Full wwPDB EM Validation Report

May 13, 2025 – 11:22 AM EDT

PDB ID	:	7RKV / pdb_00007rkv
EMDB ID	:	EMD-24504
Title	:	Structure of the SARS-CoV-2 S 6P trimer in complex with neutralizing antibody C118 (State 1)
Authors	:	Barnes, C.O.; Jette, C.A.; Bjorkman, P.J.
Deposited on	:	2021-07-22
Resolution	:	3.45 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:

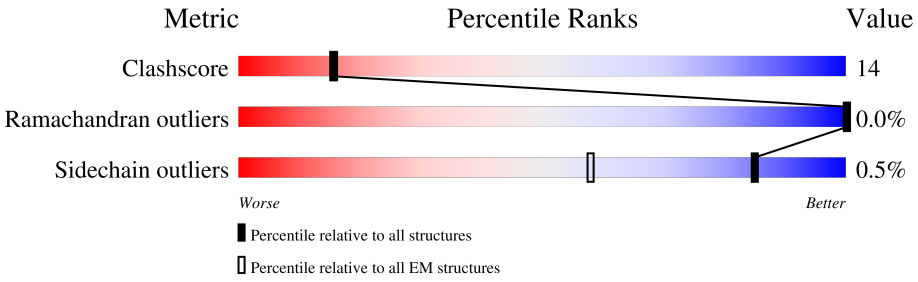
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.45 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	63% 15% • 21%
1	B	1271	62% 15% • 21%
1	C	1271	64% 13% • 21%
2	D	239	73% 66% 23% 10%
2	E	239	74% 69% 21% 10%
2	G	239	72% 68% 21% 10%
3	F	217	77% 76% 22% •
3	H	217	78% 76% 22% •

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Mol	Chain	Length	Quality of chain
3	L	217	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	1311	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31357 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	998	Total	C	N	O	S	0	0
			7064	4529	1209	1292	34		
1	B	998	Total	C	N	O	S	0	0
			7026	4501	1207	1284	34		
1	C	998	Total	C	N	O	S	0	0
			7064	4529	1209	1292	34		

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	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	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	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	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	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	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

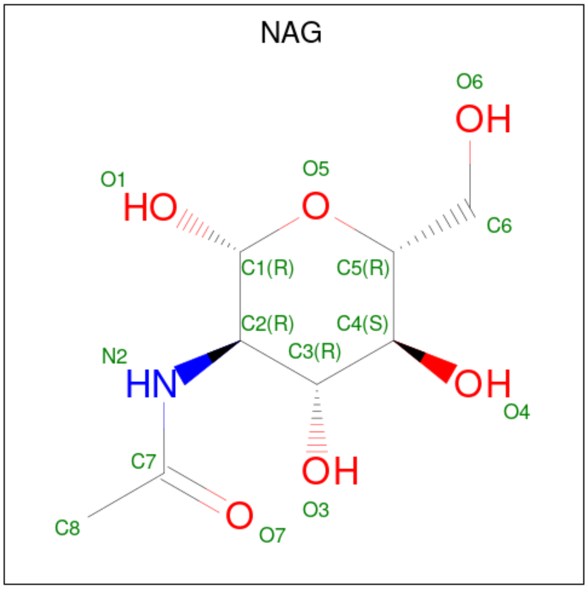
- Molecule 2 is a protein called C118 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	214	Total	C	N	O	S	0	0
			1629	1033	273	317	6		
2	E	214	Total	C	N	O	S	0	0
			1629	1033	273	317	6		
2	G	214	Total	C	N	O	S	0	0
			1629	1033	273	317	6		

- Molecule 3 is a protein called C118 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	214	Total	C	N	O	S	0	0
			1590	994	268	323	5		
3	F	214	Total	C	N	O	S	0	0
			1590	994	268	323	5		
3	L	214	Total	C	N	O	S	0	0
			1590	994	268	323	5		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0

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Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0

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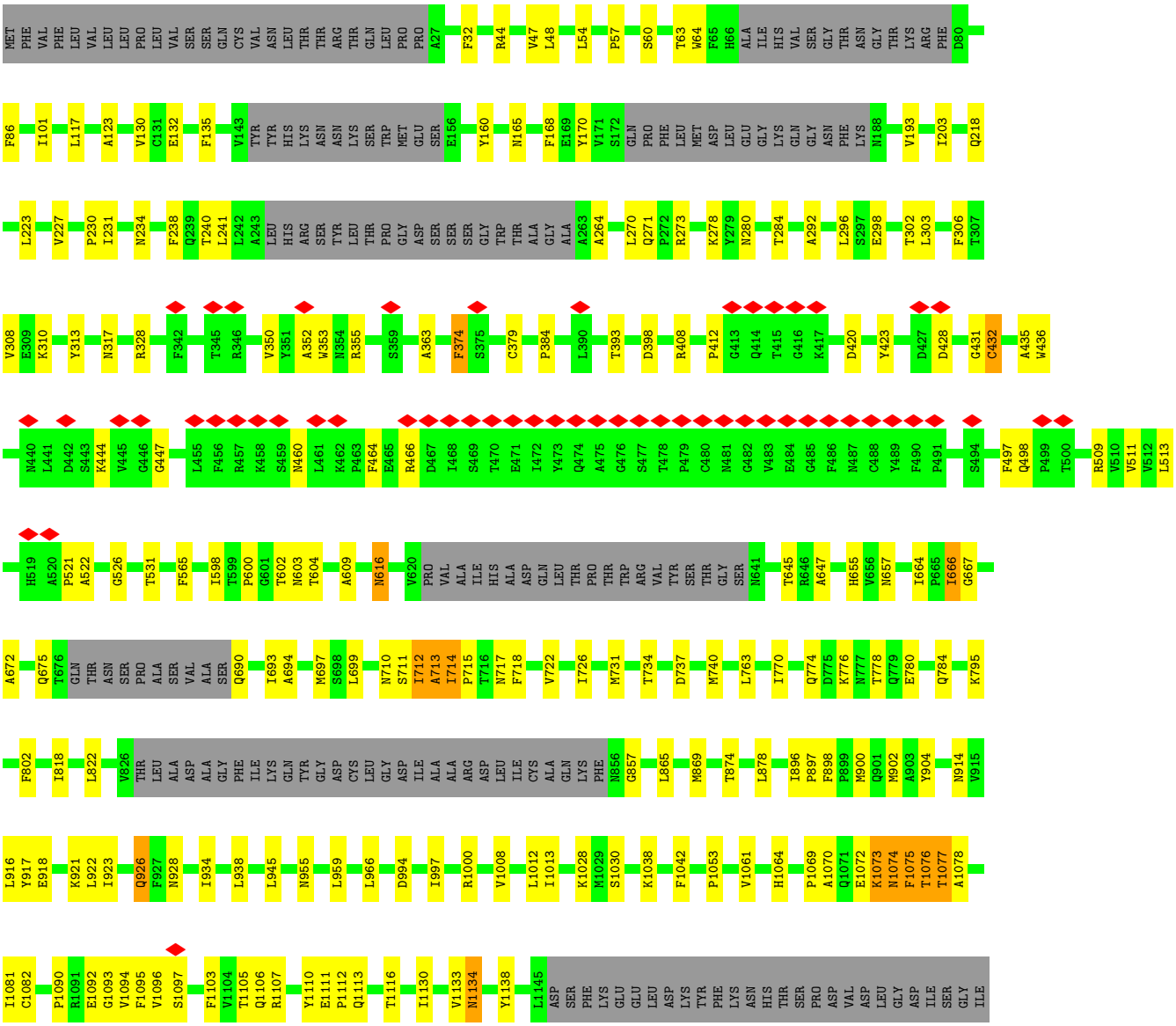
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

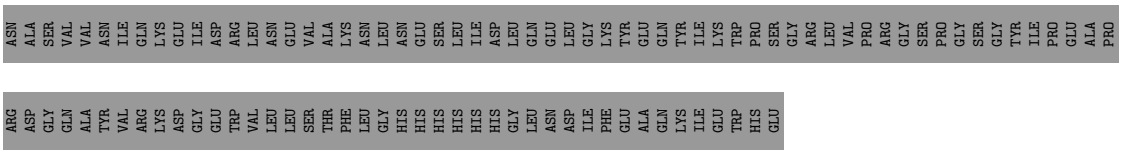
3 Residue-property plots (i)

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

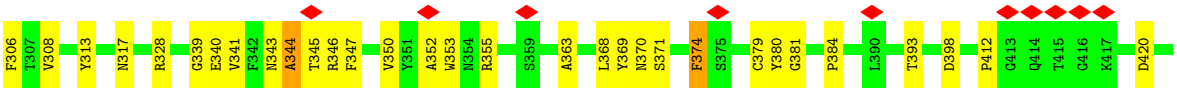
Chain A:

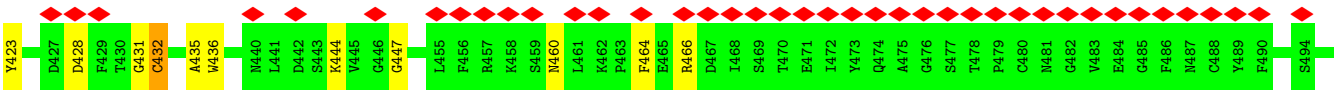


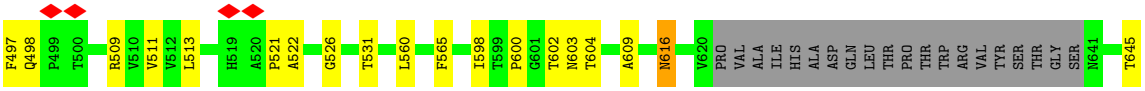


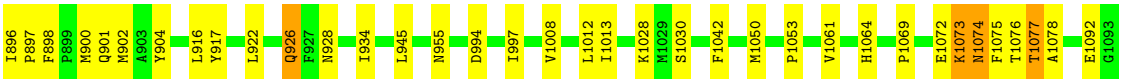
• Molecule 1: Spike glycoprotein

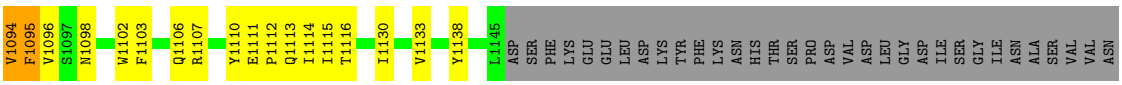
Chain B:

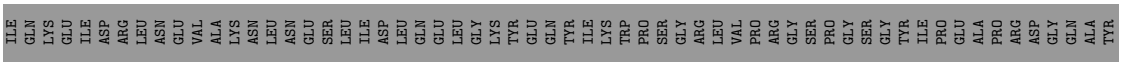


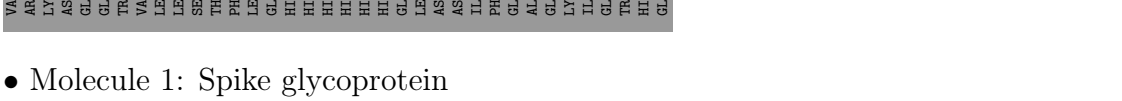






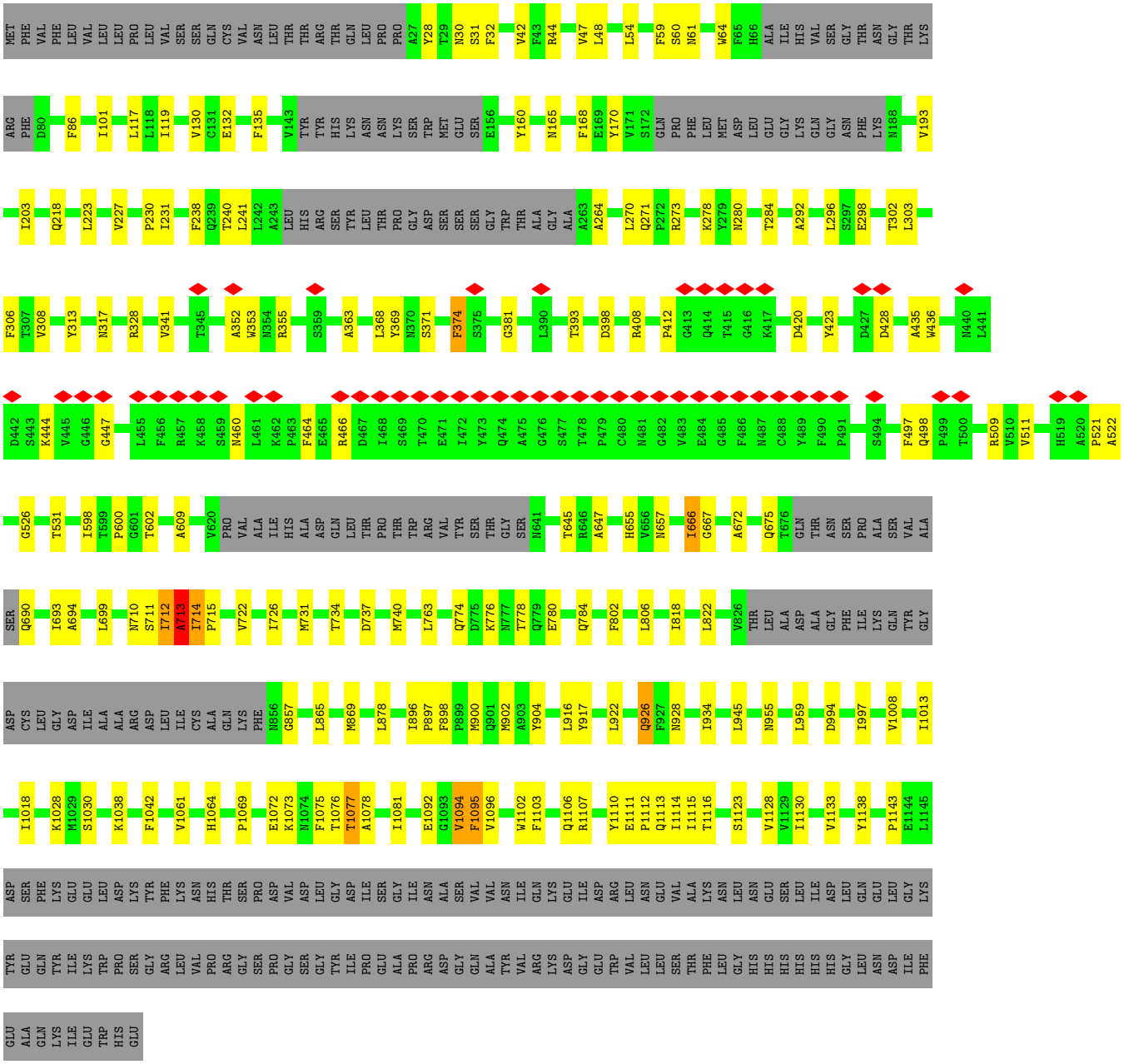






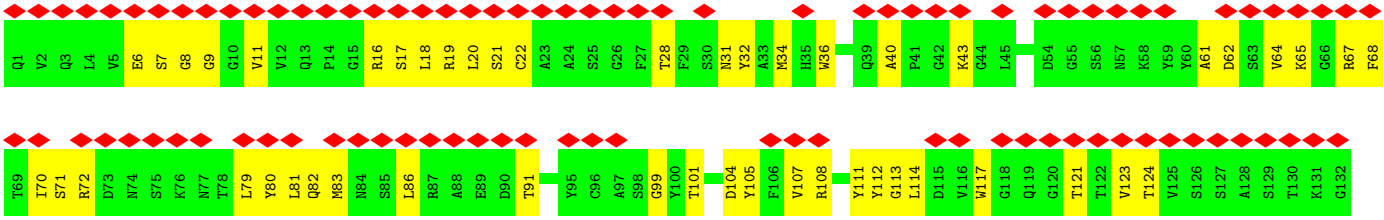
• Molecule 1: Spike glycoprotein

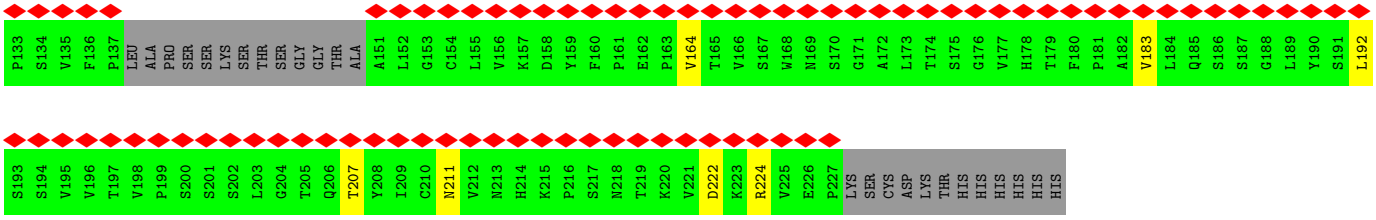
Chain C:



• Molecule 2: C118 Fab Heavy Chain

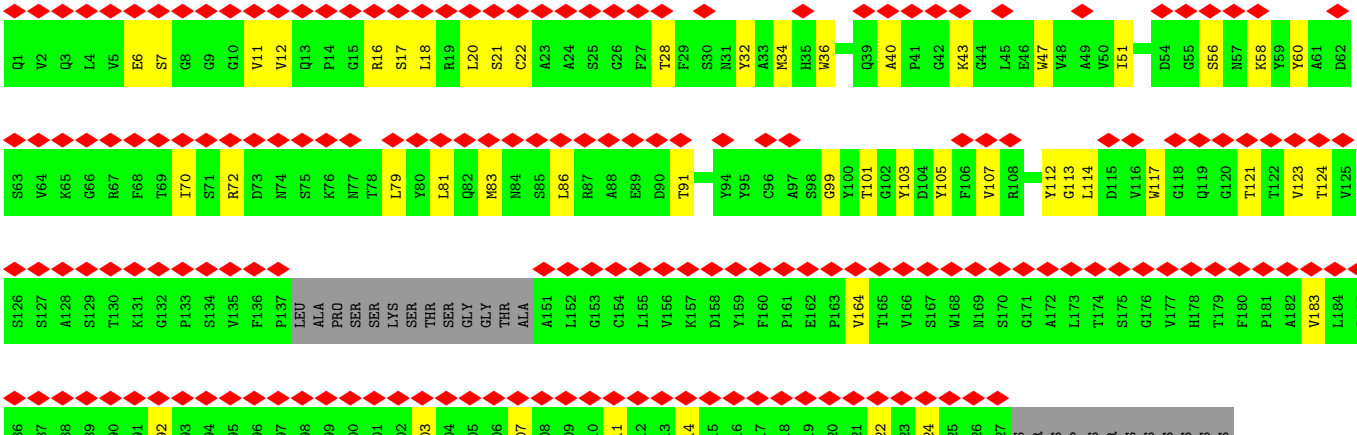
Chain D:





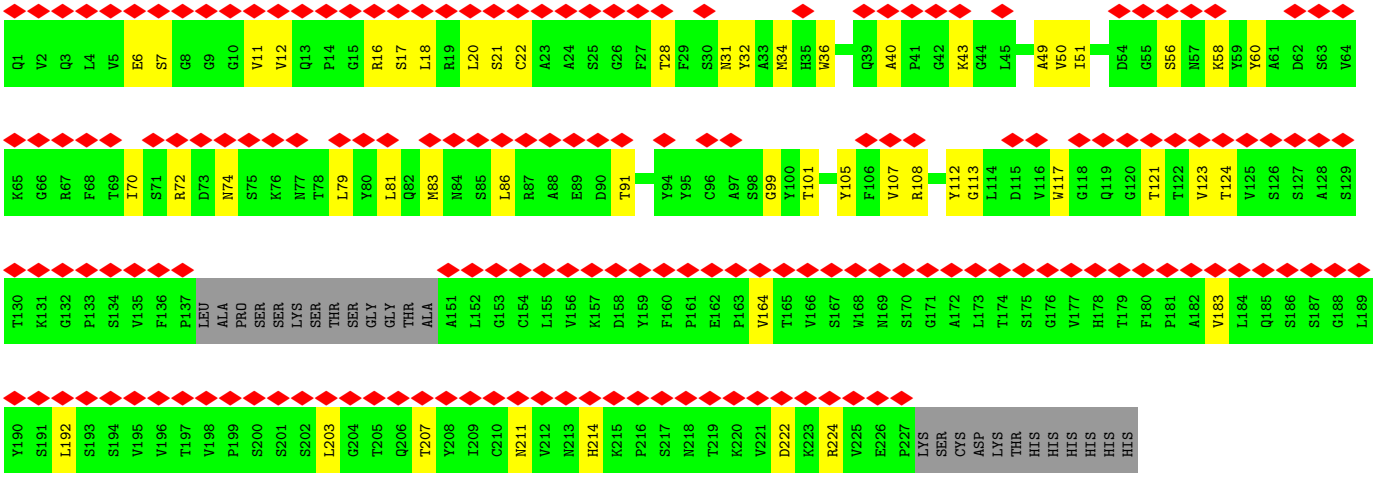
• Molecule 2: C118 Fab Heavy Chain

Chain E:



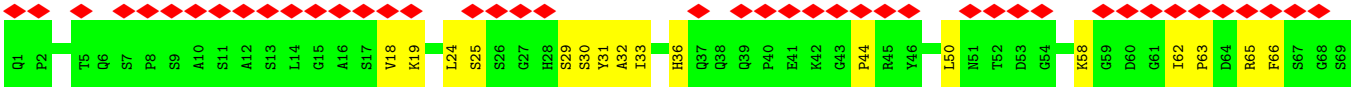
• Molecule 2: C118 Fab Heavy Chain

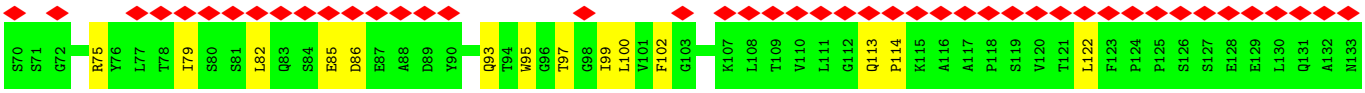
Chain G:

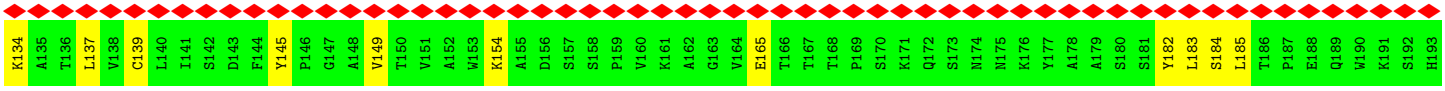


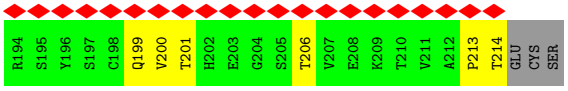
• Molecule 3: C118 Fab Light Chain

Chain H:



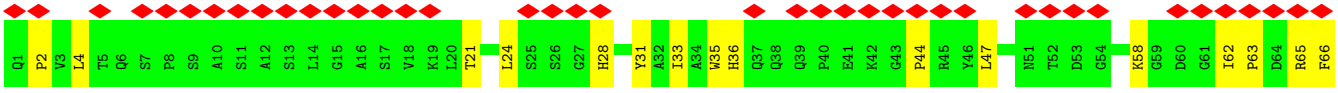


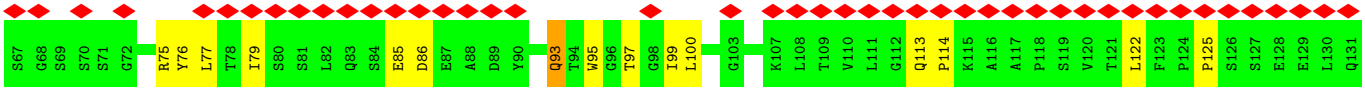


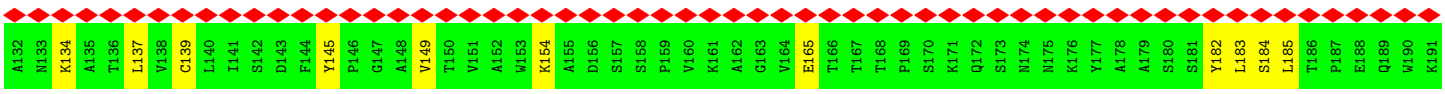


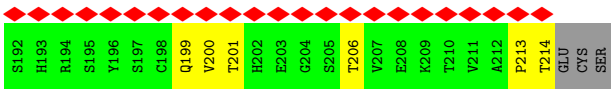
• Molecule 3: C118 Fab Light Chain

Chain F:



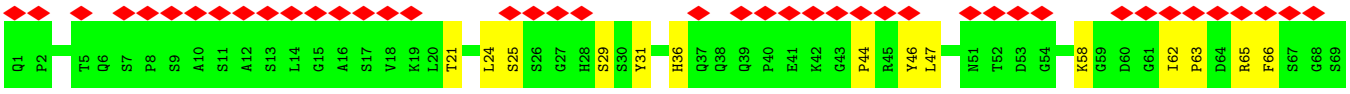


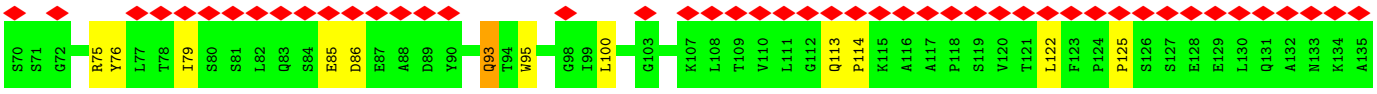


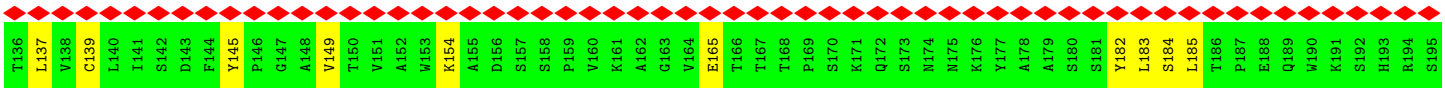


• Molecule 3: C118 Fab Light Chain

Chain L:








Y196
S197
C198
Q199
V200
T201
H202
E203
G204
S205
T206
V207
E208
K209
T210
V211
A212
P213
T214
GLU
CYS
SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	53728	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)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.395	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.09	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

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

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	0.52	3/7222 (0.0%)	0.95	36/9891 (0.4%)
1	B	0.51	3/7181 (0.0%)	0.96	38/9840 (0.4%)
1	C	0.51	3/7222 (0.0%)	0.92	26/9891 (0.3%)
2	D	0.65	0/1670	0.88	0/2275
2	E	0.53	0/1670	0.79	0/2275
2	G	0.51	0/1670	0.77	0/2275
3	F	0.45	0/1629	0.76	1/2221 (0.0%)
3	H	0.43	0/1629	0.74	1/2221 (0.0%)
3	L	0.43	0/1629	0.74	1/2221 (0.0%)
All	All	0.51	9/31522 (0.0%)	0.90	103/43110 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	2
2	D	0	1
2	G	0	1
All	All	0	7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	928	ASN	CB-CG	-8.75	1.30	1.52
1	C	928	ASN	CB-CG	-8.72	1.30	1.52
1	A	928	ASN	CB-CG	-8.71	1.30	1.52
1	A	1075	PHE	C-N	8.71	1.46	1.33
1	C	1075	PHE	C-N	8.69	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1075	PHE	C-N	8.66	1.46	1.33
1	A	1076	THR	C-N	7.43	1.43	1.33
1	B	1076	THR	C-N	7.37	1.43	1.33
1	C	1076	THR	C-N	7.37	1.43	1.33

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1075	PHE	CA-C-N	-17.20	96.63	122.09
1	A	1075	PHE	C-N-CA	-17.20	96.63	122.09
1	B	1075	PHE	CA-C-N	-17.20	96.64	122.09
1	B	1075	PHE	C-N-CA	-17.20	96.64	122.09
1	C	1075	PHE	CA-C-N	-17.20	96.64	122.09
1	C	1075	PHE	C-N-CA	-17.20	96.64	122.09
1	A	926	GLN	CA-CB-CG	14.10	142.31	114.10
1	B	926	GLN	CA-CB-CG	14.09	142.28	114.10
1	C	926	GLN	CA-CB-CG	14.09	142.28	114.10
1	B	347	PHE	CA-C-N	9.48	141.23	121.32
1	B	347	PHE	C-N-CA	9.48	141.23	121.32
1	A	713	ALA	N-CA-C	9.10	123.56	108.73
1	B	713	ALA	N-CA-C	8.97	123.55	108.20
1	C	713	ALA	N-CA-C	8.96	123.52	108.20
1	B	347	PHE	N-CA-C	8.87	129.69	110.80
1	A	926	GLN	N-CA-CB	-8.55	97.56	110.12
1	B	926	GLN	N-CA-CB	-8.54	97.57	110.12
1	C	926	GLN	N-CA-CB	-8.53	97.58	110.12
1	B	926	GLN	CB-CA-C	8.43	124.78	110.79
1	A	926	GLN	CB-CA-C	8.43	124.78	110.79
1	C	926	GLN	CB-CA-C	8.40	124.74	110.79
1	A	1133	VAL	CA-C-N	-8.20	111.52	122.42
1	A	1133	VAL	C-N-CA	-8.20	111.52	122.42
1	A	1134	ASN	CA-CB-CG	7.96	120.56	112.60
3	F	114	PRO	N-CA-C	7.76	123.42	111.15
3	L	114	PRO	N-CA-C	7.74	123.38	111.15
3	H	114	PRO	N-CA-C	7.73	123.37	111.15
1	B	1095	PHE	CB-CA-C	7.43	121.99	109.80
1	C	1095	PHE	CB-CA-C	7.40	121.93	109.80
1	A	1074	ASN	N-CA-CB	-7.24	98.69	110.21
1	B	1074	ASN	N-CA-CB	-7.23	98.71	110.21
1	C	928	ASN	CB-CA-C	-7.22	98.81	110.79
1	A	928	ASN	CB-CA-C	-7.20	98.84	110.79
1	B	928	ASN	CB-CA-C	-7.19	98.86	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	711	SER	CA-C-N	-7.11	113.06	122.94
1	A	711	SER	C-N-CA	-7.11	113.06	122.94
1	C	711	SER	CA-C-N	-7.10	113.08	122.94
1	C	711	SER	C-N-CA	-7.10	113.08	122.94
1	B	711	SER	CA-C-N	-7.09	113.08	122.94
1	B	711	SER	C-N-CA	-7.09	113.08	122.94
1	A	1134	ASN	CB-CA-C	7.05	122.44	110.81
1	C	1076	THR	CA-C-N	7.02	134.62	122.82
1	C	1076	THR	C-N-CA	7.02	134.62	122.82
1	A	1076	THR	CA-C-N	7.02	134.61	122.82
1	A	1076	THR	C-N-CA	7.02	134.61	122.82
1	B	1076	THR	CA-C-N	7.00	134.59	122.82
1	B	1076	THR	C-N-CA	7.00	134.59	122.82
1	B	1077	THR	N-CA-C	6.64	119.50	109.41
1	C	1077	THR	N-CA-C	6.63	119.49	109.41
1	A	1077	THR	N-CA-C	6.63	119.48	109.41
1	A	795	LYS	CA-C-N	-6.58	113.13	122.41
1	A	795	LYS	C-N-CA	-6.58	113.13	122.41
1	B	795	LYS	CA-C-N	-6.55	113.08	122.77
1	B	795	LYS	C-N-CA	-6.55	113.08	122.77
1	A	616	ASN	CB-CA-C	6.51	121.44	109.46
1	B	616	ASN	CB-CA-C	6.51	121.43	109.46
1	B	710	ASN	N-CA-C	6.45	120.46	111.56
1	C	710	ASN	N-CA-C	6.42	120.42	111.56
1	A	1134	ASN	N-CA-CB	6.41	120.40	110.21
1	A	710	ASN	N-CA-C	6.41	120.40	111.56
1	B	1073	LYS	CA-C-N	6.15	130.60	122.42
1	B	1073	LYS	C-N-CA	6.15	130.60	122.42
1	A	1073	LYS	CA-C-N	6.10	130.54	122.42
1	A	1073	LYS	C-N-CA	6.10	130.54	122.42
1	C	1077	THR	CA-C-N	5.77	132.63	122.08
1	C	1077	THR	C-N-CA	5.77	132.63	122.08
1	A	1077	THR	CA-C-N	5.76	132.62	122.08
1	A	1077	THR	C-N-CA	5.76	132.62	122.08
1	B	1077	THR	CA-C-N	5.74	132.59	122.08
1	B	1077	THR	C-N-CA	5.74	132.59	122.08
1	B	344	ALA	N-CA-C	-5.73	105.11	111.36
1	A	926	GLN	CB-CG-CD	5.69	122.28	112.60
1	B	926	GLN	CB-CG-CD	5.69	122.28	112.60
1	C	926	GLN	CB-CG-CD	5.67	122.24	112.60
1	A	350	VAL	N-CA-C	5.63	118.13	111.09
1	B	350	VAL	N-CA-C	5.63	118.13	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	666	ILE	N-CA-C	-5.52	107.90	113.47
1	B	666	ILE	N-CA-C	-5.48	107.94	113.47
1	A	666	ILE	N-CA-C	-5.41	108.01	113.47
1	A	667	GLY	CA-C-O	-5.41	117.91	122.29
1	B	667	GLY	CA-C-O	-5.39	117.92	122.29
1	B	1075	PHE	CA-C-O	-5.38	115.03	121.11
1	A	1075	PHE	CA-C-O	-5.37	115.04	121.11
1	C	667	GLY	CA-C-O	-5.37	117.94	122.29
1	C	1075	PHE	CA-C-O	-5.35	115.06	121.11
1	B	1094	VAL	CA-C-O	-5.33	116.35	121.63
1	C	928	ASN	CA-C-N	-5.31	112.75	120.29
1	C	928	ASN	C-N-CA	-5.31	112.75	120.29
1	C	1094	VAL	CA-C-O	-5.31	116.38	121.63
1	A	928	ASN	CA-C-N	-5.30	112.76	120.29
1	A	928	ASN	C-N-CA	-5.30	112.76	120.29
1	B	928	ASN	CA-C-N	-5.27	112.80	120.29
1	B	928	ASN	C-N-CA	-5.27	112.80	120.29
1	A	712	ILE	N-CA-C	5.27	116.32	108.46
1	B	712	ILE	N-CA-C	5.27	116.31	108.46
1	A	374	PHE	N-CA-C	5.26	118.06	109.59
1	C	374	PHE	N-CA-C	5.26	118.07	109.59
1	C	712	ILE	N-CA-C	5.26	116.29	108.46
1	B	374	PHE	N-CA-C	5.24	118.02	109.59
1	A	600	PRO	N-CA-C	-5.23	103.56	111.41
1	B	600	PRO	N-CA-C	-5.23	103.56	111.41
1	C	600	PRO	N-CA-C	-5.23	103.57	111.41
1	B	1098	ASN	N-CA-C	-5.14	105.68	111.28

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	368	LEU	Mainchain
1	B	713	ALA	Mainchain
1	B	797	PHE	Mainchain
1	C	368	LEU	Mainchain
1	C	713	ALA	Mainchain
2	D	108	ARG	Sidechain
2	G	108	ARG	Sidechain

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	7064	0	6230	195	0
1	B	7026	0	6164	227	0
1	C	7064	0	6234	199	0
2	D	1629	0	1570	94	0
2	E	1629	0	1570	60	0
2	G	1629	0	1570	70	0
3	F	1590	0	1541	50	0
3	H	1590	0	1541	59	0
3	L	1590	0	1541	50	0
4	A	196	0	182	13	0
4	B	196	0	182	19	0
4	C	154	0	143	3	0
All	All	31357	0	28468	861	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 14.

All (861) 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)
3:L:95:TRP:CD1	3:L:100:LEU:HD21	1.29	1.60
2:D:64:VAL:CG1	2:D:68:PHE:HB2	1.38	1.53
3:L:95:TRP:CD1	3:L:100:LEU:CD2	1.90	1.50
2:D:64:VAL:HG13	2:D:68:PHE:CG	1.55	1.40
1:A:428:ASP:HA	2:E:28:THR:OG1	1.19	1.35
1:A:117:LEU:HD11	1:A:231:ILE:CD1	1.60	1.30
2:D:64:VAL:CG1	2:D:68:PHE:CB	2.08	1.30
1:C:428:ASP:HA	2:G:28:THR:OG1	1.32	1.29
1:B:428:ASP:HA	2:D:28:THR:OG1	1.14	1.29
1:B:801:ASN:HA	4:B:1311:NAG:O7	1.26	1.27
1:B:412:PRO:HG2	2:D:32:TYR:OH	1.34	1.27
1:B:412:PRO:CG	2:D:32:TYR:OH	1.83	1.26
1:C:806:LEU:HD23	1:C:878:LEU:CD2	1.65	1.24
1:C:117:LEU:HD11	1:C:231:ILE:CD1	1.66	1.24
1:B:699:LEU:HD21	1:C:869:MET:CE	1.67	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:PRO:HG2	2:G:32:TYR:OH	1.40	1.22
1:A:117:LEU:CD1	1:A:231:ILE:CD1	2.18	1.21
1:A:869:MET:CE	1:C:699:LEU:HD21	1.70	1.21
3:L:95:TRP:NE1	3:L:100:LEU:HD21	1.55	1.21
1:C:412:PRO:CG	2:G:32:TYR:OH	1.92	1.18
1:B:117:LEU:HD11	1:B:231:ILE:CD1	1.73	1.17
1:A:869:MET:HE3	1:C:699:LEU:HD21	1.23	1.16
1:A:1096:VAL:HG11	1:A:1110:TYR:CE1	1.82	1.15
1:C:117:LEU:HD11	1:C:231:ILE:HD12	1.29	1.15
1:C:117:LEU:CD1	1:C:231:ILE:CD1	2.23	1.15
1:C:713:ALA:HA	1:C:1073:LYS:O	1.47	1.15
1:A:713:ALA:HA	1:A:1073:LYS:O	1.47	1.13
2:D:64:VAL:CG1	2:D:68:PHE:CG	2.30	1.12
1:B:699:LEU:HD21	1:C:869:MET:HE3	1.18	1.12
1:B:713:ALA:HA	1:B:1073:LYS:O	1.47	1.11
1:B:278:LYS:HB2	1:B:306:PHE:HE2	1.14	1.09
1:A:1096:VAL:HG11	1:A:1110:TYR:HE1	0.94	1.08
1:A:117:LEU:HD11	1:A:231:ILE:HD12	1.19	1.08
1:B:117:LEU:CD1	1:B:231:ILE:CD1	2.32	1.08
1:C:806:LEU:CD2	1:C:878:LEU:HD23	1.83	1.07
1:A:117:LEU:CD1	1:A:231:ILE:HD11	1.81	1.07
3:L:95:TRP:CD1	3:L:100:LEU:HD23	1.90	1.07
1:C:117:LEU:CD1	1:C:231:ILE:HD11	1.83	1.06
1:A:1096:VAL:CG1	1:A:1110:TYR:HE1	1.67	1.05
1:C:278:LYS:HB2	1:C:306:PHE:HE2	1.14	1.05
1:A:278:LYS:HB2	1:A:306:PHE:HE2	1.14	1.04
3:F:21:THR:HG22	3:F:76:TYR:HD2	1.21	1.04
3:L:21:THR:HG22	3:L:76:TYR:HD2	1.20	1.03
1:B:117:LEU:HD11	1:B:231:ILE:HD12	1.35	1.03
1:C:806:LEU:CD2	1:C:878:LEU:CD2	2.37	1.02
2:D:64:VAL:HG12	2:D:68:PHE:HB2	1.03	1.02
1:B:117:LEU:CD1	1:B:231:ILE:HD11	1.92	0.99
3:H:58:LYS:HD3	3:H:62:ILE:HD11	1.44	0.99
3:H:33:ILE:HG12	3:H:75:ARG:HD3	1.43	0.99
1:B:412:PRO:HG2	2:D:32:TYR:HH	1.17	0.98
1:B:699:LEU:CD2	1:C:869:MET:CE	2.40	0.98
1:B:428:ASP:CA	2:D:28:THR:OG1	2.10	0.98
1:B:699:LEU:CD2	1:C:869:MET:HE3	1.93	0.98
1:C:278:LYS:HB2	1:C:306:PHE:CE2	1.99	0.97
1:B:278:LYS:HB2	1:B:306:PHE:CE2	1.99	0.97
1:B:371:SER:O	2:D:105:TYR:CZ	2.17	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LYS:HB2	1:A:306:PHE:CE2	1.99	0.97
1:A:428:ASP:CA	2:E:28:THR:OG1	2.13	0.96
1:A:117:LEU:CD1	1:A:231:ILE:HD12	1.86	0.96
2:D:64:VAL:HG13	2:D:68:PHE:CB	1.84	0.96
1:B:801:ASN:CA	4:B:1311:NAG:O7	2.14	0.96
1:A:869:MET:CE	1:C:699:LEU:CD2	2.44	0.95
1:C:806:LEU:HD23	1:C:878:LEU:HD23	0.96	0.95
1:A:869:MET:HE3	1:C:699:LEU:CD2	1.97	0.94
1:B:117:LEU:HD11	1:B:231:ILE:HD11	1.49	0.93
1:C:117:LEU:HD21	1:C:231:ILE:HD12	1.49	0.93
1:C:428:ASP:HA	2:G:28:THR:HG1	1.14	0.92
3:H:33:ILE:HG12	3:H:75:ARG:CD	1.98	0.92
2:E:6:GLU:HB2	2:E:121:THR:HG23	1.52	0.92
1:C:117:LEU:HD11	1:C:231:ILE:HD11	1.43	0.91
3:L:47:LEU:HA	3:L:62:ILE:HD13	1.52	0.91
1:B:381:GLY:N	2:D:31:ASN:HB3	1.86	0.90
3:L:95:TRP:CG	3:L:100:LEU:CD2	2.52	0.90
1:B:428:ASP:HA	2:D:28:THR:HG1	1.35	0.90
1:C:412:PRO:HG2	2:G:32:TYR:HH	1.30	0.90
1:B:117:LEU:HD21	1:B:231:ILE:HD12	1.51	0.90
3:H:24:LEU:HD11	3:H:29:SER:HA	1.53	0.90
3:F:21:THR:HG22	3:F:76:TYR:CD2	2.06	0.90
1:A:123:ALA:HB3	4:A:1306:NAG:H82	1.55	0.89
2:G:6:GLU:HB2	2:G:121:THR:HG23	1.52	0.89
3:L:21:THR:HG22	3:L:76:TYR:CD2	2.06	0.89
1:B:123:ALA:HB3	4:B:1306:NAG:H82	1.55	0.89
1:B:801:ASN:ND2	4:B:1311:NAG:O7	2.04	0.89
1:B:339:GLY:HA2	1:B:343:ASN:HB3	1.54	0.89
1:C:117:LEU:HD13	1:C:231:ILE:HD11	1.56	0.88
2:D:19:ARG:HG2	2:D:82:GLN:OE1	1.73	0.88
3:L:24:LEU:HD11	3:L:29:SER:HA	1.53	0.88
1:B:412:PRO:HG3	2:D:32:TYR:OH	1.70	0.87
1:C:412:PRO:HG3	2:G:32:TYR:OH	1.74	0.87
1:A:428:ASP:HA	2:E:28:THR:HG1	1.33	0.87
1:A:117:LEU:HD13	1:A:231:ILE:HD11	1.53	0.86
2:G:58:LYS:HB3	2:G:70:ILE:HD11	1.55	0.86
1:B:117:LEU:CD1	1:B:231:ILE:HD12	2.01	0.85
1:C:117:LEU:CD1	1:C:231:ILE:HD12	1.93	0.85
1:C:353:TRP:HZ3	1:C:355:ARG:HB2	1.41	0.85
2:D:183:VAL:HG11	3:H:165:GLU:HB3	1.59	0.85
1:A:117:LEU:HD21	1:A:231:ILE:HD12	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TRP:HZ3	1:A:355:ARG:HB2	1.41	0.84
2:D:20:LEU:HD13	2:D:83:MET:HE2	1.60	0.83
2:E:183:VAL:HG11	3:F:165:GLU:HB3	1.58	0.83
1:C:117:LEU:CD2	1:C:231:ILE:HD12	2.07	0.83
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.41	0.83
2:G:183:VAL:HG11	3:L:165:GLU:HB3	1.58	0.83
1:B:1078:ALA:CB	1:B:1133:VAL:CG2	2.57	0.83
3:H:93:GLN:OE1	3:H:102:PHE:CZ	2.31	0.83
1:B:1078:ALA:HB2	1:B:1133:VAL:CG2	2.09	0.82
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.60	0.82
1:A:310:LYS:HG3	1:A:664:ILE:HD11	1.59	0.82
2:D:61:ALA:O	2:D:65:LYS:HG3	1.79	0.82
1:C:117:LEU:CD2	1:C:231:ILE:CD1	2.58	0.82
2:E:164:VAL:HG12	2:E:214:HIS:HD2	1.43	0.82
2:G:164:VAL:HG12	2:G:214:HIS:HD2	1.43	0.82
1:C:117:LEU:HD21	1:C:231:ILE:CD1	2.10	0.81
3:H:58:LYS:HD3	3:H:62:ILE:CD1	2.10	0.81
1:B:699:LEU:HG	1:C:869:MET:HE1	1.63	0.81
1:B:1078:ALA:CB	1:B:1133:VAL:HG23	2.10	0.80
1:A:1082:CYS:HB3	1:A:1134:ASN:HB3	1.62	0.80
3:L:47:LEU:HA	3:L:62:ILE:CD1	2.11	0.80
1:B:801:ASN:CG	4:B:1311:NAG:O7	2.24	0.80
3:H:58:LYS:CD	3:H:62:ILE:HD11	2.11	0.80
2:E:211:ASN:ND2	2:E:222:ASP:OD2	2.15	0.80
2:E:164:VAL:HG12	2:E:214:HIS:CD2	2.17	0.80
2:G:211:ASN:ND2	2:G:222:ASP:OD2	2.15	0.79
2:D:64:VAL:CG1	2:D:68:PHE:CD2	2.65	0.79
1:B:117:LEU:CD2	1:B:231:ILE:HD12	2.12	0.79
1:A:1092:GLU:OE1	1:A:1107:ARG:NH1	2.15	0.79
1:A:117:LEU:HD13	1:A:231:ILE:CD1	2.11	0.79
2:D:211:ASN:ND2	2:D:222:ASP:OD2	2.15	0.79
2:G:164:VAL:HG12	2:G:214:HIS:CD2	2.17	0.78
2:D:19:ARG:CG	2:D:82:GLN:OE1	2.32	0.78
2:D:64:VAL:HG11	2:D:68:PHE:CB	2.12	0.78
3:L:46:TYR:O	3:L:62:ILE:HD11	1.84	0.77
1:A:603:ASN:OD1	4:A:1302:NAG:H2	1.82	0.77
1:C:371:SER:O	2:G:105:TYR:CZ	2.37	0.77
2:D:64:VAL:HG13	2:D:68:PHE:CD2	2.17	0.77
1:B:117:LEU:HD21	1:B:231:ILE:CD1	2.13	0.77
1:A:117:LEU:CD2	1:A:231:ILE:HD12	2.14	0.77
1:A:869:MET:HE3	1:C:699:LEU:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:ASN:OD1	4:B:1302:NAG:H2	1.82	0.76
2:G:7:SER:HB2	2:G:21:SER:HB2	1.66	0.76
1:B:117:LEU:HD13	1:B:231:ILE:HD11	1.65	0.76
2:E:164:VAL:CG1	2:E:214:HIS:HD2	1.98	0.76
1:B:117:LEU:CD2	1:B:231:ILE:CD1	2.64	0.76
1:B:371:SER:O	2:D:105:TYR:CE1	2.39	0.76
2:G:164:VAL:CG1	2:G:214:HIS:HD2	1.98	0.76
1:A:869:MET:HE1	1:C:699:LEU:HG	1.66	0.75
1:B:1092:GLU:HA	1:B:1107:ARG:HH12	1.50	0.75
1:A:117:LEU:CD2	1:A:231:ILE:CD1	2.65	0.74
1:B:1078:ALA:HB2	1:B:1133:VAL:HG21	1.66	0.74
2:G:49:ALA:HB1	2:G:70:ILE:HG21	1.68	0.74
1:B:699:LEU:CG	1:C:869:MET:CE	2.65	0.74
3:H:24:LEU:HD12	3:H:25:SER:O	1.88	0.74
3:L:95:TRP:CG	3:L:100:LEU:HD23	2.18	0.74
2:E:7:SER:HB2	2:E:21:SER:HB2	1.66	0.74
3:F:137:LEU:HD12	3:F:183:LEU:HD23	1.70	0.74
3:L:137:LEU:HD12	3:L:183:LEU:HD23	1.70	0.74
2:G:58:LYS:CB	2:G:70:ILE:HD11	2.17	0.74
1:C:1092:GLU:HA	1:C:1107:ARG:HH12	1.51	0.73
1:A:869:MET:CE	1:C:699:LEU:CG	2.66	0.73
1:A:1096:VAL:HG21	1:A:1105:THR:CG2	2.18	0.73
3:H:137:LEU:HD12	3:H:183:LEU:HD23	1.70	0.73
1:B:1078:ALA:HB1	1:B:1133:VAL:HG23	1.71	0.73
3:L:24:LEU:HD12	3:L:25:SER:O	1.88	0.73
1:C:428:ASP:CA	2:G:28:THR:OG1	2.25	0.73
1:C:381:GLY:N	2:G:31:ASN:HB3	2.04	0.73
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.72	0.72
3:L:95:TRP:HD1	3:L:100:LEU:HD21	1.44	0.72
1:B:699:LEU:HD11	1:C:869:MET:HE3	1.70	0.72
1:B:778:THR:HG22	1:B:865:LEU:HD12	1.71	0.72
1:A:778:THR:HG22	1:A:865:LEU:HD12	1.71	0.71
1:B:1092:GLU:HA	1:B:1107:ARG:NH1	2.06	0.71
1:C:778:THR:HG22	1:C:865:LEU:HD12	1.71	0.71
2:E:6:GLU:CB	2:E:121:THR:HG23	2.20	0.71
2:G:6:GLU:CB	2:G:121:THR:HG23	2.20	0.71
2:G:49:ALA:CB	2:G:70:ILE:HG21	2.20	0.71
1:A:117:LEU:HD21	1:A:231:ILE:CD1	2.19	0.71
1:A:657:ASN:OD1	4:A:1303:NAG:N2	2.24	0.71
1:A:1106:GLN:HE21	1:A:1111:GLU:HG2	1.56	0.71
2:D:183:VAL:HG11	3:H:165:GLU:CB	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1106:GLN:HE21	1:C:1111:GLU:HG2	1.55	0.70
1:B:657:ASN:OD1	4:B:1303:NAG:N2	2.24	0.70
1:B:381:GLY:CA	2:D:31:ASN:HB3	2.21	0.70
1:A:117:LEU:HD11	1:A:231:ILE:HD11	1.43	0.70
1:A:1077:THR:HA	1:A:1095:PHE:O	1.92	0.70
1:C:353:TRP:CZ3	1:C:355:ARG:HB2	2.26	0.70
1:C:657:ASN:OD1	4:C:1302:NAG:N2	2.24	0.70
1:B:1106:GLN:HE21	1:B:1111:GLU:HG2	1.56	0.70
2:G:183:VAL:HG11	3:L:165:GLU:CB	2.21	0.70
2:E:12:VAL:HG11	2:E:18:LEU:HD11	1.74	0.69
2:G:12:VAL:HG11	2:G:18:LEU:HD11	1.74	0.69
1:C:1092:GLU:HA	1:C:1107:ARG:NH1	2.07	0.69
1:B:317:ASN:ND2	1:C:737:ASP:OD2	2.24	0.69
2:D:64:VAL:HG13	2:D:68:PHE:CD1	2.26	0.69
2:G:183:VAL:CG1	3:L:165:GLU:HB3	2.23	0.69
2:E:183:VAL:HG11	3:F:165:GLU:CB	2.21	0.69
1:A:117:LEU:HD23	1:A:130:VAL:CB	2.23	0.69
1:A:353:TRP:CZ3	1:A:355:ARG:HB2	2.26	0.68
1:B:384:PRO:CD	2:D:101:THR:HG22	2.23	0.68
2:E:183:VAL:CG1	3:F:165:GLU:HB3	2.23	0.68
1:A:869:MET:HE2	1:C:699:LEU:HD21	1.72	0.68
1:B:699:LEU:HD21	1:C:869:MET:HE2	1.71	0.68
1:B:699:LEU:CG	1:C:869:MET:HE1	2.22	0.68
2:D:183:VAL:CG1	3:H:165:GLU:HB3	2.23	0.68
2:D:62:ASP:HA	2:D:65:LYS:CD	2.24	0.68
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.76	0.67
1:C:1096:VAL:HG23	1:C:1103:PHE:HB2	1.76	0.67
1:B:353:TRP:CZ3	1:B:355:ARG:HB2	2.26	0.67
2:D:19:ARG:CD	2:D:82:GLN:OE1	2.43	0.67
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.76	0.67
1:B:278:LYS:CB	1:B:306:PHE:HE2	2.00	0.67
1:B:308:VAL:HG22	1:B:602:THR:HG23	1.77	0.67
1:C:420:ASP:O	1:C:460:ASN:HA	1.95	0.67
3:F:47:LEU:O	3:F:62:ILE:HD13	1.95	0.66
1:A:278:LYS:CB	1:A:306:PHE:HE2	2.01	0.66
1:A:420:ASP:O	1:A:460:ASN:HA	1.96	0.66
1:C:806:LEU:CD2	1:C:878:LEU:HD21	2.26	0.66
1:A:712:ILE:HD13	1:A:1094:VAL:HG21	1.76	0.66
1:B:379:CYS:HB2	2:D:101:THR:O	1.96	0.66
1:A:230:PRO:HB2	1:C:521:PRO:HG2	1.78	0.66
1:C:435:ALA:HA	1:C:509:ARG:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:95:TRP:HD1	3:L:100:LEU:CD2	1.97	0.66
1:B:398:ASP:O	1:B:511:VAL:HA	1.96	0.66
1:B:420:ASP:O	1:B:460:ASN:HA	1.95	0.66
1:C:371:SER:O	2:G:105:TYR:CE1	2.49	0.66
2:D:19:ARG:HD3	2:D:82:GLN:OE1	1.95	0.66
2:E:107:VAL:HG12	2:E:107:VAL:O	1.96	0.66
2:D:64:VAL:HG11	2:D:68:PHE:CD2	2.31	0.65
2:D:16:ARG:HG2	2:D:17:SER:H	1.61	0.65
3:F:113:GLN:HB2	3:F:145:TYR:CE2	2.32	0.65
1:A:1096:VAL:CG2	1:A:1105:THR:HG22	2.27	0.65
1:B:435:ALA:HA	1:B:509:ARG:O	1.96	0.65
3:H:113:GLN:HB2	3:H:145:TYR:CE2	2.30	0.65
2:G:164:VAL:CG1	2:G:214:HIS:CD2	2.79	0.65
1:A:435:ALA:HA	1:A:509:ARG:O	1.96	0.65
1:C:278:LYS:CB	1:C:306:PHE:HE2	2.00	0.65
1:C:381:GLY:CA	2:G:31:ASN:HB3	2.26	0.65
2:D:107:VAL:HG12	2:D:107:VAL:O	1.96	0.65
3:L:93:GLN:HE22	3:L:100:LEU:HD13	1.60	0.65
1:A:869:MET:HE1	1:C:699:LEU:CG	2.25	0.65
1:C:308:VAL:HG22	1:C:602:THR:HG23	1.77	0.65
3:L:113:GLN:HB2	3:L:145:TYR:CE2	2.32	0.65
2:E:99:GLY:HA3	2:E:113:GLY:O	1.97	0.65
1:A:308:VAL:HG22	1:A:602:THR:HG23	1.77	0.64
2:D:62:ASP:HA	2:D:65:LYS:HD2	1.79	0.64
3:F:24:LEU:HD11	3:F:33:ILE:HG21	1.78	0.64
1:B:273:ARG:HH21	1:B:292:ALA:HB3	1.62	0.64
1:A:869:MET:HE3	1:C:699:LEU:CD1	2.27	0.64
2:G:99:GLY:HA3	2:G:113:GLY:O	1.97	0.64
1:A:273:ARG:HH21	1:A:292:ALA:HB3	1.62	0.64
2:D:7:SER:HB3	2:D:21:SER:H	1.62	0.64
1:B:699:LEU:CG	1:C:869:MET:HE3	2.26	0.64
1:B:381:GLY:CA	2:D:31:ASN:CB	2.76	0.64
1:C:722:VAL:HA	1:C:1064:HIS:O	1.98	0.64
3:F:47:LEU:O	3:F:62:ILE:CD1	2.46	0.64
1:C:273:ARG:HH21	1:C:292:ALA:HB3	1.62	0.63
1:A:869:MET:HE3	1:C:699:LEU:CG	2.26	0.63
1:A:296:LEU:HD21	1:A:602:THR:HG22	1.80	0.63
1:A:722:VAL:HA	1:A:1064:HIS:O	1.98	0.63
1:B:296:LEU:HD21	1:B:602:THR:HG22	1.80	0.63
2:D:99:GLY:HA3	2:D:113:GLY:O	1.97	0.63
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:PRO:HD2	2:D:101:THR:HG22	1.79	0.63
1:A:1096:VAL:CG1	1:A:1110:TYR:CE1	2.60	0.63
1:B:722:VAL:HA	1:B:1064:HIS:O	1.98	0.63
1:C:398:ASP:O	1:C:511:VAL:HA	1.98	0.63
1:A:101:ILE:HD11	1:A:240:THR:HB	1.81	0.63
1:B:101:ILE:HD11	1:B:240:THR:HB	1.81	0.63
1:C:1095:PHE:HB3	1:C:1102:TRP:HE3	1.64	0.63
2:D:117:TRP:HE1	3:H:36:HIS:HD1	1.45	0.63
1:B:616:ASN:OD1	4:B:1305:NAG:N2	2.32	0.62
1:C:296:LEU:HD21	1:C:602:THR:HG22	1.80	0.62
1:A:776:LYS:NZ	1:A:780:GLU:OE2	2.28	0.62
1:B:802:PHE:CD2	1:B:805:ILE:HD11	2.34	0.62
1:B:1107:ARG:NE	1:C:904:TYR:CE1	2.63	0.62
1:A:398:ASP:O	1:A:511:VAL:HA	1.99	0.62
2:D:11:VAL:HG12	2:D:124:THR:HB	1.81	0.62
1:C:117:LEU:CG	1:C:231:ILE:HD12	2.30	0.62
2:G:34:MET:HG3	2:G:79:LEU:HD22	1.82	0.62
1:B:412:PRO:CG	2:D:32:TYR:HH	1.89	0.62
2:E:47:TRP:HB2	3:F:100:LEU:HD11	1.82	0.62
1:A:117:LEU:CG	1:A:231:ILE:HD12	2.30	0.62
1:A:1082:CYS:HB3	1:A:1134:ASN:CB	2.28	0.62
1:A:1096:VAL:HG21	1:A:1105:THR:HG22	1.81	0.62
2:D:20:LEU:CD1	2:D:83:MET:HE2	2.29	0.62
2:G:11:VAL:HG12	2:G:124:THR:HB	1.81	0.62
2:G:16:ARG:HG2	2:G:17:SER:H	1.64	0.62
1:B:1107:ARG:HE	1:C:904:TYR:HE1	1.42	0.62
1:A:616:ASN:OD1	4:A:1305:NAG:N2	2.32	0.61
1:B:346:ARG:HA	1:B:509:ARG:NH1	2.14	0.61
1:B:699:LEU:CD1	1:C:869:MET:HE3	2.29	0.61
1:C:101:ILE:HD11	1:C:240:THR:HB	1.81	0.61
2:E:164:VAL:CG1	2:E:214:HIS:CD2	2.79	0.61
3:L:95:TRP:NE1	3:L:100:LEU:CD2	2.38	0.61
2:D:34:MET:HG3	2:D:79:LEU:HD22	1.81	0.61
2:E:11:VAL:HG12	2:E:124:THR:HB	1.81	0.61
1:B:381:GLY:HA2	2:D:31:ASN:CB	2.30	0.61
1:C:412:PRO:CG	2:G:32:TYR:HH	1.91	0.61
2:G:50:VAL:O	2:G:70:ILE:CD1	2.49	0.61
1:B:393:THR:HA	1:B:522:ALA:HA	1.81	0.61
1:A:393:THR:HA	1:A:522:ALA:HA	1.81	0.61
1:B:1095:PHE:HB3	1:B:1102:TRP:HE3	1.66	0.61
1:B:1096:VAL:HG23	1:B:1103:PHE:HB2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:ND2	1:B:737:ASP:OD2	2.26	0.61
1:C:117:LEU:HD23	1:C:130:VAL:CB	2.30	0.61
1:C:776:LYS:NZ	1:C:780:GLU:OE2	2.28	0.61
3:H:18:VAL:HG12	3:H:19:LYS:N	2.14	0.61
2:E:34:MET:HG3	2:E:79:LEU:HD22	1.82	0.61
3:F:4:LEU:CD2	3:F:24:LEU:HG	2.31	0.61
1:C:369:TYR:O	2:G:105:TYR:CE1	2.54	0.60
1:B:776:LYS:NZ	1:B:780:GLU:OE2	2.28	0.60
2:E:16:ARG:HG2	2:E:17:SER:H	1.65	0.60
1:A:737:ASP:OD2	1:C:317:ASN:ND2	2.30	0.60
3:H:95:TRP:CD1	3:H:100:LEU:HD11	2.36	0.60
2:D:104:ASP:HB2	2:D:111:TYR:CE2	2.35	0.60
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.84	0.60
2:G:164:VAL:CG2	2:G:192:LEU:HD21	2.32	0.60
1:C:393:THR:HA	1:C:522:ALA:HA	1.81	0.60
2:E:164:VAL:CG2	2:E:192:LEU:HD21	2.31	0.60
2:G:22:CYS:HB3	2:G:79:LEU:HB3	1.84	0.60
3:H:36:HIS:NE2	3:H:93:GLN:NE2	2.49	0.59
1:A:310:LYS:CG	1:A:664:ILE:HD11	2.30	0.59
3:H:31:TYR:O	3:H:75:ARG:NH2	2.29	0.59
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.36	0.59
1:A:298:GLU:O	1:A:302:THR:HG23	2.03	0.59
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.36	0.59
1:B:801:ASN:ND2	4:B:1311:NAG:C7	2.65	0.59
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.83	0.59
1:B:117:LEU:HD23	1:B:130:VAL:CB	2.33	0.59
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.38	0.58
1:C:117:LEU:HD13	1:C:231:ILE:CD1	2.18	0.58
2:E:47:TRP:CD1	3:F:100:LEU:HG	2.38	0.58
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.36	0.58
3:H:32:ALA:HA	3:H:75:ARG:NH2	2.19	0.58
1:A:1111:GLU:OE1	1:A:1113:GLN:NE2	2.37	0.58
1:C:298:GLU:O	1:C:302:THR:HG23	2.03	0.58
2:D:9:GLY:H	2:D:121:THR:CG2	2.17	0.58
1:B:298:GLU:O	1:B:302:THR:HG23	2.03	0.58
1:C:117:LEU:CD2	1:C:231:ILE:HD13	2.32	0.58
2:D:164:VAL:CG1	2:D:192:LEU:HD21	2.34	0.58
3:L:62:ILE:HG23	3:L:63:PRO:HD2	1.85	0.58
1:B:1095:PHE:HA	1:B:1103:PHE:O	2.04	0.57
1:B:1111:GLU:OE1	1:B:1113:GLN:NE2	2.37	0.57
3:H:36:HIS:NE2	3:H:93:GLN:CD	2.62	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1095:PHE:HA	1:C:1103:PHE:O	2.04	0.57
2:D:8:GLY:HA2	2:D:121:THR:CG2	2.33	0.57
1:C:1095:PHE:HB3	1:C:1102:TRP:CE3	2.39	0.57
2:G:6:GLU:HB2	2:G:121:THR:CG2	2.30	0.57
1:A:353:TRP:O	1:A:466:ARG:HD2	2.04	0.57
1:B:381:GLY:HA2	2:D:31:ASN:HA	1.86	0.57
1:B:339:GLY:HA2	1:B:343:ASN:CB	2.32	0.57
1:B:521:PRO:HG2	1:C:230:PRO:CB	2.35	0.57
1:B:666:ILE:CD1	1:B:672:ALA:HB2	2.34	0.57
1:B:353:TRP:O	1:B:466:ARG:HD2	2.04	0.57
1:C:353:TRP:O	1:C:466:ARG:HD2	2.04	0.57
1:A:230:PRO:CB	1:C:521:PRO:HG2	2.34	0.57
1:A:1096:VAL:HG21	1:A:1105:THR:HG21	1.87	0.57
1:A:869:MET:CE	1:C:699:LEU:HD11	2.34	0.56
1:B:866:THR:HG22	1:B:867:ASP:N	2.19	0.56
1:C:1111:GLU:OE1	1:C:1113:GLN:NE2	2.37	0.56
1:A:699:LEU:HD21	1:B:869:MET:CE	2.35	0.56
1:A:731:MET:HE3	1:A:955:ASN:HD21	1.70	0.56
1:B:521:PRO:HG2	1:C:230:PRO:HB2	1.88	0.56
1:C:381:GLY:HA2	2:G:31:ASN:CB	2.34	0.56
1:C:353:TRP:CD1	1:C:353:TRP:H	2.24	0.56
1:A:234:ASN:CG	4:A:1308:NAG:N2	2.64	0.56
1:B:371:SER:O	2:D:105:TYR:OH	2.24	0.56
2:E:6:GLU:HB2	2:E:121:THR:CG2	2.30	0.56
3:F:58:LYS:HB3	3:F:62:ILE:HD11	1.88	0.56
3:H:58:LYS:CG	3:H:62:ILE:HD11	2.35	0.55
1:B:1095:PHE:HB3	1:B:1102:TRP:CE3	2.41	0.55
1:C:712:ILE:HD13	1:C:1094:VAL:HG21	1.89	0.55
1:A:353:TRP:CD1	1:A:353:TRP:H	2.24	0.55
1:B:712:ILE:HD13	1:B:1094:VAL:HG21	1.87	0.55
2:D:8:GLY:HA2	2:D:121:THR:HG21	1.88	0.55
3:F:24:LEU:HD11	3:F:33:ILE:CG2	2.35	0.55
1:A:1107:ARG:HE	1:B:904:TYR:HE1	1.51	0.55
2:E:6:GLU:CB	2:E:121:THR:CG2	2.84	0.55
1:C:818:ILE:O	1:C:822:LEU:HD23	2.07	0.55
1:B:117:LEU:HD13	1:B:231:ILE:CD1	2.26	0.55
1:B:731:MET:HE3	1:B:955:ASN:HD21	1.70	0.55
1:C:731:MET:HE3	1:C:955:ASN:HD21	1.70	0.55
2:D:104:ASP:HB2	2:D:111:TYR:CD2	2.41	0.55
1:A:966:LEU:HD12	1:A:1000:ARG:NE	2.22	0.55
2:D:7:SER:O	2:D:121:THR:HG21	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:TRP:H	1:B:353:TRP:CD1	2.24	0.54
1:B:666:ILE:HD11	1:B:672:ALA:CB	2.34	0.54
3:L:93:GLN:NE2	3:L:100:LEU:HD13	2.22	0.54
1:B:818:ILE:O	1:B:822:LEU:HD23	2.07	0.54
1:B:699:LEU:HD11	1:C:869:MET:CE	2.36	0.54
1:B:381:GLY:HA2	2:D:31:ASN:CA	2.37	0.54
2:D:22:CYS:HB3	2:D:79:LEU:HB3	1.90	0.54
1:A:48:LEU:HD22	1:A:306:PHE:CE2	2.43	0.54
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.43	0.54
1:C:48:LEU:HD22	1:C:306:PHE:CE2	2.43	0.54
1:A:117:LEU:CD2	1:A:231:ILE:HD13	2.38	0.54
1:B:778:THR:CG2	1:B:865:LEU:HD12	2.38	0.54
1:C:363:ALA:O	1:C:526:GLY:HA2	2.08	0.54
1:A:379:CYS:HB2	2:E:101:THR:O	2.07	0.54
3:L:213:PRO:O	3:L:214:THR:HG23	2.08	0.54
1:B:369:TYR:O	2:D:105:TYR:CE1	2.61	0.54
4:B:1311:NAG:O6	4:B:1311:NAG:O4	2.21	0.54
3:H:33:ILE:CG1	3:H:75:ARG:CD	2.79	0.54
3:F:213:PRO:O	3:F:214:THR:HG23	2.08	0.54
3:H:213:PRO:O	3:H:214:THR:HG23	2.08	0.54
1:A:731:MET:HB2	1:A:955:ASN:HD21	1.73	0.53
1:A:818:ILE:O	1:A:822:LEU:HD23	2.07	0.53
1:B:117:LEU:CD2	1:B:231:ILE:HD13	2.39	0.53
2:G:6:GLU:CB	2:G:121:THR:CG2	2.84	0.53
1:A:117:LEU:CD2	1:A:130:VAL:CB	2.86	0.53
1:A:363:ALA:O	1:A:526:GLY:HA2	2.08	0.53
1:B:363:ALA:O	1:B:526:GLY:HA2	2.08	0.53
1:B:800:PHE:O	1:B:801:ASN:C	2.52	0.53
1:B:713:ALA:HB1	1:B:1072:GLU:HB2	1.90	0.53
1:C:341:VAL:HG12	1:C:341:VAL:O	2.07	0.53
2:E:47:TRP:HB2	3:F:100:LEU:CD1	2.38	0.53
3:L:65:ARG:NH2	3:L:86:ASP:OD2	2.39	0.53
1:B:731:MET:HB2	1:B:955:ASN:HD21	1.73	0.53
1:B:874:THR:O	1:B:878:LEU:HG	2.08	0.53
1:C:1081:ILE:HD13	1:C:1133:VAL:CG2	2.39	0.53
2:G:72:ARG:NH2	2:G:74:ASN:OD1	2.41	0.53
1:B:48:LEU:HD22	1:B:306:PHE:CE2	2.43	0.53
1:B:117:LEU:CG	1:B:231:ILE:HD12	2.38	0.53
1:B:234:ASN:CG	4:B:1308:NAG:N2	2.64	0.53
1:C:731:MET:HB2	1:C:955:ASN:HD21	1.73	0.53
1:C:778:THR:CG2	1:C:865:LEU:HD12	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:18:VAL:CG1	3:H:19:LYS:N	2.71	0.53
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.74	0.53
1:A:715:PRO:HG3	1:A:1069:PRO:HB3	1.90	0.53
1:C:436:TRP:CZ2	1:C:509:ARG:HD2	2.44	0.53
1:A:280:ASN:ND2	1:A:284:THR:OG1	2.42	0.53
1:B:280:ASN:ND2	1:B:284:THR:OG1	2.42	0.53
1:C:806:LEU:HD23	1:C:878:LEU:HD21	1.76	0.53
1:A:521:PRO:HG2	1:B:230:PRO:HB2	1.91	0.52
2:D:6:GLU:HB3	2:D:121:THR:OG1	2.09	0.52
2:E:164:VAL:HG23	2:E:192:LEU:HD21	1.91	0.52
1:A:878:LEU:HD23	1:A:1053:PRO:HD2	1.91	0.52
2:G:164:VAL:HG23	2:G:192:LEU:HD21	1.92	0.52
1:A:713:ALA:HB1	1:A:1072:GLU:HB2	1.90	0.52
1:B:341:VAL:HG22	1:B:511:VAL:HG11	1.90	0.52
1:C:713:ALA:HB1	1:C:1072:GLU:HB2	1.90	0.52
1:C:784:GLN:HE22	1:C:1030:SER:HG	1.58	0.52
1:A:86:PHE:HB2	1:A:238:PHE:HD1	1.75	0.52
1:A:436:TRP:CZ2	1:A:509:ARG:HD2	2.44	0.52
1:C:381:GLY:CA	2:G:31:ASN:CB	2.87	0.52
1:C:672:ALA:HA	1:C:693:ILE:O	2.10	0.52
3:F:24:LEU:CD2	3:F:31:TYR:HB2	2.40	0.52
1:B:436:TRP:CZ2	1:B:509:ARG:HD2	2.44	0.52
1:A:697:MET:SD	1:B:869:MET:HE1	2.50	0.52
1:B:672:ALA:HA	1:B:693:ILE:O	2.10	0.52
1:C:280:ASN:ND2	1:C:284:THR:OG1	2.42	0.52
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.92	0.52
3:H:95:TRP:CD1	3:H:100:LEU:CD1	2.92	0.52
1:A:412:PRO:HG2	2:E:32:TYR:OH	2.10	0.51
3:H:65:ARG:NH2	3:H:86:ASP:OD2	2.39	0.51
3:H:95:TRP:HD1	3:H:100:LEU:HD11	1.76	0.51
1:A:802:PHE:HZ	1:A:898:PHE:CZ	2.27	0.51
1:A:1107:ARG:NE	1:B:904:TYR:CE1	2.67	0.51
3:F:4:LEU:HD23	3:F:24:LEU:HG	1.92	0.51
2:G:83:MET:HB3	2:G:86:LEU:HD21	1.92	0.51
1:A:54:LEU:HA	1:A:271:GLN:O	2.11	0.51
1:A:521:PRO:HG2	1:B:230:PRO:CB	2.40	0.51
1:A:712:ILE:CD1	1:A:1094:VAL:HG21	2.40	0.51
1:C:715:PRO:HG3	1:C:1069:PRO:HB3	1.93	0.51
1:A:778:THR:CG2	1:A:865:LEU:HD12	2.38	0.51
1:C:54:LEU:HA	1:C:271:GLN:O	2.11	0.51
1:A:328:ARG:NH1	1:A:531:THR:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:TYR:HB3	1:B:61:ASN:OD1	2.11	0.51
1:C:86:PHE:HB2	1:C:238:PHE:HD1	1.75	0.51
2:D:107:VAL:O	2:D:107:VAL:CG1	2.59	0.51
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.46	0.51
1:A:874:THR:O	1:A:878:LEU:HG	2.10	0.51
1:A:672:ALA:HA	1:A:693:ILE:O	2.10	0.51
1:B:54:LEU:HA	1:B:271:GLN:O	2.11	0.51
1:B:345:THR:O	1:B:509:ARG:HD3	2.11	0.51
1:C:328:ARG:NH1	1:C:531:THR:O	2.44	0.51
3:H:93:GLN:OE1	3:H:102:PHE:CE1	2.63	0.51
1:B:86:PHE:HB2	1:B:238:PHE:HD1	1.75	0.51
1:C:994:ASP:O	1:C:997:ILE:HG22	2.11	0.51
2:D:36:TRP:CE2	2:D:81:LEU:HB2	2.46	0.51
1:A:193:VAL:HG23	1:A:223:LEU:HD22	1.93	0.50
2:G:36:TRP:CE2	2:G:81:LEU:HB2	2.46	0.50
1:B:328:ARG:NH1	1:B:531:THR:O	2.44	0.50
1:B:994:ASP:O	1:B:997:ILE:HG22	2.11	0.50
1:B:384:PRO:HD2	2:D:101:THR:CG2	2.42	0.50
1:B:380:TYR:HD2	2:D:32:TYR:CE2	2.30	0.50
2:E:83:MET:HB3	2:E:86:LEU:HD21	1.92	0.50
1:B:714:ILE:HB	1:B:1110:TYR:HB2	1.93	0.50
2:E:107:VAL:HG22	3:F:31:TYR:OH	2.12	0.50
1:C:714:ILE:HB	1:C:1110:TYR:HB2	1.93	0.50
1:A:1075:PHE:HB3	1:A:1096:VAL:HG13	1.94	0.50
1:B:380:TYR:CD2	2:D:32:TYR:CE2	3.00	0.50
1:B:1078:ALA:CB	1:B:1133:VAL:HG21	2.32	0.50
2:E:107:VAL:O	2:E:107:VAL:CG1	2.59	0.50
1:A:714:ILE:HB	1:A:1110:TYR:HB2	1.93	0.50
1:A:994:ASP:O	1:A:997:ILE:HG22	2.11	0.50
3:H:33:ILE:HG12	3:H:75:ARG:HD2	1.92	0.50
1:C:28:TYR:HB3	1:C:61:ASN:OD1	2.11	0.49
2:E:114:LEU:HD12	3:F:100:LEU:HD21	1.93	0.49
1:A:666:ILE:CD1	1:A:672:ALA:HB2	2.41	0.49
1:C:1130:ILE:HG22	4:C:1307:NAG:H81	1.94	0.49
1:A:384:PRO:HB2	2:E:103:TYR:HB2	1.93	0.49
1:B:193:VAL:HG23	1:B:223:LEU:HD22	1.93	0.49
1:C:193:VAL:HG23	1:C:223:LEU:HD22	1.93	0.49
2:D:36:TRP:HD1	2:D:70:ILE:HD12	1.78	0.49
1:A:1130:ILE:HG22	4:A:1310:NAG:H81	1.94	0.49
3:H:33:ILE:CG1	3:H:75:ARG:HD3	2.29	0.49
2:D:114:LEU:HB3	3:H:93:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:900:MET:HG2	1:C:917:TYR:OH	2.13	0.49
1:B:381:GLY:CA	2:D:31:ASN:CG	2.85	0.49
1:B:802:PHE:HZ	1:B:898:PHE:CZ	2.31	0.49
1:B:1103:PHE:HB3	1:B:1113:GLN:O	2.13	0.49
1:B:1077:THR:C	1:B:1102:TRP:CZ3	2.91	0.49
2:D:107:VAL:HG22	3:H:31:TYR:OH	2.12	0.49
2:D:164:VAL:HG13	2:D:192:LEU:HD21	1.95	0.48
3:H:24:LEU:HD12	3:H:24:LEU:C	2.38	0.48
2:E:47:TRP:CD1	3:F:100:LEU:CG	2.96	0.48
1:A:900:MET:HG2	1:A:917:TYR:OH	2.13	0.48
1:A:904:TYR:CE1	1:C:1107:ARG:NE	2.72	0.48
3:L:24:LEU:HD12	3:L:24:LEU:C	2.38	0.48
1:A:374:PHE:CD1	1:A:436:TRP:HB3	2.49	0.48
1:A:699:LEU:HD21	1:B:869:MET:HE2	1.93	0.48
1:A:994:ASP:HA	1:A:997:ILE:HG22	1.95	0.48
1:C:1103:PHE:HB3	1:C:1113:GLN:O	2.13	0.48
1:B:374:PHE:CD1	1:B:436:TRP:HB3	2.49	0.48
1:B:922:LEU:O	1:B:926:GLN:HB2	2.14	0.48
1:C:168:PHE:CZ	1:C:170:TYR:HB2	2.48	0.48
1:B:1130:ILE:HG22	4:B:1310:NAG:H81	1.94	0.48
1:C:369:TYR:O	2:G:105:TYR:HE1	1.96	0.48
1:C:1077:THR:C	1:C:1102:TRP:CZ3	2.91	0.48
1:B:994:ASP:HA	1:B:997:ILE:HG22	1.95	0.48
1:C:1081:ILE:HD13	1:C:1133:VAL:HG22	1.95	0.48
1:B:715:PRO:HG3	1:B:1069:PRO:HB3	1.95	0.48
1:B:900:MET:HG2	1:B:917:TYR:OH	2.13	0.48
1:A:604:THR:OG1	4:A:1302:NAG:O7	2.31	0.48
1:A:922:LEU:O	1:A:926:GLN:HB2	2.14	0.48
1:A:1094:VAL:CG2	1:B:904:TYR:OH	2.62	0.47
1:B:801:ASN:CB	4:B:1311:NAG:O7	2.62	0.47
1:C:374:PHE:CD1	1:C:436:TRP:HB3	2.49	0.47
1:C:922:LEU:O	1:C:926:GLN:HB2	2.13	0.47
3:H:50:LEU:HB3	3:H:75:ARG:NH1	2.29	0.47
1:A:1081:ILE:HG12	1:A:1095:PHE:CE2	2.49	0.47
2:G:12:VAL:HG11	2:G:18:LEU:CD1	2.44	0.47
1:A:1094:VAL:HG12	1:A:1095:PHE:N	2.30	0.47
3:H:24:LEU:CD1	3:H:25:SER:O	2.59	0.47
2:E:56:SER:HB2	2:E:58:LYS:HZ3	1.79	0.47
1:B:384:PRO:HG3	2:D:101:THR:O	2.14	0.47
3:L:24:LEU:CD1	3:L:29:SER:HA	2.36	0.47
3:L:113:GLN:HB2	3:L:145:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:922:LEU:O	1:B:926:GLN:CB	2.63	0.47
1:C:922:LEU:O	1:C:926:GLN:CB	2.63	0.47
1:C:994:ASP:HA	1:C:997:ILE:HG22	1.95	0.47
1:A:666:ILE:HG22	1:A:666:ILE:O	2.14	0.47
2:E:112:TYR:O	3:F:95:TRP:NE1	2.46	0.46
2:E:117:TRP:CE3	3:F:44:PRO:HG2	2.50	0.46
1:A:666:ILE:HD11	1:A:672:ALA:CB	2.44	0.46
3:H:50:LEU:HB3	3:H:75:ARG:HH11	1.80	0.46
1:B:340:GLU:O	1:B:344:ALA:HB3	2.14	0.46
2:D:117:TRP:CE3	3:H:44:PRO:HG2	2.50	0.46
3:F:100:LEU:HD12	3:F:100:LEU:C	2.40	0.46
1:A:922:LEU:O	1:A:926:GLN:CB	2.63	0.46
1:B:604:THR:OG1	4:B:1302:NAG:O7	2.31	0.46
1:B:799:GLY:C	1:B:801:ASN:H	2.24	0.46
1:B:878:LEU:HD23	1:B:1053:PRO:HD2	1.96	0.46
1:C:806:LEU:HD21	1:C:878:LEU:HG	1.97	0.46
3:F:65:ARG:NH2	3:F:86:ASP:OD2	2.39	0.46
2:G:20:LEU:HG	2:G:83:MET:HE2	1.98	0.46
2:G:117:TRP:CE3	3:L:44:PRO:HG2	2.50	0.46
1:A:431:GLY:HA3	1:A:513:LEU:O	2.15	0.46
1:A:1013:ILE:HD11	1:C:1013:ILE:HD11	1.98	0.46
2:E:91:THR:HG23	2:E:124:THR:HA	1.98	0.46
3:L:184:SER:O	3:L:185:LEU:HD23	2.16	0.46
1:A:234:ASN:OD1	4:A:1308:NAG:N2	2.50	0.45
1:B:616:ASN:CG	4:B:1305:NAG:N2	2.74	0.45
2:D:207:THR:HG22	2:D:224:ARG:NH2	2.31	0.45
2:G:207:THR:HG22	2:G:224:ARG:NH2	2.31	0.45
3:H:184:SER:O	3:H:185:LEU:HD23	2.16	0.45
2:G:91:THR:HG23	2:G:124:THR:HA	1.98	0.45
1:B:1077:THR:OG1	1:B:1078:ALA:N	2.49	0.45
2:D:112:TYR:O	3:H:95:TRP:NE1	2.46	0.45
3:L:24:LEU:CD1	3:L:25:SER:O	2.59	0.45
3:L:95:TRP:HA	3:L:100:LEU:HD23	1.99	0.45
1:A:1075:PHE:CB	1:A:1096:VAL:HG13	2.46	0.45
1:C:1077:THR:OG1	1:C:1078:ALA:N	2.49	0.45
2:D:71:SER:HB2	2:D:80:TYR:HB2	1.98	0.45
1:B:234:ASN:OD1	4:B:1308:NAG:N2	2.50	0.45
1:B:431:GLY:HA3	1:B:513:LEU:O	2.16	0.45
1:B:801:ASN:O	1:B:802:PHE:HB2	2.17	0.45
2:D:83:MET:HE1	2:D:123:VAL:HG21	1.99	0.45
1:A:616:ASN:CG	4:A:1305:NAG:N2	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:TRP:HZ2	1:C:464:PHE:C	2.25	0.45
3:H:33:ILE:CG1	3:H:75:ARG:HD2	2.46	0.45
2:E:20:LEU:HG	2:E:83:MET:HE2	1.98	0.45
3:F:184:SER:O	3:F:185:LEU:HD23	2.16	0.45
1:B:797:PHE:O	1:B:800:PHE:HB2	2.17	0.45
2:D:18:LEU:HB3	2:D:83:MET:HE3	1.99	0.45
2:E:12:VAL:HG11	2:E:18:LEU:CD1	2.44	0.45
2:G:83:MET:HE1	2:G:123:VAL:HG21	1.99	0.45
1:C:135:PHE:HA	1:C:160:TYR:HA	1.99	0.45
1:C:666:ILE:O	1:C:666:ILE:HG22	2.16	0.45
3:H:33:ILE:CG2	3:H:75:ARG:HD2	2.47	0.45
2:E:20:LEU:HD12	2:E:81:LEU:HD23	1.98	0.45
3:F:113:GLN:HB2	3:F:145:TYR:CZ	2.51	0.45
1:A:914:ASN:ND2	1:C:1123:SER:OG	2.50	0.45
1:B:54:LEU:HB3	1:B:270:LEU:HB3	1.99	0.45
1:B:1013:ILE:HD11	1:C:1013:ILE:HD11	1.98	0.45
1:C:31:SER:OG	1:C:60:SER:N	2.50	0.44
1:A:353:TRP:HZ2	1:A:464:PHE:C	2.25	0.44
1:A:699:LEU:HD21	1:B:869:MET:HE3	2.00	0.44
2:D:11:VAL:HA	2:D:124:THR:O	2.17	0.44
1:B:353:TRP:HZ2	1:B:464:PHE:C	2.25	0.44
3:H:63:PRO:HG2	3:H:66:PHE:CD1	2.53	0.44
1:A:1077:THR:OG1	1:A:1094:VAL:CG1	2.65	0.44
2:E:17:SER:O	2:E:18:LEU:HD12	2.17	0.44
2:E:207:THR:HG22	2:E:224:ARG:NH2	2.31	0.44
2:G:20:LEU:HD12	2:G:81:LEU:HD23	1.99	0.44
1:A:645:THR:HG23	1:A:647:ALA:H	1.83	0.44
1:B:31:SER:OG	1:B:60:SER:N	2.50	0.44
1:B:897:PRO:HD2	1:B:900:MET:CE	2.48	0.44
2:D:91:THR:HG23	2:D:124:THR:HA	1.99	0.44
3:F:85:GLU:CD	3:F:85:GLU:H	2.25	0.44
2:G:11:VAL:HA	2:G:124:THR:O	2.17	0.44
2:G:36:TRP:NE1	2:G:81:LEU:HB2	2.33	0.44
1:A:135:PHE:HA	1:A:160:TYR:HA	1.99	0.44
1:C:896:ILE:CD1	1:C:904:TYR:HE2	2.31	0.44
1:C:117:LEU:HD22	1:C:231:ILE:HD13	1.98	0.44
1:C:897:PRO:HD2	1:C:900:MET:CE	2.48	0.44
3:H:134:LYS:HA	3:H:134:LYS:HD3	1.76	0.44
2:E:11:VAL:HA	2:E:124:THR:O	2.17	0.44
2:G:51:ILE:HB	2:G:70:ILE:HD12	1.99	0.44
1:A:303:LEU:HD21	1:A:313:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LYS:O	1:A:498:GLN:HA	2.18	0.44
1:A:869:MET:CE	1:C:699:LEU:CD1	2.93	0.44
1:A:1077:THR:OG1	1:A:1078:ALA:N	2.49	0.44
1:B:370:ASN:C	2:D:105:TYR:HE1	2.26	0.44
1:B:565:PHE:CZ	1:C:42:VAL:HG22	2.52	0.44
1:C:447:GLY:HA2	1:C:497:PHE:O	2.18	0.44
2:D:64:VAL:HG12	2:D:64:VAL:O	2.17	0.44
3:F:63:PRO:HG2	3:F:66:PHE:CD1	2.52	0.44
1:A:54:LEU:HB3	1:A:270:LEU:HB3	2.00	0.44
1:A:447:GLY:HA2	1:A:497:PHE:O	2.18	0.44
1:C:117:LEU:CD2	1:C:130:VAL:CB	2.96	0.44
2:D:36:TRP:NE1	2:D:81:LEU:HB2	2.33	0.44
3:H:95:TRP:CD1	3:H:100:LEU:HG	2.53	0.44
3:H:149:VAL:CG1	3:H:200:VAL:HG13	2.47	0.44
2:E:56:SER:HB2	2:E:58:LYS:NZ	2.32	0.44
3:F:149:VAL:CG1	3:F:200:VAL:HG13	2.47	0.44
3:L:63:PRO:HG2	3:L:66:PHE:CD1	2.52	0.44
1:C:353:TRP:CD1	1:C:423:TYR:HD1	2.36	0.43
2:E:83:MET:HE1	2:E:123:VAL:HG21	1.99	0.43
3:L:85:GLU:CD	3:L:85:GLU:H	2.25	0.43
1:A:718:PHE:HZ	1:A:923:ILE:HD11	1.83	0.43
1:A:896:ILE:CD1	1:A:904:TYR:HE2	2.31	0.43
1:B:135:PHE:HA	1:B:160:TYR:HA	1.99	0.43
1:B:353:TRP:CD1	1:B:423:TYR:HD1	2.36	0.43
1:C:1077:THR:C	1:C:1102:TRP:CH2	2.96	0.43
3:H:24:LEU:CD1	3:H:29:SER:HA	2.36	0.43
3:H:113:GLN:HB2	3:H:145:TYR:CZ	2.53	0.43
2:G:17:SER:O	2:G:18:LEU:HD12	2.17	0.43
2:G:60:TYR:OH	2:G:70:ILE:HG12	2.19	0.43
2:G:107:VAL:HG12	3:L:31:TYR:OH	2.18	0.43
3:L:149:VAL:CG1	3:L:200:VAL:HG13	2.47	0.43
1:B:896:ILE:CD1	1:B:904:TYR:HE2	2.31	0.43
1:B:1103:PHE:HA	1:B:1115:ILE:HG13	2.01	0.43
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.83	0.43
1:C:444:LYS:O	1:C:498:GLN:HA	2.18	0.43
2:G:117:TRP:CD2	3:L:44:PRO:HB2	2.53	0.43
1:A:869:MET:HE1	1:C:699:LEU:CD2	2.44	0.43
1:B:303:LEU:HD21	1:B:313:TYR:CD1	2.53	0.43
1:B:645:THR:HG23	1:B:647:ALA:H	1.83	0.43
1:B:866:THR:HG22	1:B:867:ASP:H	1.81	0.43
2:E:36:TRP:NE1	2:E:81:LEU:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:117:TRP:CD2	3:F:44:PRO:HB2	2.53	0.43
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.83	0.43
1:B:374:PHE:CZ	1:B:436:TRP:CD1	3.07	0.43
2:D:104:ASP:OD1	2:D:105:TYR:N	2.52	0.43
3:H:85:GLU:CD	3:H:85:GLU:H	2.26	0.43
1:A:353:TRP:CD1	1:A:423:TYR:HD1	2.36	0.43
3:H:29:SER:O	3:H:30:SER:OG	2.33	0.43
1:A:897:PRO:HD2	1:A:900:MET:CE	2.48	0.43
1:B:444:LYS:O	1:B:498:GLN:HA	2.18	0.43
1:C:341:VAL:O	1:C:341:VAL:CG1	2.66	0.43
1:C:352:ALA:HA	1:C:466:ARG:CG	2.49	0.43
1:C:645:THR:HG23	1:C:647:ALA:H	1.83	0.43
1:A:655:HIS:HA	1:A:694:ALA:O	2.19	0.43
1:B:352:ALA:HA	1:B:466:ARG:CG	2.49	0.43
1:B:560:LEU:HD11	1:C:284:THR:HG22	1.99	0.43
1:B:1077:THR:C	1:B:1102:TRP:CH2	2.96	0.43
2:D:117:TRP:CD2	3:H:44:PRO:HB2	2.53	0.43
3:L:122:LEU:HD13	3:L:139:CYS:HB2	2.01	0.43
1:A:352:ALA:HA	1:A:466:ARG:CG	2.49	0.43
1:A:918:GLU:HA	1:C:1128:VAL:HG12	2.00	0.43
1:B:30:ASN:OD1	1:B:59:PHE:HA	2.19	0.43
1:C:303:LEU:HD21	1:C:313:TYR:CD1	2.53	0.43
1:C:408:ARG:CB	3:L:58:LYS:O	2.66	0.43
2:D:183:VAL:HG21	3:H:182:TYR:HE2	1.84	0.43
3:H:65:ARG:O	3:H:79:ILE:HA	2.19	0.43
3:H:122:LEU:HD13	3:H:139:CYS:HB2	2.01	0.43
2:E:183:VAL:HG21	3:F:182:TYR:CE2	2.54	0.43
3:F:24:LEU:HD23	3:F:31:TYR:HB2	2.01	0.43
3:F:122:LEU:HD13	3:F:139:CYS:HB2	2.01	0.43
2:G:203:LEU:HD23	2:G:203:LEU:HA	1.88	0.43
1:A:1116:THR:HG22	1:A:1138:TYR:HD2	1.82	0.43
1:B:381:GLY:HA3	2:D:31:ASN:CG	2.44	0.43
1:B:598:ILE:HG13	1:B:609:ALA:HB3	2.01	0.43
1:B:699:LEU:CD1	1:C:869:MET:CE	2.94	0.43
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	2.01	0.43
1:C:54:LEU:HB3	1:C:270:LEU:HB3	1.99	0.43
3:F:154:LYS:HD2	3:F:199:GLN:HE22	1.84	0.43
1:B:379:CYS:HA	1:B:432:CYS:CB	2.48	0.42
1:C:381:GLY:HA2	2:G:31:ASN:HB3	1.99	0.42
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	2.01	0.42
2:D:86:LEU:HA	2:D:86:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:112:TYR:O	3:L:95:TRP:NE1	2.46	0.42
1:A:374:PHE:CZ	1:A:436:TRP:CD1	3.07	0.42
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	2.01	0.42
1:A:1097:SER:HA	1:A:1103:PHE:CD2	2.54	0.42
1:B:447:GLY:HA2	1:B:497:PHE:O	2.18	0.42
1:B:655:HIS:HA	1:B:694:ALA:O	2.19	0.42
1:C:598:ILE:HG13	1:C:609:ALA:HB3	2.01	0.42
1:C:1103:PHE:HA	1:C:1115:ILE:HG13	2.00	0.42
2:G:56:SER:HB2	2:G:58:LYS:NZ	2.33	0.42
3:L:65:ARG:O	3:L:79:ILE:HA	2.19	0.42
1:A:44:ARG:HB3	1:A:47:VAL:CG1	2.49	0.42
1:A:726:ILE:HD13	1:A:945:LEU:HG	2.02	0.42
1:A:921:LYS:HD3	1:A:921:LYS:HA	1.80	0.42
1:A:1013:ILE:HD11	1:B:1013:ILE:HD11	2.01	0.42
1:A:1074:ASN:CG	4:A:1304:NAG:C7	2.92	0.42
1:B:32:PHE:CD2	1:B:218:GLN:HG3	2.55	0.42
1:B:896:ILE:HD11	1:B:904:TYR:HE2	1.84	0.42
1:C:32:PHE:CD2	1:C:218:GLN:HG3	2.55	0.42
1:C:374:PHE:CZ	1:C:436:TRP:CD1	3.07	0.42
1:C:1110:TYR:CE2	1:C:1112:PRO:HD3	2.54	0.42
1:B:308:VAL:CG2	1:B:602:THR:HG23	2.48	0.42
2:E:40:ALA:HB3	2:E:43:LYS:HB2	2.02	0.42
2:E:183:VAL:HG21	3:F:182:TYR:HE2	1.84	0.42
2:G:49:ALA:CB	2:G:70:ILE:CG2	2.93	0.42
1:B:1110:TYR:CE2	1:B:1112:PRO:HD3	2.54	0.42
1:C:44:ARG:HB3	1:C:47:VAL:CG1	2.49	0.42
1:C:203:ILE:HB	1:C:227:VAL:HG22	2.02	0.42
1:C:726:ILE:HD13	1:C:945:LEU:HG	2.02	0.42
3:H:154:LYS:HD2	3:H:199:GLN:HE22	1.84	0.42
2:E:47:TRP:CG	3:F:100:LEU:HG	2.55	0.42
3:L:201:THR:HG23	3:L:206:THR:OG1	2.20	0.42
1:A:234:ASN:CG	4:A:1308:NAG:C7	2.93	0.42
1:B:866:THR:CG2	1:B:867:ASP:N	2.82	0.42
1:C:655:HIS:HA	1:C:694:ALA:O	2.19	0.42
3:H:201:THR:HG23	3:H:206:THR:OG1	2.20	0.42
1:A:657:ASN:CG	4:A:1303:NAG:N2	2.78	0.42
1:B:44:ARG:HB3	1:B:47:VAL:CG1	2.49	0.42
1:B:726:ILE:HD13	1:B:945:LEU:HG	2.02	0.42
1:B:1074:ASN:CG	4:B:1304:NAG:C7	2.92	0.42
1:B:1116:THR:HG22	1:B:1138:TYR:HD2	1.84	0.42
1:C:666:ILE:CD1	1:C:672:ALA:HB2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:51:ILE:HD13	2:G:72:ARG:HD2	2.01	0.42
2:G:183:VAL:HG21	3:L:182:TYR:HE2	1.84	0.42
1:B:117:LEU:CD2	1:B:130:VAL:CB	2.97	0.42
1:B:1103:PHE:CE1	1:B:1114:ILE:HD13	2.55	0.42
1:C:308:VAL:CG2	1:C:602:THR:HG23	2.48	0.42
2:D:40:ALA:HB3	2:D:43:LYS:HB2	2.02	0.42
3:L:213:PRO:O	3:L:214:THR:CG2	2.68	0.42
1:C:675:GLN:O	1:C:690:GLN:HA	2.20	0.42
1:C:896:ILE:HD11	1:C:904:TYR:HE2	1.84	0.42
2:E:47:TRP:CG	3:F:100:LEU:CD1	3.03	0.42
1:A:1076:THR:O	1:A:1097:SER:N	2.52	0.41
1:B:101:ILE:HD12	1:B:241:LEU:O	2.20	0.41
1:B:273:ARG:NH2	1:B:292:ALA:HB3	2.32	0.41
1:C:1038:LYS:HA	1:C:1038:LYS:HD2	1.91	0.41
1:A:101:ILE:HD12	1:A:241:LEU:O	2.20	0.41
1:A:722:VAL:O	1:A:934:ILE:HD11	2.21	0.41
1:A:896:ILE:HD11	1:A:904:TYR:HE2	1.84	0.41
1:A:1110:TYR:CE2	1:A:1112:PRO:HD3	2.54	0.41
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	2.02	0.41
1:C:657:ASN:CG	4:C:1302:NAG:N2	2.78	0.41
2:D:6:GLU:CB	2:D:121:THR:OG1	2.67	0.41
4:A:1313:NAG:O6	4:A:1313:NAG:O4	2.34	0.41
1:B:722:VAL:O	1:B:934:ILE:HD11	2.21	0.41
1:C:132:GLU:CD	1:C:165:ASN:HB3	2.46	0.41
2:D:183:VAL:HG21	3:H:182:TYR:CE2	2.54	0.41
2:E:51:ILE:HD13	2:E:72:ARG:HD2	2.03	0.41
2:G:183:VAL:HG21	3:L:182:TYR:CE2	2.54	0.41
3:L:154:LYS:HD2	3:L:199:GLN:HE22	1.84	0.41
1:A:32:PHE:CD2	1:A:218:GLN:HG3	2.55	0.41
1:A:48:LEU:HD22	1:A:306:PHE:CZ	2.56	0.41
1:A:203:ILE:HB	1:A:227:VAL:HG22	2.02	0.41
1:A:675:GLN:O	1:A:690:GLN:HA	2.21	0.41
1:A:1038:LYS:HA	1:A:1038:LYS:HD2	1.91	0.41
1:B:666:ILE:HG22	1:B:666:ILE:O	2.19	0.41
1:B:740:MET:HG3	1:B:857:GLY:HA3	2.02	0.41
1:C:30:ASN:OD1	1:C:59:PHE:HA	2.19	0.41
3:H:149:VAL:HG11	3:H:200:VAL:HG13	2.02	0.41
3:F:213:PRO:O	3:F:214:THR:CG2	2.68	0.41
1:A:565:PHE:CZ	1:B:42:VAL:HG22	2.56	0.41
1:A:1093:GLY:HA3	1:A:1105:THR:O	2.20	0.41
1:B:345:THR:CB	1:B:436:TRP:HE1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:GLN:HE21	1:B:1050:MET:HE1	1.86	0.41
1:C:48:LEU:HD22	1:C:306:PHE:CZ	2.56	0.41
1:C:1081:ILE:CD1	1:C:1133:VAL:CG2	2.98	0.41
1:A:598:ILE:HG13	1:A:609:ALA:HB3	2.01	0.41
1:C:731:MET:HG2	1:C:774:GLN:OE1	2.20	0.41
1:C:802:PHE:HZ	1:C:898:PHE:CZ	2.37	0.41
3:F:65:ARG:O	3:F:79:ILE:HA	2.19	0.41
3:F:97:THR:C	3:F:99:ILE:H	2.29	0.41
3:L:149:VAL:HG11	3:L:200:VAL:HG13	2.02	0.41
1:A:740:MET:HG3	1:A:857:GLY:HA3	2.02	0.41
1:B:48:LEU:HD22	1:B:306:PHE:CZ	2.55	0.41
1:B:234:ASN:CG	4:B:1308:NAG:C7	2.93	0.41
1:B:657:ASN:CG	4:B:1303:NAG:N2	2.78	0.41
1:B:675:GLN:O	1:B:690:GLN:HA	2.20	0.41
1:B:731:MET:HG2	1:B:774:GLN:OE1	2.21	0.41
1:C:101:ILE:HD12	1:C:241:LEU:O	2.20	0.41
1:C:381:GLY:HA2	2:G:31:ASN:CA	2.50	0.41
3:F:2:PRO:HB3	3:F:28:HIS:HB2	2.01	0.41
1:B:784:GLN:HE22	1:B:1030:SER:HG	1.64	0.41
1:A:57:PRO:HB2	1:A:60:SER:HB3	2.02	0.41
1:A:379:CYS:HA	1:A:432:CYS:CB	2.50	0.41
1:A:408:ARG:CB	3:F:58:LYS:O	2.69	0.41
1:A:731:MET:HG2	1:A:774:GLN:OE1	2.21	0.41
1:A:734:THR:HG21	1:A:959:LEU:HD11	2.03	0.41
1:B:203:ILE:HB	1:B:227:VAL:HG22	2.02	0.41
1:C:806:LEU:HD21	1:C:878:LEU:CD2	2.41	0.41
3:H:18:VAL:HG23	3:H:82:LEU:HD11	2.03	0.41
2:E:6:GLU:OE1	2:E:6:GLU:N	2.49	0.41
3:F:201:THR:HG23	3:F:206:THR:OG1	2.20	0.41
3:L:36:HIS:HE2	3:L:93:GLN:HG2	1.86	0.41
1:A:132:GLU:CD	1:A:165:ASN:HB3	2.46	0.41
1:C:734:THR:HG21	1:C:959:LEU:HD11	2.03	0.41
3:F:125:PRO:HD3	3:F:137:LEU:HD23	2.03	0.41
3:F:134:LYS:HD3	3:F:134:LYS:HA	1.76	0.41
1:B:132:GLU:CD	1:B:165:ASN:HB3	2.46	0.40
1:B:902:MET:HB3	1:B:916:LEU:CD2	2.51	0.40
1:C:722:VAL:O	1:C:934:ILE:HD11	2.21	0.40
1:C:1103:PHE:CE1	1:C:1114:ILE:HD13	2.55	0.40
2:D:9:GLY:H	2:D:121:THR:HG22	1.83	0.40
3:L:125:PRO:HD3	3:L:137:LEU:HD23	2.03	0.40
1:A:717:ASN:O	1:A:1070:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:LEU:CD1	1:A:945:LEU:HD21	2.52	0.40
1:A:902:MET:HB3	1:A:916:LEU:CD2	2.51	0.40
1:A:713:ALA:HB1	1:A:1072:GLU:CG	2.52	0.40
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.02	0.40
1:A:784:GLN:HE22	1:A:1030:SER:HG	1.64	0.40
1:B:713:ALA:HB1	1:B:1072:GLU:CG	2.51	0.40
1:C:1018:ILE:HD13	1:C:1018:ILE:HA	1.89	0.40
1:C:1116:THR:HG22	1:C:1138:TYR:HD2	1.86	0.40
2:E:60:TYR:OH	2:E:70:ILE:HG22	2.21	0.40
3:F:36:HIS:HE2	3:F:93:GLN:HG2	1.86	0.40
2:G:40:ALA:HB3	2:G:43:LYS:HB2	2.02	0.40
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.91	0.40
1:C:713:ALA:HB1	1:C:1072:GLU:CG	2.52	0.40
1:C:740:MET:HG3	1:C:857:GLY:HA3	2.02	0.40
1:C:902:MET:HB3	1:C:916:LEU:CD2	2.51	0.40
1:C:1138:TYR:CE1	1:C:1143:PRO:HG2	2.56	0.40
3:H:97:THR:C	3:H:99:ILE:H	2.29	0.40
3:F:149:VAL:HG11	3:F:200:VAL:HG13	2.02	0.40
2:G:34:MET:HB3	2:G:79:LEU:HD13	2.04	0.40
1:A:718:PHE:CZ	1:A:923:ILE:HD11	2.57	0.40
1:A:1074:ASN:OD1	1:A:1074:ASN:N	2.54	0.40
1:B:105:ILE:HG13	1:B:241:LEU:HD11	2.04	0.40
1:B:384:PRO:CD	2:D:101:THR:CG2	2.96	0.40
1:B:1074:ASN:OD1	1:B:1074:ASN:N	2.54	0.40
2:E:203:LEU:HD23	2:E:203:LEU:HA	1.88	0.40
3:F:35:TRP:CE2	3:F:77:LEU:HB2	2.57	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	982/1271 (77%)	948 (96%)	34 (4%)	0	100	100
1	B	982/1271 (77%)	948 (96%)	33 (3%)	1 (0%)	48	79
1	C	982/1271 (77%)	949 (97%)	33 (3%)	0	100	100
2	D	210/239 (88%)	204 (97%)	6 (3%)	0	100	100
2	E	210/239 (88%)	202 (96%)	8 (4%)	0	100	100
2	G	210/239 (88%)	202 (96%)	8 (4%)	0	100	100
3	F	212/217 (98%)	202 (95%)	10 (5%)	0	100	100
3	H	212/217 (98%)	203 (96%)	9 (4%)	0	100	100
3	L	212/217 (98%)	203 (96%)	9 (4%)	0	100	100
All	All	4212/5181 (81%)	4061 (96%)	150 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	801	ASN

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	631/1109 (57%)	628 (100%)	3 (0%)	86	92
1	B	620/1109 (56%)	617 (100%)	3 (0%)	86	92
1	C	631/1109 (57%)	629 (100%)	2 (0%)	91	96
2	D	179/201 (89%)	177 (99%)	2 (1%)	70	83
2	E	179/201 (89%)	178 (99%)	1 (1%)	84	91
2	G	179/201 (89%)	178 (99%)	1 (1%)	84	91
3	F	177/182 (97%)	175 (99%)	2 (1%)	70	83
3	H	177/182 (97%)	177 (100%)	0	100	100
3	L	177/182 (97%)	175 (99%)	2 (1%)	70	83
All	All	2950/4476 (66%)	2934 (100%)	16 (0%)	85	92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	432	CYS
1	A	714	ILE
1	B	432	CYS
1	B	714	ILE
1	B	801	ASN
1	C	119	ILE
1	C	714	ILE
2	D	67	ARG
2	D	72	ARG
2	E	105	TYR
3	F	75	ARG
3	F	93	GLN
2	G	101	THR
3	L	75	ARG
3	L	93	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	321	GLN
1	A	784	GLN
1	A	901	GLN
1	A	914	ASN
1	A	949	GLN
1	A	1005	GLN
1	A	1010	GLN
1	A	1011	GLN
1	A	1071	GLN
1	B	321	GLN
1	B	762	GLN
1	B	784	GLN
1	B	949	GLN
1	B	955	ASN
1	B	1005	GLN
1	B	1010	GLN
1	B	1071	GLN
1	C	121	ASN
1	C	321	GLN
1	C	762	GLN

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Mol	Chain	Res	Type
1	C	784	GLN
1	C	901	GLN
1	C	949	GLN
1	C	1005	GLN
1	C	1010	GLN
1	C	1011	GLN
1	C	1071	GLN
2	D	39	GLN
3	H	38	GLN
3	H	93	GLN
3	H	113	GLN
3	H	202	HIS
2	E	39	GLN
2	E	214	HIS
3	F	38	GLN
3	F	113	GLN
3	F	202	HIS
2	G	39	GLN
2	G	214	HIS
3	L	38	GLN
3	L	202	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

39 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1301	1	14,14,15	0.34	0	17,19,21	0.51	0
4	NAG	A	1306	1	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
4	NAG	B	1302	1	14,14,15	0.57	0	17,19,21	0.96	1 (5%)
4	NAG	B	1307	1	14,14,15	0.36	0	17,19,21	0.90	0
4	NAG	B	1303	1	14,14,15	0.61	0	17,19,21	0.81	0
4	NAG	A	1313	1	14,14,15	0.41	0	17,19,21	0.76	0
4	NAG	C	1310	1	14,14,15	0.28	0	17,19,21	0.67	0
4	NAG	C	1308	1	14,14,15	0.27	0	17,19,21	0.56	0
4	NAG	A	1312	1	14,14,15	0.24	0	17,19,21	0.86	1 (5%)
4	NAG	A	1311	1	14,14,15	0.29	0	17,19,21	0.66	0
4	NAG	C	1309	1	14,14,15	0.27	0	17,19,21	0.60	0
4	NAG	A	1308	1	14,14,15	0.79	1 (7%)	17,19,21	0.69	0
4	NAG	A	1314	1	14,14,15	0.40	0	17,19,21	0.75	0
4	NAG	C	1301	1	14,14,15	0.33	0	17,19,21	0.51	0
4	NAG	B	1306	1	14,14,15	0.36	0	17,19,21	0.98	1 (5%)
4	NAG	C	1311	1	14,14,15	0.28	0	17,19,21	0.70	0
4	NAG	A	1310	1	14,14,15	0.32	0	17,19,21	0.73	0
4	NAG	C	1302	1	14,14,15	0.61	0	17,19,21	0.81	0
4	NAG	C	1303	1	14,14,15	0.31	0	17,19,21	0.81	0
4	NAG	A	1309	1	14,14,15	0.33	0	17,19,21	0.71	0
4	NAG	B	1312	1	14,14,15	0.34	0	17,19,21	0.93	1 (5%)
4	NAG	B	1313	1	14,14,15	0.29	0	17,19,21	0.65	0
4	NAG	C	1305	1	14,14,15	0.35	0	17,19,21	0.90	0
4	NAG	A	1302	1	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
4	NAG	B	1314	1	14,14,15	0.29	0	17,19,21	0.67	0
4	NAG	B	1304	1	14,14,15	1.27	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	B	1305	1	14,14,15	0.39	0	17,19,21	0.83	0
4	NAG	C	1307	1	14,14,15	0.32	0	17,19,21	0.72	0
4	NAG	C	1304	1	14,14,15	0.29	0	17,19,21	0.61	0
4	NAG	B	1311	1	14,14,15	0.40	0	17,19,21	0.75	0
4	NAG	A	1303	1	14,14,15	0.59	0	17,19,21	0.81	0
4	NAG	A	1304	1	14,14,15	1.26	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	A	1307	1	14,14,15	0.34	0	17,19,21	0.90	0
4	NAG	A	1305	1	14,14,15	0.39	0	17,19,21	0.82	0
4	NAG	B	1308	1	14,14,15	0.81	1 (7%)	17,19,21	0.69	0
4	NAG	B	1310	1	14,14,15	0.32	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1306	1	14,14,15	0.34	0	17,19,21	0.71	0
4	NAG	B	1309	1	14,14,15	0.32	0	17,19,21	0.71	0
4	NAG	B	1301	1	14,14,15	0.34	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1313	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1314	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1304	NAG	O5-C1	4.53	1.51	1.43
4	A	1304	NAG	O5-C1	4.49	1.51	1.43
4	B	1308	NAG	O5-C1	2.88	1.48	1.43
4	A	1308	NAG	O5-C1	2.81	1.48	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1312	NAG	C1-O5-C5	2.52	115.56	112.19
4	B	1302	NAG	C4-C3-C2	-2.43	107.45	111.02
4	A	1302	NAG	C4-C3-C2	-2.40	107.50	111.02
4	B	1304	NAG	C1-C2-N2	2.39	114.20	110.43
4	B	1312	NAG	C1-O5-C5	2.38	115.38	112.19
4	A	1304	NAG	C1-C2-N2	2.38	114.19	110.43
4	A	1306	NAG	C4-C3-C2	-2.37	107.55	111.02
4	B	1306	NAG	C4-C3-C2	-2.34	107.59	111.02

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1312	NAG	C8-C7-N2-C2
4	A	1312	NAG	O7-C7-N2-C2
4	B	1311	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	C	1303	NAG	C8-C7-N2-C2
4	C	1303	NAG	O7-C7-N2-C2
4	C	1309	NAG	C8-C7-N2-C2
4	C	1309	NAG	O7-C7-N2-C2
4	B	1312	NAG	C8-C7-N2-C2
4	B	1312	NAG	O7-C7-N2-C2
4	A	1302	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	B	1311	NAG	O5-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	A	1309	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	A	1309	NAG	C4-C5-C6-O6
4	B	1309	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	C	1304	NAG	C8-C7-N2-C2
4	C	1304	NAG	O7-C7-N2-C2
4	A	1303	NAG	C4-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1308	NAG	O5-C5-C6-O6
4	B	1311	NAG	C4-C5-C6-O6
4	A	1311	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	A	1313	NAG	O5-C5-C6-O6
4	B	1312	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	C	1308	NAG	C8-C7-N2-C2
4	A	1312	NAG	C3-C2-N2-C7
4	B	1311	NAG	C3-C2-N2-C7
4	A	1311	NAG	O5-C5-C6-O6
4	C	1308	NAG	O7-C7-N2-C2
4	B	1313	NAG	C8-C7-N2-C2
4	C	1310	NAG	C8-C7-N2-C2
4	A	1314	NAG	C1-C2-N2-C7
4	A	1307	NAG	C3-C2-N2-C7
4	B	1307	NAG	C3-C2-N2-C7
4	C	1305	NAG	C3-C2-N2-C7
4	B	1313	NAG	O7-C7-N2-C2
4	A	1308	NAG	C4-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	C	1310	NAG	O7-C7-N2-C2

There are no ring outliers.

18 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1306	NAG	1	0
4	B	1302	NAG	2	0
4	B	1303	NAG	2	0
4	A	1313	NAG	1	0
4	A	1308	NAG	3	0
4	B	1306	NAG	1	0
4	A	1310	NAG	1	0
4	C	1302	NAG	2	0
4	A	1302	NAG	2	0
4	B	1304	NAG	1	0
4	B	1305	NAG	2	0
4	C	1307	NAG	1	0
4	B	1311	NAG	7	0
4	A	1303	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1304	NAG	1	0
4	A	1305	NAG	2	0
4	B	1308	NAG	3	0
4	B	1310	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

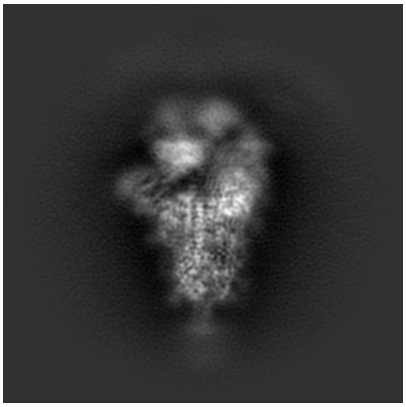
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24504. These allow visual inspection of the internal detail of the map and identification of artifacts.

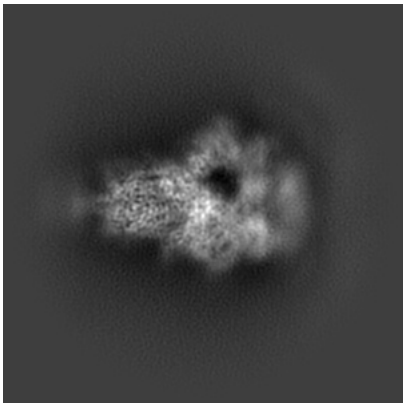
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

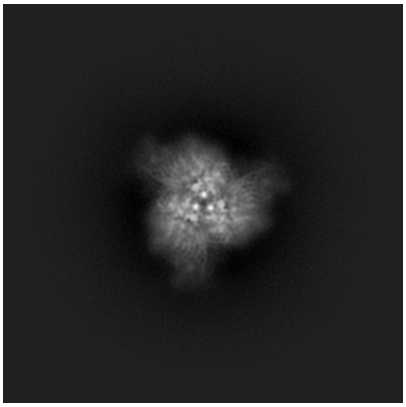
6.1.1 Primary map



X



Y

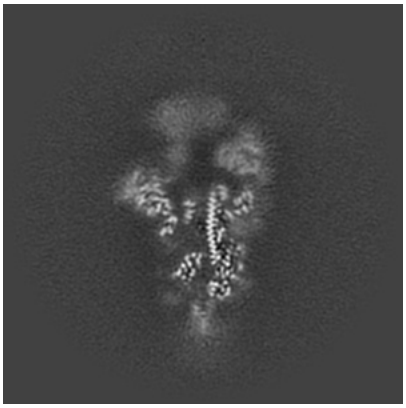


Z

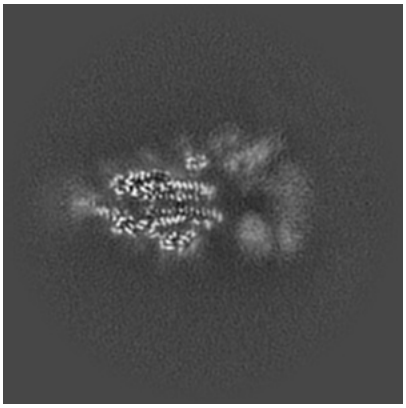
The images above show the map projected in three orthogonal directions.

6.2 Central slices

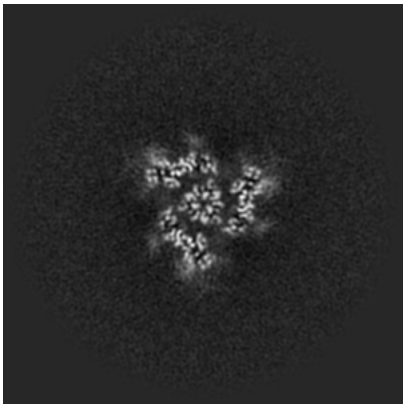
6.2.1 Primary map



X Index: 216



Y Index: 216

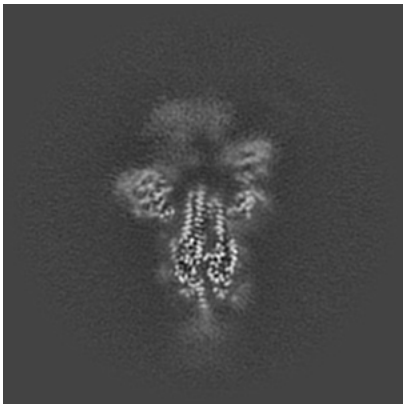


Z Index: 216

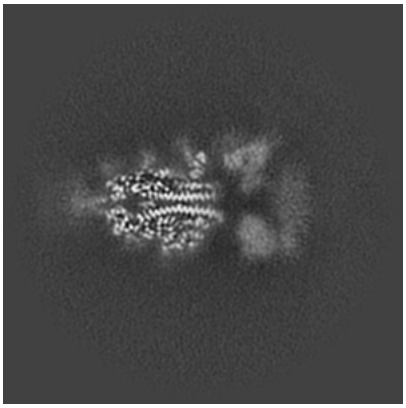
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

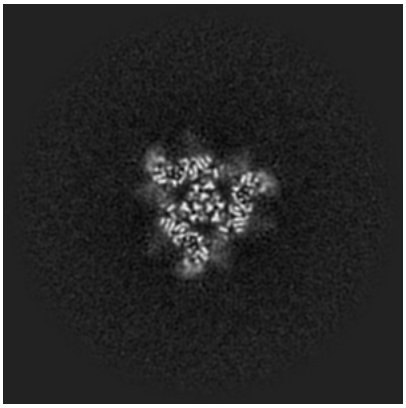
6.3.1 Primary map



X Index: 206



Y Index: 212

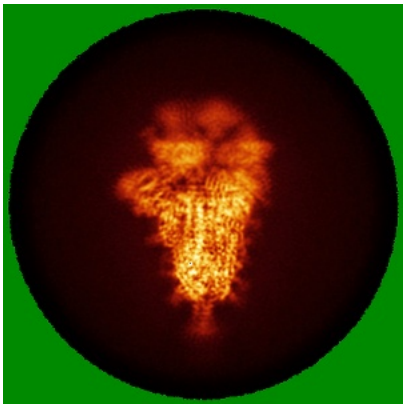


Z Index: 209

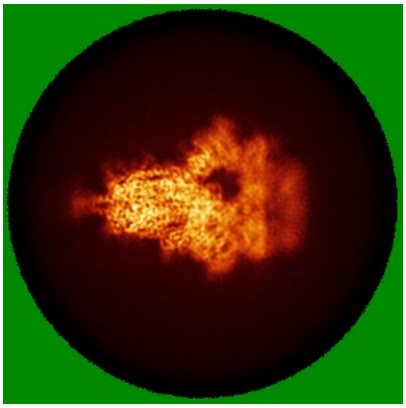
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

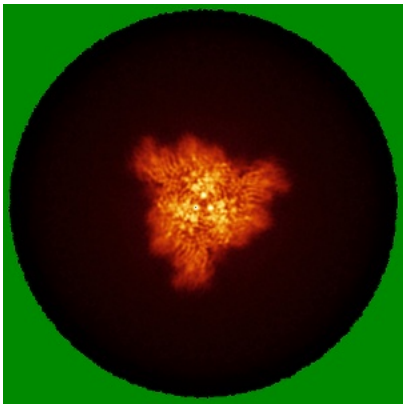
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

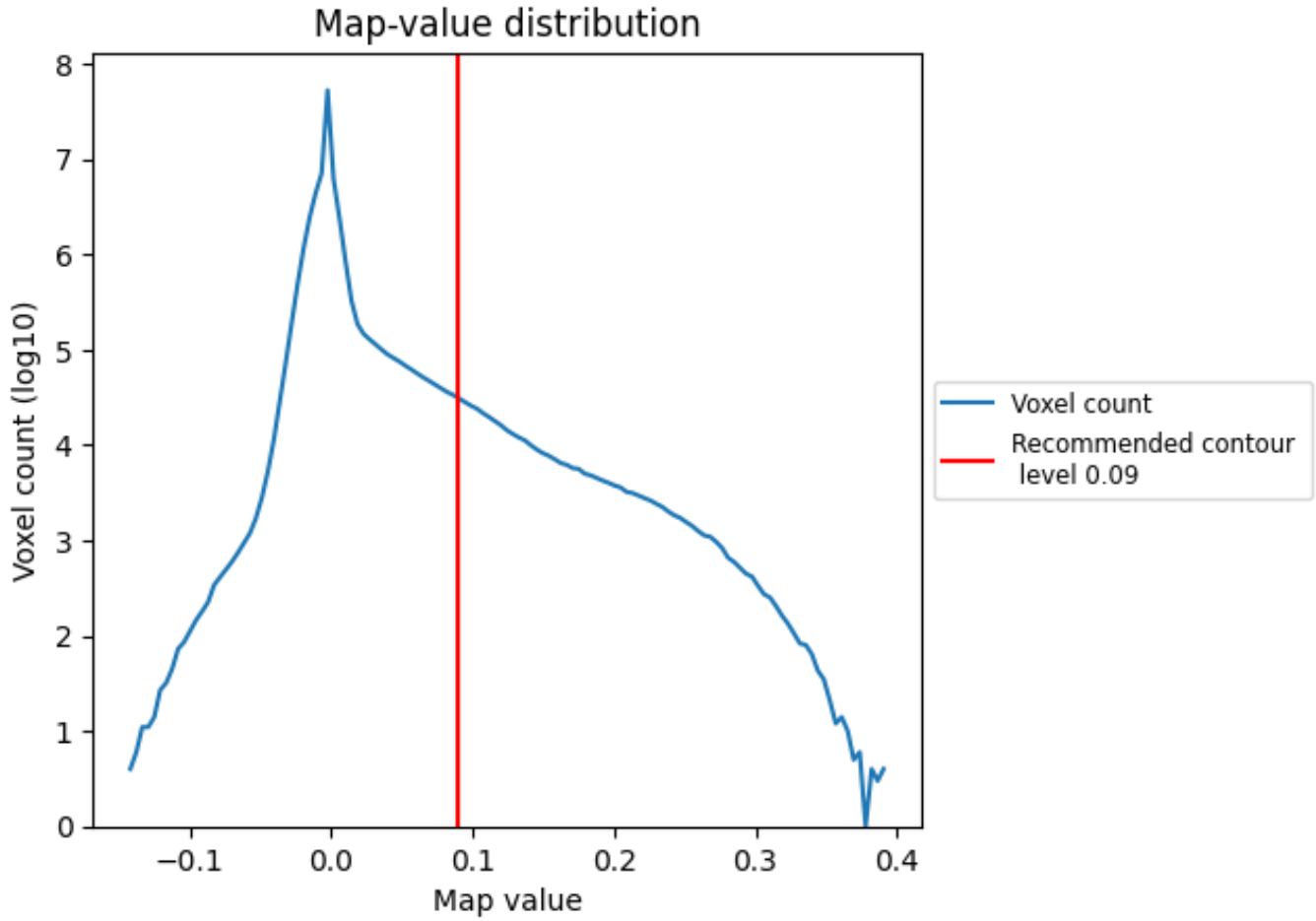
6.6 Mask visualisation (i)

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

7 Map analysis

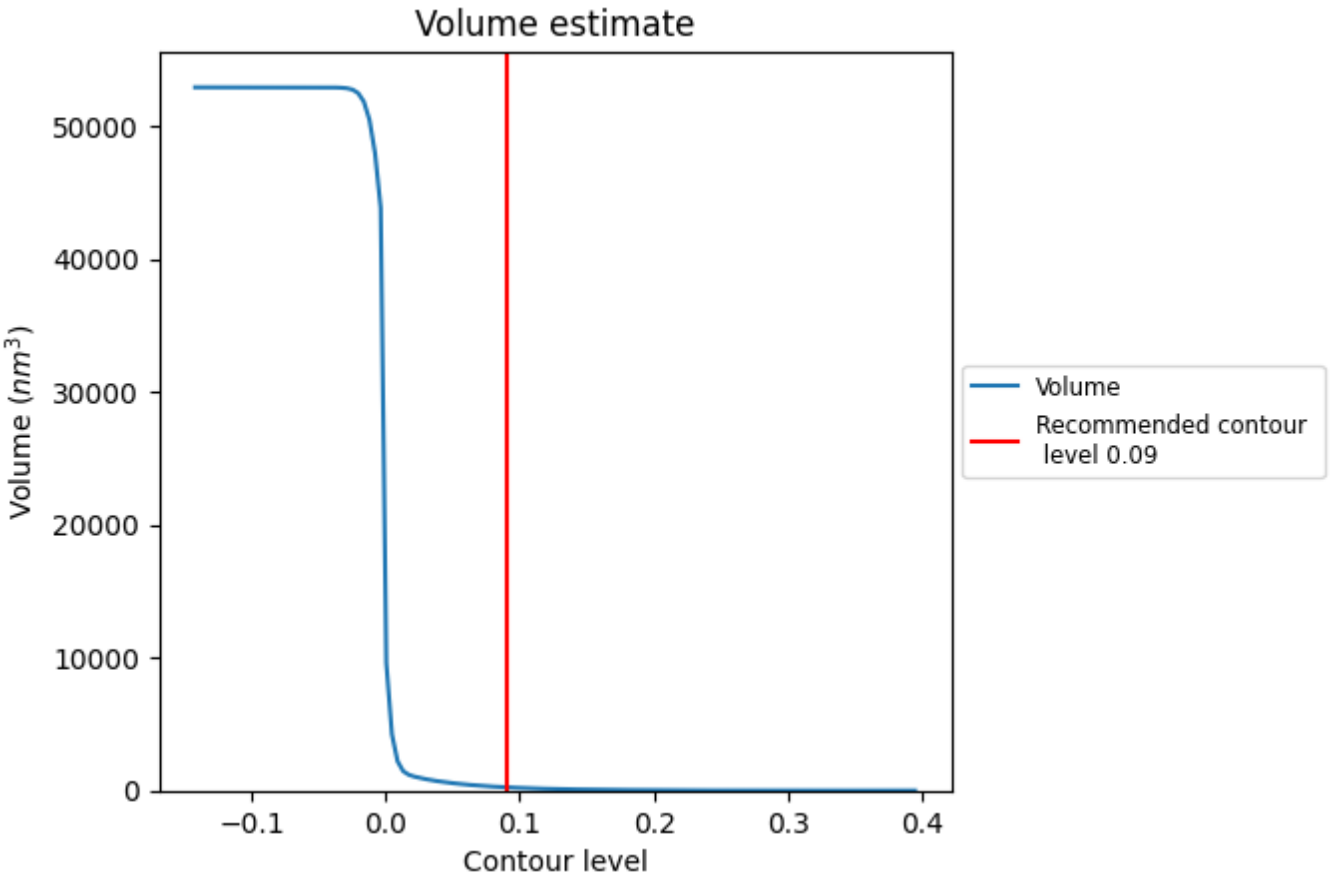
This section contains the results of statistical analysis of the map.

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.

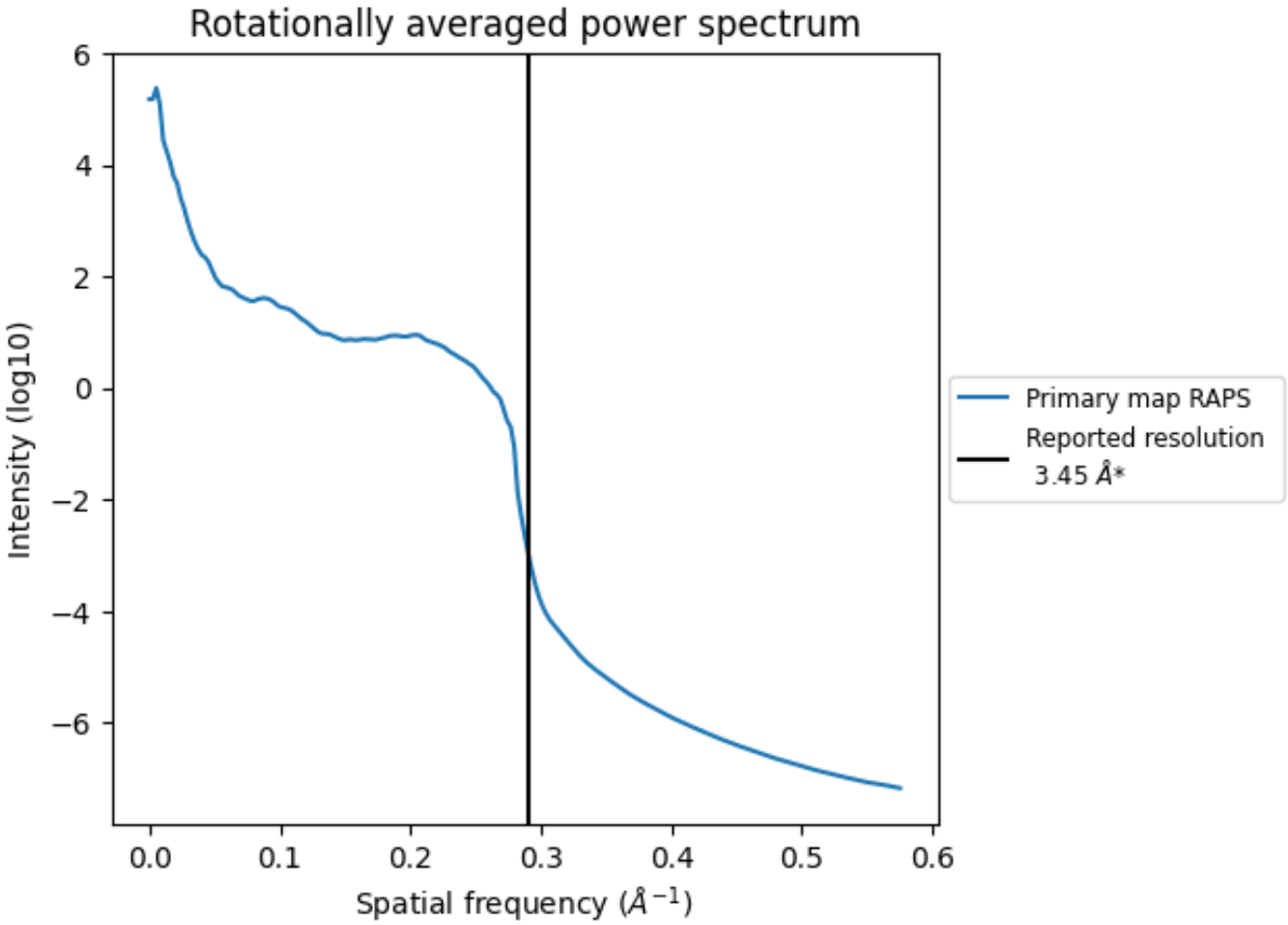
7.2 Volume estimate



The volume at the recommended contour level is 245 nm^3; this corresponds to an approximate mass of 221 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)

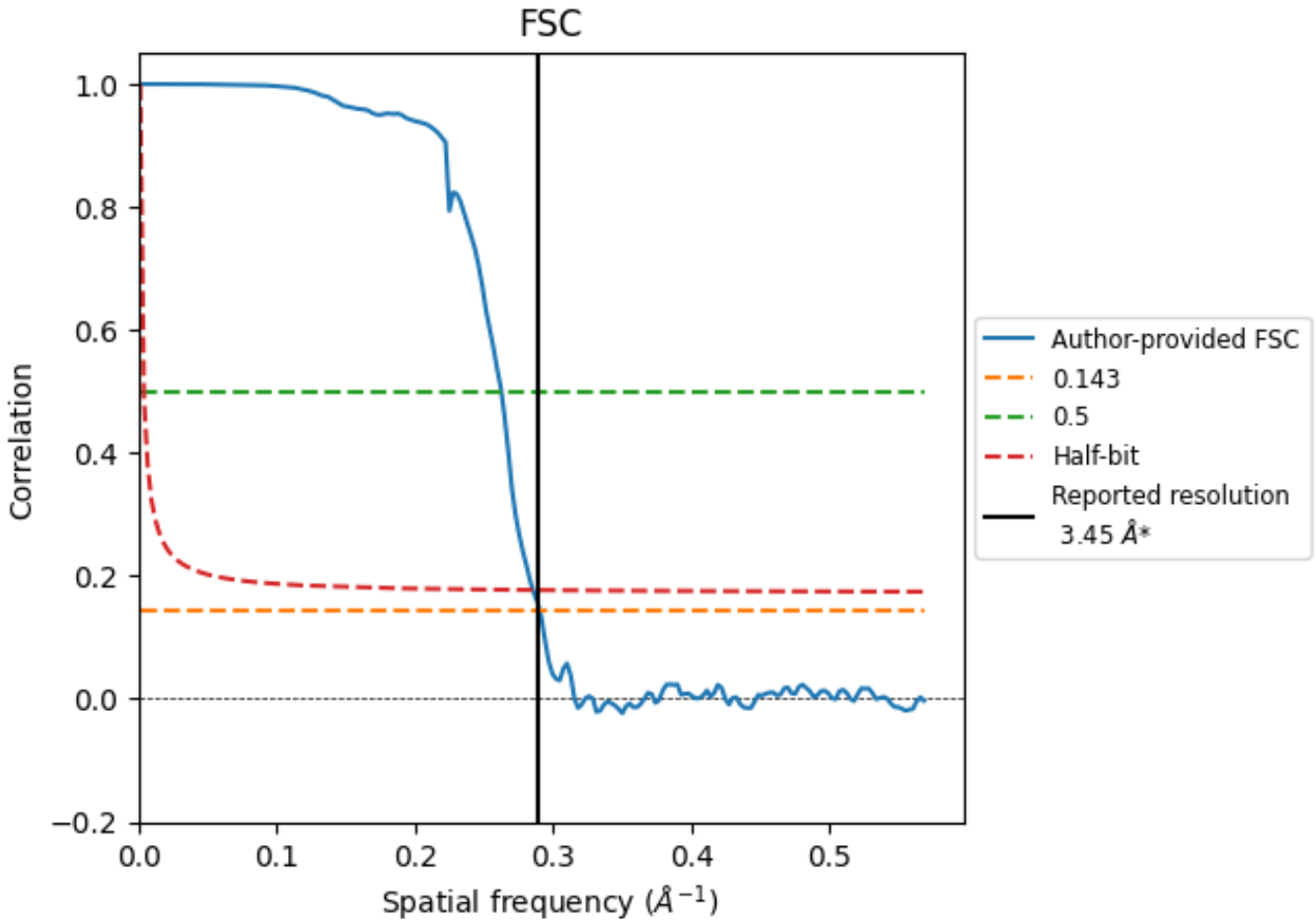


*Reported resolution corresponds to spatial frequency of 0.290 Å^{-1}

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 0.290 $Å^{-1}$

8.2 Resolution estimates (i)

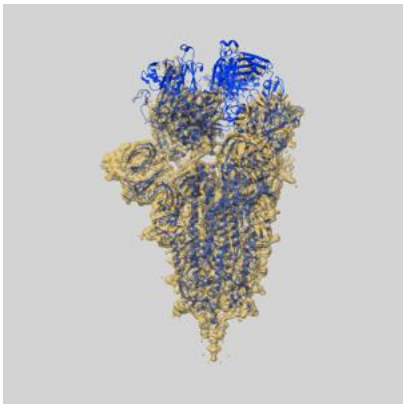
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.44	3.81	3.50
Unmasked-calculated*	-	-	-

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

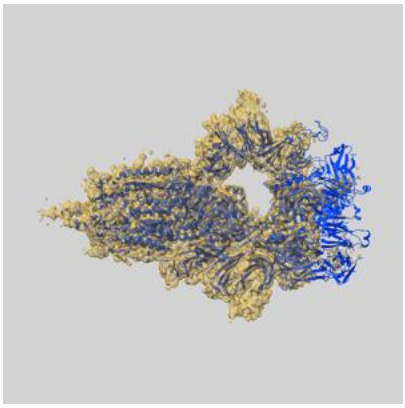
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24504 and PDB model 7RKV. Per-residue inclusion information can be found in section 3 on page 13.

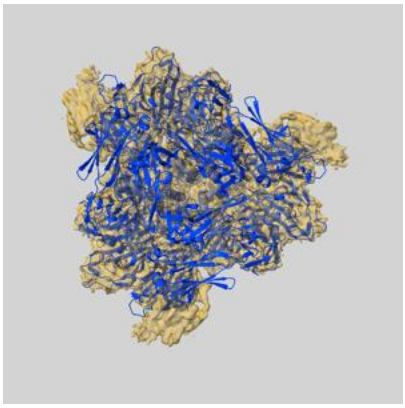
9.1 Map-model overlay



X



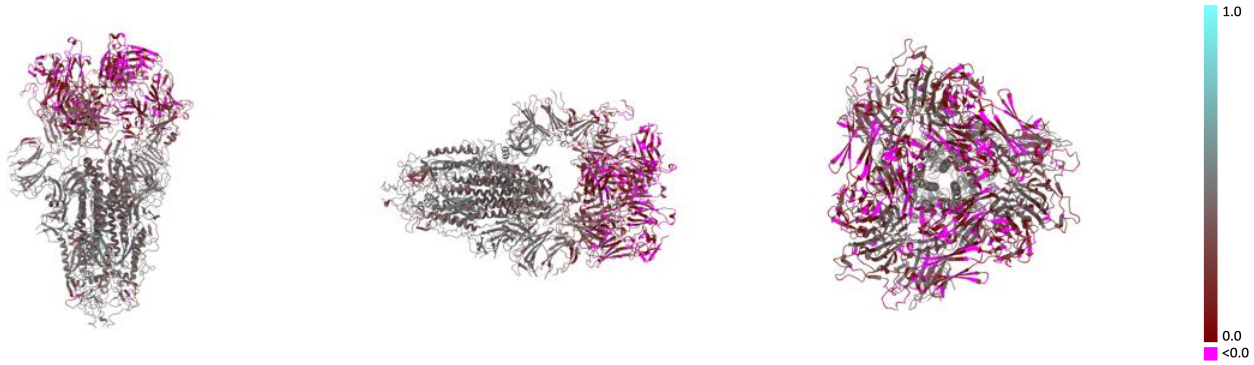
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

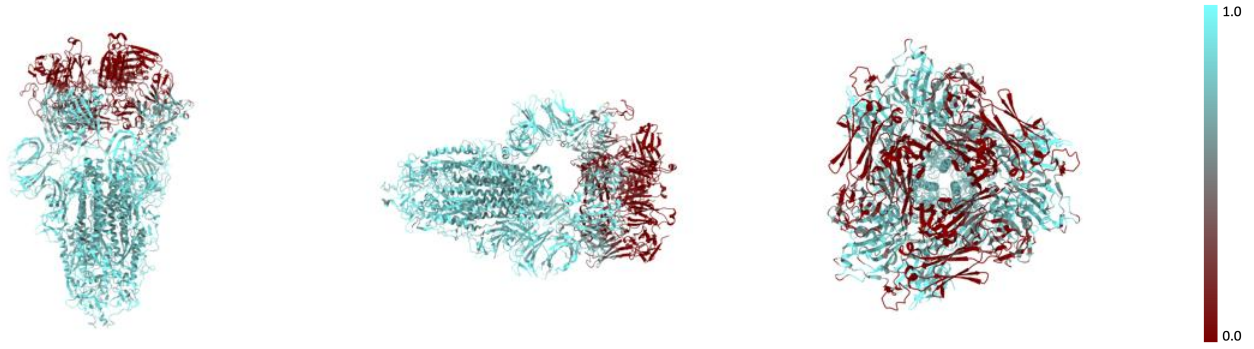
9.2 Q-score mapped to coordinate model (i)



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.

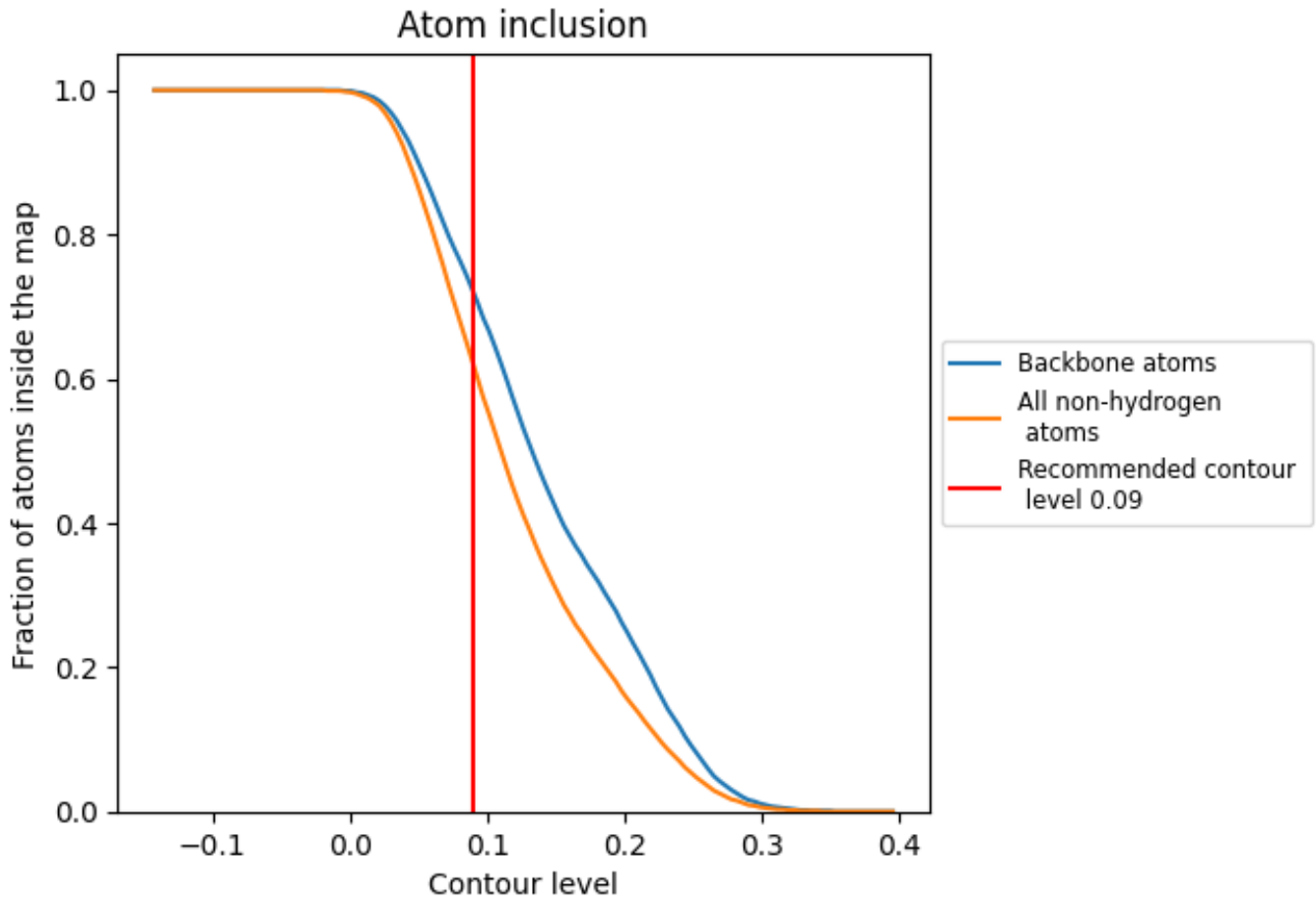
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 62% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6190	0.3000
A	0.8040	0.3970
B	0.8100	0.4000
C	0.8100	0.3990
D	0.1900	0.0830
E	0.1840	0.0810
F	0.1940	0.0700
G	0.1880	0.0830
H	0.1930	0.0730
L	0.1940	0.0720