



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:46 PM UTC

PDB ID : 8T22 / pdb_00008t22
EMDB ID : EMD-40978
Title : Cryo-EM structure of mink variant Y453F trimeric spike protein bound to one mink ACE2 receptors at downRBD conformation
Authors : Ahn, H.M.; Calderon, B.; Fan, X.; Gao, Y.; Horgan, N.; Zhou, B.; Liang, B.
Deposited on : 2023-06-05
Resolution : 3.83 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

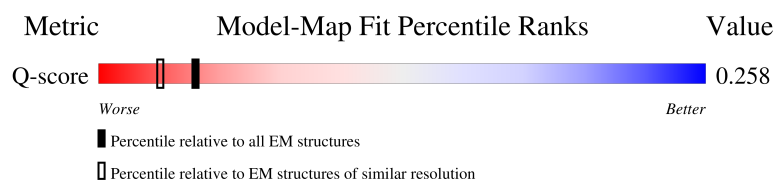
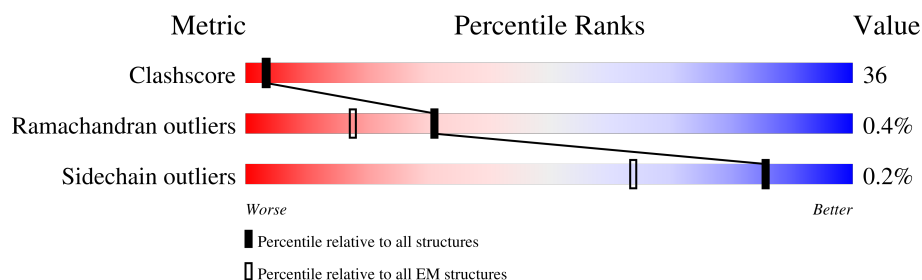
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

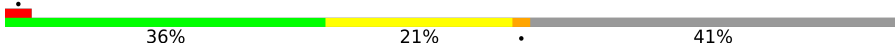
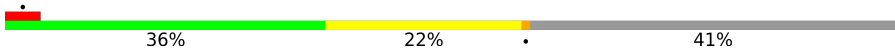
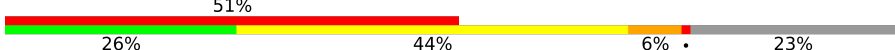
The reported resolution of this entry is 3.83 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9087 (3.33 - 4.33)

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

Mol	Chain	Length	Quality of chain
1	A	1269	
1	B	1269	
1	C	1269	
2	D	771	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23961 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	748	Total	C	N	O	S	0	0
			5813	3714	961	1112	26		
1	B	748	Total	C	N	O	S	0	0
			5813	3714	961	1112	26		
1	C	954	Total	C	N	O	S	0	0
			7431	4748	1234	1416	33		

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	453	PHE	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	SER	-	expression tag	UNP P0DTC2
A	1217	GLY	-	expression tag	UNP P0DTC2
A	1218	TYR	-	expression tag	UNP P0DTC2
A	1219	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	GLU	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	ARG	-	expression tag	UNP P0DTC2
A	1225	ASP	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	GLN	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	TYR	-	expression tag	UNP P0DTC2
A	1230	VAL	-	expression tag	UNP P0DTC2
A	1231	ARG	-	expression tag	UNP P0DTC2
A	1232	LYS	-	expression tag	UNP P0DTC2
A	1233	ASP	-	expression tag	UNP P0DTC2
A	1234	GLY	-	expression tag	UNP P0DTC2
A	1235	GLU	-	expression tag	UNP P0DTC2
A	1236	TRP	-	expression tag	UNP P0DTC2
A	1237	VAL	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	SER	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	SER	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	LEU	-	expression tag	UNP P0DTC2
A	1259	ASN	-	expression tag	UNP P0DTC2
A	1260	ASP	-	expression tag	UNP P0DTC2
A	1261	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1262	PHE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	ALA	-	expression tag	UNP P0DTC2
A	1265	GLN	-	expression tag	UNP P0DTC2
A	1266	LYS	-	expression tag	UNP P0DTC2
A	1267	ILE	-	expression tag	UNP P0DTC2
A	1268	GLU	-	expression tag	UNP P0DTC2
A	1269	TRP	-	expression tag	UNP P0DTC2
A	1270	HIS	-	expression tag	UNP P0DTC2
A	1271	GLU	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	453	PHE	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	SER	-	expression tag	UNP P0DTC2
B	1217	GLY	-	expression tag	UNP P0DTC2
B	1218	TYR	-	expression tag	UNP P0DTC2
B	1219	ILE	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	GLU	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	ARG	-	expression tag	UNP P0DTC2
B	1225	ASP	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1228	ALA	-	expression tag	UNP P0DTC2
B	1229	TYR	-	expression tag	UNP P0DTC2
B	1230	VAL	-	expression tag	UNP P0DTC2
B	1231	ARG	-	expression tag	UNP P0DTC2
B	1232	LYS	-	expression tag	UNP P0DTC2
B	1233	ASP	-	expression tag	UNP P0DTC2
B	1234	GLY	-	expression tag	UNP P0DTC2
B	1235	GLU	-	expression tag	UNP P0DTC2
B	1236	TRP	-	expression tag	UNP P0DTC2
B	1237	VAL	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	THR	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	SER	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	SER	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	GLY	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	GLY	-	expression tag	UNP P0DTC2
B	1258	LEU	-	expression tag	UNP P0DTC2
B	1259	ASN	-	expression tag	UNP P0DTC2
B	1260	ASP	-	expression tag	UNP P0DTC2
B	1261	ILE	-	expression tag	UNP P0DTC2
B	1262	PHE	-	expression tag	UNP P0DTC2
B	1263	GLU	-	expression tag	UNP P0DTC2
B	1264	ALA	-	expression tag	UNP P0DTC2
B	1265	GLN	-	expression tag	UNP P0DTC2
B	1266	LYS	-	expression tag	UNP P0DTC2
B	1267	ILE	-	expression tag	UNP P0DTC2
B	1268	GLU	-	expression tag	UNP P0DTC2
B	1269	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1270	HIS	-	expression tag	UNP P0DTC2
B	1271	GLU	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	453	PHE	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	SER	-	expression tag	UNP P0DTC2
C	1217	GLY	-	expression tag	UNP P0DTC2
C	1218	TYR	-	expression tag	UNP P0DTC2
C	1219	ILE	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	GLU	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	ARG	-	expression tag	UNP P0DTC2
C	1225	ASP	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	GLN	-	expression tag	UNP P0DTC2
C	1228	ALA	-	expression tag	UNP P0DTC2
C	1229	TYR	-	expression tag	UNP P0DTC2
C	1230	VAL	-	expression tag	UNP P0DTC2
C	1231	ARG	-	expression tag	UNP P0DTC2
C	1232	LYS	-	expression tag	UNP P0DTC2
C	1233	ASP	-	expression tag	UNP P0DTC2
C	1234	GLY	-	expression tag	UNP P0DTC2
C	1235	GLU	-	expression tag	UNP P0DTC2

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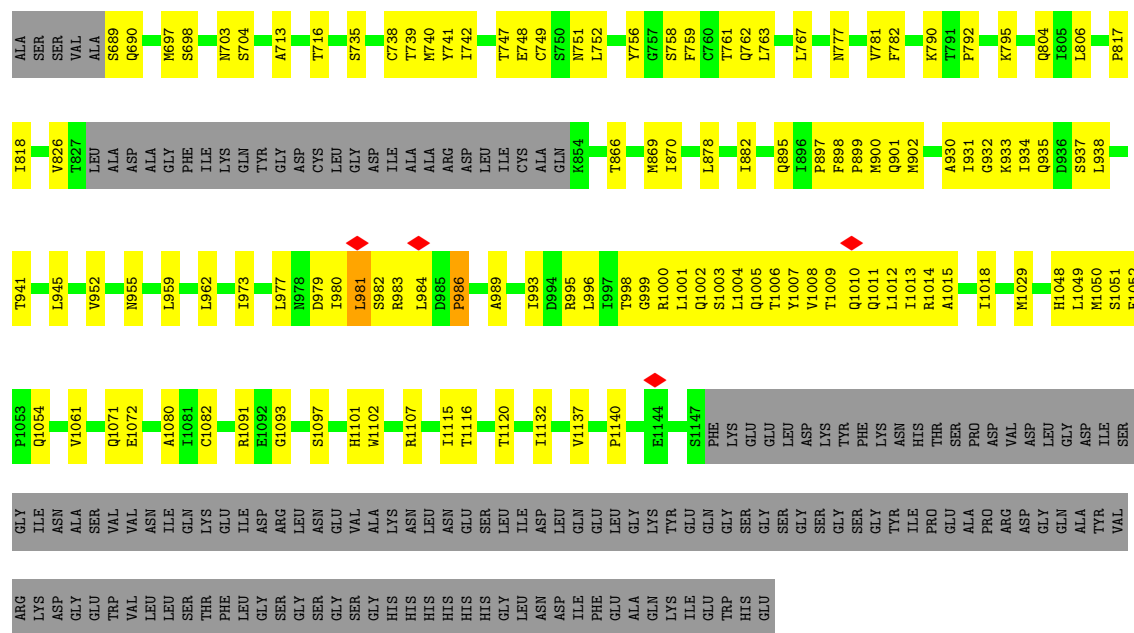
Chain	Residue	Modelled	Actual	Comment	Reference
C	1236	TRP	-	expression tag	UNP P0DTC2
C	1237	VAL	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	THR	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	SER	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	SER	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	GLY	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	GLY	-	expression tag	UNP P0DTC2
C	1258	LEU	-	expression tag	UNP P0DTC2
C	1259	ASN	-	expression tag	UNP P0DTC2
C	1260	ASP	-	expression tag	UNP P0DTC2
C	1261	ILE	-	expression tag	UNP P0DTC2
C	1262	PHE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	ALA	-	expression tag	UNP P0DTC2
C	1265	GLN	-	expression tag	UNP P0DTC2
C	1266	LYS	-	expression tag	UNP P0DTC2
C	1267	ILE	-	expression tag	UNP P0DTC2
C	1268	GLU	-	expression tag	UNP P0DTC2
C	1269	TRP	-	expression tag	UNP P0DTC2
C	1270	HIS	-	expression tag	UNP P0DTC2
C	1271	GLU	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme.

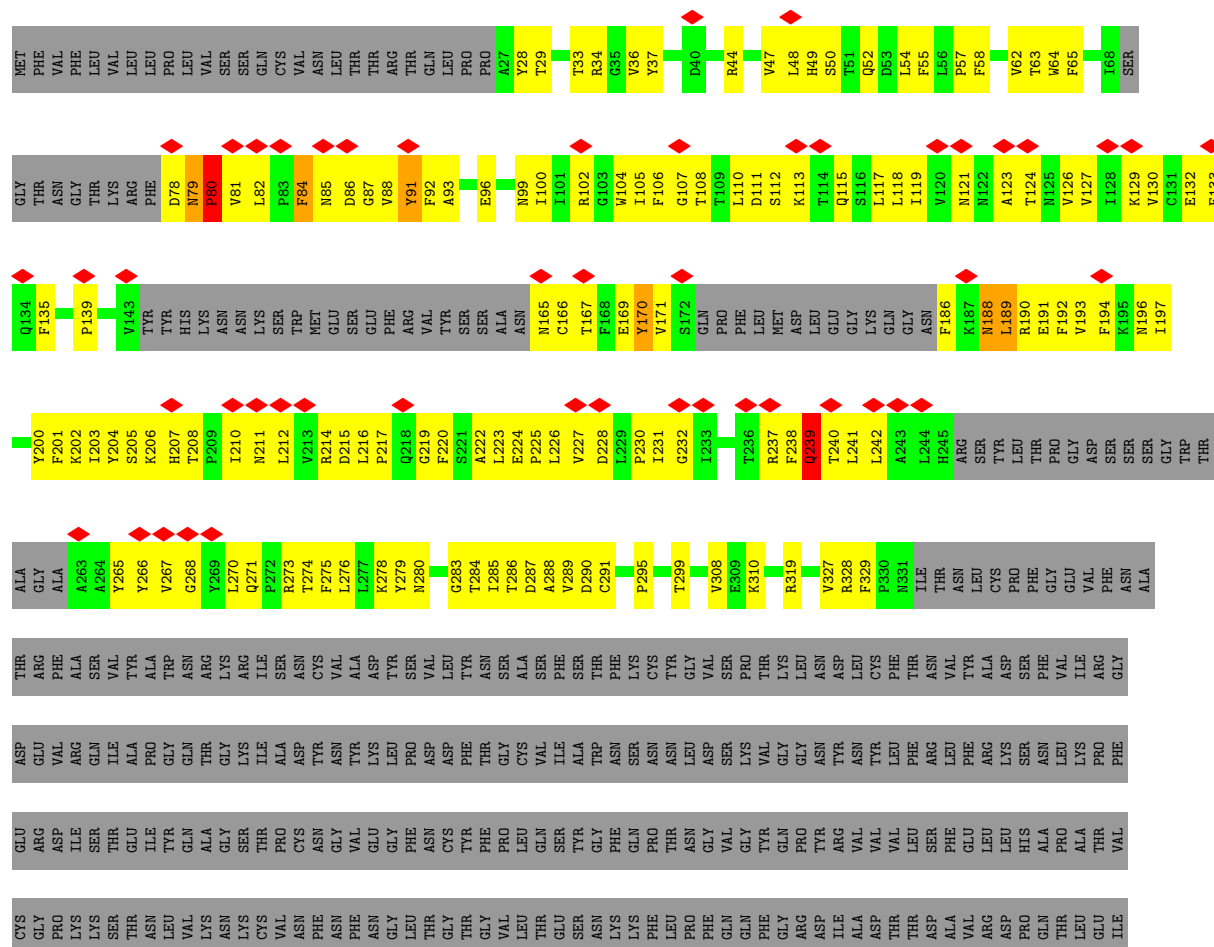
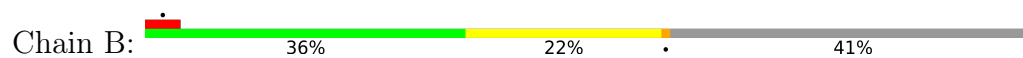
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	596	Total	C	N	O	S	0	0
			4904	3133	824	918	29		

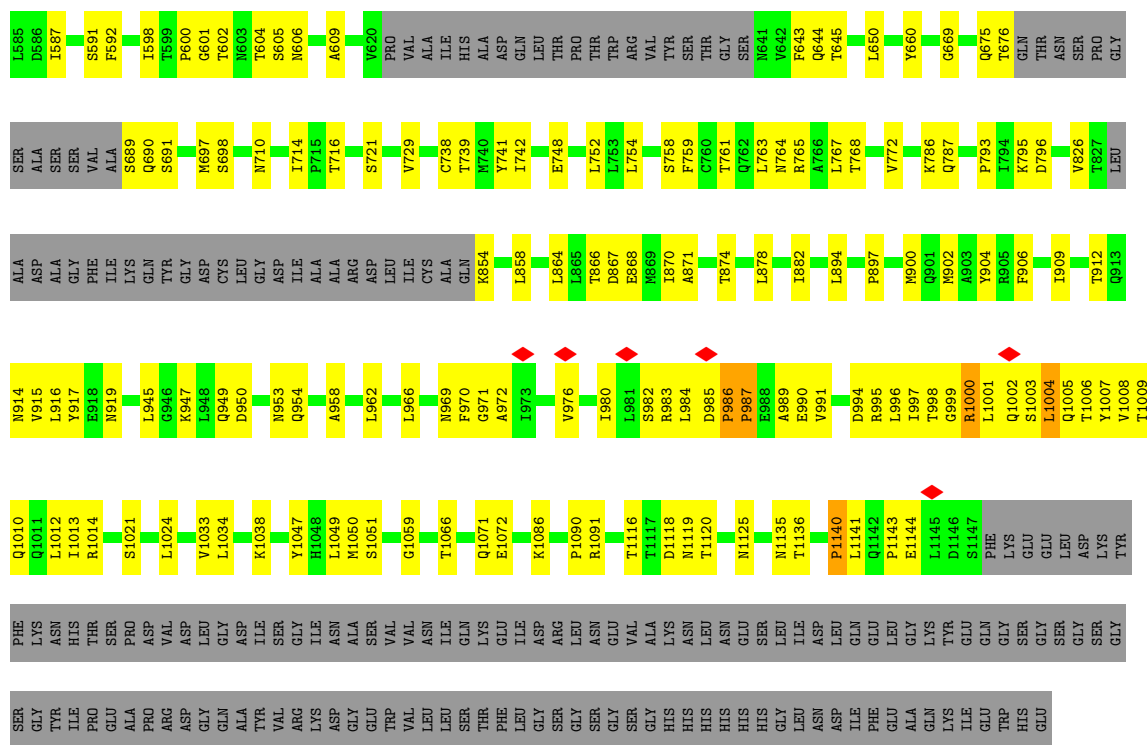
There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	740	GLY	-	expression tag	UNP A0A7T0Q2W2
D	741	SER	-	expression tag	UNP A0A7T0Q2W2
D	742	GLY	-	expression tag	UNP A0A7T0Q2W2
D	743	SER	-	expression tag	UNP A0A7T0Q2W2
D	744	GLY	-	expression tag	UNP A0A7T0Q2W2
D	745	SER	-	expression tag	UNP A0A7T0Q2W2
D	746	GLY	-	expression tag	UNP A0A7T0Q2W2
D	747	HIS	-	expression tag	UNP A0A7T0Q2W2
D	748	HIS	-	expression tag	UNP A0A7T0Q2W2
D	749	HIS	-	expression tag	UNP A0A7T0Q2W2
D	750	HIS	-	expression tag	UNP A0A7T0Q2W2
D	751	HIS	-	expression tag	UNP A0A7T0Q2W2
D	752	HIS	-	expression tag	UNP A0A7T0Q2W2
D	753	GLY	-	expression tag	UNP A0A7T0Q2W2
D	754	SER	-	expression tag	UNP A0A7T0Q2W2
D	755	GLY	-	expression tag	UNP A0A7T0Q2W2
D	756	SER	-	expression tag	UNP A0A7T0Q2W2
D	757	GLY	-	expression tag	UNP A0A7T0Q2W2
D	758	LEU	-	expression tag	UNP A0A7T0Q2W2
D	759	ASN	-	expression tag	UNP A0A7T0Q2W2
D	760	ASP	-	expression tag	UNP A0A7T0Q2W2
D	761	ILE	-	expression tag	UNP A0A7T0Q2W2
D	762	PHE	-	expression tag	UNP A0A7T0Q2W2
D	763	GLU	-	expression tag	UNP A0A7T0Q2W2
D	764	ALA	-	expression tag	UNP A0A7T0Q2W2
D	765	GLN	-	expression tag	UNP A0A7T0Q2W2
D	766	LYS	-	expression tag	UNP A0A7T0Q2W2
D	767	ILE	-	expression tag	UNP A0A7T0Q2W2
D	768	GLU	-	expression tag	UNP A0A7T0Q2W2
D	769	TRP	-	expression tag	UNP A0A7T0Q2W2
D	770	HIS	-	expression tag	UNP A0A7T0Q2W2
D	771	GLU	-	expression tag	UNP A0A7T0Q2W2

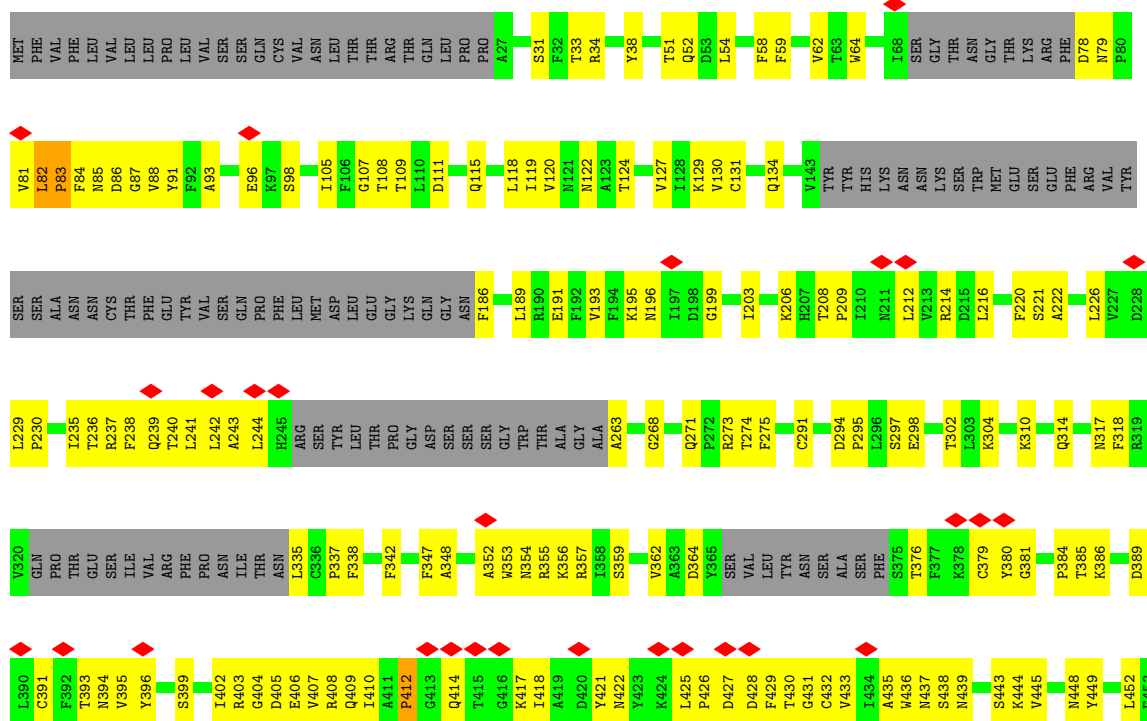


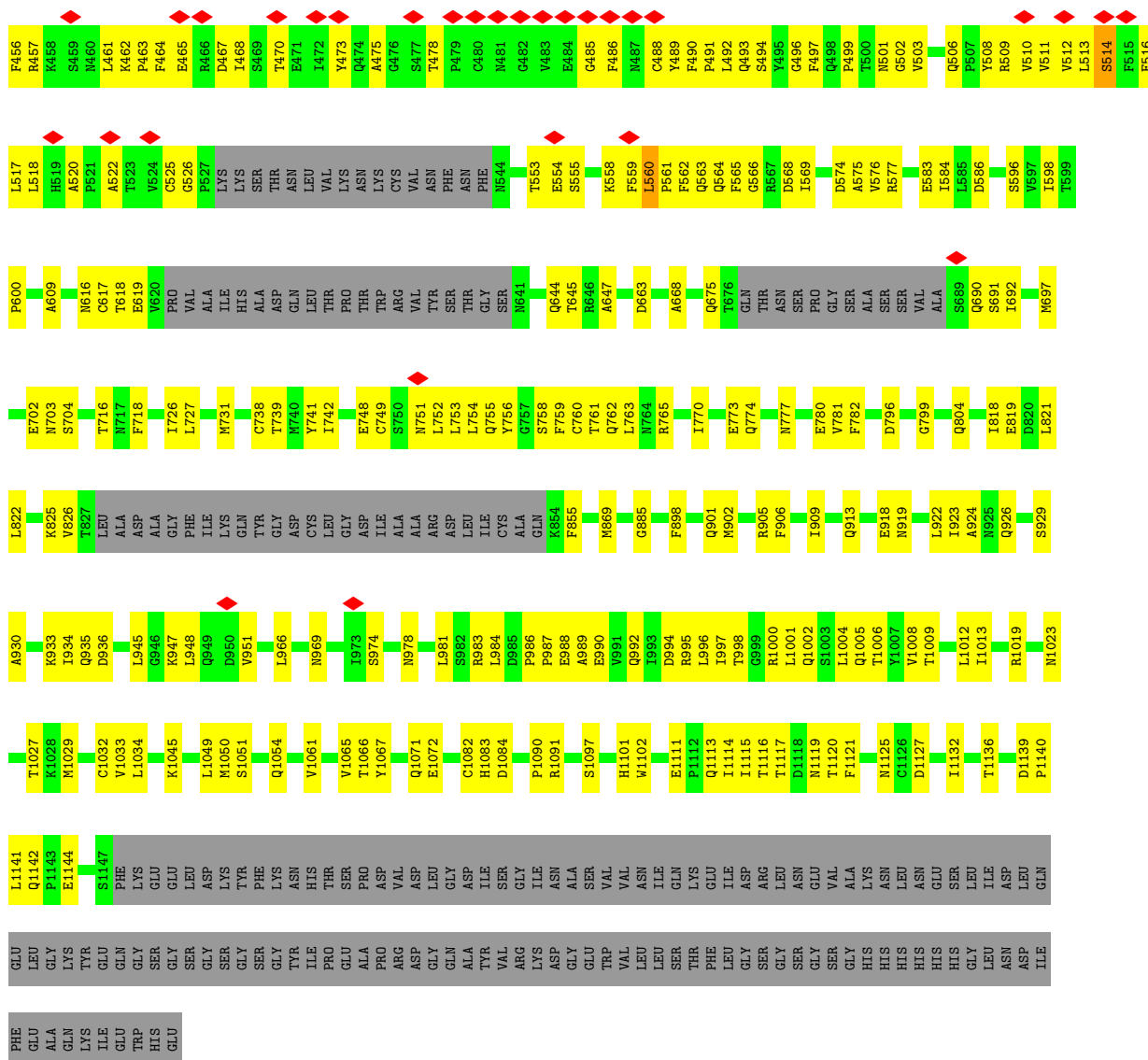
• Molecule 1: Spike glycoprotein



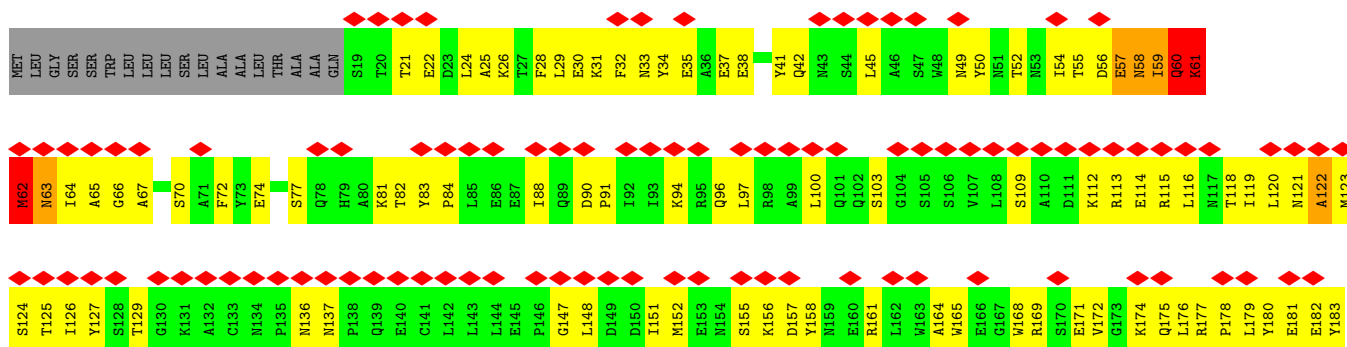


• Molecule 1: Spike glycoprotein





• Molecule 2: Angiotensin-converting enzyme



PRO	THR	VAL	ASP	D609	E549	V485	P425	T365	R305	R245	V184
LEU	GLU	ARG	GLN	V610	A550	G486	P426	M366	R306	A246	A185
PRO	VAL	VAL	GLN	G551	G551	V487	D427	D367	I307	K247	L186
PRO	SER	SER	ASP	P612	V488	D428	F428	D368	F308	L248	K187
ASP	LEU	ASP	LEU	V613	E489	S429	S429	F369	K309	M249	N188
GLN	LYS	LEU	ASP	A614	P490	E430	E430	L370	E310	D250	E189
PRO	GLN	GLN	ASP	L491	L491	D431	D431	T371	A311	A251	M190
PRO	PRO	GLN	P492	P492	P492	S432	S432	A372	E312	Y252	A191
VAL	VAL	ILE	H493	H493	H493	E433	E433	H373	K313	P253	R192
GLY	SER	ILE	D494	D494	D494	T434	T434	H374	F314	S254	A193
SER	PHE	VAL	D435	D435	D435	I436	I436	E375	F315	R255	N194
GLY	ASN	ARG	I436	I436	I436	M376	M376	G377	V316	I256	N195
SER	PHE	ILE	L560	L560	L560	G377	G377	H378	V318	S257	Y196
GLY	ILE	SER	M437	M437	M437	H378	H378	G319	E197	P258	E197
SER	VAL	LEU	F438	F438	F438	L379	L379	L320	T259	G260	D198
GLY	THR	LYS	P500	P500	P500	Q380	Q380	P321	G260	C261	G200
HIS	SER	SER	A501	A501	A501	Y381	Y381	P321	G260	C261	G200
HIS	PRO	ALA	K564	K564	K564	D382	D382	P321	G260	C261	G200
HIS	GLU	LEU	A502	A502	A502	M383	M383	P321	G260	C261	G200
HIS	ASN	GLY	A443	A443	A443	A384	A384	M323	L262	G261	D201
HIS	ASN	GLY	I444	I444	I444	Y385	Y385	T324	P263	Y202	Y202
GLY	ASP	ALA	T445	T445	T445	A386	A386	G326	A264	W203	W203
SER	ILE	TRP	I446	I446	I446	A387	A387	F327	L266	G204	G204
GLY	ILE	GLU	V447	V447	V447	Q388	Q388	W328	L267	D206	D206
SER	TRP	TRP	G448	G448	G448	P389	P389	Q329	D269	W270	Y207
ASN	ASN	ASN	L449	L449	L449	F390	F390	N330	M270	E208	E208
LEU	LEU	ALA	L450	L450	L450	L391	L391	S331	W271	E210	E210
ASN	ASN	ASN	P451	P451	P451	R392	R392	M332	G272	W211	W211
VAL	VAL	GLU	F452	F452	F452	R393	R393	L333	R273	A212	A212
ILE	GLU	MET	T453	T453	T453	G394	G394	T334	F274	D213	D213
PHE	GLU	TRP	Y454	Y454	Y454	G395	G395	E335	W275	T276	T276
ALA	ALA	PHE	L456	L456	L456	A396	A396	P336	T276	N216	N216
ILE	ILE	PHE	E457	E457	E457	N397	N397	G337	N277	Y217	Y217
GLN	ARG	GLN	L458	L458	L458	E398	E398	D338	L278	S218	S218
LYS	LYS	SER	W459	W459	W459	G399	G399	N339	Y279	R219	R219
ILE	ILE	SER	Y459	Y459	Y459	F400	F400	R340	P280	Q221	Q221
ARG	GLY	ILE	R460	R460	R460	H401	H401	K341	L281	I222	I222
GLY	ALA	ALA	W461	W461	W461	A402	A402	V342	E282	E224	E224
TRP	TRP	ALA	M462	M462	M462	A403	A403	V343	G283	D225	D225
HIS	ASN	ASN	V463	V463	V463	V404	V404	V343	F285	V226	V226
ASP	ASP	ARG	F464	F464	F464	G405	G405	C344	Q287	H228	H228
GLY	PHE	TRP	K465	K465	K465	E406	E406	H345	K288	P289	P289
LEU	LEU	PHE	G466	G466	G466	I407	I407	P346	N290	F230	F230
ASP	ASP	LYS	E467	E467	E467	M408	M408	S409	L291	T231	T231
ASN	ASN	VAL	I468	I468	I468	G409	G409	A348	Q232	Q233	Q233
LYS	LYS	LYS	P469	P469	P469	S411	S411	W349	V292	I233	I233
LEU	GLN	GLN	K470	K470	K470	A412	A412	D350	T294	K234	K234
THR	THR	ILE	E471	E471	E471	A413	A413	L351	D295	P235	P235
LEU	PRO	PRO	Q472	Q472	Q472	T414	T414	G352	A296	L236	L236
PHE	GLY	GLY	W473	W473	W473	P415	P415	K353	M297	E238	E238
ILE	ILE	PHE	M474	M474	M474	H417	H417	H354	Q300	L240	L240
VAL	VAL	VAL	Q475	Q475	Q475	L418	L418	D355	S301	H241	H241
ASP	ASP	ASP	K476	K476	K476	K419	K419	F356	W302	A242	A242
LYS	LYS	LYS	W477	W477	W477	K419	K419	R357	D303	A304	A304
GLN	GLN	GLN	W478	W478	W478	N420	N420	R357			
LYS	LYS	LYS	Y479	Y479	Y479	I421	I421	I358			
PRO	PRO	PRO	E479	E479	E479	G422	G422	K359			
GLY	GLY	GLY	M480	M480	M480	L423	L423	M360			
VAL	VAL	VAL	K481	K481	K481	G423	G423	C361			
ASP	ASP	ASP	R482	R482	R482	L424	L424	T362			
GLN	GLN	GLN	D483	D483	D483			K363			
LYS	LYS	LYS	I484	I484	I484			V364			
GLY	GLY	GLY									
ASN	ASN	ASN									
LEU	LEU	LEU									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
LYS	LYS	LYS									
ILE	ILE	ILE									
ARG	ARG	ARG									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
LYS	LYS	LYS									
ILE	ILE	ILE									
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GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
LYS	LYS	LYS									
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ARG	ARG	ARG									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
LYS	LYS	LYS									
ILE	ILE	ILE									
ARG	ARG	ARG									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
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ARG	ARG	ARG									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
LYS	LYS	LYS									
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GLN	GLN	GLN									
LYS	LYS	LYS									
ILE	ILE	ILE									
ARG	ARG	ARG									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
LYS	LYS	LYS									
ILE	ILE	ILE									
ARG	ARG	ARG									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
LYS	LYS	LYS									
ILE	ILE	ILE									
ARG	ARG	ARG									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
LYS	LYS	LYS									
ILE	ILE	ILE									
ARG	ARG	ARG									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
LYS	LYS	LYS									
ILE	ILE	ILE									
ARG	ARG	ARG									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
LYS	LYS	LYS									
ILE	ILE	ILE									
ARG	ARG	ARG									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									
GLN	GLN	GLN									
LYS	LYS	LYS									
ILE	ILE	ILE									
ARG	ARG	ARG									
GLY	GLY	GLY									
THR	THR	THR									
VAL	VAL	VAL									
ASP	ASP	ASP									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146697	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.98	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.865	Depositor
Minimum map value	-0.655	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.309	Depositor
Map size ($\text{\AA}$)	568.32, 568.32, 568.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/5938	0.68	15/8084 (0.2%)
1	B	0.22	0/5938	0.56	4/8084 (0.0%)
1	C	0.25	3/7598 (0.0%)	0.58	8/10340 (0.1%)
2	D	0.79	16/5047 (0.3%)	1.30	69/6854 (1.0%)
All	All	0.43	19/24521 (0.1%)	0.80	96/33362 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17
1	B	0	7
1	C	0	3
2	D	0	29
All	All	0	56

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	63	ASN	N-CA	19.03	1.68	1.46
2	D	62	MET	C-N	18.49	1.56	1.33
2	D	60	GLN	CA-C	15.86	1.74	1.52
2	D	542	CYS	CA-C	11.49	1.67	1.52
2	D	530	CYS	CA-C	10.08	1.67	1.52
2	D	60	GLN	N-CA	9.77	1.59	1.46
2	D	63	ASN	CA-C	9.30	1.64	1.52
2	D	60	GLN	C-N	9.27	1.46	1.33
2	D	530	CYS	N-CA	8.10	1.56	1.46
2	D	543	ASP	N-CA	8.02	1.56	1.46
1	C	412	PRO	CG-CD	-7.67	1.24	1.50
2	D	542	CYS	C-N	7.45	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	570	LEU	CA-C	6.37	1.60	1.52
2	D	530	CYS	CB-SG	6.34	2.02	1.81
1	C	83	PRO	CG-CD	-6.28	1.29	1.50
1	C	412	PRO	N-CD	5.80	1.55	1.47
2	D	62	MET	CB-CG	5.69	1.69	1.52
2	D	569	ALA	N-CA	5.46	1.52	1.46
2	D	569	ALA	CA-C	5.37	1.60	1.52

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	542	CYS	CA-C-N	15.32	150.80	121.54
2	D	542	CYS	C-N-CA	15.32	150.80	121.54
2	D	200	GLY	N-CA-C	15.00	148.73	113.18
1	C	412	PRO	CA-N-CD	-13.96	92.45	112.00
1	C	83	PRO	CA-N-CD	-13.38	93.27	112.00
2	D	62	MET	CA-C-O	-13.16	106.47	120.42
2	D	62	MET	CB-CG-SD	12.71	150.84	112.70
2	D	569	ALA	N-CA-C	12.29	127.58	112.59
2	D	532	ILE	CA-C-N	-11.70	105.15	122.24
2	D	532	ILE	C-N-CA	-11.70	105.15	122.24
2	D	530	CYS	N-CA-C	11.62	127.21	112.92
2	D	63	ASN	N-CA-CB	11.46	127.24	109.82
2	D	542	CYS	N-CA-CB	-10.84	95.60	110.67
2	D	62	MET	CA-C-N	10.02	134.72	120.79
2	D	62	MET	C-N-CA	10.02	134.72	120.79
2	D	122	ALA	CA-C-N	-9.87	106.87	122.65
2	D	122	ALA	C-N-CA	-9.87	106.87	122.65
2	D	557	MET	CA-C-N	9.78	140.22	121.54
2	D	557	MET	C-N-CA	9.78	140.22	121.54
1	C	412	PRO	N-CD-CG	-9.72	88.63	103.20
2	D	60	GLN	CA-C-N	9.33	139.36	121.54
2	D	60	GLN	C-N-CA	9.33	139.36	121.54
2	D	61	LYS	CA-CB-CG	8.87	131.84	114.10
2	D	63	ASN	N-CA-C	8.67	121.59	111.02
1	C	209	PRO	CA-N-CD	-8.61	99.95	112.00
2	D	568	PHE	N-CA-C	8.48	122.12	111.69
2	D	529	LEU	N-CA-C	8.47	120.13	111.07
1	B	1140	PRO	CA-N-CD	-8.43	100.21	112.00
1	A	215	ASP	CA-C-N	8.37	135.79	122.56
1	A	215	ASP	C-N-CA	8.37	135.79	122.56
2	D	464	PHE	N-CA-C	8.30	128.49	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	543	ASP	N-CA-C	8.29	128.46	110.80
2	D	63	ASN	CB-CA-C	-8.18	97.92	110.92
2	D	540	TYR	N-CA-C	-8.07	99.88	110.53
1	C	1032	CYS	CA-C-N	-8.04	113.06	122.63
1	C	1032	CYS	C-N-CA	-8.04	113.06	122.63
2	D	260	GLY	N-CA-C	7.84	123.84	112.55
1	A	93	ALA	N-CA-C	7.67	120.84	107.49
2	D	542	CYS	N-CA-C	7.61	123.71	113.97
2	D	60	GLN	O-C-N	-7.40	112.51	122.43
2	D	556	GLU	CA-C-N	-7.18	109.43	122.50
2	D	556	GLU	C-N-CA	-7.18	109.43	122.50
2	D	542	CYS	O-C-N	-7.18	113.80	122.48
2	D	567	THR	CA-C-N	7.17	132.84	120.58
2	D	567	THR	C-N-CA	7.17	132.84	120.58
1	B	80	PRO	N-CA-C	7.12	127.13	112.47
1	C	83	PRO	N-CD-CG	-7.09	92.56	103.20
1	A	239	GLN	N-CA-C	6.98	120.61	109.24
1	A	30	ASN	N-CA-C	6.91	121.29	110.17
2	D	60	GLN	N-CA-C	6.90	120.96	112.54
2	D	62	MET	CB-CA-C	6.89	122.56	110.85
2	D	450	LEU	N-CA-C	6.73	124.69	109.81
2	D	524	GLN	CA-CB-CG	-6.73	100.64	114.10
2	D	558	LEU	CA-CB-CG	6.70	139.76	116.30
2	D	314	PHE	N-CA-CB	-6.47	99.65	110.39
2	D	57	GLU	N-CA-C	-6.37	103.60	111.75
1	A	31	SER	CA-C-N	6.36	133.68	121.54
1	A	31	SER	C-N-CA	6.36	133.68	121.54
1	A	215	ASP	N-CA-C	6.31	119.25	109.60
1	C	412	PRO	CA-CB-CG	-6.24	92.64	104.50
1	A	86	ASP	N-CA-C	6.12	122.84	112.99
1	B	239	GLN	CA-CB-CG	6.11	126.32	114.10
1	A	98	SER	N-CA-C	6.10	123.79	110.80
2	D	569	ALA	CA-C-N	6.03	139.20	122.15
2	D	569	ALA	C-N-CA	6.03	139.20	122.15
2	D	557	MET	N-CA-C	5.98	119.81	111.56
2	D	465	LYS	CB-CA-C	-5.96	98.56	110.42
2	D	529	LEU	CA-C-O	-5.93	114.59	120.82
2	D	564	LYS	N-CA-C	-5.72	97.40	108.45
1	A	88	VAL	CA-C-N	5.70	132.42	121.54
1	A	88	VAL	C-N-CA	5.70	132.42	121.54
1	A	239	GLN	CB-CA-C	-5.69	100.37	109.75
2	D	62	MET	CA-CB-CG	5.67	125.44	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	530	CYS	CA-CB-SG	5.66	127.42	114.40
1	B	1004	LEU	CA-CB-CG	5.66	136.09	116.30
2	D	518	ARG	CA-CB-CG	-5.63	102.84	114.10
2	D	195	ASN	CA-C-N	5.57	132.17	121.54
2	D	195	ASN	C-N-CA	5.57	132.17	121.54
2	D	328	TRP	CA-CB-CG	5.56	124.17	113.60
2	D	463	VAL	CA-C-N	-5.50	111.04	121.54
2	D	463	VAL	C-N-CA	-5.50	111.04	121.54
2	D	527	GLU	CA-C-N	-5.48	111.87	122.06
2	D	527	GLU	C-N-CA	-5.48	111.87	122.06
2	D	61	LYS	CA-C-N	-5.40	112.62	120.29
2	D	61	LYS	C-N-CA	-5.40	112.62	120.29
1	A	209	PRO	N-CA-C	5.39	123.58	112.47
2	D	557	MET	N-CA-CB	-5.26	103.91	111.54
2	D	449	THR	CA-C-N	5.24	134.59	121.80
2	D	449	THR	C-N-CA	5.24	134.59	121.80
2	D	196	TYR	CA-C-N	-5.21	111.59	121.54
2	D	196	TYR	C-N-CA	-5.21	111.59	121.54
2	D	465	LYS	CA-C-N	5.19	131.59	121.41
2	D	465	LYS	C-N-CA	5.19	131.59	121.41
2	D	529	LEU	CA-CB-CG	5.19	134.47	116.30
2	D	63	ASN	O-C-N	-5.17	116.55	122.08
1	A	194	PHE	N-CA-C	-5.13	105.31	112.03

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	TRP	Peptide
1	A	119	ILE	Peptide
1	A	129	LYS	Peptide
1	A	166	CYS	Peptide
1	A	169	GLU	Peptide
1	A	214	ARG	Peptide
1	A	220	PHE	Peptide
1	A	236	THR	Peptide
1	A	238	PHE	Peptide
1	A	239	GLN	Peptide
1	A	240	THR	Peptide
1	A	29	THR	Peptide
1	A	30	ASN	Peptide
1	A	33	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	83	PRO	Peptide
1	A	91	TYR	Peptide
1	A	986	PRO	Mainchain
1	B	170	TYR	Peptide
1	B	188	ASN	Peptide
1	B	79	ASN	Peptide
1	B	84	PHE	Peptide
1	B	91	TYR	Peptide
1	B	982	SER	Peptide
1	B	987	PRO	Peptide
1	C	395	VAL	Peptide
1	C	514	SER	Peptide
1	C	560	LEU	Peptide
2	D	157	ASP	Peptide
2	D	252	TYR	Peptide
2	D	253	PRO	Peptide
2	D	264	ALA	Peptide
2	D	266	LEU	Peptide
2	D	270	MET	Peptide
2	D	311	ALA	Peptide
2	D	345	HIS	Peptide
2	D	374	HIS	Peptide
2	D	389	PRO	Peptide
2	D	408	MET	Peptide
2	D	431	ASP	Peptide
2	D	450	LEU	Peptide
2	D	470	LYS	Peptide
2	D	472	GLN	Peptide
2	D	493	HIS	Peptide
2	D	532	ILE	Peptide
2	D	540	TYR	Peptide
2	D	542	CYS	Peptide,Mainchain
2	D	553	LYS	Mainchain
2	D	564	LYS	Peptide
2	D	569	ALA	Peptide
2	D	571	GLU	Peptide
2	D	58	ASN	Mainchain
2	D	598	GLN	Peptide
2	D	60	GLN	Mainchain
2	D	61	LYS	Peptide
2	D	62	MET	Peptide

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	5813	0	5715	388	0
1	B	5813	0	5715	283	0
1	C	7431	0	7268	325	0
2	D	4904	0	4667	755	0
All	All	23961	0	23365	1709	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 36.

All (1709) 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)
2:D:60:GLN:CA	2:D:60:GLN:C	1.74	1.59
2:D:63:ASN:N	2:D:63:ASN:CA	1.68	1.52
2:D:530:CYS:SG	2:D:530:CYS:CB	2.02	1.48
2:D:558:LEU:H	2:D:570:LEU:N	1.19	1.39
2:D:531:GLN:N	2:D:543:ASP:H	1.32	1.27
2:D:531:GLN:N	2:D:543:ASP:N	1.87	1.22
2:D:61:LYS:H	2:D:63:ASN:CA	1.52	1.22
2:D:530:CYS:N	2:D:542:CYS:HB2	1.55	1.19
2:D:248:LEU:O	2:D:252:TYR:HB2	1.39	1.19
2:D:60:GLN:N	2:D:63:ASN:HA	1.57	1.16
2:D:61:LYS:H	2:D:63:ASN:N	1.41	1.16
2:D:61:LYS:O	2:D:65:ALA:HB3	1.45	1.16
2:D:203:TRP:HB2	2:D:464:PHE:HB2	1.28	1.16
2:D:531:GLN:H	2:D:542:CYS:C	1.55	1.14
2:D:61:LYS:N	2:D:63:ASN:C	2.04	1.13
2:D:59:ILE:O	2:D:62:MET:O	1.65	1.13
2:D:558:LEU:N	2:D:570:LEU:H	1.44	1.13
2:D:61:LYS:HA	2:D:65:ALA:H	1.02	1.09
2:D:526:GLN:O	2:D:542:CYS:HB3	1.53	1.09
2:D:202:TYR:H	2:D:465:LYS:HB2	0.98	1.08
2:D:530:CYS:H	2:D:542:CYS:CB	1.64	1.08
2:D:58:ASN:O	2:D:62:MET:CB	2.03	1.07
2:D:61:LYS:HD3	2:D:64:ILE:HG12	1.32	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:558:LEU:N	2:D:570:LEU:N	2.00	1.06
2:D:61:LYS:N	2:D:63:ASN:N	2.01	1.05
1:A:87:GLY:N	1:A:237:ARG:O	1.89	1.04
1:B:80:PRO:HG2	1:B:241:LEU:HB2	1.39	1.04
2:D:527:GLU:O	2:D:542:CYS:HA	1.56	1.04
1:A:84:PHE:O	1:A:238:PHE:N	1.91	1.03
2:D:60:GLN:C	2:D:63:ASN:C	2.27	1.02
2:D:533:ALA:H	2:D:543:ASP:C	1.66	1.02
2:D:307:ILE:O	2:D:311:ALA:HB3	1.60	1.02
2:D:57:GLU:O	2:D:61:LYS:HB2	1.58	1.01
2:D:123:MET:HB2	2:D:179:LEU:HG	1.39	1.01
2:D:61:LYS:N	2:D:63:ASN:CA	2.23	1.00
2:D:200:GLY:N	2:D:466:GLY:H	1.58	0.99
2:D:530:CYS:H	2:D:542:CYS:HB2	0.83	0.99
2:D:164:ALA:HB1	2:D:266:LEU:HB2	1.43	0.99
1:A:98:SER:H	1:A:209:PRO:HB2	1.28	0.99
2:D:58:ASN:O	2:D:62:MET:CA	2.11	0.99
2:D:200:GLY:H	2:D:466:GLY:H	0.99	0.99
2:D:183:TYR:O	2:D:187:LYS:HB3	1.61	0.98
1:A:187:LYS:HG2	1:A:242:LEU:HA	1.44	0.98
2:D:60:GLN:O	2:D:66:GLY:N	1.95	0.98
1:B:84:PHE:HB2	1:B:237:ARG:HA	1.43	0.98
2:D:531:GLN:H	2:D:542:CYS:CA	1.76	0.97
2:D:63:ASN:N	2:D:63:ASN:HA	1.77	0.97
2:D:61:LYS:N	2:D:62:MET:C	2.23	0.97
2:D:61:LYS:CA	2:D:65:ALA:H	1.78	0.97
2:D:58:ASN:O	2:D:62:MET:C	2.07	0.97
2:D:59:ILE:O	2:D:62:MET:C	2.07	0.97
2:D:151:ILE:O	2:D:155:SER:HB3	1.65	0.97
2:D:190:MET:O	2:D:193:ALA:C	2.08	0.96
2:D:558:LEU:HB2	2:D:571:GLU:N	1.79	0.96
2:D:529:LEU:O	2:D:543:ASP:C	2.09	0.96
2:D:60:GLN:C	2:D:62:MET:O	2.09	0.95
2:D:477:TRP:O	2:D:481:LYS:HB2	1.65	0.94
2:D:526:GLN:NE2	2:D:530:CYS:SG	2.40	0.94
2:D:531:GLN:N	2:D:542:CYS:N	2.15	0.94
2:D:202:TYR:N	2:D:465:LYS:HB2	1.81	0.94
2:D:390:PHE:HA	2:D:393:ARG:HE	1.32	0.94
2:D:61:LYS:HA	2:D:65:ALA:N	1.83	0.94
2:D:403:ALA:H	2:D:514:ARG:HH12	1.15	0.93
2:D:311:ALA:HA	2:D:314:PHE:HB3	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:177:ARG:O	2:D:181:GLU:HB2	1.69	0.92
1:A:220:PHE:HA	1:A:287:ASP:H	1.34	0.92
1:A:98:SER:HB3	1:A:210:ILE:H	1.35	0.91
2:D:238:GLU:O	2:D:599:ASN:ND2	2.04	0.91
1:A:213:VAL:HG13	1:A:214:ARG:HG2	1.53	0.91
2:D:533:ALA:N	2:D:543:ASP:O	2.04	0.91
2:D:261:CYS:H	2:D:613:TYR:HB2	1.36	0.90
1:A:187:LYS:HE3	1:A:210:ILE:HG23	1.54	0.90
1:A:126:VAL:HG22	1:A:168:PHE:HB2	1.53	0.90
1:B:1009:THR:HA	1:B:1012:LEU:HG	1.54	0.89
2:D:382:ASP:O	2:D:386:ALA:N	2.06	0.89
2:D:531:GLN:CA	2:D:543:ASP:H	1.86	0.89
2:D:61:LYS:N	2:D:64:ILE:N	2.21	0.88
1:C:83:PRO:HA	1:C:237:ARG:HA	1.54	0.88
1:A:187:LYS:HD2	1:A:208:THR:O	1.73	0.88
1:C:1050:MET:HE3	1:C:1051:SER:H	1.39	0.88
1:B:81:VAL:N	1:B:240:THR:O	2.06	0.87
2:D:553:LYS:HB2	2:D:573:VAL:HG11	1.56	0.87
1:B:79:ASN:O	1:B:239:GLN:HG2	1.74	0.87
2:D:411:SER:HB2	2:D:522:GLN:HG3	1.56	0.87
1:A:86:ASP:H	1:A:238:PHE:HA	1.40	0.86
1:B:986:PRO:HB2	1:B:987:PRO:HD2	1.53	0.86
2:D:60:GLN:C	2:D:60:GLN:HA	2.00	0.86
2:D:59:ILE:C	2:D:62:MET:C	2.44	0.86
2:D:239:HIS:HB3	2:D:595:LEU:HA	1.58	0.85
2:D:570:LEU:HD23	2:D:574:VAL:HG21	1.58	0.85
2:D:33:ASN:O	2:D:37:GLU:HB3	1.75	0.85
2:D:177:ARG:O	2:D:181:GLU:CB	2.23	0.85
2:D:532:ILE:H	2:D:542:CYS:C	1.85	0.85
2:D:529:LEU:O	2:D:543:ASP:HA	1.75	0.84
2:D:347:THR:H	2:D:361:CYS:HB2	1.43	0.84
2:D:527:GLU:O	2:D:542:CYS:CA	2.25	0.84
2:D:558:LEU:HB2	2:D:571:GLU:H	1.40	0.84
2:D:588:PHE:HA	2:D:591:LEU:HD23	1.60	0.83
1:A:1006:THR:HA	1:A:1009:THR:HB	1.59	0.83
2:D:557:MET:HA	2:D:568:PHE:O	1.78	0.83
1:C:380:TYR:HE2	1:C:430:THR:HG22	1.42	0.83
2:D:199:TYR:O	2:D:463:VAL:HA	1.79	0.83
1:A:88:VAL:HG12	1:A:91:TYR:H	1.42	0.83
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.61	0.83
2:D:161:ARG:HE	2:D:264:ALA:HA	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:530:CYS:C	2:D:542:CYS:H	1.88	0.82
2:D:530:CYS:C	2:D:542:CYS:N	2.37	0.82
2:D:241:HIS:O	2:D:245:ARG:HB2	1.79	0.82
2:D:558:LEU:H	2:D:569:ALA:C	1.88	0.82
1:A:187:LYS:HZ3	1:A:216:LEU:HG	1.44	0.81
2:D:558:LEU:H	2:D:570:LEU:H	0.83	0.81
1:A:31:SER:HB3	1:A:88:VAL:HB	1.61	0.81
1:A:30:ASN:OD1	1:A:94:SER:OG	1.99	0.81
1:B:985:ASP:O	1:B:989:ALA:HB3	1.79	0.81
2:D:558:LEU:CA	2:D:570:LEU:H	1.92	0.81
2:D:60:GLN:H	2:D:63:ASN:HA	1.40	0.81
2:D:60:GLN:CA	2:D:62:MET:O	2.29	0.80
1:A:30:ASN:HB2	1:A:32:PHE:N	1.96	0.80
1:A:87:GLY:H	1:A:237:ARG:C	1.87	0.80
2:D:178:PRO:O	2:D:181:GLU:HB3	1.82	0.80
2:D:60:GLN:C	2:D:66:GLY:H	1.90	0.80
2:D:531:GLN:H	2:D:543:ASP:N	1.64	0.80
1:C:478:THR:OG1	1:C:486:PHE:O	1.99	0.80
2:D:383:MET:HB3	2:D:387:ALA:HB3	1.62	0.80
2:D:60:GLN:C	2:D:62:MET:C	2.50	0.80
2:D:238:GLU:C	2:D:599:ASN:HD22	1.90	0.80
2:D:56:ASP:O	2:D:59:ILE:N	2.13	0.80
1:A:973:ILE:HG12	1:A:984:LEU:HD13	1.64	0.80
1:B:995:ARG:HA	1:B:998:THR:HG22	1.64	0.80
2:D:184:VAL:O	2:D:188:ASN:HB2	1.82	0.80
2:D:403:ALA:H	2:D:514:ARG:NH1	1.79	0.79
2:D:558:LEU:N	2:D:571:GLU:H	1.79	0.79
1:A:187:LYS:NZ	1:A:215:ASP:OD1	2.15	0.79
1:A:60:SER:OG	1:A:268:GLY:O	2.01	0.79
1:B:48:LEU:HD13	1:B:278:LYS:HD2	1.64	0.79
2:D:61:LYS:O	2:D:65:ALA:CB	2.27	0.79
2:D:235:PRO:O	2:D:595:LEU:HD12	1.83	0.79
2:D:549:GLU:HA	2:D:552:GLN:OE1	1.83	0.78
2:D:404:VAL:HG13	2:D:408:MET:HE1	1.65	0.78
1:A:91:TYR:HE1	1:A:270:LEU:HB3	1.47	0.78
2:D:258:PRO:HD2	2:D:610:TRP:HB3	1.66	0.78
1:A:190:ARG:HA	1:A:205:SER:HA	1.65	0.78
2:D:148:LEU:HD23	2:D:151:ILE:HD12	1.63	0.78
1:A:226:LEU:N	1:C:560:LEU:O	2.16	0.78
2:D:481:LYS:HE2	2:D:494:ASP:HB2	1.64	0.78
1:A:125:ASN:HA	1:A:168:PHE:HB3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:GLY:H	2:D:466:GLY:N	1.80	0.78
1:A:45:SER:HA	1:A:279:TYR:HB2	1.66	0.78
2:D:529:LEU:O	2:D:543:ASP:CA	2.32	0.78
1:C:393:THR:HB	1:C:520:ALA:HB3	1.65	0.77
2:D:81:LYS:NZ	2:D:100:LEU:O	2.16	0.77
2:D:582:ARG:HG3	2:D:583:PRO:HD3	1.66	0.77
1:A:87:GLY:CA	1:A:239:GLN:HA	2.15	0.77
2:D:384:ALA:HA	2:D:388:GLN:HE21	1.49	0.77
2:D:29:LEU:HA	2:D:32:PHE:HB3	1.67	0.77
1:C:1116:THR:HB	1:C:1140:PRO:HG3	1.67	0.77
2:D:293:VAL:HA	2:D:297:MET:HG2	1.65	0.77
1:A:41:LYS:HE2	1:A:230:PRO:HD3	1.67	0.77
2:D:57:GLU:HA	2:D:63:ASN:HB2	1.65	0.77
2:D:77:SER:O	2:D:81:LYS:HB2	1.85	0.77
2:D:531:GLN:N	2:D:542:CYS:CA	2.48	0.77
1:C:335:LEU:N	1:C:362:VAL:O	2.18	0.76
2:D:323:MET:HE1	2:D:359:LYS:HA	1.66	0.76
1:A:108:THR:OG1	1:A:115:GLN:O	2.02	0.76
2:D:60:GLN:CA	2:D:63:ASN:HA	2.14	0.76
2:D:524:GLN:NE2	2:D:578:THR:O	2.18	0.76
2:D:274:PHE:HD1	2:D:276:THR:H	1.33	0.76
2:D:332:MET:HE2	2:D:336:PRO:HA	1.67	0.76
1:C:84:PHE:N	1:C:236:THR:O	2.18	0.76
1:C:905:ARG:NH1	1:C:1050:MET:SD	2.59	0.76
2:D:539:LEU:HD11	2:D:582:ARG:HH12	1.50	0.75
1:C:83:PRO:O	1:C:83:PRO:HD2	1.86	0.75
2:D:191:ALA:HA	2:D:194:ASN:HA	1.67	0.75
1:B:986:PRO:HB2	1:B:987:PRO:CD	2.15	0.75
1:A:87:GLY:HA3	1:A:239:GLN:HA	1.66	0.75
2:D:239:HIS:CB	2:D:595:LEU:HA	2.17	0.75
2:D:527:GLU:OE2	2:D:582:ARG:NH2	2.20	0.75
2:D:481:LYS:HE3	2:D:496:THR:HG22	1.68	0.75
1:C:753:LEU:HD12	1:C:997:ILE:HD11	1.68	0.75
2:D:109:SER:OG	2:D:112:LYS:NZ	2.20	0.74
1:B:93:ALA:HB3	1:B:266:TYR:HE2	1.50	0.74
2:D:61:LYS:HG2	2:D:64:ILE:H	1.50	0.74
2:D:234:LYS:NZ	2:D:238:GLU:OE1	2.20	0.74
1:A:30:ASN:OD1	1:A:215:ASP:HA	1.87	0.74
1:B:50:SER:HB2	1:B:276:LEU:HD13	1.69	0.74
1:C:405:ASP:O	1:C:408:ARG:NH2	2.20	0.74
1:A:27:ALA:HB1	1:A:269:TYR:HB2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:VAL:O	1:A:1012:LEU:HB2	1.87	0.74
2:D:61:LYS:CD	2:D:64:ILE:HG12	2.14	0.74
2:D:557:MET:HE2	2:D:572:ARG:HB2	1.69	0.74
1:A:281:GLU:O	1:C:558:LYS:NZ	2.18	0.74
2:D:530:CYS:HA	2:D:543:ASP:HA	1.70	0.74
2:D:533:ALA:H	2:D:543:ASP:CA	2.00	0.74
2:D:199:TYR:C	2:D:465:LYS:H	1.95	0.74
1:C:229:LEU:HD12	1:C:230:PRO:HD2	1.70	0.74
2:D:57:GLU:HG2	2:D:61:LYS:HG3	1.68	0.73
2:D:355:ASP:HB3	2:D:357:ARG:HE	1.53	0.73
2:D:371:THR:O	2:D:375:GLU:HB2	1.88	0.73
1:A:96:GLU:OE1	1:A:215:ASP:N	2.21	0.73
1:A:758:SER:OG	1:A:761:THR:OG1	2.04	0.73
1:C:452:LEU:HD12	1:C:492:LEU:HB3	1.68	0.73
2:D:325:GLU:HA	2:D:328:TRP:HD1	1.53	0.73
2:D:558:LEU:HA	2:D:567:THR:O	1.88	0.73
2:D:583:PRO:HA	2:D:586:ASN:ND2	2.03	0.73
1:C:514:SER:HB2	1:C:516:GLU:HG3	1.70	0.73
2:D:323:MET:O	2:D:328:TRP:NE1	2.22	0.73
1:C:421:TYR:HB3	1:C:456:PHE:HA	1.69	0.72
2:D:581:VAL:O	2:D:585:LEU:N	2.21	0.72
2:D:459:TRP:CE2	2:D:463:VAL:HG21	2.24	0.72
1:A:30:ASN:ND2	1:A:94:SER:O	2.20	0.72
1:B:188:ASN:OD1	1:B:205:SER:OG	2.06	0.72
1:C:407:VAL:HA	1:C:410:ILE:HD12	1.72	0.72
2:D:58:ASN:O	2:D:62:MET:HB3	1.85	0.72
2:D:368:ASP:HA	2:D:371:THR:OG1	1.88	0.72
2:D:531:GLN:C	2:D:543:ASP:H	1.98	0.72
2:D:535:HIS:HB2	2:D:543:ASP:HB2	1.70	0.72
1:A:200:TYR:HB2	1:A:231:ILE:HD13	1.71	0.72
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.71	0.72
1:A:30:ASN:HA	1:A:92:PHE:N	2.05	0.72
2:D:60:GLN:O	2:D:65:ALA:N	2.23	0.72
2:D:187:LYS:HA	2:D:190:MET:HG3	1.71	0.72
1:C:79:ASN:ND2	1:C:240:THR:O	2.23	0.71
2:D:244:VAL:HG23	2:D:247:LYS:HE3	1.71	0.71
2:D:529:LEU:O	2:D:544:ILE:HG12	1.89	0.71
1:C:203:ILE:HB	1:C:226:LEU:HB2	1.72	0.71
2:D:386:ALA:O	2:D:393:ARG:NH1	2.22	0.71
1:C:992:GLN:O	1:C:995:ARG:NH1	2.23	0.71
2:D:239:HIS:HB3	2:D:595:LEU:HD13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:ILE:O	2:D:155:SER:CB	2.39	0.71
2:D:531:GLN:HB3	2:D:541:LYS:O	1.89	0.71
2:D:119:ILE:HG23	2:D:183:TYR:HA	1.73	0.71
2:D:571:GLU:O	2:D:573:VAL:N	2.24	0.71
1:B:1000:ARG:O	1:B:1000:ARG:NE	2.23	0.71
1:C:455:LEU:HD11	2:D:30:GLU:HG2	1.73	0.71
2:D:259:THR:H	2:D:611:SER:HA	1.56	0.71
1:A:1054:GLN:HB2	1:A:1061:VAL:HB	1.73	0.71
2:D:532:ILE:N	2:D:542:CYS:O	2.19	0.71
1:A:996:LEU:HD12	1:A:1000:ARG:HH11	1.55	0.70
1:B:644:GLN:NE2	1:B:645:THR:O	2.23	0.70
2:D:403:ALA:O	2:D:407:ILE:HG12	1.91	0.70
2:D:60:GLN:HB3	2:D:67:ALA:N	2.06	0.70
2:D:530:CYS:CA	2:D:542:CYS:HB2	2.20	0.70
2:D:57:GLU:O	2:D:63:ASN:N	2.23	0.70
2:D:123:MET:HE3	2:D:127:TYR:HA	1.73	0.70
2:D:311:ALA:HA	2:D:314:PHE:H	1.56	0.70
2:D:295:ASP:OD1	2:D:296:ALA:N	2.23	0.70
1:B:82:LEU:H	1:B:239:GLN:CB	2.04	0.70
1:C:697:MET:N	1:C:697:MET:SD	2.65	0.70
2:D:365:THR:H	2:D:368:ASP:HB2	1.56	0.70
2:D:533:ALA:N	2:D:543:ASP:C	2.45	0.70
1:B:107:GLY:O	1:B:237:ARG:NH1	2.20	0.70
1:B:205:SER:N	1:B:224:GLU:O	2.19	0.70
1:A:187:LYS:CE	1:A:210:ILE:HG23	2.21	0.70
2:D:531:GLN:NE2	2:D:537:GLY:O	2.24	0.70
1:A:47:VAL:HG11	1:C:569:ILE:HG21	1.73	0.70
1:C:741:TYR:HE1	1:C:966:LEU:HD21	1.55	0.70
2:D:520:ILE:HA	2:D:579:MET:HB3	1.73	0.70
1:B:118:LEU:HD23	1:B:127:VAL:HB	1.72	0.70
2:D:306:ARG:HB3	2:D:310:GLU:HB2	1.72	0.70
2:D:557:MET:HE2	2:D:572:ARG:HG3	1.73	0.70
1:C:81:VAL:HG13	1:C:237:ARG:HH11	1.55	0.69
2:D:60:GLN:CA	2:D:63:ASN:CA	2.70	0.69
1:A:818:ILE:HD11	1:A:938:LEU:HD23	1.74	0.69
1:C:357:ARG:NH1	1:C:357:ARG:O	2.25	0.69
2:D:327:PHE:O	2:D:331:SER:OG	2.06	0.69
1:A:208:THR:HG23	1:A:216:LEU:HD23	1.74	0.69
1:B:81:VAL:N	1:B:240:THR:H	1.90	0.69
1:B:985:ASP:O	1:B:989:ALA:CB	2.40	0.69
2:D:176:LEU:HD22	2:D:177:ARG:NH1	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:485:VAL:O	2:D:487:VAL:N	2.24	0.69
2:D:532:ILE:N	2:D:543:ASP:N	2.40	0.69
2:D:396:ALA:O	2:D:562:ARG:NH2	2.24	0.69
1:B:82:LEU:H	1:B:239:GLN:HB3	1.57	0.69
2:D:182:GLU:O	2:D:186:LEU:HB3	1.91	0.69
1:A:41:LYS:HZ2	1:C:564:GLN:HB2	1.57	0.69
2:D:26:LYS:HA	2:D:29:LEU:HG	1.75	0.69
2:D:59:ILE:C	2:D:62:MET:O	2.35	0.69
1:B:987:PRO:HA	1:B:990:GLU:OE1	1.93	0.69
1:A:735:SER:HA	1:A:767:LEU:HD21	1.75	0.68
1:C:763:LEU:HD11	1:C:1005:GLN:HE22	1.57	0.68
1:C:1090:PRO:HA	1:C:1120:THR:HG22	1.75	0.68
2:D:59:ILE:HA	2:D:62:MET:SD	2.34	0.68
2:D:558:LEU:C	2:D:569:ALA:H	2.02	0.68
2:D:431:ASP:H	2:D:435:ASP:HB2	1.59	0.68
1:C:566:GLY:H	1:C:576:VAL:HG13	1.56	0.68
2:D:35:GLU:HG3	2:D:72:PHE:HZ	1.56	0.68
2:D:60:GLN:C	2:D:63:ASN:CA	2.65	0.68
1:A:29:THR:O	1:A:91:TYR:HB3	1.94	0.68
2:D:259:THR:N	2:D:612:PRO:HD3	2.09	0.68
1:C:91:TYR:CD2	1:C:193:VAL:HG22	2.29	0.68
2:D:530:CYS:C	2:D:543:ASP:N	2.51	0.68
1:B:84:PHE:HA	1:B:238:PHE:CD2	2.28	0.68
1:B:271:GLN:HE22	1:B:273:ARG:HE	1.41	0.68
2:D:386:ALA:C	2:D:393:ARG:HD3	2.18	0.68
1:A:189:LEU:N	1:A:206:LYS:O	2.27	0.68
2:D:304:ALA:HA	2:D:307:ILE:HB	1.75	0.68
1:A:98:SER:OG	1:A:99:ASN:N	2.25	0.68
2:D:200:GLY:N	2:D:465:LYS:H	1.91	0.68
1:B:84:PHE:HB2	1:B:237:ARG:CA	2.21	0.67
2:D:283:VAL:O	2:D:441:LYS:NZ	2.26	0.67
2:D:408:MET:HA	2:D:411:SER:HB3	1.76	0.67
1:B:29:THR:N	1:B:62:VAL:O	2.25	0.67
2:D:526:GLN:O	2:D:542:CYS:CB	2.38	0.67
1:A:214:ARG:NH2	1:A:266:TYR:O	2.28	0.67
1:C:1019:ARG:O	1:C:1023:ASN:ND2	2.27	0.67
2:D:61:LYS:CA	2:D:64:ILE:N	2.57	0.67
1:A:101:ILE:HD12	1:A:243:ALA:HA	1.74	0.67
1:B:202:LYS:HE3	1:B:225:PRO:HB2	1.75	0.67
2:D:186:LEU:HA	2:D:189:GLU:OE1	1.93	0.67
2:D:234:LYS:HE3	2:D:604:VAL:HG13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:LEU:HD12	1:C:131:CYS:HB3	1.76	0.67
2:D:123:MET:SD	2:D:180:TYR:N	2.68	0.67
1:B:84:PHE:HA	1:B:238:PHE:HD2	1.59	0.67
2:D:57:GLU:OE2	2:D:58:ASN:ND2	2.28	0.67
2:D:60:GLN:HB2	2:D:63:ASN:O	1.95	0.67
2:D:244:VAL:O	2:D:248:LEU:HB2	1.95	0.67
1:B:1000:ARG:HH21	1:B:1004:LEU:N	1.93	0.67
1:C:119:ILE:HD13	1:C:127:VAL:H	1.60	0.67
1:C:493:GLN:HG2	2:D:31:LYS:NZ	2.10	0.67
2:D:381:TYR:HE2	2:D:400:PHE:HB3	1.59	0.67
1:A:1001:LEU:O	1:A:1005:GLN:HB3	1.94	0.66
2:D:313:LYS:O	2:D:317:SER:OG	2.11	0.66
1:A:206:LYS:O	1:A:207:HIS:ND1	2.27	0.66
1:A:295:PRO:O	1:A:299:THR:HG23	1.94	0.66
2:D:60:GLN:CB	2:D:63:ASN:O	2.44	0.66
2:D:120:LEU:O	2:D:124:SER:HB3	1.95	0.66
1:A:202:LYS:HE3	1:A:229:LEU:H	1.59	0.66
1:C:763:LEU:HD22	1:C:1008:VAL:HG11	1.78	0.66
1:A:28:TYR:HB3	1:A:93:ALA:HB3	1.77	0.66
1:A:225:PRO:C	1:C:563:GLN:HB2	2.20	0.66
2:D:156:LYS:HB3	2:D:251:ALA:HB1	1.76	0.66
2:D:558:LEU:CB	2:D:571:GLU:H	2.09	0.66
1:A:96:GLU:HG2	1:A:212:LEU:HB2	1.78	0.66
1:C:763:LEU:HD13	1:C:1008:VAL:HG21	1.77	0.66
1:A:118:LEU:O	1:A:121:ASN:ND2	2.29	0.66
2:D:156:LYS:HE3	2:D:248:LEU:HD12	1.78	0.66
2:D:50:TYR:CD1	2:D:62:MET:HE2	2.30	0.66
2:D:365:THR:OG1	2:D:368:ASP:OD1	2.14	0.66
1:A:31:SER:H	1:A:91:TYR:C	2.05	0.66
2:D:390:PHE:HA	2:D:393:ARG:NE	2.07	0.66
2:D:465:LYS:O	2:D:465:LYS:HG2	1.94	0.66
1:A:191:GLU:HB2	1:A:204:TYR:HB2	1.78	0.65
1:A:1005:GLN:NE2	1:A:1009:THR:OG1	2.29	0.65
1:A:30:ASN:HB3	1:A:93:ALA:HA	1.77	0.65
2:D:60:GLN:HB3	2:D:67:ALA:H	1.60	0.65
2:D:529:LEU:O	2:D:544:ILE:N	2.28	0.65
2:D:531:GLN:N	2:D:542:CYS:C	2.30	0.65
1:A:226:LEU:HA	1:C:559:PHE:HD2	1.61	0.65
1:A:226:LEU:HD23	1:A:227:VAL:HG22	1.78	0.65
1:A:986:PRO:HA	1:A:989:ALA:H	1.60	0.65
2:D:565:PRO:HG2	2:D:567:THR:OG1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ASN:CG	1:A:215:ASP:HA	2.20	0.65
1:B:190:ARG:H	1:B:190:ARG:HD3	1.61	0.65
1:B:204:TYR:HA	1:B:225:PRO:HA	1.77	0.65
1:B:592:PHE:HE1	1:C:855:PHE:HB3	1.60	0.65
2:D:32:PHE:HA	2:D:35:GLU:HG2	1.78	0.65
2:D:404:VAL:HG13	2:D:518:ARG:NH1	2.11	0.65
1:A:31:SER:N	1:A:91:TYR:O	2.30	0.65
1:A:98:SER:HB3	1:A:210:ILE:N	2.07	0.65
1:C:1125:ASN:ND2	1:C:1127:ASP:OD1	2.28	0.65
2:D:531:GLN:H	2:D:542:CYS:N	1.89	0.65
1:B:121:ASN:ND2	1:B:124:THR:OG1	2.29	0.65
1:C:376:THR:OG1	1:C:435:ALA:O	2.15	0.65
2:D:558:LEU:HA	2:D:567:THR:C	2.22	0.65
1:A:900:MET:N	1:A:900:MET:SD	2.65	0.65
1:B:79:ASN:N	1:B:105:ILE:O	2.27	0.65
2:D:365:THR:N	2:D:368:ASP:HB2	2.12	0.65
2:D:416:ASN:HD21	2:D:541:LYS:HG2	1.61	0.65
2:D:558:LEU:HD22	2:D:559:SER:OG	1.95	0.65
1:A:309:GLU:O	1:A:313:TYR:OH	2.16	0.64
2:D:60:GLN:N	2:D:63:ASN:CA	2.50	0.64
2:D:209:GLU:O	2:D:216:ASN:ND2	2.28	0.64
1:B:689:SER:OG	1:B:690:GLN:N	2.30	0.64
2:D:260:GLY:N	2:D:612:PRO:HD2	2.12	0.64
2:D:571:GLU:O	2:D:574:VAL:N	2.30	0.64
2:D:571:GLU:HA	2:D:574:VAL:HG22	1.80	0.64
1:B:1090:PRO:HA	1:B:1120:THR:HG22	1.79	0.64
2:D:472:GLN:NE2	2:D:475:GLN:HB2	2.13	0.64
1:A:85:ASN:C	1:A:237:ARG:H	2.05	0.64
1:A:62:VAL:HG11	1:A:265:TYR:CD2	2.33	0.64
2:D:58:ASN:C	2:D:62:MET:HE3	2.22	0.64
2:D:404:VAL:HG13	2:D:518:ARG:HH11	1.63	0.64
1:A:644:GLN:NE2	1:A:645:THR:O	2.31	0.64
2:D:200:GLY:N	2:D:466:GLY:N	2.40	0.64
2:D:530:CYS:N	2:D:542:CYS:CB	2.39	0.64
1:B:738:CYS:SG	1:B:739:THR:N	2.70	0.64
1:C:748:GLU:HA	1:C:751:ASN:HD21	1.63	0.64
1:B:190:ARG:HA	1:B:192:PHE:CE2	2.33	0.64
2:D:558:LEU:HG	2:D:566:TRP:O	1.98	0.64
1:A:86:ASP:H	1:A:238:PHE:CA	2.09	0.64
1:B:33:THR:OG1	1:B:219:GLY:O	2.16	0.64
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:PHE:HA	1:C:238:PHE:CZ	2.33	0.64
1:A:187:LYS:H	1:A:243:ALA:N	1.94	0.64
1:A:226:LEU:H	1:C:562:PHE:N	1.96	0.64
1:B:1140:PRO:HD2	1:B:1141:LEU:H	1.63	0.64
1:A:30:ASN:HB3	1:A:93:ALA:CA	2.28	0.63
1:A:792:PRO:O	1:A:795:LYS:NZ	2.27	0.63
1:B:949:GLN:NE2	1:B:953:ASN:OD1	2.30	0.63
1:C:1102:TRP:HB2	1:C:1115:ILE:HD11	1.80	0.63
2:D:558:LEU:N	2:D:571:GLU:N	2.45	0.63
1:B:231:ILE:HG13	1:B:232:GLY:H	1.62	0.63
2:D:34:TYR:O	2:D:38:GLU:HB2	1.99	0.63
2:D:459:TRP:HA	2:D:462:MET:SD	2.38	0.63
1:B:84:PHE:CB	1:B:237:ARG:HA	2.25	0.63
2:D:60:GLN:HA	2:D:62:MET:O	1.99	0.63
1:C:115:GLN:HB3	1:C:130:VAL:HG22	1.80	0.63
2:D:29:LEU:HD22	2:D:390:PHE:HB3	1.80	0.63
2:D:528:ALA:O	2:D:542:CYS:O	2.17	0.63
1:A:85:ASN:HB2	1:A:238:PHE:HA	1.81	0.63
1:C:186:PHE:CD2	1:C:189:LEU:HD23	2.34	0.63
2:D:194:ASN:O	2:D:196:TYR:N	2.32	0.63
2:D:530:CYS:CA	2:D:543:ASP:HA	2.29	0.63
2:D:558:LEU:CA	2:D:571:GLU:H	2.12	0.63
1:C:271:GLN:OE1	1:C:273:ARG:NH1	2.32	0.62
2:D:123:MET:HE2	2:D:180:TYR:CD1	2.34	0.62
2:D:494:ASP:O	2:D:500:PRO:HD3	1.99	0.62
1:A:227:VAL:N	1:C:563:GLN:H	1.97	0.62
1:A:996:LEU:O	1:A:1000:ARG:HG2	1.98	0.62
2:D:37:GLU:O	2:D:41:TYR:HB2	2.00	0.62
2:D:190:MET:HE1	2:D:195:ASN:HB3	1.81	0.62
2:D:557:MET:C	2:D:571:GLU:N	2.57	0.62
1:B:112:SER:HA	1:B:139:PRO:HB3	1.80	0.62
2:D:408:MET:HE1	2:D:518:ARG:HH11	1.65	0.62
1:A:96:GLU:HB3	1:A:211:ASN:H	1.64	0.62
1:C:380:TYR:CD2	1:C:430:THR:HA	2.35	0.62
2:D:70:SER:O	2:D:74:GLU:HG2	1.98	0.62
2:D:459:TRP:O	2:D:463:VAL:HB	2.00	0.62
2:D:559:SER:C	2:D:569:ALA:HB3	2.25	0.62
1:B:280:ASN:OD1	1:B:284:THR:N	2.33	0.62
2:D:473:TRP:HA	2:D:477:TRP:HD1	1.64	0.62
1:C:493:GLN:HG2	2:D:31:LYS:HZ2	1.65	0.62
2:D:304:ALA:C	2:D:307:ILE:H	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:364:VAL:HA	2:D:368:ASP:CB	2.29	0.62
2:D:472:GLN:HE22	2:D:475:GLN:HB2	1.63	0.62
1:B:196:ASN:OD1	1:B:200:TYR:N	2.33	0.62
1:B:976:VAL:HB	1:B:980:ILE:HD13	1.82	0.62
2:D:41:TYR:O	2:D:45:LEU:HG	2.00	0.62
2:D:370:LEU:HB3	2:D:412:ALA:HB3	1.80	0.62
2:D:436:ILE:HG23	2:D:440:LEU:HD12	1.82	0.62
1:A:121:ASN:HB3	1:A:126:VAL:HG12	1.82	0.61
1:A:198:ASP:O	1:C:396:TYR:OH	2.13	0.61
2:D:94:LYS:HE2	2:D:210:GLU:HG3	1.80	0.61
1:A:64:TRP:CD1	1:A:263:ALA:HA	2.35	0.61
1:A:210:ILE:HD13	1:A:242:LEU:HB2	1.81	0.61
2:D:56:ASP:O	2:D:63:ASN:CG	2.43	0.61
2:D:374:HIS:CE1	2:D:408:MET:HE2	2.35	0.61
1:A:79:ASN:HA	1:A:265:TYR:HA	1.82	0.61
1:A:664:ILE:HD12	1:A:673:SER:HA	1.82	0.61
1:C:78:ASP:N	1:C:243:ALA:O	2.34	0.61
2:D:297:MET:HG3	2:D:314:PHE:CE1	2.35	0.61
1:A:30:ASN:HB3	1:A:93:ALA:N	2.15	0.61
1:B:897:PRO:HB2	1:B:900:MET:HG3	1.83	0.61
1:C:994:ASP:O	1:C:998:THR:HG23	2.00	0.61
2:D:158:TYR:CZ	2:D:253:PRO:HA	2.35	0.61
1:A:952:VAL:O	1:A:955:ASN:ND2	2.33	0.61
1:C:335:LEU:HD12	1:C:364:ASP:HB2	1.83	0.61
2:D:291:ILE:HD12	2:D:296:ALA:HB1	1.81	0.61
2:D:481:LYS:CE	2:D:494:ASP:HB2	2.31	0.61
2:D:60:GLN:O	2:D:64:ILE:C	2.43	0.61
1:A:225:PRO:HB2	1:C:563:GLN:HG3	1.83	0.61
1:C:391:CYS:HA	1:C:522:ALA:HB2	1.83	0.61
1:C:761:THR:OG1	1:C:765:ARG:NH2	2.32	0.61
1:C:913:GLN:OE1	1:C:913:GLN:N	2.32	0.61
2:D:381:TYR:CE2	2:D:400:PHE:HB3	2.35	0.61
2:D:440:LEU:HD22	2:D:591:LEU:HD13	1.82	0.61
1:A:91:TYR:CE2	1:A:268:GLY:HA3	2.36	0.61
1:A:1049:LEU:O	1:A:1050:MET:HE2	2.01	0.61
1:A:1082:CYS:HB2	1:A:1132:ILE:HD13	1.82	0.61
2:D:96:GLN:HG3	2:D:391:LEU:HG	1.83	0.61
1:A:713:ALA:HB3	1:B:894:LEU:HB3	1.83	0.61
1:B:93:ALA:HB3	1:B:266:TYR:CE2	2.36	0.61
1:C:52:GLN:HA	1:C:274:THR:HA	1.82	0.61
2:D:61:LYS:CG	2:D:64:ILE:H	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:531:GLN:HA	2:D:535:HIS:CB	2.31	0.61
1:A:1048:HIS:NE2	1:A:1051:SER:OG	2.34	0.60
1:B:222:ALA:HB1	1:B:285:ILE:HD12	1.83	0.60
1:C:1139:ASP:HB3	1:C:1142:GLN:HB2	1.82	0.60
2:D:436:ILE:HD12	2:D:440:LEU:HD11	1.83	0.60
2:D:442:GLN:O	2:D:446:ILE:HG12	2.01	0.60
1:A:96:GLU:HB2	1:A:215:ASP:OD1	2.01	0.60
1:A:1116:THR:HB	1:A:1140:PRO:HG3	1.83	0.60
2:D:181:GLU:O	2:D:185:ALA:HB3	2.01	0.60
2:D:557:MET:O	2:D:567:THR:O	2.18	0.60
1:B:601:GLY:O	1:B:604:THR:OG1	2.18	0.60
1:A:91:TYR:CZ	1:A:92:PHE:HB2	2.35	0.60
1:B:971:GLY:C	1:B:995:ARG:HH22	2.09	0.60
1:B:1140:PRO:HD2	1:B:1141:LEU:N	2.15	0.60
2:D:524:GLN:OE1	2:D:576:ALA:HB3	2.02	0.60
1:A:112:SER:HA	1:A:116:SER:HB2	1.82	0.60
1:A:220:PHE:N	1:A:286:THR:H	1.98	0.60
1:B:105:ILE:HG12	1:B:110:LEU:HD11	1.83	0.60
1:B:295:PRO:O	1:B:299:THR:HG23	2.01	0.60
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.33	0.60
2:D:304:ALA:O	2:D:307:ILE:HG22	2.02	0.60
1:C:410:ILE:HA	1:C:425:LEU:HD13	1.83	0.60
1:C:553:THR:OG1	1:C:586:ASP:O	2.19	0.60
2:D:209:GLU:HB3	2:D:216:ASN:HB2	1.82	0.60
2:D:558:LEU:C	2:D:569:ALA:N	2.59	0.60
1:C:731:MET:HE2	1:C:951:VAL:HG22	1.83	0.60
2:D:259:THR:HB	2:D:610:TRP:O	2.01	0.60
1:A:237:ARG:HD3	1:A:241:LEU:HD21	1.84	0.60
1:A:898:PHE:O	1:A:902:MET:HG2	2.01	0.60
1:B:28:TYR:HA	1:B:63:THR:HA	1.83	0.60
2:D:194:ASN:C	2:D:196:TYR:H	2.10	0.60
1:A:97:LYS:O	1:A:211:ASN:ND2	2.27	0.60
1:A:98:SER:H	1:A:209:PRO:CB	2.09	0.60
1:B:991:VAL:O	1:B:995:ARG:HG3	2.02	0.60
1:C:716:THR:N	1:C:1071:GLN:O	2.32	0.60
1:C:758:SER:OG	1:C:761:THR:OG1	2.18	0.60
2:D:221:GLN:O	2:D:224:GLU:HG3	2.01	0.60
2:D:520:ILE:HG12	2:D:579:MET:HB3	1.84	0.60
2:D:557:MET:HE2	2:D:572:ARG:CG	2.31	0.60
1:B:81:VAL:CA	1:B:239:GLN:HB2	2.31	0.59
1:B:721:SER:OG	1:B:1066:THR:OG1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:ASP:HB3	2:D:465:LYS:O	2.01	0.59
2:D:531:GLN:HA	2:D:535:HIS:HB2	1.84	0.59
2:D:571:GLU:C	2:D:573:VAL:H	2.10	0.59
1:A:29:THR:OG1	1:A:214:ARG:HG3	2.01	0.59
1:C:517:LEU:HD23	1:C:517:LEU:H	1.67	0.59
2:D:242:ALA:HB2	2:D:599:ASN:CG	2.27	0.59
1:A:97:LYS:O	1:A:211:ASN:HB3	2.02	0.59
2:D:60:GLN:N	2:D:63:ASN:N	2.50	0.59
2:D:275:TRP:HB2	2:D:444:LEU:HD21	1.84	0.59
2:D:473:TRP:O	2:D:477:TRP:HB2	2.01	0.59
1:B:82:LEU:HD11	1:B:238:PHE:CZ	2.38	0.59
1:B:86:ASP:HB2	1:B:270:LEU:HB2	1.83	0.59
1:A:1091:ARG:NH1	1:A:1120:THR:O	2.36	0.59
1:B:793:PRO:O	1:B:795:LYS:NZ	2.34	0.59
1:B:983:ARG:HH21	1:B:984:LEU:HB2	1.68	0.59
1:A:28:TYR:HA	1:A:91:TYR:CE2	2.38	0.59
1:A:84:PHE:CG	1:A:236:THR:HB	2.37	0.59
1:A:878:LEU:HD11	1:A:1052:PHE:HB3	1.85	0.59
1:C:433:VAL:HG21	1:C:512:VAL:HA	1.83	0.59
2:D:22:GLU:O	2:D:26:LYS:CB	2.51	0.59
2:D:57:GLU:CA	2:D:63:ASN:HB2	2.33	0.59
2:D:353:LYS:HB2	2:D:357:ARG:HH12	1.68	0.59
2:D:532:ILE:N	2:D:542:CYS:C	2.59	0.59
2:D:236:LEU:HA	2:D:595:LEU:HD12	1.85	0.59
2:D:266:LEU:C	2:D:268:GLY:H	2.09	0.59
2:D:543:ASP:CG	2:D:545:SER:H	2.10	0.59
1:A:28:TYR:HA	1:A:91:TYR:HE2	1.68	0.59
1:A:83:PRO:HD3	1:A:265:TYR:CD2	2.37	0.59
1:C:111:ASP:O	1:C:134:GLN:NE2	2.29	0.59
1:C:118:LEU:N	1:C:129:LYS:O	2.23	0.59
2:D:258:PRO:O	2:D:602:SER:HA	2.02	0.59
1:B:80:PRO:O	1:B:239:GLN:HG3	2.02	0.59
1:C:986:PRO:N	1:C:987:PRO:HD3	2.17	0.59
2:D:176:LEU:HD22	2:D:177:ARG:CZ	2.32	0.59
2:D:414:THR:HG22	2:D:530:CYS:HB3	1.83	0.59
1:A:930:ALA:HA	1:A:933:LYS:HD3	1.85	0.58
2:D:316:VAL:HA	2:D:369:PHE:CE1	2.38	0.58
2:D:557:MET:HE2	2:D:572:ARG:CB	2.33	0.58
1:A:46:SER:N	1:A:279:TYR:O	2.35	0.58
1:A:96:GLU:HB2	1:A:215:ASP:CG	2.28	0.58
1:B:54:LEU:HG	1:B:270:LEU:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:540:TYR:O	2:D:541:LYS:HB2	2.01	0.58
1:C:405:ASP:N	1:C:405:ASP:OD1	2.34	0.58
2:D:120:LEU:HA	2:D:183:TYR:CE1	2.37	0.58
2:D:302:TRP:HB3	2:D:314:PHE:CE2	2.38	0.58
1:A:44:ARG:HH22	1:A:277:LEU:HD12	1.68	0.58
1:A:88:VAL:H	1:A:240:THR:H	1.51	0.58
1:A:202:LYS:HG2	1:A:203:ILE:H	1.68	0.58
1:B:80:PRO:HB2	1:B:241:LEU:HD13	1.86	0.58
1:C:437:ASN:OD1	1:C:438:SER:N	2.37	0.58
1:C:1127:ASP:OD1	1:C:1127:ASP:N	2.36	0.58
2:D:374:HIS:CE1	2:D:408:MET:CE	2.86	0.58
2:D:418:LEU:O	2:D:422:GLY:N	2.36	0.58
2:D:558:LEU:HB3	2:D:570:LEU:HB3	1.84	0.58
1:A:738:CYS:SG	1:A:739:THR:N	2.76	0.58
1:A:290:ASP:OD1	1:A:291:CYS:N	2.36	0.58
1:C:438:SER:HB2	1:C:509:ARG:HG3	1.86	0.58
1:A:220:PHE:HA	1:A:287:ASP:N	2.13	0.58
1:C:431:GLY:HA3	1:C:514:SER:HA	1.85	0.58
2:D:252:TYR:HB3	2:D:253:PRO:HD3	1.86	0.58
2:D:189:GLU:HA	2:D:192:ARG:HG2	1.84	0.58
1:C:403:ARG:HB3	1:C:405:ASP:OD1	2.04	0.58
1:C:994:ASP:O	1:C:997:ILE:HG22	2.04	0.58
2:D:125:THR:O	2:D:129:THR:HG23	2.04	0.58
2:D:199:TYR:H	2:D:466:GLY:N	2.02	0.58
2:D:293:VAL:O	2:D:297:MET:HB2	2.03	0.58
2:D:371:THR:O	2:D:375:GLU:CB	2.51	0.58
2:D:592:PHE:HD2	2:D:596:LYS:NZ	2.01	0.58
1:C:1111:GLU:OE2	1:C:1113:GLN:NE2	2.37	0.57
2:D:203:TRP:CE3	2:D:461:TRP:HA	2.39	0.57
2:D:316:VAL:HA	2:D:369:PHE:HE1	1.69	0.57
2:D:399:GLY:C	2:D:514:ARG:HG2	2.29	0.57
1:B:1007:TYR:HA	1:B:1010:GLN:HE21	1.69	0.57
2:D:528:ALA:C	2:D:542:CYS:O	2.47	0.57
1:A:937:SER:O	1:A:941:THR:HG22	2.04	0.57
1:C:91:TYR:HB2	1:C:193:VAL:HG13	1.86	0.57
2:D:60:GLN:C	2:D:63:ASN:O	2.45	0.57
2:D:203:TRP:HB2	2:D:464:PHE:CB	2.19	0.57
1:A:96:GLU:HG2	1:A:212:LEU:N	2.20	0.57
1:A:121:ASN:HA	1:A:126:VAL:HA	1.85	0.57
1:B:697:MET:SD	1:B:697:MET:N	2.65	0.57
2:D:276:THR:O	2:D:279:TYR:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:O	1:B:239:GLN:HB3	2.04	0.57
1:B:110:LEU:HD22	1:B:139:PRO:HG2	1.85	0.57
2:D:558:LEU:HB2	2:D:571:GLU:HB2	1.85	0.57
2:D:583:PRO:HA	2:D:586:ASN:HD22	1.68	0.57
1:C:294:ASP:OD1	1:C:297:SER:OG	2.19	0.57
2:D:355:ASP:HB3	2:D:357:ARG:NE	2.18	0.57
2:D:385:TYR:C	2:D:393:ARG:HB3	2.30	0.57
1:B:37:TYR:HA	1:B:223:LEU:O	2.05	0.57
1:C:422:ASN:HD22	1:C:454:ARG:HB3	1.70	0.57
2:D:58:ASN:O	2:D:62:MET:CG	2.51	0.57
1:C:437:ASN:HA	1:C:508:TYR:HA	1.86	0.57
2:D:190:MET:O	2:D:193:ALA:O	2.21	0.57
2:D:194:ASN:OD1	2:D:195:ASN:ND2	2.37	0.57
1:A:115:GLN:HE21	1:A:235:ILE:HA	1.68	0.57
2:D:201:ASP:OD2	2:D:465:LYS:HD3	2.05	0.57
1:A:716:THR:N	1:A:1071:GLN:O	2.33	0.57
1:C:54:LEU:HD11	1:C:86:ASP:OD2	2.05	0.57
1:C:1091:ARG:NH2	1:C:1120:THR:O	2.38	0.57
2:D:190:MET:O	2:D:193:ALA:CA	2.53	0.57
2:D:305:ARG:NE	2:D:305:ARG:HA	2.20	0.57
1:B:761:THR:OG1	1:B:765:ARG:NH2	2.38	0.56
1:C:418:ILE:HD12	1:C:422:ASN:HB3	1.87	0.56
2:D:260:GLY:HA3	2:D:612:PRO:HD2	1.87	0.56
2:D:593:THR:O	2:D:597:GLU:HG2	2.04	0.56
1:A:88:VAL:H	1:A:240:THR:N	2.02	0.56
1:A:213:VAL:HG22	1:A:214:ARG:HD2	1.86	0.56
2:D:120:LEU:HA	2:D:183:TYR:CZ	2.40	0.56
2:D:261:CYS:N	2:D:613:TYR:HD2	2.03	0.56
2:D:588:PHE:O	2:D:591:LEU:HB2	2.04	0.56
1:A:1072:GLU:N	1:A:1072:GLU:OE1	2.37	0.56
2:D:34:TYR:O	2:D:38:GLU:CB	2.53	0.56
2:D:199:TYR:HA	2:D:463:VAL:O	2.04	0.56
2:D:263:PRO:HB3	2:D:490:PRO:HD3	1.87	0.56
2:D:592:PHE:HD2	2:D:596:LYS:HZ1	1.52	0.56
1:A:299:THR:HG22	1:A:597:VAL:HG11	1.86	0.56
1:C:302:THR:O	1:C:304:LYS:NZ	2.39	0.56
1:C:692:ILE:HD12	1:C:692:ILE:H	1.70	0.56
2:D:164:ALA:CB	2:D:266:LEU:HB2	2.27	0.56
2:D:371:THR:HB	2:D:375:GLU:HG2	1.87	0.56
1:A:189:LEU:HG	1:A:206:LYS:HB2	1.88	0.56
1:B:111:ASP:HB3	1:B:132:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:ILE:C	2:D:63:ASN:N	2.63	0.56
2:D:241:HIS:O	2:D:245:ARG:CB	2.49	0.56
2:D:366:MET:O	2:D:370:LEU:HG	2.06	0.56
2:D:526:GLN:O	2:D:529:LEU:HB3	2.05	0.56
2:D:557:MET:CE	2:D:568:PHE:HA	2.35	0.56
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.86	0.56
2:D:316:VAL:HG11	2:D:320:LEU:HB2	1.86	0.56
2:D:364:VAL:HA	2:D:368:ASP:HB3	1.88	0.56
1:A:30:ASN:HD21	1:A:215:ASP:HB2	1.71	0.56
1:A:999:GLY:HA2	1:A:1002:GLN:OE1	2.05	0.56
1:B:81:VAL:H	1:B:240:THR:H	1.53	0.56
1:C:1019:ARG:NH2	1:C:1023:ASN:OD1	2.39	0.56
1:A:86:ASP:C	1:A:239:GLN:HB3	2.31	0.56
1:A:91:TYR:CG	1:A:92:PHE:N	2.72	0.56
1:A:115:GLN:OE1	1:A:115:GLN:N	2.39	0.56
1:A:227:VAL:O	1:C:562:PHE:HA	2.06	0.56
1:B:166:CYS:SG	1:B:171:VAL:N	2.79	0.56
1:B:203:ILE:HD11	1:B:226:LEU:HD23	1.87	0.56
1:B:1001:LEU:HA	1:B:1004:LEU:HG	1.87	0.56
1:C:433:VAL:HB	1:C:511:VAL:HG12	1.88	0.56
2:D:191:ALA:HA	2:D:194:ASN:CA	2.33	0.56
1:A:167:THR:HB	1:A:170:TYR:HA	1.87	0.56
1:A:759:PHE:O	1:A:762:GLN:HG2	2.06	0.56
2:D:121:ASN:OD1	2:D:122:ALA:N	2.38	0.56
1:A:85:ASN:HB2	1:A:238:PHE:CA	2.35	0.55
1:B:79:ASN:HD21	1:B:238:PHE:HD1	1.53	0.55
1:B:915:VAL:O	1:B:919:ASN:ND2	2.39	0.55
2:D:188:ASN:HA	2:D:191:ALA:HB3	1.87	0.55
2:D:204:ARG:HD3	2:D:462:MET:HA	1.87	0.55
2:D:235:PRO:O	2:D:238:GLU:HB2	2.06	0.55
2:D:260:GLY:CA	2:D:612:PRO:HD2	2.36	0.55
1:A:96:GLU:CD	1:A:215:ASP:H	2.13	0.55
2:D:282:MET:SD	2:D:441:LYS:HE2	2.45	0.55
2:D:473:TRP:HA	2:D:477:TRP:CD1	2.40	0.55
2:D:416:ASN:ND2	2:D:541:LYS:HE2	2.22	0.55
1:A:30:ASN:HB2	1:A:32:PHE:H	1.68	0.55
1:A:209:PRO:HB3	1:A:245:HIS:HA	1.88	0.55
1:B:81:VAL:N	1:B:239:GLN:HB2	2.21	0.55
2:D:187:LYS:HA	2:D:190:MET:CG	2.36	0.55
1:A:986:PRO:HA	1:A:989:ALA:HB3	1.89	0.55
2:D:242:ALA:HB2	2:D:599:ASN:ND2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:255:ARG:HG3	2:D:612:PRO:O	2.07	0.55
1:A:30:ASN:CG	1:A:94:SER:N	2.64	0.55
1:A:86:ASP:HB2	1:A:239:GLN:CD	2.31	0.55
1:A:91:TYR:CE2	1:A:92:PHE:HB2	2.41	0.55
1:A:689:SER:OG	1:A:690:GLN:N	2.35	0.55
1:B:995:ARG:HA	1:B:998:THR:CG2	2.36	0.55
1:A:219:GLY:HA3	1:A:286:THR:HG23	1.89	0.55
1:B:205:SER:HA	1:B:223:LEU:HD11	1.89	0.55
1:C:475:ALA:HB3	1:C:489:TYR:CD2	2.42	0.55
2:D:379:ILE:O	2:D:383:MET:HG3	2.06	0.55
2:D:557:MET:O	2:D:572:ARG:N	2.37	0.55
2:D:50:TYR:CG	2:D:62:MET:HE2	2.42	0.55
1:A:98:SER:N	1:A:209:PRO:HB2	2.10	0.55
1:C:718:PHE:HE2	1:C:923:ILE:HD11	1.71	0.55
1:C:1116:THR:OG1	1:C:1119:ASN:ND2	2.40	0.55
2:D:524:GLN:HB3	2:D:576:ALA:H	1.71	0.55
1:A:82:LEU:HB3	1:A:83:PRO:HD2	1.90	0.54
1:A:208:THR:HG21	1:A:217:PRO:HG3	1.89	0.54
1:B:206:LYS:HD3	1:B:222:ALA:O	2.07	0.54
2:D:61:LYS:HD3	2:D:64:ILE:CG1	2.22	0.54
2:D:236:LEU:O	2:D:240:LEU:HB2	2.06	0.54
2:D:288:LYS:HD2	2:D:289:PRO:HD2	1.88	0.54
2:D:376:MET:HA	2:D:376:MET:HE3	1.88	0.54
2:D:455:MET:SD	2:D:456:LEU:N	2.80	0.54
1:A:84:PHE:HA	1:A:237:ARG:HA	1.89	0.54
1:A:826:VAL:HG22	1:A:945:LEU:HG	1.89	0.54
1:B:764:ASN:HA	1:B:767:LEU:HD12	1.88	0.54
2:D:323:MET:HE2	2:D:323:MET:HA	1.89	0.54
2:D:557:MET:H	2:D:570:LEU:HA	1.72	0.54
1:A:30:ASN:HA	1:A:91:TYR:C	2.32	0.54
1:B:1010:GLN:O	1:B:1014:ARG:HB2	2.06	0.54
2:D:403:ALA:N	2:D:514:ARG:HH12	1.96	0.54
1:A:32:PHE:C	1:A:34:ARG:H	2.15	0.54
1:A:804:GLN:HG3	1:A:935:GLN:HE21	1.71	0.54
1:B:119:ILE:HG12	1:B:123:ALA:H	1.72	0.54
1:C:1049:LEU:HD11	1:C:1067:TYR:HB2	1.88	0.54
2:D:527:GLU:O	2:D:542:CYS:O	2.25	0.54
1:A:28:TYR:HB3	1:A:93:ALA:CB	2.37	0.54
1:A:97:LYS:C	1:A:211:ASN:HD22	2.16	0.54
2:D:199:TYR:H	2:D:466:GLY:HA2	1.72	0.54
1:A:31:SER:HB2	1:A:240:THR:OG1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:CA	1:A:287:ASP:H	2.14	0.54
2:D:199:TYR:H	2:D:466:GLY:CA	2.20	0.54
2:D:210:GLU:H	2:D:210:GLU:CD	2.16	0.54
2:D:239:HIS:ND1	2:D:239:HIS:O	2.41	0.54
2:D:199:TYR:O	2:D:463:VAL:CA	2.52	0.54
2:D:261:CYS:N	2:D:613:TYR:HB2	2.14	0.54
2:D:519:THR:O	2:D:522:GLN:HB3	2.07	0.54
1:A:1002:GLN:O	1:A:1006:THR:OG1	2.16	0.54
2:D:439:LEU:O	2:D:442:GLN:HG2	2.08	0.54
2:D:544:ILE:HG22	2:D:544:ILE:O	2.08	0.54
1:A:29:THR:N	1:A:93:ALA:H	2.05	0.53
1:A:1012:LEU:HD21	1:C:1013:ILE:HG21	1.91	0.53
1:B:1086:LYS:HA	1:B:1125:ASN:HA	1.88	0.53
1:C:437:ASN:ND2	1:C:503:VAL:HG23	2.23	0.53
2:D:459:TRP:CD2	2:D:463:VAL:HG21	2.42	0.53
1:B:950:ASP:OD1	1:B:954:GLN:NE2	2.40	0.53
1:C:433:VAL:HG11	1:C:513:LEU:H	1.73	0.53
1:C:444:LYS:O	1:C:499:PRO:HA	2.07	0.53
1:C:1117:THR:H	1:C:1140:PRO:CD	2.21	0.53
2:D:458:LYS:O	2:D:462:MET:HG3	2.08	0.53
2:D:550:ALA:HA	2:D:553:LYS:HG2	1.91	0.53
1:A:209:PRO:HG3	1:A:245:HIS:ND1	2.23	0.53
2:D:199:TYR:O	2:D:462:MET:O	2.26	0.53
2:D:199:TYR:N	2:D:466:GLY:N	2.56	0.53
1:A:32:PHE:CG	1:A:33:THR:N	2.76	0.53
2:D:239:HIS:HD2	2:D:594:TRP:O	1.91	0.53
2:D:260:GLY:HA2	2:D:611:SER:HB3	1.89	0.53
2:D:431:ASP:O	2:D:435:ASP:HB3	2.08	0.53
1:A:108:THR:H	1:A:116:SER:HA	1.74	0.53
1:A:124:THR:O	1:A:169:GLU:HG3	2.09	0.53
1:A:202:LYS:NZ	1:A:228:ASP:OD2	2.41	0.53
1:A:237:ARG:NH2	1:A:242:LEU:HD21	2.23	0.53
1:A:1107:ARG:HD3	1:B:904:TYR:CE2	2.43	0.53
2:D:257:SER:HB2	2:D:611:SER:O	2.08	0.53
2:D:528:ALA:HA	2:D:542:CYS:O	2.08	0.53
1:A:41:LYS:HZ1	1:A:228:ASP:C	2.17	0.53
1:C:918:GLU:OE1	1:C:919:ASN:ND2	2.42	0.53
2:D:61:LYS:CA	2:D:64:ILE:H	2.22	0.53
2:D:194:ASN:C	2:D:196:TYR:N	2.67	0.53
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.91	0.53
2:D:41:TYR:CZ	2:D:351:LEU:HD13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:PHE:HB2	1:B:273:ARG:HB2	1.91	0.53
2:D:57:GLU:O	2:D:61:LYS:CB	2.46	0.53
2:D:257:SER:HB2	2:D:611:SER:C	2.34	0.53
2:D:297:MET:HG3	2:D:314:PHE:HE1	1.73	0.53
2:D:414:THR:HB	2:D:417:HIS:HB3	1.90	0.53
1:C:58:PHE:HB3	1:C:59:PHE:HD1	1.74	0.53
1:C:485:GLY:H	1:C:488:CYS:HB2	1.74	0.53
2:D:123:MET:CB	2:D:179:LEU:HG	2.27	0.53
2:D:158:TYR:CE2	2:D:253:PRO:HA	2.44	0.53
1:A:113:LYS:HD2	1:A:114:THR:HG23	1.89	0.53
1:C:1117:THR:HA	1:C:1120:THR:OG1	2.09	0.53
2:D:191:ALA:O	2:D:194:ASN:HB2	2.09	0.53
2:D:519:THR:HG23	2:D:522:GLN:NE2	2.24	0.53
1:A:222:ALA:HB3	1:A:279:TYR:CE2	2.44	0.52
1:A:982:SER:HB2	1:A:983:ARG:NH2	2.24	0.52
1:B:186:PHE:HA	1:B:226:LEU:HB2	1.89	0.52
2:D:165:TRP:HE1	2:D:169:ARG:HD3	1.73	0.52
2:D:241:HIS:HA	2:D:244:VAL:HG12	1.91	0.52
2:D:557:MET:C	2:D:571:GLU:H	2.16	0.52
1:A:32:PHE:N	1:A:91:TYR:O	2.42	0.52
1:A:977:LEU:HA	1:A:980:ILE:HD12	1.91	0.52
1:C:618:THR:OG1	1:C:619:GLU:OE1	2.26	0.52
2:D:61:LYS:CB	2:D:64:ILE:H	2.22	0.52
2:D:165:TRP:HA	2:D:265:HIS:HB3	1.91	0.52
2:D:544:ILE:HD12	2:D:550:ALA:HB1	1.90	0.52
1:A:28:TYR:CD2	1:A:92:PHE:HB3	2.44	0.52
1:C:449:TYR:HB3	1:C:494:SER:HB2	1.91	0.52
1:A:897:PRO:HB2	1:A:899:PRO:HD2	1.90	0.52
1:B:84:PHE:HB2	1:B:238:PHE:H	1.73	0.52
1:B:906:PHE:O	1:B:909:ILE:HG22	2.10	0.52
1:C:822:LEU:HA	1:C:825:LYS:HD2	1.90	0.52
1:C:969:ASN:ND2	1:C:974:SER:O	2.42	0.52
2:D:336:PRO:HD2	2:D:342:VAL:O	2.10	0.52
2:D:554:LEU:HA	2:D:570:LEU:HG	1.91	0.52
1:A:198:ASP:CG	1:C:396:TYR:HE2	2.18	0.52
1:B:78:ASP:OD1	1:B:106:PHE:N	2.42	0.52
1:B:132:GLU:O	1:B:169:GLU:HG2	2.09	0.52
1:C:439:ASN:OD1	1:C:506:GLN:NE2	2.42	0.52
2:D:210:GLU:OE1	2:D:210:GLU:N	2.32	0.52
2:D:370:LEU:HD13	2:D:412:ALA:C	2.35	0.52
1:B:108:THR:H	1:B:113:LYS:NZ	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:O	1:C:240:THR:HB	2.10	0.52
2:D:114:GLU:O	2:D:118:THR:HG23	2.09	0.52
1:C:1033:VAL:HG13	1:C:1034:LEU:HD12	1.92	0.52
2:D:165:TRP:CD1	2:D:265:HIS:HB2	2.45	0.52
2:D:207:TYR:H	2:D:219:ARG:NH2	2.07	0.52
2:D:152:MET:HE3	2:D:152:MET:O	2.10	0.52
2:D:556:GLU:OE1	2:D:557:MET:HB2	2.10	0.52
1:A:1007:TYR:O	1:A:1011:GLN:HB2	2.10	0.52
1:B:63:THR:H	1:B:267:VAL:HG22	1.75	0.52
1:B:1001:LEU:HA	1:B:1004:LEU:CD1	2.40	0.52
1:C:1005:GLN:O	1:C:1009:THR:HG23	2.10	0.52
2:D:22:GLU:O	2:D:26:LYS:HB2	2.09	0.52
2:D:375:GLU:HA	2:D:378:HIS:HB3	1.92	0.52
1:A:86:ASP:O	1:A:239:GLN:HB3	2.10	0.52
1:B:969:ASN:HB3	1:B:972:ALA:HB3	1.91	0.52
1:C:214:ARG:H	1:C:214:ARG:HD2	1.74	0.52
2:D:49:ASN:O	2:D:52:THR:HB	2.10	0.52
2:D:123:MET:HB2	2:D:179:LEU:CG	2.27	0.52
2:D:275:TRP:CE3	2:D:444:LEU:HG	2.45	0.52
2:D:297:MET:HA	2:D:300:GLN:HB2	1.92	0.52
1:A:901:GLN:HB3	1:A:902:MET:HE2	1.92	0.51
1:B:54:LEU:HG	1:B:270:LEU:HD12	1.90	0.51
1:B:188:ASN:ND2	1:B:206:LYS:HA	2.25	0.51
2:D:25:ALA:O	2:D:29:LEU:HG	2.09	0.51
2:D:290:ASN:OD1	2:D:291:ILE:N	2.42	0.51
2:D:558:LEU:O	2:D:565:PRO:O	2.28	0.51
1:A:88:VAL:HG12	1:A:91:TYR:N	2.18	0.51
1:B:200:TYR:HB3	1:B:228:ASP:OD1	2.10	0.51
1:B:970:PHE:HE2	1:B:999:GLY:HA3	1.74	0.51
1:A:221:SER:HB3	1:A:285:ILE:HD12	1.92	0.51
1:B:194:PHE:HB3	1:B:201:PHE:CZ	2.46	0.51
2:D:494:ASP:N	2:D:499:ASP:OD1	2.40	0.51
2:D:543:ASP:OD1	2:D:544:ILE:N	2.42	0.51
2:D:553:LYS:HA	2:D:556:GLU:HB3	1.91	0.51
1:A:54:LEU:HD23	1:A:54:LEU:H	1.75	0.51
1:A:165:ASN:ND2	1:A:166:CYS:SG	2.83	0.51
1:C:85:ASN:HD22	1:C:86:ASP:H	1.59	0.51
2:D:55:THR:O	2:D:58:ASN:HB2	2.11	0.51
1:A:104:TRP:CH2	1:A:118:LEU:HA	2.45	0.51
1:B:1072:GLU:OE1	1:B:1072:GLU:N	2.43	0.51
2:D:557:MET:HE3	2:D:567:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:581:VAL:HG13	2:D:585:LEU:HG	1.93	0.51
1:A:226:LEU:HD22	1:C:561:PRO:HA	1.92	0.51
1:C:402:ILE:HG13	1:C:403:ARG:H	1.75	0.51
1:A:188:ASN:O	1:A:190:ARG:N	2.37	0.51
1:C:898:PHE:O	1:C:902:MET:HG2	2.11	0.51
2:D:352:GLY:O	2:D:357:ARG:NH1	2.43	0.51
2:D:531:GLN:OE1	2:D:537:GLY:N	2.43	0.51
2:D:570:LEU:O	2:D:574:VAL:HG13	2.10	0.51
1:A:53:ASP:HB2	1:A:55:PHE:HE2	1.76	0.51
1:A:747:THR:O	1:A:751:ASN:ND2	2.44	0.51
1:A:804:GLN:HG3	1:A:935:GLN:NE2	2.26	0.51
1:B:86:ASP:CB	1:B:270:LEU:HB2	2.41	0.51
1:A:32:PHE:HD2	1:A:217:PRO:O	1.94	0.51
1:A:43:PHE:HB2	1:A:225:PRO:HG3	1.93	0.51
1:C:462:LYS:HE3	1:C:463:PRO:HD2	1.93	0.51
1:C:1117:THR:H	1:C:1140:PRO:HD3	1.75	0.51
2:D:223:ILE:H	2:D:223:ILE:HD12	1.76	0.51
2:D:556:GLU:O	2:D:569:ALA:HA	2.11	0.51
1:A:239:GLN:HB2	1:A:240:THR:HA	1.92	0.51
1:A:995:ARG:HA	1:A:998:THR:HG22	1.93	0.51
1:C:427:ASP:N	1:C:427:ASP:OD2	2.42	0.51
1:C:560:LEU:HB3	1:C:561:PRO:HD3	1.93	0.51
2:D:364:VAL:HA	2:D:368:ASP:HB2	1.93	0.51
1:A:30:ASN:CG	1:A:94:SER:H	2.18	0.50
1:A:34:ARG:HH22	1:A:217:PRO:HG2	1.74	0.50
1:A:98:SER:HA	1:A:211:ASN:HB3	1.92	0.50
1:A:191:GLU:HB2	1:A:204:TYR:HD2	1.76	0.50
2:D:56:ASP:C	2:D:63:ASN:ND2	2.69	0.50
2:D:557:MET:HE1	2:D:564:LYS:NZ	2.26	0.50
1:A:666:ILE:HG12	1:A:670:ILE:O	2.11	0.50
1:B:308:VAL:O	1:B:602:THR:OG1	2.25	0.50
1:B:319:ARG:NH1	1:B:591:SER:O	2.44	0.50
1:A:228:ASP:HB2	1:C:562:PHE:HB2	1.92	0.50
1:B:1143:PRO:HG2	1:B:1144:GLU:OE2	2.11	0.50
1:C:930:ALA:O	1:C:934:ILE:HG22	2.11	0.50
2:D:151:ILE:HG22	2:D:155:SER:HB3	1.93	0.50
1:A:1029:MET:HE2	1:A:1029:MET:HA	1.93	0.50
2:D:38:GLU:O	2:D:42:GLN:HG2	2.11	0.50
2:D:147:GLY:O	2:D:151:ILE:HG13	2.11	0.50
2:D:168:TRP:HA	2:D:171:GLU:OE1	2.12	0.50
2:D:191:ALA:C	2:D:193:ALA:N	2.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:ASP:O	2:D:464:PHE:HA	2.12	0.50
2:D:558:LEU:N	2:D:569:ALA:N	2.60	0.50
1:A:91:TYR:OH	1:A:269:TYR:O	2.28	0.50
1:A:169:GLU:O	1:A:170:TYR:HD1	1.93	0.50
1:A:187:LYS:HB3	1:A:209:PRO:HA	1.92	0.50
1:A:931:ILE:HG22	1:A:935:GLN:HE21	1.76	0.50
1:B:34:ARG:NH2	1:B:217:PRO:O	2.44	0.50
1:B:79:ASN:CG	1:B:239:GLN:O	2.54	0.50
1:B:186:PHE:C	1:B:226:LEU:HD22	2.37	0.50
1:B:669:GLY:HA2	1:B:697:MET:HE1	1.93	0.50
1:C:525:CYS:SG	1:C:526:GLY:N	2.84	0.50
1:A:44:ARG:NH1	1:A:49:HIS:HB3	2.26	0.50
1:A:979:ASP:HA	1:A:982:SER:OG	2.12	0.50
1:C:467:ASP:OD1	1:C:467:ASP:N	2.43	0.50
1:C:749:CYS:O	1:C:752:LEU:HG	2.12	0.50
2:D:60:GLN:O	2:D:65:ALA:C	2.54	0.50
2:D:244:VAL:HG11	2:D:275:TRP:CD1	2.47	0.50
2:D:316:VAL:CG1	2:D:320:LEU:HB2	2.41	0.50
1:B:166:CYS:SG	1:B:171:VAL:HG13	2.52	0.50
1:C:88:VAL:HG23	1:C:268:GLY:O	2.11	0.50
1:C:564:GLN:HG3	1:C:565:PHE:HD2	1.76	0.50
1:A:83:PRO:HD3	1:A:265:TYR:CE2	2.47	0.50
1:B:84:PHE:CD1	1:B:238:PHE:HB3	2.47	0.50
2:D:21:THR:HG21	2:D:97:LEU:HD11	1.94	0.50
2:D:261:CYS:H	2:D:613:TYR:HD2	1.59	0.50
2:D:523:PHE:HZ	2:D:583:PRO:HD2	1.76	0.50
2:D:529:LEU:C	2:D:543:ASP:HA	2.37	0.50
2:D:559:SER:H	2:D:570:LEU:N	2.09	0.50
1:C:193:VAL:HG12	1:C:195:LYS:HB2	1.94	0.50
2:D:457:GLU:HG2	2:D:513:ILE:HB	1.94	0.50
2:D:571:GLU:C	2:D:573:VAL:N	2.69	0.50
1:A:32:PHE:O	1:A:34:ARG:N	2.45	0.49
1:A:41:LYS:HD2	1:C:563:GLN:HA	1.94	0.49
1:A:118:LEU:O	1:A:118:LEU:HD12	2.12	0.49
2:D:291:ILE:HG12	2:D:423:LEU:O	2.12	0.49
2:D:370:LEU:HD13	2:D:413:ALA:N	2.27	0.49
2:D:432:SER:O	2:D:436:ILE:HG12	2.12	0.49
2:D:530:CYS:CB	2:D:542:CYS:HB2	2.40	0.49
1:A:32:PHE:HA	1:A:92:PHE:C	2.36	0.49
1:A:86:ASP:HB2	1:A:239:GLN:CG	2.42	0.49
1:B:710:ASN:OD1	1:B:710:ASN:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1144:GLU:OE2	1:B:1144:GLU:N	2.34	0.49
1:C:79:ASN:HB2	1:C:242:LEU:HA	1.93	0.49
2:D:116:LEU:O	2:D:120:LEU:HG	2.12	0.49
2:D:565:PRO:C	2:D:567:THR:N	2.67	0.49
1:A:273:ARG:HG2	1:A:291:CYS:HB2	1.94	0.49
1:A:675:GLN:OE1	1:A:690:GLN:NE2	2.44	0.49
1:B:115:GLN:HG3	1:B:130:VAL:HG23	1.94	0.49
1:B:165:ASN:O	1:B:169:GLU:HB2	2.12	0.49
1:B:1033:VAL:HA	1:B:1051:SER:HB2	1.94	0.49
2:D:55:THR:OG1	2:D:58:ASN:ND2	2.46	0.49
2:D:185:ALA:HA	2:D:188:ASN:HB2	1.93	0.49
2:D:387:ALA:HA	2:D:393:ARG:NH1	2.27	0.49
2:D:531:GLN:C	2:D:543:ASP:N	2.66	0.49
2:D:557:MET:HE3	2:D:568:PHE:HA	1.92	0.49
1:A:40:ASP:OD1	1:A:41:LYS:N	2.42	0.49
1:B:81:VAL:H	1:B:240:THR:C	2.14	0.49
1:B:290:ASP:OD1	1:B:291:CYS:N	2.43	0.49
1:C:426:PRO:HB2	1:C:428:ASP:OD1	2.12	0.49
1:C:936:ASP:OD1	1:C:936:ASP:N	2.44	0.49
1:C:1054:GLN:N	1:C:1061:VAL:O	2.41	0.49
2:D:91:PRO:HG3	2:D:211:TRP:CZ3	2.47	0.49
2:D:239:HIS:ND1	2:D:242:ALA:HB3	2.27	0.49
2:D:407:ILE:HG21	2:D:518:ARG:C	2.38	0.49
2:D:437:ASN:O	2:D:441:LYS:HG3	2.13	0.49
1:A:41:LYS:HE2	1:A:230:PRO:CD	2.41	0.49
1:A:320:VAL:HG23	1:A:592:PHE:HA	1.93	0.49
1:B:44:ARG:HB2	1:B:279:TYR:HD2	1.76	0.49
1:B:84:PHE:HD1	1:B:238:PHE:HB3	1.78	0.49
1:B:196:ASN:OD1	1:B:197:ILE:N	2.45	0.49
1:B:319:ARG:HD2	1:B:592:PHE:HB2	1.94	0.49
2:D:239:HIS:H	2:D:595:LEU:HD13	1.76	0.49
2:D:257:SER:O	2:D:612:PRO:HG3	2.12	0.49
1:A:49:HIS:NE2	1:A:51:THR:OG1	2.46	0.49
1:A:88:VAL:CG1	1:A:91:TYR:H	2.17	0.49
1:A:96:GLU:OE1	1:A:210:ILE:HG22	2.13	0.49
1:A:191:GLU:HB2	1:A:204:TYR:CD2	2.47	0.49
1:A:193:VAL:HB	1:A:202:LYS:O	2.12	0.49
1:B:207:HIS:O	1:B:208:THR:OG1	2.29	0.49
1:C:473:TYR:HB3	1:C:491:PRO:HD3	1.94	0.49
1:C:819:GLU:O	1:C:822:LEU:HD12	2.12	0.49
2:D:347:THR:O	2:D:361:CYS:N	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:525:PHE:CE1	2:D:571:GLU:HG3	2.48	0.49
1:B:36:VAL:HG21	1:B:220:PHE:CZ	2.47	0.49
1:B:310:LYS:HZ3	1:B:601:GLY:H	1.60	0.49
2:D:307:ILE:O	2:D:311:ALA:CB	2.46	0.49
2:D:531:GLN:CA	2:D:543:ASP:HB2	2.42	0.49
1:A:213:VAL:C	1:A:214:ARG:HD2	2.38	0.49
1:B:52:GLN:HB2	1:B:274:THR:HG22	1.94	0.49
1:B:80:PRO:CG	1:B:241:LEU:HB2	2.28	0.49
1:C:109:THR:HA	1:C:237:ARG:HH21	1.77	0.49
1:C:406:GLU:OE1	1:C:409:GLN:HG3	2.13	0.49
2:D:261:CYS:SG	2:D:488:VAL:HG21	2.52	0.49
2:D:431:ASP:O	2:D:435:ASP:CB	2.60	0.49
1:B:64:TRP:O	1:B:64:TRP:HE3	1.96	0.49
1:B:118:LEU:HB3	1:B:127:VAL:H	1.76	0.49
1:B:194:PHE:HA	1:B:203:ILE:HG22	1.95	0.49
1:B:759:PHE:O	1:B:763:LEU:HG	2.12	0.49
1:C:554:GLU:HG3	1:C:555:SER:H	1.77	0.49
1:C:929:SER:O	1:C:933:LYS:HG3	2.12	0.49
1:C:1097:SER:OG	1:C:1101:HIS:O	2.30	0.49
2:D:206:ASP:H	2:D:219:ARG:HH22	1.61	0.49
2:D:348:ALA:HA	2:D:360:MET:HA	1.95	0.49
1:A:221:SER:H	1:A:286:THR:N	2.11	0.49
1:A:1000:ARG:HA	1:A:1003:SER:OG	2.12	0.49
1:B:82:LEU:N	1:B:239:GLN:CB	2.75	0.49
1:B:276:LEU:HB2	1:B:289:VAL:HB	1.94	0.49
1:C:947:LYS:O	1:C:951:VAL:HG12	2.13	0.49
2:D:168:TRP:O	2:D:172:VAL:HG13	2.12	0.49
2:D:177:ARG:O	2:D:181:GLU:HB3	2.08	0.49
2:D:524:GLN:O	2:D:527:GLU:HB3	2.13	0.49
2:D:526:GLN:O	2:D:529:LEU:N	2.45	0.49
2:D:531:GLN:O	2:D:531:GLN:HG3	2.13	0.49
1:A:187:LYS:NZ	1:A:216:LEU:HG	2.22	0.48
1:B:994:ASP:OD1	1:B:995:ARG:N	2.46	0.48
1:C:574:ASP:OD1	1:C:575:ALA:N	2.46	0.48
2:D:459:TRP:O	2:D:463:VAL:CB	2.61	0.48
1:A:186:PHE:O	1:A:189:LEU:HA	2.13	0.48
1:B:119:ILE:CD1	1:B:124:THR:H	2.25	0.48
1:C:96:GLU:OE1	1:C:98:SER:OG	2.27	0.48
1:C:449:TYR:HA	1:C:496:GLY:H	1.78	0.48
2:D:35:GLU:HG3	2:D:72:PHE:CZ	2.45	0.48
1:A:189:LEU:O	1:A:189:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:PHE:O	2:D:32:PHE:CB	2.61	0.48
1:A:28:TYR:CZ	1:A:92:PHE:HD2	2.30	0.48
1:A:61:ASN:OD1	1:A:62:VAL:N	2.45	0.48
2:D:275:TRP:HE3	2:D:444:LEU:HG	1.79	0.48
2:D:462:MET:O	2:D:462:MET:HE2	2.13	0.48
2:D:557:MET:O	2:D:571:GLU:N	2.46	0.48
1:A:220:PHE:O	1:A:221:SER:HB2	2.13	0.48
1:A:225:PRO:HB2	1:C:563:GLN:CG	2.43	0.48
1:A:596:SER:OG	1:A:613:GLN:OE1	2.32	0.48
1:C:756:TYR:HB3	1:C:759:PHE:CZ	2.48	0.48
1:C:773:GLU:OE1	1:C:774:GLN:NE2	2.46	0.48
1:A:108:THR:HG23	1:A:117:LEU:N	2.28	0.48
1:A:225:PRO:HB2	1:C:563:GLN:CB	2.44	0.48
1:B:57:PRO:HA	1:B:275:PHE:HZ	1.78	0.48
1:B:202:LYS:HD2	1:B:227:VAL:O	2.14	0.48
1:B:796:ASP:OD1	1:B:796:ASP:N	2.44	0.48
1:A:97:LYS:H	1:A:211:ASN:ND2	2.11	0.48
2:D:399:GLY:HA2	2:D:514:ARG:HG2	1.96	0.48
2:D:528:ALA:HB3	2:D:574:VAL:O	2.14	0.48
2:D:531:GLN:HB3	2:D:541:LYS:C	2.38	0.48
1:B:132:GLU:HG3	1:B:169:GLU:HA	1.95	0.48
1:C:421:TYR:CG	1:C:456:PHE:HD1	2.31	0.48
1:C:1097:SER:HB2	1:C:1102:TRP:CE3	2.48	0.48
2:D:196:TYR:HD2	2:D:202:TYR:HE2	1.62	0.48
2:D:278:LEU:C	2:D:280:PRO:HD2	2.38	0.48
2:D:441:LYS:O	2:D:444:LEU:HB3	2.14	0.48
2:D:530:CYS:N	2:D:542:CYS:C	2.72	0.48
2:D:557:MET:O	2:D:557:MET:HE3	2.14	0.48
1:B:675:GLN:HG2	1:B:676:THR:H	1.79	0.48
1:C:409:GLN:O	1:C:414:GLN:HG3	2.14	0.48
1:C:433:VAL:HG21	1:C:513:LEU:H	1.78	0.48
1:C:644:GLN:NE2	1:C:645:THR:O	2.46	0.48
1:C:748:GLU:HA	1:C:751:ASN:ND2	2.27	0.48
2:D:297:MET:O	2:D:302:TRP:HB2	2.14	0.48
2:D:520:ILE:HG23	2:D:578:THR:C	2.39	0.48
1:A:91:TYR:CE1	1:A:270:LEU:HB3	2.38	0.48
1:B:1116:THR:HB	1:B:1118:ASP:OD1	2.14	0.48
1:C:86:ASP:O	1:C:195:LYS:NZ	2.40	0.48
1:C:983:ARG:HH12	1:C:984:LEU:HD22	1.78	0.48
2:D:443:ALA:O	2:D:447:VAL:HG23	2.13	0.48
2:D:543:ASP:OD1	2:D:545:SER:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:554:LEU:C	2:D:556:GLU:H	2.22	0.48
1:A:81:VAL:HB	1:A:84:PHE:CE1	2.49	0.47
1:A:86:ASP:O	1:A:241:LEU:HG	2.13	0.47
1:A:104:TRP:HA	1:A:106:PHE:CE2	2.49	0.47
1:A:1005:GLN:O	1:A:1009:THR:OG1	2.23	0.47
1:C:465:GLU:OE1	1:C:465:GLU:N	2.46	0.47
1:C:598:ILE:HG23	1:C:609:ALA:HB3	1.95	0.47
2:D:200:GLY:CA	2:D:465:LYS:H	2.27	0.47
2:D:382:ASP:O	2:D:385:TYR:N	2.47	0.47
1:C:490:PHE:CG	1:C:491:PRO:HD2	2.49	0.47
2:D:560:LEU:HD13	2:D:568:PHE:CE1	2.49	0.47
1:A:96:GLU:HG2	1:A:212:LEU:CB	2.44	0.47
1:A:293:LEU:HD23	1:A:297:SER:OG	2.14	0.47
1:C:62:VAL:HG12	1:C:268:GLY:HA3	1.97	0.47
1:C:389:ASP:OD1	1:C:389:ASP:N	2.46	0.47
1:C:796:ASP:N	1:C:796:ASP:OD1	2.47	0.47
1:C:1050:MET:HE3	1:C:1051:SER:N	2.19	0.47
2:D:148:LEU:O	2:D:268:GLY:HA3	2.15	0.47
2:D:239:HIS:CB	2:D:595:LEU:HD13	2.40	0.47
2:D:252:TYR:HB3	2:D:253:PRO:CD	2.44	0.47
2:D:407:ILE:HD11	2:D:515:TYR:HA	1.97	0.47
1:A:294:ASP:O	1:A:298:GLU:HG3	2.15	0.47
1:A:931:ILE:HG22	1:A:935:GLN:NE2	2.29	0.47
1:A:986:PRO:HA	1:A:989:ALA:N	2.28	0.47
1:B:79:ASN:HA	1:B:80:PRO:HD3	1.67	0.47
1:B:82:LEU:HG	1:B:239:GLN:HA	1.96	0.47
1:B:88:VAL:O	1:B:91:TYR:C	2.58	0.47
1:B:1049:LEU:O	1:B:1050:MET:HE2	2.14	0.47
1:C:759:PHE:O	1:C:763:LEU:HG	2.14	0.47
2:D:169:ARG:HB3	2:D:493:HIS:CG	2.50	0.47
2:D:323:MET:HB2	2:D:328:TRP:CZ2	2.50	0.47
2:D:446:ILE:HB	2:D:588:PHE:HZ	1.79	0.47
2:D:564:LYS:HD2	2:D:565:PRO:HD2	1.96	0.47
1:A:30:ASN:CB	1:A:32:PHE:H	2.28	0.47
1:A:96:GLU:HG2	1:A:212:LEU:H	1.78	0.47
1:A:193:VAL:HG21	1:A:202:LYS:HB3	1.95	0.47
1:A:756:TYR:HB3	1:A:759:PHE:HE2	1.79	0.47
1:A:759:PHE:O	1:A:763:LEU:HG	2.13	0.47
1:B:748:GLU:O	1:B:752:LEU:HG	2.15	0.47
1:C:107:GLY:HA2	1:C:235:ILE:HD12	1.97	0.47
1:C:237:ARG:NH2	1:C:239:GLN:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:ASP:OD2	2:D:354:HIS:ND1	2.47	0.47
2:D:28:PHE:O	2:D:32:PHE:HB2	2.14	0.47
2:D:379:ILE:O	2:D:382:ASP:N	2.48	0.47
2:D:558:LEU:HB2	2:D:571:GLU:CB	2.45	0.47
1:A:85:ASN:C	1:A:237:ARG:N	2.71	0.47
1:A:187:LYS:HB2	1:A:243:ALA:O	2.14	0.47
1:A:294:ASP:HB2	1:A:295:PRO:HD2	1.95	0.47
2:D:30:GLU:HG3	2:D:31:LYS:HE2	1.95	0.47
2:D:184:VAL:O	2:D:188:ASN:CB	2.58	0.47
2:D:549:GLU:O	2:D:552:GLN:NE2	2.48	0.47
2:D:557:MET:HG3	2:D:572:ARG:N	2.28	0.47
1:A:64:TRP:HD1	1:A:263:ALA:HA	1.77	0.47
1:A:200:TYR:HB2	1:A:231:ILE:CD1	2.42	0.47
1:A:319:ARG:NH1	1:A:592:PHE:HB3	2.29	0.47
1:A:790:LYS:HZ2	1:C:702:GLU:HG2	1.79	0.47
1:A:982:SER:HB2	1:A:983:ARG:CZ	2.45	0.47
1:B:189:LEU:C	1:B:191:GLU:H	2.23	0.47
1:B:273:ARG:HB3	1:B:275:PHE:CE1	2.50	0.47
1:B:980:ILE:O	1:B:983:ARG:N	2.47	0.47
1:C:751:ASN:HA	1:C:754:LEU:HD23	1.97	0.47
1:C:901:GLN:O	1:C:905:ARG:HG2	2.15	0.47
2:D:50:TYR:HE1	2:D:54:ILE:HG23	1.80	0.47
2:D:201:ASP:HA	2:D:204:ARG:HG2	1.96	0.47
2:D:236:LEU:HA	2:D:595:LEU:CD1	2.44	0.47
2:D:474:MET:SD	2:D:475:GLN:HG3	2.55	0.47
1:A:32:PHE:CE1	1:A:33:THR:HG23	2.50	0.47
1:A:758:SER:OG	1:A:758:SER:O	2.24	0.47
1:B:33:THR:HG22	1:B:58:PHE:CZ	2.50	0.47
1:B:186:PHE:O	1:B:205:SER:OG	2.33	0.47
1:C:906:PHE:HA	1:C:909:ILE:HG22	1.96	0.47
2:D:64:ILE:HG13	2:D:65:ALA:N	2.29	0.47
2:D:126:ILE:HG13	2:D:179:LEU:HD23	1.97	0.47
2:D:380:GLN:HA	2:D:383:MET:HE3	1.95	0.47
2:D:451:PRO:O	2:D:454:TYR:HB3	2.14	0.47
2:D:561:GLY:HA2	2:D:562:ARG:HH11	1.80	0.47
1:A:86:ASP:HA	1:A:237:ARG:H	1.79	0.47
1:A:194:PHE:CD1	1:A:194:PHE:O	2.68	0.47
1:A:237:ARG:HH21	1:A:242:LEU:HD21	1.79	0.47
1:B:108:THR:HA	1:B:237:ARG:HH22	1.80	0.47
1:B:119:ILE:HD11	1:B:124:THR:H	1.79	0.47
1:B:186:PHE:HA	1:B:226:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:LEU:HA	1:B:1007:TYR:HB3	1.97	0.47
1:B:1005:GLN:O	1:B:1009:THR:OG1	2.26	0.47
1:C:244:LEU:HD23	1:C:244:LEU:HA	1.73	0.47
2:D:201:ASP:O	2:D:204:ARG:N	2.48	0.47
2:D:303:ASP:HB3	2:D:306:ARG:HB2	1.95	0.47
2:D:407:ILE:HG21	2:D:518:ARG:O	2.15	0.47
1:A:225:PRO:C	1:C:560:LEU:O	2.58	0.47
1:B:132:GLU:N	1:B:169:GLU:O	2.48	0.47
1:B:754:LEU:HD23	1:B:754:LEU:H	1.80	0.47
1:C:186:PHE:CE2	1:C:189:LEU:HA	2.50	0.47
2:D:532:ILE:HA	2:D:534:LYS:H	1.79	0.47
1:A:697:MET:HE3	1:A:698:SER:H	1.80	0.46
1:B:78:ASP:HB3	1:B:104:TRP:C	2.39	0.46
1:B:86:ASP:OD1	1:B:87:GLY:N	2.48	0.46
1:C:317:ASN:OD1	1:C:318:PHE:N	2.47	0.46
1:C:562:PHE:CG	1:C:562:PHE:O	2.68	0.46
2:D:303:ASP:O	2:D:307:ILE:HB	2.15	0.46
2:D:559:SER:H	2:D:569:ALA:C	2.23	0.46
1:A:192:PHE:O	1:A:233:ILE:HG12	2.15	0.46
1:B:190:ARG:HH22	1:B:210:ILE:HG23	1.81	0.46
1:C:448:ASN:H	1:C:497:PHE:H	1.64	0.46
2:D:56:ASP:HA	2:D:59:ILE:HG12	1.96	0.46
2:D:58:ASN:O	2:D:63:ASN:N	2.48	0.46
2:D:123:MET:HG3	2:D:127:TYR:N	2.29	0.46
2:D:164:ALA:HB1	2:D:266:LEU:HD12	1.97	0.46
2:D:368:ASP:HA	2:D:371:THR:HG1	1.76	0.46
2:D:418:LEU:CD1	2:D:423:LEU:HB3	2.45	0.46
1:A:41:LYS:NZ	1:A:228:ASP:O	2.45	0.46
1:A:221:SER:CB	1:A:285:ILE:HB	2.45	0.46
1:B:592:PHE:CE1	1:C:855:PHE:HB3	2.45	0.46
1:B:854:LYS:HA	1:B:858:LEU:HB2	1.96	0.46
1:C:978:ASN:HA	1:C:981:LEU:HD23	1.96	0.46
1:A:749:CYS:O	1:A:752:LEU:HG	2.16	0.46
1:A:866:THR:N	1:A:869:MET:SD	2.84	0.46
1:B:33:THR:HG22	1:B:58:PHE:HZ	1.80	0.46
1:C:240:THR:OG1	1:C:241:LEU:N	2.41	0.46
2:D:266:LEU:HD23	2:D:269:ASP:HA	1.96	0.46
2:D:408:MET:HA	2:D:411:SER:CB	2.45	0.46
2:D:524:GLN:HE21	2:D:578:THR:C	2.19	0.46
2:D:564:LYS:HG3	2:D:568:PHE:HB2	1.98	0.46
1:A:84:PHE:C	1:A:237:ARG:HA	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:THR:OG1	1:B:287:ASP:N	2.47	0.46
1:C:1004:LEU:O	1:C:1008:VAL:HG23	2.16	0.46
2:D:439:LEU:HA	2:D:442:GLN:NE2	2.31	0.46
2:D:531:GLN:HA	2:D:535:HIS:HB3	1.97	0.46
2:D:557:MET:H	2:D:570:LEU:CA	2.27	0.46
2:D:570:LEU:CD2	2:D:574:VAL:HG21	2.39	0.46
1:A:81:VAL:HB	1:A:84:PHE:HE1	1.80	0.46
1:A:605:SER:OG	1:A:606:ASN:N	2.49	0.46
2:D:174:LYS:HA	2:D:177:ARG:HG2	1.96	0.46
2:D:200:GLY:O	2:D:204:ARG:HG2	2.15	0.46
2:D:269:ASP:HB2	2:D:270:MET:SD	2.56	0.46
1:A:88:VAL:N	1:A:238:PHE:O	2.49	0.46
1:B:79:ASN:ND2	1:B:238:PHE:HD1	2.13	0.46
1:B:241:LEU:HG	1:B:242:LEU:H	1.80	0.46
1:C:703:ASN:OD1	1:C:704:SER:N	2.48	0.46
2:D:181:GLU:HA	2:D:185:ALA:HB3	1.97	0.46
2:D:234:LYS:O	2:D:237:TYR:HB3	2.15	0.46
2:D:239:HIS:N	2:D:595:LEU:HD13	2.31	0.46
2:D:306:ARG:NH2	2:D:310:GLU:HG2	2.30	0.46
2:D:311:ALA:HA	2:D:314:PHE:N	2.28	0.46
1:C:93:ALA:HA	1:C:191:GLU:HA	1.97	0.46
1:C:355:ARG:HG3	1:C:357:ARG:HB2	1.96	0.46
1:C:380:TYR:CE2	1:C:430:THR:HG22	2.34	0.46
1:C:412:PRO:HA	1:C:427:ASP:HA	1.97	0.46
2:D:123:MET:HE2	2:D:180:TYR:CG	2.50	0.46
2:D:385:TYR:HB3	2:D:395:GLY:N	2.31	0.46
1:B:82:LEU:HD23	1:B:240:THR:CG2	2.45	0.46
1:B:826:VAL:HG22	1:B:945:LEU:HD13	1.98	0.46
2:D:266:LEU:C	2:D:268:GLY:N	2.74	0.46
1:A:226:LEU:HA	1:C:559:PHE:CD2	2.46	0.46
1:A:804:GLN:O	1:A:817:PRO:HD2	2.15	0.46
1:B:871:ALA:HA	1:B:874:THR:HG22	1.98	0.46
1:B:958:ALA:O	1:B:962:LEU:HG	2.16	0.46
1:C:738:CYS:SG	1:C:739:THR:N	2.88	0.46
1:C:948:LEU:HD12	1:C:948:LEU:H	1.81	0.46
2:D:60:GLN:CA	2:D:63:ASN:C	2.89	0.46
1:A:97:LYS:O	1:A:97:LYS:HD3	2.16	0.45
1:A:125:ASN:HB3	1:A:169:GLU:CD	2.41	0.45
1:B:1004:LEU:O	1:B:1008:VAL:HG22	2.15	0.45
1:C:119:ILE:CD1	1:C:127:VAL:H	2.28	0.45
1:C:195:LYS:HA	1:C:195:LYS:HD2	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ILE:HG22	1:C:429:PHE:CE1	2.51	0.45
2:D:119:ILE:HA	2:D:182:GLU:CD	2.41	0.45
2:D:442:GLN:HG3	2:D:587:TYR:OH	2.15	0.45
2:D:481:LYS:HG2	2:D:495:GLU:HB2	1.98	0.45
2:D:565:PRO:O	2:D:568:PHE:N	2.45	0.45
1:A:30:ASN:ND2	1:A:94:SER:H	2.15	0.45
1:A:66:HIS:CG	1:A:67:ALA:N	2.84	0.45
1:A:87:GLY:HA3	1:A:239:GLN:CA	2.42	0.45
1:A:703:ASN:OD1	1:A:704:SER:N	2.48	0.45
1:A:898:PHE:CD1	1:A:899:PRO:HD3	2.52	0.45
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.69	0.45
2:D:552:GLN:O	2:D:556:GLU:HB2	2.16	0.45
1:A:58:PHE:CE1	1:A:269:TYR:HB3	2.52	0.45
1:A:986:PRO:CA	1:A:989:ALA:HB3	2.47	0.45
1:A:1115:ILE:HG22	1:A:1137:VAL:HG23	1.99	0.45
1:B:84:PHE:H	1:B:237:ARG:HB2	1.80	0.45
1:B:206:LYS:NZ	1:B:207:HIS:H	2.15	0.45
1:B:660:TYR:O	1:B:698:SER:N	2.49	0.45
1:B:949:GLN:HE21	1:B:953:ASN:CG	2.25	0.45
1:C:675:GLN:O	1:C:691:SER:OG	2.28	0.45
2:D:349:TRP:CD1	2:D:359:LYS:HB2	2.51	0.45
2:D:481:LYS:NZ	2:D:494:ASP:OD2	2.36	0.45
2:D:535:HIS:CD2	2:D:536:GLU:H	2.34	0.45
1:A:53:ASP:HB2	1:A:55:PHE:CE2	2.52	0.45
1:A:1097:SER:HB2	1:A:1102:TRP:CE3	2.51	0.45
1:B:1047:TYR:O	1:B:1066:THR:HA	2.16	0.45
1:A:998:THR:O	1:A:1002:GLN:OE1	2.35	0.45
1:C:468:ILE:O	1:C:470:THR:HG23	2.16	0.45
2:D:56:ASP:C	2:D:59:ILE:H	2.21	0.45
2:D:349:TRP:HD1	2:D:359:LYS:HB2	1.82	0.45
2:D:380:GLN:CA	2:D:383:MET:HE3	2.47	0.45
2:D:446:ILE:HG21	2:D:584:LEU:HD22	1.98	0.45
2:D:528:ALA:O	2:D:542:CYS:C	2.60	0.45
1:A:120:VAL:HG13	1:A:127:VAL:HB	1.98	0.45
1:B:80:PRO:HG2	1:B:241:LEU:CB	2.29	0.45
1:B:643:PHE:HB3	1:B:650:LEU:HB3	1.98	0.45
2:D:374:HIS:ND1	2:D:408:MET:HE2	2.32	0.45
2:D:558:LEU:CB	2:D:570:LEU:H	2.29	0.45
1:A:878:LEU:O	1:A:882:ILE:HG22	2.16	0.45
1:A:1000:ARG:O	1:A:1004:LEU:HG	2.16	0.45
1:C:818:ILE:HG13	1:C:935:GLN:HE22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:VAL:C	2:D:318:VAL:N	2.74	0.45
2:D:472:GLN:NE2	2:D:475:GLN:OE1	2.45	0.45
1:A:97:LYS:HE2	1:A:245:HIS:HE1	1.81	0.45
1:A:777:ASN:O	1:A:781:VAL:HG12	2.16	0.45
1:A:932:GLY:HA2	1:A:935:GLN:CD	2.42	0.45
1:B:212:LEU:HG	1:B:214:ARG:H	1.80	0.45
1:B:998:THR:O	1:B:1002:GLN:HG2	2.16	0.45
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.44	0.45
1:C:436:TRP:O	1:C:508:TYR:HB3	2.17	0.45
2:D:188:ASN:HA	2:D:191:ALA:CB	2.47	0.45
2:D:259:THR:H	2:D:612:PRO:HD3	1.82	0.45
2:D:560:LEU:HD13	2:D:568:PHE:HE1	1.81	0.45
1:A:41:LYS:HD3	1:A:228:ASP:HB3	1.99	0.45
1:B:100:ILE:O	1:B:102:ARG:NH1	2.50	0.45
1:C:214:ARG:HD2	1:C:214:ARG:N	2.32	0.45
1:C:826:VAL:HB	1:C:945:LEU:HD13	1.98	0.45
1:C:1002:GLN:O	1:C:1006:THR:HG23	2.17	0.45
2:D:375:GLU:O	2:D:379:ILE:HG12	2.17	0.45
2:D:550:ALA:HA	2:D:553:LYS:CD	2.47	0.45
1:A:41:LYS:HD2	1:C:563:GLN:CA	2.47	0.45
1:A:186:PHE:HA	1:A:243:ALA:CB	2.47	0.45
1:A:931:ILE:O	1:A:935:GLN:HG3	2.17	0.45
1:B:57:PRO:HD2	1:B:91:TYR:CZ	2.51	0.45
1:B:78:ASP:C	1:B:104:TRP:HB2	2.42	0.45
1:C:455:LEU:HD22	2:D:31:LYS:HE3	1.99	0.45
1:C:1091:ARG:HH21	1:C:1121:PHE:HB3	1.82	0.45
2:D:203:TRP:CB	2:D:464:PHE:HB2	2.21	0.45
2:D:259:THR:HG21	2:D:606:TRP:HA	1.99	0.45
2:D:558:LEU:HD13	2:D:570:LEU:HD22	1.99	0.45
1:A:32:PHE:CE2	1:A:218:GLN:HG3	2.52	0.44
1:B:55:PHE:O	1:B:270:LEU:HD13	2.17	0.44
1:B:81:VAL:O	1:B:240:THR:HG22	2.16	0.44
1:B:914:ASN:HA	1:B:917:TYR:HD2	1.81	0.44
1:C:502:GLY:H	2:D:357:ARG:CZ	2.30	0.44
1:C:577:ARG:HG2	1:C:583:GLU:C	2.42	0.44
1:C:752:LEU:HD22	1:C:990:GLU:OE2	2.17	0.44
2:D:56:ASP:C	2:D:58:ASN:N	2.72	0.44
1:A:32:PHE:HA	1:A:92:PHE:O	2.17	0.44
1:A:740:MET:SD	1:A:741:TYR:N	2.90	0.44
1:B:1001:LEU:HA	1:B:1004:LEU:CG	2.46	0.44
1:A:186:PHE:N	1:A:241:LEU:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:SER:N	1:A:285:ILE:HB	2.32	0.44
1:A:742:ILE:HG22	1:A:993:ILE:HD11	1.99	0.44
1:B:44:ARG:NH1	1:B:49:HIS:HB3	2.31	0.44
1:B:675:GLN:HG3	1:B:689:SER:N	2.32	0.44
1:C:508:TYR:O	1:C:510:VAL:HG23	2.16	0.44
1:C:758:SER:OG	1:C:758:SER:O	2.24	0.44
1:C:1082:CYS:HB2	1:C:1132:ILE:HG12	1.97	0.44
2:D:83:TYR:HB3	2:D:97:LEU:HD22	1.99	0.44
2:D:259:THR:CG2	2:D:606:TRP:HA	2.47	0.44
2:D:350:ASP:OD1	2:D:350:ASP:N	2.50	0.44
2:D:564:LYS:HZ3	2:D:568:PHE:HB2	1.83	0.44
1:A:84:PHE:HB3	1:A:236:THR:HB	1.99	0.44
1:B:675:GLN:HB2	1:B:691:SER:N	2.32	0.44
1:B:1038:LYS:HA	1:B:1038:LYS:HD3	1.79	0.44
1:B:1118:ASP:OD1	1:B:1119:ASN:N	2.50	0.44
1:C:457:ARG:NH2	1:C:461:LEU:HD22	2.32	0.44
1:C:869:MET:HA	1:C:869:MET:HE3	1.99	0.44
2:D:296:ALA:HB3	2:D:297:MET:HE2	2.00	0.44
2:D:306:ARG:CZ	2:D:310:GLU:HG2	2.47	0.44
2:D:325:GLU:HA	2:D:328:TRP:CD1	2.43	0.44
2:D:382:ASP:HA	2:D:385:TYR:CE1	2.52	0.44
2:D:450:LEU:HD23	2:D:451:PRO:HA	2.00	0.44
2:D:494:ASP:N	2:D:494:ASP:OD1	2.47	0.44
2:D:554:LEU:HD12	2:D:574:VAL:CG1	2.47	0.44
1:A:127:VAL:HG13	1:A:166:CYS:HB2	2.00	0.44
1:B:190:ARG:HD3	1:B:190:ARG:N	2.29	0.44
1:C:51:THR:OG1	1:C:52:GLN:N	2.50	0.44
2:D:60:GLN:C	2:D:63:ASN:N	2.69	0.44
1:A:96:GLU:HG2	1:A:212:LEU:CA	2.48	0.44
1:A:931:ILE:O	1:A:934:ILE:HG22	2.18	0.44
1:B:91:TYR:HD2	1:B:270:LEU:HD22	1.81	0.44
1:B:866:THR:O	1:B:870:ILE:HG12	2.18	0.44
1:B:983:ARG:HE	1:B:984:LEU:HB2	1.83	0.44
1:C:33:THR:HG21	1:C:220:PHE:HD2	1.83	0.44
1:C:78:ASP:N	1:C:243:ALA:HB3	2.33	0.44
1:C:804:GLN:CD	1:C:804:GLN:H	2.25	0.44
1:C:885:GLY:HA2	1:C:901:GLN:HE22	1.83	0.44
2:D:297:MET:HE2	2:D:297:MET:N	2.33	0.44
2:D:388:GLN:N	2:D:393:ARG:HG2	2.33	0.44
2:D:531:GLN:HA	2:D:543:ASP:HB2	1.99	0.44
1:A:86:ASP:OD1	1:A:235:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:ASN:ND2	1:C:454:ARG:HB3	2.32	0.44
1:C:445:VAL:HG23	1:C:499:PRO:HB3	1.99	0.44
1:C:753:LEU:O	1:C:755:GLN:N	2.51	0.44
2:D:56:ASP:OD2	2:D:57:GLU:N	2.51	0.44
2:D:265:HIS:CE1	2:D:266:LEU:HD23	2.52	0.44
2:D:525:PHE:HD1	2:D:575:GLY:HA3	1.83	0.44
1:B:96:GLU:OE2	1:B:99:ASN:N	2.50	0.44
1:B:912:THR:HG23	1:B:915:VAL:HG23	1.98	0.44
1:C:295:PRO:HA	1:C:298:GLU:HG2	2.00	0.44
1:A:32:PHE:CD1	1:A:33:THR:N	2.84	0.44
1:A:983:ARG:HH21	1:C:386:LYS:HE3	1.83	0.44
1:B:78:ASP:HB3	1:B:104:TRP:HB2	1.99	0.44
2:D:25:ALA:HA	2:D:28:PHE:HB3	1.98	0.44
2:D:50:TYR:HA	2:D:58:ASN:OD1	2.18	0.44
2:D:56:ASP:HA	2:D:59:ILE:CG1	2.48	0.44
2:D:81:LYS:HE3	2:D:103:SER:HB2	2.00	0.44
2:D:172:VAL:O	2:D:175:GLN:HG3	2.18	0.44
2:D:550:ALA:O	2:D:554:LEU:HD13	2.18	0.44
2:D:557:MET:C	2:D:568:PHE:C	2.85	0.44
1:A:959:LEU:O	1:A:962:LEU:HG	2.18	0.43
1:B:205:SER:HA	1:B:223:LEU:CD1	2.47	0.43
1:B:605:SER:OG	1:B:606:ASN:N	2.51	0.43
1:C:692:ILE:HD12	1:C:692:ILE:N	2.33	0.43
2:D:194:ASN:O	2:D:196:TYR:HB2	2.18	0.43
2:D:270:MET:HE2	2:D:271:TRP:CD1	2.53	0.43
2:D:325:GLU:OE1	2:D:325:GLU:N	2.50	0.43
2:D:592:PHE:O	2:D:596:LYS:HG3	2.18	0.43
1:A:87:GLY:HA2	1:A:241:LEU:HA	1.99	0.43
1:B:80:PRO:C	1:B:239:GLN:HG3	2.44	0.43
1:C:404:GLY:HA3	1:C:508:TYR:CE1	2.53	0.43
2:D:148:LEU:HB3	2:D:268:GLY:O	2.18	0.43
2:D:240:LEU:O	2:D:244:VAL:HG12	2.18	0.43
2:D:402:GLU:H	2:D:514:ARG:NH1	2.16	0.43
1:A:273:ARG:CZ	1:A:292:ALA:HB3	2.48	0.43
1:A:273:ARG:HB2	1:A:290:ASP:OD2	2.18	0.43
1:A:1010:GLN:HB3	1:A:1014:ARG:HH21	1.81	0.43
1:B:84:PHE:HD1	1:B:238:PHE:CD2	2.36	0.43
1:C:436:TRP:CZ2	1:C:509:ARG:HD3	2.53	0.43
1:C:763:LEU:HD11	1:C:1005:GLN:NE2	2.29	0.43
2:D:198:ASP:HB3	2:D:465:LYS:C	2.42	0.43
2:D:531:GLN:N	2:D:541:LYS:C	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:SER:HB3	1:A:285:ILE:HB	2.01	0.43
1:B:191:GLU:HB2	1:B:223:LEU:HD11	2.01	0.43
1:C:1023:ASN:O	1:C:1027:THR:HG22	2.19	0.43
2:D:58:ASN:C	2:D:63:ASN:H	2.26	0.43
2:D:88:ILE:HG23	2:D:90:ASP:OD1	2.19	0.43
2:D:230:PHE:HA	2:D:233:ILE:HG22	2.00	0.43
2:D:253:PRO:O	2:D:255:ARG:HG2	2.18	0.43
2:D:255:ARG:HH21	2:D:614:ALA:HA	1.82	0.43
2:D:402:GLU:C	2:D:404:VAL:N	2.74	0.43
2:D:557:MET:HE1	2:D:564:LYS:HZ1	1.82	0.43
2:D:612:PRO:HB2	2:D:613:TYR:CD1	2.53	0.43
1:A:662:CYS:N	1:A:697:MET:HE1	2.33	0.43
1:B:1003:SER:HA	1:B:1006:THR:HG22	1.99	0.43
1:C:762:GLN:O	1:C:765:ARG:HG2	2.19	0.43
1:C:1083:HIS:ND1	1:C:1084:ASP:OD2	2.51	0.43
2:D:60:GLN:C	2:D:66:GLY:N	2.57	0.43
2:D:261:CYS:H	2:D:613:TYR:CB	2.20	0.43
2:D:530:CYS:CA	2:D:543:ASP:N	2.82	0.43
2:D:558:LEU:CB	2:D:571:GLU:N	2.64	0.43
1:A:216:LEU:HD13	1:A:240:THR:OG1	2.17	0.43
1:A:606:ASN:N	1:A:606:ASN:OD1	2.50	0.43
1:A:895:GLN:OE1	1:A:895:GLN:N	2.50	0.43
1:C:122:ASN:ND2	1:C:124:THR:OG1	2.52	0.43
1:C:335:LEU:O	1:C:337:PRO:HD3	2.18	0.43
1:C:380:TYR:CE2	1:C:430:THR:HA	2.53	0.43
1:C:1050:MET:O	1:C:1065:VAL:N	2.50	0.43
1:C:1141:LEU:HA	1:C:1144:GLU:OE1	2.18	0.43
2:D:113:ARG:HD2	2:D:116:LEU:HD13	1.99	0.43
1:A:222:ALA:HB3	1:A:279:TYR:HE2	1.83	0.43
1:A:977:LEU:O	1:A:981:LEU:HD23	2.19	0.43
1:B:167:THR:O	1:B:170:TYR:HB3	2.18	0.43
1:B:962:LEU:HD22	1:B:1000:ARG:HH12	1.83	0.43
1:B:1000:ARG:HE	1:B:1000:ARG:C	2.25	0.43
1:C:34:ARG:HD2	1:C:216:LEU:HD12	2.01	0.43
1:C:353:TRP:CZ3	1:C:396:TYR:HB2	2.54	0.43
1:C:1054:GLN:HB2	1:C:1061:VAL:HB	1.99	0.43
1:C:1139:ASP:OD1	1:C:1140:PRO:HD2	2.18	0.43
2:D:165:TRP:NE1	2:D:493:HIS:CD2	2.87	0.43
2:D:169:ARG:HE	2:D:493:HIS:HB3	1.83	0.43
2:D:232:GLN:O	2:D:235:PRO:HD2	2.18	0.43
2:D:245:ARG:O	2:D:249:MET:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:459:TRP:CZ3	2:D:463:VAL:HG11	2.54	0.43
1:B:133:PHE:C	1:B:135:PHE:H	2.27	0.43
1:B:878:LEU:O	1:B:882:ILE:HG22	2.18	0.43
1:C:34:ARG:CZ	1:C:221:SER:HB2	2.49	0.43
1:C:1029:MET:O	1:C:1033:VAL:HG12	2.18	0.43
2:D:366:MET:SD	2:D:367:ASP:N	2.92	0.43
2:D:388:GLN:H	2:D:393:ARG:HG2	1.83	0.43
2:D:532:ILE:HG22	2:D:532:ILE:O	2.18	0.43
2:D:591:LEU:O	2:D:595:LEU:HD23	2.19	0.43
1:A:87:GLY:CA	1:A:237:ARG:O	2.66	0.43
1:A:87:GLY:C	1:A:238:PHE:O	2.61	0.43
1:A:186:PHE:HB3	1:A:188:ASN:O	2.18	0.43
1:A:215:ASP:O	1:A:216:LEU:HG	2.19	0.43
1:A:654:GLU:O	1:A:656:VAL:HG23	2.19	0.43
1:A:1009:THR:O	1:A:1013:ILE:HG12	2.19	0.43
1:B:970:PHE:CD2	1:B:996:LEU:HA	2.54	0.43
1:C:91:TYR:HD2	1:C:193:VAL:HG22	1.80	0.43
1:C:781:VAL:HG13	1:C:782:PHE:HD2	1.84	0.43
2:D:320:LEU:HD12	2:D:321:PRO:HD2	2.00	0.43
2:D:531:GLN:HB2	2:D:541:LYS:HB3	1.99	0.43
1:A:228:ASP:CG	1:C:562:PHE:HB2	2.44	0.43
1:B:84:PHE:HD1	1:B:238:PHE:HD2	1.65	0.43
1:B:211:ASN:OD1	1:B:212:LEU:N	2.52	0.43
2:D:50:TYR:CE1	2:D:54:ILE:HG12	2.54	0.43
2:D:190:MET:O	2:D:193:ALA:N	2.52	0.43
2:D:554:LEU:C	2:D:556:GLU:N	2.76	0.43
1:A:95:THR:C	1:A:215:ASP:HB3	2.44	0.42
1:A:99:ASN:HB2	1:A:245:HIS:HE2	1.82	0.42
1:A:187:LYS:HG3	1:A:210:ILE:HG12	2.01	0.42
1:A:194:PHE:HB3	1:A:234:ASN:O	2.19	0.42
1:A:1015:ALA:HA	1:A:1018:ILE:HG22	1.99	0.42
1:A:1080:ALA:HB3	1:A:1132:ILE:HG13	2.00	0.42
1:A:1093:GLY:H	1:A:1107:ARG:NH2	2.17	0.42
1:B:129:LYS:HA	1:B:129:LYS:HD3	1.80	0.42
1:C:314:GLN:HA	1:C:596:SER:HA	2.01	0.42
1:C:452:LEU:HD13	1:C:493:GLN:C	2.44	0.42
2:D:31:LYS:HD3	2:D:31:LYS:HA	1.36	0.42
2:D:60:GLN:CA	2:D:62:MET:C	2.92	0.42
2:D:115:ARG:NH1	2:D:186:LEU:HG	2.33	0.42
2:D:238:GLU:HB3	2:D:599:ASN:HB3	2.01	0.42
2:D:305:ARG:HE	2:D:333:LEU:HD11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:452:PHE:HA	2:D:455:MET:HG3	2.01	0.42
2:D:489:GLU:OE2	2:D:493:HIS:N	2.26	0.42
2:D:528:ALA:CA	2:D:542:CYS:O	2.66	0.42
2:D:556:GLU:C	2:D:569:ALA:HA	2.44	0.42
1:A:91:TYR:CD2	1:A:92:PHE:N	2.86	0.42
1:A:202:LYS:HE3	1:A:229:LEU:C	2.44	0.42
1:A:205:SER:O	1:A:206:LYS:HG3	2.19	0.42
1:B:200:TYR:HA	1:B:230:PRO:HA	2.01	0.42
2:D:349:TRP:O	2:D:358:ILE:HD12	2.19	0.42
1:A:186:PHE:HA	1:A:243:ALA:HB3	1.99	0.42
1:A:189:LEU:CD1	1:A:206:LYS:HB2	2.49	0.42
1:B:675:GLN:HB2	1:B:690:GLN:C	2.44	0.42
1:C:108:THR:HG22	1:C:109:THR:HG23	2.01	0.42
2:D:61:LYS:HG2	2:D:64:ILE:HG23	2.00	0.42
1:A:219:GLY:N	1:A:286:THR:OG1	2.52	0.42
1:B:1001:LEU:O	1:B:1004:LEU:HD12	2.19	0.42
1:B:1009:THR:O	1:B:1013:ILE:HG12	2.19	0.42
1:C:380:TYR:OH	1:C:412:PRO:HG3	2.19	0.42
1:C:559:PHE:C	1:C:560:LEU:HD12	2.44	0.42
1:C:988:GLU:HG2	1:C:989:ALA:N	2.35	0.42
1:C:995:ARG:HH11	1:C:996:LEU:H	1.68	0.42
2:D:257:SER:N	2:D:612:PRO:HA	2.34	0.42
1:A:121:ASN:OD1	1:A:126:VAL:HB	2.20	0.42
1:B:44:ARG:HG3	1:B:47:VAL:HG12	2.01	0.42
2:D:57:GLU:O	2:D:63:ASN:HB2	2.19	0.42
2:D:239:HIS:CA	2:D:595:LEU:HD13	2.50	0.42
2:D:259:THR:OG1	2:D:603:PHE:HB3	2.18	0.42
2:D:302:TRP:CE3	2:D:314:PHE:CD1	3.07	0.42
2:D:389:PRO:O	2:D:393:ARG:HG3	2.19	0.42
2:D:412:ALA:O	2:D:414:THR:HG23	2.20	0.42
2:D:557:MET:CE	2:D:572:ARG:HB2	2.45	0.42
1:C:196:ASN:ND2	1:C:199:GLY:O	2.52	0.42
1:C:353:TRP:CH2	1:C:464:PHE:HB3	2.54	0.42
1:C:417:LYS:NZ	2:D:30:GLU:OE2	2.44	0.42
1:C:443:SER:CB	1:C:506:GLN:HE21	2.33	0.42
1:C:770:ILE:HD11	1:C:1012:LEU:HD22	2.01	0.42
1:C:1072:GLU:OE1	1:C:1072:GLU:N	2.52	0.42
2:D:396:ALA:HB1	2:D:566:TRP:NE1	2.34	0.42
2:D:419:LYS:HE2	2:D:423:LEU:N	2.35	0.42
1:A:31:SER:HB3	1:A:88:VAL:C	2.45	0.42
1:A:101:ILE:O	1:A:244:LEU:HD21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:N	1:A:125:ASN:O	2.50	0.42
1:A:1010:GLN:O	1:A:1014:ARG:HB2	2.19	0.42
1:B:108:THR:H	1:B:113:LYS:HZ1	1.68	0.42
1:B:202:LYS:CE	1:B:225:PRO:HB2	2.45	0.42
1:C:379:CYS:SG	1:C:384:PRO:HG3	2.59	0.42
1:C:1083:HIS:CD2	1:C:1136:THR:HA	2.55	0.42
2:D:60:GLN:N	2:D:62:MET:C	2.77	0.42
2:D:383:MET:HA	2:D:387:ALA:N	2.34	0.42
2:D:473:TRP:CA	2:D:477:TRP:HD1	2.30	0.42
1:A:28:TYR:CE2	1:A:92:PHE:HD2	2.38	0.42
1:A:226:LEU:HB3	1:C:561:PRO:HA	2.01	0.42
1:B:82:LEU:N	1:B:239:GLN:HB2	2.35	0.42
1:B:716:THR:N	1:B:1071:GLN:O	2.52	0.42
1:B:854:LYS:N	1:B:858:LEU:HD13	2.35	0.42
1:B:1004:LEU:HA	1:B:1007:TYR:CB	2.50	0.42
1:C:31:SER:O	1:C:34:ARG:N	2.49	0.42
1:C:380:TYR:HB3	1:C:431:GLY:O	2.20	0.42
2:D:377:GLY:HA2	2:D:380:GLN:HB3	2.02	0.42
1:A:29:THR:HA	1:A:93:ALA:O	2.20	0.42
1:A:31:SER:HA	1:A:216:LEU:HB2	2.01	0.42
1:A:32:PHE:C	1:A:34:ARG:N	2.78	0.42
1:A:62:VAL:HG21	1:A:265:TYR:CE2	2.55	0.42
1:A:124:THR:OG1	1:A:169:GLU:OE2	2.24	0.42
1:A:667:GLY:HA2	1:B:864:LEU:HD13	2.01	0.42
1:A:782:PHE:HD2	1:A:870:ILE:HD12	1.84	0.42
1:B:188:ASN:HB2	1:B:207:HIS:HA	2.01	0.42
1:B:196:ASN:HB2	1:B:201:PHE:HD1	1.85	0.42
1:B:327:VAL:HA	1:B:329:PHE:CE2	2.55	0.42
1:B:741:TYR:HE1	1:B:966:LEU:HD11	1.85	0.42
1:C:58:PHE:CE1	1:C:275:PHE:HZ	2.38	0.42
1:C:189:LEU:HB2	1:C:206:LYS:O	2.20	0.42
1:C:353:TRP:CZ2	1:C:464:PHE:HB3	2.55	0.42
1:C:379:CYS:HA	1:C:432:CYS:CB	2.49	0.42
1:C:726:ILE:O	1:C:947:LYS:HE2	2.20	0.42
2:D:81:LYS:HA	2:D:81:LYS:HD3	1.72	0.42
2:D:198:ASP:OD2	2:D:466:GLY:HA2	2.19	0.42
2:D:199:TYR:N	2:D:465:LYS:C	2.77	0.42
2:D:241:HIS:HA	2:D:244:VAL:CG1	2.49	0.42
1:B:188:ASN:CG	1:B:206:LYS:HA	2.45	0.42
1:B:190:ARG:H	1:B:190:ARG:CD	2.28	0.42
1:B:1034:LEU:HD12	1:B:1034:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1091:ARG:H	1:B:1120:THR:HA	1.85	0.42
1:C:898:PHE:CE2	1:C:902:MET:SD	3.13	0.42
2:D:305:ARG:NE	2:D:333:LEU:HD11	2.35	0.42
2:D:399:GLY:O	2:D:514:ARG:HA	2.20	0.42
2:D:411:SER:CB	2:D:522:GLN:HG3	2.38	0.42
2:D:513:ILE:HD12	2:D:516:TYR:HD2	1.85	0.42
2:D:527:GLU:O	2:D:542:CYS:C	2.62	0.42
2:D:544:ILE:HG23	2:D:550:ALA:HB3	2.01	0.42
1:B:55:PHE:C	1:B:270:LEU:HD13	2.44	0.41
1:B:994:ASP:HA	1:B:997:ILE:HG22	2.00	0.41
1:C:84:PHE:CE1	1:C:87:GLY:HA2	2.55	0.41
1:C:503:VAL:HG12	2:D:355:ASP:OD2	2.20	0.41
1:C:616:ASN:OD1	1:C:617:CYS:N	2.53	0.41
1:C:738:CYS:HB3	1:C:760:CYS:HB2	1.95	0.41
2:D:239:HIS:HA	2:D:242:ALA:HB3	2.02	0.41
2:D:481:LYS:HA	2:D:484:ILE:HG22	2.00	0.41
2:D:564:LYS:NZ	2:D:568:PHE:HB2	2.34	0.41
1:A:748:GLU:HA	1:A:751:ASN:HD21	1.85	0.41
1:B:202:LYS:HA	1:B:227:VAL:O	2.20	0.41
1:B:729:VAL:HG23	1:B:1059:GLY:HA2	2.01	0.41
1:B:1021:SER:O	1:B:1024:LEU:HG	2.20	0.41
1:C:444:LYS:H	1:C:444:LYS:HD2	1.85	0.41
1:C:821:LEU:HD23	1:C:821:LEU:HA	1.86	0.41
2:D:61:LYS:CA	2:D:65:ALA:N	2.60	0.41
2:D:176:LEU:HD23	2:D:177:ARG:HA	2.02	0.41
2:D:473:TRP:HE3	2:D:477:TRP:HE1	1.68	0.41
2:D:535:HIS:CG	2:D:536:GLU:H	2.38	0.41
1:A:34:ARG:NE	1:A:286:THR:HB	2.35	0.41
1:A:68:ILE:HD12	1:A:68:ILE:HA	1.97	0.41
1:A:1097:SER:OG	1:A:1101:HIS:O	2.36	0.41
1:B:764:ASN:O	1:B:768:THR:HG23	2.20	0.41
1:B:997:ILE:O	1:B:1001:LEU:HG	2.20	0.41
1:C:82:LEU:O	1:C:238:PHE:N	2.53	0.41
1:C:274:THR:HG23	1:C:291:CYS:HB2	2.02	0.41
1:C:356:LYS:HD2	1:C:356:LYS:HA	1.82	0.41
1:C:357:ARG:NH1	1:C:359:SER:O	2.49	0.41
1:C:409:GLN:HA	1:C:414:GLN:HG3	2.03	0.41
1:C:1019:ARG:HG3	1:C:1023:ASN:HD21	1.84	0.41
2:D:58:ASN:C	2:D:63:ASN:N	2.79	0.41
2:D:199:TYR:O	2:D:463:VAL:C	2.62	0.41
2:D:307:ILE:C	2:D:311:ALA:HB3	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:533:ALA:C	2:D:543:ASP:HB3	2.45	0.41
2:D:558:LEU:HB2	2:D:571:GLU:CA	2.47	0.41
1:A:806:LEU:HD12	1:A:806:LEU:HA	1.86	0.41
1:B:738:CYS:O	1:B:742:ILE:HG23	2.20	0.41
1:B:1000:ARG:HH21	1:B:1003:SER:C	2.29	0.41
1:B:1010:GLN:HA	1:B:1013:ILE:HG12	2.03	0.41
1:C:84:PHE:HZ	1:C:195:LYS:HZ2	1.68	0.41
1:C:393:THR:HG23	1:C:518:LEU:HB2	2.02	0.41
1:C:759:PHE:CE1	1:C:1001:LEU:HD11	2.55	0.41
2:D:61:LYS:H	2:D:63:ASN:C	1.84	0.41
2:D:371:THR:O	2:D:375:GLU:HG2	2.21	0.41
1:C:118:LEU:HD23	1:C:118:LEU:HA	1.82	0.41
1:C:428:ASP:OD1	1:C:428:ASP:N	2.39	0.41
1:C:759:PHE:HE1	1:C:1001:LEU:HD11	1.86	0.41
2:D:84:PRO:O	2:D:97:LEU:HD13	2.20	0.41
2:D:165:TRP:HE1	2:D:169:ARG:CD	2.32	0.41
2:D:312:GLU:HA	2:D:316:VAL:CG1	2.50	0.41
1:A:46:SER:O	1:A:278:LYS:NZ	2.53	0.41
1:B:49:HIS:CG	1:B:50:SER:N	2.89	0.41
1:B:986:PRO:CB	1:B:987:PRO:HD2	2.39	0.41
1:C:212:LEU:HG	1:C:214:ARG:HD2	2.03	0.41
1:C:338:PHE:HB3	1:C:342:PHE:CE2	2.55	0.41
1:C:497:PHE:HA	1:C:501:ASN:HD21	1.86	0.41
1:C:568:ASP:HB3	1:C:574:ASP:OD1	2.20	0.41
2:D:38:GLU:O	2:D:41:TYR:HB3	2.21	0.41
2:D:57:GLU:C	2:D:63:ASN:HB2	2.45	0.41
2:D:550:ALA:HA	2:D:553:LYS:HD3	2.01	0.41
1:A:29:THR:CA	1:A:93:ALA:H	2.33	0.41
1:A:1006:THR:HB	1:A:1010:GLN:OE1	2.21	0.41
1:B:947:LYS:NZ	1:B:947:LYS:H	2.19	0.41
1:C:105:ILE:HB	1:C:240:THR:HA	2.02	0.41
1:C:206:LYS:HG2	1:C:222:ALA:O	2.20	0.41
1:C:647:ALA:HB2	1:C:668:ALA:HB2	2.02	0.41
1:C:1114:ILE:O	1:C:1116:THR:HG23	2.20	0.41
2:D:209:GLU:HG2	2:D:210:GLU:N	2.34	0.41
2:D:239:HIS:HB3	2:D:595:LEU:HD22	2.03	0.41
2:D:239:HIS:HA	2:D:242:ALA:CB	2.51	0.41
2:D:382:ASP:HA	2:D:385:TYR:CZ	2.55	0.41
1:A:31:SER:N	1:A:91:TYR:C	2.75	0.41
1:A:120:VAL:O	1:A:120:VAL:HG22	2.20	0.41
1:B:287:ASP:OD1	1:B:288:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:TYR:HE1	1:C:222:ALA:HB1	1.85	0.41
1:C:393:THR:OG1	1:C:394:ASN:N	2.54	0.41
2:D:203:TRP:C	2:D:205:GLY:H	2.29	0.41
2:D:310:GLU:O	2:D:314:PHE:HB3	2.21	0.41
2:D:399:GLY:CA	2:D:514:ARG:HG2	2.51	0.41
2:D:459:TRP:CZ2	2:D:463:VAL:HG21	2.56	0.41
1:A:195:LYS:HG3	1:A:197:ILE:HG12	2.03	0.41
1:A:272:PRO:O	1:A:273:ARG:HD2	2.21	0.41
1:A:290:ASP:HB3	1:A:293:LEU:HD21	2.03	0.41
1:A:295:PRO:HA	1:A:298:GLU:HG3	2.01	0.41
1:B:78:ASP:O	1:B:104:TRP:HB2	2.20	0.41
1:B:92:PHE:CD1	1:B:193:VAL:HA	2.55	0.41
1:B:188:ASN:OD1	1:B:188:ASN:N	2.50	0.41
1:B:758:SER:HB2	1:B:761:THR:OG1	2.21	0.41
1:B:768:THR:O	1:B:772:VAL:HG13	2.21	0.41
1:B:985:ASP:N	1:B:986:PRO:HD3	2.35	0.41
1:C:78:ASP:OD1	1:C:240:THR:HG23	2.20	0.41
1:C:347:PHE:HB3	1:C:399:SER:O	2.21	0.41
1:C:381:GLY:HA3	1:C:431:GLY:N	2.35	0.41
1:C:384:PRO:HG2	1:C:385:THR:HG23	2.03	0.41
1:C:405:ASP:HB3	2:D:354:HIS:HB3	2.02	0.41
1:C:436:TRP:CH2	1:C:509:ARG:HD3	2.56	0.41
1:C:555:SER:OG	1:C:584:ILE:O	2.32	0.41
1:C:922:LEU:O	1:C:926:GLN:HG3	2.21	0.41
2:D:355:ASP:HB2	2:D:357:ARG:HH21	1.86	0.41
2:D:374:HIS:CE1	2:D:408:MET:HE3	2.55	0.41
2:D:528:ALA:C	2:D:542:CYS:C	2.88	0.41
1:A:86:ASP:N	1:A:237:ARG:C	2.79	0.41
1:A:167:THR:HB	1:A:170:TYR:CA	2.49	0.41
1:A:220:PHE:H	1:A:285:ILE:HA	1.86	0.41
1:B:91:TYR:CD2	1:B:270:LEU:HD22	2.56	0.41
1:B:117:LEU:HB2	1:B:126:VAL:HG22	2.03	0.41
1:B:786:LYS:HG3	1:B:787:GLN:HG3	2.03	0.41
1:B:1144:GLU:N	1:B:1144:GLU:CD	2.79	0.41
1:C:64:TRP:O	1:C:263:ALA:HA	2.21	0.41
1:C:119:ILE:HD12	1:C:120:VAL:H	1.86	0.41
1:C:348:ALA:HB1	1:C:352:ALA:O	2.21	0.41
1:C:348:ALA:HB3	1:C:354:ASN:OD1	2.21	0.41
1:C:799:GLY:O	1:C:924:ALA:HB1	2.21	0.41
2:D:156:LYS:HE2	2:D:251:ALA:HB3	2.02	0.41
2:D:276:THR:N	2:D:444:LEU:HD21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:553:LYS:HA	2:D:556:GLU:CB	2.50	0.41
1:A:63:THR:O	1:A:264:ALA:HB3	2.21	0.40
1:A:293:LEU:HD22	1:A:293:LEU:H	1.85	0.40
1:B:81:VAL:HA	1:B:239:GLN:HB2	2.02	0.40
1:C:220:PHE:CZ	1:C:222:ALA:HB2	2.56	0.40
1:C:405:ASP:CB	2:D:354:HIS:HB3	2.51	0.40
1:C:690:GLN:OE1	1:C:690:GLN:HA	2.21	0.40
2:D:24:LEU:HD23	2:D:24:LEU:HA	1.91	0.40
2:D:306:ARG:NE	2:D:310:GLU:HG2	2.36	0.40
1:A:41:LYS:HZ2	1:C:564:GLN:CB	2.31	0.40
1:B:88:VAL:HG12	1:B:238:PHE:CZ	2.56	0.40
1:B:216:LEU:HD12	1:B:217:PRO:HD2	2.04	0.40
1:B:867:ASP:OD1	1:B:868:GLU:N	2.54	0.40
1:C:1045:LYS:O	1:C:1066:THR:HG21	2.22	0.40
2:D:22:GLU:OE1	2:D:22:GLU:N	2.54	0.40
2:D:136:ASN:OD1	2:D:137:ASN:N	2.48	0.40
2:D:226:VAL:HG13	2:D:450:LEU:HD11	2.04	0.40
2:D:291:ILE:HG13	2:D:423:LEU:HD12	2.03	0.40
2:D:419:LYS:C	2:D:422:GLY:H	2.29	0.40
2:D:584:LEU:HA	2:D:587:TYR:HB2	2.02	0.40
1:B:212:LEU:HB3	1:B:215:ASP:O	2.21	0.40
1:B:280:ASN:OD1	1:B:283:GLY:N	2.55	0.40
1:B:986:PRO:CB	1:B:987:PRO:CD	2.94	0.40
1:C:503:VAL:HG12	2:D:355:ASP:CG	2.46	0.40
1:C:726:ILE:C	1:C:727:LEU:HD22	2.46	0.40
2:D:403:ALA:HB2	2:D:515:TYR:CD1	2.56	0.40
2:D:527:GLU:C	2:D:542:CYS:HB3	2.47	0.40
2:D:531:GLN:O	2:D:534:LYS:N	2.54	0.40
2:D:531:GLN:CB	2:D:541:LYS:C	2.94	0.40
2:D:558:LEU:HB3	2:D:570:LEU:H	1.86	0.40
1:A:276:LEU:O	1:A:288:ALA:HA	2.21	0.40
1:B:238:PHE:C	1:B:239:GLN:OE1	2.64	0.40
1:B:902:MET:HB3	1:B:916:LEU:HD21	2.02	0.40
1:C:189:LEU:HD12	1:C:208:THR:H	1.86	0.40
1:C:777:ASN:O	1:C:780:GLU:HG3	2.21	0.40
2:D:240:LEU:HD23	2:D:240:LEU:HA	1.83	0.40
1:A:97:LYS:HA	1:A:209:PRO:HG2	2.04	0.40
1:B:65:PHE:HB3	1:B:265:TYR:O	2.20	0.40
1:B:91:TYR:CE1	1:B:268:GLY:HA3	2.57	0.40
1:B:328:ARG:HG2	1:B:587:ILE:HD11	2.03	0.40
1:B:714:ILE:HD13	1:B:714:ILE:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:ALA:HB1	1:C:586:ASP:OD1	2.21	0.40
1:C:663:ASP:N	1:C:663:ASP:OD1	2.45	0.40
2:D:52:THR:HA	2:D:340:ARG:HD3	2.02	0.40
2:D:82:THR:O	2:D:82:THR:OG1	2.34	0.40
2:D:419:LYS:HD3	2:D:419:LYS:O	2.22	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	730/1269 (58%)	636 (87%)	92 (13%)	2 (0%)	36	69
1	B	730/1269 (58%)	653 (90%)	73 (10%)	4 (0%)	24	59
1	C	934/1269 (74%)	834 (89%)	100 (11%)	0	100	100
2	D	594/771 (77%)	461 (78%)	128 (22%)	5 (1%)	16	50
All	All	2988/4578 (65%)	2584 (86%)	393 (13%)	11 (0%)	31	64

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	ASN
1	B	189	LEU
1	B	986	PRO
2	D	198	ASP
2	D	566	TRP
2	D	543	ASP
2	D	59	ILE
1	A	84	PHE
1	A	221	SER
2	D	565	PRO

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Mol	Chain	Res	Type
1	B	80	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	657/1101 (60%)	655 (100%)	2 (0%)	86	85
1	B	657/1101 (60%)	655 (100%)	2 (0%)	86	85
1	C	831/1101 (76%)	830 (100%)	1 (0%)	88	89
2	D	524/676 (78%)	523 (100%)	1 (0%)	87	87
All	All	2669/3979 (67%)	2663 (100%)	6 (0%)	85	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	TYR
1	A	981	LEU
1	B	239	GLN
1	B	1000	ARG
1	C	82	LEU
2	D	361	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	211	ASN
1	A	234	ASN
1	A	751	ASN
1	A	935	GLN
1	A	954	GLN
1	A	955	ASN
1	A	1005	GLN
1	A	1011	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	A	1054	GLN
1	A	1106	GLN
1	B	121	ASN
1	B	271	GLN
1	B	949	GLN
1	B	1002	GLN
1	C	85	ASN
1	C	388	ASN
1	C	422	ASN
1	C	439	ASN
1	C	506	GLN
1	C	606	ASN
1	C	613	GLN
1	C	675	GLN
1	C	751	ASN
1	C	957	GLN
1	C	1048	HIS
2	D	58	ASN
2	D	63	ASN
2	D	195	ASN
2	D	339	ASN
2	D	345	HIS
2	D	374	HIS
2	D	388	GLN
2	D	401	HIS
2	D	416	ASN
2	D	420	ASN
2	D	493	HIS
2	D	535	HIS
2	D	586	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

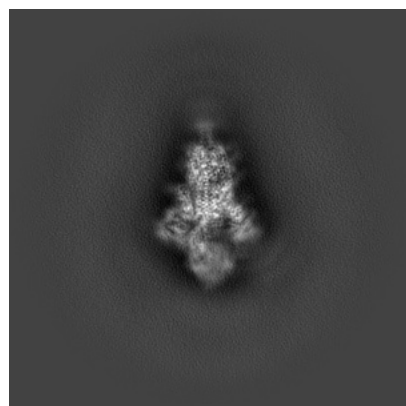
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40978. These allow visual inspection of the internal detail of the map and identification of artifacts.

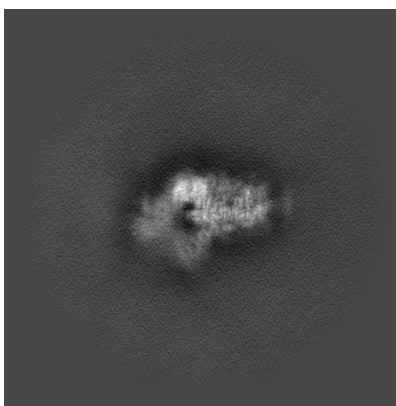
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

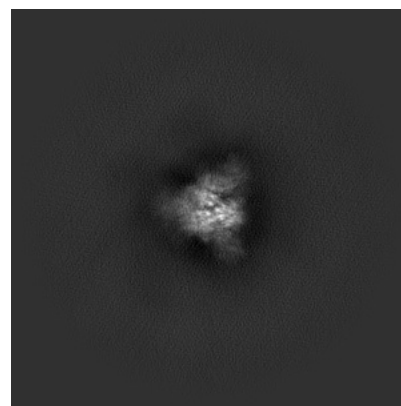
6.1.1 Primary map



X

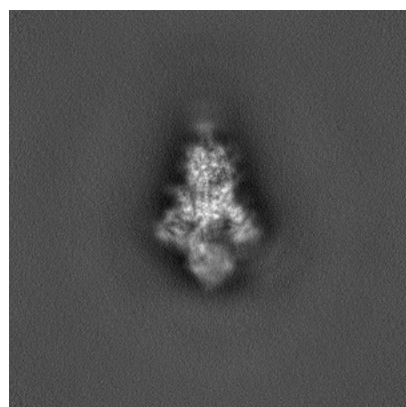


Y

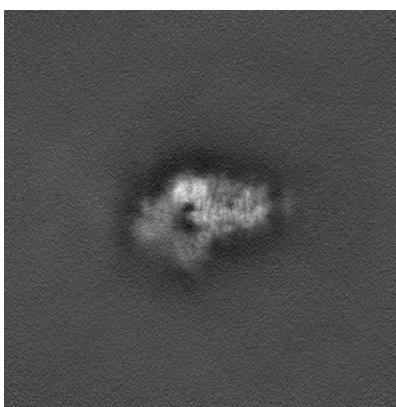


Z

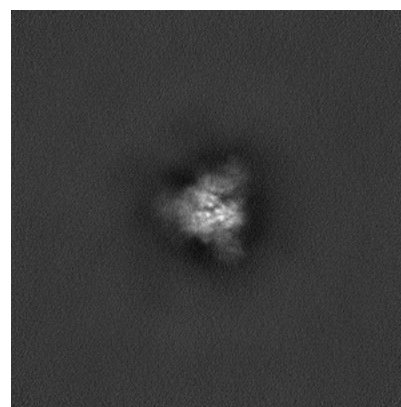
6.1.2 Raw map



X



Y

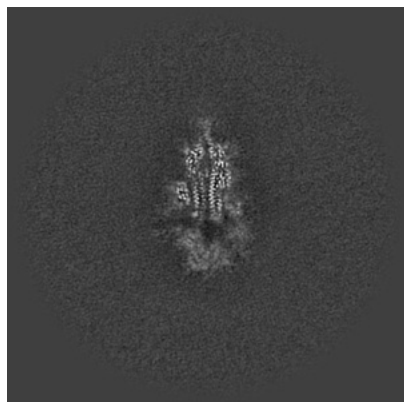


Z

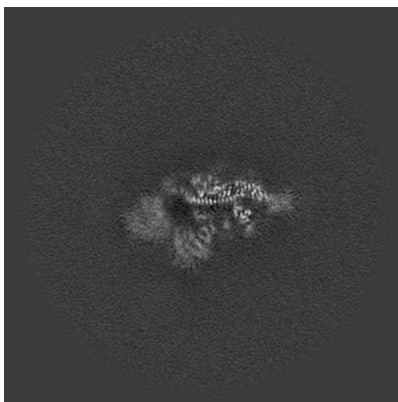
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

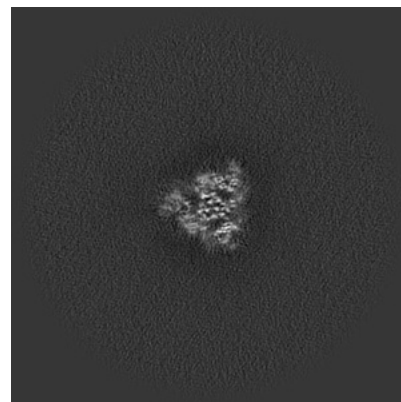
6.2.1 Primary map



X Index: 256

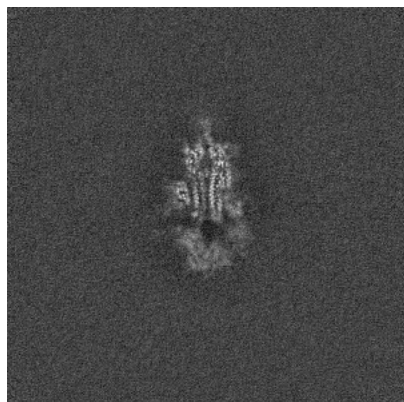


Y Index: 256

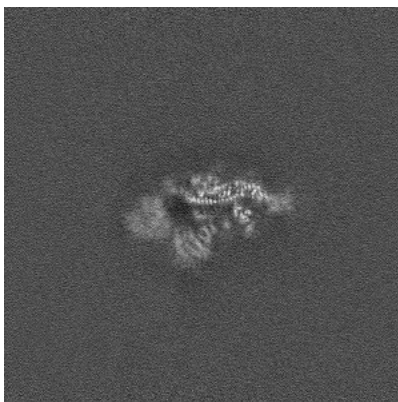


Z Index: 256

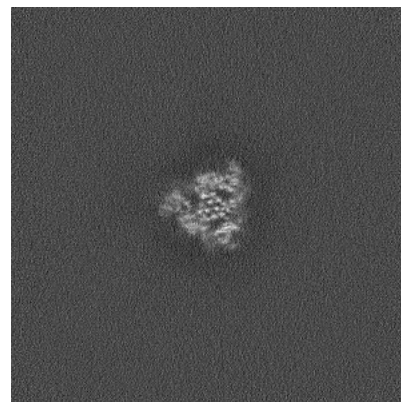
6.2.2 Raw map



X Index: 256



Y Index: 256

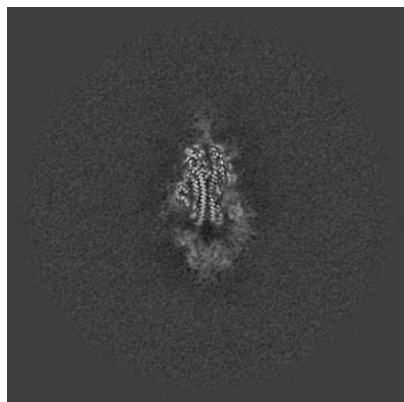


Z Index: 256

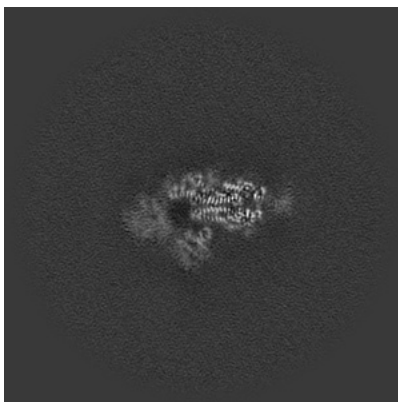
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

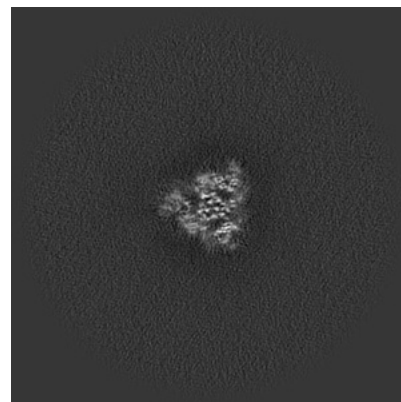
6.3.1 Primary map



X Index: 252

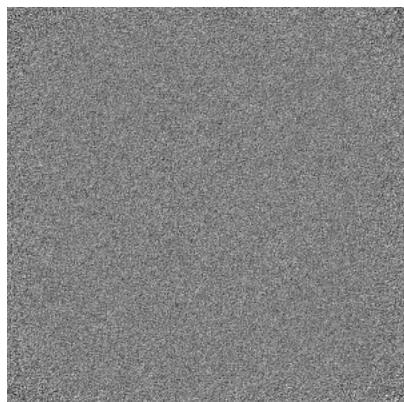


Y Index: 252

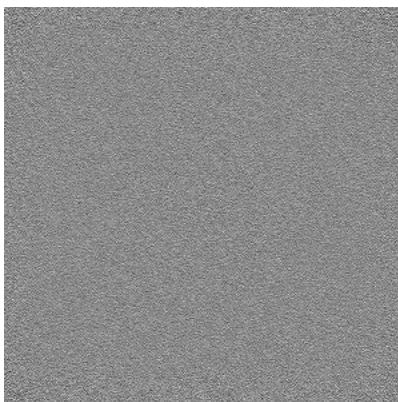


Z Index: 256

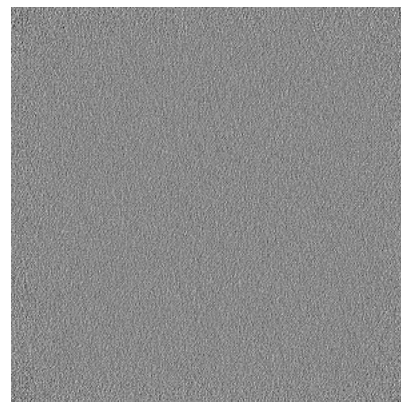
6.3.2 Raw map



X Index: 0



Y Index: 0

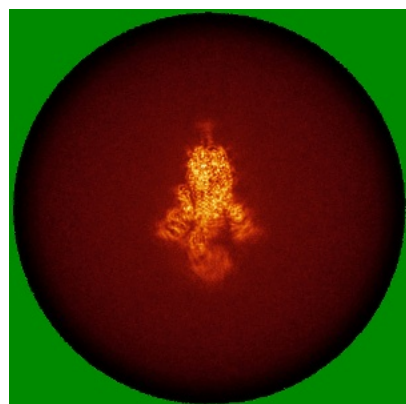


Z Index: 0

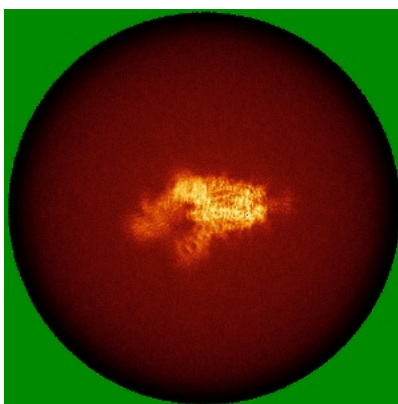
The images above show the largest variance slices of the map in three orthogonal directions.

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

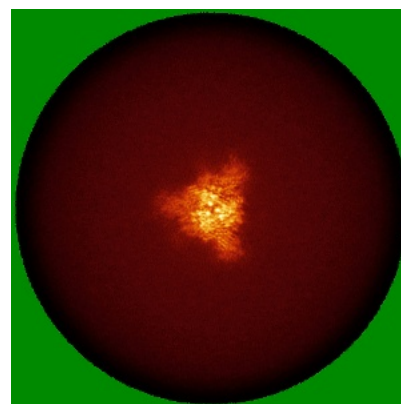
6.4.1 Primary map



X

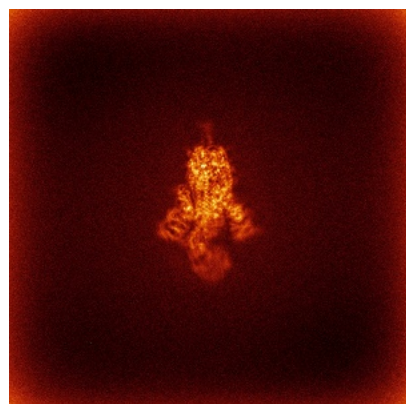


Y

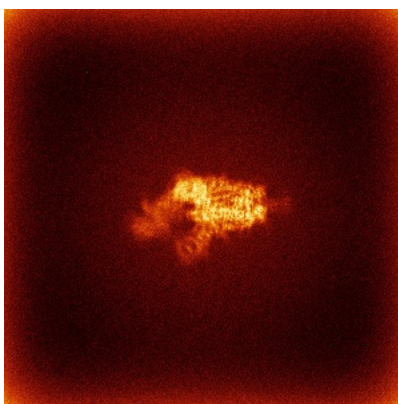


Z

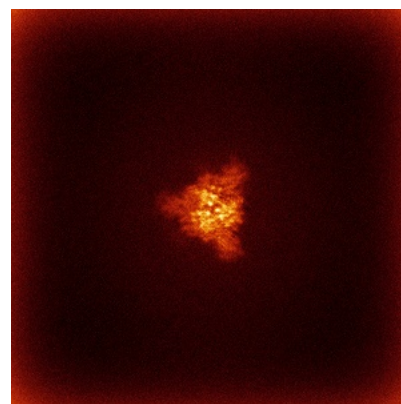
6.4.2 Raw map



X



Y

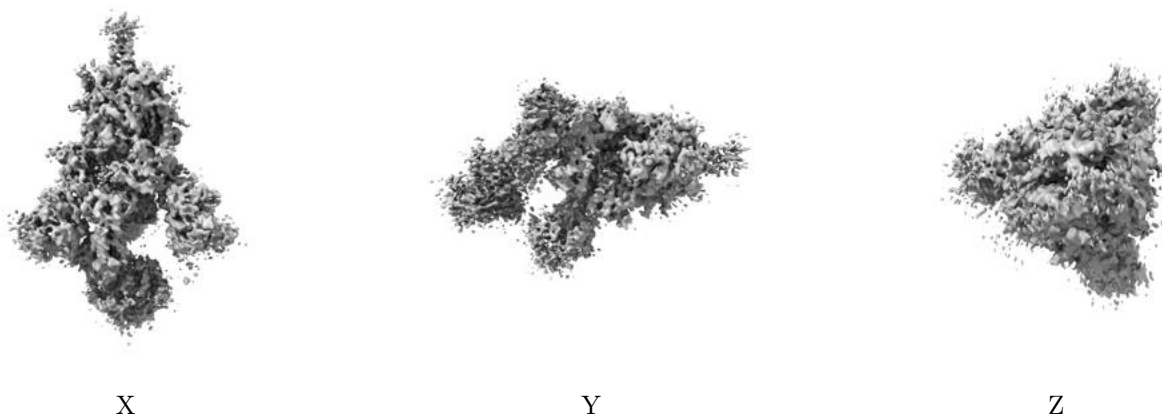


Z

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

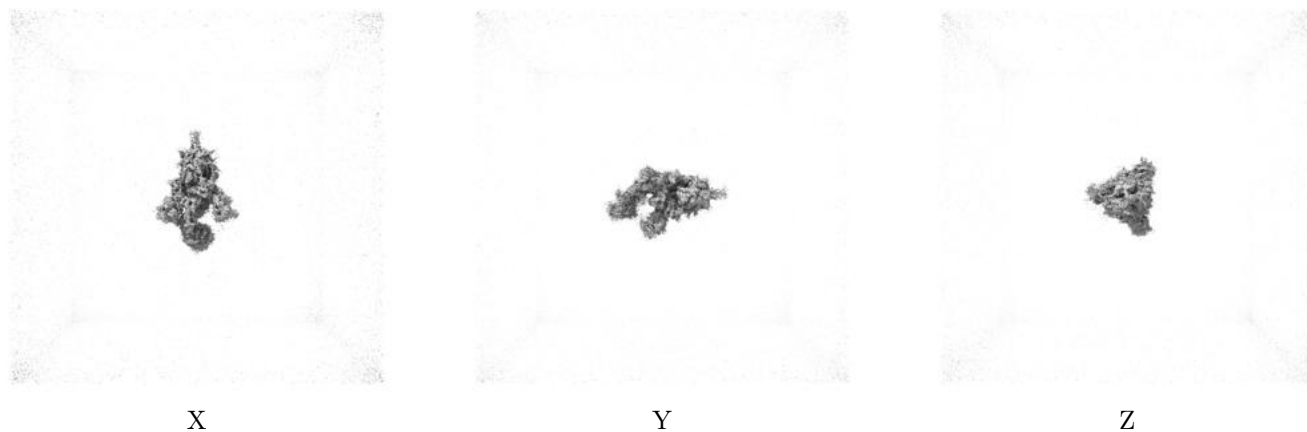
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.309. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

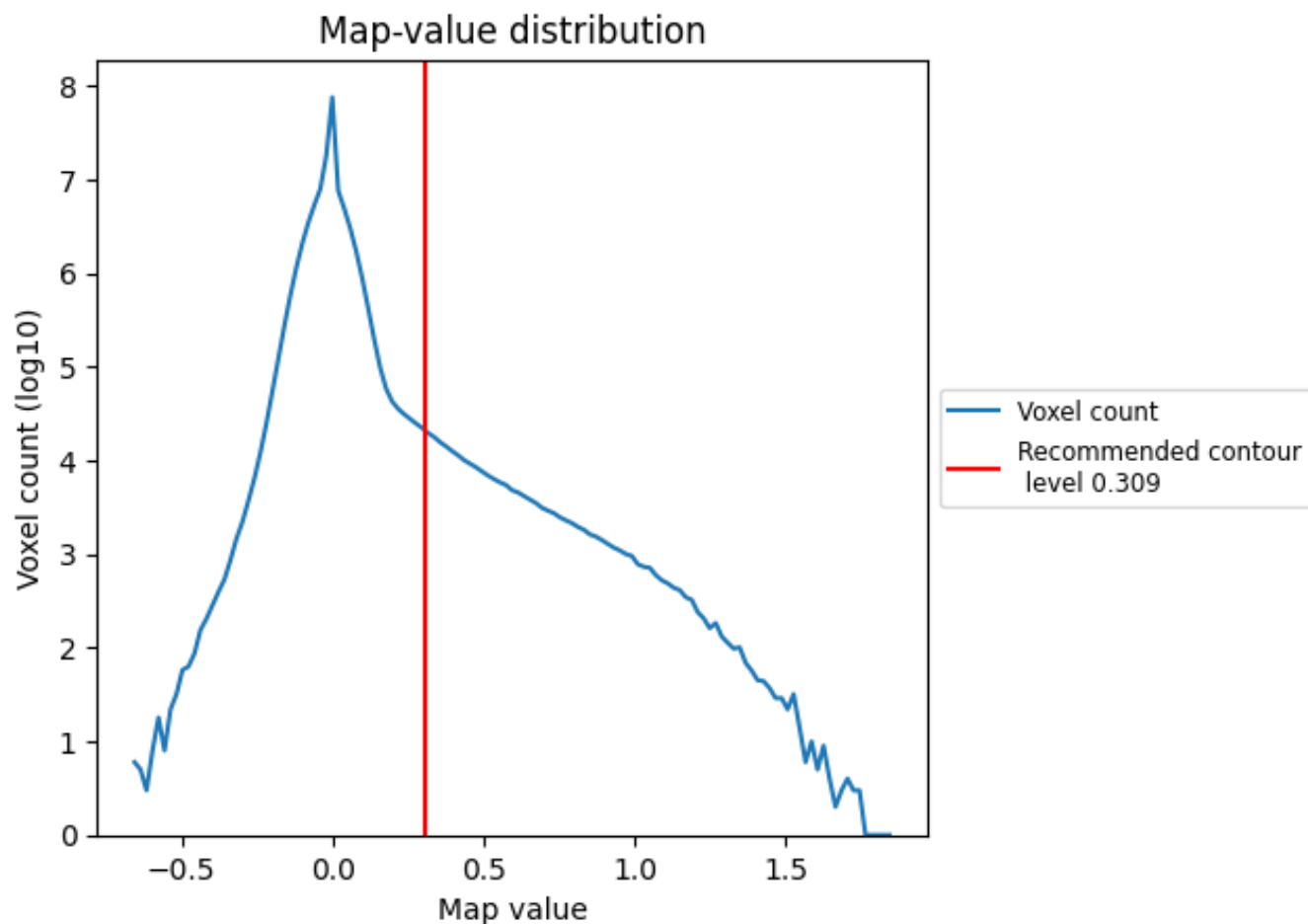
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

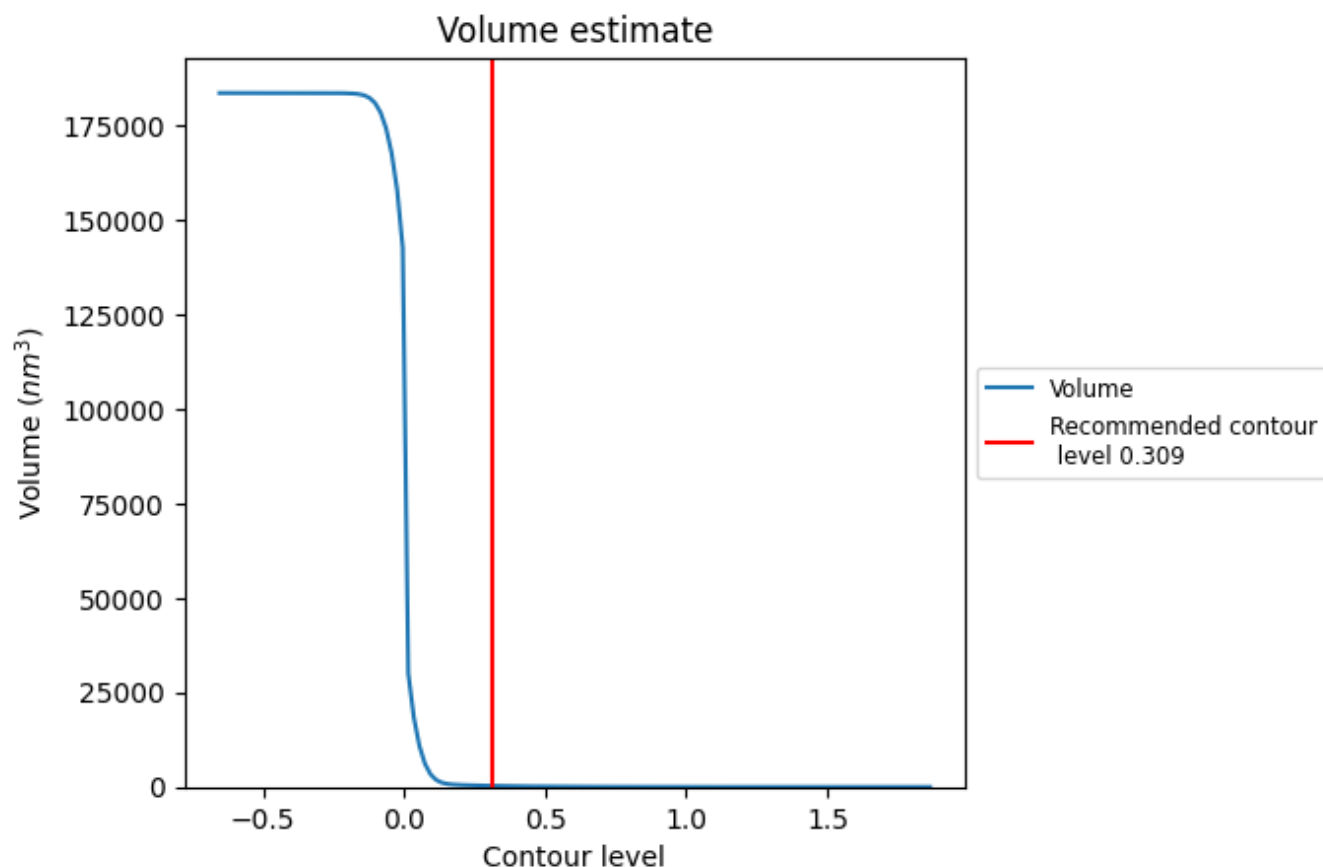
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

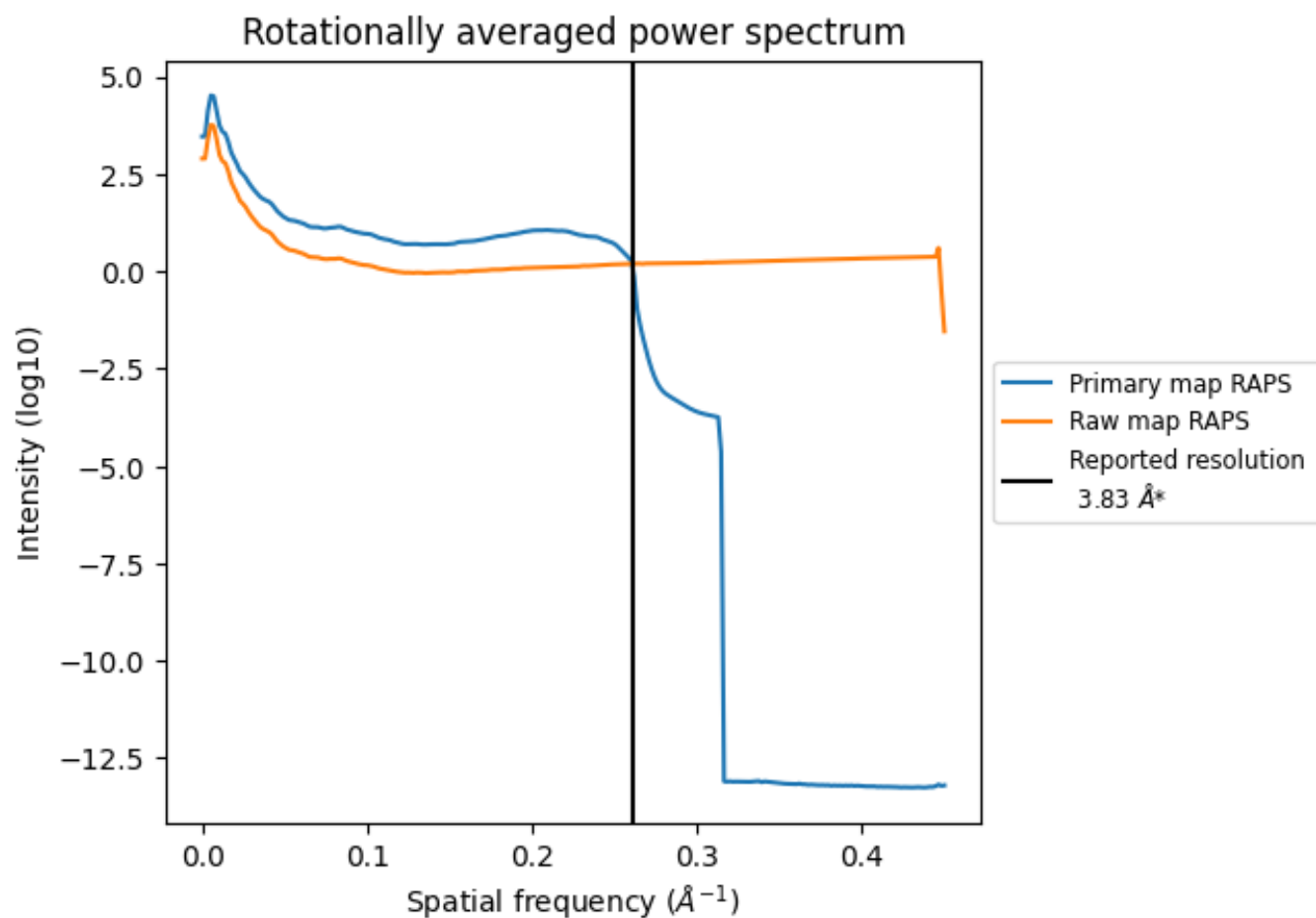
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 298 nm^3 ; this corresponds to an approximate mass of 269 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

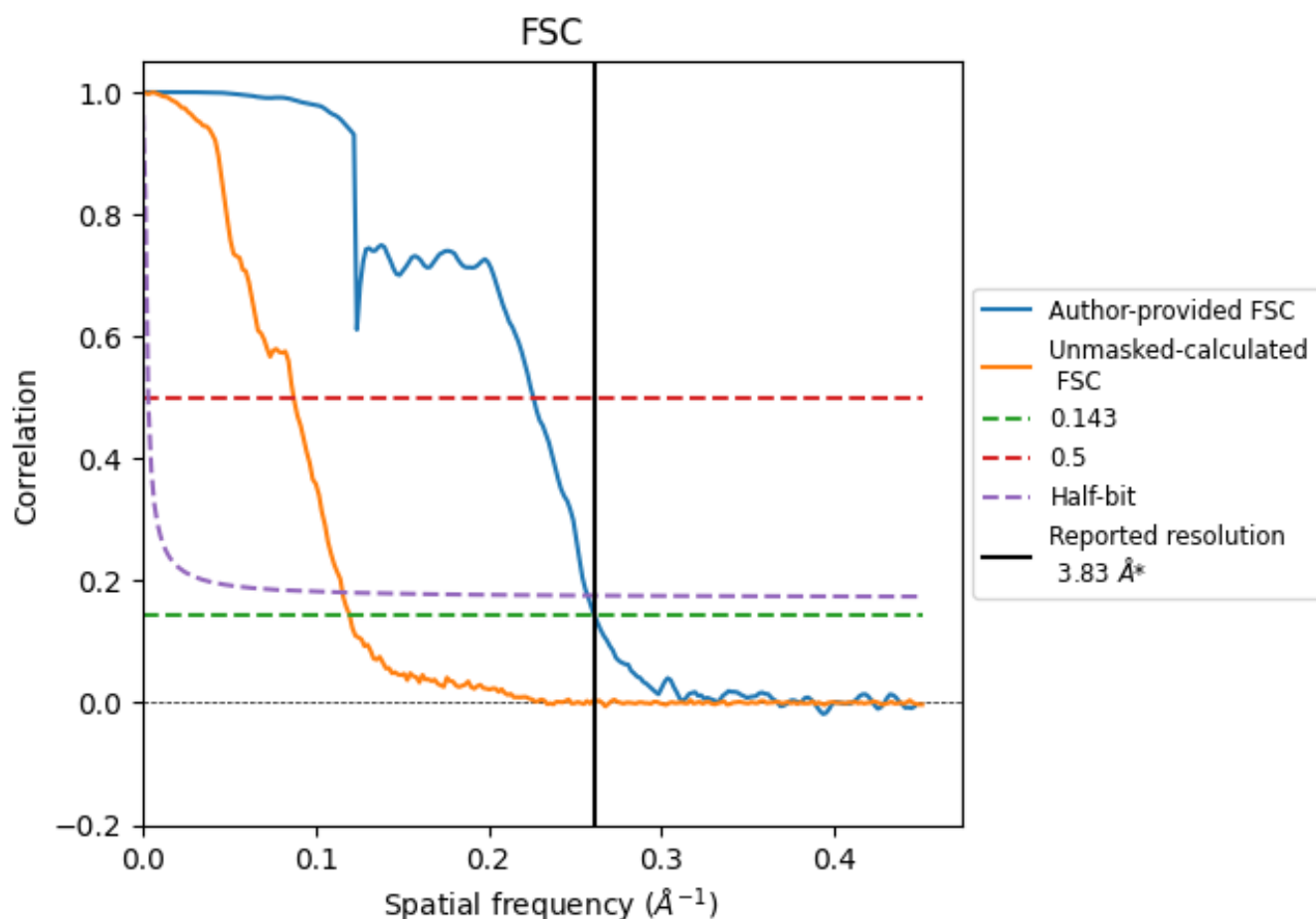


*Reported resolution corresponds to spatial frequency of 0.261 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.261 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

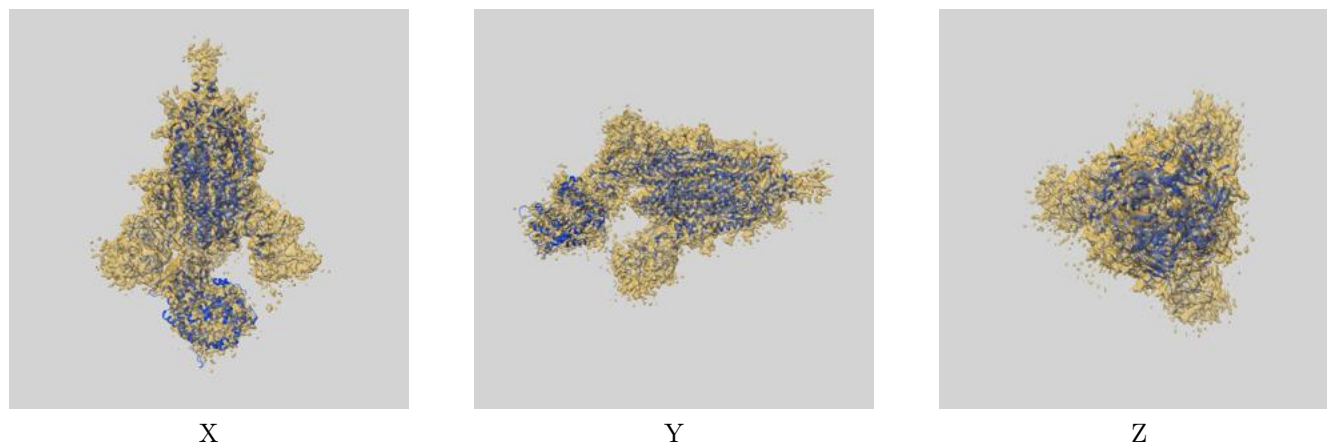
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.83	-	-
Author-provided FSC curve	3.83	4.43	3.89
Unmasked-calculated*	8.35	11.43	8.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.35 differs from the reported value 3.83 by more than 10 %

9 Map-model fit [i](#)

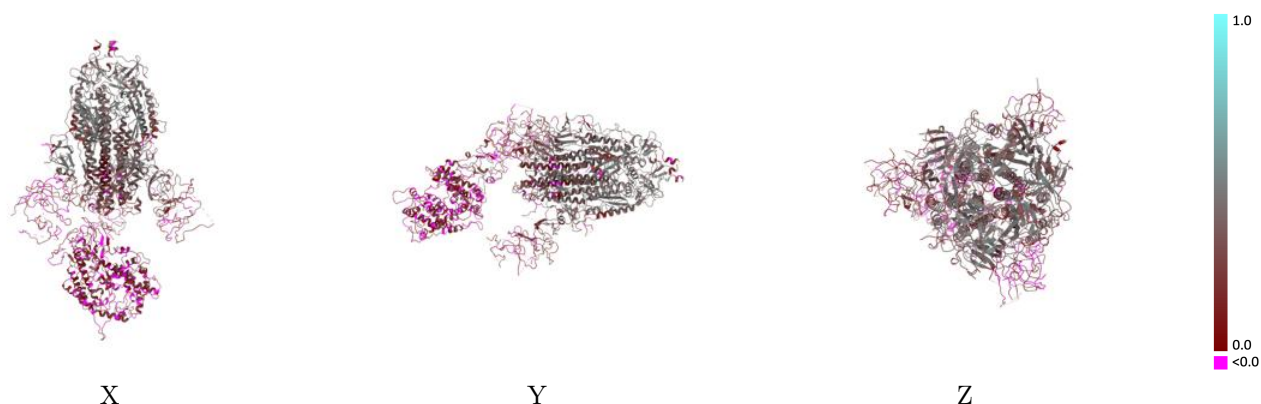
This section contains information regarding the fit between EMDB map EMD-40978 and PDB model 8T22. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



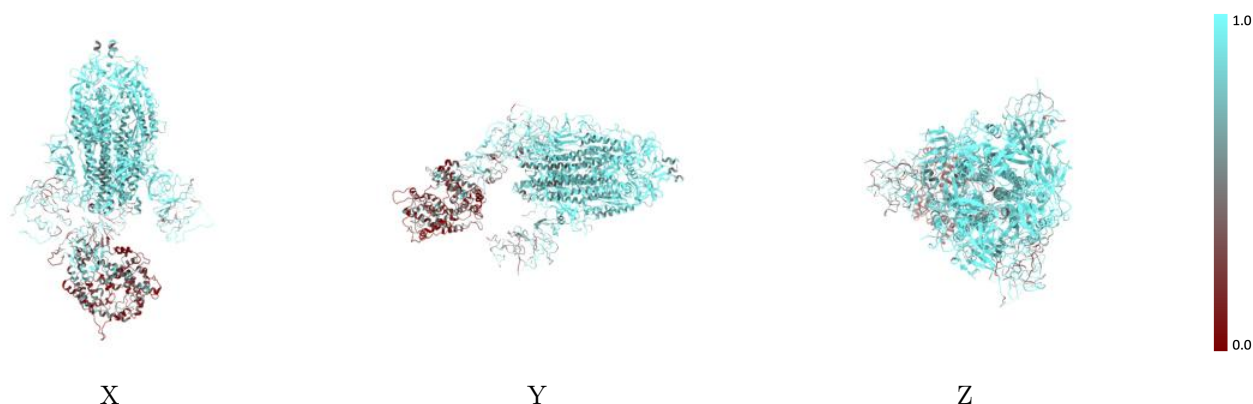
The images above show the 3D surface view of the map at the recommended contour level 0.309 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



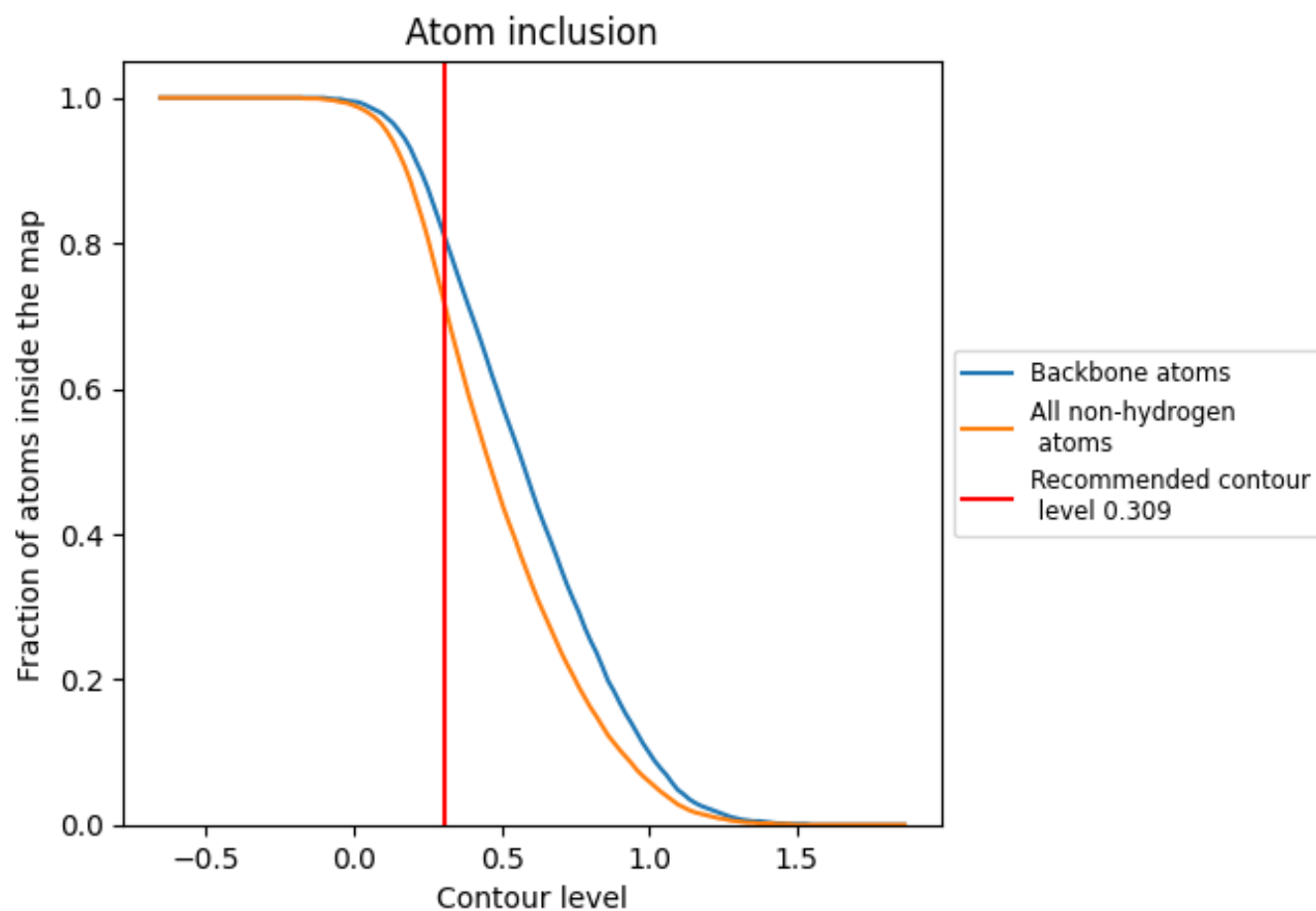
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.309).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.309) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.2580
A	0.8290	0.3040
B	0.8050	0.3120
C	0.8220	0.2940
D	0.3020	0.0840

