Full wwPDB EM Validation Report (i)

Nov 23, 2022 – 06:32 PM JST

PDB ID	:	7WOW
EMDB ID	:	EMD-32661
Title	:	The state 6 of Omicron Spike with bispecific antibody FD01
Authors	:	Zhang, X.; Zhan, W.Q.; Chen, Z.G.; Sun, L.
Deposited on	:	2022-01-22
Resolution	:	6.11 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 (i) 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 (i)) were used in the production of this report:

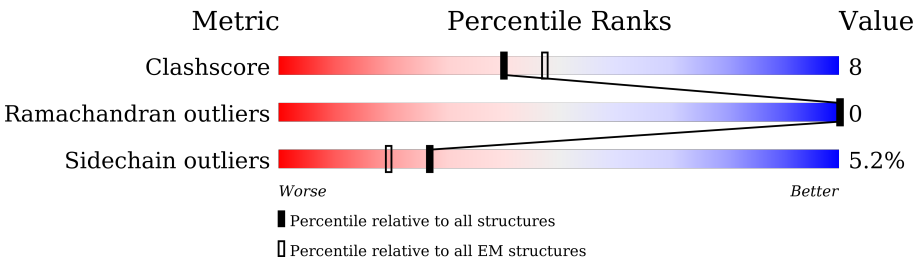
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.11 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1285	64% 16% • 20%
1	B	1285	63% 16% • 20%
1	C	1285	63% 15% • 20%
1	J	1285	14% 64% 15% • 20%
1	K	1285	13% 63% 16% • 20%
1	L	1285	14% 63% 16% • 20%
2	D	247	18% 68% 25% • •
2	F	247	5% 66% 26% • •

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Mol	Chain	Length	Quality of chain
2	H	247	67% 25%
2	M	247	35% 69% 23%
2	O	247	14% 66% 27%
2	Q	247	15% 66% 26%
3	E	251	17% 73% 20% 6%
3	G	251	71% 22% 6%
3	I	251	71% 22% 6%
3	N	251	48% 74% 19% 6%
3	P	251	22% 74% 20% 6%
3	R	251	30% 73% 21% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 69264 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
			Total	C	N	O	S		
1	A	1033	8043	5158	1338	1510	37	0	0
1	B	1033	8043	5158	1338	1510	37	0	0
1	C	1026	7989	5124	1326	1502	37	0	0
1	J	1033	8043	5158	1338	1510	37	0	0
1	K	1033	8043	5158	1338	1510	37	0	0
1	L	1026	7989	5124	1326	1502	37	0	0

There are 768 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	145	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	209	ILE	LEU	variant	UNP P0DTC2
A	212	GLU	-	insertion	UNP P0DTC2
A	213	PRO	-	insertion	UNP P0DTC2
A	214	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	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	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	856	LYS	ASN	variant	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	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	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	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	PHE	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	145	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	209	ILE	LEU	variant	UNP P0DTC2
B	212	GLU	-	insertion	UNP P0DTC2
B	213	PRO	-	insertion	UNP P0DTC2
B	214	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	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	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	856	LYS	ASN	variant	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	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	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	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	145	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	209	ILE	LEU	variant	UNP P0DTC2
C	212	GLU	-	insertion	UNP P0DTC2
C	213	PRO	-	insertion	UNP P0DTC2
C	214	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	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	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	856	LYS	ASN	variant	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	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	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	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	PHE	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2
J	67	VAL	ALA	variant	UNP P0DTC2
J	?	-	HIS	deletion	UNP P0DTC2
J	?	-	VAL	deletion	UNP P0DTC2
J	95	ILE	THR	variant	UNP P0DTC2
J	145	ASP	GLY	variant	UNP P0DTC2
J	?	-	VAL	deletion	UNP P0DTC2
J	?	-	TYR	deletion	UNP P0DTC2
J	?	-	TYR	deletion	UNP P0DTC2
J	?	-	ASN	deletion	UNP P0DTC2
J	209	ILE	LEU	variant	UNP P0DTC2
J	212	GLU	-	insertion	UNP P0DTC2
J	213	PRO	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	214	GLU	-	insertion	UNP P0DTC2
J	339	ASP	GLY	variant	UNP P0DTC2
J	371	LEU	SER	variant	UNP P0DTC2
J	373	PRO	SER	variant	UNP P0DTC2
J	375	PHE	SER	variant	UNP P0DTC2
J	417	ASN	LYS	variant	UNP P0DTC2
J	440	LYS	ASN	variant	UNP P0DTC2
J	446	SER	GLY	variant	UNP P0DTC2
J	477	ASN	SER	variant	UNP P0DTC2
J	478	LYS	THR	variant	UNP P0DTC2
J	484	ALA	GLU	variant	UNP P0DTC2
J	493	ARG	GLN	variant	UNP P0DTC2
J	496	SER	GLY	variant	UNP P0DTC2
J	498	ARG	GLN	variant	UNP P0DTC2
J	501	TYR	ASN	variant	UNP P0DTC2
J	505	HIS	TYR	variant	UNP P0DTC2
J	547	LYS	THR	variant	UNP P0DTC2
J	614	GLY	ASP	variant	UNP P0DTC2
J	655	TYR	HIS	variant	UNP P0DTC2
J	679	LYS	ASN	variant	UNP P0DTC2
J	681	HIS	PRO	variant	UNP P0DTC2
J	682	GLY	ARG	engineered mutation	UNP P0DTC2
J	683	SER	ARG	engineered mutation	UNP P0DTC2
J	685	SER	ARG	engineered mutation	UNP P0DTC2
J	764	LYS	ASN	variant	UNP P0DTC2
J	796	TYR	ASP	variant	UNP P0DTC2
J	817	PRO	PHE	variant	UNP P0DTC2
J	856	LYS	ASN	variant	UNP P0DTC2
J	892	PRO	ALA	engineered mutation	UNP P0DTC2
J	899	PRO	ALA	engineered mutation	UNP P0DTC2
J	942	PRO	ALA	engineered mutation	UNP P0DTC2
J	954	HIS	GLN	variant	UNP P0DTC2
J	969	LYS	ASN	variant	UNP P0DTC2
J	981	PHE	LEU	variant	UNP P0DTC2
J	986	PRO	LYS	engineered mutation	UNP P0DTC2
J	987	PRO	VAL	engineered mutation	UNP P0DTC2
J	1209	GLY	-	expression tag	UNP P0DTC2
J	1210	SER	-	expression tag	UNP P0DTC2
J	1211	GLY	-	expression tag	UNP P0DTC2
J	1212	TYR	-	expression tag	UNP P0DTC2
J	1213	ILE	-	expression tag	UNP P0DTC2
J	1214	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1215	GLU	-	expression tag	UNP P0DTC2
J	1216	ALA	-	expression tag	UNP P0DTC2
J	1217	PRO	-	expression tag	UNP P0DTC2
J	1218	ARG	-	expression tag	UNP P0DTC2
J	1219	ASP	-	expression tag	UNP P0DTC2
J	1220	GLY	-	expression tag	UNP P0DTC2
J	1221	GLN	-	expression tag	UNP P0DTC2
J	1222	ALA	-	expression tag	UNP P0DTC2
J	1223	TYR	-	expression tag	UNP P0DTC2
J	1224	VAL	-	expression tag	UNP P0DTC2
J	1225	ARG	-	expression tag	UNP P0DTC2
J	1226	LYS	-	expression tag	UNP P0DTC2
J	1227	ASP	-	expression tag	UNP P0DTC2
J	1228	GLY	-	expression tag	UNP P0DTC2
J	1229	GLU	-	expression tag	UNP P0DTC2
J	1230	TRP	-	expression tag	UNP P0DTC2
J	1231	VAL	-	expression tag	UNP P0DTC2
J	1232	PHE	-	expression tag	UNP P0DTC2
J	1233	LEU	-	expression tag	UNP P0DTC2
J	1234	SER	-	expression tag	UNP P0DTC2
J	1235	THR	-	expression tag	UNP P0DTC2
J	1236	PHE	-	expression tag	UNP P0DTC2
J	1237	LEU	-	expression tag	UNP P0DTC2
J	1238	SER	-	expression tag	UNP P0DTC2
J	1239	GLY	-	expression tag	UNP P0DTC2
J	1240	LEU	-	expression tag	UNP P0DTC2
J	1241	GLU	-	expression tag	UNP P0DTC2
J	1242	VAL	-	expression tag	UNP P0DTC2
J	1243	LEU	-	expression tag	UNP P0DTC2
J	1244	PHE	-	expression tag	UNP P0DTC2
J	1245	GLN	-	expression tag	UNP P0DTC2
J	1246	GLY	-	expression tag	UNP P0DTC2
J	1247	PRO	-	expression tag	UNP P0DTC2
J	1248	GLY	-	expression tag	UNP P0DTC2
J	1249	GLY	-	expression tag	UNP P0DTC2
J	1250	TRP	-	expression tag	UNP P0DTC2
J	1251	SER	-	expression tag	UNP P0DTC2
J	1252	HIS	-	expression tag	UNP P0DTC2
J	1253	PRO	-	expression tag	UNP P0DTC2
J	1254	GLN	-	expression tag	UNP P0DTC2
J	1255	PHE	-	expression tag	UNP P0DTC2
J	1256	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1257	LYS	-	expression tag	UNP P0DTC2
J	1258	GLY	-	expression tag	UNP P0DTC2
J	1259	GLY	-	expression tag	UNP P0DTC2
J	1260	GLY	-	expression tag	UNP P0DTC2
J	1261	SER	-	expression tag	UNP P0DTC2
J	1262	GLY	-	expression tag	UNP P0DTC2
J	1263	GLY	-	expression tag	UNP P0DTC2
J	1264	GLY	-	expression tag	UNP P0DTC2
J	1265	SER	-	expression tag	UNP P0DTC2
J	1266	GLY	-	expression tag	UNP P0DTC2
J	1267	GLY	-	expression tag	UNP P0DTC2
J	1268	SER	-	expression tag	UNP P0DTC2
J	1269	ALA	-	expression tag	UNP P0DTC2
J	1270	TRP	-	expression tag	UNP P0DTC2
J	1271	SER	-	expression tag	UNP P0DTC2
J	1272	HIS	-	expression tag	UNP P0DTC2
J	1273	PRO	-	expression tag	UNP P0DTC2
J	1274	GLN	-	expression tag	UNP P0DTC2
J	1275	PHE	-	expression tag	UNP P0DTC2
J	1276	GLU	-	expression tag	UNP P0DTC2
J	1277	LYS	-	expression tag	UNP P0DTC2
J	1278	GLY	-	expression tag	UNP P0DTC2
J	1279	GLY	-	expression tag	UNP P0DTC2
J	1280	SER	-	expression tag	UNP P0DTC2
J	1281	HIS	-	expression tag	UNP P0DTC2
J	1282	HIS	-	expression tag	UNP P0DTC2
J	1283	HIS	-	expression tag	UNP P0DTC2
J	1284	HIS	-	expression tag	UNP P0DTC2
J	1285	HIS	-	expression tag	UNP P0DTC2
J	1286	HIS	-	expression tag	UNP P0DTC2
J	1287	HIS	-	expression tag	UNP P0DTC2
J	1288	HIS	-	expression tag	UNP P0DTC2
K	67	VAL	ALA	variant	UNP P0DTC2
K	?	-	HIS	deletion	UNP P0DTC2
K	?	-	VAL	deletion	UNP P0DTC2
K	95	ILE	THR	variant	UNP P0DTC2
K	145	ASP	GLY	variant	UNP P0DTC2
K	?	-	VAL	deletion	UNP P0DTC2
K	?	-	TYR	deletion	UNP P0DTC2
K	?	-	TYR	deletion	UNP P0DTC2
K	?	-	ASN	deletion	UNP P0DTC2
K	209	ILE	LEU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	212	GLU	-	insertion	UNP P0DTC2
K	213	PRO	-	insertion	UNP P0DTC2
K	214	GLU	-	insertion	UNP P0DTC2
K	339	ASP	GLY	variant	UNP P0DTC2
K	371	LEU	SER	variant	UNP P0DTC2
K	373	PRO	SER	variant	UNP P0DTC2
K	375	PHE	SER	variant	UNP P0DTC2
K	417	ASN	LYS	variant	UNP P0DTC2
K	440	LYS	ASN	variant	UNP P0DTC2
K	446	SER	GLY	variant	UNP P0DTC2
K	477	ASN	SER	variant	UNP P0DTC2
K	478	LYS	THR	variant	UNP P0DTC2
K	484	ALA	GLU	variant	UNP P0DTC2
K	493	ARG	GLN	variant	UNP P0DTC2
K	496	SER	GLY	variant	UNP P0DTC2
K	498	ARG	GLN	variant	UNP P0DTC2
K	501	TYR	ASN	variant	UNP P0DTC2
K	505	HIS	TYR	variant	UNP P0DTC2
K	547	LYS	THR	variant	UNP P0DTC2
K	614	GLY	ASP	variant	UNP P0DTC2
K	655	TYR	HIS	variant	UNP P0DTC2
K	679	LYS	ASN	variant	UNP P0DTC2
K	681	HIS	PRO	variant	UNP P0DTC2
K	682	GLY	ARG	engineered mutation	UNP P0DTC2
K	683	SER	ARG	engineered mutation	UNP P0DTC2
K	685	SER	ARG	engineered mutation	UNP P0DTC2
K	764	LYS	ASN	variant	UNP P0DTC2
K	796	TYR	ASP	variant	UNP P0DTC2
K	817	PRO	PHE	variant	UNP P0DTC2
K	856	LYS	ASN	variant	UNP P0DTC2
K	892	PRO	ALA	engineered mutation	UNP P0DTC2
K	899	PRO	ALA	engineered mutation	UNP P0DTC2
K	942	PRO	ALA	engineered mutation	UNP P0DTC2
K	954	HIS	GLN	variant	UNP P0DTC2
K	969	LYS	ASN	variant	UNP P0DTC2
K	981	PHE	LEU	variant	UNP P0DTC2
K	986	PRO	LYS	engineered mutation	UNP P0DTC2
K	987	PRO	VAL	engineered mutation	UNP P0DTC2
K	1209	GLY	-	expression tag	UNP P0DTC2
K	1210	SER	-	expression tag	UNP P0DTC2
K	1211	GLY	-	expression tag	UNP P0DTC2
K	1212	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1213	ILE	-	expression tag	UNP P0DTC2
K	1214	PRO	-	expression tag	UNP P0DTC2
K	1215	GLU	-	expression tag	UNP P0DTC2
K	1216	ALA	-	expression tag	UNP P0DTC2
K	1217	PRO	-	expression tag	UNP P0DTC2
K	1218	ARG	-	expression tag	UNP P0DTC2
K	1219	ASP	-	expression tag	UNP P0DTC2
K	1220	GLY	-	expression tag	UNP P0DTC2
K	1221	GLN	-	expression tag	UNP P0DTC2
K	1222	ALA	-	expression tag	UNP P0DTC2
K	1223	TYR	-	expression tag	UNP P0DTC2
K	1224	VAL	-	expression tag	UNP P0DTC2
K	1225	ARG	-	expression tag	UNP P0DTC2
K	1226	LYS	-	expression tag	UNP P0DTC2
K	1227	ASP	-	expression tag	UNP P0DTC2
K	1228	GLY	-	expression tag	UNP P0DTC2
K	1229	GLU	-	expression tag	UNP P0DTC2
K	1230	TRP	-	expression tag	UNP P0DTC2
K	1231	VAL	-	expression tag	UNP P0DTC2
K	1232	PHE	-	expression tag	UNP P0DTC2
K	1233	LEU	-	expression tag	UNP P0DTC2
K	1234	SER	-	expression tag	UNP P0DTC2
K	1235	THR	-	expression tag	UNP P0DTC2
K	1236	PHE	-	expression tag	UNP P0DTC2
K	1237	LEU	-	expression tag	UNP P0DTC2
K	1238	SER	-	expression tag	UNP P0DTC2
K	1239	GLY	-	expression tag	UNP P0DTC2
K	1240	LEU	-	expression tag	UNP P0DTC2
K	1241	GLU	-	expression tag	UNP P0DTC2
K	1242	VAL	-	expression tag	UNP P0DTC2
K	1243	LEU	-	expression tag	UNP P0DTC2
K	1244	PHE	-	expression tag	UNP P0DTC2
K	1245	GLN	-	expression tag	UNP P0DTC2
K	1246	GLY	-	expression tag	UNP P0DTC2
K	1247	PRO	-	expression tag	UNP P0DTC2
K	1248	GLY	-	expression tag	UNP P0DTC2
K	1249	GLY	-	expression tag	UNP P0DTC2
K	1250	TRP	-	expression tag	UNP P0DTC2
K	1251	SER	-	expression tag	UNP P0DTC2
K	1252	HIS	-	expression tag	UNP P0DTC2
K	1253	PRO	-	expression tag	UNP P0DTC2
K	1254	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1255	PHE	-	expression tag	UNP P0DTC2
K	1256	GLU	-	expression tag	UNP P0DTC2
K	1257	LYS	-	expression tag	UNP P0DTC2
K	1258	GLY	-	expression tag	UNP P0DTC2
K	1259	GLY	-	expression tag	UNP P0DTC2
K	1260	GLY	-	expression tag	UNP P0DTC2
K	1261	SER	-	expression tag	UNP P0DTC2
K	1262	GLY	-	expression tag	UNP P0DTC2
K	1263	GLY	-	expression tag	UNP P0DTC2
K	1264	GLY	-	expression tag	UNP P0DTC2
K	1265	SER	-	expression tag	UNP P0DTC2
K	1266	GLY	-	expression tag	UNP P0DTC2
K	1267	GLY	-	expression tag	UNP P0DTC2
K	1268	SER	-	expression tag	UNP P0DTC2
K	1269	ALA	-	expression tag	UNP P0DTC2
K	1270	TRP	-	expression tag	UNP P0DTC2
K	1271	SER	-	expression tag	UNP P0DTC2
K	1272	HIS	-	expression tag	UNP P0DTC2
K	1273	PRO	-	expression tag	UNP P0DTC2
K	1274	GLN	-	expression tag	UNP P0DTC2
K	1275	PHE	-	expression tag	UNP P0DTC2
K	1276	GLU	-	expression tag	UNP P0DTC2
K	1277	LYS	-	expression tag	UNP P0DTC2
K	1278	GLY	-	expression tag	UNP P0DTC2
K	1279	GLY	-	expression tag	UNP P0DTC2
K	1280	SER	-	expression tag	UNP P0DTC2
K	1281	HIS	-	expression tag	UNP P0DTC2
K	1282	HIS	-	expression tag	UNP P0DTC2
K	1283	HIS	-	expression tag	UNP P0DTC2
K	1284	HIS	-	expression tag	UNP P0DTC2
K	1285	HIS	-	expression tag	UNP P0DTC2
K	1286	HIS	-	expression tag	UNP P0DTC2
K	1287	HIS	-	expression tag	UNP P0DTC2
K	1288	HIS	-	expression tag	UNP P0DTC2
L	67	VAL	ALA	variant	UNP P0DTC2
L	?	-	HIS	deletion	UNP P0DTC2
L	?	-	VAL	deletion	UNP P0DTC2
L	95	ILE	THR	variant	UNP P0DTC2
L	145	ASP	GLY	variant	UNP P0DTC2
L	?	-	VAL	deletion	UNP P0DTC2
L	?	-	TYR	deletion	UNP P0DTC2
L	?	-	TYR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	ASN	deletion	UNP P0DTC2
L	209	ILE	LEU	variant	UNP P0DTC2
L	212	GLU	-	insertion	UNP P0DTC2
L	213	PRO	-	insertion	UNP P0DTC2
L	214	GLU	-	insertion	UNP P0DTC2
L	339	ASP	GLY	variant	UNP P0DTC2
L	371	LEU	SER	variant	UNP P0DTC2
L	373	PRO	SER	variant	UNP P0DTC2
L	375	PHE	SER	variant	UNP P0DTC2
L	417	ASN	LYS	variant	UNP P0DTC2
L	440	LYS	ASN	variant	UNP P0DTC2
L	446	SER	GLY	variant	UNP P0DTC2
L	477	ASN	SER	variant	UNP P0DTC2
L	478	LYS	THR	variant	UNP P0DTC2
L	484	ALA	GLU	variant	UNP P0DTC2
L	493	ARG	GLN	variant	UNP P0DTC2
L	496	SER	GLY	variant	UNP P0DTC2
L	498	ARG	GLN	variant	UNP P0DTC2
L	501	TYR	ASN	variant	UNP P0DTC2
L	505	HIS	TYR	variant	UNP P0DTC2
L	547	LYS	THR	variant	UNP P0DTC2
L	614	GLY	ASP	variant	UNP P0DTC2
L	655	TYR	HIS	variant	UNP P0DTC2
L	679	LYS	ASN	variant	UNP P0DTC2
L	681	HIS	PRO	variant	UNP P0DTC2
L	682	GLY	ARG	engineered mutation	UNP P0DTC2
L	683	SER	ARG	engineered mutation	UNP P0DTC2
L	685	SER	ARG	engineered mutation	UNP P0DTC2
L	764	LYS	ASN	variant	UNP P0DTC2
L	796	TYR	ASP	variant	UNP P0DTC2
L	817	PRO	PHE	variant	UNP P0DTC2
L	856	LYS	ASN	variant	UNP P0DTC2
L	892	PRO	ALA	engineered mutation	UNP P0DTC2
L	899	PRO	ALA	engineered mutation	UNP P0DTC2
L	942	PRO	ALA	engineered mutation	UNP P0DTC2
L	954	HIS	GLN	variant	UNP P0DTC2
L	969	LYS	ASN	variant	UNP P0DTC2
L	981	PHE	LEU	variant	UNP P0DTC2
L	986	PRO	LYS	engineered mutation	UNP P0DTC2
L	987	PRO	VAL	engineered mutation	UNP P0DTC2
L	1209	GLY	-	expression tag	UNP P0DTC2
L	1210	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	1211	GLY	-	expression tag	UNP P0DTC2
L	1212	TYR	-	expression tag	UNP P0DTC2
L	1213	ILE	-	expression tag	UNP P0DTC2
L	1214	PRO	-	expression tag	UNP P0DTC2
L	1215	GLU	-	expression tag	UNP P0DTC2
L	1216	ALA	-	expression tag	UNP P0DTC2
L	1217	PRO	-	expression tag	UNP P0DTC2
L	1218	ARG	-	expression tag	UNP P0DTC2
L	1219	ASP	-	expression tag	UNP P0DTC2
L	1220	GLY	-	expression tag	UNP P0DTC2
L	1221	GLN	-	expression tag	UNP P0DTC2
L	1222	ALA	-	expression tag	UNP P0DTC2
L	1223	TYR	-	expression tag	UNP P0DTC2
L	1224	VAL	-	expression tag	UNP P0DTC2
L	1225	ARG	-	expression tag	UNP P0DTC2
L	1226	LYS	-	expression tag	UNP P0DTC2
L	1227	ASP	-	expression tag	UNP P0DTC2
L	1228	GLY	-	expression tag	UNP P0DTC2
L	1229	GLU	-	expression tag	UNP P0DTC2
L	1230	TRP	-	expression tag	UNP P0DTC2
L	1231	VAL	-	expression tag	UNP P0DTC2
L	1232	PHE	-	expression tag	UNP P0DTC2
L	1233	LEU	-	expression tag	UNP P0DTC2
L	1234	SER	-	expression tag	UNP P0DTC2
L	1235	THR	-	expression tag	UNP P0DTC2
L	1236	PHE	-	expression tag	UNP P0DTC2
L	1237	LEU	-	expression tag	UNP P0DTC2
L	1238	SER	-	expression tag	UNP P0DTC2
L	1239	GLY	-	expression tag	UNP P0DTC2
L	1240	LEU	-	expression tag	UNP P0DTC2
L	1241	GLU	-	expression tag	UNP P0DTC2
L	1242	VAL	-	expression tag	UNP P0DTC2
L	1243	LEU	-	expression tag	UNP P0DTC2
L	1244	PHE	-	expression tag	UNP P0DTC2
L	1245	GLN	-	expression tag	UNP P0DTC2
L	1246	GLY	-	expression tag	UNP P0DTC2
L	1247	PRO	-	expression tag	UNP P0DTC2
L	1248	GLY	-	expression tag	UNP P0DTC2
L	1249	GLY	-	expression tag	UNP P0DTC2
L	1250	TRP	-	expression tag	UNP P0DTC2
L	1251	SER	-	expression tag	UNP P0DTC2
L	1252	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	1253	PRO	-	expression tag	UNP P0DTC2
L	1254	GLN	-	expression tag	UNP P0DTC2
L	1255	PHE	-	expression tag	UNP P0DTC2
L	1256	GLU	-	expression tag	UNP P0DTC2
L	1257	LYS	-	expression tag	UNP P0DTC2
L	1258	GLY	-	expression tag	UNP P0DTC2
L	1259	GLY	-	expression tag	UNP P0DTC2
L	1260	GLY	-	expression tag	UNP P0DTC2
L	1261	SER	-	expression tag	UNP P0DTC2
L	1262	GLY	-	expression tag	UNP P0DTC2
L	1263	GLY	-	expression tag	UNP P0DTC2
L	1264	GLY	-	expression tag	UNP P0DTC2
L	1265	SER	-	expression tag	UNP P0DTC2
L	1266	GLY	-	expression tag	UNP P0DTC2
L	1267	GLY	-	expression tag	UNP P0DTC2
L	1268	SER	-	expression tag	UNP P0DTC2
L	1269	ALA	-	expression tag	UNP P0DTC2
L	1270	TRP	-	expression tag	UNP P0DTC2
L	1271	SER	-	expression tag	UNP P0DTC2
L	1272	HIS	-	expression tag	UNP P0DTC2
L	1273	PRO	-	expression tag	UNP P0DTC2
L	1274	GLN	-	expression tag	UNP P0DTC2
L	1275	PHE	-	expression tag	UNP P0DTC2
L	1276	GLU	-	expression tag	UNP P0DTC2
L	1277	LYS	-	expression tag	UNP P0DTC2
L	1278	GLY	-	expression tag	UNP P0DTC2
L	1279	GLY	-	expression tag	UNP P0DTC2
L	1280	SER	-	expression tag	UNP P0DTC2
L	1281	HIS	-	expression tag	UNP P0DTC2
L	1282	HIS	-	expression tag	UNP P0DTC2
L	1283	HIS	-	expression tag	UNP P0DTC2
L	1284	HIS	-	expression tag	UNP P0DTC2
L	1285	HIS	-	expression tag	UNP P0DTC2
L	1286	HIS	-	expression tag	UNP P0DTC2
L	1287	HIS	-	expression tag	UNP P0DTC2
L	1288	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called 16L9 Fv.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	236	1754	1092	292	362	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	236	1754	1092	292	362	8	0	0
2	H	236	1754	1092	292	362	8	0	0
2	M	236	1754	1092	292	362	8	0	0
2	O	236	1754	1092	292	362	8	0	0
2	Q	236	1754	1092	292	362	8	0	0

- Molecule 3 is a protein called GW01 Fv.

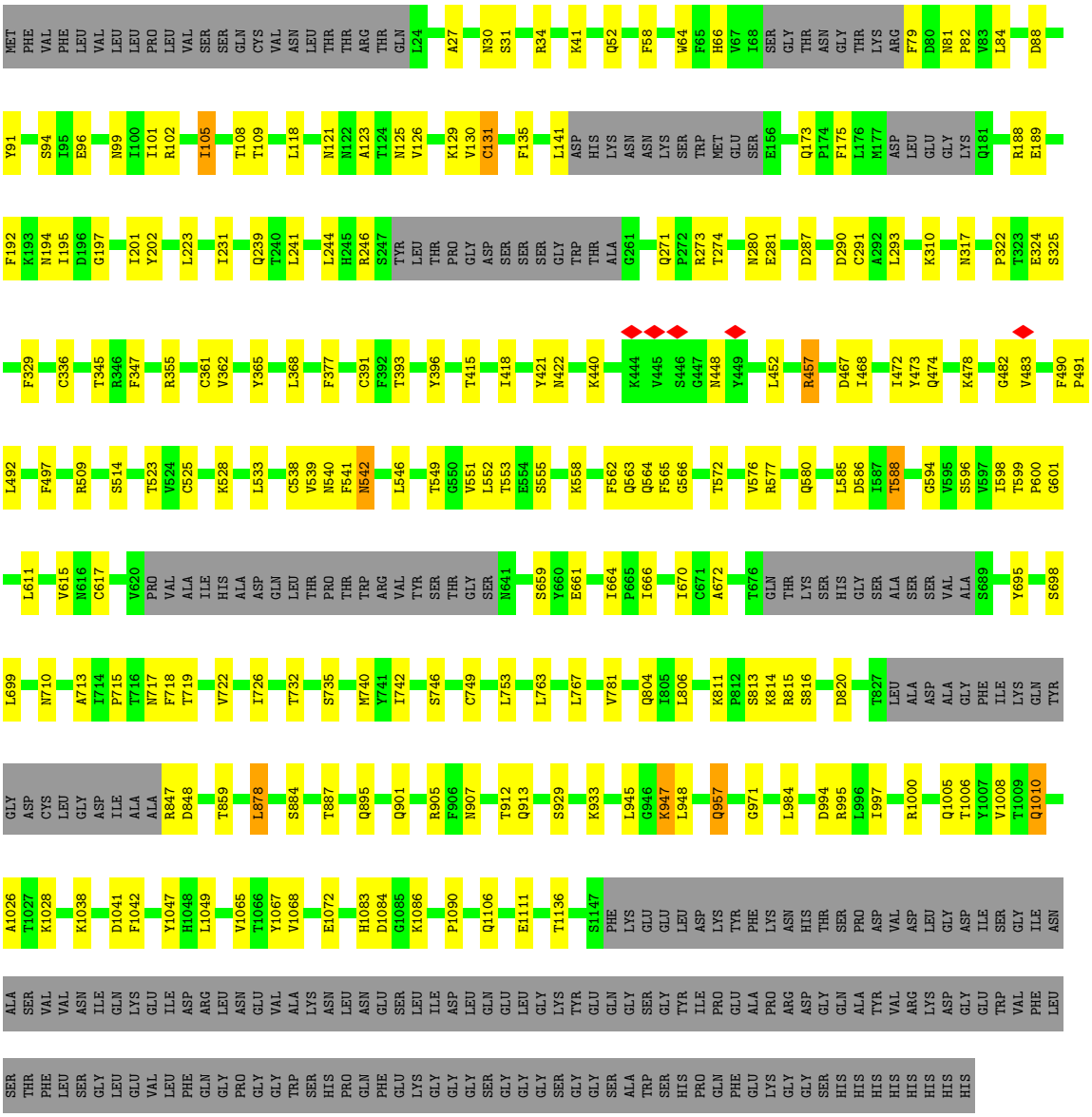
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	235	1765	1096	302	360	7	0	0
3	G	235	1765	1096	302	360	7	0	0
3	I	235	1765	1096	302	360	7	0	0
3	N	235	1765	1096	302	360	7	0	0
3	P	235	1765	1096	302	360	7	0	0
3	R	235	1765	1096	302	360	7	0	0

3 Residue-property plots (i)

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

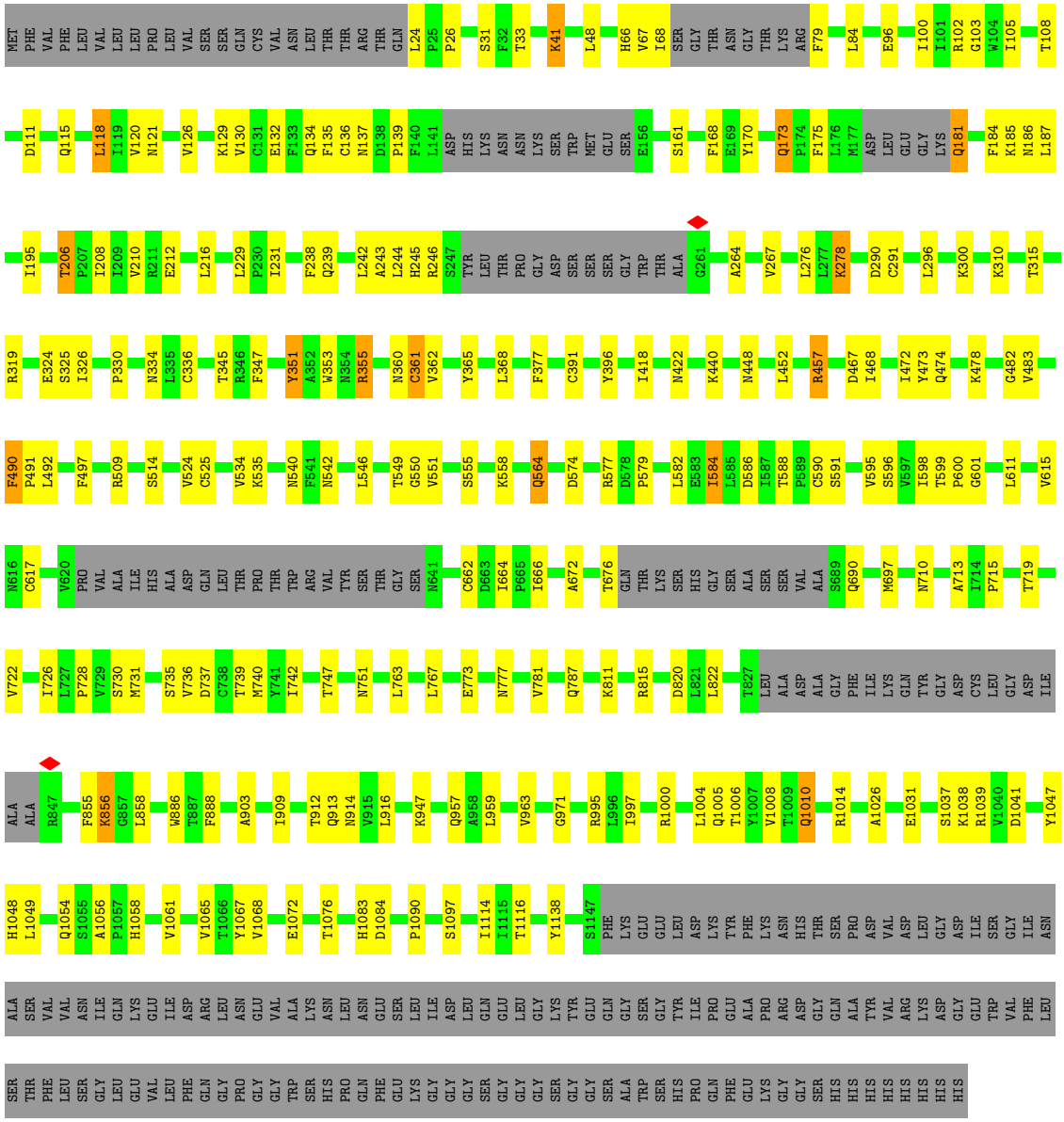
- Molecule 1: Spike glycoprotein

Chain A:



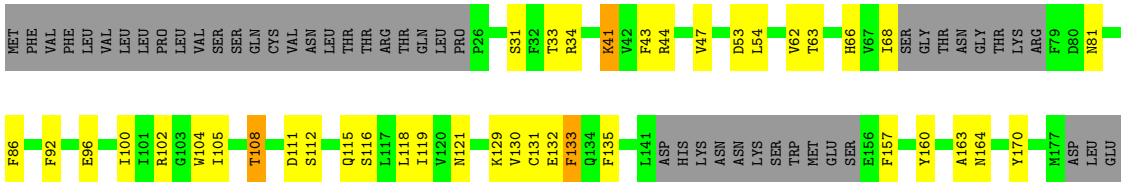
• Molecule 1: Spike glycoprotein

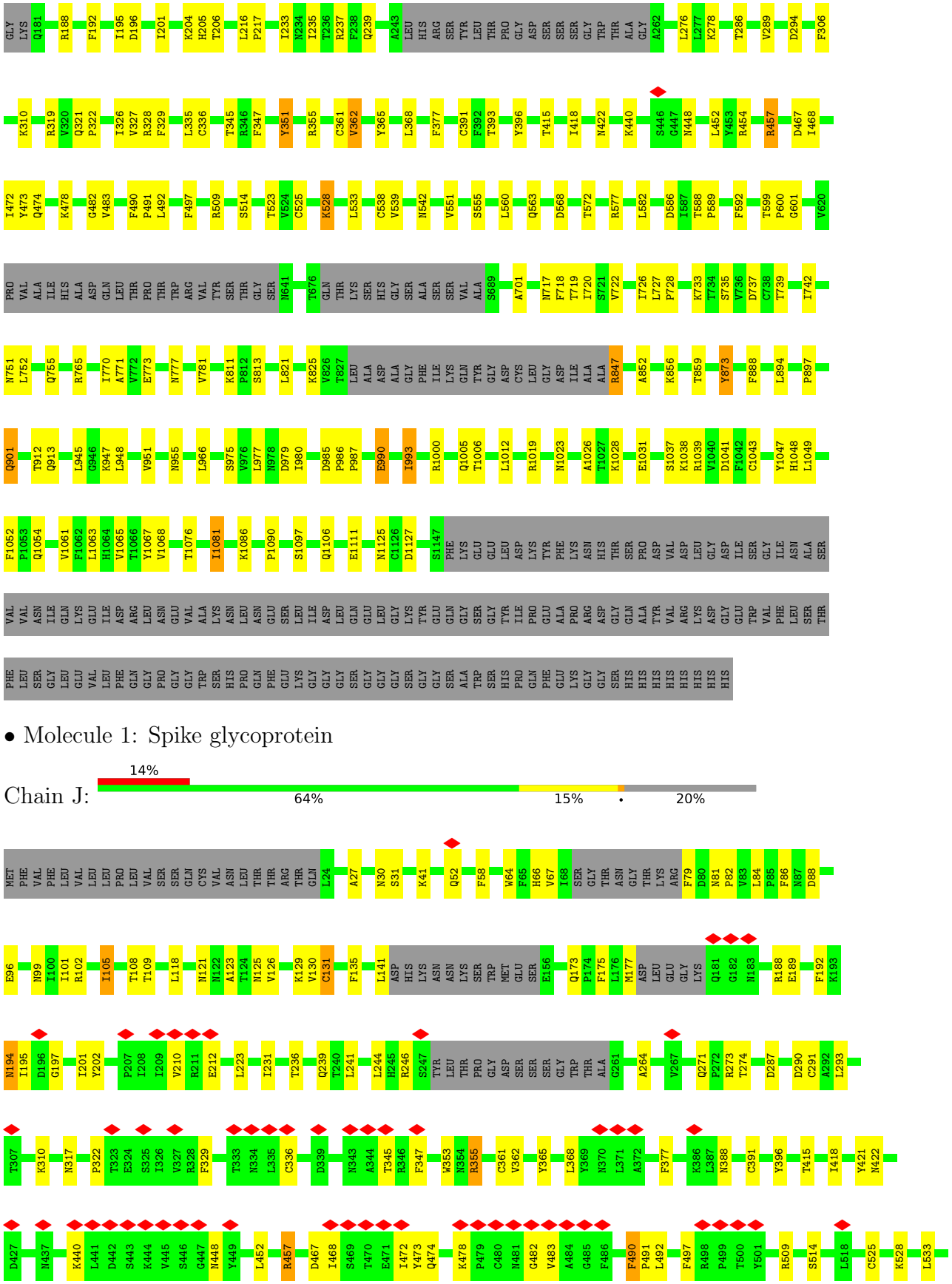
Chain B: 63% 16% • 20%



• Molecule 1: Spike glycoprotein

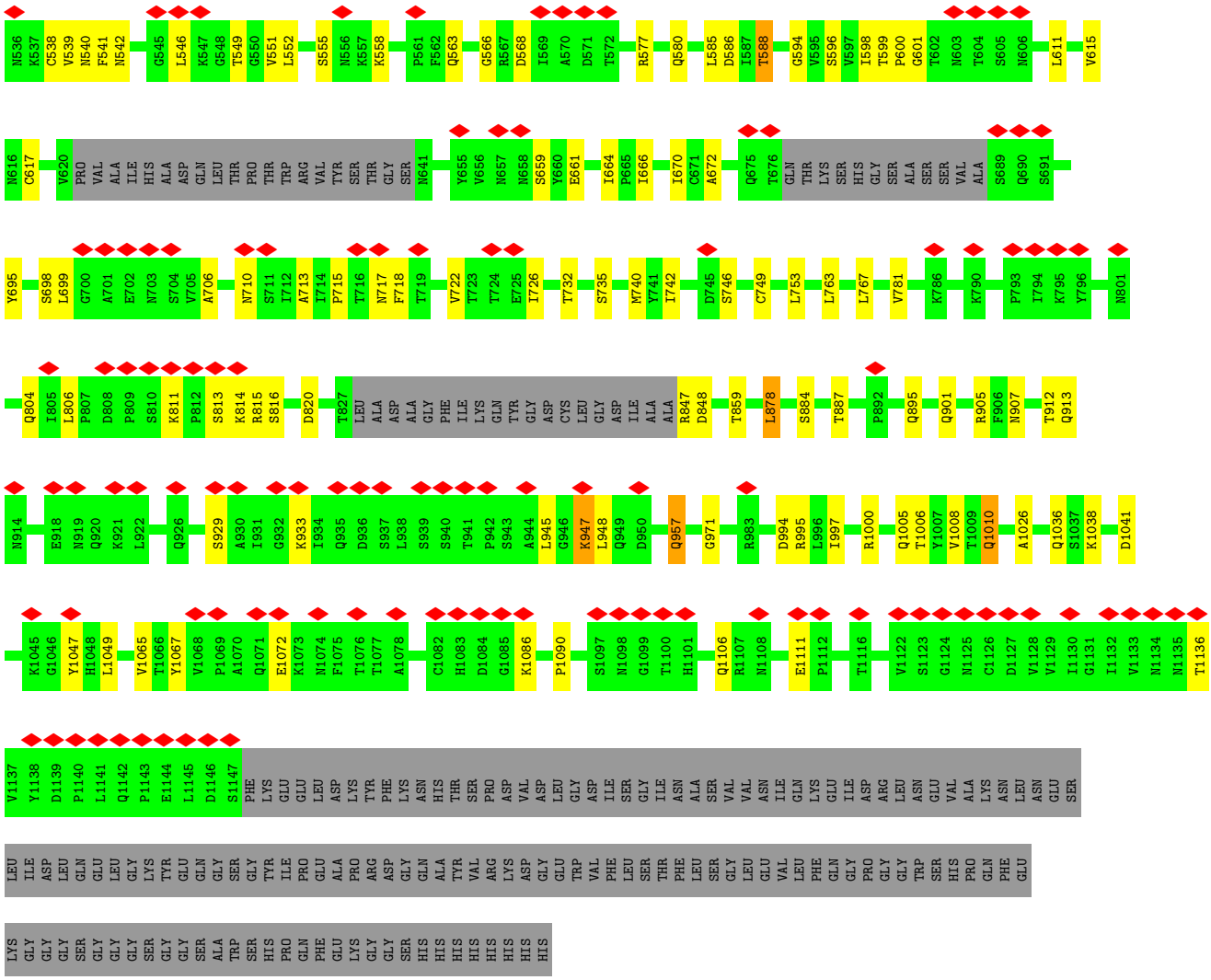
Chain C: 63% 15% • 20%





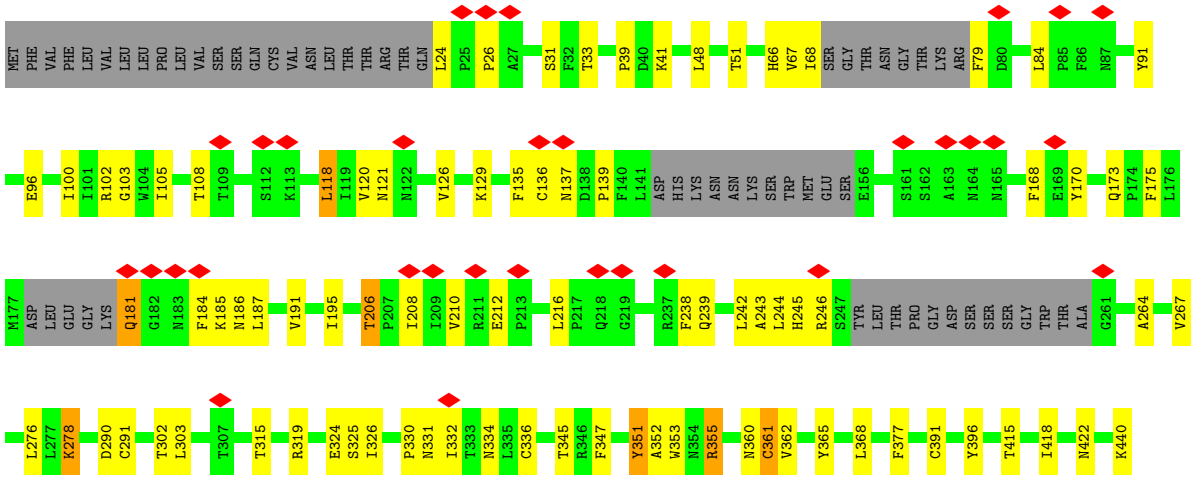
• Molecule 1: Spike glycoprotein

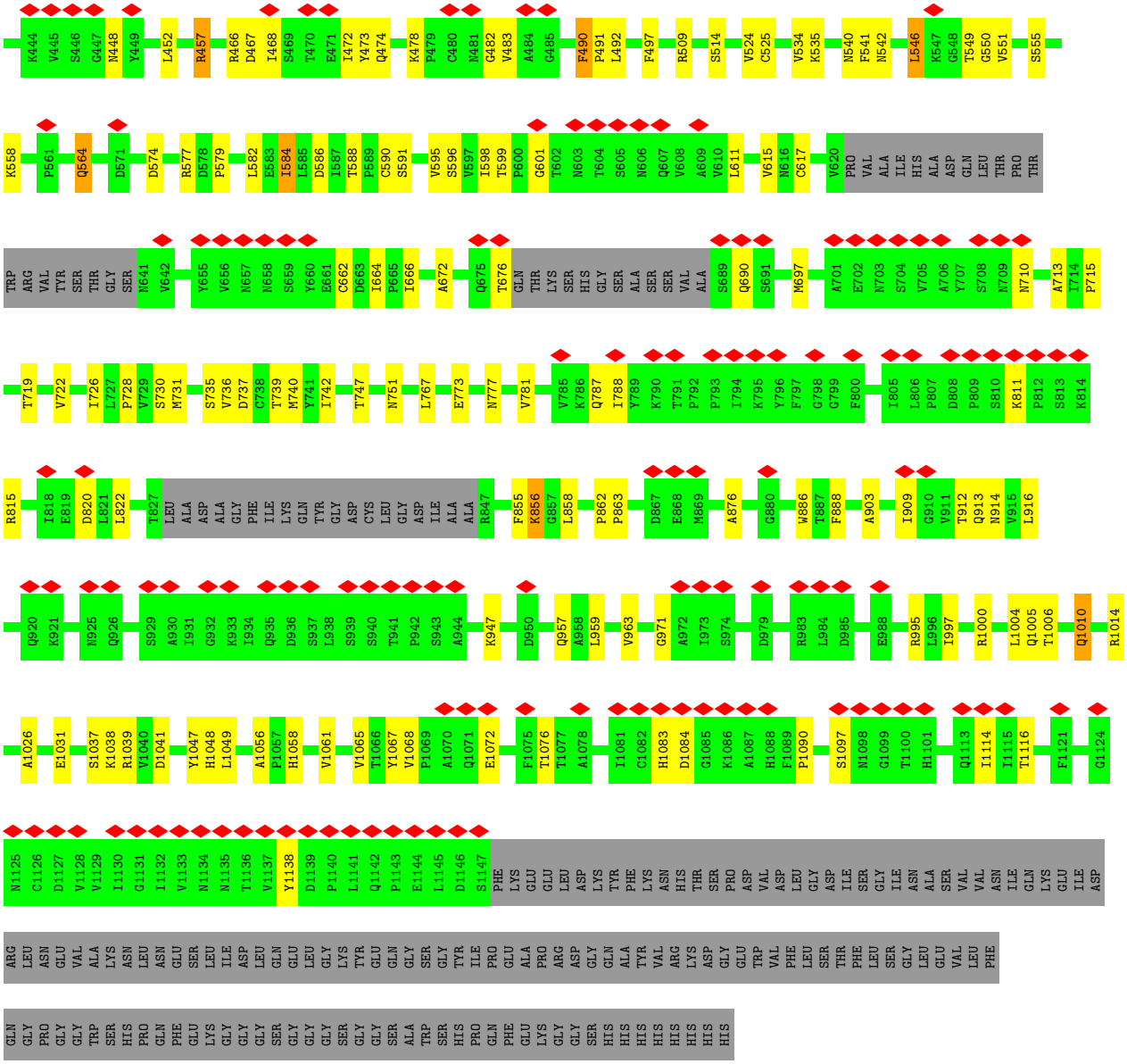
Chain J: 14% 64% 15% 20%



- Molecule 1: Spike glycoprotein

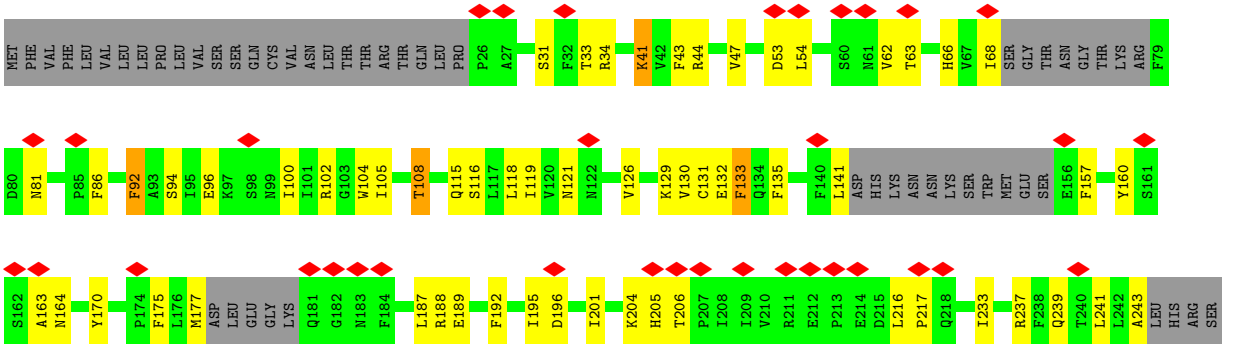
Chain K:

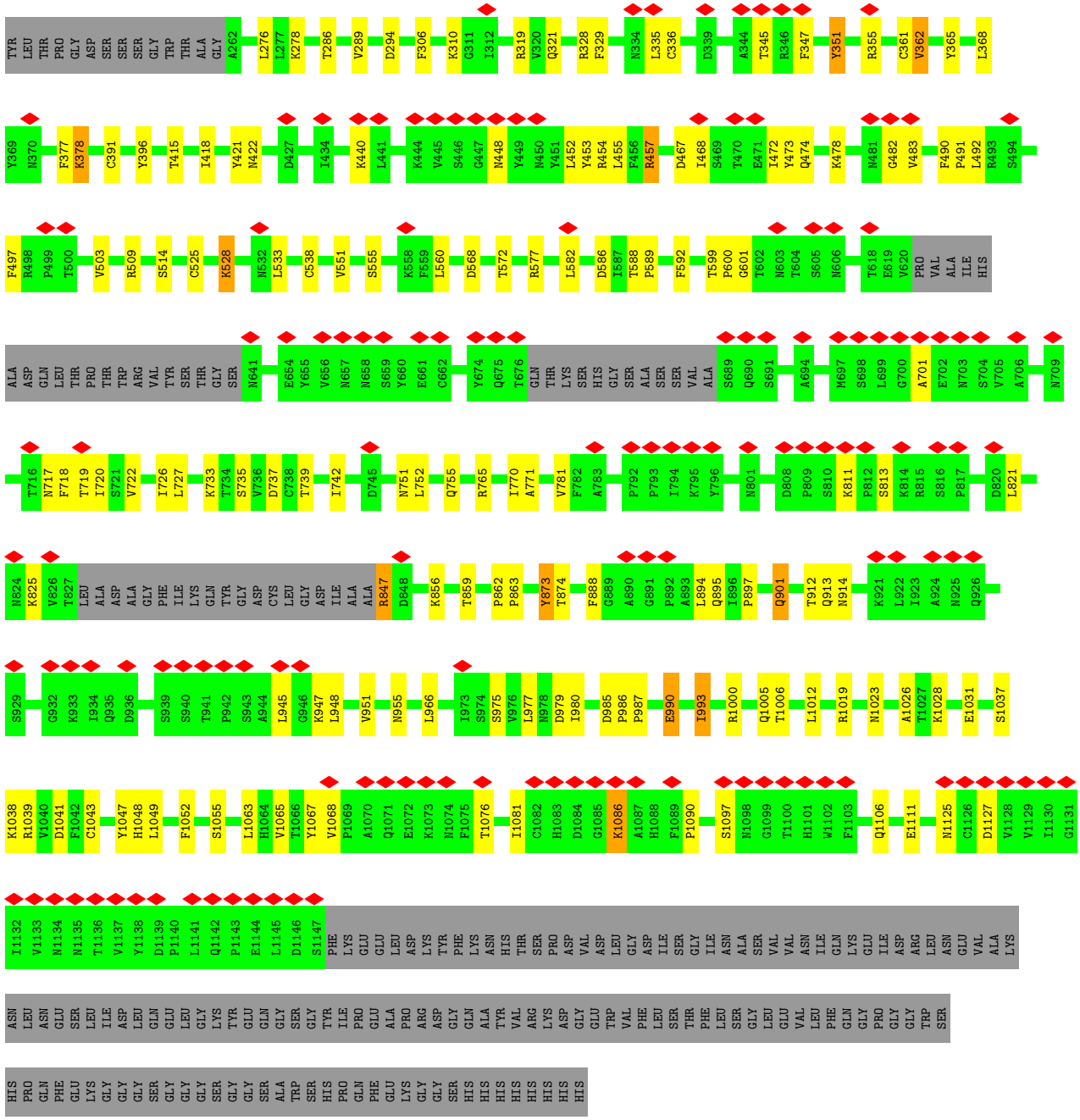




- Molecule 1: Spike glycoprotein

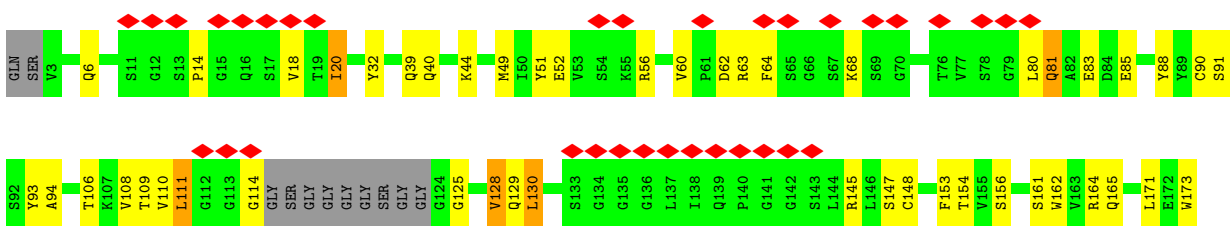
Chain L:

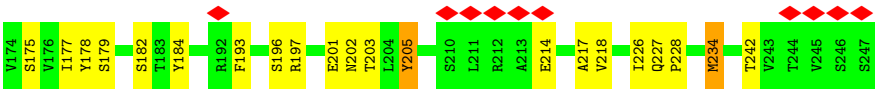




- Molecule 2: 16L9 Fv

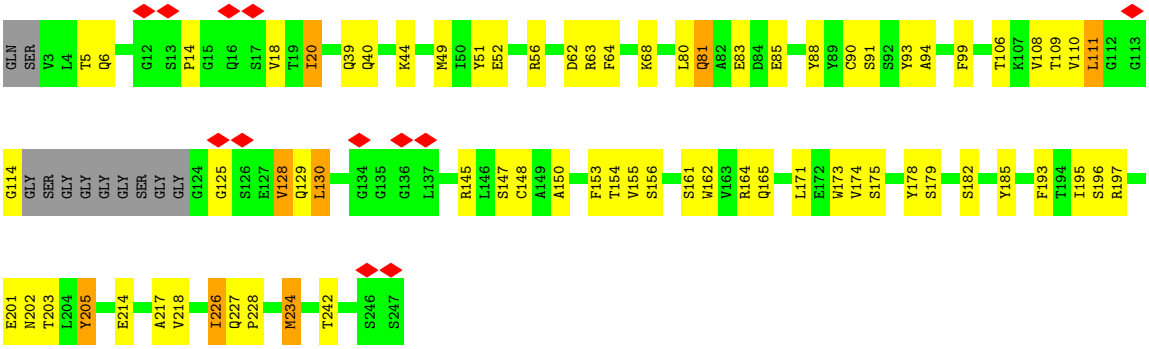
Chain D:





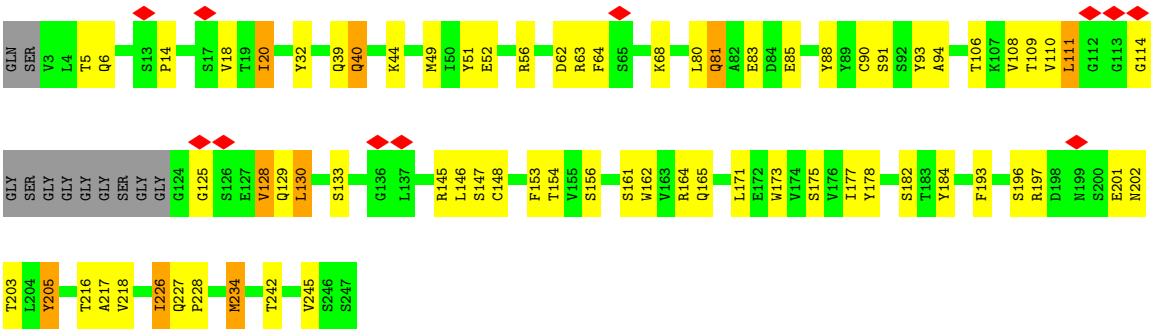
• Molecule 2: 16L9 Fv

Chain F:



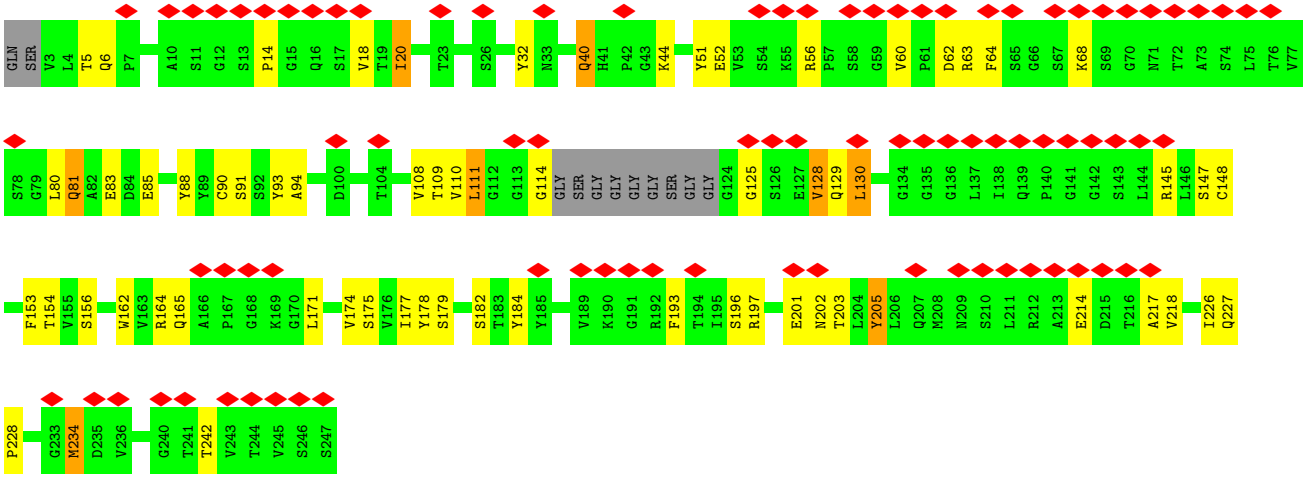
• Molecule 2: 16L9 Fv

Chain H:



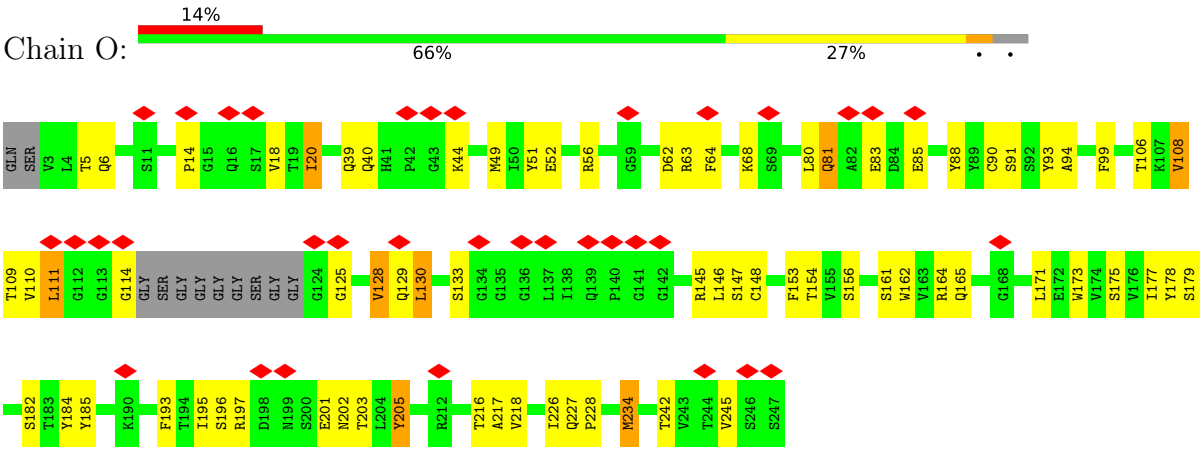
• Molecule 2: 16L9 Fv

Chain M:



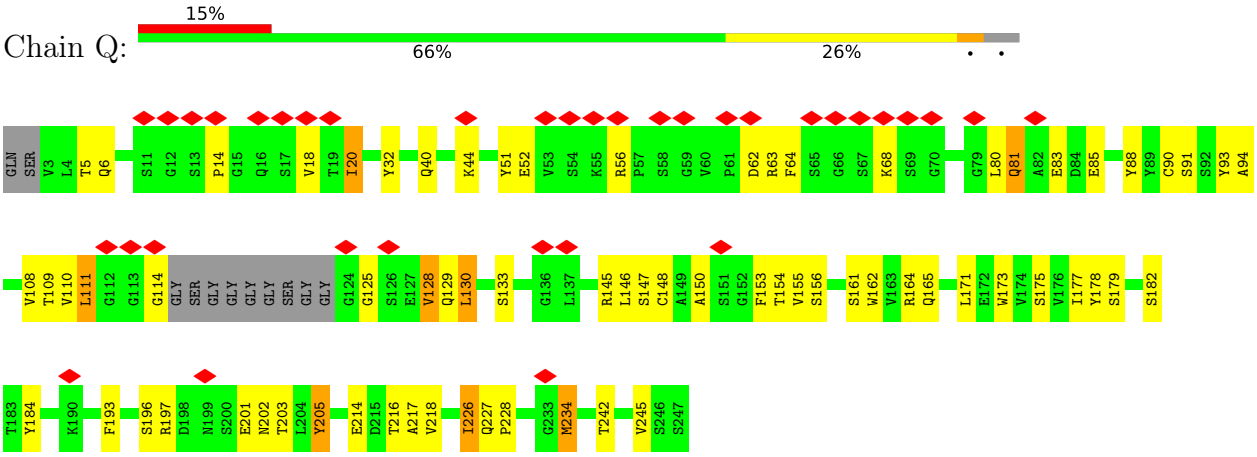
- Molecule 2: 16L9 Fv

Chain O:



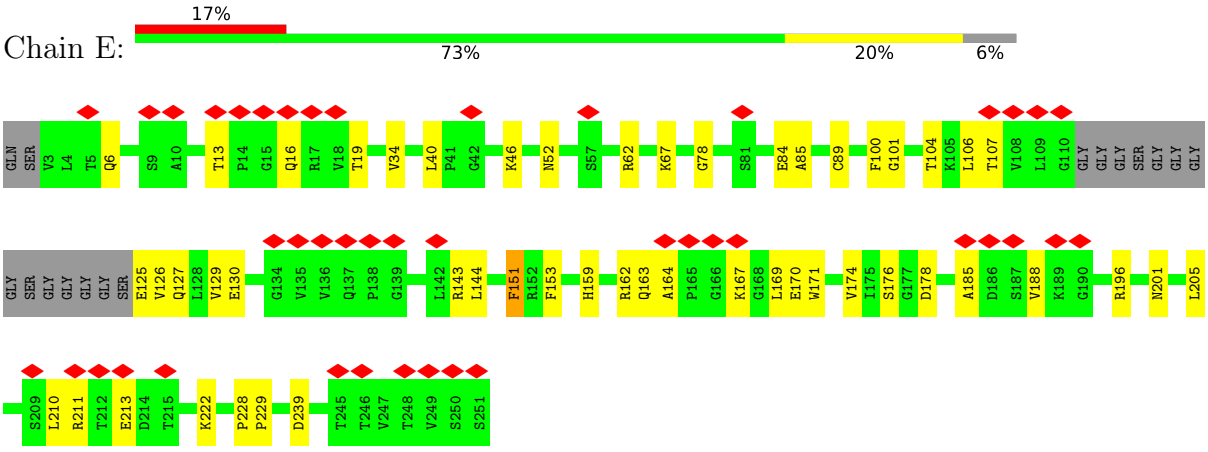
- Molecule 2: 16L9 Fv

Chain Q:



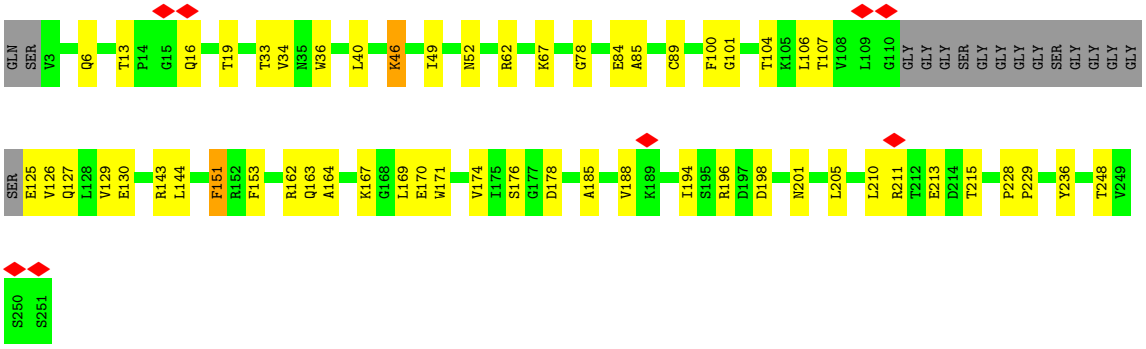
- Molecule 3: GW01 Fv

Chain E:



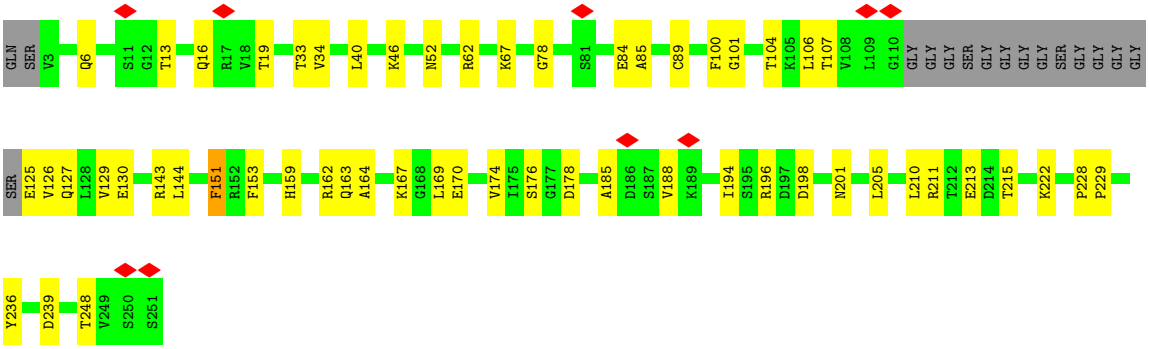
- Molecule 3: GW01 Fv

Chain G:



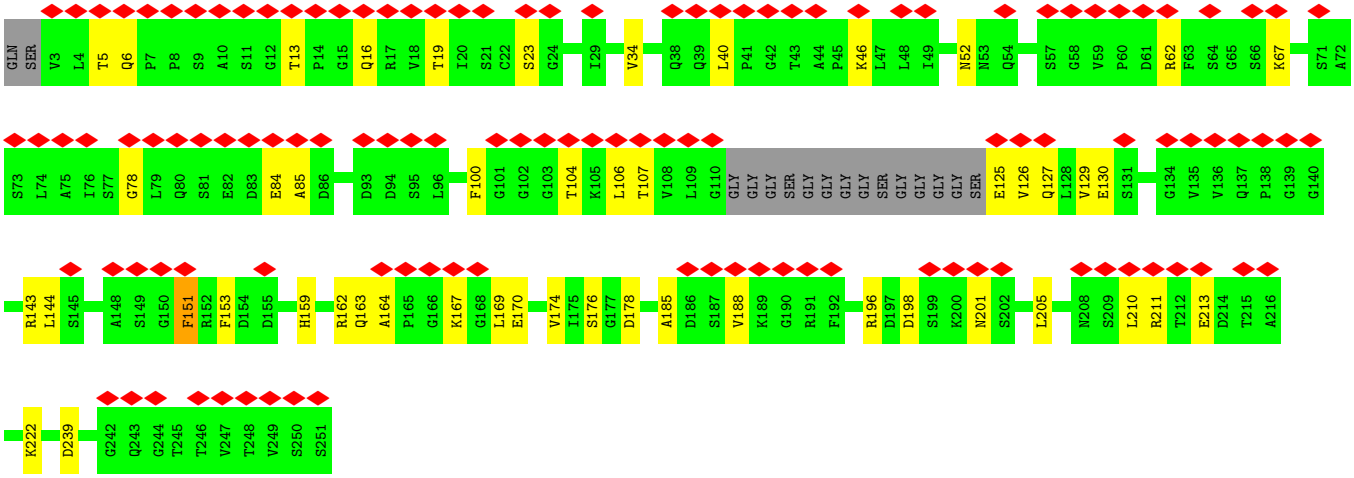
- Molecule 3: GW01 Fv

Chain I:



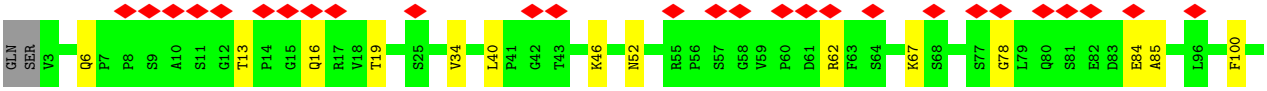
- Molecule 3: GW01 Fv

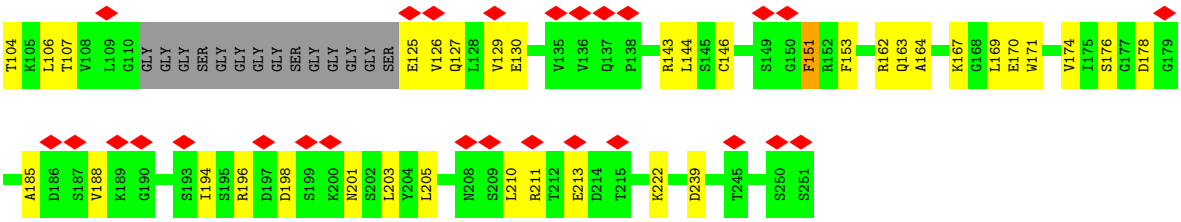
Chain N:



- Molecule 3: GW01 Fv

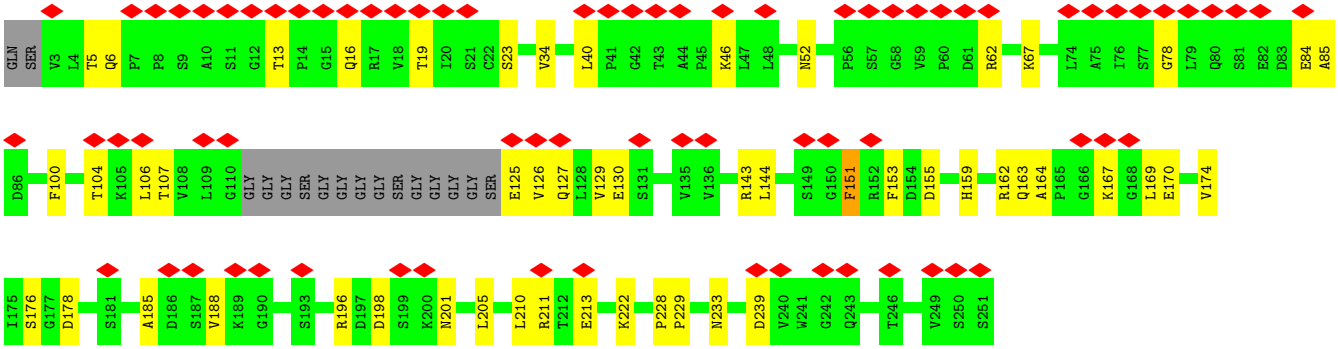
Chain P:





- Molecule 3: GW01 Fv

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71568	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 ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	574.56, 574.56, 574.56	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.24	0/8235	0.42	0/11214
1	B	0.24	0/8235	0.42	0/11214
1	C	0.25	0/8179	0.42	0/11137
1	J	0.24	0/8235	0.42	0/11214
1	K	0.24	0/8235	0.42	0/11214
1	L	0.24	0/8179	0.42	0/11137
2	D	0.24	0/1794	0.45	0/2434
2	F	0.24	0/1794	0.45	0/2434
2	H	0.24	0/1794	0.45	0/2434
2	M	0.24	0/1794	0.45	0/2434
2	O	0.24	0/1794	0.45	0/2434
2	Q	0.24	0/1794	0.45	0/2434
3	E	0.24	0/1806	0.44	0/2453
3	G	0.24	0/1806	0.44	0/2453
3	I	0.24	0/1806	0.43	0/2453
3	N	0.24	0/1806	0.44	0/2453
3	P	0.24	0/1806	0.43	0/2453
3	R	0.24	0/1806	0.43	0/2453
All	All	0.24	0/70898	0.42	0/96452

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	8043	0	7834	120	0
1	B	8043	0	7834	123	0
1	C	7989	0	7778	117	0
1	J	8043	0	7834	118	0
1	K	8043	0	7834	121	0
1	L	7989	0	7778	120	0
2	D	1754	0	1647	38	0
2	F	1754	0	1647	40	0
2	H	1754	0	1647	40	0
2	M	1754	0	1647	37	0
2	O	1754	0	1647	41	0
2	Q	1754	0	1647	41	0
3	E	1765	0	1659	24	0
3	G	1765	0	1659	28	0
3	I	1765	0	1659	27	0
3	N	1765	0	1659	23	0
3	P	1765	0	1659	24	0
3	R	1765	0	1659	26	0
All	All	69264	0	66728	1037	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 8.

All (1037) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HB2	1:B:238:PHE:HB3	1.72	0.72
1:K:84:LEU:HB2	1:K:238:PHE:HB3	1.72	0.70
1:B:96:GLU:HB2	1:B:100:ILE:HB	1.74	0.70
1:K:96:GLU:HB2	1:K:100:ILE:HB	1.74	0.69
1:J:1047:TYR:HB2	1:J:1067:TYR:HB3	1.75	0.69
1:L:1047:TYR:HB2	1:L:1067:TYR:HB3	1.76	0.68
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.74	0.68
1:L:811:LYS:NZ	1:L:813:SER:OG	2.27	0.68
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.75	0.67
1:C:811:LYS:NZ	1:C:813:SER:OG	2.26	0.67
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	1.75	0.67
1:K:391:CYS:HA	1:K:525:CYS:HA	1.77	0.67
1:B:391:CYS:HA	1:B:525:CYS:HA	1.77	0.66
1:B:781:VAL:HG22	1:B:1026:ALA:HB2	1.78	0.66
1:B:730:SER:HB3	1:B:1058:HIS:HA	1.77	0.66
1:K:1047:TYR:HB2	1:K:1067:TYR:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:126:VAL:HG11	3:P:151:PHE:HB3	1.77	0.66
1:J:244:LEU:HG	1:J:246:ARG:HG2	1.78	0.66
1:K:781:VAL:HG22	1:K:1026:ALA:HB2	1.77	0.66
1:B:1006:THR:O	1:B:1010:GLN:NE2	2.29	0.65
2:F:154:THR:HG22	2:F:156:SER:H	1.61	0.65
1:J:599:THR:HG22	1:J:601:GLY:H	1.61	0.65
1:A:391:CYS:HA	1:A:525:CYS:HA	1.79	0.65
1:L:751:ASN:O	1:L:755:GLN:NE2	2.27	0.65
3:G:126:VAL:HG11	3:G:151:PHE:HB3	1.79	0.65
1:K:1006:THR:O	1:K:1010:GLN:NE2	2.30	0.65
1:A:1006:THR:O	1:A:1010:GLN:NE2	2.29	0.65
2:D:154:THR:HG22	2:D:156:SER:H	1.61	0.65
2:H:154:THR:HG22	2:H:156:SER:H	1.62	0.65
1:A:599:THR:HG22	1:A:601:GLY:H	1.61	0.65
1:C:391:CYS:HA	1:C:525:CYS:HA	1.78	0.65
1:B:577:ARG:HH21	1:B:582:LEU:HD12	1.61	0.64
1:C:105:ILE:HG12	1:C:118:LEU:HA	1.78	0.64
1:L:105:ILE:HG12	1:L:118:LEU:HA	1.80	0.64
2:O:154:THR:HG22	2:O:156:SER:H	1.61	0.64
3:I:126:VAL:HG11	3:I:151:PHE:HB3	1.80	0.64
1:K:577:ARG:HH21	1:K:582:LEU:HD12	1.63	0.64
1:L:391:CYS:HA	1:L:525:CYS:HA	1.79	0.64
1:K:730:SER:HB3	1:K:1058:HIS:HA	1.79	0.64
3:E:126:VAL:HG11	3:E:151:PHE:HB3	1.78	0.64
1:J:1006:THR:O	1:J:1010:GLN:NE2	2.31	0.64
2:O:111:LEU:HD12	2:O:114:GLY:H	1.61	0.64
1:C:1019:ARG:O	1:C:1023:ASN:ND2	2.31	0.64
1:J:391:CYS:HA	1:J:525:CYS:HA	1.80	0.64
3:R:126:VAL:HG11	3:R:151:PHE:HB3	1.78	0.64
2:M:154:THR:HG22	2:M:156:SER:H	1.61	0.64
2:Q:154:THR:HG22	2:Q:156:SER:H	1.63	0.64
1:C:452:LEU:HD13	1:C:492:LEU:HD22	1.80	0.64
1:C:751:ASN:O	1:C:755:GLN:NE2	2.27	0.64
3:G:34:VAL:H	3:G:52:ASN:HD21	1.46	0.64
1:J:123:ALA:O	1:J:125:ASN:ND2	2.31	0.63
1:K:396:TYR:HB2	1:K:514:SER:HB2	1.81	0.63
1:A:244:LEU:HG	1:A:246:ARG:HG2	1.80	0.63
1:C:1037:SER:H	1:C:1048:HIS:HD2	1.45	0.63
1:K:555:SER:HB3	1:K:586:ASP:HB2	1.79	0.63
1:A:1090:PRO:O	1:C:913:GLN:NE2	2.32	0.63
1:K:452:LEU:HD13	1:K:492:LEU:HD22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ALA:O	1:A:125:ASN:ND2	2.30	0.63
1:L:452:LEU:HD13	1:L:492:LEU:HD22	1.80	0.63
2:D:94:ALA:HB2	2:D:227:GLN:HE21	1.64	0.63
1:A:740:MET:HB2	1:B:319:ARG:HH22	1.63	0.62
1:B:452:LEU:HD13	1:B:492:LEU:HD22	1.81	0.62
1:J:452:LEU:HD13	1:J:492:LEU:HD22	1.79	0.62
1:J:1090:PRO:O	1:L:913:GLN:NE2	2.31	0.62
1:B:555:SER:HB3	1:B:586:ASP:HB2	1.81	0.62
1:J:555:SER:HB3	1:J:586:ASP:HB2	1.81	0.62
1:K:185:LYS:HB2	1:K:208:ILE:HD11	1.82	0.62
2:Q:111:LEU:HD12	2:Q:114:GLY:H	1.63	0.62
1:B:747:THR:O	1:B:751:ASN:ND2	2.33	0.62
1:J:58:PHE:HB2	1:J:293:LEU:HD11	1.80	0.62
1:J:901:GLN:HE21	1:J:905:ARG:HE	1.48	0.62
1:L:1037:SER:H	1:L:1048:HIS:HD2	1.47	0.62
1:B:596:SER:HB2	1:B:611:LEU:HB3	1.82	0.62
2:F:162:TRP:HB2	2:F:175:SER:HB2	1.82	0.62
1:A:452:LEU:HD13	1:A:492:LEU:HD22	1.80	0.61
1:C:560:LEU:O	1:C:577:ARG:NH2	2.33	0.61
2:H:94:ALA:HB2	2:H:227:GLN:HE21	1.65	0.61
1:B:396:TYR:HB2	1:B:514:SER:HB2	1.81	0.61
1:L:1019:ARG:O	1:L:1023:ASN:ND2	2.32	0.61
3:N:126:VAL:HG11	3:N:151:PHE:HB3	1.80	0.61
2:O:94:ALA:HB2	2:O:227:GLN:HE21	1.65	0.61
1:K:596:SER:HB2	1:K:611:LEU:HB3	1.82	0.61
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.49	0.61
1:B:103:GLY:HA2	1:B:120:VAL:HA	1.83	0.61
2:H:111:LEU:HD12	2:H:114:GLY:H	1.66	0.61
2:M:111:LEU:HD12	2:M:114:GLY:H	1.65	0.61
1:A:58:PHE:HB2	1:A:293:LEU:HD11	1.83	0.61
2:F:111:LEU:HD12	2:F:114:GLY:H	1.65	0.61
1:B:811:LYS:HD3	1:B:815:ARG:H	1.66	0.61
2:D:111:LEU:HD12	2:D:114:GLY:H	1.65	0.61
2:F:94:ALA:HB2	2:F:227:GLN:HE21	1.66	0.60
1:L:119:ILE:O	1:L:121:ASN:ND2	2.35	0.60
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.82	0.60
1:J:740:MET:HB2	1:K:319:ARG:HH22	1.66	0.60
1:C:951:VAL:O	1:C:955:ASN:ND2	2.32	0.60
3:P:34:VAL:H	3:P:52:ASN:HD21	1.50	0.60
2:Q:94:ALA:HB2	2:Q:227:GLN:HE21	1.66	0.60
1:K:903:ALA:HB2	1:K:916:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:555:SER:HB3	1:L:586:ASP:HB2	1.83	0.60
1:L:1038:LYS:HB2	1:L:1038:LYS:HZ2	1.67	0.60
2:M:94:ALA:HB2	2:M:227:GLN:HE21	1.66	0.60
3:N:164:ALA:HB3	3:N:167:LYS:HB2	1.84	0.60
1:B:418:ILE:HG23	1:B:422:ASN:HD22	1.67	0.59
1:C:1038:LYS:HZ2	1:C:1038:LYS:HB2	1.66	0.59
1:K:747:THR:O	1:K:751:ASN:ND2	2.33	0.59
2:F:145:ARG:NH2	2:F:196:SER:OG	2.35	0.59
1:L:418:ILE:HG23	1:L:422:ASN:HD22	1.67	0.59
2:H:145:ARG:NH2	2:H:196:SER:OG	2.35	0.59
2:O:145:ARG:NH2	2:O:196:SER:OG	2.35	0.59
1:B:185:LYS:HB2	1:B:208:ILE:HD11	1.82	0.59
1:C:119:ILE:O	1:C:121:ASN:ND2	2.36	0.59
2:H:125:GLY:HA2	2:H:130:LEU:HD21	1.85	0.59
1:K:103:GLY:HA2	1:K:120:VAL:HA	1.83	0.59
1:L:560:LEU:O	1:L:577:ARG:NH2	2.35	0.59
2:Q:145:ARG:NH2	2:Q:196:SER:OG	2.35	0.59
1:A:913:GLN:NE2	1:B:1090:PRO:O	2.35	0.59
1:C:418:ILE:HG23	1:C:422:ASN:HD22	1.67	0.59
2:M:18:VAL:HG12	2:M:20:ILE:HG23	1.85	0.59
2:O:162:TRP:HB2	2:O:175:SER:HB2	1.85	0.59
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.83	0.59
3:I:84:GLU:HG3	3:I:107:THR:HA	1.83	0.59
2:M:125:GLY:HA2	2:M:130:LEU:HD21	1.85	0.59
2:Q:178:TYR:HB2	2:Q:182:SER:HB2	1.85	0.59
1:A:189:GLU:HG2	1:A:223:LEU:HD21	1.85	0.58
1:A:912:THR:OG1	1:A:1106:GLN:NE2	2.35	0.58
2:O:125:GLY:HA2	2:O:130:LEU:HD21	1.85	0.58
3:I:164:ALA:HB3	3:I:167:LYS:HB2	1.85	0.58
1:J:847:ARG:NH1	1:K:574:ASP:OD1	2.36	0.58
2:D:18:VAL:HG12	2:D:20:ILE:HG23	1.86	0.58
2:D:145:ARG:NH2	2:D:196:SER:OG	2.36	0.58
1:A:847:ARG:NH1	1:B:574:ASP:OD1	2.36	0.58
2:Q:162:TRP:HB2	2:Q:175:SER:HB2	1.85	0.58
1:J:27:ALA:HB3	1:J:64:TRP:HB3	1.86	0.58
1:B:540:ASN:HD22	1:B:549:THR:HG22	1.69	0.58
1:B:903:ALA:HB2	1:B:916:LEU:HD22	1.85	0.58
3:G:164:ALA:HB3	3:G:167:LYS:HB2	1.86	0.58
2:M:145:ARG:NH2	2:M:196:SER:OG	2.37	0.58
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.37	0.58
2:H:18:VAL:HG12	2:H:20:ILE:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:913:GLN:NE2	1:K:1090:PRO:O	2.36	0.58
2:H:162:TRP:HB2	2:H:175:SER:HB2	1.85	0.58
1:J:141:LEU:HD21	1:J:241:LEU:HB3	1.85	0.58
1:J:912:THR:OG1	1:J:1106:GLN:NE2	2.35	0.58
1:K:811:LYS:HD3	1:K:815:ARG:H	1.68	0.58
1:B:345:THR:O	1:B:509:ARG:NH2	2.37	0.57
3:G:84:GLU:HG3	3:G:107:THR:HA	1.85	0.57
3:R:84:GLU:HG3	3:R:107:THR:HA	1.86	0.57
1:A:971:GLY:HA3	1:A:995:ARG:HE	1.69	0.57
2:F:91:SER:OG	2:F:227:GLN:OE1	2.22	0.57
2:H:85:GLU:HA	2:H:109:THR:HG22	1.86	0.57
2:H:178:TYR:HB2	2:H:182:SER:HB2	1.85	0.57
1:K:735:SER:HA	1:K:767:LEU:HD13	1.86	0.57
1:L:742:ILE:O	1:L:1000:ARG:NH1	2.37	0.57
3:P:164:ALA:HB3	3:P:167:LYS:HB2	1.86	0.57
1:L:473:TYR:HB2	1:L:491:PRO:HB3	1.86	0.57
1:B:599:THR:HG22	1:B:601:GLY:H	1.69	0.57
3:I:62:ARG:NH2	3:I:78:GLY:O	2.37	0.57
1:K:105:ILE:HB	1:K:239:GLN:HB3	1.87	0.57
1:L:599:THR:HG22	1:L:601:GLY:H	1.67	0.57
2:H:91:SER:OG	2:H:227:GLN:OE1	2.22	0.57
1:C:599:THR:HG22	1:C:601:GLY:H	1.69	0.57
2:D:178:TYR:HB2	2:D:182:SER:HB2	1.87	0.57
1:A:141:LEU:HD21	1:A:241:LEU:HB3	1.86	0.57
1:C:351:TYR:HB2	1:C:454:ARG:HH11	1.70	0.57
2:Q:18:VAL:HG12	2:Q:20:ILE:HG23	1.85	0.57
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.87	0.57
1:J:533:LEU:HD21	1:J:585:LEU:HD21	1.87	0.57
1:K:1037:SER:H	1:K:1048:HIS:HD2	1.53	0.57
3:N:84:GLU:HG3	3:N:107:THR:HA	1.87	0.57
3:E:164:ALA:HB3	3:E:167:LYS:HB2	1.85	0.57
2:F:18:VAL:HG12	2:F:20:ILE:HG23	1.87	0.57
1:J:1106:GLN:NE2	1:J:1111:GLU:OE1	2.38	0.57
1:L:951:VAL:O	1:L:955:ASN:ND2	2.33	0.57
2:O:18:VAL:HG12	2:O:20:ILE:HG23	1.86	0.57
3:G:62:ARG:NH2	3:G:78:GLY:O	2.38	0.57
1:K:811:LYS:NZ	1:K:820:ASP:OD1	2.33	0.57
1:B:105:ILE:HB	1:B:239:GLN:HB3	1.88	0.56
1:B:735:SER:HA	1:B:767:LEU:HD13	1.87	0.56
3:E:84:GLU:HG3	3:E:107:THR:HA	1.86	0.56
2:Q:91:SER:OG	2:Q:227:GLN:OE1	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1037:SER:H	1:B:1048:HIS:HD2	1.52	0.56
1:J:971:GLY:HA3	1:J:995:ARG:HE	1.70	0.56
1:K:599:THR:HG22	1:K:601:GLY:H	1.70	0.56
2:O:91:SER:OG	2:O:227:GLN:OE1	2.22	0.56
2:O:178:TYR:HB2	2:O:182:SER:HB2	1.87	0.56
1:A:1106:GLN:NE2	1:A:1111:GLU:OE1	2.39	0.56
2:F:85:GLU:HA	2:F:109:THR:HG22	1.87	0.56
2:F:178:TYR:HB2	2:F:182:SER:HB2	1.87	0.56
1:K:418:ILE:HG23	1:K:422:ASN:HD22	1.71	0.56
3:N:62:ARG:NH2	3:N:78:GLY:O	2.39	0.56
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.38	0.56
1:J:457:ARG:NH1	1:J:467:ASP:OD2	2.39	0.56
1:L:396:TYR:HB2	1:L:514:SER:HB2	1.87	0.56
1:L:457:ARG:NH1	1:L:467:ASP:OD2	2.38	0.56
2:O:85:GLU:HA	2:O:109:THR:HG22	1.87	0.56
2:D:162:TRP:HB2	2:D:175:SER:HB2	1.87	0.56
2:M:162:TRP:HB2	2:M:175:SER:HB2	1.87	0.56
3:R:62:ARG:NH2	3:R:78:GLY:O	2.38	0.56
1:A:365:TYR:HA	1:A:368:LEU:HD13	1.88	0.56
1:B:474:GLN:NE2	1:B:478:LYS:O	2.39	0.56
1:L:1076:THR:HB	1:L:1097:SER:HB3	1.87	0.56
3:P:62:ARG:NH2	3:P:78:GLY:O	2.39	0.56
1:A:551:VAL:HB	1:A:588:THR:HG23	1.87	0.56
1:K:822:LEU:HD13	1:K:1061:VAL:HG21	1.88	0.56
3:R:164:ALA:HB3	3:R:167:LYS:HB2	1.86	0.56
1:C:115:GLN:HB2	1:C:233:ILE:HD12	1.87	0.56
1:C:473:TYR:HB2	1:C:491:PRO:HB3	1.88	0.56
3:E:62:ARG:NH2	3:E:78:GLY:O	2.38	0.56
1:J:202:TYR:HB3	1:J:223:LEU:HB3	1.88	0.56
1:A:52:GLN:NE2	1:A:274:THR:OG1	2.38	0.56
2:D:85:GLU:HA	2:D:109:THR:HG22	1.89	0.56
1:J:763:LEU:HD22	1:J:1008:VAL:HG21	1.87	0.56
1:A:41:LYS:HE2	1:B:564:GLN:HE22	1.70	0.55
1:J:418:ILE:HG23	1:J:422:ASN:HD22	1.71	0.55
3:P:153:PHE:HB2	3:P:201:ASN:HD22	1.71	0.55
1:B:457:ARG:NH1	1:B:467:ASP:OD2	2.38	0.55
1:B:811:LYS:NZ	1:B:820:ASP:OD1	2.33	0.55
1:J:317:ASN:HA	1:J:594:GLY:HA2	1.88	0.55
1:L:31:SER:HA	1:L:216:LEU:HD23	1.88	0.55
2:Q:85:GLU:HA	2:Q:109:THR:HG22	1.87	0.55
1:J:189:GLU:HG2	1:J:223:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:396:TYR:HB2	1:J:514:SER:HB2	1.88	0.55
1:L:115:GLN:HB2	1:L:233:ILE:HD12	1.89	0.55
1:A:27:ALA:HB3	1:A:64:TRP:HB3	1.88	0.55
1:A:541:PHE:HB3	1:A:552:LEU:HD11	1.87	0.55
1:A:1005:GLN:NE2	1:B:1006:THR:OG1	2.39	0.55
1:C:278:LYS:NZ	1:C:286:THR:OG1	2.37	0.55
1:C:474:GLN:NE2	1:C:478:LYS:O	2.39	0.55
1:K:457:ARG:NH1	1:K:467:ASP:OD2	2.39	0.55
1:B:473:TYR:HB2	1:B:491:PRO:HB3	1.87	0.55
1:J:563:GLN:O	1:J:577:ARG:NH1	2.37	0.55
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.89	0.55
1:K:1005:GLN:NE2	1:L:1006:THR:OG1	2.40	0.55
1:C:34:ARG:HH22	1:C:206:THR:HG21	1.72	0.55
1:C:115:GLN:HG3	1:C:132:GLU:HB2	1.88	0.55
1:C:1125:ASN:ND2	1:C:1127:ASP:OD2	2.39	0.55
3:G:153:PHE:HB2	3:G:201:ASN:HD22	1.71	0.55
1:J:551:VAL:HB	1:J:588:THR:HG23	1.88	0.55
1:J:1005:GLN:NE2	1:K:1006:THR:OG1	2.39	0.55
1:A:473:TYR:HB2	1:A:491:PRO:HB3	1.87	0.55
1:B:181:GLN:HB3	1:B:184:PHE:HB2	1.89	0.55
1:J:541:PHE:HB3	1:J:552:LEU:HD11	1.89	0.55
1:J:811:LYS:NZ	1:J:820:ASP:OD1	2.40	0.55
3:N:211:ARG:NH1	3:N:213:GLU:OE1	2.40	0.55
3:G:211:ARG:NH1	3:G:213:GLU:OE1	2.40	0.55
1:K:474:GLN:NE2	1:K:478:LYS:O	2.40	0.55
1:C:396:TYR:HB2	1:C:514:SER:HB2	1.89	0.54
1:J:290:ASP:HB3	1:J:293:LEU:HD13	1.89	0.54
3:N:162:ARG:NE	3:N:170:GLU:OE2	2.40	0.54
3:N:5:THR:HB	3:N:23:SER:HB3	1.89	0.54
3:P:211:ARG:NH1	3:P:213:GLU:OE1	2.40	0.54
1:C:457:ARG:NH1	1:C:467:ASP:OD2	2.40	0.54
3:E:211:ARG:NH1	3:E:213:GLU:OE1	2.40	0.54
3:I:211:ARG:NH1	3:I:213:GLU:OE1	2.41	0.54
1:L:474:GLN:NE2	1:L:478:LYS:O	2.40	0.54
1:A:418:ILE:HG23	1:A:422:ASN:HD22	1.71	0.54
1:C:81:ASN:HB3	1:C:239:GLN:HE22	1.73	0.54
3:E:162:ARG:NE	3:E:170:GLU:OE2	2.40	0.54
1:K:361:CYS:H	1:K:524:VAL:HG12	1.73	0.54
1:A:781:VAL:HG22	1:A:1026:ALA:HB2	1.90	0.54
1:C:1052:PHE:HB2	1:C:1063:LEU:HB2	1.89	0.54
3:E:153:PHE:HB2	3:E:201:ASN:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:540:ASN:HD22	1:K:549:THR:HG22	1.72	0.54
1:L:912:THR:OG1	1:L:1106:GLN:NE2	2.40	0.54
1:A:290:ASP:HB3	1:A:293:LEU:HD13	1.89	0.54
1:B:1005:GLN:NE2	1:C:1006:THR:OG1	2.40	0.54
1:C:980:ILE:HD12	1:C:993:ILE:HG12	1.90	0.54
1:K:67:VAL:HG23	1:K:264:ALA:HA	1.89	0.54
1:L:204:LYS:NZ	1:L:205:HIS:O	2.40	0.54
1:J:742:ILE:O	1:J:1000:ARG:NH1	2.40	0.54
1:B:67:VAL:HG23	1:B:264:ALA:HA	1.89	0.54
1:L:421:TYR:HH	2:Q:179:SER:HG	1.51	0.54
1:J:473:TYR:HB2	1:J:491:PRO:HB3	1.89	0.54
1:J:740:MET:SD	1:K:319:ARG:NH1	2.81	0.54
1:K:345:THR:O	1:K:509:ARG:NH2	2.40	0.54
3:N:153:PHE:HB2	3:N:201:ASN:HD22	1.73	0.54
1:C:345:THR:O	1:C:509:ARG:NH2	2.41	0.54
3:P:162:ARG:NE	3:P:170:GLU:OE2	2.40	0.54
3:R:211:ARG:NH1	3:R:213:GLU:OE1	2.41	0.54
2:Q:125:GLY:HA2	2:Q:130:LEU:HD21	1.89	0.53
1:A:474:GLN:NE2	1:A:478:LYS:O	2.41	0.53
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.90	0.53
1:B:822:LEU:HD13	1:B:1061:VAL:HG21	1.89	0.53
2:F:234:MET:N	2:F:234:MET:SD	2.81	0.53
2:Q:165:GLN:HB3	2:Q:171:LEU:HG	1.90	0.53
1:C:735:SER:OG	1:C:859:THR:OG1	2.26	0.53
1:C:1125:ASN:OD1	1:C:1125:ASN:N	2.42	0.53
1:K:473:TYR:HB2	1:K:491:PRO:HB3	1.90	0.53
2:M:178:TYR:HB2	2:M:182:SER:HB2	1.91	0.53
1:A:533:LEU:HD21	1:A:585:LEU:HD21	1.89	0.53
1:B:365:TYR:HA	1:B:368:LEU:HD13	1.91	0.53
2:H:63:ARG:NH2	2:H:88:TYR:OH	2.42	0.53
1:J:365:TYR:HA	1:J:368:LEU:HD13	1.89	0.53
1:J:1038:LYS:HZ1	1:K:1038:LYS:HE2	1.72	0.53
1:K:102:ARG:HD2	1:K:121:ASN:HD22	1.71	0.53
1:L:452:LEU:HD22	1:L:492:LEU:HD13	1.91	0.53
1:A:108:THR:HG23	1:A:109:THR:HG23	1.91	0.53
1:A:811:LYS:NZ	1:A:820:ASP:OD1	2.42	0.53
2:D:91:SER:OG	2:D:227:GLN:OE1	2.22	0.53
2:F:93:TYR:OH	3:G:178:ASP:O	2.26	0.53
3:I:40:LEU:HD13	3:I:85:ALA:HB2	1.90	0.53
1:L:34:ARG:HH22	1:L:206:THR:HG21	1.72	0.53
1:A:202:TYR:HB3	1:A:223:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:THR:O	1:A:509:ARG:NH2	2.42	0.53
1:A:1038:LYS:HZ1	1:B:1038:LYS:HE2	1.73	0.53
1:C:977:LEU:HD21	1:C:1000:ARG:HH12	1.74	0.53
1:C:1031:GLU:OE1	1:C:1039:ARG:NH1	2.41	0.53
1:L:811:LYS:HZ3	1:L:813:SER:HG	1.54	0.53
2:M:85:GLU:HA	2:M:109:THR:HG22	1.89	0.53
3:R:162:ARG:NE	3:R:170:GLU:OE2	2.40	0.53
2:D:63:ARG:NH2	2:D:88:TYR:OH	2.42	0.53
3:I:153:PHE:HB2	3:I:201:ASN:HD22	1.73	0.53
1:A:1006:THR:OG1	1:C:1005:GLN:NE2	2.42	0.53
1:C:31:SER:HA	1:C:216:LEU:HD23	1.90	0.53
1:K:912:THR:OG1	1:K:914:ASN:ND2	2.42	0.53
1:L:977:LEU:HD21	1:L:1000:ARG:HH12	1.73	0.53
2:O:234:MET:SD	2:O:234:MET:N	2.82	0.53
3:P:84:GLU:HG3	3:P:107:THR:HA	1.90	0.53
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.41	0.53
1:J:52:GLN:NE2	1:J:274:THR:OG1	2.41	0.53
1:J:130:VAL:HG11	1:J:231:ILE:HG12	1.91	0.53
2:M:91:SER:OG	2:M:227:GLN:OE1	2.22	0.53
3:G:185:ALA:HB3	3:G:188:VAL:HG22	1.90	0.53
2:D:234:MET:SD	2:D:234:MET:N	2.82	0.52
2:F:63:ARG:NH2	2:F:88:TYR:OH	2.42	0.52
1:J:474:GLN:NE2	1:J:478:LYS:O	2.42	0.52
1:J:666:ILE:HD11	1:J:672:ALA:HB2	1.91	0.52
1:K:452:LEU:HD22	1:K:492:LEU:HD13	1.91	0.52
1:L:912:THR:OG1	1:L:914:ASN:ND2	2.42	0.52
2:O:63:ARG:NH2	2:O:88:TYR:OH	2.42	0.52
3:P:185:ALA:HB3	3:P:188:VAL:HG22	1.91	0.52
2:Q:234:MET:SD	2:Q:234:MET:N	2.82	0.52
1:A:929:SER:O	1:A:933:LYS:NZ	2.40	0.52
1:B:472:ILE:HD12	1:B:482:GLY:HA2	1.91	0.52
1:B:1076:THR:HB	1:B:1097:SER:HB3	1.91	0.52
1:C:1106:GLN:NE2	1:C:1111:GLU:OE1	2.42	0.52
1:K:584:ILE:H	1:K:584:ILE:HD13	1.74	0.52
3:E:185:ALA:HB3	3:E:188:VAL:HG22	1.91	0.52
1:J:41:LYS:HE2	1:K:564:GLN:HE22	1.73	0.52
1:K:365:TYR:HA	1:K:368:LEU:HD13	1.91	0.52
3:R:40:LEU:HD13	3:R:85:ALA:HB2	1.91	0.52
2:D:62:ASP:HB2	2:D:80:LEU:HD12	1.92	0.52
3:G:162:ARG:NE	3:G:170:GLU:OE2	2.40	0.52
1:L:108:THR:HA	1:L:237:ARG:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:115:GLN:HG3	1:L:132:GLU:HB2	1.91	0.52
2:H:234:MET:SD	2:H:234:MET:N	2.82	0.52
1:K:472:ILE:HD12	1:K:482:GLY:HA2	1.91	0.52
2:M:234:MET:SD	2:M:234:MET:N	2.83	0.52
3:R:153:PHE:HB2	3:R:201:ASN:HD22	1.74	0.52
1:B:361:CYS:H	1:B:524:VAL:HG12	1.74	0.52
2:M:14:PRO:HB3	2:M:110:VAL:HB	1.92	0.52
3:R:6:GLN:NE2	3:R:104:THR:OG1	2.43	0.52
1:A:130:VAL:HG11	1:A:231:ILE:HG12	1.92	0.52
3:E:6:GLN:NE2	3:E:104:THR:OG1	2.42	0.52
3:E:127:GLN:HE21	3:E:129:VAL:HB	1.74	0.52
2:M:63:ARG:NH2	2:M:88:TYR:OH	2.43	0.52
1:J:596:SER:HB2	1:J:611:LEU:HB3	1.91	0.52
1:L:472:ILE:HD12	1:L:482:GLY:HA2	1.91	0.52
2:M:62:ASP:HB2	2:M:80:LEU:HD12	1.90	0.52
1:B:855:PHE:HB3	1:C:589:PRO:HG2	1.92	0.52
1:C:912:THR:OG1	1:C:1106:GLN:NE2	2.43	0.52
1:J:568:ASP:OD1	1:L:847:ARG:N	2.43	0.52
1:J:781:VAL:HG22	1:J:1026:ALA:HB2	1.92	0.52
1:J:1006:THR:OG1	1:L:1005:GLN:NE2	2.43	0.52
1:L:1125:ASN:OD1	1:L:1125:ASN:N	2.43	0.52
1:J:108:THR:HG23	1:J:109:THR:HG23	1.92	0.52
1:K:181:GLN:HB3	1:K:184:PHE:HB2	1.91	0.52
1:K:1031:GLU:OE1	1:K:1039:ARG:NH1	2.43	0.52
1:L:448:ASN:HD22	1:L:497:PHE:HB2	1.74	0.52
1:L:1031:GLU:OE1	1:L:1039:ARG:NH1	2.42	0.52
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.91	0.51
1:C:204:LYS:NZ	1:C:205:HIS:O	2.39	0.51
3:E:34:VAL:H	3:E:52:ASN:HD21	1.58	0.51
2:H:93:TYR:OH	3:I:178:ASP:O	2.27	0.51
1:L:735:SER:OG	1:L:859:THR:OG1	2.28	0.51
3:N:40:LEU:HD13	3:N:85:ALA:HB2	1.92	0.51
2:D:125:GLY:HA2	2:D:130:LEU:HD21	1.92	0.51
1:B:96:GLU:OE2	1:B:186:ASN:ND2	2.44	0.51
3:I:185:ALA:HB3	3:I:188:VAL:HG22	1.91	0.51
1:J:715:PRO:HA	1:J:1072:GLU:HA	1.92	0.51
1:K:742:ILE:O	1:K:1000:ARG:NH1	2.43	0.51
2:O:62:ASP:HB2	2:O:80:LEU:HD12	1.92	0.51
2:Q:63:ARG:NH2	2:Q:88:TYR:OH	2.42	0.51
2:F:62:ASP:HB2	2:F:80:LEU:HD12	1.92	0.51
1:L:351:TYR:HB2	1:L:454:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.43	0.51
1:C:452:LEU:HD22	1:C:492:LEU:HD13	1.92	0.51
1:L:278:LYS:NZ	1:L:286:THR:OG1	2.38	0.51
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.91	0.51
1:J:452:LEU:HD22	1:J:492:LEU:HD13	1.93	0.51
1:J:806:LEU:HD23	1:J:878:LEU:HD13	1.91	0.51
3:I:162:ARG:NE	3:I:170:GLU:OE2	2.40	0.51
3:I:176:SER:O	3:I:196:ARG:NH2	2.44	0.51
1:J:929:SER:O	1:J:933:LYS:NZ	2.40	0.51
1:L:821:LEU:O	1:L:825:LYS:NZ	2.43	0.51
3:R:185:ALA:HB3	3:R:188:VAL:HG22	1.92	0.51
1:B:584:ILE:HD13	1:B:584:ILE:H	1.74	0.51
3:E:40:LEU:HD13	3:E:85:ALA:HB2	1.93	0.51
3:E:163:GLN:HB2	3:E:169:LEU:HG	1.93	0.51
1:J:811:LYS:HD3	1:J:815:ARG:H	1.76	0.51
1:K:719:THR:OG1	1:K:1068:VAL:O	2.27	0.51
3:P:40:LEU:HD13	3:P:85:ALA:HB2	1.92	0.51
1:A:884:SER:OG	1:A:887:THR:OG1	2.28	0.51
3:G:40:LEU:HD13	3:G:85:ALA:HB2	1.92	0.51
3:G:176:SER:O	3:G:196:ARG:NH2	2.44	0.51
3:I:163:GLN:HB2	3:I:169:LEU:HG	1.93	0.51
3:N:185:ALA:HB3	3:N:188:VAL:HG22	1.91	0.51
3:R:127:GLN:HE21	3:R:129:VAL:HB	1.75	0.51
1:C:821:LEU:O	1:C:825:LYS:NZ	2.44	0.51
1:L:104:TRP:HB2	1:L:119:ILE:HD12	1.93	0.51
1:L:1125:ASN:ND2	1:L:1127:ASP:OD2	2.43	0.51
2:O:161:SER:OG	2:O:173:TRP:NE1	2.42	0.51
3:G:163:GLN:HB2	3:G:169:LEU:HG	1.92	0.50
1:J:472:ILE:HD12	1:J:482:GLY:HA2	1.92	0.50
1:L:365:TYR:HA	1:L:368:LEU:HD13	1.94	0.50
2:M:20:ILE:HD13	2:M:20:ILE:H	1.76	0.50
3:P:163:GLN:HB2	3:P:169:LEU:HG	1.93	0.50
1:A:740:MET:SD	1:B:319:ARG:NH1	2.83	0.50
1:A:804:GLN:O	1:A:816:SER:OG	2.29	0.50
2:H:20:ILE:HD13	2:H:20:ILE:H	1.76	0.50
2:M:165:GLN:HB3	2:M:171:LEU:HG	1.93	0.50
3:R:5:THR:HB	3:R:23:SER:HB3	1.93	0.50
1:A:753:LEU:HD13	1:A:997:ILE:HD11	1.91	0.50
1:B:48:LEU:HD21	1:B:278:LYS:HZ2	1.76	0.50
1:B:912:THR:OG1	1:B:914:ASN:ND2	2.44	0.50
1:B:1031:GLU:OE1	1:B:1039:ARG:NH1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:ASP:HB2	2:H:80:LEU:HD12	1.93	0.50
2:M:177:ILE:HD11	2:M:197:ARG:HH11	1.76	0.50
3:I:127:GLN:HE21	3:I:129:VAL:HB	1.76	0.50
1:J:322:PRO:HB3	1:J:539:VAL:HA	1.93	0.50
1:L:44:ARG:HD3	1:L:47:VAL:HG21	1.93	0.50
1:L:310:LYS:HG3	1:L:600:PRO:HA	1.93	0.50
1:A:472:ILE:HD12	1:A:482:GLY:HA2	1.93	0.50
1:B:971:GLY:HA3	1:B:995:ARG:HE	1.77	0.50
2:H:205:TYR:HD1	2:H:205:TYR:H	1.60	0.50
1:K:39:PRO:HG3	1:K:51:THR:HG21	1.93	0.50
2:D:51:TYR:HD1	2:D:52:GLU:HG2	1.77	0.50
3:E:13:THR:OG1	3:E:16:GLN:NE2	2.45	0.50
2:F:165:GLN:HB3	2:F:171:LEU:HG	1.93	0.50
2:H:165:GLN:HB3	2:H:171:LEU:HG	1.93	0.50
1:K:726:ILE:HB	1:K:947:LYS:HD3	1.93	0.50
1:K:1076:THR:HB	1:K:1097:SER:HB3	1.92	0.50
1:L:345:THR:O	1:L:509:ARG:NH2	2.45	0.50
2:D:147:SER:HG	2:D:203:THR:HG1	1.58	0.50
2:F:125:GLY:HA2	2:F:130:LEU:HD21	1.92	0.50
3:N:127:GLN:HE21	3:N:129:VAL:HB	1.77	0.50
2:Q:20:ILE:HD13	2:Q:20:ILE:H	1.76	0.50
1:C:1049:LEU:HD11	1:C:1067:TYR:HB2	1.94	0.50
1:L:781:VAL:HG22	1:L:1026:ALA:HB2	1.94	0.50
2:O:20:ILE:HD13	2:O:20:ILE:H	1.77	0.50
3:P:13:THR:OG1	3:P:16:GLN:NE2	2.45	0.50
3:R:13:THR:OG1	3:R:16:GLN:NE2	2.45	0.50
1:A:806:LEU:HD23	1:A:878:LEU:HD13	1.93	0.50
1:B:615:VAL:HG12	1:B:617:CYS:H	1.77	0.50
1:C:41:LYS:H	1:C:41:LYS:HD2	1.76	0.50
2:D:20:ILE:HD13	2:D:20:ILE:H	1.76	0.50
1:J:957:GLN:OE1	1:L:765:ARG:NH2	2.39	0.50
1:C:781:VAL:HG22	1:C:1026:ALA:HB2	1.93	0.49
3:E:144:LEU:HD12	3:E:205:LEU:HD23	1.93	0.49
1:K:615:VAL:HG12	1:K:617:CYS:H	1.76	0.49
1:A:322:PRO:HB3	1:A:539:VAL:HA	1.93	0.49
1:A:452:LEU:HD22	1:A:492:LEU:HD13	1.94	0.49
1:B:290:ASP:OD1	1:B:291:CYS:N	2.38	0.49
1:C:365:TYR:HA	1:C:368:LEU:HD13	1.93	0.49
3:G:13:THR:OG1	3:G:16:GLN:NE2	2.45	0.49
1:J:884:SER:OG	1:J:887:THR:OG1	2.28	0.49
1:A:30:ASN:OD1	1:A:31:SER:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:ILE:HB	1:B:947:LYS:HD3	1.95	0.49
2:F:161:SER:OG	2:F:173:TRP:NE1	2.43	0.49
2:Q:205:TYR:HD1	2:Q:205:TYR:H	1.60	0.49
3:R:163:GLN:HB2	3:R:169:LEU:HG	1.95	0.49
2:H:14:PRO:HB3	2:H:110:VAL:HB	1.95	0.49
2:Q:62:ASP:HB2	2:Q:80:LEU:HD12	1.94	0.49
3:R:144:LEU:HD12	3:R:205:LEU:HD23	1.95	0.49
3:I:6:GLN:NE2	3:I:104:THR:OG1	2.42	0.49
2:O:205:TYR:HD1	2:O:205:TYR:H	1.61	0.49
2:Q:93:TYR:OH	3:R:178:ASP:O	2.28	0.49
2:F:20:ILE:HD13	2:F:20:ILE:H	1.77	0.49
1:J:722:VAL:HG22	1:J:1065:VAL:HG22	1.93	0.49
2:M:205:TYR:HD1	2:M:205:TYR:H	1.61	0.49
1:B:452:LEU:HD22	1:B:492:LEU:HD13	1.95	0.49
1:C:335:LEU:HD13	1:C:362:VAL:HG23	1.94	0.49
2:D:205:TYR:HD1	2:D:205:TYR:H	1.60	0.49
3:N:13:THR:OG1	3:N:16:GLN:NE2	2.45	0.49
3:P:6:GLN:NE2	3:P:104:THR:OG1	2.45	0.49
3:P:144:LEU:HD12	3:P:205:LEU:HD23	1.94	0.49
1:A:811:LYS:HD3	1:A:815:ARG:H	1.77	0.49
1:C:1076:THR:HB	1:C:1097:SER:HB3	1.95	0.49
1:L:568:ASP:OD1	1:L:572:THR:N	2.46	0.49
3:P:127:GLN:HE21	3:P:129:VAL:HB	1.77	0.49
1:B:913:GLN:NE2	1:C:1090:PRO:O	2.46	0.49
1:C:568:ASP:OD1	1:C:572:THR:N	2.46	0.49
2:O:51:TYR:HD1	2:O:52:GLU:HG2	1.78	0.49
1:C:472:ILE:HD12	1:C:482:GLY:HA2	1.94	0.49
1:J:310:LYS:HG3	1:J:600:PRO:HA	1.95	0.49
2:Q:51:TYR:HD1	2:Q:52:GLU:HG2	1.78	0.49
1:C:44:ARG:HD3	1:C:47:VAL:HG21	1.94	0.48
1:C:322:PRO:HB3	1:C:539:VAL:HA	1.95	0.48
2:D:14:PRO:HB3	2:D:110:VAL:HB	1.95	0.48
2:D:177:ILE:HD11	2:D:197:ARG:HH11	1.78	0.48
3:G:144:LEU:HD12	3:G:205:LEU:HD23	1.94	0.48
3:I:13:THR:OG1	3:I:16:GLN:NE2	2.45	0.48
1:K:736:VAL:HG21	1:K:1004:LEU:HD11	1.95	0.48
1:L:722:VAL:HG22	1:L:1065:VAL:HG22	1.95	0.48
3:N:144:LEU:HD12	3:N:205:LEU:HD23	1.94	0.48
1:B:24:LEU:O	1:B:26:PRO:HD3	2.13	0.48
1:B:590:CYS:SG	1:B:591:SER:N	2.86	0.48
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:14:PRO:HB3	2:F:110:VAL:HB	1.96	0.48
1:J:804:GLN:O	1:J:816:SER:OG	2.31	0.48
1:K:666:ILE:HD11	1:K:672:ALA:HB2	1.95	0.48
1:K:737:ASP:OD2	1:K:739:THR:OG1	2.26	0.48
1:L:41:LYS:H	1:L:41:LYS:HD2	1.78	0.48
1:L:1106:GLN:NE2	1:L:1111:GLU:OE1	2.46	0.48
2:Q:14:PRO:HB3	2:Q:110:VAL:HB	1.95	0.48
1:A:99:ASN:HB3	1:A:102:ARG:HE	1.77	0.48
1:A:659:SER:HB3	1:A:698:SER:HB2	1.95	0.48
1:J:421:TYR:HH	2:M:179:SER:HG	1.57	0.48
1:J:421:TYR:OH	2:M:179:SER:OG	2.31	0.48
1:J:753:LEU:HD13	1:J:997:ILE:HD11	1.94	0.48
1:K:787:GLN:HG2	1:L:701:ALA:HB3	1.95	0.48
1:K:855:PHE:HB3	1:L:589:PRO:HG2	1.95	0.48
1:A:421:TYR:HH	2:D:179:SER:HG	1.59	0.48
1:A:735:SER:OG	1:A:859:THR:OG1	2.26	0.48
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.94	0.48
2:D:93:TYR:OH	3:E:178:ASP:O	2.27	0.48
2:F:51:TYR:HD1	2:F:52:GLU:HG2	1.78	0.48
1:J:551:VAL:N	1:J:588:THR:O	2.47	0.48
1:C:104:TRP:HB2	1:C:119:ILE:HD12	1.94	0.48
1:C:737:ASP:OD2	1:C:739:THR:OG1	2.24	0.48
1:J:99:ASN:HB3	1:J:102:ARG:HE	1.78	0.48
1:K:971:GLY:HA3	1:K:995:ARG:HE	1.78	0.48
3:N:163:GLN:HB2	3:N:169:LEU:HG	1.95	0.48
1:A:271:GLN:OE1	1:A:273:ARG:NH2	2.47	0.48
1:B:334:ASN:ND2	1:B:360:ASN:O	2.47	0.48
2:D:165:GLN:HB3	2:D:171:LEU:HG	1.95	0.48
1:K:290:ASP:OD1	1:K:291:CYS:N	2.38	0.48
1:A:96:GLU:OE1	1:A:101:ILE:N	2.42	0.48
1:C:86:PHE:H	1:C:237:ARG:HA	1.79	0.48
3:G:6:GLN:NE2	3:G:104:THR:OG1	2.43	0.48
3:I:144:LEU:HD12	3:I:205:LEU:HD23	1.94	0.48
1:L:770:ILE:HD11	1:L:1012:LEU:HD23	1.94	0.48
1:L:945:LEU:HD12	1:L:948:LEU:HD12	1.96	0.48
1:B:244:LEU:HG	1:B:246:ARG:HG2	1.94	0.48
2:F:63:ARG:HB2	2:F:80:LEU:HD13	1.96	0.48
1:K:909:ILE:HG21	1:K:1047:TYR:HB3	1.95	0.48
3:P:146:CYS:HB3	3:P:203:LEU:HB3	1.95	0.48
1:C:726:ILE:HB	1:C:947:LYS:HD3	1.95	0.48
1:K:67:VAL:HG12	1:K:242:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:96:GLU:OE2	1:K:186:ASN:ND2	2.47	0.48
1:K:1056:ALA:HB2	1:K:1061:VAL:HG23	1.95	0.48
1:L:980:ILE:HD12	1:L:993:ILE:HG12	1.96	0.48
2:Q:5:THR:OG1	3:R:198:ASP:OD2	2.30	0.48
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.96	0.47
1:A:563:GLN:O	1:A:577:ARG:NH1	2.38	0.47
1:C:966:LEU:O	1:C:975:SER:OG	2.31	0.47
1:A:329:PHE:O	1:A:580:GLN:NE2	2.47	0.47
1:B:909:ILE:HG21	1:B:1047:TYR:HB3	1.96	0.47
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.96	0.47
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.96	0.47
1:K:24:LEU:O	1:K:26:PRO:HD3	2.13	0.47
2:O:93:TYR:OH	3:P:178:ASP:O	2.28	0.47
1:J:105:ILE:HG22	1:J:239:GLN:HB3	1.96	0.47
1:K:448:ASN:HD22	1:K:497:PHE:HB2	1.79	0.47
3:R:34:VAL:H	3:R:52:ASN:HD21	1.63	0.47
1:J:566:GLY:HA2	1:L:43:PHE:H	1.80	0.47
1:K:598:ILE:HG23	1:K:664:ILE:HG21	1.96	0.47
1:A:726:ILE:HB	1:A:947:LYS:HD3	1.96	0.47
2:F:205:TYR:HD1	2:F:205:TYR:H	1.61	0.47
3:G:127:GLN:HE21	3:G:129:VAL:HB	1.78	0.47
2:H:51:TYR:HD1	2:H:52:GLU:HG2	1.79	0.47
2:M:51:TYR:HD1	2:M:52:GLU:HG2	1.79	0.47
1:A:947:LYS:H	1:A:947:LYS:HD2	1.79	0.47
1:B:598:ILE:HG23	1:B:664:ILE:HG21	1.95	0.47
2:H:218:VAL:HG12	2:H:242:THR:HA	1.96	0.47
1:K:48:LEU:HD21	1:K:278:LYS:HZ2	1.79	0.47
1:L:966:LEU:O	1:L:975:SER:OG	2.32	0.47
1:A:192:PHE:HE1	1:A:201:ILE:HG23	1.80	0.47
1:B:126:VAL:HG23	1:B:175:PHE:HA	1.96	0.47
2:F:147:SER:HG	2:F:203:THR:HG1	1.61	0.47
2:H:80:LEU:HG	2:H:81:GLN:HG3	1.96	0.47
3:I:144:LEU:HB2	3:I:205:LEU:HB3	1.97	0.47
1:J:895:GLN:HG2	1:K:713:ALA:HB2	1.96	0.47
1:K:334:ASN:ND2	1:K:360:ASN:O	2.48	0.47
1:L:737:ASP:OD2	1:L:739:THR:OG1	2.25	0.47
1:L:752:LEU:HD21	1:L:990:GLU:HG3	1.96	0.47
2:O:80:LEU:HG	2:O:81:GLN:HG3	1.97	0.47
2:O:218:VAL:HG12	2:O:242:THR:HA	1.97	0.47
1:A:421:TYR:OH	2:D:179:SER:OG	2.32	0.47
1:B:1114:ILE:H	1:B:1114:ILE:HG13	1.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:726:ILE:HB	1:J:947:LYS:HD3	1.96	0.47
1:J:994:ASP:HB3	1:K:995:ARG:HH22	1.80	0.47
2:F:39:GLN:NE2	2:F:49:MET:SD	2.87	0.47
1:L:421:TYR:OH	2:Q:179:SER:OG	2.28	0.47
1:A:615:VAL:HG12	1:A:617:CYS:H	1.80	0.47
1:A:994:ASP:HB3	1:B:995:ARG:HH22	1.80	0.47
1:B:102:ARG:HD2	1:B:121:ASN:HD22	1.80	0.47
1:A:848:ASP:OD1	1:A:848:ASP:N	2.47	0.46
1:C:108:THR:HA	1:C:237:ARG:HB2	1.97	0.46
2:Q:63:ARG:HH21	2:Q:80:LEU:HD21	1.80	0.46
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.98	0.46
1:B:1056:ALA:HB2	1:B:1061:VAL:HG23	1.96	0.46
1:C:811:LYS:HZ3	1:C:813:SER:HG	1.59	0.46
1:A:551:VAL:N	1:A:588:THR:O	2.47	0.46
1:B:326:ILE:HD13	1:B:534:VAL:HG22	1.98	0.46
1:C:897:PRO:O	1:C:901:GLN:N	2.47	0.46
3:E:144:LEU:HB2	3:E:205:LEU:HB3	1.97	0.46
1:L:551:VAL:HB	1:L:588:THR:HG23	1.96	0.46
2:F:63:ARG:HH21	2:F:80:LEU:HD21	1.81	0.46
2:H:63:ARG:HB2	2:H:80:LEU:HD13	1.96	0.46
1:J:30:ASN:OD1	1:J:31:SER:N	2.47	0.46
1:J:329:PHE:O	1:J:580:GLN:NE2	2.49	0.46
1:J:717:ASN:OD1	1:J:718:PHE:N	2.48	0.46
2:O:39:GLN:NE2	2:O:49:MET:SD	2.87	0.46
1:B:787:GLN:HG2	1:C:701:ALA:HB3	1.97	0.46
1:C:1037:SER:OG	1:C:1043:CYS:SG	2.71	0.46
1:J:945:LEU:HB3	1:J:948:LEU:HB2	1.98	0.46
2:O:63:ARG:HB2	2:O:80:LEU:HD13	1.97	0.46
1:A:396:TYR:HB2	1:A:514:SER:HB2	1.98	0.46
1:B:118:LEU:HD11	1:B:129:LYS:HB2	1.98	0.46
2:F:5:THR:OG1	3:G:198:ASP:OD2	2.32	0.46
2:F:80:LEU:HG	2:F:81:GLN:HG3	1.98	0.46
1:K:126:VAL:HG23	1:K:175:PHE:HA	1.97	0.46
1:K:244:LEU:HG	1:K:246:ARG:HG2	1.98	0.46
1:K:1037:SER:H	1:K:1048:HIS:CD2	2.34	0.46
2:M:56:ARG:HD3	2:M:64:PHE:HB3	1.98	0.46
3:N:6:GLN:NE2	3:N:104:THR:OG1	2.48	0.46
2:O:63:ARG:HH21	2:O:80:LEU:HD21	1.81	0.46
1:A:666:ILE:HD12	1:A:670:ILE:HG22	1.98	0.46
1:A:717:ASN:OD1	1:A:718:PHE:N	2.48	0.46
1:C:551:VAL:HB	1:C:588:THR:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:ARG:HH21	2:D:80:LEU:HD21	1.80	0.46
3:E:222:LYS:O	3:E:239:ASP:N	2.45	0.46
1:J:848:ASP:OD1	1:J:848:ASP:N	2.47	0.46
1:K:590:CYS:SG	1:K:591:SER:N	2.89	0.46
1:L:335:LEU:HD13	1:L:362:VAL:HG23	1.98	0.46
1:A:105:ILE:HG22	1:A:239:GLN:HB3	1.97	0.46
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.98	0.46
1:J:947:LYS:H	1:J:947:LYS:HD2	1.80	0.46
1:C:415:THR:O	2:H:184:TYR:OH	2.33	0.46
1:C:448:ASN:HD22	1:C:497:PHE:HB2	1.81	0.46
1:K:662:CYS:HB2	1:K:697:MET:HG2	1.98	0.46
1:K:913:GLN:NE2	1:L:1090:PRO:O	2.49	0.46
1:L:86:PHE:H	1:L:237:ARG:HA	1.80	0.46
2:O:14:PRO:HB3	2:O:110:VAL:HB	1.98	0.46
1:A:566:GLY:HA2	1:C:43:PHE:H	1.82	0.45
1:B:67:VAL:HG12	1:B:242:LEU:HD13	1.98	0.45
1:B:473:TYR:H	1:B:491:PRO:HD3	1.80	0.45
1:C:328:ARG:HH21	1:C:533:LEU:H	1.64	0.45
2:H:63:ARG:HH21	2:H:80:LEU:HD21	1.80	0.45
1:L:727:LEU:HD11	1:L:1028:LYS:HD2	1.97	0.45
1:A:94:SER:HB2	1:A:188:ARG:HG3	1.98	0.45
1:B:315:THR:OG1	1:B:595:VAL:O	2.30	0.45
1:J:192:PHE:HE1	1:J:201:ILE:HG23	1.81	0.45
1:J:195:ILE:HG22	1:J:197:GLY:H	1.82	0.45
1:K:315:THR:OG1	1:K:595:VAL:O	2.28	0.45
1:L:141:LEU:HB2	1:L:243:ALA:HA	1.97	0.45
1:B:577:ARG:HA	1:B:584:ILE:HA	1.98	0.45
1:C:133:PHE:HA	1:C:164:ASN:HB2	1.97	0.45
1:K:722:VAL:HG22	1:K:1065:VAL:HG22	1.99	0.45
1:B:662:CYS:HB2	1:B:697:MET:HG2	1.99	0.45
2:F:218:VAL:HG12	2:F:242:THR:HA	1.98	0.45
2:H:128:VAL:HG13	2:H:129:GLN:H	1.82	0.45
1:B:48:LEU:HB3	1:B:276:LEU:HD11	1.99	0.45
1:B:324:GLU:OE1	1:B:325:SER:N	2.47	0.45
1:B:719:THR:OG1	1:B:1068:VAL:O	2.26	0.45
1:B:858:LEU:HD13	1:B:959:LEU:HD22	1.98	0.45
1:C:393:THR:O	1:C:523:THR:OG1	2.33	0.45
2:H:147:SER:OG	2:H:203:THR:OG1	2.30	0.45
2:H:201:GLU:OE2	2:H:202:ASN:ND2	2.50	0.45
1:A:746:SER:O	1:A:749:CYS:N	2.48	0.45
1:J:659:SER:HB3	1:J:698:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:666:ILE:HD12	1:J:670:ILE:HG22	1.99	0.45
1:K:1049:LEU:HD11	1:K:1067:TYR:HB2	1.99	0.45
1:L:192:PHE:HE1	1:L:201:ILE:HG23	1.81	0.45
1:A:126:VAL:HB	1:A:175:PHE:HA	1.98	0.45
2:Q:56:ARG:HD3	2:Q:64:PHE:HB3	1.98	0.45
2:Q:128:VAL:HG13	2:Q:129:GLN:H	1.82	0.45
1:A:324:GLU:OE1	1:A:325:SER:N	2.49	0.45
1:B:187:LEU:HB3	1:B:206:THR:HG23	1.99	0.45
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.99	0.45
1:J:345:THR:O	1:J:509:ARG:NH2	2.50	0.45
1:K:210:VAL:HG22	1:K:212:GLU:H	1.82	0.45
1:K:324:GLU:OE1	1:K:325:SER:N	2.50	0.45
1:L:216:LEU:HD12	1:L:217:PRO:HD2	1.99	0.45
1:L:1037:SER:OG	1:L:1043:CYS:SG	2.74	0.45
2:Q:80:LEU:HG	2:Q:81:GLN:HG3	1.99	0.45
1:B:731:MET:HE3	1:B:1014:ARG:HD2	1.99	0.45
1:C:328:ARG:HH21	1:C:533:LEU:N	2.14	0.45
1:J:82:PRO:HG2	1:J:84:LEU:HD11	1.99	0.45
1:A:596:SER:HB2	1:A:611:LEU:HB3	1.98	0.45
1:A:710:ASN:OD1	1:A:710:ASN:N	2.50	0.45
1:B:296:LEU:HG	1:B:300:LYS:HE2	1.99	0.45
2:F:201:GLU:OE2	2:F:202:ASN:ND2	2.50	0.45
1:J:746:SER:O	1:J:749:CYS:N	2.49	0.45
2:Q:20:ILE:HD12	2:Q:108:VAL:HG11	2.00	0.45
1:A:195:ILE:HG22	1:A:197:GLY:H	1.82	0.44
2:D:201:GLU:OE2	2:D:202:ASN:ND2	2.51	0.44
2:D:218:VAL:HG12	2:D:242:THR:HA	1.98	0.44
1:K:135:PHE:CZ	1:K:139:PRO:HG3	2.52	0.44
2:H:39:GLN:NE2	2:H:49:MET:SD	2.90	0.44
2:H:161:SER:OG	2:H:173:TRP:NE1	2.49	0.44
1:J:710:ASN:N	1:J:710:ASN:OD1	2.50	0.44
1:K:856:LYS:HZ3	1:K:856:LYS:HB2	1.81	0.44
2:Q:218:VAL:HG12	2:Q:242:THR:HA	1.98	0.44
1:A:473:TYR:H	1:A:491:PRO:HD3	1.82	0.44
3:G:130:GLU:OE1	3:G:130:GLU:N	2.51	0.44
1:L:129:LYS:HG2	1:L:131:CYS:H	1.83	0.44
2:M:128:VAL:HG13	2:M:129:GLN:H	1.82	0.44
1:A:895:GLN:HG2	1:B:713:ALA:HB2	1.99	0.44
1:C:752:LEU:HD21	1:C:990:GLU:HG3	1.98	0.44
2:H:133:SER:HB2	2:H:146:LEU:HA	1.98	0.44
1:K:1083:HIS:CG	1:K:1084:ASP:H	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PHE:HD2	1:A:528:LYS:HB3	1.82	0.44
1:C:129:LYS:HG2	1:C:131:CYS:H	1.83	0.44
3:I:130:GLU:OE1	3:I:130:GLU:N	2.50	0.44
1:K:48:LEU:HB3	1:K:276:LEU:HD11	2.00	0.44
1:L:351:TYR:CG	1:L:452:LEU:HD11	2.53	0.44
2:O:128:VAL:HG13	2:O:129:GLN:H	1.82	0.44
1:A:562:PHE:O	1:A:564:GLN:NE2	2.50	0.44
2:H:5:THR:OG1	3:I:198:ASP:OD2	2.30	0.44
2:O:177:ILE:HD11	2:O:197:ARG:HH11	1.82	0.44
1:C:727:LEU:HD11	1:C:1028:LYS:HD2	1.99	0.44
2:D:56:ARG:HD3	2:D:64:PHE:HB3	2.00	0.44
3:G:194:ILE:HB	3:G:205:LEU:HD13	1.98	0.44
1:K:676:THR:OG1	1:K:690:GLN:OE1	2.35	0.44
1:L:726:ILE:HB	1:L:947:LYS:HD3	2.00	0.44
3:N:130:GLU:OE1	3:N:130:GLU:N	2.51	0.44
1:B:710:ASN:OD1	1:B:710:ASN:N	2.51	0.44
1:B:856:LYS:HG2	1:B:963:VAL:HG23	1.99	0.44
1:B:1037:SER:H	1:B:1048:HIS:CD2	2.33	0.44
2:D:63:ARG:HB2	2:D:80:LEU:HD13	1.99	0.44
1:K:187:LEU:HB3	1:K:206:THR:HG23	2.00	0.44
1:A:735:SER:O	1:A:859:THR:OG1	2.34	0.44
1:B:1083:HIS:CG	1:B:1084:ASP:H	2.36	0.44
3:E:228:PRO:HA	3:E:229:PRO:HD3	1.91	0.44
1:J:1049:LEU:HD11	1:J:1067:TYR:HB2	2.00	0.44
2:O:147:SER:OG	2:O:203:THR:OG1	2.30	0.44
1:A:82:PRO:HG2	1:A:84:LEU:HD11	2.00	0.43
1:A:811:LYS:HG3	1:A:814:LYS:H	1.83	0.43
1:B:31:SER:HA	1:B:216:LEU:HD12	2.00	0.43
1:B:210:VAL:HG22	1:B:212:GLU:H	1.82	0.43
1:B:856:LYS:HB2	1:B:856:LYS:HZ3	1.82	0.43
1:C:327:VAL:HG13	1:C:542:ASN:HB3	1.99	0.43
3:E:130:GLU:N	3:E:130:GLU:OE1	2.51	0.43
3:I:34:VAL:H	3:I:52:ASN:HD21	1.66	0.43
3:R:130:GLU:N	3:R:130:GLU:OE1	2.51	0.43
1:B:351:TYR:CG	1:B:452:LEU:HD11	2.52	0.43
1:C:102:ARG:NH1	1:C:121:ASN:O	2.50	0.43
1:C:351:TYR:CG	1:C:452:LEU:HD11	2.53	0.43
1:C:577:ARG:HH11	1:C:582:LEU:HD22	1.84	0.43
2:D:20:ILE:HD12	2:D:108:VAL:HG11	2.01	0.43
3:G:89:CYS:O	3:G:101:GLY:N	2.51	0.43
3:I:89:CYS:O	3:I:101:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:731:MET:HE3	1:K:1014:ARG:HD2	2.00	0.43
1:L:276:LEU:HB3	1:L:289:VAL:HB	2.00	0.43
1:L:717:ASN:OD1	1:L:718:PHE:N	2.51	0.43
1:L:719:THR:OG1	1:L:1068:VAL:O	2.30	0.43
1:L:897:PRO:O	1:L:901:GLN:N	2.51	0.43
3:N:222:LYS:O	3:N:239:ASP:N	2.47	0.43
3:P:176:SER:O	3:P:196:ARG:NH2	2.51	0.43
2:Q:63:ARG:HB2	2:Q:80:LEU:HD13	2.00	0.43
1:A:945:LEU:HB3	1:A:948:LEU:HB2	1.99	0.43
2:D:80:LEU:HG	2:D:81:GLN:HG3	1.99	0.43
3:G:171:TRP:HZ2	3:G:174:VAL:HG12	1.83	0.43
1:K:715:PRO:HA	1:K:1072:GLU:HA	1.99	0.43
1:L:1049:LEU:HD11	1:L:1067:TYR:HB2	2.00	0.43
3:R:176:SER:O	3:R:196:ARG:NH2	2.51	0.43
3:R:222:LYS:O	3:R:239:ASP:N	2.45	0.43
1:A:102:ARG:O	1:A:121:ASN:N	2.46	0.43
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.48	0.43
1:B:855:PHE:HA	1:C:592:PHE:HZ	1.84	0.43
1:C:329:PHE:CD2	1:C:528:LYS:HB2	2.53	0.43
2:F:164:ARG:HD2	2:F:217:ALA:HB3	2.01	0.43
1:J:96:GLU:OE1	1:J:101:ILE:N	2.43	0.43
1:K:541:PHE:HE2	1:K:546:LEU:HD12	1.82	0.43
1:L:1052:PHE:HB2	1:L:1063:LEU:HB2	1.99	0.43
2:M:93:TYR:OH	3:N:178:ASP:O	2.29	0.43
3:R:144:LEU:HB2	3:R:205:LEU:HB3	2.00	0.43
1:B:448:ASN:HD22	1:B:497:PHE:HB2	1.83	0.43
2:O:201:GLU:OE2	2:O:202:ASN:ND2	2.51	0.43
3:P:130:GLU:N	3:P:130:GLU:OE1	2.50	0.43
1:B:135:PHE:CZ	1:B:139:PRO:HG3	2.54	0.43
1:B:736:VAL:HG21	1:B:1004:LEU:HD11	2.01	0.43
2:H:164:ARG:HD2	2:H:217:ALA:HB3	2.01	0.43
1:K:473:TYR:H	1:K:491:PRO:HD3	1.82	0.43
1:K:773:GLU:OE2	1:K:777:ASN:ND2	2.52	0.43
1:L:126:VAL:HG22	1:L:175:PHE:HA	2.00	0.43
3:N:144:LEU:HB2	3:N:205:LEU:HB3	2.00	0.43
2:O:165:GLN:HB3	2:O:171:LEU:HG	2.00	0.43
2:O:179:SER:O	2:O:197:ARG:NH1	2.45	0.43
1:A:393:THR:O	1:A:523:THR:OG1	2.33	0.43
3:E:89:CYS:O	3:E:101:GLY:N	2.52	0.43
2:F:128:VAL:HG13	2:F:129:GLN:H	1.82	0.43
2:F:173:TRP:CE2	2:F:226:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:222:LYS:O	3:I:239:ASP:N	2.45	0.43
1:K:551:VAL:HB	1:K:588:THR:HG23	2.01	0.43
1:K:710:ASN:OD1	1:K:710:ASN:N	2.51	0.43
1:L:195:ILE:HG22	1:L:196:ASP:H	1.84	0.43
2:M:80:LEU:HG	2:M:81:GLN:HG3	2.00	0.43
3:N:34:VAL:H	3:N:52:ASN:HD21	1.65	0.43
3:N:176:SER:O	3:N:196:ARG:NH2	2.51	0.43
2:Q:133:SER:HB2	2:Q:146:LEU:HA	2.01	0.43
1:A:553:THR:O	1:A:586:ASP:N	2.46	0.43
1:A:572:THR:OG1	1:C:847:ARG:NH2	2.52	0.43
1:B:564:GLN:HE21	1:B:564:GLN:HB2	1.67	0.43
1:C:986:PRO:N	1:C:987:PRO:HD2	2.34	0.43
3:I:159:HIS:CD2	3:I:174:VAL:HG23	2.54	0.43
1:J:126:VAL:HB	1:J:175:PHE:HA	1.99	0.43
1:A:957:GLN:OE1	1:C:765:ARG:NH2	2.39	0.43
2:D:128:VAL:HG13	2:D:129:GLN:H	1.83	0.43
1:J:615:VAL:HG12	1:J:617:CYS:H	1.83	0.43
1:K:118:LEU:HD11	1:K:129:LYS:HB2	2.01	0.43
1:L:718:PHE:HB2	1:L:720:ILE:HD12	2.00	0.43
3:P:222:LYS:O	3:P:239:ASP:N	2.46	0.43
2:Q:161:SER:OG	2:Q:173:TRP:NE1	2.48	0.43
1:C:195:ILE:HG22	1:C:196:ASP:H	1.84	0.43
1:J:713:ALA:HB3	1:L:894:LEU:HB3	2.00	0.43
1:K:331:ASN:OD1	1:K:332:ILE:N	2.52	0.43
1:K:415:THR:O	2:O:184:TYR:OH	2.36	0.43
1:K:811:LYS:HE3	1:K:811:LYS:HB2	1.86	0.43
2:M:40:GLN:HE21	2:M:40:GLN:HB3	1.70	0.43
2:O:99:PHE:HB3	2:O:173:TRP:HB3	2.01	0.43
2:Q:227:GLN:HB3	2:Q:228:PRO:HD3	2.01	0.43
1:B:136:CYS:SG	1:B:137:ASN:N	2.92	0.42
1:B:490:PHE:HD1	1:B:491:PRO:HD2	1.82	0.42
1:B:1049:LEU:HD11	1:B:1067:TYR:HB2	2.01	0.42
2:D:60:VAL:HG22	2:D:62:ASP:H	1.84	0.42
3:E:176:SER:O	3:E:196:ARG:NH2	2.53	0.42
2:F:185:TYR:HE1	2:F:195:ILE:H	1.67	0.42
1:J:329:PHE:HD2	1:J:528:LYS:HB3	1.84	0.42
2:O:133:SER:HB2	2:O:146:LEU:HA	2.00	0.42
2:Q:164:ARG:HD2	2:Q:217:ALA:HB3	2.01	0.42
1:A:448:ASN:HD22	1:A:497:PHE:HB2	1.84	0.42
1:B:676:THR:OG1	1:B:690:GLN:OE1	2.34	0.42
2:H:20:ILE:HD12	2:H:108:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:811:LYS:HE2	1:J:813:SER:HB2	2.01	0.42
2:M:63:ARG:HH21	2:M:80:LEU:HD21	1.83	0.42
2:Q:201:GLU:OE2	2:Q:202:ASN:ND2	2.52	0.42
1:A:81:ASN:HB2	1:A:239:GLN:NE2	2.34	0.42
1:A:129:LYS:HG2	1:A:131:CYS:H	1.84	0.42
1:C:847:ARG:HE	1:C:852:ALA:HA	1.83	0.42
1:J:81:ASN:HB2	1:J:239:GLN:NE2	2.34	0.42
1:J:811:LYS:HG3	1:J:814:LYS:H	1.83	0.42
2:M:201:GLU:OE2	2:M:202:ASN:ND2	2.52	0.42
1:A:415:THR:O	2:D:184:TYR:OH	2.35	0.42
1:C:473:TYR:H	1:C:491:PRO:HD3	1.85	0.42
2:D:39:GLN:NE2	2:D:49:MET:SD	2.93	0.42
3:G:228:PRO:HA	3:G:229:PRO:HD3	1.91	0.42
1:J:735:SER:OG	1:J:859:THR:OG1	2.29	0.42
1:L:160:TYR:HE1	1:L:163:ALA:HB2	1.84	0.42
2:Q:177:ILE:HD11	2:Q:197:ARG:HH11	1.84	0.42
1:A:1049:LEU:HD11	1:A:1067:TYR:HB2	2.00	0.42
1:C:96:GLU:HA	1:C:100:ILE:HD12	1.99	0.42
2:M:147:SER:OG	2:M:203:THR:OG1	2.34	0.42
1:A:565:PHE:HA	1:A:576:VAL:HG23	2.02	0.42
1:B:130:VAL:HG21	1:B:231:ILE:HG12	2.02	0.42
1:C:718:PHE:HB2	1:C:720:ILE:HD12	2.01	0.42
1:K:243:ALA:HB1	1:K:245:HIS:CD2	2.55	0.42
1:K:1114:ILE:H	1:K:1114:ILE:HG13	1.52	0.42
2:O:227:GLN:HB3	2:O:228:PRO:HD3	2.02	0.42
1:A:713:ALA:HB3	1:C:894:LEU:HB3	2.01	0.42
1:C:1037:SER:H	1:C:1048:HIS:CD2	2.32	0.42
3:G:36:TRP:HB2	3:G:49:ILE:HB	2.02	0.42
2:H:216:THR:HG23	2:H:245:VAL:H	1.84	0.42
3:I:228:PRO:HA	3:I:229:PRO:HD3	1.91	0.42
1:K:351:TYR:CG	1:K:452:LEU:HD11	2.54	0.42
1:C:111:ASP:OD1	1:C:112:SER:N	2.52	0.42
1:C:773:GLU:OE2	1:C:777:ASN:ND2	2.53	0.42
2:F:179:SER:O	2:F:197:ARG:NH1	2.47	0.42
1:J:735:SER:HA	1:J:767:LEU:HD13	2.02	0.42
1:K:136:CYS:SG	1:K:137:ASN:N	2.93	0.42
1:K:302:THR:HG23	1:K:303:LEU:HG	2.02	0.42
1:K:856:LYS:HG2	1:K:963:VAL:HG23	2.01	0.42
2:M:218:VAL:HG12	2:M:242:THR:HA	2.01	0.42
1:A:661:GLU:O	1:A:695:TYR:OH	2.34	0.42
1:K:31:SER:HA	1:K:216:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:294:ASP:OD1	1:L:294:ASP:N	2.52	0.42
1:L:378:LYS:HE3	3:R:233:ASN:HD21	1.85	0.42
1:A:118:LEU:HD21	1:A:129:LYS:HB3	2.02	0.42
1:B:115:GLN:HA	1:B:132:GLU:HB3	2.01	0.42
1:B:728:PRO:HD3	1:B:947:LYS:HZ3	1.85	0.42
1:C:192:PHE:HE1	1:C:201:ILE:HG23	1.83	0.42
1:C:278:LYS:HB2	1:C:306:PHE:CE1	2.55	0.42
1:C:717:ASN:OD1	1:C:718:PHE:N	2.52	0.42
2:F:150:ALA:HB3	2:F:155:VAL:HG22	2.02	0.42
1:J:353:TRP:HZ3	1:J:355:ARG:HG2	1.85	0.42
1:J:448:ASN:HD22	1:J:497:PHE:HB2	1.83	0.42
1:J:947:LYS:HE2	1:J:947:LYS:HB3	1.91	0.42
1:L:986:PRO:N	1:L:987:PRO:HD2	2.34	0.42
3:P:171:TRP:HZ2	3:P:174:VAL:HG12	1.85	0.42
1:A:735:SER:HA	1:A:767:LEU:HD13	2.01	0.41
1:C:62:VAL:HG12	1:C:63:THR:H	1.85	0.41
1:K:490:PHE:HD1	1:K:491:PRO:HD2	1.85	0.41
2:M:60:VAL:HG22	2:M:62:ASP:H	1.84	0.41
2:M:164:ARG:HD2	2:M:217:ALA:HB3	2.02	0.41
2:M:227:GLN:HB3	2:M:228:PRO:HD3	2.02	0.41
2:O:164:ARG:HD2	2:O:217:ALA:HB3	2.01	0.41
3:R:159:HIS:CD2	3:R:174:VAL:HG23	2.55	0.41
1:A:907:ASN:HD21	1:A:913:GLN:HB3	1.84	0.41
1:C:719:THR:OG1	1:C:1068:VAL:O	2.30	0.41
1:J:129:LYS:HG2	1:J:131:CYS:H	1.85	0.41
1:J:598:ILE:HG23	1:J:664:ILE:HG21	2.02	0.41
1:L:328:ARG:HH21	1:L:533:LEU:N	2.17	0.41
3:R:228:PRO:HA	3:R:229:PRO:HD3	1.91	0.41
1:A:34:ARG:NH1	1:A:91:TYR:OH	2.54	0.41
1:B:173:GLN:HE21	1:B:173:GLN:HB3	1.69	0.41
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	2.01	0.41
1:C:53:ASP:OD1	1:C:54:LEU:N	2.47	0.41
2:F:106:THR:HG22	2:F:108:VAL:HG22	2.03	0.41
3:I:33:THR:O	3:I:236:TYR:OH	2.29	0.41
1:J:365:TYR:H	1:J:388:ASN:HD21	1.67	0.41
1:L:415:THR:O	2:Q:184:TYR:OH	2.32	0.41
2:O:56:ARG:HD3	2:O:64:PHE:HB3	2.01	0.41
3:P:144:LEU:HB2	3:P:205:LEU:HB3	2.03	0.41
1:B:353:TRP:HZ3	1:B:355:ARG:HG2	1.85	0.41
1:C:216:LEU:HD12	1:C:217:PRO:HD2	2.01	0.41
1:C:728:PRO:HD3	1:C:947:LYS:HZ3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:177:ILE:HD11	2:H:197:ARG:HH11	1.86	0.41
1:J:271:GLN:OE1	1:J:273:ARG:NH2	2.53	0.41
1:K:330:PRO:HG3	1:K:579:PRO:HB2	2.02	0.41
1:K:550:GLY:HA2	1:K:590:CYS:N	2.35	0.41
2:M:20:ILE:HD12	2:M:108:VAL:HG11	2.01	0.41
1:C:160:TYR:HE1	1:C:163:ALA:HB2	1.85	0.41
1:L:329:PHE:CD2	1:L:528:LYS:HB2	2.56	0.41
1:A:280:ASN:OD1	1:A:281:GLU:N	2.48	0.41
1:C:294:ASP:OD1	1:C:294:ASP:N	2.53	0.41
1:J:194:ASN:O	1:J:194:ASN:ND2	2.50	0.41
1:K:326:ILE:HD13	1:K:534:VAL:HG22	2.01	0.41
1:K:353:TRP:HZ3	1:K:355:ARG:HG2	1.85	0.41
1:K:740:MET:HB2	1:L:319:ARG:NH2	2.35	0.41
2:Q:161:SER:HG	2:Q:173:TRP:HE1	1.68	0.41
1:A:598:ILE:HG23	1:A:664:ILE:HG21	2.01	0.41
1:B:551:VAL:HB	1:B:588:THR:HG23	2.03	0.41
3:G:215:THR:HG23	3:G:248:THR:HG22	2.03	0.41
1:K:858:LEU:HD13	1:K:959:LEU:HD22	2.01	0.41
1:L:81:ASN:HB3	1:L:239:GLN:HE22	1.85	0.41
1:L:102:ARG:NH1	1:L:121:ASN:O	2.54	0.41
1:L:733:LYS:HD2	1:L:771:ALA:HB1	2.02	0.41
2:Q:147:SER:OG	2:Q:203:THR:OG1	2.31	0.41
1:A:811:LYS:HE2	1:A:813:SER:HB2	2.02	0.41
2:D:227:GLN:HB3	2:D:228:PRO:HD3	2.02	0.41
3:E:171:TRP:HZ2	3:E:174:VAL:HG12	1.86	0.41
2:H:173:TRP:CE2	2:H:226:ILE:HD11	2.55	0.41
2:H:227:GLN:HB3	2:H:228:PRO:HD3	2.02	0.41
1:J:490:PHE:HD1	1:J:491:PRO:HD2	1.84	0.41
1:J:540:ASN:HD22	1:J:549:THR:HG22	1.85	0.41
1:K:855:PHE:HA	1:L:592:PHE:HZ	1.86	0.41
1:L:1037:SER:H	1:L:1048:HIS:CD2	2.34	0.41
2:O:20:ILE:HD12	2:O:108:VAL:HG11	2.02	0.41
2:O:106:THR:HG22	2:O:108:VAL:HG22	2.03	0.41
1:A:719:THR:OG1	1:A:1068:VAL:O	2.29	0.41
1:B:41:LYS:HB2	1:C:563:GLN:HA	2.02	0.41
1:B:41:LYS:HE3	1:B:41:LYS:HB3	1.88	0.41
1:B:111:ASP:HA	1:B:134:GLN:HG3	2.03	0.41
1:B:737:ASP:OD2	1:B:739:THR:OG1	2.25	0.41
1:C:116:SER:O	1:C:130:VAL:HA	2.20	0.41
1:C:1054:GLN:N	1:C:1061:VAL:O	2.51	0.41
2:F:227:GLN:HB3	2:F:228:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:33:THR:O	3:G:236:TYR:OH	2.27	0.41
3:G:46:LYS:HE2	3:G:46:LYS:HB2	1.95	0.41
2:H:106:THR:HG22	2:H:108:VAL:HG22	2.03	0.41
3:I:194:ILE:HB	3:I:205:LEU:HD13	2.03	0.41
1:J:67:VAL:HG23	1:J:264:ALA:HA	2.03	0.41
1:J:177:MET:SD	1:J:188:ARG:NH1	2.93	0.41
1:J:415:THR:O	2:M:184:TYR:OH	2.38	0.41
1:J:713:ALA:HB2	1:L:895:GLN:HG2	2.03	0.41
1:K:91:TYR:HD1	1:K:191:VAL:HG22	1.86	0.41
1:K:540:ASN:ND2	1:K:549:THR:HG22	2.34	0.41
1:L:133:PHE:HA	1:L:164:ASN:HB2	2.03	0.41
1:A:540:ASN:HD22	1:A:549:THR:HG22	1.85	0.41
1:B:229:LEU:H	1:B:229:LEU:HD22	1.86	0.41
1:C:326:ILE:HD13	1:C:539:VAL:HG21	2.02	0.41
2:F:20:ILE:HD12	2:F:108:VAL:HG11	2.03	0.41
2:F:56:ARG:HD3	2:F:64:PHE:HB3	2.02	0.41
1:J:210:VAL:HG13	1:J:212:GLU:H	1.86	0.41
1:J:661:GLU:O	1:J:695:TYR:OH	2.36	0.41
1:J:907:ASN:HD21	1:J:913:GLN:HB3	1.85	0.41
1:L:62:VAL:HG12	1:L:63:THR:H	1.85	0.41
1:L:862:PRO:HA	1:L:863:PRO:HD3	1.97	0.41
2:O:185:TYR:HE1	2:O:195:ILE:H	1.69	0.41
1:C:1081:ILE:H	1:C:1081:ILE:HD13	1.86	0.40
2:H:40:GLN:HE21	2:H:40:GLN:HB3	1.71	0.40
1:J:706:ALA:HB3	1:L:895:GLN:HE22	1.86	0.40
1:J:905:ARG:O	1:J:1036:GLN:NE2	2.53	0.40
1:K:728:PRO:HD3	1:K:947:LYS:HZ3	1.85	0.40
1:L:53:ASP:OD1	1:L:54:LEU:N	2.48	0.40
1:L:92:PHE:HE1	1:L:94:SER:HB2	1.86	0.40
1:L:278:LYS:HB2	1:L:306:PHE:CE1	2.56	0.40
2:O:5:THR:OG1	3:P:198:ASP:OD2	2.36	0.40
1:B:136:CYS:HB3	1:B:161:SER:N	2.36	0.40
1:B:773:GLU:OE2	1:B:777:ASN:ND2	2.55	0.40
1:J:86:PHE:N	1:J:236:THR:O	2.43	0.40
1:J:118:LEU:HD21	1:J:129:LYS:HB3	2.02	0.40
1:J:699:LEU:HD22	1:L:873:TYR:CZ	2.57	0.40
1:K:352:ALA:HA	1:K:466:ARG:HD2	2.02	0.40
1:L:453:TYR:HE2	1:L:455:LEU:HD23	1.86	0.40
2:Q:150:ALA:HB3	2:Q:155:VAL:HG22	2.04	0.40
2:Q:216:THR:HG23	2:Q:245:VAL:H	1.87	0.40
1:A:542:ASN:O	1:A:542:ASN:ND2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:PRO:HG3	1:B:579:PRO:HB2	2.03	0.40
1:B:550:GLY:HA2	1:B:590:CYS:N	2.37	0.40
1:C:276:LEU:HB3	1:C:289:VAL:HB	2.03	0.40
1:C:733:LYS:HD2	1:C:771:ALA:HB1	2.04	0.40
2:D:106:THR:HG22	2:D:108:VAL:HG22	2.04	0.40
1:K:862:PRO:HA	1:K:863:PRO:HD3	1.95	0.40
1:L:96:GLU:HA	1:L:100:ILE:HD12	2.02	0.40
1:L:187:LEU:HG	1:L:189:GLU:HG2	2.03	0.40
1:L:1086:LYS:HE2	1:L:1086:LYS:HB3	1.92	0.40
2:M:5:THR:OG1	3:N:198:ASP:OD2	2.35	0.40
3:P:194:ILE:HB	3:P:205:LEU:HD13	2.04	0.40
1:B:1054:GLN:HB2	1:B:1061:VAL:HB	2.04	0.40
2:F:99:PHE:HB3	2:F:173:TRP:HB3	2.03	0.40
2:F:164:ARG:HG2	2:F:174:VAL:HG21	2.03	0.40
3:G:144:LEU:HB2	3:G:205:LEU:HB3	2.04	0.40
3:I:215:THR:HG23	3:I:248:THR:HG22	2.04	0.40
1:L:116:SER:O	1:L:130:VAL:HA	2.21	0.40
1:L:503:VAL:HG22	3:R:155:ASP:HB3	2.03	0.40
1:L:577:ARG:HH11	1:L:582:LEU:HD22	1.86	0.40
2:M:164:ARG:HG2	2:M:174:VAL:HG21	2.02	0.40
1:A:699:LEU:HD22	1:C:873:TYR:CZ	2.57	0.40
1:A:1083:HIS:CG	1:A:1084:ASP:H	2.40	0.40
1:B:243:ALA:HB1	1:B:245:HIS:CD2	2.55	0.40
1:B:740:MET:HB2	1:C:319:ARG:NH2	2.36	0.40
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	2.03	0.40
2:D:161:SER:OG	2:D:173:TRP:NE1	2.53	0.40
2:D:164:ARG:HD2	2:D:217:ALA:HB3	2.02	0.40
3:E:159:HIS:CD2	3:E:174:VAL:HG23	2.56	0.40
2:H:56:ARG:HD3	2:H:64:PHE:HB3	2.04	0.40
1:J:102:ARG:O	1:J:121:ASN:N	2.46	0.40
1:K:577:ARG:HA	1:K:584:ILE:HA	2.03	0.40
1:K:788:ILE:HG23	1:K:876:ALA:HB2	2.04	0.40
1:L:141:LEU:HD21	1:L:241:LEU:HD12	2.03	0.40
1:L:874:THR:HG21	1:L:1055:SER:HB3	2.03	0.40
3:N:159:HIS:CD2	3:N:174:VAL:HG23	2.56	0.40
2:O:216:THR:HG23	2:O:245:VAL:H	1.87	0.40
2:Q:173:TRP:CE2	2:Q:226:ILE:HD11	2.56	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	1017/1285 (79%)	959 (94%)	58 (6%)	0	100	100
1	B	1017/1285 (79%)	947 (93%)	70 (7%)	0	100	100
1	C	1010/1285 (79%)	935 (93%)	75 (7%)	0	100	100
1	J	1017/1285 (79%)	959 (94%)	58 (6%)	0	100	100
1	K	1017/1285 (79%)	949 (93%)	68 (7%)	0	100	100
1	L	1010/1285 (79%)	938 (93%)	72 (7%)	0	100	100
2	D	232/247 (94%)	211 (91%)	21 (9%)	0	100	100
2	F	232/247 (94%)	210 (90%)	22 (10%)	0	100	100
2	H	232/247 (94%)	208 (90%)	24 (10%)	0	100	100
2	M	232/247 (94%)	210 (90%)	22 (10%)	0	100	100
2	O	232/247 (94%)	211 (91%)	21 (9%)	0	100	100
2	Q	232/247 (94%)	211 (91%)	21 (9%)	0	100	100
3	E	231/251 (92%)	222 (96%)	9 (4%)	0	100	100
3	G	231/251 (92%)	221 (96%)	10 (4%)	0	100	100
3	I	231/251 (92%)	221 (96%)	10 (4%)	0	100	100
3	N	231/251 (92%)	221 (96%)	10 (4%)	0	100	100
3	P	231/251 (92%)	222 (96%)	9 (4%)	0	100	100
3	R	231/251 (92%)	222 (96%)	9 (4%)	0	100	100
All	All	8866/10698 (83%)	8277 (93%)	589 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	891/1115 (80%)	856 (96%)	35 (4%)	32	56
1	B	891/1115 (80%)	849 (95%)	42 (5%)	26	51
1	C	885/1115 (79%)	846 (96%)	39 (4%)	28	53
1	J	891/1115 (80%)	857 (96%)	34 (4%)	33	57
1	K	891/1115 (80%)	849 (95%)	42 (5%)	26	51
1	L	885/1115 (79%)	845 (96%)	40 (4%)	27	52
2	D	190/194 (98%)	171 (90%)	19 (10%)	7	26
2	F	190/194 (98%)	172 (90%)	18 (10%)	8	28
2	H	190/194 (98%)	172 (90%)	18 (10%)	8	28
2	M	190/194 (98%)	171 (90%)	19 (10%)	7	26
2	O	190/194 (98%)	172 (90%)	18 (10%)	8	28
2	Q	190/194 (98%)	171 (90%)	19 (10%)	7	26
3	E	192/197 (98%)	183 (95%)	9 (5%)	26	51
3	G	192/197 (98%)	183 (95%)	9 (5%)	26	51
3	I	192/197 (98%)	183 (95%)	9 (5%)	26	51
3	N	192/197 (98%)	183 (95%)	9 (5%)	26	51
3	P	192/197 (98%)	183 (95%)	9 (5%)	26	51
3	R	192/197 (98%)	183 (95%)	9 (5%)	26	51
All	All	7626/9036 (84%)	7229 (95%)	397 (5%)	27	48

All (397) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	79	PHE
1	A	88	ASP
1	A	105	ILE
1	A	131	CYS
1	A	135	PHE
1	A	173	GLN
1	A	194	ASN
1	A	287	ASP
1	A	291	CYS
1	A	336	CYS

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Mol	Chain	Res	Type
1	A	347	PHE
1	A	355	ARG
1	A	361	CYS
1	A	362	VAL
1	A	377	PHE
1	A	440	LYS
1	A	457	ARG
1	A	468	ILE
1	A	483	VAL
1	A	490	PHE
1	A	538	CYS
1	A	542	ASN
1	A	546	LEU
1	A	558	LYS
1	A	588	THR
1	A	732	THR
1	A	878	LEU
1	A	947	LYS
1	A	957	GLN
1	A	984	LEU
1	A	1010	GLN
1	A	1041	ASP
1	A	1086	LYS
1	A	1136	THR
1	B	33	THR
1	B	41	LYS
1	B	66	HIS
1	B	68	ILE
1	B	79	PHE
1	B	108	THR
1	B	118	LEU
1	B	168	PHE
1	B	170	TYR
1	B	173	GLN
1	B	181	GLN
1	B	195	ILE
1	B	206	THR
1	B	267	VAL
1	B	278	LYS
1	B	336	CYS
1	B	347	PHE
1	B	351	TYR

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Mol	Chain	Res	Type
1	B	355	ARG
1	B	361	CYS
1	B	362	VAL
1	B	377	PHE
1	B	440	LYS
1	B	457	ARG
1	B	468	ILE
1	B	483	VAL
1	B	490	PHE
1	B	535	LYS
1	B	542	ASN
1	B	546	LEU
1	B	558	LYS
1	B	564	GLN
1	B	584	ILE
1	B	856	LYS
1	B	886	TRP
1	B	888	PHE
1	B	957	GLN
1	B	997	ILE
1	B	1010	GLN
1	B	1041	ASP
1	B	1116	THR
1	B	1138	TYR
1	C	33	THR
1	C	41	LYS
1	C	66	HIS
1	C	68	ILE
1	C	92	PHE
1	C	108	THR
1	C	133	PHE
1	C	135	PHE
1	C	157	PHE
1	C	170	TYR
1	C	188	ARG
1	C	235	ILE
1	C	321	GLN
1	C	336	CYS
1	C	347	PHE
1	C	351	TYR
1	C	355	ARG
1	C	361	CYS

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Mol	Chain	Res	Type
1	C	362	VAL
1	C	377	PHE
1	C	440	LYS
1	C	457	ARG
1	C	468	ILE
1	C	483	VAL
1	C	490	PHE
1	C	528	LYS
1	C	538	CYS
1	C	847	ARG
1	C	856	LYS
1	C	873	TYR
1	C	888	PHE
1	C	901	GLN
1	C	979	ASP
1	C	985	ASP
1	C	990	GLU
1	C	993	ILE
1	C	1041	ASP
1	C	1081	ILE
1	C	1086	LYS
2	D	6	GLN
2	D	20	ILE
2	D	32	TYR
2	D	40	GLN
2	D	44	LYS
2	D	68	LYS
2	D	81	GLN
2	D	83	GLU
2	D	90	CYS
2	D	111	LEU
2	D	128	VAL
2	D	130	LEU
2	D	148	CYS
2	D	153	PHE
2	D	193	PHE
2	D	205	TYR
2	D	214	GLU
2	D	226	ILE
2	D	234	MET
3	E	19	THR
3	E	46	LYS

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Mol	Chain	Res	Type
3	E	67	LYS
3	E	100	PHE
3	E	106	LEU
3	E	125	GLU
3	E	143	ARG
3	E	151	PHE
3	E	210	LEU
2	F	6	GLN
2	F	20	ILE
2	F	40	GLN
2	F	44	LYS
2	F	68	LYS
2	F	81	GLN
2	F	83	GLU
2	F	90	CYS
2	F	111	LEU
2	F	128	VAL
2	F	130	LEU
2	F	148	CYS
2	F	153	PHE
2	F	193	PHE
2	F	205	TYR
2	F	214	GLU
2	F	226	ILE
2	F	234	MET
3	G	19	THR
3	G	46	LYS
3	G	67	LYS
3	G	100	PHE
3	G	106	LEU
3	G	125	GLU
3	G	143	ARG
3	G	151	PHE
3	G	210	LEU
2	H	6	GLN
2	H	20	ILE
2	H	32	TYR
2	H	40	GLN
2	H	44	LYS
2	H	68	LYS
2	H	81	GLN
2	H	83	GLU

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Mol	Chain	Res	Type
2	H	90	CYS
2	H	111	LEU
2	H	128	VAL
2	H	130	LEU
2	H	148	CYS
2	H	153	PHE
2	H	193	PHE
2	H	205	TYR
2	H	226	ILE
2	H	234	MET
3	I	19	THR
3	I	46	LYS
3	I	67	LYS
3	I	100	PHE
3	I	106	LEU
3	I	125	GLU
3	I	143	ARG
3	I	151	PHE
3	I	210	LEU
1	J	66	HIS
1	J	79	PHE
1	J	88	ASP
1	J	105	ILE
1	J	131	CYS
1	J	135	PHE
1	J	173	GLN
1	J	194	ASN
1	J	287	ASP
1	J	291	CYS
1	J	336	CYS
1	J	347	PHE
1	J	355	ARG
1	J	361	CYS
1	J	362	VAL
1	J	377	PHE
1	J	440	LYS
1	J	457	ARG
1	J	468	ILE
1	J	483	VAL
1	J	490	PHE
1	J	538	CYS
1	J	542	ASN

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Mol	Chain	Res	Type
1	J	546	LEU
1	J	558	LYS
1	J	588	THR
1	J	732	THR
1	J	878	LEU
1	J	947	LYS
1	J	957	GLN
1	J	1010	GLN
1	J	1041	ASP
1	J	1086	LYS
1	J	1136	THR
1	K	33	THR
1	K	41	LYS
1	K	66	HIS
1	K	68	ILE
1	K	79	PHE
1	K	108	THR
1	K	118	LEU
1	K	168	PHE
1	K	170	TYR
1	K	173	GLN
1	K	181	GLN
1	K	195	ILE
1	K	206	THR
1	K	267	VAL
1	K	278	LYS
1	K	336	CYS
1	K	347	PHE
1	K	351	TYR
1	K	355	ARG
1	K	361	CYS
1	K	362	VAL
1	K	377	PHE
1	K	440	LYS
1	K	457	ARG
1	K	468	ILE
1	K	483	VAL
1	K	490	PHE
1	K	535	LYS
1	K	542	ASN
1	K	546	LEU
1	K	558	LYS

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Mol	Chain	Res	Type
1	K	564	GLN
1	K	584	ILE
1	K	856	LYS
1	K	886	TRP
1	K	888	PHE
1	K	957	GLN
1	K	997	ILE
1	K	1010	GLN
1	K	1041	ASP
1	K	1116	THR
1	K	1138	TYR
1	L	33	THR
1	L	41	LYS
1	L	66	HIS
1	L	68	ILE
1	L	92	PHE
1	L	108	THR
1	L	133	PHE
1	L	135	PHE
1	L	157	PHE
1	L	170	TYR
1	L	177	MET
1	L	188	ARG
1	L	321	GLN
1	L	336	CYS
1	L	347	PHE
1	L	351	TYR
1	L	355	ARG
1	L	361	CYS
1	L	362	VAL
1	L	377	PHE
1	L	378	LYS
1	L	440	LYS
1	L	457	ARG
1	L	468	ILE
1	L	483	VAL
1	L	490	PHE
1	L	528	LYS
1	L	538	CYS
1	L	847	ARG
1	L	856	LYS
1	L	873	TYR

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Mol	Chain	Res	Type
1	L	888	PHE
1	L	901	GLN
1	L	979	ASP
1	L	985	ASP
1	L	990	GLU
1	L	993	ILE
1	L	1041	ASP
1	L	1081	ILE
1	L	1086	LYS
2	M	6	GLN
2	M	20	ILE
2	M	32	TYR
2	M	40	GLN
2	M	44	LYS
2	M	68	LYS
2	M	81	GLN
2	M	83	GLU
2	M	90	CYS
2	M	111	LEU
2	M	128	VAL
2	M	130	LEU
2	M	148	CYS
2	M	153	PHE
2	M	193	PHE
2	M	205	TYR
2	M	214	GLU
2	M	226	ILE
2	M	234	MET
3	N	19	THR
3	N	46	LYS
3	N	67	LYS
3	N	100	PHE
3	N	106	LEU
3	N	125	GLU
3	N	143	ARG
3	N	151	PHE
3	N	210	LEU
2	O	6	GLN
2	O	20	ILE
2	O	40	GLN
2	O	44	LYS
2	O	68	LYS

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Mol	Chain	Res	Type
2	O	81	GLN
2	O	83	GLU
2	O	90	CYS
2	O	108	VAL
2	O	111	LEU
2	O	128	VAL
2	O	130	LEU
2	O	148	CYS
2	O	153	PHE
2	O	193	PHE
2	O	205	TYR
2	O	226	ILE
2	O	234	MET
3	P	19	THR
3	P	46	LYS
3	P	67	LYS
3	P	100	PHE
3	P	106	LEU
3	P	125	GLU
3	P	143	ARG
3	P	151	PHE
3	P	210	LEU
2	Q	6	GLN
2	Q	20	ILE
2	Q	32	TYR
2	Q	40	GLN
2	Q	44	LYS
2	Q	68	LYS
2	Q	81	GLN
2	Q	83	GLU
2	Q	90	CYS
2	Q	111	LEU
2	Q	128	VAL
2	Q	130	LEU
2	Q	148	CYS
2	Q	153	PHE
2	Q	193	PHE
2	Q	205	TYR
2	Q	214	GLU
2	Q	226	ILE
2	Q	234	MET
3	R	19	THR

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Mol	Chain	Res	Type
3	R	46	LYS
3	R	67	LYS
3	R	100	PHE
3	R	106	LEU
3	R	125	GLU
3	R	143	ARG
3	R	151	PHE
3	R	210	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (249) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	87	ASN
1	A	173	GLN
1	A	354	ASN
1	A	370	ASN
1	A	388	ASN
1	A	409	GLN
1	A	448	ASN
1	A	540	ASN
1	A	563	GLN
1	A	564	GLN
1	A	613	GLN
1	A	690	GLN
1	A	762	GLN
1	A	784	GLN
1	A	853	GLN
1	A	901	GLN
1	A	965	GLN
1	A	1005	GLN
1	A	1011	GLN
1	A	1048	HIS
1	A	1125	ASN
1	B	121	ASN
1	B	173	GLN
1	B	181	GLN
1	B	186	ASN
1	B	234	ASN
1	B	245	HIS
1	B	354	ASN
1	B	370	ASN

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Mol	Chain	Res	Type
1	B	388	ASN
1	B	409	GLN
1	B	422	ASN
1	B	448	ASN
1	B	477	ASN
1	B	563	GLN
1	B	564	GLN
1	B	784	GLN
1	B	853	GLN
1	B	872	GLN
1	B	907	ASN
1	B	913	GLN
1	B	914	ASN
1	B	1005	GLN
1	B	1010	GLN
1	B	1011	GLN
1	B	1048	HIS
1	B	1125	ASN
1	C	164	ASN
1	C	218	GLN
1	C	321	GLN
1	C	334	ASN
1	C	354	ASN
1	C	370	ASN
1	C	388	ASN
1	C	409	GLN
1	C	448	ASN
1	C	477	ASN
1	C	540	ASN
1	C	580	GLN
1	C	784	GLN
1	C	853	GLN
1	C	895	GLN
1	C	913	GLN
1	C	914	ASN
1	C	1005	GLN
1	C	1011	GLN
1	C	1048	HIS
2	D	6	GLN
2	D	33	ASN
2	D	40	GLN
2	D	81	GLN

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Mol	Chain	Res	Type
2	D	129	GLN
2	D	165	GLN
2	D	202	ASN
2	D	207	GLN
2	D	209	ASN
3	E	6	GLN
3	E	16	GLN
3	E	52	ASN
3	E	80	GLN
3	E	97	ASN
3	E	127	GLN
3	E	137	GLN
3	E	159	HIS
3	E	201	ASN
3	E	206	GLN
3	E	233	ASN
2	F	6	GLN
2	F	33	ASN
2	F	40	GLN
2	F	81	GLN
2	F	129	GLN
2	F	165	GLN
2	F	202	ASN
2	F	207	GLN
2	F	209	ASN
3	G	16	GLN
3	G	52	ASN
3	G	80	GLN
3	G	97	ASN
3	G	127	GLN
3	G	137	GLN
3	G	159	HIS
3	G	201	ASN
3	G	206	GLN
3	G	233	ASN
2	H	33	ASN
2	H	40	GLN
2	H	81	GLN
2	H	129	GLN
2	H	165	GLN
2	H	202	ASN
2	H	207	GLN

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Mol	Chain	Res	Type
2	H	209	ASN
3	I	16	GLN
3	I	52	ASN
3	I	80	GLN
3	I	97	ASN
3	I	127	GLN
3	I	137	GLN
3	I	159	HIS
3	I	201	ASN
3	I	206	GLN
3	I	233	ASN
1	J	52	GLN
1	J	87	ASN
1	J	173	GLN
1	J	354	ASN
1	J	370	ASN
1	J	388	ASN
1	J	409	GLN
1	J	448	ASN
1	J	540	ASN
1	J	563	GLN
1	J	564	GLN
1	J	690	GLN
1	J	762	GLN
1	J	784	GLN
1	J	853	GLN
1	J	901	GLN
1	J	965	GLN
1	J	1005	GLN
1	J	1010	GLN
1	J	1011	GLN
1	J	1048	HIS
1	J	1125	ASN
1	K	121	ASN
1	K	165	ASN
1	K	173	GLN
1	K	181	GLN
1	K	186	ASN
1	K	234	ASN
1	K	245	HIS
1	K	354	ASN
1	K	370	ASN

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Mol	Chain	Res	Type
1	K	388	ASN
1	K	409	GLN
1	K	448	ASN
1	K	477	ASN
1	K	563	GLN
1	K	564	GLN
1	K	784	GLN
1	K	853	GLN
1	K	872	GLN
1	K	907	ASN
1	K	914	ASN
1	K	1005	GLN
1	K	1010	GLN
1	K	1011	GLN
1	K	1048	HIS
1	K	1125	ASN
1	L	164	ASN
1	L	218	GLN
1	L	321	GLN
1	L	334	ASN
1	L	354	ASN
1	L	370	ASN
1	L	388	ASN
1	L	409	GLN
1	L	448	ASN
1	L	477	ASN
1	L	540	ASN
1	L	580	GLN
1	L	784	GLN
1	L	853	GLN
1	L	895	GLN
1	L	913	GLN
1	L	914	ASN
1	L	1005	GLN
1	L	1011	GLN
1	L	1048	HIS
2	M	6	GLN
2	M	33	ASN
2	M	40	GLN
2	M	81	GLN
2	M	129	GLN
2	M	165	GLN

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Mol	Chain	Res	Type
2	M	202	ASN
2	M	207	GLN
2	M	209	ASN
3	N	6	GLN
3	N	16	GLN
3	N	52	ASN
3	N	80	GLN
3	N	97	ASN
3	N	127	GLN
3	N	137	GLN
3	N	159	HIS
3	N	201	ASN
3	N	206	GLN
3	N	233	ASN
2	O	6	GLN
2	O	33	ASN
2	O	40	GLN
2	O	81	GLN
2	O	129	GLN
2	O	165	GLN
2	O	202	ASN
2	O	207	GLN
2	O	209	ASN
3	P	16	GLN
3	P	52	ASN
3	P	80	GLN
3	P	97	ASN
3	P	127	GLN
3	P	137	GLN
3	P	159	HIS
3	P	201	ASN
3	P	206	GLN
3	P	233	ASN
2	Q	6	GLN
2	Q	33	ASN
2	Q	40	GLN
2	Q	81	GLN
2	Q	129	GLN
2	Q	165	GLN
2	Q	207	GLN
2	Q	209	ASN
3	R	16	GLN

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Mol	Chain	Res	Type
3	R	52	ASN
3	R	80	GLN
3	R	97	ASN
3	R	127	GLN
3	R	137	GLN
3	R	159	HIS
3	R	201	ASN
3	R	206	GLN
3	R	233	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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.

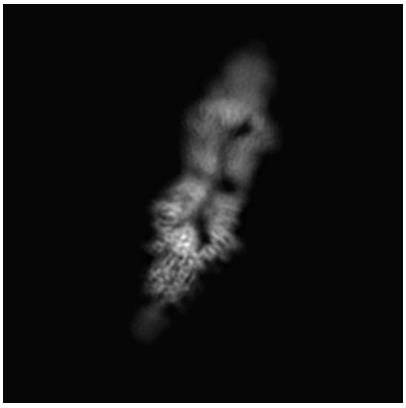
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32661. These allow visual inspection of the internal detail of the map and identification of artifacts.

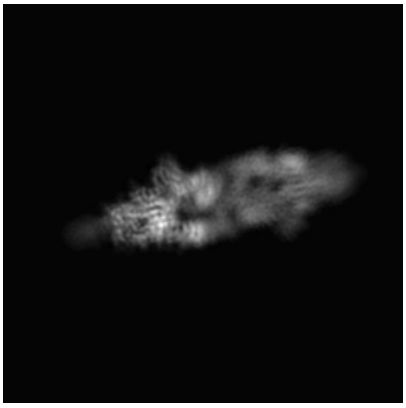
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

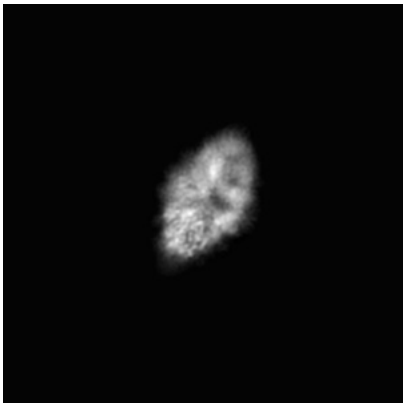
6.1.1 Primary map



X



Y



Z

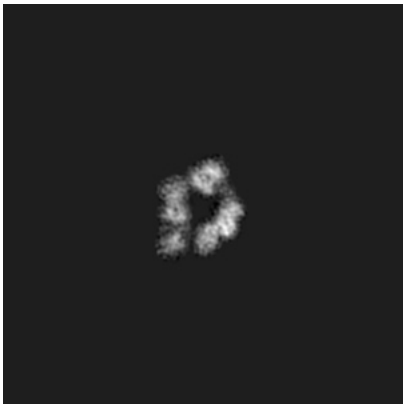
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

X Index: 270

Y Index: 270



Z Index: 270

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: 242

Y Index: 245

Z Index: 213

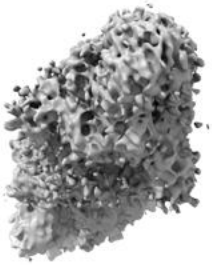
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

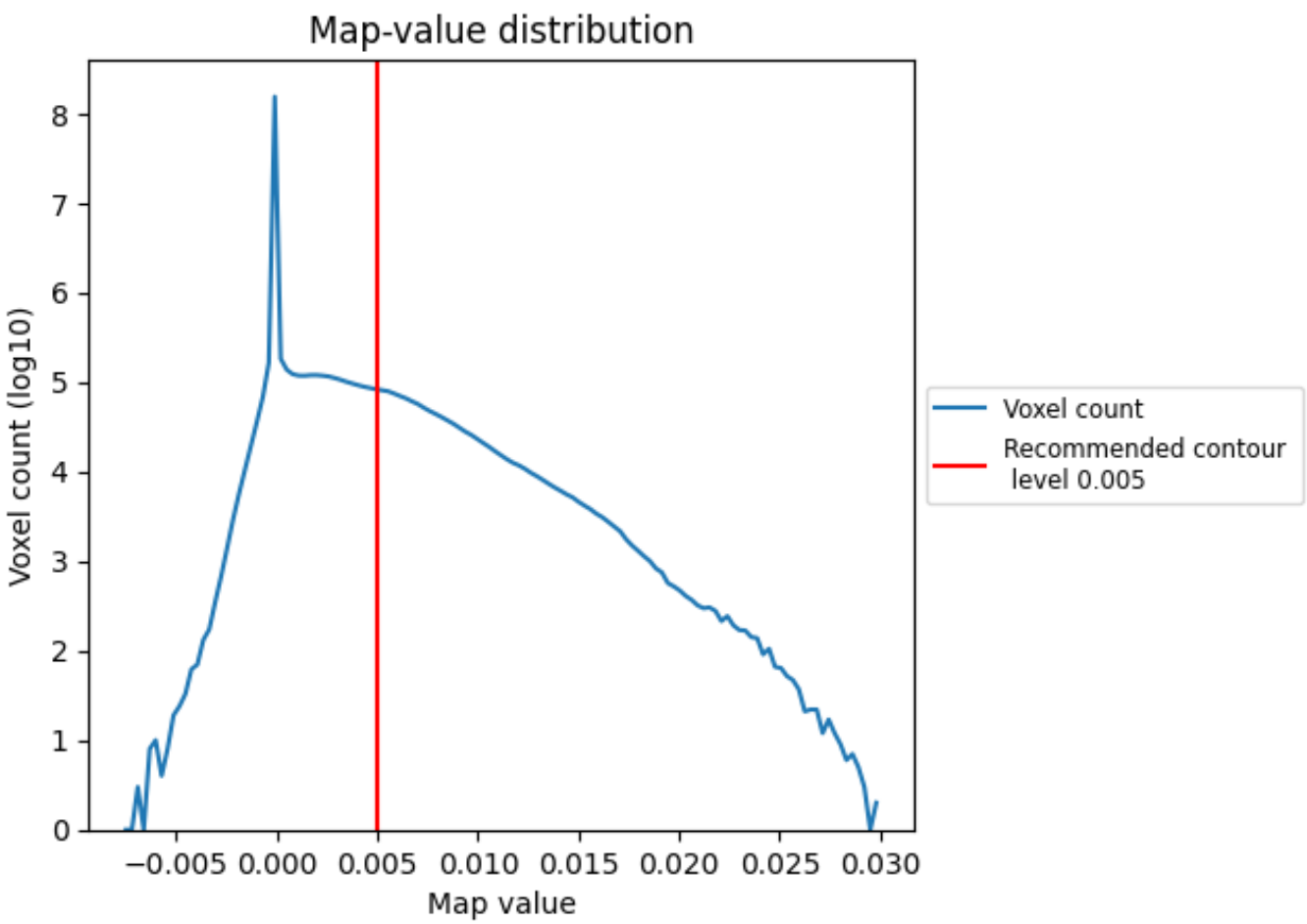
6.5 Mask visualisation (i)

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

7 Map analysis (i)

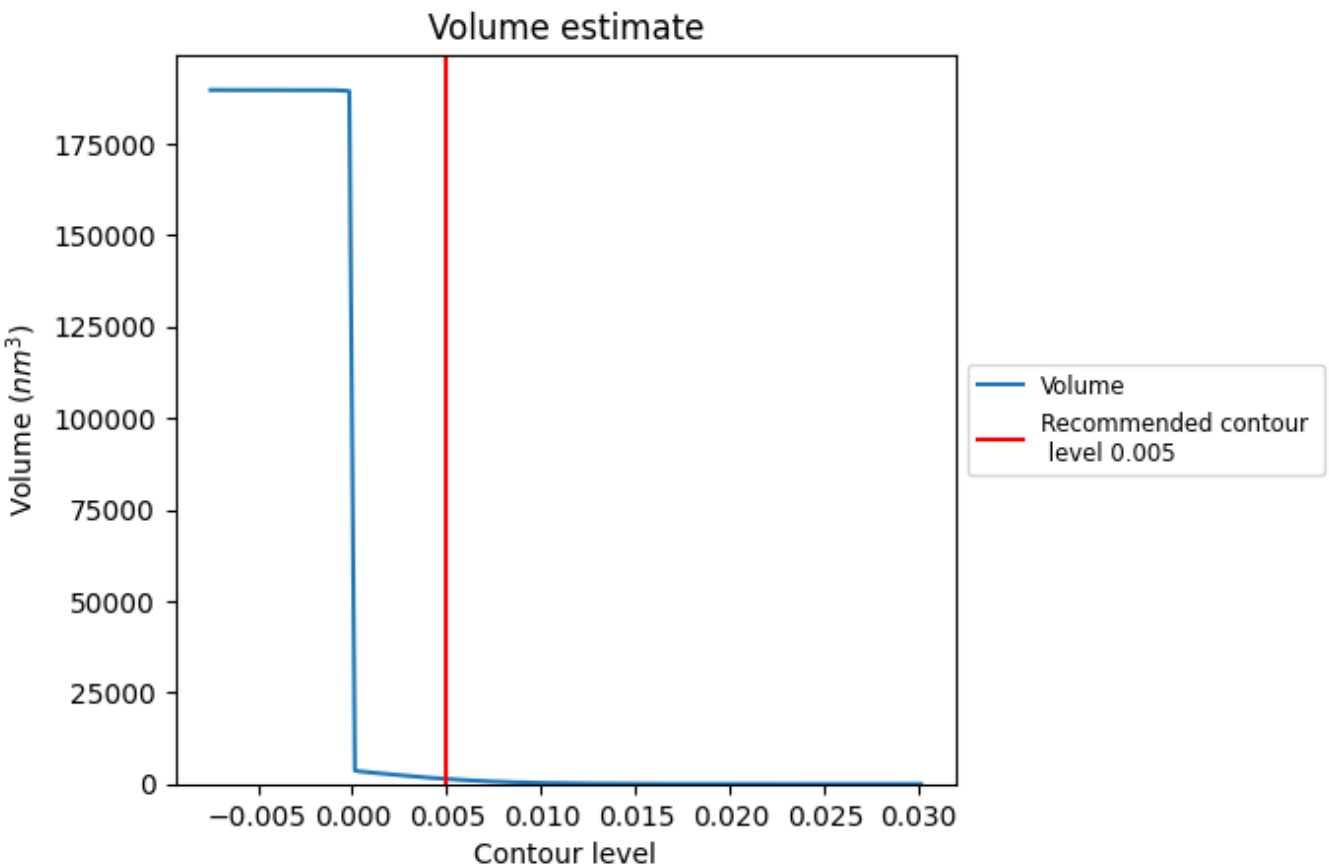
This section contains the results of statistical analysis of the map.

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.

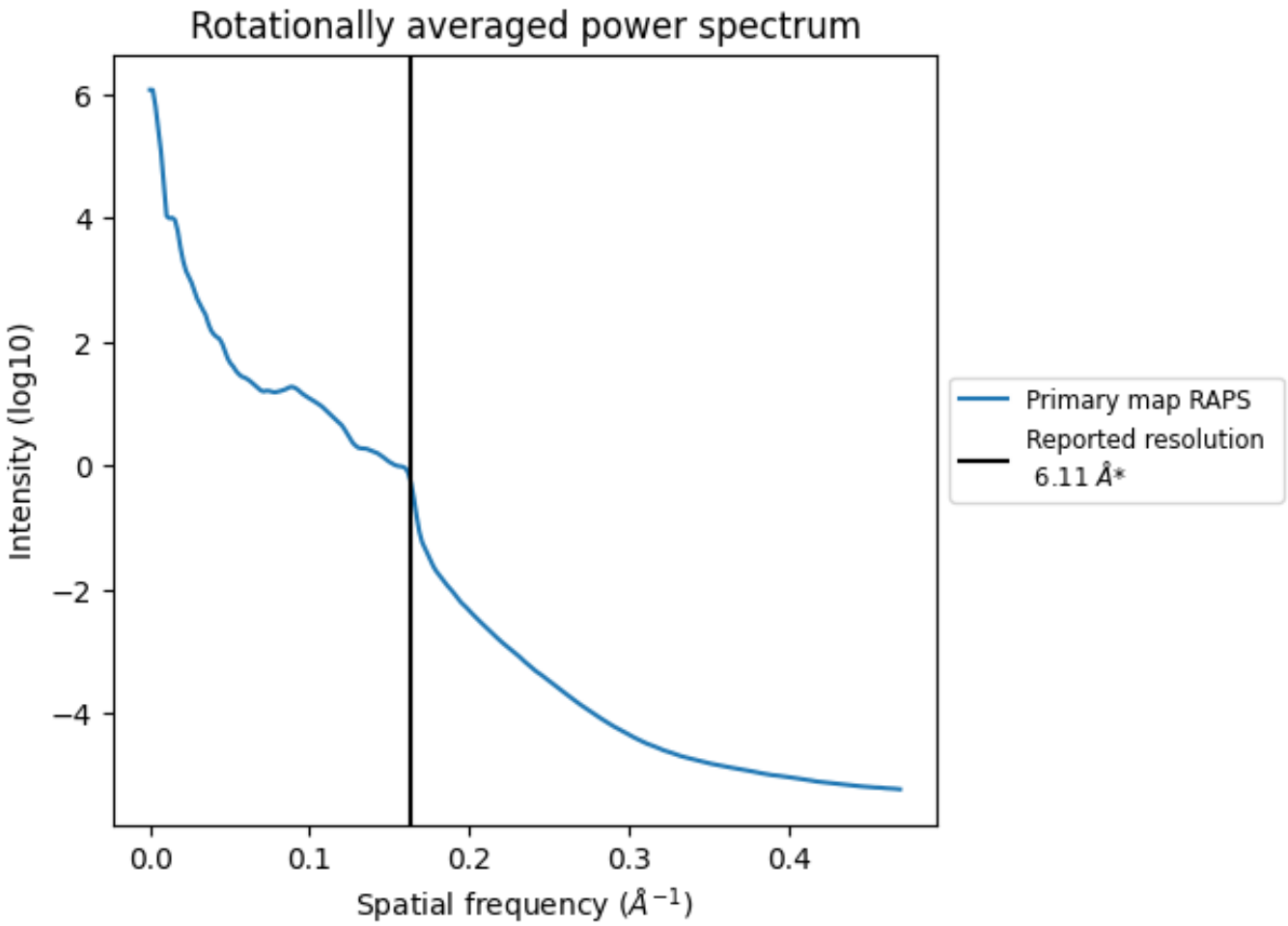
7.2 Volume estimate (i)



The volume at the recommended contour level is 1367 nm^3; this corresponds to an approximate mass of 1235 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 (i)



*Reported resolution corresponds to spatial frequency of 0.164 Å^{-1}

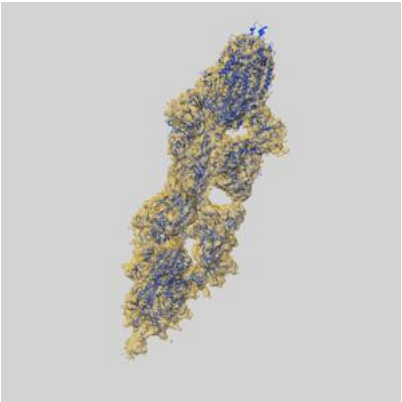
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

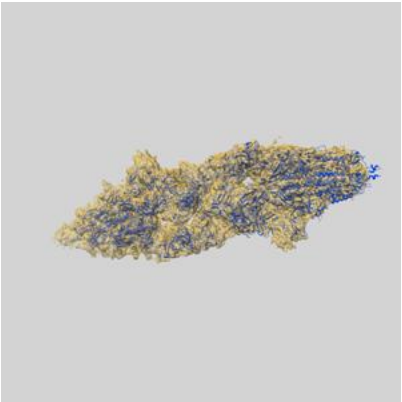
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32661 and PDB model 7WOW. Per-residue inclusion information can be found in section 3 on page 24.

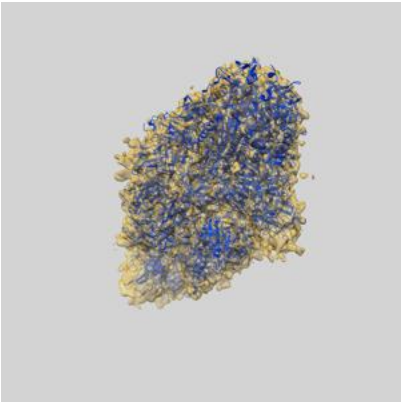
9.1 Map-model overlay (i)



X



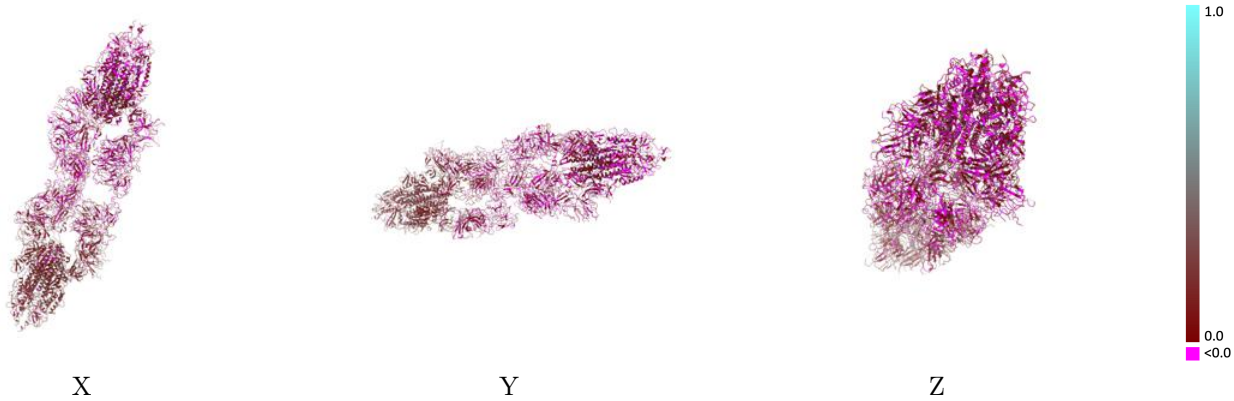
Y



Z

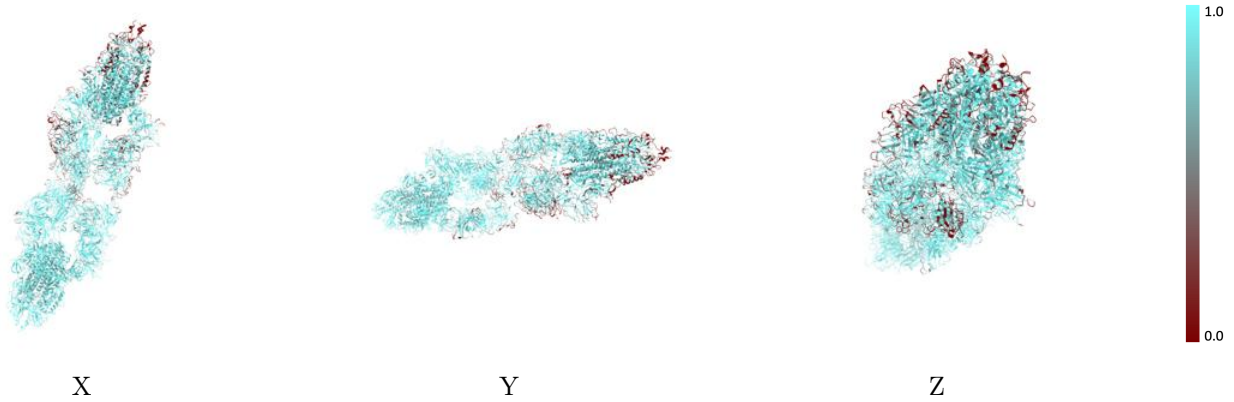
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



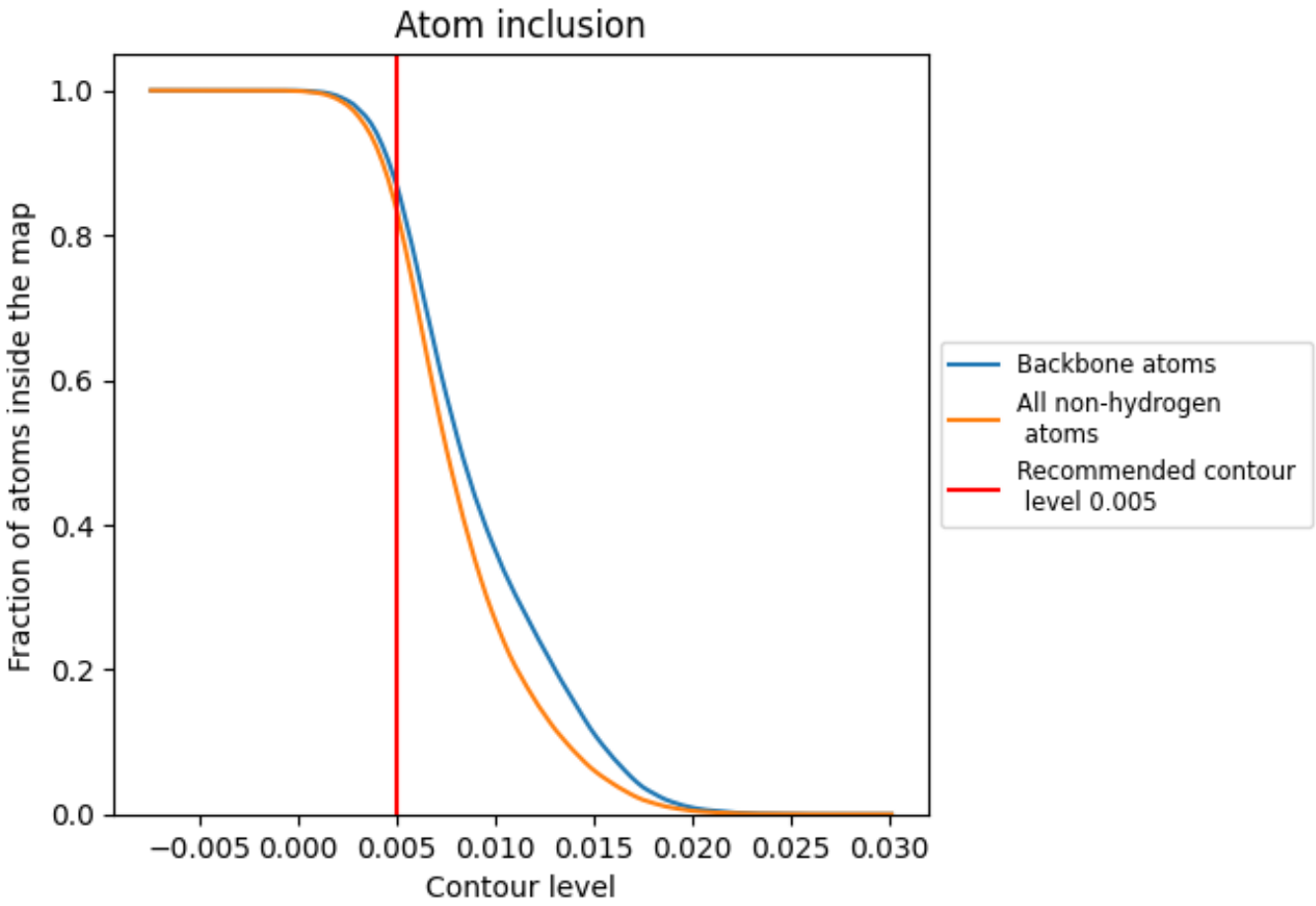
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8327	0.1020
A	0.9421	0.1740
B	0.9410	0.1790
C	0.9412	0.1740
D	0.7927	0.0530
E	0.7817	0.0710
F	0.9272	0.1030
G	0.9317	0.1190
H	0.9307	0.0890
I	0.9160	0.0970
J	0.7699	0.0590
K	0.7797	0.0620
L	0.7500	0.0650
M	0.6203	0.0250
N	0.4661	0.0190
O	0.8125	0.0560
P	0.7516	0.0440
Q	0.8340	0.0530
R	0.6410	0.0430