Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 07:41 AM EST

PDB ID	:	7S0D
EMDB ID	:	EMD-24787
Title	:	Structure of the SARS-CoV-2 S 6P trimer in complex with neutralizing antibody N-612-014
Authors	:	Barnes, C.O.; Bjorkman, P.J.
Deposited on	:	2021-08-30
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

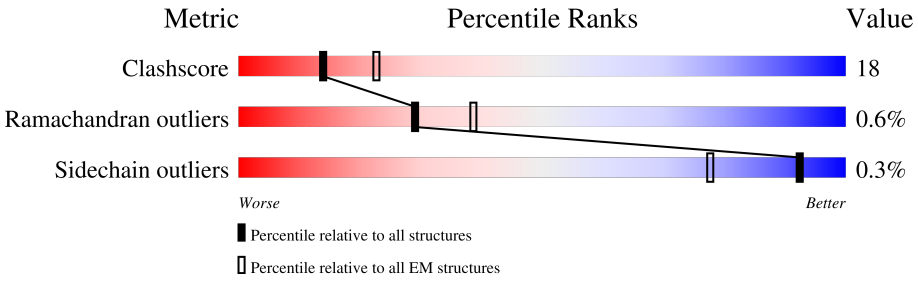
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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	1271	19% 53% 26% 20%
1	B	1271	9% 55% 26% 19%
1	C	1271	6% 55% 26% 19%
2	H	228	68% 61% 35%
2	M	228	81% 61% 34%
2	O	228	77% 57% 38%
3	L	214	89% 62% 37%
3	N	214	92% 61% 39%

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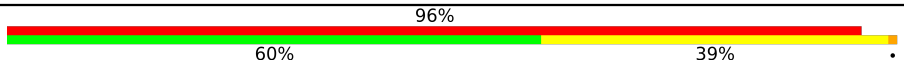
Mol	Chain	Length	Quality of chain
3	P	214	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 33623 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1013	Total	C	N	O	S	0	0
			7844	5018	1305	1485	36		
1	B	1033	Total	C	N	O	S	0	0
			7976	5097	1330	1512	37		
1	C	1026	Total	C	N	O	S	0	0
			7882	5039	1316	1490	37		

There are 213 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1270	ILE	-	expression tag	UNP P0DTC2
A	1271	GLU	-	expression tag	UNP P0DTC2
A	1272	TRP	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	GLU	-	expression tag	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	VAL	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	SER	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	ILE	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	PRO	-	expression tag	UNP P0DTC2
B	1233	ARG	-	expression tag	UNP P0DTC2
B	1234	ASP	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	GLN	-	expression tag	UNP P0DTC2
B	1237	ALA	-	expression tag	UNP P0DTC2
B	1238	TYR	-	expression tag	UNP P0DTC2
B	1239	VAL	-	expression tag	UNP P0DTC2
B	1240	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	GLU	-	expression tag	UNP P0DTC2
B	1245	TRP	-	expression tag	UNP P0DTC2
B	1246	VAL	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	THR	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	LEU	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	LEU	-	expression tag	UNP P0DTC2
B	1262	ASN	-	expression tag	UNP P0DTC2
B	1263	ASP	-	expression tag	UNP P0DTC2
B	1264	ILE	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	ALA	-	expression tag	UNP P0DTC2
B	1268	GLN	-	expression tag	UNP P0DTC2
B	1269	LYS	-	expression tag	UNP P0DTC2
B	1270	ILE	-	expression tag	UNP P0DTC2
B	1271	GLU	-	expression tag	UNP P0DTC2
B	1272	TRP	-	expression tag	UNP P0DTC2
B	1273	HIS	-	expression tag	UNP P0DTC2
B	1274	GLU	-	expression tag	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	VAL	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	SER	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	ILE	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	PRO	-	expression tag	UNP P0DTC2
C	1233	ARG	-	expression tag	UNP P0DTC2
C	1234	ASP	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	GLN	-	expression tag	UNP P0DTC2
C	1237	ALA	-	expression tag	UNP P0DTC2
C	1238	TYR	-	expression tag	UNP P0DTC2
C	1239	VAL	-	expression tag	UNP P0DTC2
C	1240	ARG	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	GLU	-	expression tag	UNP P0DTC2
C	1245	TRP	-	expression tag	UNP P0DTC2
C	1246	VAL	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	THR	-	expression tag	UNP P0DTC2
C	1251	PHE	-	expression tag	UNP P0DTC2
C	1252	LEU	-	expression tag	UNP P0DTC2
C	1253	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	LEU	-	expression tag	UNP P0DTC2
C	1262	ASN	-	expression tag	UNP P0DTC2
C	1263	ASP	-	expression tag	UNP P0DTC2
C	1264	ILE	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	ALA	-	expression tag	UNP P0DTC2
C	1268	GLN	-	expression tag	UNP P0DTC2
C	1269	LYS	-	expression tag	UNP P0DTC2
C	1270	ILE	-	expression tag	UNP P0DTC2
C	1271	GLU	-	expression tag	UNP P0DTC2
C	1272	TRP	-	expression tag	UNP P0DTC2
C	1273	HIS	-	expression tag	UNP P0DTC2
C	1274	GLU	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called N-612-014 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	223	Total	C	N	O	S	0	0
			1657	1046	279	326	6		
2	M	223	Total	C	N	O	S	0	0
			1657	1046	279	326	6		
2	O	223	Total	C	N	O	S	0	0
			1657	1046	279	326	6		

- Molecule 3 is a protein called N-612-014 Light Chain.

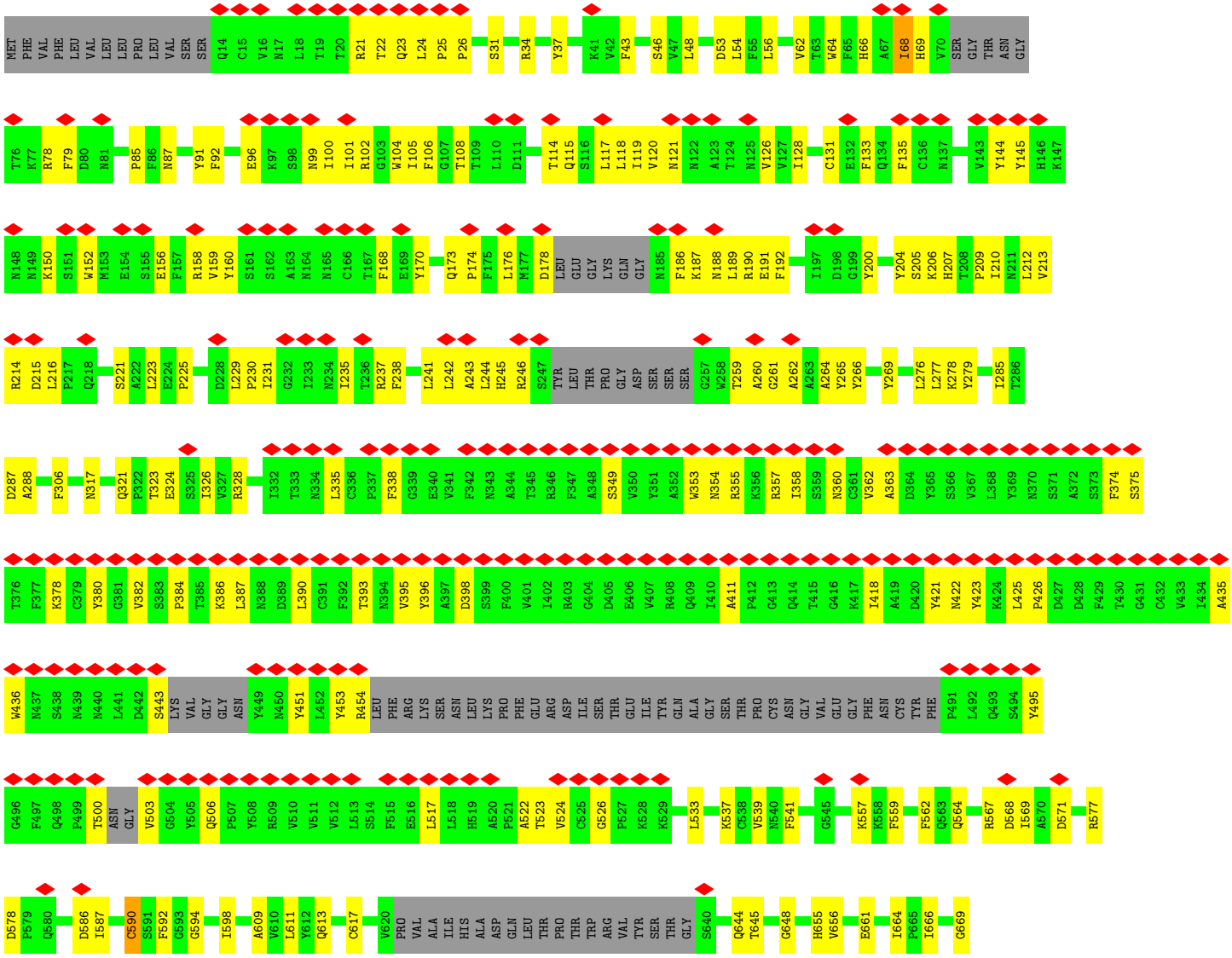
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	214	Total	C	N	O	S	1	0
			1650	1032	272	339	7		
3	N	214	Total	C	N	O	S	1	0
			1650	1032	272	339	7		
3	P	214	Total	C	N	O	S	1	0
			1650	1032	272	339	7		

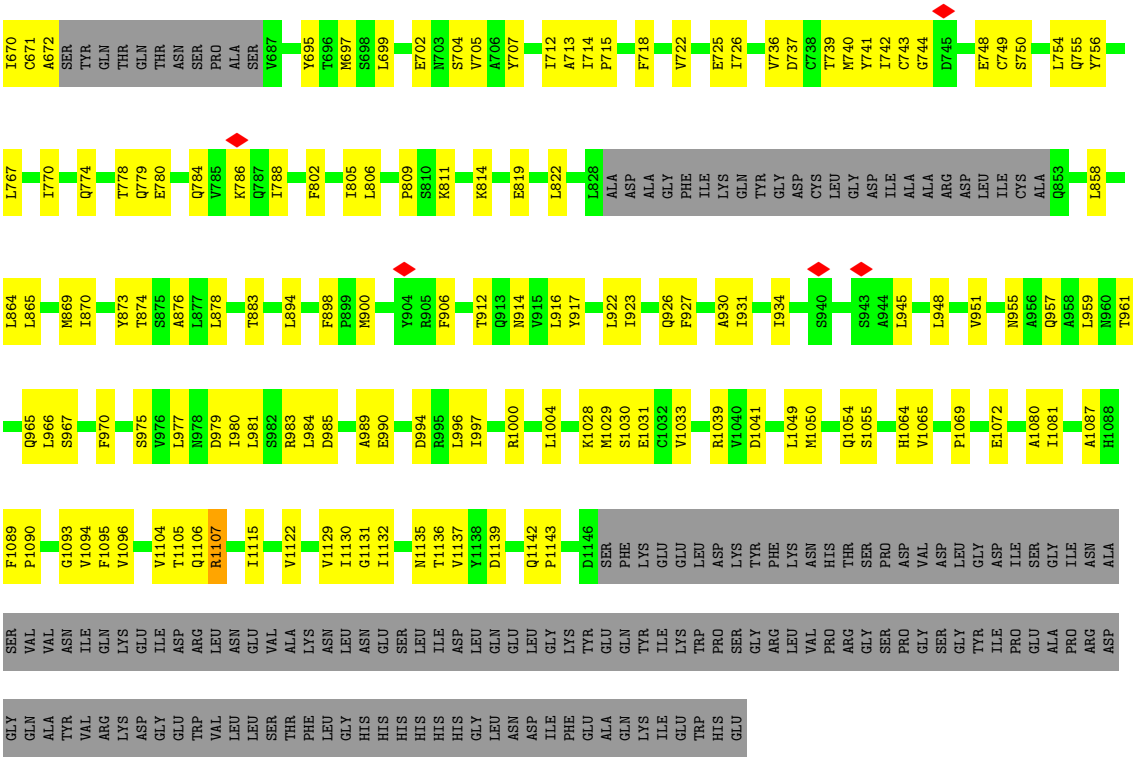
3 Residue-property plots (i)

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

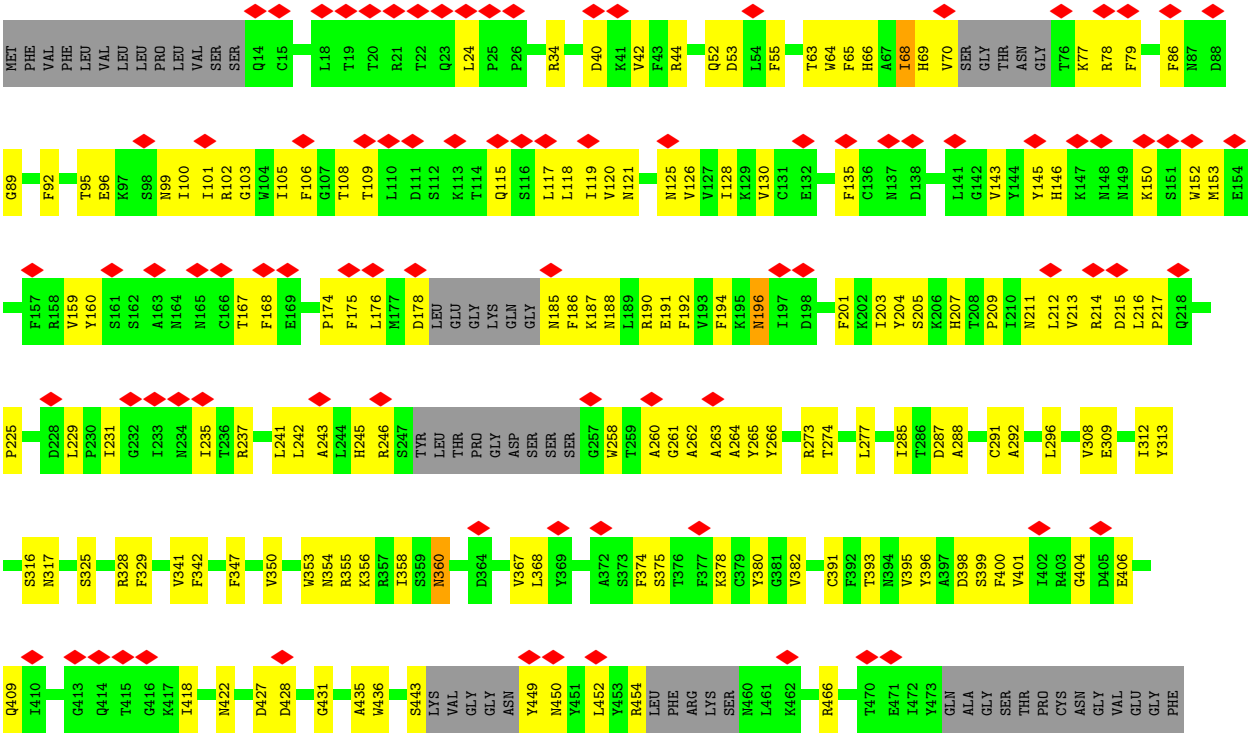
Chain A:

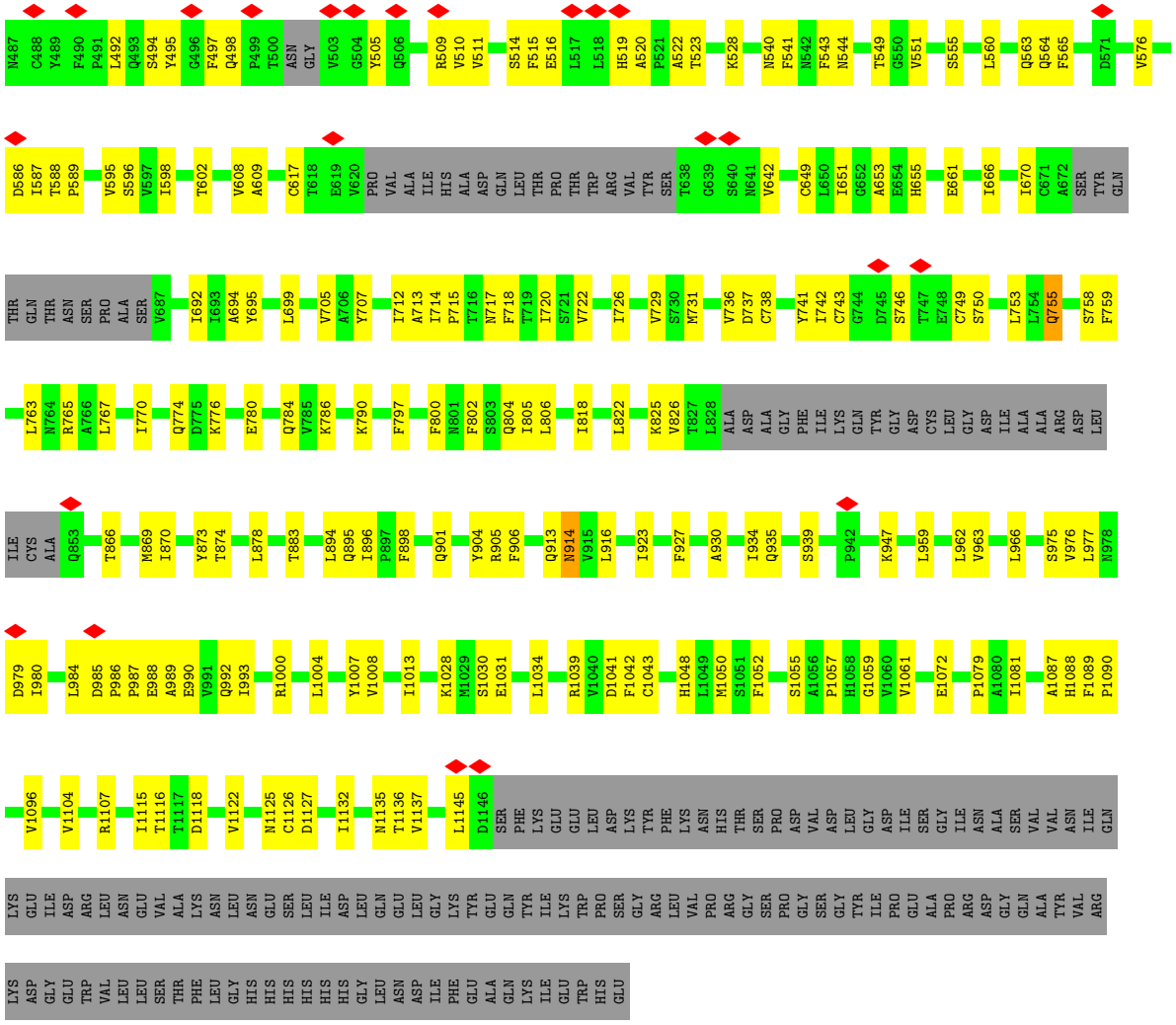




• Molecule 1: Spike glycoprotein

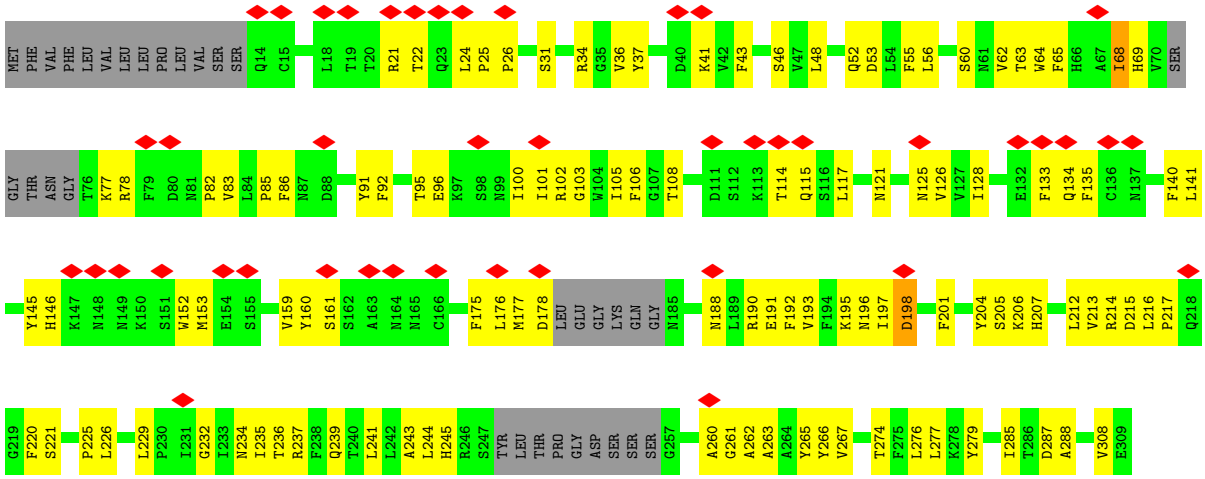
Chain B:

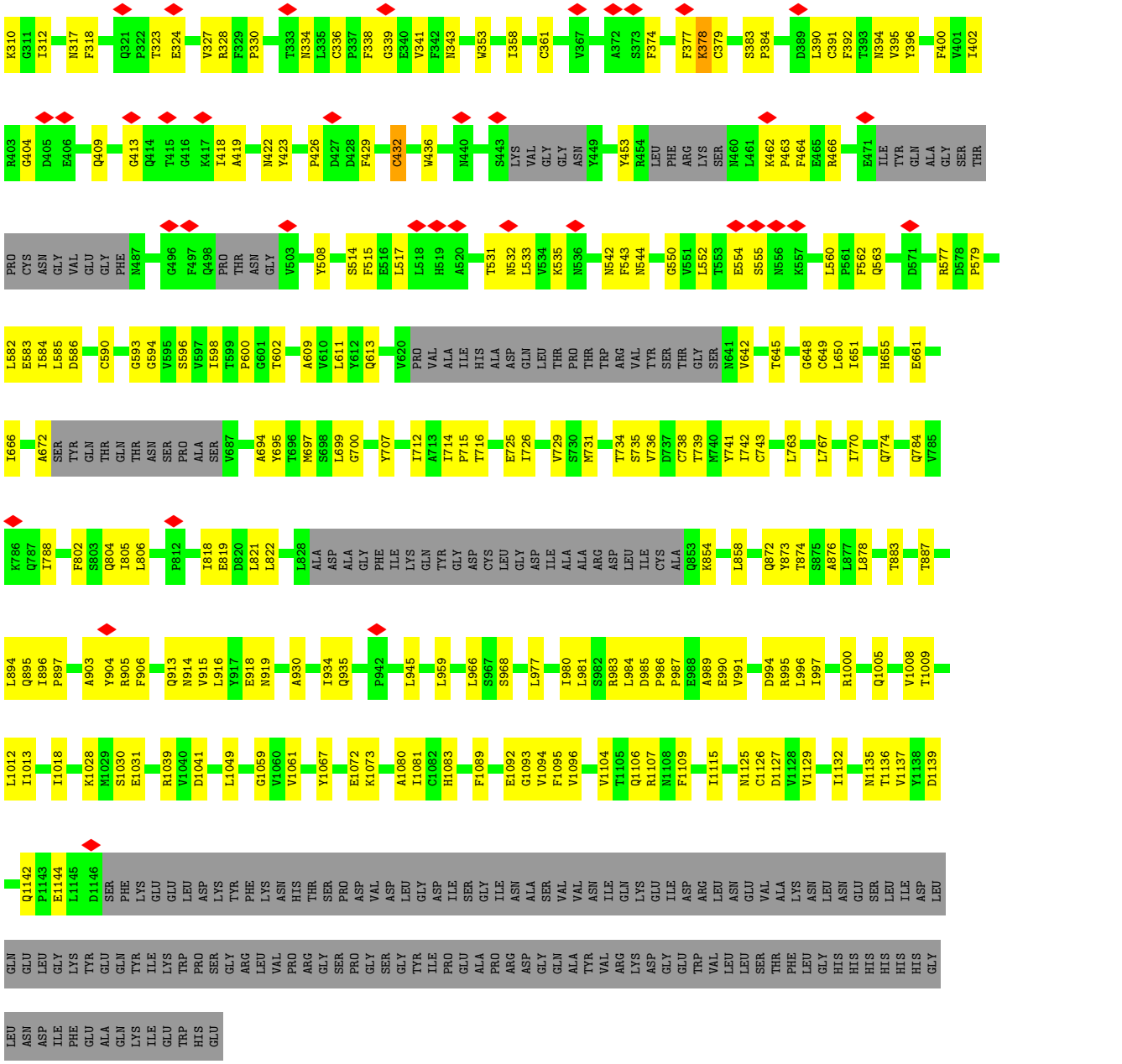




• Molecule 1: Spike glycoprotein

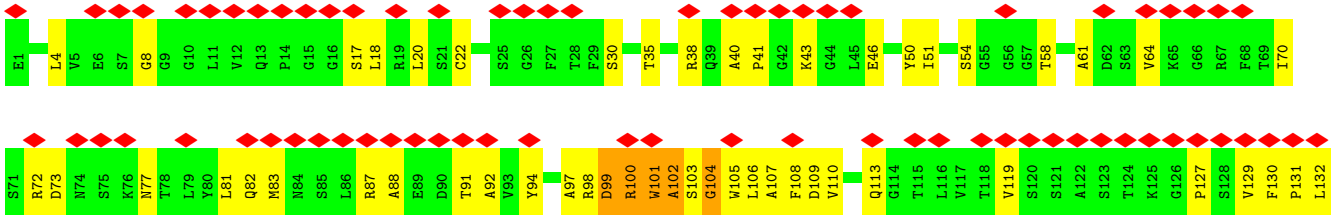
Chain C:

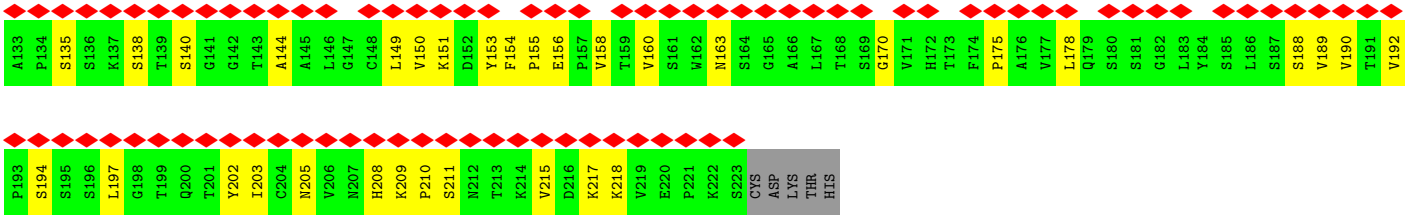




• Molecule 2: N-612-014 Fab Heavy Chain

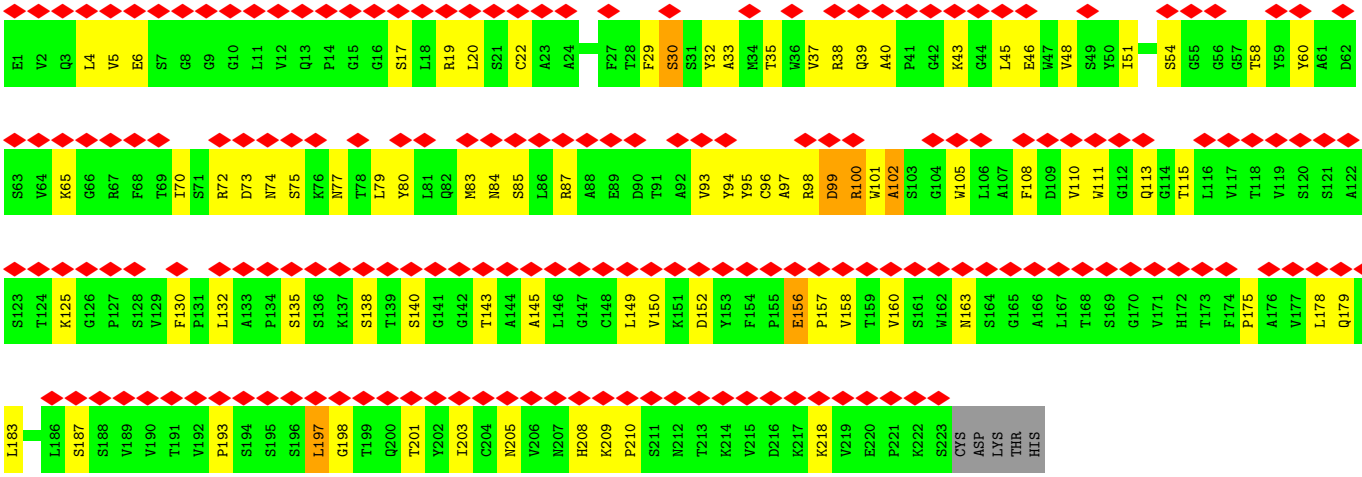
Chain H:





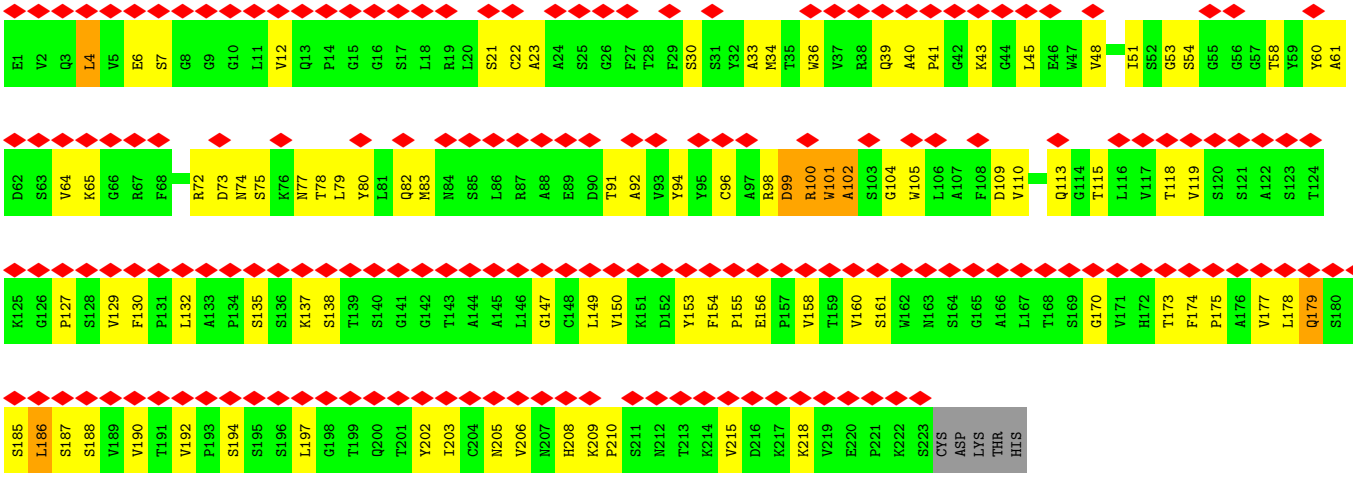
• Molecule 2: N-612-014 Fab Heavy Chain

Chain M:



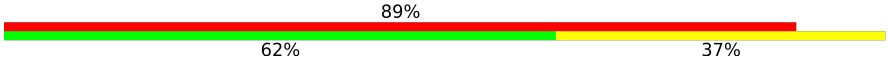
• Molecule 2: N-612-014 Fab Heavy Chain

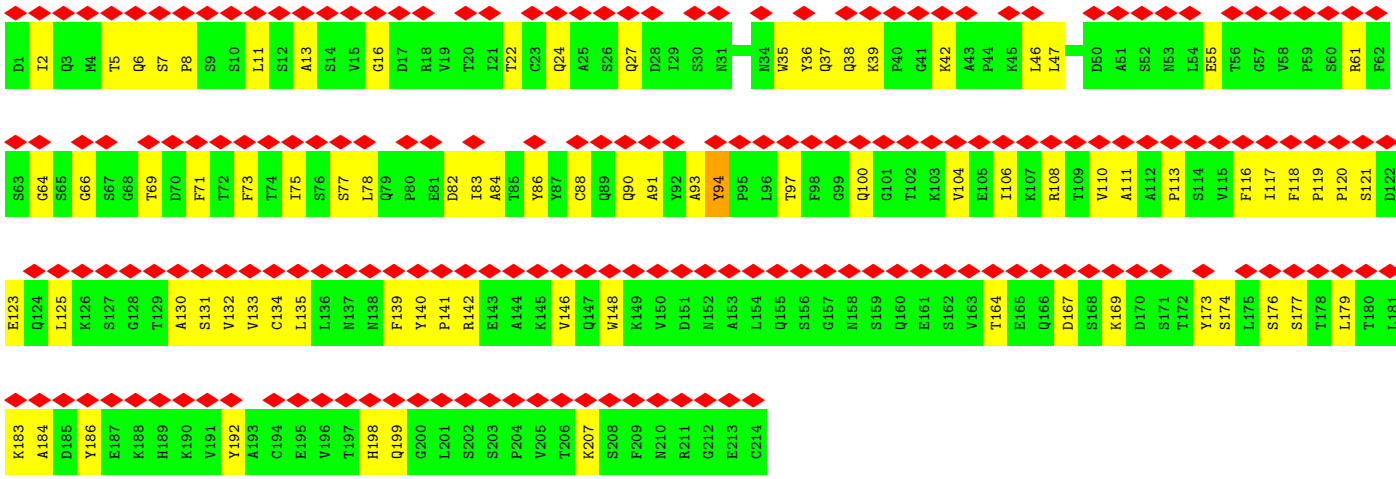
Chain O:



• Molecule 3: N-612-014 Light Chain

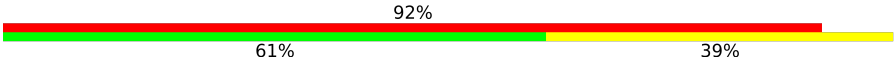
Chain L:

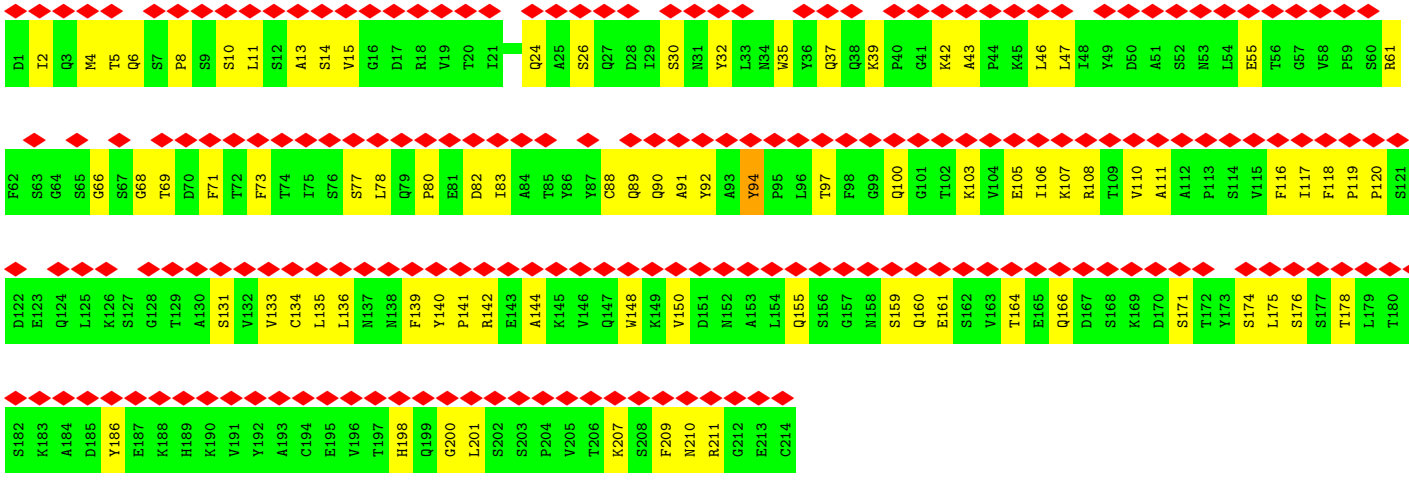




- Molecule 3: N-612-014 Light Chain

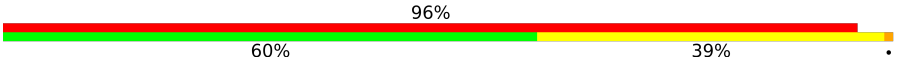
Chain N:

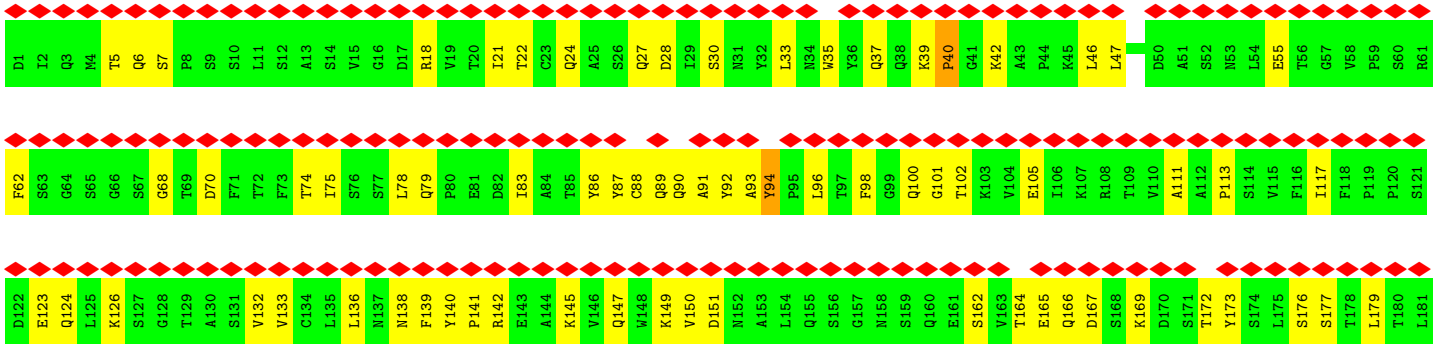


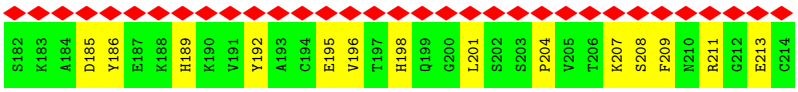


- Molecule 3: N-612-014 Light Chain

Chain P:






S182
K183
A184
D185
Y186
E187
K188
H189
K190
V191
Y192
A193
C194
E195
V196
T197
H198
Q199
G200
L201
S202
S203
P204
V205
T206
K207
S208
F209
N210
R211
G212
E213
C214

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	137684	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.795	Depositor
Minimum map value	-0.386	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	375.40802, 375.40802, 375.40802	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.869, 0.869, 0.869	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/8025	0.57	2/10937 (0.0%)
1	B	0.31	2/8157 (0.0%)	0.56	1/11113 (0.0%)
1	C	0.31	0/8060	0.57	3/10986 (0.0%)
2	H	0.29	0/1698	0.62	1/2313 (0.0%)
2	M	0.29	0/1698	0.64	2/2313 (0.1%)
2	O	0.30	0/1698	0.67	2/2313 (0.1%)
3	L	0.28	0/1688	0.58	0/2294
3	N	0.31	0/1688	0.63	1/2294 (0.0%)
3	P	0.35	1/1688 (0.1%)	0.69	3/2294 (0.1%)
All	All	0.31	3/34400 (0.0%)	0.59	15/46857 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	78	LEU	C-N	5.90	1.47	1.34
1	B	617	CYS	CB-SG	-5.35	1.73	1.81
1	B	649	CYS	CB-SG	-5.01	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	649	CYS	CA-CB-SG	14.04	139.26	114.00
3	P	40	PRO	CA-N-CD	-8.02	100.28	111.50
1	B	1079	PRO	CA-N-CD	-7.87	100.48	111.50
1	C	432	CYS	CA-CB-SG	7.80	128.04	114.00
2	M	197	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	590	CYS	CA-CB-SG	5.94	124.69	114.00
2	O	186	LEU	CA-CB-CG	5.89	128.85	115.30
1	C	198	ASP	CB-CG-OD1	5.76	123.48	118.30
2	M	156	GLU	C-N-CD	-5.60	108.28	120.60
2	H	101	TRP	CB-CA-C	5.36	121.12	110.40
2	O	4	LEU	CB-CG-CD1	-5.36	101.89	111.00
3	P	40	PRO	N-CD-CG	-5.32	95.22	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	80	PRO	CA-N-CD	-5.30	104.08	111.50
3	P	28	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	743	CYS	C-N-CA	-5.08	111.64	122.30

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	7844	0	7602	273	0
1	B	7976	0	7710	284	0
1	C	7882	0	7594	275	0
2	H	1657	0	1618	81	0
2	M	1657	0	1618	76	0
2	O	1657	0	1618	89	0
3	L	1650	0	1593	68	0
3	N	1650	0	1593	75	0
3	P	1650	0	1593	64	0
All	All	33623	0	32539	1166	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 18.

All (1166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:203:ILE:CG1	2:O:218:LYS:HG2	1.56	1.32
2:H:203:ILE:HG12	2:H:218:LYS:CG	1.76	1.15
2:H:203:ILE:CG1	2:H:218:LYS:HG2	1.75	1.14
2:M:203:ILE:HG12	2:M:218:LYS:HG2	1.16	1.08
2:M:203:ILE:CG1	2:M:218:LYS:HG2	1.92	1.00
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.41	0.99
2:O:203:ILE:CG1	2:O:218:LYS:CG	2.42	0.97
2:O:203:ILE:HG13	2:O:218:LYS:CG	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:203:ILE:HG13	2:O:218:LYS:HG2	0.97	0.96
2:M:35:THR:OG1	2:M:97:ALA:HB3	1.67	0.95
1:A:212:LEU:HD22	1:A:215:ASP:H	1.33	0.94
2:H:87:ARG:HD2	2:H:88:ALA:H	1.33	0.91
2:O:160:VAL:HB	2:O:188:SER:HB3	1.54	0.90
1:A:245:HIS:HB2	1:A:260:ALA:HB3	1.54	0.90
1:A:200:TYR:OH	1:C:394:ASN:ND2	2.06	0.88
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.53	0.88
2:O:22:CYS:HB3	2:O:79:LEU:HB3	1.54	0.87
1:A:101:ILE:O	1:A:190:ARG:NH2	2.07	0.86
2:O:203:ILE:HG12	2:O:218:LYS:HG2	1.55	0.86
2:H:100:ARG:HG3	2:H:101:TRP:HD1	1.40	0.85
2:O:98:ARG:HG2	2:O:99:ASP:H	1.41	0.85
1:A:21:ARG:NH1	1:A:22:THR:O	2.09	0.85
3:N:140:TYR:O	3:N:198:HIS:NE2	2.12	0.83
2:O:203:ILE:HG12	2:O:218:LYS:CG	2.07	0.82
1:A:214:ARG:O	1:A:266:TYR:OH	1.97	0.81
1:C:245:HIS:HB2	1:C:260:ALA:HB3	1.63	0.81
3:L:113:PRO:HB3	3:L:139:PHE:HB3	1.62	0.80
3:N:78:LEU:HD21	3:N:106:ILE:HG12	1.63	0.80
3:P:113:PRO:HB3	3:P:139:PHE:HB3	1.65	0.79
3:P:105:GLU:HB3	3:P:142:ARG:HH12	1.47	0.79
1:C:358:ILE:HB	1:C:395:VAL:HB	1.63	0.78
1:A:189:LEU:HB2	1:A:210:ILE:HD13	1.64	0.78
1:A:755:GLN:O	1:C:968:SER:OG	2.02	0.78
1:C:742:ILE:HA	1:C:1000:ARG:HD2	1.66	0.78
2:O:135:SER:HB3	2:O:138:SER:HB2	1.66	0.78
3:P:83:ILE:HG21	3:P:166:GLN:HE22	1.47	0.77
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.48	0.77
1:A:611:LEU:HD11	1:A:666:ILE:HG23	1.66	0.77
1:A:858:LEU:HD21	1:A:959:LEU:HD22	1.65	0.77
2:M:152:ASP:OD1	2:M:179:GLN:NE2	2.17	0.77
2:H:98:ARG:HG2	2:H:99:ASP:H	1.49	0.77
1:B:866:THR:H	1:B:869:MET:HE2	1.49	0.77
2:H:132:LEU:HD22	3:L:118:PHE:HB3	1.65	0.77
2:O:36:TRP:HZ3	2:O:96:CYS:HB3	1.49	0.76
1:C:379:CYS:HA	1:C:432:CYS:CB	2.15	0.76
1:A:317:ASN:ND2	1:B:737:ASP:OD2	2.20	0.75
2:O:4:LEU:HD11	2:O:22:CYS:SG	2.26	0.75
1:B:130:VAL:HG21	1:B:231:ILE:HD12	1.69	0.75
1:B:245:HIS:NE2	2:O:53:GLY:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:HIS:HB3	1:B:260:ALA:HB3	1.69	0.74
1:B:966:LEU:O	1:B:975:SER:OG	2.04	0.73
2:H:135:SER:HB3	2:H:138:SER:HB2	1.69	0.73
1:A:131:CYS:HB2	1:A:133:PHE:CE1	2.23	0.73
1:C:736:VAL:HG22	1:C:858:LEU:HD23	1.71	0.73
3:P:5:THR:HB	3:P:24:GLN:HB2	1.69	0.73
1:A:355:ARG:NH2	1:A:423:TYR:OH	2.21	0.73
2:O:100:ARG:HH21	2:O:101:TRP:HE1	1.36	0.73
1:B:1030:SER:HA	1:B:1034:LEU:HD12	1.71	0.73
1:A:740:MET:SD	1:C:317:ASN:ND2	2.62	0.72
1:A:983:ARG:HH11	1:C:517:LEU:HD22	1.55	0.72
2:O:60:TYR:HB2	2:O:65:LYS:HD2	1.68	0.72
1:C:214:ARG:HD2	2:H:105:TRP:CD1	2.25	0.72
1:B:69:HIS:CD2	1:B:70:VAL:HG12	2.25	0.71
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.73	0.71
1:B:382:VAL:HG12	1:C:983:ARG:HB2	1.72	0.71
3:L:39:LYS:HD2	3:L:84:ALA:HB2	1.72	0.71
1:C:68:ILE:HD11	2:H:101:TRP:HB2	1.71	0.70
3:N:120:PRO:O	3:N:211:ARG:NH2	2.25	0.70
1:A:739:THR:O	1:A:744:GLY:N	2.25	0.69
2:H:100:ARG:HG3	2:H:101:TRP:CD1	2.27	0.69
3:P:151:ASP:OD2	3:P:189:HIS:ND1	2.20	0.69
2:O:92:ALA:HB3	2:O:94:TYR:HE1	1.57	0.69
1:B:214:ARG:HG3	2:O:104:GLY:HA2	1.74	0.69
3:L:5:THR:HB	3:L:24:GLN:HB2	1.75	0.68
1:A:119:ILE:HG13	1:A:128:ILE:HG12	1.74	0.68
1:B:977:LEU:HD11	1:B:1000:ARG:HH12	1.59	0.68
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.27	0.68
1:B:68:ILE:HG13	1:B:69:HIS:H	1.59	0.68
2:H:35:THR:OG1	2:H:97:ALA:HB3	1.94	0.68
1:A:425:LEU:HD12	1:A:426:PRO:HD2	1.76	0.68
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.74	0.68
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.75	0.67
1:A:1089:PHE:HE2	1:B:914:ASN:HA	1.58	0.67
1:B:287:ASP:OD1	1:B:288:ALA:N	2.26	0.67
3:N:106:ILE:H	3:N:142:ARG:HH12	1.40	0.67
1:B:452:LEU:HD12	1:B:492:LEU:HG	1.76	0.67
1:B:722:VAL:HG22	1:B:930:ALA:HB1	1.77	0.67
1:B:1088:HIS:HD2	1:B:1137:VAL:HG21	1.59	0.67
1:C:788:ILE:HG23	1:C:876:ALA:HB2	1.76	0.67
2:M:135:SER:HB3	2:M:138:SER:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:149:LEU:HD13	2:M:187:SER:HB3	1.76	0.67
2:O:22:CYS:SG	2:O:34:MET:HE1	2.35	0.67
2:O:130:PHE:N	2:O:149:LEU:O	2.27	0.67
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.76	0.66
1:A:894:LEU:HD21	1:C:715:PRO:HD3	1.78	0.66
2:M:98:ARG:HG2	2:M:99:ASP:H	1.61	0.66
2:M:203:ILE:CD1	2:M:218:LYS:HG2	2.25	0.66
1:A:214:ARG:HD3	2:M:105:TRP:CZ3	2.31	0.66
2:H:150:VAL:HG21	2:H:158:VAL:HG21	1.75	0.66
2:H:192:VAL:HG21	2:H:202:TYR:HE2	1.61	0.66
3:L:61:ARG:NH2	3:L:82:ASP:OD2	2.29	0.66
2:H:208:HIS:HD1	2:H:211:SER:HG	1.42	0.66
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.76	0.66
3:P:18:ARG:HD2	3:P:74:THR:HB	1.77	0.66
1:B:68:ILE:HD11	2:O:101:TRP:HB2	1.78	0.66
1:B:1090:PRO:HD2	1:C:913:GLN:HE22	1.60	0.66
1:C:135:PHE:HA	1:C:160:TYR:HA	1.77	0.65
1:B:642:VAL:HG12	1:B:651:ILE:HG12	1.78	0.65
2:H:153:TYR:HE2	2:H:156:GLU:HA	1.61	0.65
1:C:328:ARG:HD3	1:C:543:PHE:HE1	1.60	0.65
2:M:4:LEU:HD12	2:M:110:VAL:HG11	1.79	0.65
2:M:40:ALA:HB3	2:M:43:LYS:HB2	1.79	0.65
1:A:523:THR:HG23	1:A:524:VAL:HG13	1.77	0.65
1:B:214:ARG:NH2	1:B:266:TYR:OH	2.30	0.65
1:C:323:THR:OG1	1:C:324:GLU:OE1	2.15	0.65
2:H:98:ARG:HB2	2:H:110:VAL:HG12	1.79	0.65
2:O:7:SER:OG	2:O:21:SER:OG	2.13	0.65
2:M:19:ARG:HH21	2:M:80:TYR:HD2	1.45	0.65
3:N:161:GLU:HG2	3:N:175:LEU:HD21	1.77	0.64
2:O:41:PRO:HD3	2:O:92:ALA:HA	1.77	0.64
3:P:21:ILE:HD12	3:P:102:THR:HG21	1.79	0.64
1:C:712:ILE:HG21	1:C:1096:VAL:HG12	1.78	0.64
3:L:198:HIS:HD2	3:L:199:GLN:H	1.44	0.64
1:A:213:VAL:HG11	2:M:105:TRP:HA	1.78	0.64
1:A:335:LEU:HD13	1:A:362:VAL:HG23	1.80	0.64
1:B:1104:VAL:HG23	1:B:1115:ILE:HG13	1.77	0.64
1:A:1039:ARG:NE	1:B:1031:GLU:OE1	2.30	0.64
2:O:23:ALA:HA	2:O:78:THR:HG22	1.79	0.64
2:O:178:LEU:HD12	2:O:179:GLN:H	1.61	0.64
3:P:111:ALA:H	3:P:140:TYR:HB3	1.63	0.64
1:B:108:THR:O	1:B:237:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:HG12	1:B:152:TRP:HE3	1.63	0.64
2:H:149:LEU:HD21	2:H:151:LYS:HE3	1.80	0.64
1:B:308:VAL:HG22	1:B:602:THR:HG23	1.80	0.64
1:A:957:GLN:HE22	1:B:765:ARG:NH1	1.96	0.64
1:B:96:GLU:OE1	1:B:190:ARG:NH1	2.30	0.64
2:O:51:ILE:HA	2:O:58:THR:HG22	1.79	0.64
1:C:64:TRP:CD1	1:C:266:TYR:HE1	2.16	0.63
3:N:6:GLN:O	3:N:100:GLN:NE2	2.31	0.63
1:B:707:TYR:HB2	1:C:883:THR:HG23	1.79	0.63
1:C:327:VAL:HG12	1:C:542:ASN:HB3	1.79	0.63
1:A:749:CYS:HB2	1:A:997:ILE:HD11	1.79	0.63
1:B:1087:ALA:O	1:B:1088:HIS:ND1	2.31	0.63
2:H:61:ALA:HB3	2:H:64:VAL:HG12	1.79	0.63
1:B:186:PHE:HD2	1:B:209:PRO:HB2	1.62	0.63
2:H:203:ILE:HG12	2:H:218:LYS:HG2	0.82	0.63
1:A:145:TYR:HB2	1:A:152:TRP:CE2	2.34	0.63
1:A:786:LYS:HE3	1:A:786:LYS:HA	1.81	0.63
1:C:92:PHE:CE1	1:C:265:TYR:HB2	2.33	0.63
1:C:83:VAL:HG11	1:C:237:ARG:HH12	1.64	0.63
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.81	0.62
1:C:68:ILE:HG13	1:C:69:HIS:H	1.65	0.62
2:O:149:LEU:HG	2:O:187:SER:HB3	1.81	0.62
2:O:192:VAL:HG21	2:O:202:TYR:HE2	1.63	0.62
1:C:802:PHE:HB3	1:C:806:LEU:HD23	1.81	0.62
1:B:109:THR:HA	1:B:237:ARG:HH22	1.64	0.62
1:C:96:GLU:OE1	1:C:190:ARG:NH1	2.31	0.62
1:C:731:MET:HE3	1:C:1018:ILE:HG13	1.82	0.62
2:M:51:ILE:HA	2:M:58:THR:HG22	1.80	0.62
2:M:51:ILE:HG12	2:M:72:ARG:HH21	1.64	0.62
1:B:699:LEU:CB	1:C:788:ILE:HD11	2.30	0.62
1:C:65:PHE:HE1	1:C:82:PRO:HG3	1.65	0.62
3:P:79:GLN:OE1	3:P:79:GLN:N	2.33	0.62
3:P:117:ILE:HB	3:P:207:LYS:HE2	1.82	0.62
1:A:1104:VAL:HG23	1:A:1115:ILE:HG13	1.81	0.62
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.82	0.62
3:L:2:ILE:H	3:L:97:THR:HG22	1.65	0.62
1:A:914:ASN:HA	1:C:1089:PHE:HE2	1.65	0.62
1:B:34:ARG:NE	1:B:191:GLU:OE2	2.32	0.62
3:P:123:GLU:HA	3:P:126:LYS:HE3	1.82	0.62
1:C:1094:VAL:HG13	1:C:1107:ARG:HG2	1.82	0.61
3:P:40:PRO:HD2	3:P:40:PRO:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:160:VAL:HG22	2:O:206:VAL:HG22	1.83	0.61
1:A:715:PRO:HG3	1:A:1069:PRO:HB3	1.82	0.61
1:A:809:PRO:O	1:A:814:LYS:NZ	2.31	0.61
1:B:146:HIS:HB2	1:B:153:MET:HE1	1.83	0.61
1:C:400:PHE:CE2	1:C:402:ILE:HD11	2.36	0.61
2:H:203:ILE:HD11	2:H:218:LYS:HD2	1.82	0.61
1:A:780:GLU:O	1:A:784:GLN:NE2	2.33	0.61
3:L:164:THR:HB	3:L:174:SER:HB2	1.81	0.61
1:B:378:LYS:NZ	1:B:380:TYR:OH	2.31	0.61
1:C:645:THR:OG1	1:C:648:GLY:O	2.13	0.61
2:M:100:ARG:HG3	2:M:101:TRP:HE3	1.66	0.61
2:O:36:TRP:CZ3	2:O:96:CYS:HB3	2.33	0.61
1:A:106:PHE:HD2	1:A:238:PHE:HB2	1.65	0.61
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.49	0.60
1:C:1129:VAL:HG13	1:C:1132:ILE:HG21	1.83	0.60
1:A:191:GLU:O	1:A:205:SER:HA	2.02	0.60
1:A:722:VAL:HG12	1:A:1065:VAL:HG22	1.84	0.60
1:A:742:ILE:HA	1:A:1000:ARG:HD2	1.84	0.60
1:B:780:GLU:O	1:B:784:GLN:NE2	2.34	0.60
2:M:156:GLU:OE1	2:M:157:PRO:HG3	2.02	0.60
3:N:134:CYS:HB2	3:N:148:TRP:CZ2	2.36	0.60
1:B:367:VAL:HG23	1:B:368:LEU:HD12	1.83	0.60
1:B:987:PRO:HB3	1:C:413:GLY:HA3	1.84	0.60
1:A:883:THR:HG23	1:C:707:TYR:HB2	1.84	0.60
1:A:912:THR:OG1	1:A:1106:GLN:NE2	2.34	0.60
1:B:347:PHE:HD2	1:B:399:SER:HB2	1.67	0.60
3:P:136:LEU:HD11	3:P:196:VAL:HG13	1.83	0.60
1:A:121:ASN:HA	1:A:126:VAL:HG22	1.82	0.60
1:A:736:VAL:HG21	1:A:1004:LEU:HD11	1.84	0.60
1:B:736:VAL:HG21	1:B:1004:LEU:HD11	1.84	0.60
3:P:211:ARG:NE	3:P:211:ARG:HA	2.17	0.60
1:A:102:ARG:HG3	1:A:102:ARG:HH11	1.66	0.60
1:B:347:PHE:CD2	1:B:399:SER:HB2	2.37	0.60
1:B:393:THR:HB	1:B:520:ALA:HB3	1.83	0.60
1:C:409:GLN:OE1	1:C:418:ILE:HB	2.02	0.60
2:H:153:TYR:HB2	2:H:208:HIS:CE1	2.37	0.60
1:A:128:ILE:HD13	1:A:229:LEU:HD11	1.83	0.59
1:B:360:ASN:ND2	1:B:523:THR:OG1	2.33	0.59
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.37	0.59
2:M:98:ARG:HB2	2:M:110:VAL:HG12	1.83	0.59
3:N:24:GLN:OE1	3:N:69:THR:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:118:PHE:HE2	3:N:135:LEU:HB2	1.67	0.59
1:A:567:ARG:HD3	1:A:571:ASP:HA	1.84	0.59
1:B:431:GLY:HA2	1:B:515:PHE:HD2	1.66	0.59
1:B:191:GLU:O	1:B:205:SER:HA	2.02	0.59
1:C:930:ALA:O	1:C:934:ILE:HG12	2.02	0.59
2:M:39:GLN:HE22	2:M:45:LEU:HD12	1.65	0.59
1:A:66:HIS:HD2	1:A:68:ILE:HB	1.68	0.59
1:B:395:VAL:HG23	1:B:514:SER:O	2.02	0.59
3:P:24:GLN:NE2	3:P:70:ASP:OD1	2.31	0.59
1:B:214:ARG:HD3	2:O:105:TRP:CZ3	2.38	0.59
2:H:140:SER:HB2	3:L:207:LYS:HG3	1.85	0.59
3:L:132:VAL:HB	3:L:179:LEU:HB3	1.83	0.59
1:A:357:ARG:NH1	1:B:167:THR:OG1	2.22	0.59
1:B:145:TYR:HB2	1:B:152:TRP:CE2	2.38	0.59
2:H:20:LEU:HD12	2:H:81:LEU:HD23	1.85	0.59
3:N:32:TYR:HE2	3:N:91:ALA:HB3	1.67	0.59
1:A:215:ASP:HA	1:A:266:TYR:OH	2.03	0.59
1:C:68:ILE:O	1:C:78:ARG:N	2.35	0.59
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.85	0.59
1:C:583:GLU:OE1	1:C:585:LEU:HD23	2.02	0.59
2:H:87:ARG:HD2	2:H:88:ALA:N	2.13	0.59
1:A:564:GLN:O	1:A:577:ARG:HG2	2.03	0.58
2:H:91:THR:HG22	2:H:119:VAL:H	1.68	0.58
3:L:75:ILE:HD12	3:L:78:LEU:HD13	1.85	0.58
2:H:98:ARG:O	2:H:108:PHE:HA	2.03	0.58
2:M:132:LEU:HD22	3:N:118:PHE:HB3	1.86	0.58
3:N:61:ARG:NH2	3:N:82:ASP:OD1	2.36	0.58
1:B:24:LEU:HB2	1:B:78:ARG:NH1	2.18	0.58
2:O:61:ALA:HB1	3:P:96:LEU:HD11	1.86	0.58
1:A:966:LEU:O	1:A:975:SER:OG	2.20	0.58
1:C:68:ILE:CD1	2:H:101:TRP:HB2	2.33	0.58
3:P:37:GLN:HB2	3:P:47:LEU:HD21	1.85	0.58
1:A:748:GLU:HG2	1:A:981:LEU:HD21	1.85	0.58
1:C:102:ARG:HB2	1:C:141:LEU:HD21	1.85	0.58
1:A:1080:ALA:HB3	1:A:1132:ILE:HG12	1.84	0.58
1:B:422:ASN:HD21	1:B:454:ARG:H	1.50	0.58
1:B:720:ILE:HD12	1:B:923:ILE:HG23	1.85	0.58
1:C:742:ILE:HG22	1:C:1000:ARG:HG2	1.85	0.58
2:H:208:HIS:CD2	2:H:210:PRO:HD2	2.39	0.58
2:M:100:ARG:HG3	2:M:101:TRP:CE3	2.39	0.58
2:O:135:SER:HB2	3:P:209:PHE:HE1	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:MET:HB2	1:C:699:LEU:HD11	1.84	0.58
1:B:106:PHE:HB3	1:B:235:ILE:HD12	1.85	0.58
1:A:655:HIS:HD2	1:A:656:VAL:N	2.02	0.57
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.87	0.57
1:C:858:LEU:HD22	1:C:959:LEU:HD11	1.85	0.57
2:H:170:GLY:HA3	2:H:190:VAL:HG23	1.86	0.57
3:L:111:ALA:H	3:L:140:TYR:HB3	1.69	0.57
2:M:145:ALA:HB3	3:N:116:PHE:CD2	2.39	0.57
2:M:150:VAL:HG21	2:M:158:VAL:HG21	1.85	0.57
2:O:7:SER:HG	2:O:21:SER:HG	1.48	0.57
1:C:336:CYS:HB3	1:C:358:ILE:HD12	1.87	0.57
1:B:216:LEU:HG	1:B:266:TYR:HE2	1.70	0.57
1:C:986:PRO:O	1:C:990:GLU:HG2	2.04	0.57
1:A:92:PHE:CE1	1:A:265:TYR:HB2	2.39	0.57
1:B:64:TRP:HE1	1:B:264:ALA:CB	2.17	0.57
1:B:92:PHE:CE1	1:B:265:TYR:HB2	2.39	0.57
2:M:130:PHE:HD2	2:M:149:LEU:HD23	1.70	0.57
1:C:145:TYR:HB2	1:C:152:TRP:CE2	2.40	0.57
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.86	0.57
2:O:130:PHE:CE1	3:P:124:GLN:HB2	2.39	0.57
1:A:34:ARG:HD3	1:A:216:LEU:HD23	1.86	0.57
1:A:702:GLU:OE2	1:B:790:LYS:NZ	2.37	0.57
1:C:577:ARG:HD3	1:C:582:LEU:HD22	1.85	0.57
2:H:41:PRO:HD3	2:H:92:ALA:HA	1.86	0.57
1:A:68:ILE:HG12	1:A:69:HIS:H	1.69	0.57
1:B:52:GLN:HG2	1:B:274:THR:HG22	1.86	0.57
3:L:64:GLY:HA2	3:L:73:PHE:HA	1.85	0.57
1:B:64:TRP:NE1	1:B:264:ALA:HB1	2.19	0.57
1:B:187:LYS:NZ	1:B:213:VAL:O	2.36	0.57
2:O:4:LEU:HD23	2:O:110:VAL:HG11	1.85	0.57
1:B:443:SER:OG	1:B:498:GLN:N	2.37	0.57
1:C:214:ARG:HD2	2:H:105:TRP:NE1	2.19	0.57
1:C:874:THR:O	1:C:878:LEU:HG	2.05	0.57
1:A:788:ILE:HG23	1:A:876:ALA:HB2	1.86	0.56
1:B:1089:PHE:HE2	1:C:914:ASN:HA	1.70	0.56
3:P:33:LEU:HG	3:P:89:GLN:O	2.05	0.56
3:P:105:GLU:CB	3:P:142:ARG:HH12	2.15	0.56
1:C:213:VAL:HG11	2:H:105:TRP:HA	1.87	0.56
3:N:111:ALA:H	3:N:140:TYR:HB3	1.70	0.56
3:P:142:ARG:HH21	3:P:173:TYR:HE1	1.50	0.56
1:A:661:GLU:O	1:A:695:TYR:OH	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:HG23	1:C:135:PHE:HE2	1.71	0.56
1:C:716:THR:HG21	1:C:1073:LYS:HD3	1.86	0.56
2:O:129:VAL:HG21	2:O:215:VAL:HG11	1.88	0.56
2:H:51:ILE:HA	2:H:58:THR:HG22	1.88	0.56
1:A:722:VAL:HG22	1:A:930:ALA:HB1	1.88	0.56
1:C:896:ILE:HD12	1:C:897:PRO:HD2	1.87	0.56
2:M:32:TYR:CD1	2:M:100:ARG:HA	2.41	0.56
3:N:106:ILE:H	3:N:142:ARG:NH1	2.03	0.56
1:B:1039:ARG:NE	1:C:1031:GLU:OE2	2.38	0.56
1:C:994:ASP:HA	1:C:997:ILE:HG22	1.88	0.56
3:L:27:GLN:N	3:L:27:GLN:OE1	2.39	0.56
2:M:51:ILE:HD11	2:M:72:ARG:HE	1.71	0.56
1:B:66:HIS:HD2	1:B:68:ILE:HB	1.70	0.56
1:C:613:GLN:HA	1:C:648:GLY:HA3	1.87	0.56
1:B:746:SER:HB2	1:B:749:CYS:SG	2.45	0.56
3:N:61:ARG:HD2	3:N:77:SER:O	2.06	0.56
2:O:153:TYR:HE2	2:O:156:GLU:HA	1.70	0.56
1:C:68:ILE:HD13	2:H:103:SER:OG	2.05	0.55
1:C:308:VAL:HG22	1:C:602:THR:HG23	1.88	0.55
1:A:48:LEU:HB3	1:A:276:LEU:HD11	1.87	0.55
1:A:278:LYS:HZ2	1:A:287:ASP:HB2	1.70	0.55
1:A:822:LEU:HD23	1:A:945:LEU:HD21	1.87	0.55
1:B:401:VAL:HG22	1:B:509:ARG:HD3	1.88	0.55
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.88	0.55
1:C:37:TYR:OH	1:C:195:LYS:NZ	2.27	0.55
1:C:1115:ILE:HG22	1:C:1137:VAL:HG13	1.87	0.55
3:L:6:GLN:NE2	3:L:86:TYR:O	2.35	0.55
3:N:14:SER:HA	3:N:107:LYS:HB2	1.87	0.55
3:N:108:ARG:N	3:N:140:TYR:OH	2.36	0.55
1:B:176:LEU:O	1:B:207:HIS:NE2	2.37	0.55
1:C:46:SER:HA	1:C:279:TYR:O	2.06	0.55
3:N:61:ARG:HH11	3:N:61:ARG:HG2	1.71	0.55
1:A:37:TYR:OH	1:A:53:ASP:OD2	2.20	0.55
3:L:66:GLY:HA3	3:L:71:PHE:HA	1.89	0.55
2:M:160:VAL:HA	2:M:205:ASN:O	2.07	0.55
3:N:83:ILE:HD11	3:N:106:ILE:H	1.70	0.55
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.88	0.55
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.88	0.55
1:A:503:VAL:HA	1:A:506:GLN:HG2	1.88	0.55
1:A:562:PHE:CD2	1:B:225:PRO:HG3	2.42	0.55
1:B:277:LEU:HD23	1:B:285:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:GLY:HA2	1:B:505:TYR:HA	1.88	0.55
1:C:312:ILE:HD13	1:C:598:ILE:HG13	1.89	0.55
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.88	0.55
1:B:990:GLU:HA	1:B:993:ILE:HG22	1.88	0.55
1:C:287:ASP:OD2	1:C:288:ALA:N	2.39	0.55
1:C:396:TYR:HB2	1:C:514:SER:OG	2.07	0.55
3:P:35:TRP:CZ3	3:P:88:CYS:HB3	2.42	0.55
1:A:328:ARG:NH2	1:A:533:LEU:HG	2.22	0.55
1:B:213:VAL:HG11	2:O:105:TRP:HA	1.89	0.55
2:O:48:VAL:HG13	2:O:64:VAL:HG21	1.88	0.55
1:A:152:TRP:CZ2	2:M:54:SER:HB2	2.41	0.54
1:C:52:GLN:OE1	1:C:274:THR:OG1	2.24	0.54
1:C:598:ILE:HB	1:C:609:ALA:HB3	1.88	0.54
1:A:152:TRP:HZ2	2:M:54:SER:HB2	1.72	0.54
1:B:767:LEU:HD23	1:B:770:ILE:HD12	1.88	0.54
1:C:1106:GLN:HE21	1:C:1109:PHE:HB3	1.72	0.54
1:A:64:TRP:CD1	1:A:266:TYR:CE1	2.95	0.54
1:A:984:LEU:HB3	1:A:989:ALA:HB2	1.89	0.54
1:B:342:PHE:HE1	1:B:511:VAL:HG11	1.73	0.54
3:N:32:TYR:CE2	3:N:91:ALA:HB3	2.43	0.54
1:B:34:ARG:HD3	1:B:216:LEU:HD22	1.89	0.54
3:N:164:THR:HB	3:N:174:SER:HB2	1.90	0.54
3:P:62:PHE:CD1	3:P:75:ILE:HD12	2.42	0.54
1:C:178:ASP:HB3	1:C:188:ASN:HB2	1.90	0.54
3:L:198:HIS:HD2	3:L:199:GLN:N	2.06	0.54
1:A:712:ILE:HD12	1:B:895:GLN:O	2.08	0.54
1:B:927:PHE:HZ	1:B:1052:PHE:HE2	1.55	0.54
2:H:129:VAL:HG21	2:H:215:VAL:HG11	1.90	0.54
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.42	0.54
1:C:146:HIS:HB2	1:C:153:MET:CE	2.38	0.54
1:A:957:GLN:HE22	1:B:765:ARG:CZ	2.21	0.54
1:B:354:ASN:O	1:B:398:ASP:HA	2.07	0.54
1:C:22:THR:O	1:C:78:ARG:NH1	2.40	0.54
1:A:69:HIS:HA	1:A:78:ARG:H	1.73	0.54
1:A:382:VAL:HA	1:A:386:LYS:HZ1	1.73	0.54
1:B:92:PHE:HZ	1:B:101:ILE:HG21	1.73	0.54
1:B:146:HIS:HB2	1:B:153:MET:CE	2.37	0.54
1:C:277:LEU:HD23	1:C:285:ILE:HD13	1.88	0.54
1:B:1116:THR:OG1	1:B:1118:ASP:OD1	2.24	0.53
2:O:127:PRO:HB3	2:O:153:TYR:HB3	1.89	0.53
1:C:31:SER:OG	1:C:60:SER:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PHE:CD1	1:A:117:LEU:HD22	2.43	0.53
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.41	0.53
1:B:40:ASP:OD2	1:B:44:ARG:NH2	2.41	0.53
2:M:38:ARG:HD2	2:M:94:TYR:CE1	2.43	0.53
1:A:970:PHE:HE1	1:B:759:PHE:HE2	1.56	0.53
1:B:121:ASN:HA	1:B:126:VAL:HG22	1.90	0.53
1:C:338:PHE:HA	1:C:341:VAL:HG22	1.89	0.53
3:P:133:VAL:HG11	3:P:176:SER:HB2	1.91	0.53
1:A:68:ILE:HG13	2:M:101:TRP:CD1	2.43	0.53
1:C:661:GLU:O	1:C:695:TYR:OH	2.27	0.53
1:A:278:LYS:NZ	1:A:287:ASP:HB2	2.24	0.53
1:A:705:VAL:HG13	1:B:883:THR:HG21	1.91	0.53
1:B:466:ARG:HG2	1:C:232:GLY:O	2.09	0.53
1:C:176:LEU:O	1:C:207:HIS:NE2	2.41	0.53
2:O:54:SER:HA	2:O:72:ARG:HD2	1.91	0.53
2:O:173:THR:HA	2:O:188:SER:HA	1.90	0.53
1:B:92:PHE:CZ	1:B:101:ILE:HG21	2.44	0.53
1:B:763:LEU:HD12	1:B:1008:VAL:HG21	1.90	0.53
2:H:130:PHE:HD2	2:H:149:LEU:HD23	1.74	0.53
3:L:90:GLN:NE2	3:L:97:THR:OG1	2.41	0.53
3:N:66:GLY:HA3	3:N:71:PHE:HA	1.91	0.53
3:P:47:LEU:HD11	3:P:86:TYR:HD1	1.74	0.53
1:A:168:PHE:CE2	1:A:170:TYR:HB2	2.43	0.53
1:C:64:TRP:CD1	1:C:266:TYR:CE1	2.96	0.53
3:L:120:PRO:HD2	3:L:186:TYR:CZ	2.44	0.53
1:A:37:TYR:OH	1:A:54:LEU:O	2.27	0.53
1:A:212:LEU:HD22	1:A:215:ASP:N	2.14	0.53
1:B:135:PHE:HA	1:B:160:TYR:HA	1.91	0.53
1:C:63:THR:HG22	1:C:65:PHE:HE2	1.73	0.53
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.49	0.53
3:N:133:VAL:HG22	3:N:178:THR:HG23	1.91	0.53
2:H:160:VAL:HA	2:H:205:ASN:O	2.09	0.52
1:B:699:LEU:HB2	1:C:788:ILE:HD11	1.89	0.52
1:B:729:VAL:HG22	1:B:1059:GLY:HA2	1.91	0.52
1:C:85:PRO:HA	1:C:237:ARG:HA	1.90	0.52
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.44	0.52
1:B:105:ILE:HD11	1:B:241:LEU:HD21	1.91	0.52
1:B:353:TRP:N	1:B:466:ARG:HH12	2.08	0.52
1:C:214:ARG:HG2	2:H:104:GLY:HA2	1.91	0.52
1:C:819:GLU:HA	1:C:822:LEU:HD12	1.92	0.52
3:N:160:GLN:HG3	3:N:178:THR:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PHE:CD2	1:B:231:ILE:HD11	2.45	0.52
1:A:819:GLU:HA	1:A:822:LEU:HD12	1.92	0.52
1:B:1089:PHE:HB3	1:C:913:GLN:HE21	1.75	0.52
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.91	0.52
3:P:39:LYS:HE3	3:P:40:PRO:HD3	1.92	0.52
1:A:102:ARG:NH2	1:A:121:ASN:O	2.42	0.52
1:A:1115:ILE:HG22	1:A:1137:VAL:HG13	1.90	0.52
1:B:776:LYS:O	1:B:780:GLU:HG3	2.09	0.52
1:C:729:VAL:HG22	1:C:1059:GLY:HA2	1.92	0.52
1:A:767:LEU:HD23	1:A:770:ILE:HD11	1.90	0.52
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	1.91	0.52
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.91	0.52
1:C:212:LEU:HD23	1:C:217:PRO:HB3	1.91	0.52
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.24	0.52
1:A:802:PHE:HB3	1:A:806:LEU:HD23	1.91	0.52
1:A:873:TYR:CZ	1:C:699:LEU:HD22	2.45	0.52
1:A:977:LEU:H	1:A:977:LEU:HD23	1.74	0.52
1:B:95:THR:O	1:B:263:ALA:HB1	2.10	0.52
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.92	0.52
3:P:195:GLU:OE2	3:P:204:PRO:HB2	2.10	0.52
1:A:533:LEU:HD11	1:A:578:ASP:OD2	2.09	0.52
1:B:435:ALA:HB2	1:B:510:VAL:HG12	1.92	0.52
1:B:742:ILE:HA	1:B:1000:ARG:HD2	1.92	0.52
1:C:330:PRO:HD3	1:C:544:ASN:ND2	2.25	0.52
1:C:409:GLN:NE2	1:C:419:ALA:H	2.07	0.52
1:C:1009:THR:O	1:C:1013:ILE:HG12	2.10	0.52
1:B:802:PHE:HB3	1:B:806:LEU:HD23	1.92	0.51
1:B:874:THR:HG21	1:B:1055:SER:HB3	1.91	0.51
1:C:105:ILE:CG2	1:C:135:PHE:HE2	2.23	0.51
3:L:16:GLY:H	3:L:78:LEU:HB3	1.75	0.51
3:L:113:PRO:HD3	3:L:198:HIS:ND1	2.24	0.51
3:N:13:ALA:HA	3:N:107:LYS:HE2	1.91	0.51
2:O:150:VAL:HG21	2:O:158:VAL:HG21	1.92	0.51
1:A:156:GLU:OE1	1:A:158:ARG:NH2	2.44	0.51
1:A:244:LEU:HD23	1:A:259:THR:HG22	1.92	0.51
3:L:39:LYS:HB2	3:L:42:LYS:HB3	1.92	0.51
3:N:30:SER:HA	3:N:68:GLY:H	1.75	0.51
2:M:208:HIS:CD2	2:M:210:PRO:HD2	2.45	0.51
2:O:101:TRP:HE3	2:O:102:ALA:H	1.57	0.51
1:A:104:TRP:HB2	1:A:119:ILE:CG2	2.40	0.51
1:B:353:TRP:HZ3	1:B:355:ARG:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:VAL:HB	1:C:883:THR:HG21	1.93	0.51
1:C:560:LEU:H	1:C:563:GLN:HE22	1.58	0.51
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.93	0.51
2:M:6:GLU:OE2	2:M:96:CYS:N	2.31	0.51
2:O:137:LYS:NZ	3:P:213:GLU:HB3	2.26	0.51
1:C:192:PHE:HE1	1:C:205:SER:HG	1.59	0.51
3:N:39:LYS:HB3	3:N:42:LYS:HB3	1.93	0.51
2:O:92:ALA:HB3	2:O:94:TYR:CE1	2.43	0.51
1:A:357:ARG:HH22	1:B:168:PHE:H	1.58	0.51
1:A:384:PRO:HA	1:A:387:LEU:HD23	1.92	0.51
1:B:186:PHE:CD2	1:B:209:PRO:HB2	2.43	0.51
1:B:215:ASP:HA	1:B:266:TYR:OH	2.11	0.51
1:B:563:GLN:HG3	1:C:43:PHE:HB2	1.93	0.51
1:C:1081:ILE:HG23	1:C:1135:ASN:HB3	1.91	0.51
2:M:125:LYS:HD2	2:M:183:LEU:HD11	1.92	0.51
3:P:150:VAL:HG13	3:P:192:TYR:HE1	1.75	0.51
1:A:212:LEU:CD2	1:A:215:ASP:H	2.13	0.51
1:A:278:LYS:HZ2	1:A:306:PHE:HE2	1.59	0.51
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.45	0.51
1:B:296:LEU:HB2	1:B:608:VAL:HG11	1.91	0.51
1:C:742:ILE:HD12	1:C:997:ILE:HD11	1.92	0.51
1:C:903:ALA:HB1	1:C:913:GLN:HB2	1.93	0.51
1:B:68:ILE:CG2	1:B:78:ARG:HE	2.22	0.51
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.46	0.51
2:M:60:TYR:HB2	2:M:65:LYS:HE2	1.93	0.51
3:P:6:GLN:NE2	3:P:100:GLN:HB2	2.26	0.51
1:A:34:ARG:NH2	1:A:221:SER:OG	2.44	0.51
1:A:1093:GLY:HA3	1:A:1105:THR:O	2.11	0.51
1:A:1129:VAL:HB	1:A:1132:ILE:HD11	1.93	0.51
2:O:178:LEU:HD12	2:O:179:GLN:N	2.25	0.51
1:A:1094:VAL:HG12	1:B:904:TYR:OH	2.10	0.50
1:C:146:HIS:HB2	1:C:153:MET:HE3	1.93	0.50
3:N:186:TYR:CE2	3:N:211:ARG:HB2	2.46	0.50
1:B:699:LEU:HB3	1:C:788:ILE:HD11	1.93	0.50
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.46	0.50
1:C:1126:CYS:HB2	1:C:1132:ILE:HD11	1.93	0.50
2:H:203:ILE:CD1	2:H:218:LYS:HD2	2.40	0.50
1:C:339:GLY:O	1:C:343:ASN:HB2	2.11	0.50
3:N:118:PHE:CE2	3:N:135:LEU:HB2	2.46	0.50
3:P:149:LYS:HZ1	3:P:195:GLU:HB2	1.77	0.50
1:A:64:TRP:NE1	1:A:264:ALA:HB1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:ASP:OD1	1:A:980:ILE:N	2.44	0.50
1:B:1125:ASN:ND2	1:B:1127:ASP:OD2	2.45	0.50
1:C:215:ASP:HA	1:C:266:TYR:OH	2.11	0.50
1:C:328:ARG:HD3	1:C:543:PHE:CE1	2.45	0.50
2:H:4:LEU:HB2	2:H:110:VAL:HG21	1.94	0.50
3:L:125:LEU:HD22	3:L:183:LYS:HA	1.93	0.50
2:M:70:ILE:HD11	2:M:79:LEU:HD11	1.94	0.50
2:O:61:ALA:HB3	2:O:64:VAL:HG22	1.93	0.50
1:B:341:VAL:HB	1:B:356:LYS:HD3	1.94	0.50
1:C:69:HIS:CD2	1:C:77:LYS:HD2	2.47	0.50
1:C:391:CYS:HB2	1:C:544:ASN:O	2.11	0.50
1:C:532:ASN:OD1	1:C:533:LEU:N	2.43	0.50
2:M:38:ARG:NH1	2:M:46:GLU:HB3	2.25	0.50
3:N:2:ILE:HG23	3:N:26:SER:HB2	1.94	0.50
2:O:209:LYS:HB2	2:O:210:PRO:HD3	1.92	0.50
3:P:90:GLN:OE1	3:P:91:ALA:N	2.45	0.50
1:A:31:SER:HB3	1:A:62:VAL:HG13	1.93	0.50
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.76	0.50
1:C:739:THR:O	1:C:743:CYS:C	2.50	0.50
3:L:6:GLN:O	3:L:100:GLN:NE2	2.45	0.50
2:M:4:LEU:HD22	2:M:22:CYS:SG	2.52	0.50
2:O:34:MET:SD	2:O:79:LEU:HD22	2.52	0.50
2:O:150:VAL:HB	2:O:158:VAL:HG11	1.92	0.50
1:A:878:LEU:HD11	1:A:1054:GLN:HE22	1.77	0.50
1:B:126:VAL:HG21	1:B:175:PHE:H	1.76	0.50
1:B:274:THR:OG1	1:B:291:CYS:HB2	2.12	0.50
1:B:393:THR:OG1	1:B:516:GLU:O	2.18	0.50
1:B:713:ALA:O	1:C:894:LEU:HB3	2.11	0.50
1:C:966:LEU:HD22	1:C:1000:ARG:HD3	1.93	0.50
3:N:5:THR:HB	3:N:24:GLN:HB3	1.94	0.50
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.94	0.50
3:L:118:PHE:HZ	3:L:135:LEU:HD22	1.77	0.50
1:A:21:ARG:HA	1:A:79:PHE:CE2	2.46	0.50
1:A:980:ILE:O	1:A:984:LEU:HB2	2.12	0.50
1:B:211:ASN:OD1	1:B:212:LEU:N	2.45	0.50
1:B:743:CYS:SG	1:B:750:SER:N	2.85	0.50
1:C:159:VAL:HG23	1:C:160:TYR:CD2	2.47	0.50
1:C:177:MET:HB2	1:C:190:ARG:HH21	1.77	0.50
1:C:426:PRO:HG2	1:C:429:PHE:HB2	1.94	0.50
1:B:393:THR:HA	1:B:522:ALA:HA	1.94	0.49
3:L:46:LEU:HB3	3:L:55:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:2:ILE:H	3:N:97:THR:HG22	1.77	0.49
3:P:62:PHE:HD1	3:P:75:ILE:HD12	1.76	0.49
1:B:312:ILE:HD11	1:B:596:SER:HB3	1.93	0.49
1:B:738:CYS:HB3	1:B:753:LEU:HD21	1.93	0.49
1:C:65:PHE:HE1	1:C:82:PRO:CG	2.25	0.49
2:O:12:VAL:HG23	2:O:119:VAL:HG22	1.95	0.49
1:A:106:PHE:CD2	1:A:238:PHE:HB2	2.45	0.49
1:B:449:TYR:N	1:B:495:TYR:O	2.46	0.49
2:M:152:ASP:HB3	2:M:183:LEU:HD12	1.95	0.49
2:O:6:GLU:OE1	2:O:115:THR:HG22	2.12	0.49
3:P:132:VAL:CG1	3:P:179:LEU:HB3	2.43	0.49
1:A:87:ASN:HD22	1:A:269:TYR:HD2	1.60	0.49
1:A:96:GLU:OE2	1:A:101:ILE:HB	2.12	0.49
1:C:220:PHE:CD1	1:C:221:SER:N	2.81	0.49
2:H:92:ALA:HB3	2:H:94:TYR:HE1	1.77	0.49
1:A:324:GLU:O	1:A:539:VAL:HG13	2.11	0.49
1:A:378:LYS:HG3	1:A:380:TYR:HE1	1.76	0.49
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.38	0.49
3:L:13:ALA:O	3:L:106:ILE:HA	2.11	0.49
3:L:167:ASP:OD2	3:L:169:LYS:HG2	2.12	0.49
3:N:83:ILE:HG12	3:N:105:GLU:HA	1.93	0.49
3:N:198:HIS:CE1	3:N:200:GLY:H	2.31	0.49
1:C:64:TRP:HD1	1:C:266:TYR:CE1	2.30	0.49
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	1.95	0.49
3:N:136:LEU:HD21	3:N:144:ALA:HB3	1.93	0.49
1:B:69:HIS:HA	1:B:78:ARG:H	1.77	0.49
1:B:358:ILE:HB	1:B:395:VAL:HG13	1.95	0.49
1:B:395:VAL:C	1:B:396:TYR:HD2	2.14	0.49
2:H:38:ARG:HD2	2:H:94:TYR:CE1	2.48	0.49
2:H:127:PRO:HB3	2:H:153:TYR:CB	2.43	0.49
1:A:1139:ASP:O	1:A:1143:PRO:HD2	2.12	0.49
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.40	0.49
1:C:86:PHE:N	1:C:236:THR:O	2.43	0.49
1:C:318:PHE:N	1:C:593:GLY:O	2.36	0.49
1:C:336:CYS:SG	1:C:358:ILE:HG23	2.53	0.49
1:C:552:LEU:HD12	1:C:585:LEU:HB3	1.94	0.49
2:M:145:ALA:HB3	3:N:116:PHE:CG	2.48	0.49
3:N:117:ILE:O	3:N:119:PRO:HD3	2.12	0.49
1:B:212:LEU:HD23	1:B:217:PRO:HB3	1.94	0.49
3:N:120:PRO:HG3	3:N:131:SER:N	2.28	0.49
1:A:714:ILE:HD12	1:A:1096:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:PRO:O	1:B:913:GLN:NE2	2.45	0.49
1:C:915:VAL:O	1:C:919:ASN:HB2	2.12	0.49
2:O:153:TYR:CE1	2:O:185:SER:HA	2.48	0.49
1:B:69:HIS:HA	1:B:77:LYS:HA	1.95	0.48
1:B:192:PHE:HA	1:B:204:TYR:O	2.13	0.48
3:L:120:PRO:HG3	3:L:131:SER:N	2.28	0.48
3:N:150:VAL:HG23	3:N:155:GLN:HG3	1.95	0.48
1:A:192:PHE:HA	1:A:204:TYR:O	2.13	0.48
1:C:105:ILE:HB	1:C:239:GLN:HB3	1.94	0.48
1:C:611:LEU:HD21	1:C:613:GLN:HB3	1.94	0.48
1:C:714:ILE:HD12	1:C:1096:VAL:HG11	1.94	0.48
1:C:1106:GLN:NE2	1:C:1109:PHE:HB3	2.28	0.48
3:N:15:VAL:HA	3:N:78:LEU:HD22	1.95	0.48
3:N:83:ILE:HD12	3:N:166:GLN:OE1	2.12	0.48
1:A:655:HIS:CD2	1:A:656:VAL:N	2.81	0.48
1:A:707:TYR:HD1	1:B:883:THR:HG23	1.78	0.48
1:B:178:ASP:HB3	1:B:188:ASN:HB2	1.95	0.48
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.44	0.48
1:C:741:TYR:CE1	1:C:966:LEU:HD21	2.48	0.48
2:H:129:VAL:HG12	2:H:217:LYS:NZ	2.29	0.48
3:L:118:PHE:HB2	3:L:133:VAL:HB	1.94	0.48
3:L:142:ARG:HE	3:L:173:TYR:HD1	1.61	0.48
2:O:175:PRO:HG2	3:P:165:GLU:HG2	1.95	0.48
1:A:985:ASP:HB2	1:C:383:SER:HB2	1.95	0.48
1:C:106:PHE:HB3	1:C:235:ILE:HD12	1.95	0.48
1:C:991:VAL:O	1:C:995:ARG:HG2	2.14	0.48
2:H:38:ARG:NH1	2:H:46:GLU:HB3	2.29	0.48
2:M:132:LEU:HB3	3:N:118:PHE:CD1	2.49	0.48
1:B:196:ASN:HB3	1:B:201:PHE:CD1	2.48	0.48
1:B:985:ASP:N	1:B:985:ASP:OD1	2.45	0.48
3:L:134:CYS:HB2	3:L:148:TRP:CZ2	2.48	0.48
1:A:1030:SER:HB3	1:C:1041:ASP:OD1	2.13	0.48
1:C:103:GLY:HA3	1:C:241:LEU:HD12	1.94	0.48
2:H:50:TYR:CZ	2:H:106:LEU:HD13	2.48	0.48
1:B:63:THR:HG22	1:B:65:PHE:CE1	2.49	0.48
1:C:985:ASP:OD1	1:C:985:ASP:N	2.47	0.48
2:H:109:ASP:HA	3:L:46:LEU:HD11	1.96	0.48
2:H:144:ALA:HB3	2:H:197:LEU:HD11	1.95	0.48
1:A:788:ILE:HD11	1:C:699:LEU:C	2.34	0.48
1:A:770:ILE:O	1:A:774:GLN:HG2	2.14	0.48
1:A:1087:ALA:O	1:A:1122:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:GLY:HA2	1:A:1107:ARG:HD2	1.94	0.48
1:B:353:TRP:CZ3	1:B:355:ARG:HD2	2.48	0.48
1:C:82:PRO:O	1:C:239:GLN:NE2	2.47	0.48
3:P:150:VAL:HG13	3:P:192:TYR:CE1	2.49	0.48
1:B:100:ILE:HA	1:B:243:ALA:HB3	1.96	0.48
1:C:68:ILE:HG23	1:C:69:HIS:N	2.29	0.48
3:L:135:LEU:HD13	3:L:176:SER:HB3	1.95	0.48
1:A:338:PHE:HE1	1:A:358:ILE:HG13	1.79	0.47
1:A:357:ARG:HH22	1:B:167:THR:HA	1.77	0.47
1:C:34:ARG:HE	1:C:217:PRO:HD2	1.79	0.47
1:C:125:ASN:OD1	1:C:126:VAL:N	2.47	0.47
1:A:277:LEU:HD23	1:A:285:ILE:HD13	1.96	0.47
1:C:767:LEU:HD21	1:C:1008:VAL:HG22	1.95	0.47
1:C:1139:ASP:HB3	1:C:1142:GLN:HG2	1.96	0.47
1:A:85:PRO:HA	1:A:237:ARG:HA	1.96	0.47
1:A:206:LYS:HE2	1:A:221:SER:HB2	1.96	0.47
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.49	0.47
1:C:770:ILE:O	1:C:774:GLN:HG2	2.14	0.47
1:C:996:LEU:HD22	1:C:1000:ARG:HH21	1.78	0.47
3:L:24:GLN:HA	3:L:69:THR:O	2.14	0.47
3:L:116:PHE:HD2	3:L:118:PHE:CE1	2.32	0.47
3:L:198:HIS:CD2	3:L:199:GLN:H	2.29	0.47
2:M:100:ARG:HE	2:M:101:TRP:HZ3	1.62	0.47
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.31	0.47
3:N:135:LEU:HD13	3:N:176:SER:HB3	1.96	0.47
1:B:86:PHE:CZ	1:B:89:GLY:HA2	2.50	0.47
1:C:31:SER:HB3	1:C:62:VAL:HG23	1.94	0.47
2:M:140:SER:HB2	3:N:207:LYS:HG3	1.97	0.47
2:O:153:TYR:OH	2:O:186:LEU:HD13	2.15	0.47
1:B:427:ASP:OD1	1:B:428:ASP:N	2.47	0.47
1:B:986:PRO:HA	1:B:989:ALA:HB3	1.96	0.47
1:B:1031:GLU:OE2	1:B:1039:ARG:HD3	2.14	0.47
1:B:1145:LEU:HD11	1:C:1144:GLU:OE2	2.15	0.47
3:L:2:ILE:H	3:L:97:THR:CG2	2.26	0.47
2:M:39:GLN:N	2:M:93:VAL:O	2.36	0.47
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.97	0.47
3:N:105:GLU:HB2	3:N:142:ARG:NH1	2.29	0.47
2:O:33:ALA:HB1	2:O:51:ILE:O	2.15	0.47
1:A:46:SER:N	1:A:279:TYR:O	2.47	0.47
1:A:557:LYS:HD2	1:A:559:PHE:HE1	1.80	0.47
1:A:704:SER:HB3	1:B:790:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:HA	1:B:258:TRP:HB2	1.96	0.47
1:B:391:CYS:HB2	1:B:544:ASN:O	2.15	0.47
1:B:712:ILE:HG21	1:B:1096:VAL:HG12	1.96	0.47
1:B:916:LEU:HD12	1:B:923:ILE:HD12	1.96	0.47
1:C:1083:HIS:ND1	1:C:1136:THR:HA	2.30	0.47
3:P:89:GLN:HG2	3:P:98:PHE:CD1	2.49	0.47
3:P:145:LYS:HD3	3:P:147:GLN:NE2	2.30	0.47
1:B:103:GLY:HA3	1:B:241:LEU:HD12	1.97	0.47
1:B:731:MET:N	1:B:774:GLN:OE1	2.32	0.47
2:M:132:LEU:HB3	3:N:118:PHE:HD1	1.80	0.47
3:P:138:ASN:HA	3:P:172:THR:HG21	1.96	0.47
1:A:349:SER:HA	1:A:451:TYR:CE1	2.50	0.47
1:A:453:TYR:HB3	1:A:495:TYR:CE2	2.49	0.47
1:B:64:TRP:CD1	1:B:266:TYR:CE1	3.03	0.47
1:B:185:ASN:O	1:B:186:PHE:HD1	1.98	0.47
1:C:34:ARG:HD2	1:C:216:LEU:HD22	1.96	0.47
1:C:133:PHE:HB3	1:C:135:PHE:CE1	2.50	0.47
2:H:203:ILE:HD11	2:H:218:LYS:CD	2.45	0.47
3:L:117:ILE:O	3:L:119:PRO:HD3	2.14	0.47
3:N:61:ARG:HG2	3:N:61:ARG:NH1	2.30	0.47
1:A:64:TRP:HE1	1:A:264:ALA:CB	2.27	0.47
1:A:102:ARG:HG3	1:A:102:ARG:NH1	2.29	0.47
1:B:196:ASN:HB3	1:B:201:PHE:HD1	1.80	0.47
1:C:41:LYS:HE2	1:C:225:PRO:HB2	1.97	0.47
2:H:192:VAL:HG21	2:H:202:TYR:CE2	2.46	0.47
3:N:135:LEU:HA	3:N:176:SER:HA	1.97	0.47
1:B:770:ILE:O	1:B:774:GLN:HG2	2.14	0.46
1:C:609:ALA:HB1	1:C:650:LEU:HD11	1.96	0.46
3:P:27:GLN:N	3:P:27:GLN:OE1	2.48	0.46
1:A:1130:ILE:HG13	1:A:1131:GLY:N	2.30	0.46
1:C:134:GLN:O	1:C:161:SER:N	2.36	0.46
1:C:353:TRP:O	1:C:466:ARG:NH1	2.48	0.46
2:M:209:LYS:HB2	2:M:210:PRO:HD3	1.97	0.46
2:O:170:GLY:O	2:O:190:VAL:HG12	2.16	0.46
1:A:517:LEU:HD23	1:A:517:LEU:H	1.80	0.46
2:M:175:PRO:CD	3:N:164:THR:HA	2.45	0.46
1:A:874:THR:HG21	1:A:1055:SER:HB3	1.96	0.46
1:B:125:ASN:OD1	1:B:126:VAL:N	2.49	0.46
1:B:802:PHE:HZ	1:B:898:PHE:CZ	2.33	0.46
1:B:986:PRO:O	1:B:990:GLU:OE1	2.34	0.46
1:C:62:VAL:HG13	1:C:267:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:977:LEU:O	1:C:981:LEU:HD23	2.15	0.46
2:H:35:THR:HG21	2:H:106:LEU:HD21	1.96	0.46
2:H:108:PHE:HD2	3:L:36:TYR:HE2	1.64	0.46
2:M:111:TRP:O	3:N:43:ALA:HB1	2.15	0.46
2:O:161:SER:OG	2:O:205:ASN:HB2	2.15	0.46
1:B:64:TRP:CD1	1:B:266:TYR:HE1	2.34	0.46
1:B:350:VAL:HG12	1:B:400:PHE:CD2	2.51	0.46
1:B:398:ASP:O	1:B:511:VAL:HA	2.15	0.46
1:B:514:SER:OG	1:B:515:PHE:N	2.49	0.46
1:B:666:ILE:HB	1:B:670:ILE:HB	1.97	0.46
1:B:742:ILE:HG22	1:B:1000:ARG:HG2	1.97	0.46
1:B:1090:PRO:HD2	1:C:913:GLN:NE2	2.28	0.46
1:C:400:PHE:CD2	1:C:402:ILE:HD11	2.50	0.46
1:B:565:PHE:HB3	1:B:576:VAL:HG23	1.97	0.46
1:B:984:LEU:HD21	1:B:988:GLU:OE1	2.16	0.46
2:H:8:GLY:O	2:H:18:LEU:HD21	2.16	0.46
3:L:140:TYR:O	3:L:198:HIS:NE2	2.46	0.46
2:M:163:ASN:ND2	2:M:201:THR:O	2.49	0.46
1:A:718:PHE:HE1	1:A:923:ILE:HD13	1.81	0.46
1:A:741:TYR:CE1	1:A:966:LEU:HD11	2.51	0.46
1:B:99:ASN:HB3	1:B:102:ARG:NH2	2.30	0.46
1:B:273:ARG:NH1	1:B:292:ALA:HB3	2.31	0.46
2:M:39:GLN:NE2	2:M:45:LEU:HD12	2.31	0.46
1:C:92:PHE:HZ	1:C:101:ILE:HG21	1.81	0.46
1:C:328:ARG:NH1	1:C:531:THR:O	2.49	0.46
2:M:33:ALA:HB1	2:M:51:ILE:O	2.15	0.46
3:P:145:LYS:HD3	3:P:147:GLN:HE22	1.81	0.46
1:A:354:ASN:O	1:A:398:ASP:HA	2.16	0.46
2:H:209:LYS:HB2	2:H:210:PRO:HD3	1.97	0.46
3:P:186:TYR:O	3:P:192:TYR:OH	2.26	0.46
1:A:204:TYR:CD2	1:A:225:PRO:HA	2.51	0.46
1:C:96:GLU:OE2	1:C:101:ILE:HB	2.16	0.46
3:N:118:PHE:HB2	3:N:133:VAL:HB	1.98	0.46
1:A:100:ILE:HA	1:A:243:ALA:HB3	1.98	0.45
1:A:375:SER:H	1:A:436:TRP:HA	1.81	0.45
1:B:551:VAL:HG22	1:B:588:THR:O	2.16	0.45
2:O:91:THR:HG23	2:O:118:THR:HA	1.99	0.45
3:P:47:LEU:HD11	3:P:86:TYR:CD1	2.51	0.45
1:B:1088:HIS:CE1	1:B:1122:VAL:HG12	2.51	0.45
1:C:887:THR:HG21	1:C:894:LEU:HD12	1.98	0.45
3:L:141:PRO:HD2	3:L:198:HIS:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:83:ILE:HB	3:N:166:GLN:OE1	2.16	0.45
3:P:133:VAL:HA	3:P:177:SER:O	2.16	0.45
1:A:669:GLY:O	1:A:697:MET:HG2	2.16	0.45
1:A:712:ILE:HG21	1:A:1096:VAL:HG12	1.97	0.45
1:B:870:ILE:O	1:B:874:THR:HG23	2.17	0.45
1:C:69:HIS:HA	1:C:78:ARG:H	1.81	0.45
3:N:108:ARG:HG3	3:N:171:SER:HB3	1.97	0.45
2:O:132:LEU:HD12	2:O:147:GLY:HA3	1.98	0.45
1:A:321:GLN:HA	1:A:321:GLN:OE1	2.17	0.45
1:B:143:VAL:CG1	1:B:152:TRP:HB3	2.47	0.45
3:L:83:ILE:HG23	3:L:104:VAL:O	2.16	0.45
2:M:60:TYR:HB2	2:M:65:LYS:CE	2.46	0.45
2:M:98:ARG:O	2:M:108:PHE:HA	2.16	0.45
3:N:8:PRO:HG2	3:N:11:LEU:HD23	1.99	0.45
1:A:159:VAL:HG23	1:A:160:TYR:CD1	2.52	0.45
1:A:173:GLN:HG2	1:A:174:PRO:HD2	1.99	0.45
1:A:360:ASN:N	1:A:523:THR:OG1	2.37	0.45
1:A:874:THR:O	1:A:878:LEU:HG	2.16	0.45
1:B:316:SER:OG	1:B:317:ASN:N	2.49	0.45
1:B:1041:ASP:HB2	1:C:1030:SER:HB3	1.97	0.45
1:C:377:PHE:HE2	1:C:384:PRO:HB3	1.82	0.45
1:A:355:ARG:HD3	1:A:396:TYR:HD2	1.82	0.45
1:A:864:LEU:HD21	1:C:697:MET:HE3	1.98	0.45
1:A:967:SER:O	1:A:967:SER:OG	2.29	0.45
1:C:105:ILE:HD11	1:C:241:LEU:HD21	1.98	0.45
2:H:175:PRO:HD3	3:L:164:THR:HG23	1.98	0.45
3:L:7:SER:OG	3:L:22:THR:OG1	2.35	0.45
2:M:84:ASN:OD1	2:M:85:SER:N	2.50	0.45
2:O:194:SER:HA	2:O:197:LEU:HG	1.97	0.45
3:P:46:LEU:HB3	3:P:55:GLU:OE2	2.17	0.45
1:A:811:LYS:HB2	1:A:811:LYS:HE2	1.74	0.45
1:A:961:THR:O	1:A:965:GLN:HG2	2.16	0.45
1:A:996:LEU:HD11	1:A:1000:ARG:NH2	2.31	0.45
1:B:699:LEU:HD22	1:C:873:TYR:CZ	2.52	0.45
1:B:717:ASN:OD1	1:B:718:PHE:N	2.44	0.45
1:B:741:TYR:HD2	1:B:742:ILE:HG23	1.82	0.45
1:B:1081:ILE:HG23	1:B:1135:ASN:HB3	1.98	0.45
1:C:177:MET:HB2	1:C:190:ARG:NH2	2.31	0.45
3:L:134:CYS:HB2	3:L:148:TRP:CE2	2.52	0.45
3:L:198:HIS:CD2	3:L:199:GLN:N	2.84	0.45
2:M:37:VAL:CG1	2:M:95:TYR:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:99:ASP:O	2:O:100:ARG:HB2	2.17	0.45
1:C:379:CYS:CA	1:C:432:CYS:HB3	2.22	0.45
1:C:544:ASN:HD21	1:C:579:PRO:HG2	1.82	0.45
2:M:5:VAL:HG12	2:M:113:GLN:HE22	1.82	0.45
3:N:83:ILE:HD11	3:N:106:ILE:N	2.31	0.45
2:O:192:VAL:HG21	2:O:202:TYR:CE2	2.49	0.45
1:A:68:ILE:O	1:A:78:ARG:N	2.50	0.45
1:A:205:SER:HA	1:A:223:LEU:HD23	1.97	0.45
1:B:541:PHE:CZ	1:B:587:ILE:HD13	2.52	0.45
1:B:986:PRO:O	1:B:989:ALA:N	2.49	0.45
3:L:108:ARG:N	3:L:140:TYR:OH	2.50	0.45
3:N:136:LEU:HG	3:N:139:PHE:HB3	1.99	0.45
2:O:82:GLN:NE2	2:O:83:MET:O	2.50	0.45
1:A:418:ILE:O	1:A:422:ASN:HB3	2.17	0.45
1:A:713:ALA:O	1:B:894:LEU:HB3	2.17	0.45
1:B:128:ILE:HD13	1:B:229:LEU:HD11	1.99	0.45
1:C:193:VAL:HB	1:C:204:TYR:HB2	1.99	0.45
1:C:206:LYS:HE2	1:C:221:SER:HB2	1.98	0.45
2:O:45:LEU:HD13	3:P:87:TYR:CE2	2.52	0.45
1:B:409:GLN:NE2	1:B:418:ILE:HB	2.32	0.44
1:B:738:CYS:O	1:B:742:ILE:HG12	2.16	0.44
1:B:759:PHE:O	1:B:763:LEU:HD23	2.16	0.44
1:C:21:ARG:NH1	1:C:22:THR:O	2.49	0.44
1:C:69:HIS:HA	1:C:77:LYS:HA	1.97	0.44
1:C:642:VAL:HG22	1:C:651:ILE:HG22	1.98	0.44
3:L:186:TYR:O	3:L:192:TYR:OH	2.35	0.44
1:A:1142:GLN:HA	1:A:1142:GLN:OE1	2.17	0.44
1:B:712:ILE:HD12	1:C:895:GLN:O	2.17	0.44
1:C:784:GLN:OE1	1:C:1030:SER:OG	2.35	0.44
2:O:4:LEU:HD12	2:O:23:ALA:O	2.18	0.44
1:A:46:SER:HA	1:A:279:TYR:O	2.17	0.44
1:B:96:GLU:OE2	1:B:101:ILE:HB	2.17	0.44
1:B:117:LEU:HD21	1:B:119:ILE:HG13	1.99	0.44
1:C:68:ILE:HD11	2:H:101:TRP:HE3	1.82	0.44
2:H:105:TRP:CZ3	3:L:91:ALA:O	2.70	0.44
2:O:185:SER:O	2:O:186:LEU:HD12	2.17	0.44
2:O:208:HIS:HE1	2:O:210:PRO:HB2	1.83	0.44
1:A:176:LEU:O	1:A:207:HIS:NE2	2.51	0.44
1:A:726:ILE:HG22	1:A:948:LEU:HD13	1.99	0.44
1:B:101:ILE:HG13	1:B:242:LEU:CD1	2.48	0.44
1:B:329:PHE:CE2	1:B:528:LYS:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:SER:OG	1:B:436:TRP:HA	2.18	0.44
1:C:63:THR:CG2	1:C:65:PHE:HE2	2.30	0.44
1:C:804:GLN:HE21	1:C:818:ILE:HD11	1.83	0.44
2:H:73:ASP:O	2:H:77:ASN:HA	2.15	0.44
3:L:134:CYS:N	3:L:148:TRP:HE1	2.16	0.44
2:M:48:VAL:O	2:M:60:TYR:HA	2.18	0.44
1:A:104:TRP:N	1:A:241:LEU:HD13	2.32	0.44
1:A:1031:GLU:OE1	1:A:1039:ARG:HD3	2.16	0.44
1:B:196:ASN:O	1:B:196:ASN:ND2	2.31	0.44
1:C:68:ILE:CG1	2:H:101:TRP:HB2	2.47	0.44
1:C:201:PHE:O	1:C:229:LEU:N	2.49	0.44
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.98	0.44
1:C:422:ASN:HD21	1:C:453:TYR:HB2	1.83	0.44
1:C:1094:VAL:HG23	1:C:1096:VAL:HG13	2.00	0.44
2:M:203:ILE:CD1	2:M:218:LYS:CG	2.94	0.44
2:O:175:PRO:HD2	3:P:164:THR:HA	2.00	0.44
1:A:393:THR:HA	1:A:522:ALA:HA	1.98	0.44
1:B:329:PHE:CE1	1:B:391:CYS:SG	3.11	0.44
1:C:48:LEU:HB3	1:C:276:LEU:HD11	1.99	0.44
2:O:177:VAL:HG11	3:P:162:SER:HA	1.99	0.44
1:B:309:GLU:O	1:B:313:TYR:OH	2.30	0.44
1:B:350:VAL:O	1:B:353:TRP:HD1	2.00	0.44
1:B:555:SER:HB3	1:B:586:ASP:HB2	1.99	0.44
1:B:726:ILE:O	1:B:947:LYS:HD3	2.18	0.44
2:O:74:ASN:C	2:O:75:SER:HG	2.20	0.44
3:P:93:ALA:O	3:P:94:TYR:HB2	2.18	0.44
1:A:225:PRO:HG3	1:C:562:PHE:CD2	2.53	0.44
1:A:382:VAL:HG23	1:A:386:LYS:HZ1	1.82	0.44
1:C:83:VAL:HG11	1:C:237:ARG:NH1	2.32	0.44
1:C:214:ARG:O	1:C:266:TYR:OH	2.36	0.44
1:C:312:ILE:HD11	1:C:596:SER:HB3	1.99	0.44
1:C:802:PHE:CD1	1:C:805:ILE:HD11	2.53	0.44
1:A:187:LYS:HG3	3:N:94:TYR:OH	2.18	0.44
1:A:900:MET:HG2	1:A:917:TYR:OH	2.17	0.44
1:B:519:HIS:O	1:C:41:LYS:HD2	2.18	0.44
1:B:874:THR:O	1:B:878:LEU:HG	2.17	0.44
1:B:1043:CYS:HB2	1:B:1048:HIS:CG	2.53	0.44
1:C:140:PHE:CD2	1:C:244:LEU:HD13	2.53	0.44
1:C:378:LYS:O	1:C:432:CYS:HB2	2.18	0.44
2:M:29:PHE:O	2:M:30:SER:OG	2.32	0.44
3:N:35:TRP:CZ3	3:N:88:CYS:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:40:ALA:HB3	2:O:43:LYS:HB2	2.00	0.44
1:A:24:LEU:HD12	1:A:78:ARG:HD3	1.99	0.43
1:B:382:VAL:HA	1:C:983:ARG:O	2.18	0.43
2:M:197:LEU:HD12	2:M:198:GLY:N	2.33	0.43
3:N:140:TYR:CD2	3:N:141:PRO:HA	2.53	0.43
2:O:113:GLN:OE1	2:O:113:GLN:N	2.51	0.43
1:A:1031:GLU:OE2	1:C:1039:ARG:HB3	2.18	0.43
1:B:560:LEU:HB2	1:B:563:GLN:OE1	2.18	0.43
1:C:69:HIS:HD2	1:C:77:LYS:HD2	1.83	0.43
1:A:115:GLN:OE1	1:A:115:GLN:HA	2.19	0.43
1:A:977:LEU:HA	1:A:980:ILE:HG12	2.01	0.43
1:C:46:SER:CA	1:C:279:TYR:O	2.66	0.43
2:H:189:VAL:HG22	2:H:190:VAL:H	1.82	0.43
3:P:167:ASP:OD2	3:P:169:LYS:HG2	2.18	0.43
1:A:1029:MET:O	1:A:1033:VAL:HB	2.19	0.43
1:B:589:PRO:HB2	1:C:854:LYS:HZ1	1.83	0.43
1:B:985:ASP:O	1:B:989:ALA:HB2	2.17	0.43
1:C:68:ILE:HG13	1:C:69:HIS:N	2.31	0.43
1:C:197:ILE:O	1:C:198:ASP:OD1	2.36	0.43
3:L:38:GLN:O	3:L:84:ALA:HB1	2.19	0.43
1:A:557:LYS:HE3	1:A:586:ASP:OD2	2.18	0.43
1:B:393:THR:HG21	1:B:520:ALA:H	1.83	0.43
2:H:130:PHE:HE1	3:L:121:SER:H	1.66	0.43
3:N:120:PRO:HB2	3:N:211:ARG:HH22	1.83	0.43
1:A:594:GLY:C	1:A:613:GLN:HE21	2.21	0.43
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.53	0.43
1:B:406:GLU:O	1:B:409:GLN:HG2	2.19	0.43
1:C:56:LEU:HD22	1:C:91:TYR:CD2	2.54	0.43
1:C:106:PHE:HD2	1:C:235:ILE:HG21	1.82	0.43
1:C:115:GLN:OE1	1:C:115:GLN:HA	2.18	0.43
1:C:655:HIS:HA	1:C:694:ALA:O	2.18	0.43
1:C:738:CYS:O	1:C:742:ILE:HG12	2.19	0.43
3:L:8:PRO:HG2	3:L:11:LEU:HD23	2.01	0.43
1:A:34:ARG:NE	1:A:191:GLU:OE2	2.43	0.43
1:A:118:LEU:HG	1:A:120:VAL:HG23	2.01	0.43
1:A:671:CYS:SG	1:A:697:MET:HB3	2.59	0.43
1:A:786:LYS:O	1:C:700:GLY:HA3	2.19	0.43
1:A:814:LYS:HA	1:A:814:LYS:HD3	1.87	0.43
1:B:101:ILE:HA	1:B:242:LEU:HD12	2.01	0.43
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.88	0.43
1:C:178:ASP:HB2	1:C:207:HIS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:PHE:HE2	1:C:402:ILE:HD11	1.81	0.43
1:C:984:LEU:HB3	1:C:989:ALA:HB2	2.00	0.43
2:M:178:LEU:HD23	2:M:178:LEU:H	1.84	0.43
2:O:36:TRP:CZ2	2:O:94:TYR:HB3	2.54	0.43
2:O:79:LEU:O	2:O:80:TYR:HD1	2.02	0.43
3:P:141:PRO:HD2	3:P:198:HIS:CE1	2.54	0.43
1:A:699:LEU:HD22	1:B:873:TYR:CZ	2.53	0.43
1:B:77:LYS:O	1:B:79:PHE:N	2.51	0.43
1:B:1088:HIS:ND1	1:B:1122:VAL:HG12	2.34	0.43
1:C:196:ASN:ND2	1:C:235:ILE:HB	2.33	0.43
1:C:577:ARG:HB3	1:C:584:ILE:HD13	2.01	0.43
3:N:110:VAL:HA	3:N:140:TYR:HB3	2.01	0.43
1:A:53:ASP:CG	1:A:54:LEU:H	2.22	0.43
1:A:144:TYR:CE2	1:A:246:ARG:HB3	2.54	0.43
1:A:323:THR:OG1	1:A:324:GLU:OE1	2.23	0.43
1:A:778:THR:HG22	1:A:865:LEU:HD12	2.00	0.43
1:A:898:PHE:HZ	1:A:1050:MET:HE1	1.84	0.43
1:B:159:VAL:HG23	1:B:160:TYR:CD1	2.54	0.43
1:B:354:ASN:HB3	1:B:399:SER:OG	2.19	0.43
2:H:194:SER:HA	2:H:197:LEU:HG	2.01	0.43
3:N:35:TRP:CE2	3:N:73:PHE:HB2	2.53	0.43
3:N:140:TYR:HA	3:N:141:PRO:C	2.38	0.43
3:P:30:SER:HA	3:P:68:GLY:H	1.84	0.43
1:A:666:ILE:HD13	1:A:670:ILE:HG22	2.00	0.43
1:A:736:VAL:HG12	1:A:858:LEU:HG	2.00	0.43
1:A:1081:ILE:HG23	1:A:1135:ASN:HB3	2.00	0.43
1:B:540:ASN:HB3	1:B:549:THR:HG22	2.00	0.43
1:C:100:ILE:HA	1:C:243:ALA:HB3	2.01	0.43
3:L:183:LYS:HG3	3:L:184:ALA:N	2.33	0.43
2:M:101:TRP:CG	2:M:102:ALA:N	2.87	0.43
1:A:108:THR:OG1	1:A:114:THR:HG21	2.18	0.42
1:A:363:ALA:O	1:A:526:GLY:HA2	2.18	0.42
1:A:722:VAL:O	1:A:934:ILE:HD11	2.19	0.42
1:B:68:ILE:HG23	1:B:69:HIS:N	2.34	0.42
2:M:37:VAL:HG13	2:M:95:TYR:HB2	2.01	0.42
1:A:1089:PHE:CE2	1:B:914:ASN:HA	2.47	0.42
1:B:168:PHE:HZ	1:B:229:LEU:HD22	1.83	0.42
1:B:977:LEU:HD23	1:B:993:ILE:HD11	2.01	0.42
1:C:128:ILE:HD13	1:C:229:LEU:HD11	2.01	0.42
1:C:1080:ALA:O	1:C:1081:ILE:HD13	2.19	0.42
2:H:131:PRO:HG2	3:L:123:GLU:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:47:LEU:HD13	3:L:73:PHE:CZ	2.53	0.42
3:L:93:ALA:O	3:L:94:TYR:HB2	2.19	0.42
2:O:154:PHE:HA	2:O:155:PRO:HA	1.81	0.42
1:A:46:SER:CA	1:A:279:TYR:O	2.67	0.42
1:A:168:PHE:CE1	1:A:231:ILE:HG13	2.54	0.42
1:A:443:SER:OG	1:A:500:THR:O	2.37	0.42
1:A:712:ILE:HD13	1:B:896:ILE:CD1	2.49	0.42
1:B:818:ILE:O	1:B:822:LEU:HG	2.19	0.42
1:C:1049:LEU:HD11	1:C:1067:TYR:HB2	2.00	0.42
2:M:45:LEU:HD22	3:N:89:GLN:HE22	1.85	0.42
3:P:207:LYS:HE3	3:P:207:LYS:HB3	1.87	0.42
1:B:53:ASP:HB2	1:B:55:PHE:CE1	2.54	0.42
1:B:959:LEU:O	1:B:963:VAL:HG23	2.20	0.42
1:B:962:LEU:HD22	1:B:1007:TYR:CD2	2.55	0.42
1:C:741:TYR:HD2	1:C:742:ILE:HG23	1.85	0.42
2:H:101:TRP:O	2:H:102:ALA:HB3	2.19	0.42
2:H:178:LEU:HD23	2:H:178:LEU:H	1.84	0.42
1:A:150:LYS:HA	1:A:150:LYS:HD3	1.78	0.42
1:B:1115:ILE:HG22	1:B:1137:VAL:HG13	2.00	0.42
1:C:423:TYR:HH	1:C:464:PHE:HE1	1.66	0.42
1:C:731:MET:HG2	1:C:774:GLN:OE1	2.18	0.42
2:H:40:ALA:HA	2:H:92:ALA:HA	2.01	0.42
3:L:134:CYS:HB3	3:L:146:VAL:HG11	2.02	0.42
3:P:132:VAL:HG12	3:P:179:LEU:HB3	2.02	0.42
1:A:326:ILE:HG12	1:A:539:VAL:HG11	2.00	0.42
1:A:645:THR:OG1	1:A:648:GLY:N	2.53	0.42
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.34	0.42
1:B:755:GLN:HE21	1:B:755:GLN:HB3	1.57	0.42
1:B:797:PHE:CD2	1:B:802:PHE:HD2	2.38	0.42
1:A:21:ARG:O	1:A:23:GLN:NE2	2.53	0.42
1:A:568:ASP:CG	1:A:569:ILE:H	2.22	0.42
1:A:715:PRO:HA	1:A:1072:GLU:HA	2.01	0.42
1:C:24:LEU:HG	1:C:78:ARG:NH1	2.35	0.42
1:C:36:VAL:HB	1:C:220:PHE:HE1	1.85	0.42
1:C:1095:PHE:CE1	1:C:1104:VAL:HG22	2.55	0.42
2:H:101:TRP:CZ3	2:H:104:GLY:HA3	2.55	0.42
2:H:215:VAL:HG22	2:H:217:LYS:HG3	2.02	0.42
3:L:133:VAL:HA	3:L:177:SER:O	2.20	0.42
3:P:87:TYR:CE1	3:P:101:GLY:HA3	2.55	0.42
1:A:870:ILE:O	1:A:874:THR:HG23	2.20	0.42
1:A:906:PHE:HD2	1:A:916:LEU:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:HG23	1:B:174:PRO:HA	2.00	0.42
1:B:450:ASN:H	1:B:497:PHE:HE1	1.66	0.42
1:B:1107:ARG:NH1	1:C:904:TYR:HB2	2.35	0.42
1:C:552:LEU:HD12	1:C:585:LEU:CB	2.50	0.42
2:M:38:ARG:HB2	2:M:94:TYR:CD1	2.55	0.42
3:P:198:HIS:HB3	3:P:201:LEU:HD12	2.01	0.42
1:A:126:VAL:HG23	1:A:174:PRO:HA	2.01	0.42
1:A:276:LEU:O	1:A:288:ALA:HA	2.19	0.42
1:A:537:LYS:O	1:A:539:VAL:HG23	2.20	0.42
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.85	0.42
1:A:922:LEU:O	1:A:926:GLN:HG3	2.20	0.42
1:A:927:PHE:O	1:A:931:ILE:HG12	2.20	0.42
1:A:1094:VAL:HG12	1:B:904:TYR:CE1	2.55	0.42
1:B:66:HIS:CD2	1:B:68:ILE:HB	2.52	0.42
1:C:25:PRO:HA	1:C:26:PRO:HD3	1.86	0.42
2:H:88:ALA:O	2:H:91:THR:HG23	2.20	0.42
3:L:61:ARG:NH2	3:L:77:SER:O	2.46	0.42
2:M:143:THR:HG22	2:M:193:PRO:HA	2.01	0.42
1:A:326:ILE:HG13	1:A:541:PHE:HA	2.01	0.42
1:A:421:TYR:HB2	1:A:454:ARG:C	2.41	0.42
1:A:541:PHE:CZ	1:A:587:ILE:HD13	2.55	0.42
1:A:750:SER:O	1:A:754:LEU:HD23	2.19	0.42
1:B:329:PHE:HE2	1:B:528:LYS:HD3	1.83	0.42
1:B:661:GLU:O	1:B:695:TYR:OH	2.36	0.42
1:B:825:LYS:HE3	1:B:939:SER:HA	2.02	0.42
1:C:905:ARG:HD3	1:C:1049:LEU:O	2.20	0.42
3:N:10:SER:HA	3:N:103:LYS:O	2.19	0.42
1:A:56:LEU:HD22	1:A:91:TYR:CD2	2.55	0.41
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.84	0.41
1:B:150:LYS:HD3	1:B:150:LYS:HA	1.77	0.41
1:B:178:ASP:HB3	1:B:188:ASN:CB	2.49	0.41
1:B:452:LEU:HA	1:B:494:SER:HA	2.01	0.41
1:B:653:ALA:HA	1:B:692:ILE:O	2.20	0.41
1:C:804:GLN:HE21	1:C:804:GLN:HB3	1.65	0.41
1:C:980:ILE:O	1:C:984:LEU:HB2	2.20	0.41
2:H:50:TYR:O	2:H:70:ILE:HG21	2.20	0.41
2:M:4:LEU:HB2	2:M:110:VAL:HG21	2.02	0.41
3:N:4:MET:CE	3:N:90:GLN:HG2	2.50	0.41
3:N:78:LEU:HD21	3:N:106:ILE:CG1	2.41	0.41
2:O:39:GLN:N	2:O:39:GLN:OE1	2.53	0.41
1:A:353:TRP:NE1	1:A:423:TYR:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:SER:N	1:A:435:ALA:O	2.53	0.41
1:A:382:VAL:HG21	1:A:390:LEU:HD22	2.02	0.41
1:A:737:ASP:OD1	1:A:737:ASP:N	2.53	0.41
1:A:985:ASP:H	1:C:383:SER:HB3	1.84	0.41
1:B:106:PHE:HZ	1:B:194:PHE:HD2	1.66	0.41
1:B:901:GLN:O	1:B:905:ARG:HG3	2.20	0.41
1:B:1050:MET:HE3	1:B:1052:PHE:CE1	2.55	0.41
1:C:121:ASN:ND2	1:C:175:PHE:HB2	2.35	0.41
1:C:462:LYS:HD3	1:C:463:PRO:HD2	2.02	0.41
2:H:99:ASP:HA	2:H:107:ALA:O	2.20	0.41
2:M:17:SER:HA	2:M:83:MET:O	2.19	0.41
2:O:101:TRP:HZ3	2:O:105:TRP:O	2.03	0.41
1:A:101:ILE:HG13	1:A:242:LEU:CD1	2.51	0.41
1:A:105:ILE:HG13	1:A:241:LEU:HD11	2.02	0.41
1:A:159:VAL:HG23	1:A:160:TYR:HD1	1.85	0.41
1:A:168:PHE:CZ	1:A:230:PRO:HD2	2.55	0.41
1:A:567:ARG:NH1	1:B:42:VAL:HG11	2.36	0.41
1:A:712:ILE:HD13	1:B:896:ILE:HD12	2.01	0.41
1:A:983:ARG:HB3	1:C:390:LEU:HD21	2.02	0.41
1:A:990:GLU:O	1:A:994:ASP:HB2	2.21	0.41
2:M:6:GLU:OE1	2:M:115:THR:HG22	2.20	0.41
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.83	0.41
1:A:178:ASP:HB3	1:A:188:ASN:CG	2.40	0.41
1:B:77:LYS:HD2	1:B:77:LYS:H	1.85	0.41
1:B:976:VAL:HG12	1:B:979:ASP:H	1.85	0.41
1:C:217:PRO:HD2	1:C:217:PRO:O	2.20	0.41
1:C:404:GLY:HA2	1:C:508:TYR:CD1	2.55	0.41
1:C:763:LEU:HD21	1:C:1005:GLN:NE2	2.35	0.41
2:O:6:GLU:HG2	2:O:96:CYS:SG	2.60	0.41
1:A:43:PHE:HB2	1:C:563:GLN:HG3	2.02	0.41
1:A:133:PHE:HB2	1:A:135:PHE:CE1	2.56	0.41
1:A:215:ASP:OD2	1:A:266:TYR:OH	2.39	0.41
1:A:1115:ILE:HG21	1:A:1137:VAL:HG22	2.02	0.41
1:C:535:LYS:NZ	1:C:554:GLU:OE2	2.37	0.41
3:L:120:PRO:HB3	3:L:130:ALA:HA	2.03	0.41
3:N:159:SER:HA	3:N:178:THR:O	2.20	0.41
3:N:186:TYR:O	3:N:211:ARG:HB3	2.20	0.41
2:O:73:ASP:O	2:O:77:ASN:HA	2.19	0.41
2:O:109:ASP:HA	3:P:46:LEU:HD11	2.02	0.41
3:P:7:SER:O	3:P:22:THR:N	2.54	0.41
1:A:106:PHE:HB3	1:A:235:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ALA:C	1:A:425:LEU:HD23	2.41	0.41
1:A:948:LEU:HA	1:A:951:VAL:HG12	2.03	0.41
1:B:115:GLN:OE1	1:B:115:GLN:HA	2.21	0.41
1:B:325:SER:HA	1:B:540:ASN:O	2.20	0.41
1:C:317:ASN:HA	1:C:594:GLY:HA2	2.01	0.41
1:C:996:LEU:HD23	1:C:996:LEU:HA	1.93	0.41
2:O:100:ARG:NH2	2:O:101:TRP:NE1	2.69	0.41
1:A:99:ASN:OD1	1:A:102:ARG:NH1	2.52	0.41
1:A:326:ILE:HG12	1:A:539:VAL:CG1	2.50	0.41
1:B:99:ASN:O	1:B:102:ARG:NH2	2.53	0.41
1:B:316:SER:O	1:B:595:VAL:HG12	2.19	0.41
1:B:980:ILE:HD11	1:B:992:GLN:HB3	2.03	0.41
1:C:276:LEU:O	1:C:288:ALA:HA	2.21	0.41
1:C:418:ILE:HA	1:C:422:ASN:ND2	2.36	0.41
1:C:734:THR:HG22	1:C:735:SER:N	2.36	0.41
2:M:20:LEU:O	2:M:80:TYR:HA	2.20	0.41
3:P:21:ILE:CD1	3:P:102:THR:HG21	2.50	0.41
1:A:1041:ASP:HB3	1:B:1030:SER:HB3	2.03	0.41
1:B:714:ILE:HD12	1:B:1096:VAL:HG11	2.02	0.41
1:C:53:ASP:HB2	1:C:55:PHE:CE1	2.56	0.41
1:C:108:THR:OG1	1:C:114:THR:HG21	2.20	0.41
3:L:140:TYR:HA	3:L:141:PRO:C	2.40	0.41
2:M:4:LEU:HD23	2:M:4:LEU:HA	1.90	0.41
3:N:30:SER:CA	3:N:68:GLY:H	2.33	0.41
2:O:154:PHE:HB2	2:O:183:LEU:HD22	2.02	0.41
3:P:39:LYS:HB2	3:P:42:LYS:HB3	2.03	0.41
3:P:185:ASP:O	3:P:189:HIS:HD2	2.03	0.41
1:A:590:CYS:O	1:A:592:PHE:HD1	2.03	0.41
1:A:1081:ILE:HG12	1:A:1095:PHE:CE2	2.56	0.41
1:B:826:VAL:HG11	1:B:1057:PRO:HB2	2.03	0.41
1:B:1013:ILE:HD13	1:C:1012:LEU:HD23	2.01	0.41
1:C:108:THR:HG23	1:C:234:ASN:O	2.20	0.41
1:C:205:SER:HB3	1:C:226:LEU:HD11	2.02	0.41
1:C:334:ASN:O	1:C:361:CYS:HB2	2.21	0.41
1:C:392:PHE:CD2	1:C:515:PHE:CD1	3.09	0.41
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.50	0.41
2:H:82:GLN:NE2	2:H:83:MET:O	2.54	0.41
3:L:110:VAL:HG13	3:L:140:TYR:O	2.21	0.41
2:M:73:ASP:O	2:M:77:ASN:HA	2.21	0.41
2:M:87:ARG:HA	2:M:87:ARG:HD3	1.70	0.41
2:M:101:TRP:CD1	2:M:102:ALA:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:60:TYR:HB2	2:O:65:LYS:CD	2.46	0.41
2:O:100:ARG:NH2	2:O:101:TRP:HE1	2.12	0.41
3:P:192:TYR:O	3:P:208:SER:HA	2.20	0.41
1:A:355:ARG:HD3	1:A:396:TYR:CD2	2.56	0.41
1:A:664:ILE:O	1:A:666:ILE:HD12	2.21	0.41
1:A:779:GLN:HE21	1:A:864:LEU:HD22	1.86	0.41
1:C:95:THR:O	1:C:263:ALA:HB1	2.21	0.41
1:C:550:GLY:HA2	1:C:590:CYS:SG	2.61	0.41
1:C:966:LEU:CD2	1:C:1000:ARG:HD3	2.51	0.41
1:C:1092:GLU:OE1	1:C:1093:GLY:N	2.54	0.41
3:P:117:ILE:HG13	3:P:133:VAL:O	2.21	0.41
1:A:664:ILE:HB	1:A:672:ALA:HB3	2.03	0.40
1:B:118:LEU:HG	1:B:120:VAL:HG23	2.02	0.40
1:B:328:ARG:HG3	1:B:543:PHE:CE1	2.56	0.40
2:O:154:PHE:CB	2:O:183:LEU:HD22	2.51	0.40
1:A:186:PHE:CD2	1:A:209:PRO:HB2	2.56	0.40
1:A:617:CYS:N	1:A:644:GLN:OE1	2.48	0.40
1:B:201:PHE:CD2	1:B:203:ILE:HD11	2.56	0.40
1:B:214:ARG:CG	2:O:104:GLY:HA2	2.46	0.40
1:B:435:ALA:HA	1:B:509:ARG:O	2.20	0.40
1:B:564:GLN:HG2	1:B:565:PHE:H	1.86	0.40
1:B:934:ILE:HD13	1:B:934:ILE:HA	1.92	0.40
1:C:788:ILE:HD13	1:C:872:GLN:HE21	1.86	0.40
1:C:821:LEU:HD22	1:C:935:GLN:HG3	2.03	0.40
2:O:174:PHE:HA	2:O:175:PRO:HD3	1.93	0.40
1:A:69:HIS:CE1	2:M:32:TYR:HH	2.39	0.40
1:A:965:GLN:OE1	1:B:758:SER:OG	2.30	0.40
1:B:825:LYS:HA	1:B:825:LYS:HD3	1.90	0.40
1:B:1050:MET:HE3	1:B:1052:PHE:CZ	2.56	0.40
1:C:145:TYR:HB2	1:C:152:TRP:CZ2	2.56	0.40
1:C:220:PHE:HD2	1:C:287:ASP:HA	1.86	0.40
2:H:154:PHE:HA	2:H:155:PRO:HA	1.94	0.40
3:L:55:GLU:OE1	3:L:55:GLU:N	2.52	0.40
3:N:198:HIS:HB3	3:N:201:LEU:HD12	2.02	0.40
3:N:209:PHE:CG	3:N:210:ASN:N	2.89	0.40
1:A:979:ASP:O	1:A:983:ARG:HG2	2.22	0.40
1:B:718:PHE:HE1	1:B:923:ILE:HG12	1.86	0.40
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.83	0.40
1:C:914:ASN:O	1:C:918:GLU:HG2	2.22	0.40
1:C:985:ASP:C	1:C:987:PRO:HD2	2.42	0.40
2:H:17:SER:HA	2:H:83:MET:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:160:VAL:HG21	2:H:188:SER:HB3	2.04	0.40
3:N:46:LEU:HB3	3:N:55:GLU:OE2	2.20	0.40
1:B:655:HIS:HA	1:B:694:ALA:O	2.21	0.40
1:B:786:LYS:H	1:B:786:LYS:HG2	1.72	0.40
1:C:191:GLU:O	1:C:205:SER:HA	2.22	0.40
1:C:1125:ASN:ND2	1:C:1127:ASP:OD2	2.55	0.40
2:H:54:SER:HA	2:H:72:ARG:HD2	2.03	0.40
2:H:175:PRO:CD	3:L:164:THR:HA	2.52	0.40
2:H:203:ILE:CD1	2:H:218:LYS:CD	3.00	0.40
2:M:74:ASN:C	2:M:75:SER:HG	2.24	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	993/1271 (78%)	935 (94%)	55 (6%)	3 (0%)	41	75
1	B	1011/1271 (80%)	957 (95%)	51 (5%)	3 (0%)	41	75
1	C	1004/1271 (79%)	953 (95%)	48 (5%)	3 (0%)	41	75
2	H	221/228 (97%)	194 (88%)	22 (10%)	5 (2%)	6	36
2	M	221/228 (97%)	195 (88%)	22 (10%)	4 (2%)	8	41
2	O	221/228 (97%)	195 (88%)	22 (10%)	4 (2%)	8	41
3	L	213/214 (100%)	199 (93%)	13 (6%)	1 (0%)	29	68
3	N	213/214 (100%)	198 (93%)	13 (6%)	2 (1%)	17	56
3	P	213/214 (100%)	198 (93%)	13 (6%)	2 (1%)	17	56
All	All	4310/5139 (84%)	4024 (93%)	259 (6%)	27 (1%)	29	64

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	100	ARG
2	M	100	ARG
2	O	100	ARG
1	A	262	ALA
1	B	262	ALA
1	C	262	ALA
2	H	30	SER
2	M	30	SER
2	O	30	SER
3	N	92	TYR
3	P	92	TYR
2	H	99	ASP
3	L	94	TYR
2	M	99	ASP
3	N	94	TYR
2	O	99	ASP
1	A	68	ILE
1	B	68	ILE
1	C	68	ILE
2	M	102	ALA
2	O	102	ALA
3	P	94	TYR
2	H	102	ALA
1	A	261	GLY
1	B	261	GLY
1	C	261	GLY
2	H	104	GLY

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	867/1109 (78%)	865 (100%)	2 (0%)	93 98
1	B	879/1109 (79%)	875 (100%)	4 (0%)	88 94
1	C	861/1109 (78%)	860 (100%)	1 (0%)	93 98
2	H	183/188 (97%)	181 (99%)	2 (1%)	73 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	M	183/188 (97%)	183 (100%)	0	100 100
2	O	183/188 (97%)	181 (99%)	2 (1%)	73 88
3	L	189/188 (100%)	189 (100%)	0	100 100
3	N	189/188 (100%)	189 (100%)	0	100 100
3	P	189/188 (100%)	189 (100%)	0	100 100
All	All	3723/4455 (84%)	3712 (100%)	11 (0%)	92 97

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	955	ASN
1	A	1107	ARG
1	B	196	ASN
1	B	360	ASN
1	B	755	GLN
1	B	914	ASN
1	C	378	LYS
2	H	113	GLN
2	H	163	ASN
2	O	101	TRP
2	O	179	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	703	ASN
1	A	957	GLN
1	A	1002	GLN
1	B	66	HIS
1	B	360	ASN
1	C	196	ASN
1	C	394	ASN
1	C	544	ASN
1	C	913	GLN
3	L	90	GLN
2	M	39	GLN
3	P	166	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

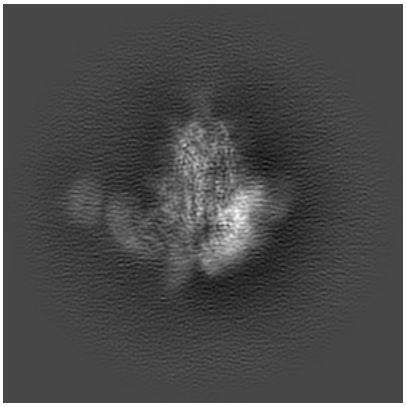
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24787. These allow visual inspection of the internal detail of the map and identification of artifacts.

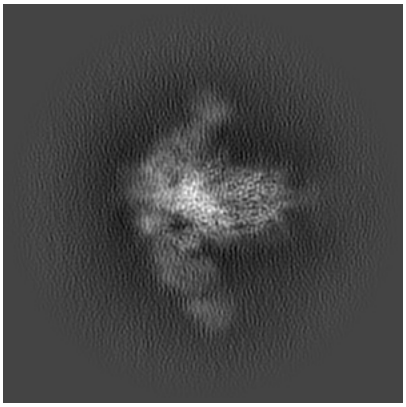
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

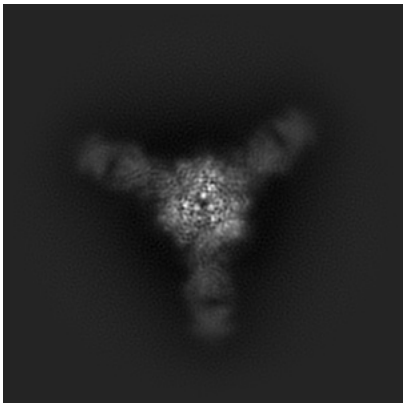
6.1.1 Primary map



X



Y

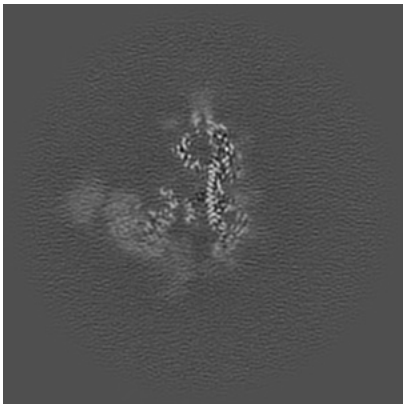


Z

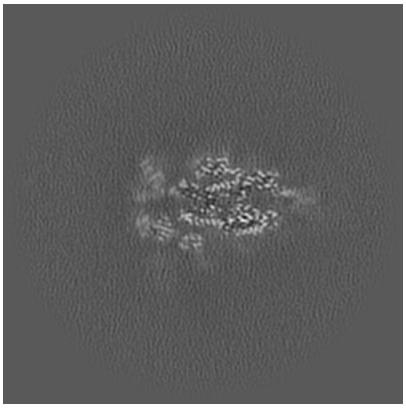
The images above show the map projected in three orthogonal directions.

6.2 Central slices

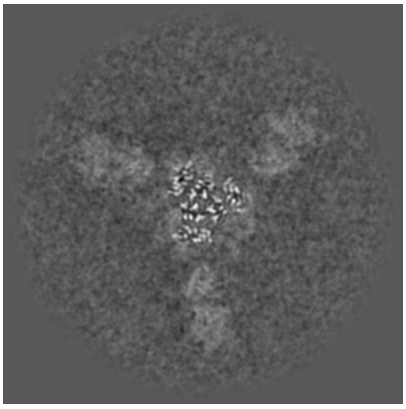
6.2.1 Primary map



X Index: 216



Y Index: 216

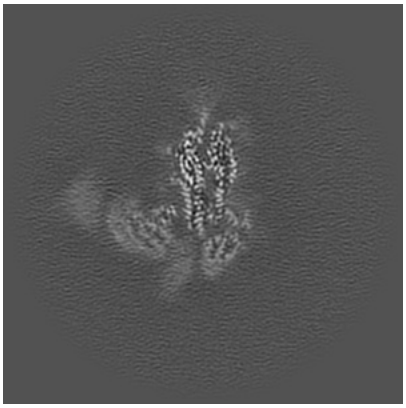


Z Index: 216

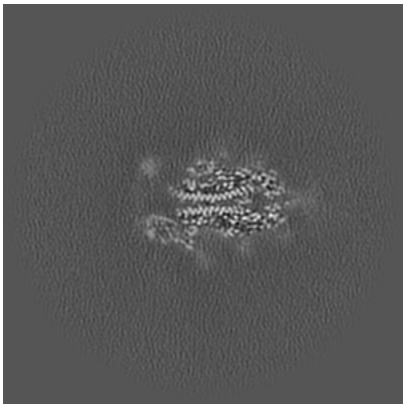
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

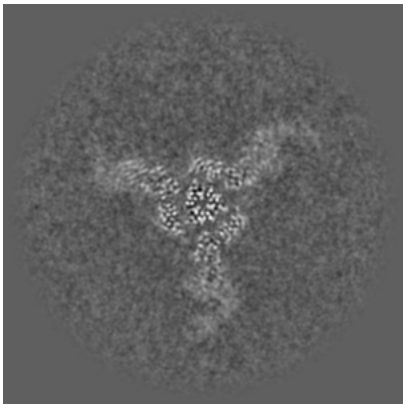
6.3.1 Primary map



X Index: 226



Y Index: 211

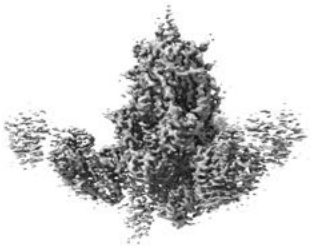


Z Index: 200

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 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

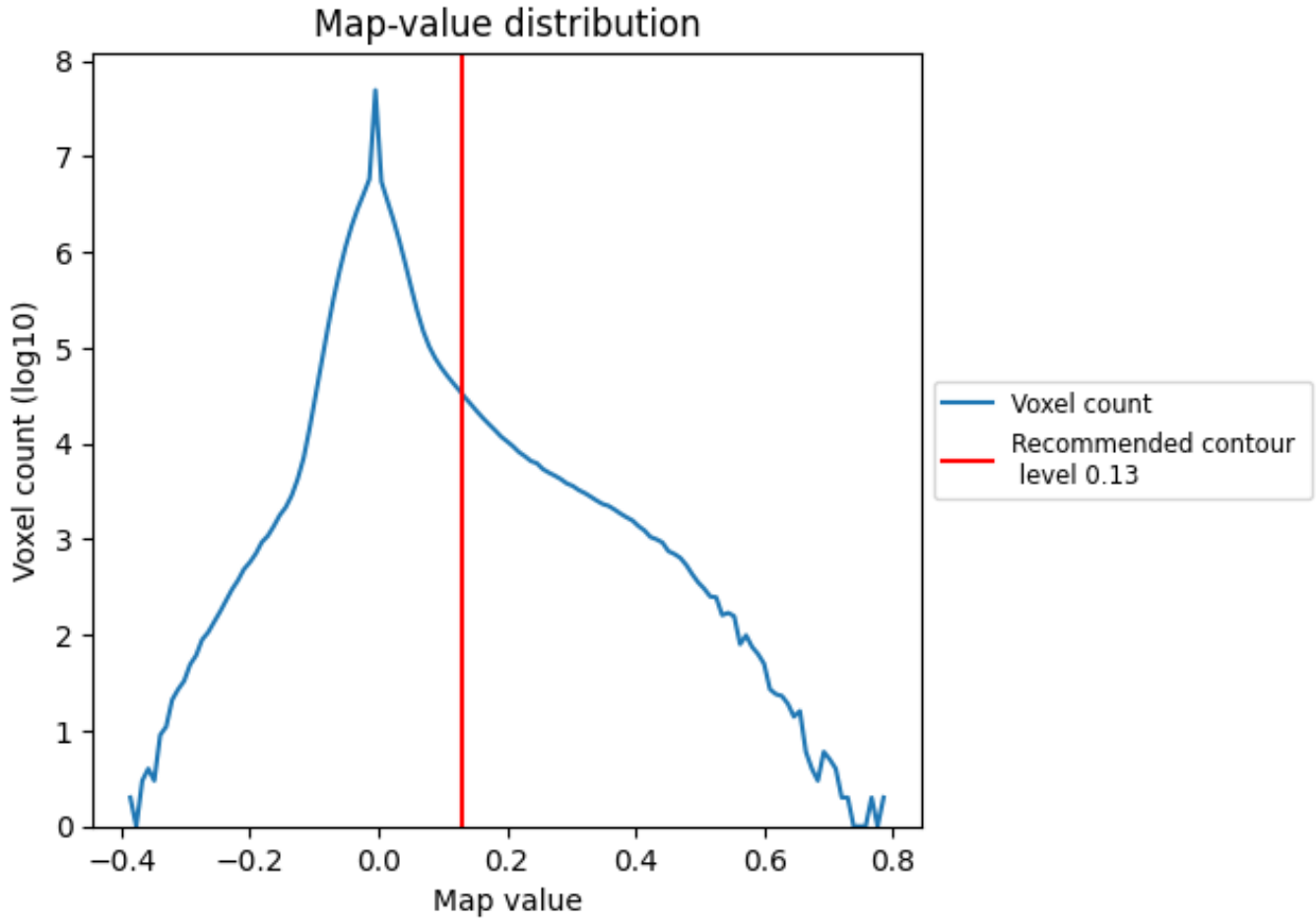
6.5 Mask visualisation (i)

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

7 Map analysis

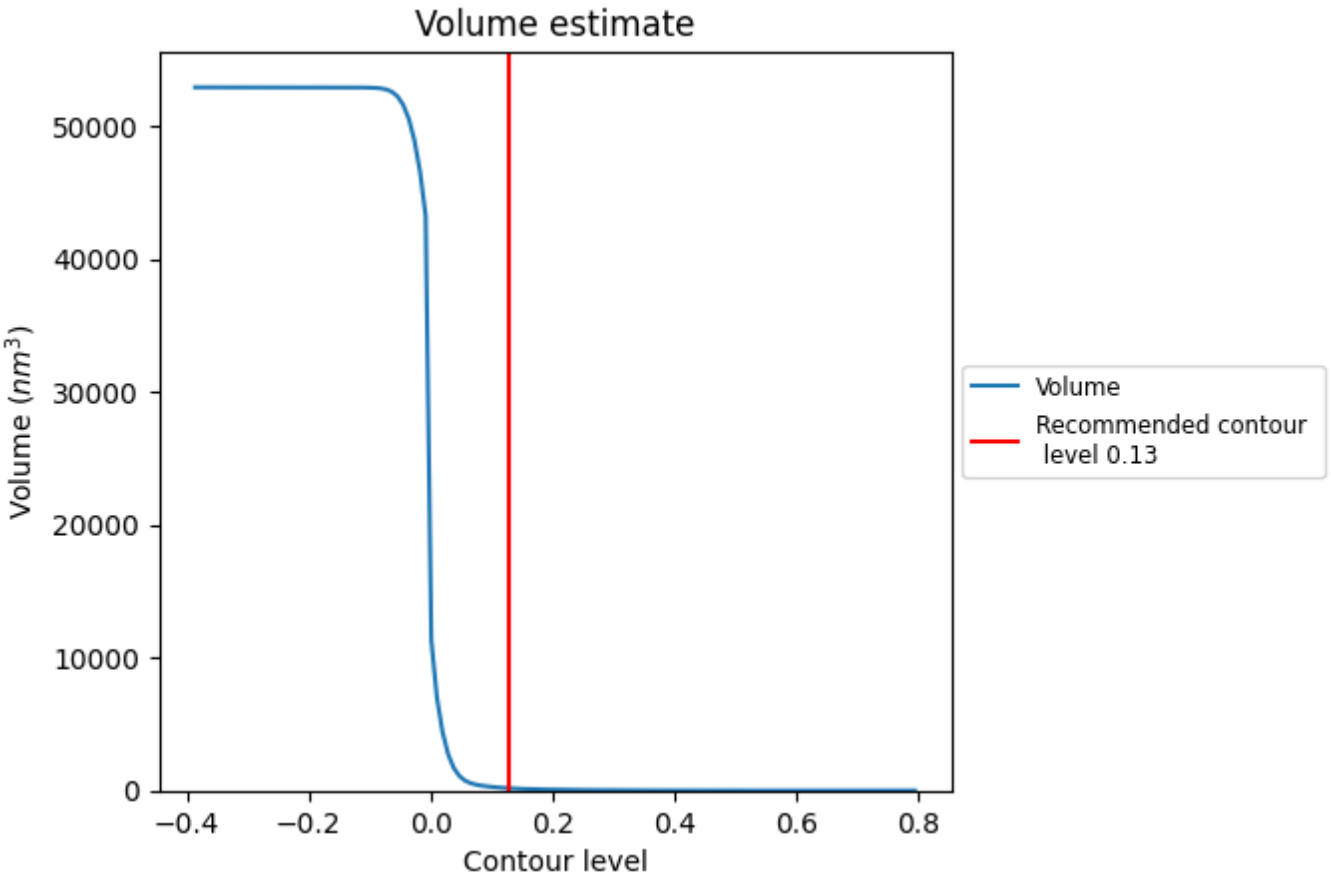
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

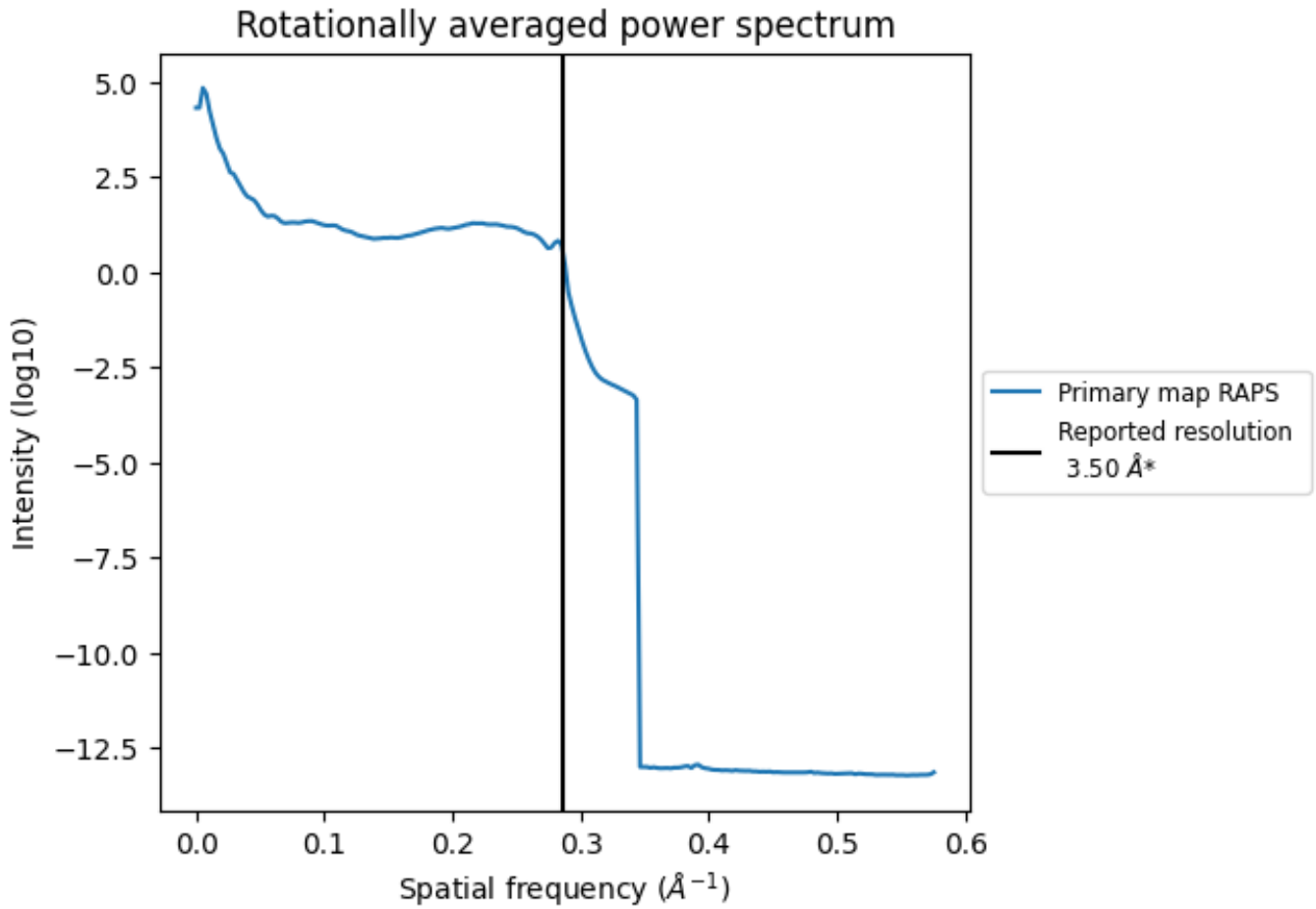
7.2 Volume estimate



The volume at the recommended contour level is 174 nm^3; this corresponds to an approximate mass of 157 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)

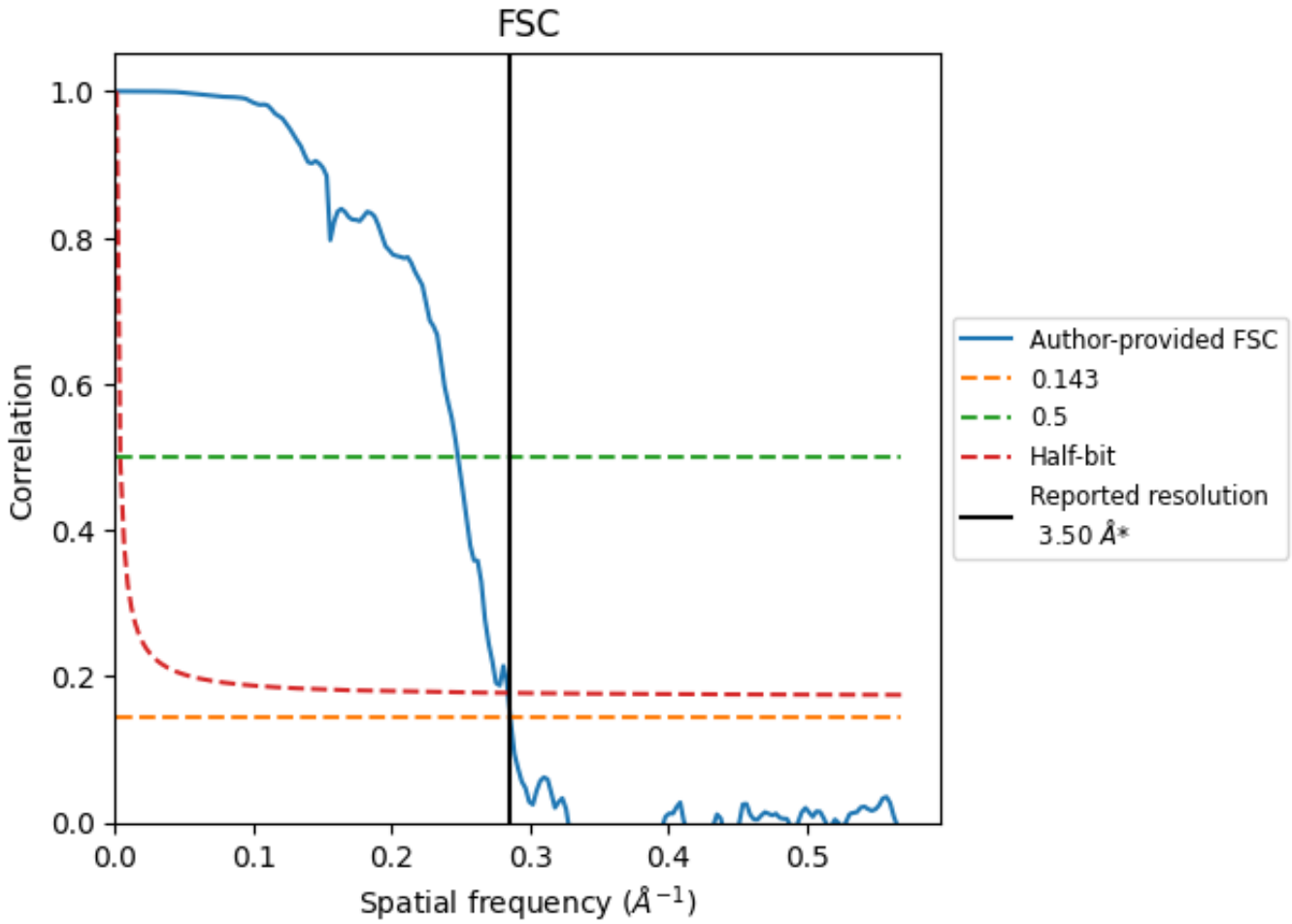


*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

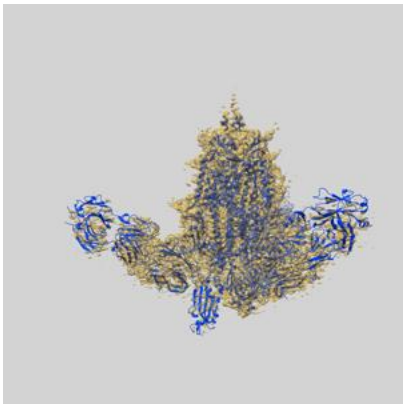
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.03	3.52
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

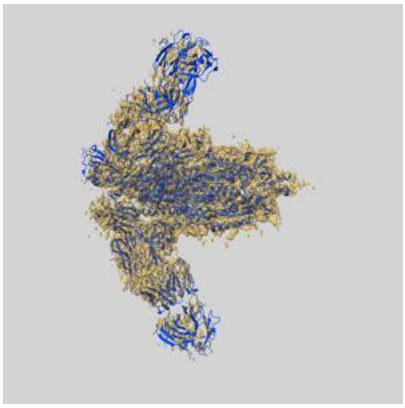
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24787 and PDB model 7S0D. Per-residue inclusion information can be found in section 3 on page 10.

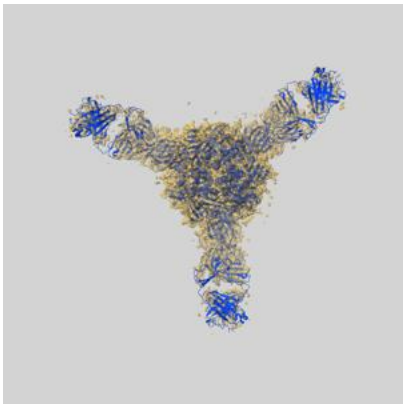
9.1 Map-model overlay



X



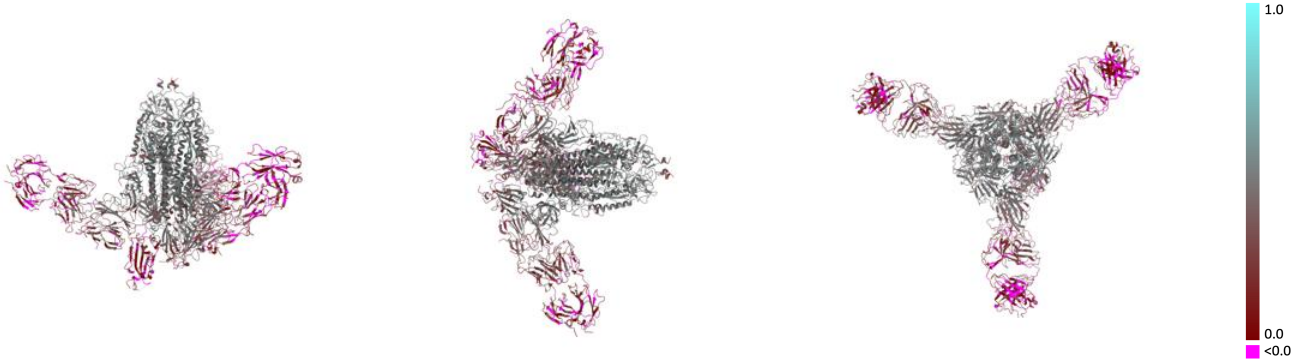
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

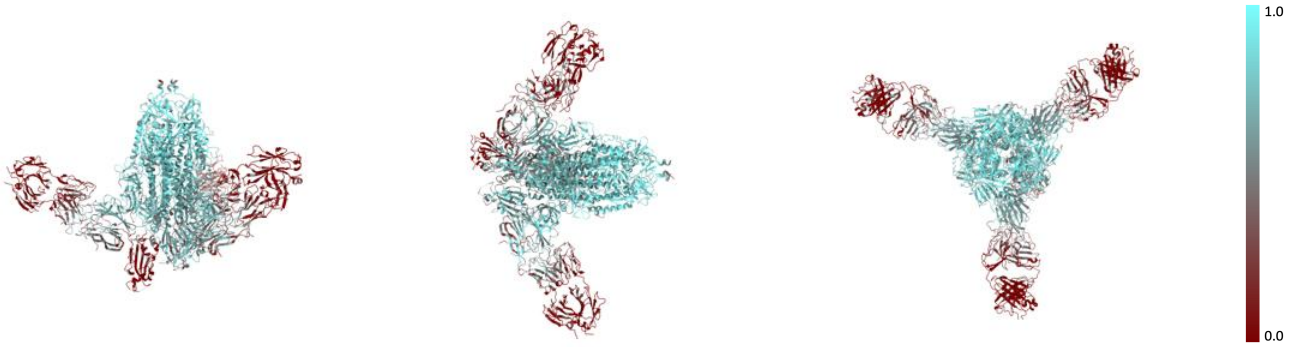
9.2 Q-score mapped to coordinate model



X Y Z

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.

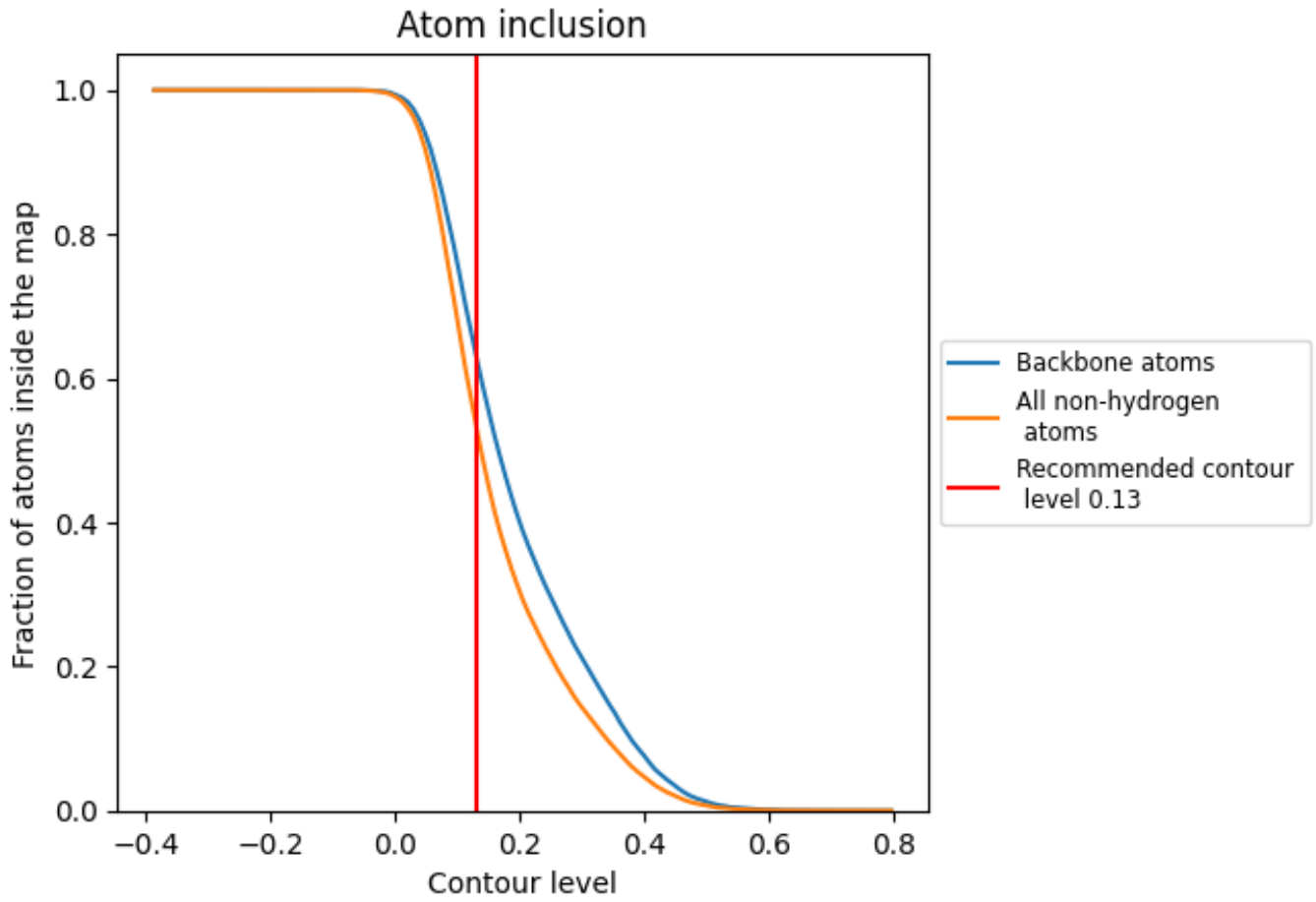
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5327	0.3310
A	0.6160	0.3660
B	0.7091	0.4140
C	0.7289	0.4300
H	0.2526	0.2140
L	0.1595	0.2000
M	0.1782	0.1330
N	0.1145	0.1300
O	0.2096	0.1530
P	0.0942	0.1200