.50
1:A:382:ASN:OD1	1:A:385:ASN:N	2.45	0.50
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.24	0.50
1:A:80:ALA:O	1:A:88:VAL:HG23	2.11	0.50
1:A:335:ALA:CB	3:A:811:NDG:C6	2.90	0.50
1:C:109:THR:HG22	1:C:110:GLN:CG	2.42	0.50
1:C:327:ASN:OD1	1:C:360:ASP:OD1	2.30	0.50
1:A:338:ARG:HB3	1:A:339:VAL:HG22	1.92	0.49
1:B:109:THR:HG22	1:B:110:GLN:HG3	1.94	0.49
1:B:155:PRO:HG2	2:B:801:NAG:C7	2.42	0.49
1:B:27:ASN:C	1:B:29:ASP:H	2.15	0.49
1:B:496:LEU:HD21	1:B:509:ILE:CD1	2.38	0.49
1:C:155:PRO:HG2	2:C:801:NAG:C7	2.42	0.49
1:C:27:ASN:C	1:C:29:ASP:H	2.16	0.49
1:C:457:LEU:HD23	1:C:494:MET:SD	2.52	0.49
1:A:44:ASP:CG	1:C:79:HIS:ND1	2.63	0.49
1:A:27:ASN:C	1:A:29:ASP:H	2.15	0.49
1:A:419:VAL:HG22	2:A:809:NAG:H81	1.94	0.49
1:B:151:LEU:H	1:B:151:LEU:HD12	1.78	0.49
1:C:216:ASP:HB2	1:C:217:ASN:ND2	2.27	0.49
1:C:397:GLU:N	1:C:397:GLU:OE1	2.44	0.49
1:A:155:PRO:O	1:A:157:GLU:N	2.43	0.49
1:A:432:ASP:CB	1:A:464:ILE:CG2	2.89	0.49
1:A:76:LEU:O	1:A:94:ILE:N	2.44	0.49
1:B:252:THR:CG2	1:B:253:PRO:HD2	2.43	0.49
1:B:273:THR:H	2:B:803:NAG:HN2	1.61	0.49
1:A:352:ILE:HG13	1:A:388:VAL:CB	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:THR:H	2:A:803:NAG:HN2	1.60	0.49
1:B:216:ASP:HB2	1:B:217:ASN:ND2	2.27	0.49
1:B:402:LYS:C	1:B:403:ASN:O	2.46	0.49
1:B:76:LEU:O	1:B:94:ILE:N	2.44	0.49
1:A:82:SER:H	1:B:90:GLU:C	2.15	0.49
1:C:252:THR:CG2	1:C:253:PRO:HD2	2.43	0.49
1:A:261:ILE:HD11	1:A:264:ASN:HD22	1.77	0.49
1:A:290:PHE:CE2	1:A:293:ARG:CB	2.92	0.49
1:A:327:ASN:OD1	1:A:360:ASP:OD1	2.30	0.49
1:A:363:GLN:C	1:A:364:ILE:HG23	2.32	0.49
1:A:368:SER:OG	1:A:370:PHE:HE1	1.94	0.49
1:A:512:LEU:HD11	1:A:519:ASN:ND2	2.28	0.49
1:B:234:GLU:HB2	1:B:235:ILE:HG22	1.93	0.49
1:C:367:LEU:HB2	1:C:413:THR:O	2.12	0.49
1:A:282:LEU:CD2	1:A:283:THR:N	2.76	0.49
1:A:482:THR:O	1:A:482:THR:HG22	2.09	0.49
1:C:76:LEU:O	1:C:94:ILE:N	2.44	0.49
1:C:273:THR:H	2:C:803:NAG:HN2	1.61	0.49
1:A:352:ILE:CG1	1:A:388:VAL:HB	2.33	0.49
1:A:451:ASN:O	1:A:534:GLY:CA	2.60	0.49
2:A:807:NAG:H3	2:A:807:NAG:O7	2.11	0.49
1:B:281:ILE:O	1:B:281:ILE:HG23	2.13	0.49
1:B:282:LEU:CD2	1:B:283:THR:N	2.76	0.49
1:B:373:ASN:ND2	1:B:374:ASP:OD1	2.45	0.49
1:B:320:THR:CG2	2:B:807:NAG:C2	2.76	0.49
1:C:226:TYR:C	1:C:227:THR:HG23	2.33	0.49
1:C:310:VAL:HG12	1:C:312:LEU:HG	1.95	0.49
1:C:512:LEU:HD11	1:C:519:ASN:ND2	2.28	0.49
1:A:268:PHE:CD2	1:A:268:PHE:N	2.75	0.49
1:A:68:ARG:HD3	1:A:100:ASP:CA	2.43	0.49
1:B:109:THR:HG22	1:B:110:GLN:CG	2.42	0.49
1:B:192:GLN:HA	1:B:203:VAL:O	2.13	0.49
2:B:809:NAG:H62	2:B:810:NAG:O6	2.13	0.49
1:B:82:SER:HB3	1:C:2:TRP:CA	2.42	0.49
1:C:192:GLN:HA	1:C:203:VAL:O	2.13	0.49
1:C:336:VAL:CG1	1:C:338:ARG:HB2	2.43	0.49
1:A:151:LEU:HD12	1:A:151:LEU:H	1.78	0.49
1:A:226:TYR:C	1:A:227:THR:HG23	2.33	0.49
1:B:335:ALA:CB	3:B:811:NDG:C6	2.90	0.49
1:B:33:LYS:HB3	1:B:83:GLU:CG	2.40	0.49
1:B:327:ASN:OD1	1:B:360:ASP:OD1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLU:OE2	1:B:69:GLU:OE1	2.30	0.49
1:C:151:LEU:H	1:C:151:LEU:HD12	1.78	0.49
1:C:281:ILE:HG23	1:C:281:ILE:O	2.13	0.49
1:C:449:ASP:CB	1:C:532:CYS:N	2.74	0.49
2:C:812:NAG:O7	2:C:812:NAG:C1	2.60	0.49
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.95	0.49
1:A:336:VAL:CG1	1:A:338:ARG:HB2	2.43	0.49
1:A:397:GLU:OE1	1:A:397:GLU:N	2.45	0.49
1:A:423:THR:HB	2:A:810:NAG:H83	1.94	0.49
1:A:432:ASP:CB	1:A:464:ILE:HG21	2.43	0.49
1:B:310:VAL:HG12	1:B:312:LEU:HG	1.95	0.49
1:C:224:LYS:HE3	2:C:806:NAG:H82	1.95	0.49
1:A:365:GLN:HA	1:A:416:GLY:HA3	1.95	0.48
2:A:809:NAG:H62	2:A:810:NAG:O6	2.13	0.48
1:A:8:LYS:CD	1:A:8:LYS:N	2.51	0.48
1:B:154:ASP:CG	1:B:155:PRO:HD2	2.33	0.48
1:B:186:GLU:OE1	2:B:801:NAG:C6	2.59	0.48
1:B:512:LEU:HD11	1:B:519:ASN:ND2	2.28	0.48
1:C:266:GLY:N	1:C:268:PHE:CE2	2.76	0.48
1:C:68:ARG:HD3	1:C:100:ASP:CA	2.43	0.48
1:A:367:LEU:HD13	1:A:412:VAL:CG2	2.43	0.48
1:A:41:GLN:HA	1:A:45:ASN:HB2	1.95	0.48
1:B:266:GLY:N	1:B:268:PHE:CE2	2.76	0.48
1:B:41:GLN:HA	1:B:45:ASN:HB2	1.96	0.48
1:C:368:SER:OG	1:C:370:PHE:HE1	1.94	0.48
1:C:371:ILE:HA	1:C:371:ILE:HD12	1.65	0.48
1:C:365:GLN:HA	1:C:416:GLY:HA3	1.95	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:224:LYS:CE	2:A:806:NAG:C8	2.91	0.48
1:A:224:LYS:HE3	2:A:806:NAG:H82	1.95	0.48
1:A:89:GLU:OE2	1:B:3:VAL:CG1	2.55	0.48
1:B:336:VAL:CG1	1:B:338:ARG:HB2	2.43	0.48
1:B:224:LYS:CE	2:B:806:NAG:C8	2.91	0.48
1:C:250:PRO:O	1:C:255:TRP:CE3	2.66	0.48
1:C:261:ILE:HD11	1:C:264:ASN:HD22	1.77	0.48
2:C:807:NAG:H3	2:C:807:NAG:O7	2.11	0.48
1:A:43:ALA:HB3	1:C:79:HIS:HD1	1.63	0.48
1:B:432:ASP:CB	1:B:464:ILE:HG21	2.43	0.48
1:C:186:GLU:OE1	2:C:801:NAG:C6	2.59	0.48
1:C:119:GLU:OE2	1:C:216:ASP:OD1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PRO:O	1:A:255:TRP:CE3	2.66	0.48
1:C:11:GLU:OE2	1:C:69:GLU:OE1	2.30	0.48
1:A:373:ASN:ND2	1:A:374:ASP:OD1	2.45	0.48
1:B:151:LEU:O	1:B:152:LYS:HB2	2.13	0.48
1:C:41:GLN:HA	1:C:45:ASN:HB2	1.95	0.48
1:C:432:ASP:CB	1:C:464:ILE:HG21	2.43	0.48
1:A:109:THR:HG22	1:A:110:GLN:CG	2.42	0.48
1:A:109:THR:HG22	1:A:110:GLN:HG3	1.94	0.48
1:A:281:ILE:HG23	1:A:281:ILE:O	2.13	0.48
1:B:155:PRO:O	1:B:157:GLU:N	2.43	0.48
1:B:119:GLU:OE2	1:B:216:ASP:OD1	2.32	0.48
1:B:352:ILE:HG13	1:B:388:VAL:CB	2.33	0.48
1:B:367:LEU:HD13	1:B:412:VAL:CG2	2.43	0.48
1:A:192:GLN:HA	1:A:203:VAL:O	2.13	0.48
1:A:252:THR:CG2	1:A:253:PRO:HD2	2.43	0.48
1:A:333:VAL:CB	1:A:334:PRO:CD	2.88	0.48
1:B:150:ILE:HD11	1:B:165:ILE:HB	1.96	0.48
1:B:367:LEU:HB2	1:B:413:THR:O	2.12	0.48
1:B:67:ASP:OD2	1:B:69:GLU:HB2	2.13	0.48
2:B:812:NAG:O7	2:B:812:NAG:C1	2.60	0.48
1:C:154:ASP:CG	1:C:155:PRO:HD2	2.33	0.48
1:C:224:LYS:CE	2:C:806:NAG:C8	2.91	0.48
1:A:46:PRO:CB	1:C:35:TYR:CD2	2.72	0.48
1:A:151:LEU:O	1:A:152:LYS:HB2	2.13	0.48
1:A:79:HIS:HD1	1:A:91:PRO:HG3	1.79	0.48
1:B:226:TYR:C	1:B:227:THR:HG23	2.33	0.48
1:C:366:LYS:HG2	1:C:367:LEU:H	1.75	0.48
1:C:514:SER:CA	1:C:517:GLN:O	2.62	0.48
1:A:367:LEU:HB2	1:A:413:THR:O	2.12	0.48
1:A:48:GLN:CG	1:C:37:SER:CB	2.92	0.48
1:B:250:PRO:O	1:B:255:TRP:CE3	2.66	0.48
1:B:225:THR:HA	1:B:318:THR:O	2.14	0.48
1:B:365:GLN:HA	1:B:416:GLY:HA3	1.95	0.48
1:C:150:ILE:HD11	1:C:165:ILE:HB	1.96	0.48
1:C:418:SER:O	1:C:419:VAL:HG23	2.14	0.48
1:C:482:THR:O	1:C:482:THR:HG22	2.08	0.48
1:C:335:ALA:CB	3:C:811:NDG:C6	2.90	0.48
1:A:366:LYS:HG2	1:A:367:LEU:H	1.75	0.47
2:A:809:NAG:H61	2:A:810:NAG:C6	2.39	0.47
1:B:68:ARG:HD3	1:B:100:ASP:CA	2.43	0.47
1:B:81:VAL:HA	1:C:2:TRP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ASP:OD2	1:C:69:GLU:HB2	2.13	0.47
1:C:8:LYS:CD	1:C:8:LYS:N	2.51	0.47
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.32	0.47
1:A:246:ASP:C	1:A:247:LEU:HD12	2.35	0.47
1:A:67:ASP:OD2	1:A:69:GLU:HB2	2.13	0.47
1:B:224:LYS:HE3	2:B:806:NAG:H82	1.95	0.47
1:B:418:SER:O	1:B:419:VAL:HG23	2.14	0.47
2:B:809:NAG:C6	2:B:810:NAG:C6	2.92	0.47
1:C:451:ASN:O	1:C:534:GLY:CA	2.60	0.47
2:C:809:NAG:C6	2:C:810:NAG:C6	2.92	0.47
1:A:226:TYR:O	1:A:227:THR:HG23	2.15	0.47
1:A:448:CYS:SG	1:A:537:ILE:CG2	3.01	0.47
1:A:450:GLN:CB	1:A:533:GLU:HA	2.29	0.47
1:A:537:ILE:CG1	1:A:538:LYS:N	2.77	0.47
1:A:82:SER:C	1:B:90:GLU:HG3	2.21	0.47
1:B:537:ILE:CG1	1:B:538:LYS:N	2.77	0.47
1:C:151:LEU:O	1:C:152:LYS:HB2	2.13	0.47
1:A:514:SER:HG	1:A:519:ASN:HA	1.79	0.47
2:A:809:NAG:C6	2:A:810:NAG:C6	2.92	0.47
1:B:300:ILE:N	1:B:300:ILE:HD12	2.29	0.47
1:C:226:TYR:O	1:C:227:THR:HG23	2.15	0.47
1:A:76:LEU:N	1:C:87:PRO:HG2	2.26	0.47
1:A:77:SER:OG	1:C:90:GLU:OE1	2.30	0.47
1:A:227:THR:CG2	2:A:807:NAG:H83	2.32	0.47
1:B:514:SER:CA	1:B:517:GLN:O	2.62	0.47
1:C:261:ILE:CD1	1:C:264:ASN:ND2	2.77	0.47
1:C:367:LEU:HD13	1:C:412:VAL:CG2	2.43	0.47
1:A:117:VAL:O	1:A:212:THR:N	2.46	0.47
1:B:268:PHE:CA	1:B:285:ALA:HB3	2.45	0.47
1:B:301:THR:CG2	1:B:316:THR:HG23	2.45	0.47
1:C:320:THR:CB	2:C:807:NAG:N2	2.78	0.47
1:A:261:ILE:CD1	1:A:264:ASN:ND2	2.77	0.47
1:A:301:THR:CG2	1:A:316:THR:HG23	2.45	0.47
1:A:402:LYS:C	1:A:403:ASN:O	2.46	0.47
1:A:514:SER:CA	1:A:517:GLN:O	2.62	0.47
2:A:812:NAG:C1	2:A:812:NAG:O7	2.60	0.47
1:B:261:ILE:CD1	1:B:264:ASN:ND2	2.77	0.47
1:C:23:GLN:HB2	1:C:59:TRP:CE3	2.50	0.47
1:C:50:VAL:HB	1:C:51:PHE:CD1	2.50	0.47
1:A:225:THR:HA	1:A:318:THR:O	2.14	0.47
1:A:300:ILE:HD12	1:A:300:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:PHE:HE1	1:B:203:VAL:HG23	1.80	0.47
1:B:246:ASP:C	1:B:247:LEU:HD12	2.35	0.47
1:B:449:ASP:CB	1:B:532:CYS:N	2.74	0.47
1:B:80:ALA:HB3	1:C:1:ASP:CA	2.40	0.47
1:C:300:ILE:HD12	1:C:300:ILE:N	2.30	0.47
1:C:352:ILE:CG1	1:C:388:VAL:HB	2.33	0.47
1:A:44:ASP:HB3	1:C:77:SER:C	2.32	0.47
1:C:423:THR:HB	2:C:810:NAG:H83	1.93	0.47
1:A:108:PHE:HE1	1:A:203:VAL:HG23	1.80	0.47
1:C:225:THR:HA	1:C:318:THR:O	2.14	0.47
1:C:282:LEU:CD2	1:C:283:THR:N	2.76	0.47
1:C:481:LEU:HD12	1:C:481:LEU:HA	1.50	0.47
1:C:36:TYR:O	1:C:55:TRP:HA	2.15	0.47
1:A:150:ILE:HD11	1:A:165:ILE:HB	1.96	0.47
1:A:23:GLN:HB2	1:A:59:TRP:CE3	2.50	0.47
1:A:276:GLU:HG3	1:A:277:SER:N	2.25	0.47
1:A:39:THR:HA	1:C:79:HIS:HD1	1.79	0.47
1:C:246:ASP:C	1:C:247:LEU:HD12	2.35	0.47
1:A:268:PHE:CA	1:A:285:ALA:HB3	2.45	0.47
1:A:320:THR:CB	2:A:807:NAG:N2	2.78	0.47
1:B:310:VAL:HG12	1:B:311:PRO:O	2.15	0.47
1:B:36:TYR:O	1:B:55:TRP:HA	2.15	0.47
1:C:301:THR:CG2	1:C:316:THR:HG23	2.45	0.47
1:C:448:CYS:SG	1:C:537:ILE:CG2	3.01	0.47
1:C:496:LEU:HD21	1:C:509:ILE:CD1	2.38	0.47
1:C:537:ILE:CG1	1:C:538:LYS:N	2.77	0.47
1:A:262:ARG:HG3	1:A:299:GLN:HB2	1.98	0.46
1:B:226:TYR:O	1:B:227:THR:HG23	2.15	0.46
1:B:379:LEU:CD2	1:B:379:LEU:H	2.22	0.46
1:C:402:LYS:C	1:C:403:ASN:O	2.46	0.46
1:A:310:VAL:HG12	1:A:311:PRO:O	2.15	0.46
1:B:272:THR:HG23	2:B:803:NAG:HN2	1.81	0.46
1:C:272:THR:HG23	2:C:803:NAG:HN2	1.80	0.46
1:A:41:GLN:CA	1:C:81:VAL:CG1	2.92	0.46
1:A:27:ASN:ND2	1:A:28:LYS:N	2.50	0.46
1:B:50:VAL:HB	1:B:51:PHE:CD1	2.50	0.46
1:C:100:ASP:OD1	1:C:101:GLN:N	2.49	0.46
1:C:271:ILE:HG23	1:C:271:ILE:O	2.15	0.46
1:C:268:PHE:CA	1:C:285:ALA:HB3	2.45	0.46
1:C:374:ASP:N	1:C:374:ASP:OD1	2.49	0.46
1:C:408:VAL:O	1:C:426:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:GLU:HB2	1:C:57:THR:OG1	2.16	0.46
2:C:809:NAG:H61	2:C:810:NAG:C6	2.39	0.46
1:B:270:ASN:OD1	1:B:271:ILE:N	2.49	0.46
1:B:371:ILE:HD12	1:B:371:ILE:HA	1.65	0.46
1:C:363:GLN:O	1:C:364:ILE:CG2	2.63	0.46
1:C:373:ASN:CG	1:C:374:ASP:H	2.18	0.46
1:C:421:THR:HG21	2:C:809:NAG:H61	1.98	0.46
1:A:241:ARG:HE	1:A:281:ILE:CD1	2.24	0.46
1:A:272:THR:HG23	2:A:803:NAG:HN2	1.81	0.46
1:A:374:ASP:OD1	1:A:374:ASP:N	2.49	0.46
1:A:418:SER:O	1:A:419:VAL:HG23	2.14	0.46
1:B:290:PHE:CE2	1:B:293:ARG:CB	2.92	0.46
1:B:54:GLU:HB2	1:B:57:THR:OG1	2.16	0.46
1:B:227:THR:N	2:B:812:NAG:H2	2.31	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:76:LEU:CA	1:C:87:PRO:HG2	2.45	0.46
1:A:194:THR:CG2	1:A:195:ASP:N	2.79	0.46
1:A:270:ASN:OD1	1:A:271:ILE:N	2.49	0.46
1:B:374:ASP:OD1	1:B:374:ASP:N	2.49	0.46
1:A:187:TYR:HE1	1:A:211:ILE:HD11	1.81	0.46
1:A:415:ASP:CG	1:A:416:GLY:H	2.16	0.46
1:A:50:VAL:HB	1:A:51:PHE:CD1	2.50	0.46
1:B:109:THR:CB	1:B:131:SER:HB2	2.46	0.46
1:B:23:GLN:HB2	1:B:59:TRP:CE3	2.50	0.46
1:B:363:GLN:O	1:B:364:ILE:CG2	2.63	0.46
1:B:371:ILE:HD13	1:B:381:VAL:HG11	1.95	0.46
1:B:415:ASP:CG	1:B:416:GLY:H	2.17	0.46
1:B:459:ILE:HD12	1:B:459:ILE:N	2.31	0.46
1:B:320:THR:CB	2:B:807:NAG:N2	2.78	0.46
1:C:117:VAL:O	1:C:212:THR:N	2.46	0.46
1:A:64:ARG:HH12	1:C:44:ASP:HB2	1.80	0.46
1:A:373:ASN:CG	1:A:374:ASP:H	2.18	0.46
1:A:5:PRO:HA	1:A:6:PRO:HD3	1.86	0.46
1:B:271:ILE:HG23	1:B:271:ILE:O	2.15	0.46
1:C:374:ASP:C	1:C:375:PRO:O	2.54	0.46
1:A:506:ASP:OD1	1:A:506:ASP:N	2.49	0.46
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.16	0.46
1:B:100:ASP:OD1	1:B:101:GLN:N	2.49	0.46
1:B:187:TYR:HE1	1:B:211:ILE:HD11	1.81	0.46
1:B:373:ASN:CG	1:B:374:ASP:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASN:O	1:B:79:HIS:CE1	2.69	0.46
1:C:310:VAL:HG12	1:C:311:PRO:O	2.15	0.46
1:C:459:ILE:HD12	1:C:459:ILE:N	2.31	0.46
1:A:40:GLY:CA	1:C:79:HIS:HB3	2.45	0.46
1:C:227:THR:N	2:C:812:NAG:H2	2.31	0.46
1:A:461:ASP:HB3	1:A:468:THR:CG2	2.46	0.46
1:A:36:TYR:O	1:A:55:TRP:HA	2.15	0.46
1:B:227:THR:HG22	1:B:320:THR:HB	1.98	0.46
2:B:805:NAG:C5	2:B:806:NAG:H83	2.46	0.46
1:C:109:THR:CB	1:C:131:SER:HB2	2.46	0.46
1:C:514:SER:HG	1:C:519:ASN:HA	1.81	0.46
1:A:227:THR:HG22	1:A:320:THR:HB	1.98	0.45
1:A:227:THR:N	2:A:812:NAG:H2	2.31	0.45
1:B:194:THR:CG2	1:B:195:ASP:N	2.79	0.45
1:C:270:ASN:OD1	1:C:271:ILE:N	2.49	0.45
1:C:272:THR:CG2	1:C:273:THR:N	2.76	0.45
1:C:473:VAL:CG2	1:C:487:LEU:HD21	2.47	0.45
1:A:100:ASP:OD1	1:A:101:GLN:N	2.49	0.45
1:A:152:LYS:O	1:A:189:LEU:HA	2.17	0.45
1:A:363:GLN:O	1:A:364:ILE:CG2	2.64	0.45
1:A:44:ASP:OD1	1:C:91:PRO:HA	2.16	0.45
1:A:473:VAL:CG2	1:A:487:LEU:HD21	2.47	0.45
1:A:511:VAL:N	1:A:523:THR:O	2.46	0.45
1:B:506:ASP:N	1:B:506:ASP:OD1	2.49	0.45
1:C:79:HIS:HD1	1:C:91:PRO:HG3	1.79	0.45
1:A:408:VAL:O	1:A:426:LEU:N	2.49	0.45
1:A:459:ILE:HD12	1:A:459:ILE:N	2.31	0.45
1:B:421:THR:HG21	2:B:809:NAG:H61	1.98	0.45
1:C:262:ARG:HG3	1:C:299:GLN:HB2	1.98	0.45
1:A:380:THR:CG2	1:A:381:VAL:N	2.79	0.45
1:C:155:PRO:CB	2:C:801:NAG:C8	2.94	0.45
1:B:252:THR:HA	1:B:253:PRO:HD3	1.81	0.45
1:C:152:LYS:O	1:C:189:LEU:HA	2.17	0.45
1:C:469:TYR:CD2	1:C:470:PRO:N	2.85	0.45
1:A:162:LEU:HB2	1:A:163:PHE:CE1	2.52	0.45
1:B:261:ILE:HD11	1:B:264:ASN:ND2	2.32	0.45
1:B:380:THR:CG2	1:B:381:VAL:N	2.79	0.45
1:C:336:VAL:HG11	1:C:338:ARG:HD2	1.99	0.45
1:C:450:GLN:CB	1:C:533:GLU:OE2	2.64	0.45
1:A:109:THR:CB	1:A:131:SER:HB2	2.46	0.45
1:A:155:PRO:CB	2:A:801:NAG:C8	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:VAL:HA	1:B:387:ILE:O	2.16	0.45
1:B:461:ASP:HB3	1:B:468:THR:CG2	2.46	0.45
1:B:469:TYR:CD2	1:B:470:PRO:N	2.85	0.45
1:B:88:VAL:H	1:C:1:ASP:H3	1.62	0.45
1:C:461:ASP:HB3	1:C:468:THR:CG2	2.46	0.45
1:A:271:ILE:O	1:A:271:ILE:HG23	2.15	0.45
1:A:380:THR:HG22	1:A:381:VAL:N	2.32	0.45
1:A:469:TYR:CE2	1:A:470:PRO:HB2	2.52	0.45
1:A:469:TYR:CD2	1:A:470:PRO:N	2.85	0.45
1:B:109:THR:HB	1:B:131:SER:HB2	1.99	0.45
1:B:286:LYS:C	1:B:287:GLY:O	2.55	0.45
1:B:408:VAL:O	1:B:426:LEU:N	2.49	0.45
1:C:227:THR:HG22	1:C:320:THR:HB	1.98	0.45
1:C:482:THR:O	1:C:483:TRP:CD2	2.70	0.45
1:A:44:ASP:O	1:C:78:SER:HA	2.17	0.45
1:A:336:VAL:HG11	1:A:338:ARG:HD2	1.99	0.45
2:A:805:NAG:C5	2:A:806:NAG:H83	2.46	0.45
1:B:272:THR:CG2	1:B:273:THR:N	2.76	0.45
1:B:426:LEU:C	1:B:426:LEU:HD13	2.37	0.45
1:B:469:TYR:CE2	1:B:470:PRO:HB2	2.52	0.45
1:B:482:THR:O	1:B:483:TRP:CD2	2.70	0.45
1:C:162:LEU:HB2	1:C:163:PHE:CE1	2.52	0.45
1:C:286:LYS:C	1:C:287:GLY:O	2.55	0.45
1:C:380:THR:CG2	1:C:381:VAL:N	2.79	0.45
1:C:450:GLN:CB	1:C:533:GLU:HA	2.29	0.45
2:C:805:NAG:C5	2:C:806:NAG:H83	2.46	0.45
1:A:109:THR:HB	1:A:131:SER:HB2	1.99	0.45
1:A:312:LEU:O	3:A:804:NDG:H8C1	2.17	0.45
1:A:421:THR:HG21	2:A:809:NAG:H61	1.98	0.45
1:A:450:GLN:CB	1:A:533:GLU:OE2	2.64	0.45
1:B:339:VAL:HG11	1:B:351:ILE:HG23	1.98	0.45
1:B:450:GLN:CB	1:B:533:GLU:OE2	2.64	0.45
1:C:469:TYR:CE2	1:C:470:PRO:HB2	2.52	0.45
1:C:468:THR:C	1:C:469:TYR:O	2.54	0.45
1:C:519:ASN:O	1:C:519:ASN:CG	2.55	0.45
1:A:32:ASN:HD22	1:A:83:GLU:N	2.13	0.44
1:A:440:PRO:HB3	1:A:457:LEU:CD2	2.43	0.44
1:A:482:THR:O	1:A:483:TRP:CD2	2.70	0.44
1:B:152:LYS:O	1:B:189:LEU:HA	2.17	0.44
1:B:473:VAL:CG2	1:B:487:LEU:HD21	2.47	0.44
1:B:449:ASP:CB	1:B:532:CYS:H	2.22	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:LEU:HD13	1:C:426:LEU:C	2.37	0.44
1:B:440:PRO:HB3	1:B:457:LEU:CD2	2.43	0.44
1:B:80:ALA:HB3	1:C:1:ASP:N	2.32	0.44
1:B:82:SER:H	1:C:2:TRP:CA	1.92	0.44
1:C:194:THR:CG2	1:C:195:ASP:N	2.79	0.44
1:C:108:PHE:HE1	1:C:203:VAL:HG23	1.80	0.44
1:C:261:ILE:HD11	1:C:264:ASN:ND2	2.32	0.44
1:C:312:LEU:O	3:C:804:NDG:H8C1	2.17	0.44
1:C:440:PRO:HB3	1:C:457:LEU:CD2	2.43	0.44
1:C:67:ASP:OD1	1:C:69:GLU:HB2	2.18	0.44
1:A:187:TYR:CE1	1:A:211:ILE:HD11	2.52	0.44
1:B:299:GLN:CG	1:B:318:THR:HG23	2.42	0.44
1:B:32:ASN:ND2	1:B:83:GLU:CB	2.62	0.44
1:C:232:GLU:HA	1:C:288:LEU:HD12	1.99	0.44
1:A:45:ASN:HA	1:C:37:SER:O	2.18	0.44
1:A:64:ARG:NH1	1:C:44:ASP:HB2	2.33	0.44
1:C:442:PRO:HD2	1:C:457:LEU:HD12	2.00	0.44
1:A:339:VAL:HG11	1:A:351:ILE:HG23	1.98	0.44
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.44
1:B:241:ARG:HE	1:B:281:ILE:CD1	2.24	0.44
1:B:232:GLU:HA	1:B:288:LEU:HD12	1.99	0.44
1:B:461:ASP:HB3	1:B:468:THR:HG22	2.00	0.44
1:B:485:ALA:O	1:B:486:GLU:OE1	2.35	0.44
1:C:187:TYR:CE1	1:C:211:ILE:HD11	2.52	0.44
1:C:485:ALA:O	1:C:486:GLU:OE1	2.35	0.44
1:A:374:ASP:C	1:A:375:PRO:O	2.54	0.44
1:A:461:ASP:HB3	1:A:468:THR:HG22	2.00	0.44
1:B:162:LEU:HB2	1:B:163:PHE:CE1	2.52	0.44
1:B:448:CYS:SG	1:B:537:ILE:CG2	3.01	0.44
1:B:519:ASN:O	1:B:519:ASN:CG	2.55	0.44
1:B:312:LEU:O	3:B:804:NDG:H8C1	2.17	0.44
1:C:151:LEU:HD12	1:C:151:LEU:N	2.33	0.44
1:C:224:LYS:HE3	2:C:806:NAG:C8	2.48	0.44
1:C:339:VAL:HG11	1:C:351:ILE:HG23	1.98	0.44
1:A:4:ILE:HA	1:A:5:PRO:HD3	1.72	0.44
1:B:336:VAL:HG11	1:B:338:ARG:HD2	1.99	0.44
1:B:380:THR:HG22	1:B:381:VAL:N	2.32	0.44
1:B:67:ASP:OD1	1:B:69:GLU:HB2	2.18	0.44
1:B:86:SER:HA	1:B:87:PRO:HD3	1.83	0.44
1:A:381:VAL:HA	1:A:387:ILE:O	2.17	0.44
1:A:224:LYS:HE3	2:A:806:NAG:C8	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:VAL:O	1:B:212:THR:N	2.46	0.44
1:B:151:LEU:N	1:B:151:LEU:HD12	2.33	0.44
1:B:187:TYR:CE1	1:B:211:ILE:HD11	2.52	0.44
1:B:374:ASP:C	1:B:375:PRO:O	2.54	0.44
1:B:396:ARG:NH2	1:B:464:ILE:HG22	2.12	0.44
1:C:134:ASP:HB2	1:C:146:LEU:HD11	1.99	0.44
1:C:380:THR:HG22	1:C:381:VAL:N	2.32	0.44
1:C:381:VAL:HA	1:C:387:ILE:O	2.17	0.44
1:A:151:LEU:HD12	1:A:151:LEU:N	2.33	0.44
1:A:426:LEU:HD13	1:A:426:LEU:C	2.38	0.44
1:A:49:GLY:HA2	1:C:39:THR:HB	0.85	0.44
1:C:461:ASP:HB3	1:C:468:THR:HG22	2.00	0.44
1:A:261:ILE:HD11	1:A:264:ASN:ND2	2.32	0.44
1:A:485:ALA:O	1:A:486:GLU:OE1	2.35	0.44
1:B:262:ARG:HG3	1:B:299:GLN:HB2	1.98	0.44
1:C:109:THR:HB	1:C:131:SER:HB2	1.99	0.44
1:C:194:THR:HG23	1:C:201:LEU:O	2.18	0.44
1:C:27:ASN:ND2	1:C:28:LYS:N	2.50	0.44
1:A:45:ASN:HA	1:C:37:SER:C	2.37	0.44
1:C:354:LEU:HD12	1:C:386:GLY:O	2.18	0.44
1:C:86:SER:HA	1:C:87:PRO:HD3	1.83	0.44
1:B:220:ILE:O	1:B:220:ILE:HG22	2.18	0.43
1:B:290:PHE:CD2	1:B:293:ARG:O	2.71	0.43
1:B:468:THR:C	1:B:469:TYR:O	2.54	0.43
1:C:371:ILE:HD13	1:C:381:VAL:HG11	1.95	0.43
1:A:286:LYS:C	1:A:287:GLY:O	2.55	0.43
1:A:28:LYS:CD	1:A:88:VAL:HG12	2.38	0.43
1:B:134:ASP:HB2	1:B:146:LEU:HD11	1.99	0.43
1:B:247:LEU:N	1:B:247:LEU:HD12	2.33	0.43
1:B:27:ASN:ND2	1:B:28:LYS:N	2.50	0.43
1:B:366:LYS:HG2	1:B:367:LEU:H	1.75	0.43
1:B:442:PRO:HD2	1:B:457:LEU:HD12	2.00	0.43
1:B:502:LEU:HA	1:B:502:LEU:HD23	1.82	0.43
1:B:524:VAL:HG21	2:B:904:NAG:C8	2.44	0.43
1:B:34:VAL:HG22	1:C:2:TRP:HB2	2.00	0.43
1:A:134:ASP:HB2	1:A:146:LEU:HD11	1.99	0.43
1:A:220:ILE:O	1:A:220:ILE:HG22	2.18	0.43
1:A:247:LEU:HD12	1:A:247:LEU:N	2.33	0.43
1:A:421:THR:CG2	1:A:422:GLY:N	2.81	0.43
1:B:155:PRO:CB	2:B:801:NAG:C8	2.94	0.43
1:C:247:LEU:N	1:C:247:LEU:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:LYS:HB3	1:C:260:LYS:HE3	1.81	0.43
1:B:194:THR:HG23	1:B:201:LEU:O	2.18	0.43
1:B:354:LEU:HD12	1:B:386:GLY:O	2.18	0.43
1:B:224:LYS:HE3	2:B:806:NAG:C8	2.48	0.43
1:B:297:VAL:HG21	2:B:807:NAG:H62	2.01	0.43
1:A:35:TYR:HB3	1:B:90:GLU:CD	2.38	0.43
1:A:232:GLU:HA	1:A:288:LEU:HD12	1.99	0.43
1:A:468:THR:C	1:A:469:TYR:O	2.54	0.43
1:A:297:VAL:HG21	2:A:807:NAG:H62	2.01	0.43
1:A:82:SER:HG	1:B:91:PRO:C	2.19	0.43
1:B:421:THR:CG2	1:B:422:GLY:N	2.81	0.43
1:B:4:ILE:HA	1:B:5:PRO:HD3	1.72	0.43
1:C:220:ILE:HG22	1:C:220:ILE:O	2.18	0.43
1:A:290:PHE:CD2	1:A:293:ARG:O	2.71	0.43
1:B:195:ASP:HB3	1:B:196:LEU:HG	2.01	0.43
1:A:344:ASP:CG	1:A:344:ASP:O	2.57	0.43
1:A:354:LEU:HD12	1:A:386:GLY:O	2.18	0.43
1:A:519:ASN:CG	1:A:519:ASN:O	2.55	0.43
1:B:1:ASP:CG	1:B:2:TRP:N	2.70	0.43
1:B:518:ASN:C	1:B:520:PRO:CD	2.87	0.43
1:C:290:PHE:CD2	1:C:293:ARG:O	2.71	0.43
1:C:368:SER:CB	1:C:370:PHE:HE1	2.31	0.43
1:C:441:SER:CB	1:C:442:PRO:HD3	2.47	0.43
1:C:539:CYS:HB3	1:C:540:GLN:H	1.45	0.43
2:A:805:NAG:H62	2:A:806:NAG:N2	2.31	0.43
1:B:239:VAL:HG13	1:B:240:GLN:N	2.34	0.43
1:A:46:PRO:HD2	1:C:35:TYR:O	2.19	0.43
1:A:194:THR:HG23	1:A:201:LEU:O	2.18	0.43
1:A:239:VAL:HG13	1:A:240:GLN:N	2.33	0.43
1:A:419:VAL:HG13	1:A:420:GLY:N	2.34	0.43
1:C:239:VAL:HG13	1:C:240:GLN:N	2.33	0.43
1:B:367:LEU:HG	1:B:367:LEU:H	1.41	0.43
1:B:419:VAL:HG13	1:B:420:GLY:N	2.34	0.43
1:B:188:THR:H	2:B:801:NAG:H83	1.84	0.43
2:B:810:NAG:O7	2:B:810:NAG:C1	2.67	0.43
1:C:175:ILE:CG2	1:C:176:GLY:N	2.82	0.43
1:C:333:VAL:HG23	1:C:334:PRO:HD3	2.01	0.43
1:C:421:THR:CG2	1:C:422:GLY:N	2.81	0.43
1:A:48:GLN:O	1:C:44:ASP:HB3	2.18	0.43
1:A:264:ASN:HB3	1:A:267:GLY:HA2	2.01	0.42
1:A:347:ARG:HG3	1:A:392:GLY:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:LEU:HD23	1:B:522:LEU:HA	1.36	0.42
1:C:195:ASP:HB3	1:C:196:LEU:HG	2.01	0.42
1:C:22:VAL:CG2	1:C:23:GLN:N	2.81	0.42
1:C:344:ASP:CG	1:C:344:ASP:O	2.57	0.42
1:C:522:LEU:HA	1:C:522:LEU:HD23	1.36	0.42
1:C:409:ILE:HD13	3:C:811:NDG:H8C3	2.01	0.42
1:A:368:SER:CB	1:A:370:PHE:HE1	2.31	0.42
1:A:371:ILE:HG13	1:A:410:MET:SD	2.59	0.42
1:A:40:GLY:O	1:A:45:ASN:HB2	2.19	0.42
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.81	0.42
1:A:32:ASN:ND2	1:A:83:GLU:CB	2.62	0.42
1:A:90:GLU:O	1:A:91:PRO:O	2.37	0.42
1:A:89:GLU:CD	1:B:1:ASP:N	2.37	0.42
1:B:22:VAL:CG2	1:B:23:GLN:N	2.81	0.42
1:B:32:ASN:HD22	1:B:83:GLU:N	2.13	0.42
1:C:419:VAL:HG13	1:C:420:GLY:N	2.33	0.42
1:A:154:ASP:HB3	2:A:801:NAG:C7	2.48	0.42
1:A:450:GLN:HG3	1:A:532:CYS:O	2.10	0.42
1:B:451:ASN:O	1:B:534:GLY:CA	2.60	0.42
1:C:90:GLU:O	1:C:91:PRO:O	2.37	0.42
1:A:22:VAL:CG2	1:A:23:GLN:N	2.81	0.42
1:A:347:ARG:HD2	1:A:392:GLY:CA	2.50	0.42
1:A:371:ILE:HA	1:A:410:MET:HB3	2.02	0.42
1:A:442:PRO:HD2	1:A:457:LEU:HD12	2.00	0.42
1:A:522:LEU:HB3	1:A:523:THR:H	1.57	0.42
1:B:138:ASN:C	1:B:138:ASN:ND2	2.73	0.42
1:B:261:ILE:H	1:B:261:ILE:HD13	1.85	0.42
1:B:333:VAL:HG23	1:B:334:PRO:HD3	2.01	0.42
1:B:368:SER:CB	1:B:370:PHE:HE1	2.31	0.42
1:C:127:VAL:HG13	1:C:128:MET:N	2.25	0.42
1:C:138:ASN:C	1:C:138:ASN:ND2	2.73	0.42
1:C:371:ILE:HG13	1:C:410:MET:SD	2.59	0.42
1:A:298:LEU:CD2	1:A:298:LEU:N	2.75	0.42
1:A:409:ILE:HD13	3:A:811:NDG:H8C3	2.01	0.42
1:A:518:ASN:C	1:A:520:PRO:CD	2.87	0.42
1:B:30:ARG:HH12	1:C:25:LYS:CG	2.31	0.42
1:B:482:THR:HG22	1:B:499:THR:H	1.70	0.42
1:B:7:ILE:O	1:B:96:ILE:HG23	2.20	0.42
1:C:250:PRO:HA	1:C:255:TRP:CG	2.55	0.42
1:B:88:VAL:HG21	1:C:2:TRP:HB2	1.85	0.42
1:C:230:VAL:O	1:C:323:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:ASP:OD1	1:C:516:ALA:N	2.53	0.42
1:A:138:ASN:C	1:A:138:ASN:ND2	2.73	0.42
1:A:333:VAL:HG23	1:A:334:PRO:HD3	2.01	0.42
1:A:84:ASN:O	1:B:79:HIS:ND1	2.53	0.42
1:B:371:ILE:HG13	1:B:410:MET:SD	2.59	0.42
1:C:67:ASP:CG	1:C:69:GLU:HB2	2.40	0.42
1:A:515:ASP:OD1	1:A:516:ALA:N	2.53	0.42
1:B:347:ARG:HD2	1:B:392:GLY:CA	2.50	0.42
1:B:441:SER:CB	1:B:442:PRO:HD3	2.47	0.42
1:B:511:VAL:N	1:B:523:THR:O	2.46	0.42
1:B:83:GLU:CD	1:C:2:TRP:CH2	2.93	0.42
1:A:44:ASP:C	1:C:38:ILE:HA	2.38	0.42
1:C:40:GLY:O	1:C:45:ASN:HB2	2.19	0.42
2:C:805:NAG:H62	2:C:806:NAG:N2	2.31	0.42
1:A:339:VAL:HG21	1:A:351:ILE:HG22	2.01	0.42
1:B:235:ILE:HG21	1:B:235:ILE:HD13	1.84	0.42
1:B:250:PRO:HA	1:B:255:TRP:CG	2.55	0.42
1:B:339:VAL:HG21	1:B:351:ILE:HG22	2.01	0.42
1:B:469:TYR:CE2	1:B:470:PRO:HD2	2.54	0.42
1:B:515:ASP:OD1	1:B:516:ALA:N	2.53	0.42
1:C:415:ASP:CG	1:C:416:GLY:H	2.16	0.42
1:C:7:ILE:O	1:C:96:ILE:HG23	2.20	0.42
1:A:469:TYR:CE2	1:A:470:PRO:HD2	2.54	0.42
1:A:3:VAL:HB	1:A:4:ILE:H	1.51	0.42
1:A:539:CYS:HB3	1:A:540:GLN:H	1.45	0.42
1:A:524:VAL:HG21	2:A:904:NAG:C8	2.44	0.42
1:B:67:ASP:CG	1:B:69:GLU:HB2	2.40	0.42
1:B:335:ALA:HB3	3:B:811:NDG:O6	2.15	0.42
1:C:188:THR:H	2:C:801:NAG:H83	1.84	0.42
1:C:239:VAL:HG11	1:C:282:LEU:HD22	2.02	0.42
1:C:32:ASN:HD22	1:C:83:GLU:N	2.13	0.42
1:C:347:ARG:HD2	1:C:392:GLY:CA	2.50	0.42
1:C:439:VAL:HA	1:C:440:PRO:HD3	1.81	0.42
1:C:505:GLY:H	1:C:529:VAL:HB	1.85	0.42
1:C:4:ILE:HA	1:C:5:PRO:HD3	1.72	0.42
1:A:195:ASP:HB3	1:A:196:LEU:HG	2.01	0.42
1:A:441:SER:CB	1:A:442:PRO:HD3	2.47	0.42
1:B:175:ILE:CG2	1:B:176:GLY:N	2.82	0.42
1:B:230:VAL:O	1:B:323:VAL:HA	2.20	0.42
1:B:344:ASP:O	1:B:344:ASP:CG	2.57	0.42
1:B:40:GLY:O	1:B:45:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ILE:HD13	1:C:261:ILE:H	1.85	0.42
1:A:45:ASN:CA	1:C:37:SER:C	2.88	0.42
1:A:108:PHE:HA	1:A:132:ALA:CB	2.50	0.41
1:A:239:VAL:HG11	1:A:282:LEU:HD22	2.02	0.41
1:A:502:LEU:HD22	1:A:503:LYS:H	1.85	0.41
1:B:108:PHE:HA	1:B:132:ALA:CB	2.50	0.41
1:B:264:ASN:HB3	1:B:267:GLY:HA2	2.01	0.41
1:B:371:ILE:HA	1:B:410:MET:HB3	2.02	0.41
1:B:514:SER:HG	1:B:519:ASN:HA	1.85	0.41
1:B:505:GLY:H	1:B:529:VAL:HB	1.85	0.41
1:C:108:PHE:HA	1:C:132:ALA:CB	2.50	0.41
1:C:264:ASN:HB3	1:C:267:GLY:HA2	2.01	0.41
1:C:367:LEU:HG	1:C:367:LEU:H	1.41	0.41
1:C:449:ASP:N	1:C:532:CYS:HB3	2.19	0.41
1:A:35:TYR:CZ	1:C:93:GLU:OE2	2.69	0.41
1:A:250:PRO:HA	1:A:255:TRP:CG	2.55	0.41
1:A:188:THR:H	2:A:801:NAG:H83	1.84	0.41
2:A:810:NAG:C1	2:A:810:NAG:O7	2.67	0.41
1:B:127:VAL:HG13	1:B:128:MET:N	2.25	0.41
1:B:231:PRO:O	1:B:235:ILE:HD13	2.21	0.41
1:B:347:ARG:HG3	1:B:392:GLY:N	2.33	0.41
1:C:231:PRO:O	1:C:288:LEU:HD12	2.20	0.41
1:A:127:VAL:HG22	1:A:128:MET:HG3	2.03	0.41
1:A:505:GLY:H	1:A:529:VAL:HB	1.85	0.41
1:A:86:SER:HB3	1:B:92:MET:HB2	1.39	0.41
1:B:154:ASP:HB3	2:B:801:NAG:C7	2.48	0.41
1:B:231:PRO:O	1:B:288:LEU:HD12	2.20	0.41
1:B:449:ASP:N	1:B:532:CYS:HB3	2.19	0.41
1:B:409:ILE:HD13	3:B:811:NDG:H8C3	2.01	0.41
1:C:154:ASP:HB3	2:C:801:NAG:C7	2.48	0.41
1:A:48:GLN:CG	1:C:37:SER:HB2	2.45	0.41
1:B:128:MET:HB3	1:B:129:ALA:H	1.62	0.41
1:B:33:LYS:O	1:C:2:TRP:CG	2.73	0.41
1:C:230:VAL:HG23	1:C:323:VAL:HA	2.03	0.41
1:C:297:VAL:HG21	2:C:807:NAG:H62	2.01	0.41
1:C:518:ASN:C	1:C:520:PRO:CD	2.87	0.41
1:A:175:ILE:CG2	1:A:176:GLY:N	2.82	0.41
1:A:42:GLY:CA	1:A:47:PRO:O	2.69	0.41
1:B:502:LEU:HD22	1:B:503:LYS:H	1.85	0.41
1:C:119:GLU:CG	1:C:214:ALA:HB3	2.51	0.41
1:C:3:VAL:HB	1:C:4:ILE:H	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:HG23	1:A:323:VAL:HA	2.03	0.41
1:A:231:PRO:O	1:A:235:ILE:HD13	2.21	0.41
1:A:230:VAL:O	1:A:323:VAL:HA	2.20	0.41
1:A:474:SER:N	1:A:512:LEU:O	2.53	0.41
1:B:230:VAL:HG23	1:B:323:VAL:HA	2.03	0.41
1:B:19:LYS:HB3	1:B:62:VAL:HG12	2.03	0.41
1:C:319:VAL:CG1	1:C:320:THR:N	2.84	0.41
1:C:502:LEU:HD22	1:C:503:LYS:H	1.85	0.41
2:C:810:NAG:C1	2:C:810:NAG:O7	2.67	0.41
1:A:400:TYR:O	1:A:401:VAL:C	2.59	0.41
1:A:33:LYS:NZ	1:A:56:GLU:OE1	2.42	0.41
1:B:474:SER:N	1:B:512:LEU:O	2.53	0.41
1:C:62:VAL:O	1:C:62:VAL:HG13	2.21	0.41
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.51	0.41
1:A:261:ILE:H	1:A:261:ILE:HD13	1.85	0.41
1:A:82:SER:OG	1:B:91:PRO:CD	2.68	0.41
1:B:68:ARG:HD3	1:B:100:ASP:CB	2.51	0.41
1:B:108:PHE:CZ	1:B:191:VAL:HG23	2.56	0.41
1:C:23:GLN:HB2	1:C:59:TRP:CD2	2.55	0.41
1:C:423:THR:CG2	2:C:810:NAG:N2	2.84	0.41
1:A:23:GLN:HA	1:A:58:GLY:O	2.21	0.41
1:A:290:PHE:CG	1:A:292:LEU:HB2	2.56	0.41
1:A:345:LEU:HD22	1:A:349:GLU:HB2	2.03	0.41
1:A:316:THR:OG1	2:A:806:NAG:H83	2.21	0.41
1:A:7:ILE:O	1:A:96:ILE:HG23	2.20	0.41
1:B:448:CYS:C	1:B:452:PRO:HG3	2.40	0.41
1:C:339:VAL:HG21	1:C:351:ILE:HG22	2.01	0.41
1:C:483:TRP:CZ2	1:C:507:TYR:CE1	2.87	0.41
1:A:108:PHE:HA	1:A:132:ALA:HB2	2.03	0.41
1:A:138:ASN:N	1:A:138:ASN:HD22	2.19	0.41
1:A:235:ILE:HD13	1:A:235:ILE:HG21	1.84	0.41
1:A:62:VAL:HG13	1:A:62:VAL:O	2.21	0.41
1:B:25:LYS:NZ	1:B:29:ASP:OD2	2.39	0.41
1:B:373:ASN:CG	1:B:374:ASP:N	2.75	0.41
1:B:449:ASP:HB2	1:B:531:SER:HA	2.03	0.41
1:B:33:LYS:NZ	1:B:56:GLU:OE1	2.43	0.41
1:C:108:PHE:HA	1:C:132:ALA:HB2	2.03	0.41
1:C:231:PRO:O	1:C:235:ILE:HD13	2.21	0.41
1:C:23:GLN:HA	1:C:58:GLY:O	2.21	0.41
1:C:336:VAL:H	1:C:336:VAL:HG23	1.52	0.41
1:C:345:LEU:HD22	1:C:349:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:TYR:CE2	1:C:470:PRO:HD2	2.54	0.41
1:A:193:ALA:O	1:A:202:SER:HA	2.21	0.41
1:A:45:ASN:ND2	1:C:80:ALA:C	2.48	0.41
1:A:297:VAL:HG22	2:A:807:NAG:H62	2.03	0.41
1:B:108:PHE:HA	1:B:132:ALA:HB2	2.03	0.41
1:B:111:ASP:O	1:B:112:VAL:HG13	2.21	0.41
1:B:193:ALA:O	1:B:202:SER:HA	2.21	0.41
1:B:319:VAL:CG1	1:B:320:THR:N	2.84	0.41
1:C:111:ASP:O	1:C:112:VAL:HG13	2.21	0.41
1:C:127:VAL:HG22	1:C:128:MET:HG3	2.03	0.41
1:C:118:ARG:CA	1:C:212:THR:HB	2.51	0.41
1:C:290:PHE:CG	1:C:292:LEU:HB2	2.56	0.41
1:C:448:CYS:C	1:C:452:PRO:HG3	2.40	0.41
1:C:68:ARG:HD3	1:C:100:ASP:CB	2.51	0.41
1:A:231:PRO:O	1:A:288:LEU:HD12	2.20	0.40
1:A:67:ASP:CG	1:A:69:GLU:HB2	2.40	0.40
1:B:378:TRP:HB2	1:B:379:LEU:H	1.64	0.40
2:B:805:NAG:H62	2:B:806:NAG:N2	2.31	0.40
1:C:138:ASN:HD22	1:C:138:ASN:N	2.19	0.40
1:C:226:TYR:O	1:C:227:THR:HG22	2.21	0.40
1:C:274:ASP:O	1:C:278:ASN:CA	2.51	0.40
1:C:438:PRO:HB2	1:C:513:LEU:CD1	2.51	0.40
1:C:474:SER:N	1:C:512:LEU:O	2.53	0.40
1:C:449:ASP:HB2	1:C:531:SER:HA	2.03	0.40
1:A:119:GLU:CG	1:A:214:ALA:HB3	2.51	0.40
1:A:409:ILE:HD13	3:A:811:NDG:C8	2.51	0.40
1:A:23:GLN:HB2	1:A:59:TRP:CD2	2.55	0.40
1:B:540:GLN:NE2	1:B:540:GLN:O	2.47	0.40
1:B:316:THR:OG1	2:B:806:NAG:H83	2.21	0.40
1:C:445:PHE:CD2	1:C:445:PHE:N	2.89	0.40
1:C:19:LYS:HB3	1:C:62:VAL:HG12	2.03	0.40
1:C:297:VAL:HG22	2:C:807:NAG:H62	2.03	0.40
1:A:108:PHE:CZ	1:A:191:VAL:HG23	2.56	0.40
1:A:373:ASN:CG	1:A:374:ASP:N	2.75	0.40
1:A:466:PRO:O	1:A:469:TYR:N	2.46	0.40
1:B:127:VAL:HG22	1:B:128:MET:HG3	2.03	0.40
1:B:272:THR:O	1:B:281:ILE:HG22	2.21	0.40
1:B:239:VAL:HG11	1:B:282:LEU:HD22	2.02	0.40
1:B:400:TYR:O	1:B:401:VAL:C	2.59	0.40
1:C:108:PHE:CZ	1:C:191:VAL:HG23	2.56	0.40
1:C:193:ALA:O	1:C:202:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:THR:CG2	1:C:213:ASP:N	2.83	0.40
1:C:223:PRO:HB2	1:C:226:TYR:CZ	2.56	0.40
1:C:371:ILE:HA	1:C:410:MET:HB3	2.02	0.40
1:C:432:ASP:CG	1:C:433:VAL:N	2.74	0.40
1:C:316:THR:OG1	2:C:806:NAG:H83	2.21	0.40
1:A:249:MET:HA	1:A:250:PRO:HD3	1.85	0.40
1:A:319:VAL:CG1	1:A:320:THR:N	2.84	0.40
1:A:371:ILE:HA	1:A:371:ILE:HD12	1.65	0.40
1:A:78:SER:C	1:C:90:GLU:CD	2.79	0.40
1:A:423:THR:CG2	2:A:810:NAG:N2	2.84	0.40
1:B:23:GLN:HA	1:B:58:GLY:O	2.21	0.40
1:B:23:GLN:HB2	1:B:59:TRP:CD2	2.55	0.40
1:B:298:LEU:N	1:B:298:LEU:CD2	2.75	0.40
1:B:396:ARG:HH21	1:B:432:ASP:CG	2.25	0.40
1:A:28:LYS:NZ	1:B:4:ILE:HG22	2.37	0.40
1:B:423:THR:CG2	2:B:810:NAG:N2	2.84	0.40
1:C:42:GLY:CA	1:C:47:PRO:O	2.69	0.40
1:C:490:LYS:CG	1:C:490:LYS:O	2.67	0.40
1:A:111:ASP:O	1:A:112:VAL:HG13	2.21	0.40
1:B:432:ASP:CG	1:B:433:VAL:N	2.74	0.40
1:B:409:ILE:HD13	3:B:811:NDG:C8	2.51	0.40
1:C:235:ILE:CD1	1:C:287:GLY:HA2	2.50	0.40
1:C:400:TYR:O	1:C:401:VAL:C	2.59	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	15
1	B	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	15
All	All	1614/2640 (61%)	1203 (74%)	276 (17%)	135 (8%)	2	15

All (135) 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	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	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

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Mol	Chain	Res	Type
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	A	152	LYS
1	A	223	PRO
1	A	359	PRO
1	A	375	PRO
1	B	152	LYS
1	B	223	PRO
1	B	359	PRO
1	B	375	PRO
1	C	152	LYS
1	C	223	PRO
1	C	359	PRO
1	C	375	PRO
1	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	A	498	PRO
1	A	523	THR
1	B	498	PRO
1	B	523	THR
1	C	498	PRO
1	C	523	THR
1	A	154	ASP
1	A	307	PRO
1	B	154	ASP

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Mol	Chain	Res	Type
1	B	307	PRO
1	C	154	ASP
1	C	307	PRO
1	A	222	ASP
1	B	222	ASP
1	C	222	ASP
1	A	200	GLY
1	B	200	GLY
1	C	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

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	8
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	8
1	C	480/779 (62%)	381 (79%)	99 (21%)	1	8
All	All	1440/2337 (62%)	1143 (79%)	297 (21%)	4	8

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	18	PRO
1	A	19	LYS
1	A	27	ASN
1	A	52	ARG
1	A	61	LEU
1	A	66	LEU

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Mol	Chain	Res	Type
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
1	A	315	SER
1	A	316	THR
1	A	318	THR
1	A	333	VAL

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Mol	Chain	Res	Type
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
1	A	477	HIS
1	A	492	THR
1	A	509	ILE
1	A	512	LEU

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Mol	Chain	Res	Type
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
1	B	237	PHE
1	B	250	PRO
1	B	253	PRO
1	B	261	ILE

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Mol	Chain	Res	Type
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
1	B	407	THR
1	B	410	MET
1	B	423	THR
1	B	425	THR

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Mol	Chain	Res	Type
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
1	C	155	PRO
1	C	156	GLU
1	C	161	ASN
1	C	163	PHE

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Mol	Chain	Res	Type
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
1	C	365	GLN
1	C	371	ILE
1	C	373	ASN
1	C	375	PRO

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) 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	48	GLN
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	404	ASN
1	A	455	GLN
1	A	467	ASN
1	A	517	GLN
1	A	519	ASN
1	B	12	ASN
1	B	27	ASN
1	B	32	ASN
1	B	45	ASN
1	B	79	HIS
1	B	84	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

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Mol	Chain	Res	Type
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	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
1	C	467	ASN
1	C	517	GLN
1	C	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 81 ligands modelled in this entry, 36 are monoatomic - leaving 45 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	0.67	0	15,19,21	0.99	1 (6%)
2	NAG	A	802	1	14,14,15	0.73	0	15,19,21	0.92	0
2	NAG	A	803	1	14,14,15	0.94	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	A	804	1	14,14,15	0.63	0	15,19,21	0.82	0
2	NAG	A	805	1	14,14,15	0.69	0	15,19,21	1.07	1 (6%)
2	NAG	A	806	1	14,14,15	0.55	0	15,19,21	1.44	3 (20%)
2	NAG	A	807	1	14,14,15	0.65	0	15,19,21	1.25	2 (13%)
2	NAG	A	808	1	14,14,15	0.66	0	15,19,21	0.68	0
2	NAG	A	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.86	0
2	NAG	A	810	1	14,14,15	0.65	0	15,19,21	1.40	4 (26%)
3	NDG	A	811	1	14,14,15	0.86	0	15,19,21	1.95	1 (6%)
2	NAG	A	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.75	1 (6%)
3	NDG	A	902	1	14,14,15	1.10	1 (7%)	15,19,21	1.14	1 (6%)
3	NDG	A	903	1	14,14,15	0.52	0	15,19,21	0.80	0
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.64	0
2	NAG	B	801	1	14,14,15	0.66	0	15,19,21	1.00	1 (6%)
2	NAG	B	802	1	14,14,15	0.74	0	15,19,21	0.91	0
2	NAG	B	803	1	14,14,15	0.94	1 (7%)	15,19,21	1.21	2 (13%)
3	NDG	B	804	1	14,14,15	0.62	0	15,19,21	0.82	0
2	NAG	B	805	1	14,14,15	0.70	0	15,19,21	1.07	1 (6%)
2	NAG	B	806	1	14,14,15	0.55	0	15,19,21	1.45	3 (20%)
2	NAG	B	807	1	14,14,15	0.64	0	15,19,21	1.25	2 (13%)
2	NAG	B	808	1	14,14,15	0.68	0	15,19,21	0.67	0
2	NAG	B	809	1	14,14,15	0.77	1 (7%)	15,19,21	0.86	0
2	NAG	B	810	1	14,14,15	0.64	0	15,19,21	1.40	4 (26%)
3	NDG	B	811	1	14,14,15	0.84	0	15,19,21	1.96	1 (6%)
2	NAG	B	812	1	14,14,15	0.85	1 (7%)	15,19,21	0.75	0

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	1.09	1 (7%)	15,19,21	1.14	1 (6%)
3	NDG	B	903	1	14,14,15	0.52	0	15,19,21	0.80	0
2	NAG	B	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.65	0
2	NAG	C	801	1	14,14,15	0.66	0	15,19,21	1.00	0
2	NAG	C	802	1	14,14,15	0.74	0	15,19,21	0.92	0
2	NAG	C	803	1	14,14,15	0.94	1 (7%)	15,19,21	1.21	2 (13%)
3	NDG	C	804	1	14,14,15	0.63	0	15,19,21	0.81	0
2	NAG	C	805	1	14,14,15	0.70	0	15,19,21	1.07	1 (6%)
2	NAG	C	806	1	14,14,15	0.55	0	15,19,21	1.44	3 (20%)
2	NAG	C	807	1	14,14,15	0.64	0	15,19,21	1.25	2 (13%)
2	NAG	C	808	1	14,14,15	0.66	0	15,19,21	0.67	0
2	NAG	C	809	1	14,14,15	0.78	1 (7%)	15,19,21	0.87	0
2	NAG	C	810	1	14,14,15	0.64	0	15,19,21	1.40	4 (26%)
3	NDG	C	811	1	14,14,15	0.85	0	15,19,21	1.95	1 (6%)
2	NAG	C	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.75	0
3	NDG	C	902	1	14,14,15	1.10	1 (7%)	15,19,21	1.13	1 (6%)
3	NDG	C	903	1	14,14,15	0.52	0	15,19,21	0.80	0
2	NAG	C	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	904	NAG	C1-C2	-2.46	1.49	1.52
2	B	904	NAG	C1-C2	-2.44	1.49	1.52
2	A	904	NAG	C1-C2	-2.42	1.49	1.52
2	C	812	NAG	C1-C2	-2.38	1.49	1.52
2	B	812	NAG	C1-C2	-2.37	1.49	1.52
2	A	812	NAG	C1-C2	-2.36	1.49	1.52
2	C	809	NAG	C1-C2	-2.07	1.49	1.52
2	B	809	NAG	C1-C2	-2.05	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	809	NAG	C1-C2	-2.01	1.49	1.52
2	A	803	NAG	O5-C5	2.42	1.48	1.43
2	B	803	NAG	O5-C5	2.42	1.48	1.43
2	C	803	NAG	O5-C5	2.44	1.48	1.43
3	B	902	NDG	C1-C2	3.20	1.56	1.52
3	C	902	NDG	C1-C2	3.26	1.56	1.52
3	A	902	NDG	C1-C2	3.27	1.57	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-6.87	112.92	122.94
3	A	811	NDG	C2-N2-C7	-6.85	112.95	122.94
3	C	811	NDG	C2-N2-C7	-6.84	112.96	122.94
2	A	806	NAG	C2-N2-C7	-3.36	118.04	122.94
2	B	806	NAG	C2-N2-C7	-3.35	118.05	122.94
2	C	806	NAG	C2-N2-C7	-3.34	118.07	122.94
2	B	805	NAG	C2-N2-C7	-2.97	118.61	122.94
2	A	805	NAG	C2-N2-C7	-2.94	118.66	122.94
2	C	805	NAG	C2-N2-C7	-2.92	118.68	122.94
2	C	807	NAG	C2-N2-C7	-2.85	118.78	122.94
2	B	807	NAG	C2-N2-C7	-2.83	118.81	122.94
2	A	807	NAG	C2-N2-C7	-2.83	118.82	122.94
2	C	803	NAG	C2-N2-C7	-2.79	118.87	122.94
2	A	810	NAG	O5-C1-C2	-2.78	107.60	111.47
2	B	810	NAG	O5-C1-C2	-2.78	107.61	111.47
2	A	803	NAG	C2-N2-C7	-2.75	118.93	122.94
2	B	803	NAG	C2-N2-C7	-2.75	118.94	122.94
2	C	810	NAG	O5-C1-C2	-2.73	107.68	111.47
2	C	810	NAG	C4-C3-C2	-2.46	107.41	111.02
2	B	810	NAG	C4-C3-C2	-2.46	107.41	111.02
2	A	810	NAG	C4-C3-C2	-2.45	107.42	111.02
2	B	807	NAG	O5-C1-C2	-2.45	108.06	111.47
2	A	806	NAG	C4-C3-C2	-2.45	107.43	111.02
2	B	806	NAG	C4-C3-C2	-2.44	107.44	111.02
2	C	807	NAG	O5-C1-C2	-2.44	108.08	111.47
2	A	807	NAG	O5-C1-C2	-2.43	108.08	111.47
2	C	806	NAG	C4-C3-C2	-2.43	107.45	111.02
2	B	806	NAG	O5-C1-C2	-2.39	108.15	111.47
2	A	806	NAG	O5-C1-C2	-2.38	108.17	111.47
2	C	806	NAG	O5-C1-C2	-2.35	108.20	111.47
2	B	810	NAG	C1-O5-C5	-2.17	109.17	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	810	NAG	C1-O5-C5	-2.17	109.17	112.17
2	A	810	NAG	C1-O5-C5	-2.16	109.19	112.17
2	A	812	NAG	C2-N2-C7	-2.01	120.01	122.94
2	A	801	NAG	C1-C2-N2	-2.00	107.07	110.49
2	B	801	NAG	C1-C2-N2	-2.00	107.07	110.49
3	C	902	NDG	O-C1-C2	2.22	114.57	111.47
3	A	902	NDG	O-C1-C2	2.27	114.63	111.47
2	B	810	NAG	C1-C2-N2	2.28	114.38	110.49
3	B	902	NDG	O-C1-C2	2.28	114.65	111.47
2	A	810	NAG	C1-C2-N2	2.30	114.41	110.49
2	C	810	NAG	C1-C2-N2	2.32	114.45	110.49
2	A	803	NAG	C1-O5-C5	2.37	115.44	112.17
2	B	803	NAG	C1-O5-C5	2.38	115.45	112.17
2	C	803	NAG	C1-O5-C5	2.41	115.49	112.17

All (6) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

39 monomers are involved in 300 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	12	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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	NDG	8	0
2	A	904	NAG	8	0
2	B	801	NAG	21	0
2	B	803	NAG	4	0
3	B	804	NDG	2	0
2	B	805	NAG	7	0
2	B	806	NAG	12	0
2	B	807	NAG	16	0
2	B	808	NAG	2	0
2	B	809	NAG	8	0
2	B	810	NAG	13	0
3	B	811	NDG	7	0
2	B	812	NAG	3	0
3	B	902	NDG	8	0
2	B	904	NAG	8	0
2	C	801	NAG	20	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	17	0
2	C	808	NAG	2	0
2	C	809	NAG	8	0
2	C	810	NAG	13	0
3	C	811	NDG	5	0
2	C	812	NAG	3	0
3	C	902	NDG	8	0
2	C	904	NAG	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.