Full wwPDB EM Validation Report (i)

Oct 1, 2024 – 01:25 PM JST

PDB ID	:	7WO4
EMDB ID	:	EMD-32638
Title	:	SARS-CoV-2 Spike in complex with IgG 553-15 (S-553-15 dimer trimer)
Authors	:	Zhan, W.Q.; Zhang, X.; Chen, Z.G.; Sun, L.
Deposited on	:	2022-01-20
Resolution	:	4.47 Å(reported)

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

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

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

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

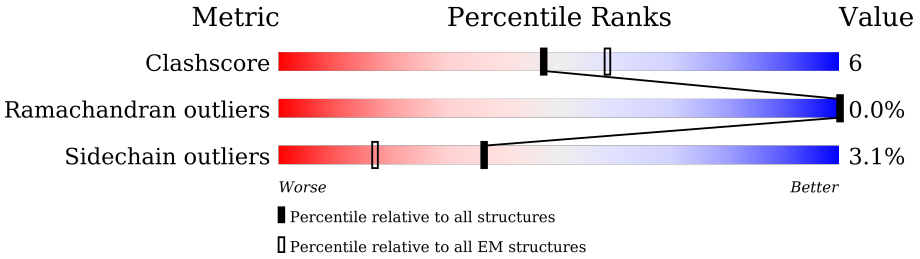
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.47 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	1288	70% 12% • 16%
1	B	1288	71% 12% • 16%
1	C	1288	71% 12% • 16%
1	J	1288	70% 12% • 16%
1	K	1288	70% 13% 16%
1	L	1288	71% 12% • 16%
2	D	225	80% 20%
2	F	225	76% 23%

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Mol	Chain	Length	Quality of chain
2	H	225	80% 19%
2	M	225	80% 20%
2	O	225	75% 24%
2	Q	225	78% 21%
3	E	218	79% 18%
3	G	218	82% 15%
3	I	218	77% 21%
3	N	218	81% 16%
3	P	218	80% 16%
3	R	218	80% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 71208 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1076	8338	5318	1396	1586	38	0	0
1	B	1076	8338	5318	1396	1586	38	0	0
1	C	1076	8338	5318	1396	1586	38	0	0
1	J	1076	8338	5318	1396	1586	38	0	0
1	K	1076	8338	5318	1396	1586	38	0	0
1	L	1076	8338	5318	1396	1586	38	0	0

There are 516 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2
J	614	GLY	ASP	variant	UNP P0DTC2
J	682	GLY	ARG	conflict	UNP P0DTC2
J	683	SER	ARG	conflict	UNP P0DTC2
J	685	SER	ARG	conflict	UNP P0DTC2
J	986	PRO	LYS	conflict	UNP P0DTC2
J	987	PRO	VAL	conflict	UNP P0DTC2
J	1209	GLY	-	expression tag	UNP P0DTC2
J	1210	SER	-	expression tag	UNP P0DTC2
J	1211	GLY	-	expression tag	UNP P0DTC2
J	1212	TYR	-	expression tag	UNP P0DTC2
J	1213	ILE	-	expression tag	UNP P0DTC2
J	1214	PRO	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1257	LYS	-	expression tag	UNP P0DTC2
J	1258	GLY	-	expression tag	UNP P0DTC2
J	1259	GLY	-	expression tag	UNP P0DTC2
J	1260	GLY	-	expression tag	UNP P0DTC2
J	1261	SER	-	expression tag	UNP P0DTC2
J	1262	GLY	-	expression tag	UNP P0DTC2
J	1263	GLY	-	expression tag	UNP P0DTC2
J	1264	GLY	-	expression tag	UNP P0DTC2
J	1265	SER	-	expression tag	UNP P0DTC2
J	1266	GLY	-	expression tag	UNP P0DTC2
J	1267	GLY	-	expression tag	UNP P0DTC2
J	1268	SER	-	expression tag	UNP P0DTC2
J	1269	ALA	-	expression tag	UNP P0DTC2
J	1270	TRP	-	expression tag	UNP P0DTC2
J	1271	SER	-	expression tag	UNP P0DTC2
J	1272	HIS	-	expression tag	UNP P0DTC2
J	1273	PRO	-	expression tag	UNP P0DTC2
J	1274	GLN	-	expression tag	UNP P0DTC2
J	1275	PHE	-	expression tag	UNP P0DTC2
J	1276	GLU	-	expression tag	UNP P0DTC2
J	1277	LYS	-	expression tag	UNP P0DTC2
J	1278	GLY	-	expression tag	UNP P0DTC2
J	1279	GLY	-	expression tag	UNP P0DTC2
J	1280	SER	-	expression tag	UNP P0DTC2
J	1281	HIS	-	expression tag	UNP P0DTC2
J	1282	HIS	-	expression tag	UNP P0DTC2
J	1283	HIS	-	expression tag	UNP P0DTC2
J	1284	HIS	-	expression tag	UNP P0DTC2
J	1285	HIS	-	expression tag	UNP P0DTC2
J	1286	HIS	-	expression tag	UNP P0DTC2
J	1287	HIS	-	expression tag	UNP P0DTC2
J	1288	HIS	-	expression tag	UNP P0DTC2
K	614	GLY	ASP	variant	UNP P0DTC2
K	682	GLY	ARG	conflict	UNP P0DTC2
K	683	SER	ARG	conflict	UNP P0DTC2
K	685	SER	ARG	conflict	UNP P0DTC2
K	986	PRO	LYS	conflict	UNP P0DTC2
K	987	PRO	VAL	conflict	UNP P0DTC2
K	1209	GLY	-	expression tag	UNP P0DTC2
K	1210	SER	-	expression tag	UNP P0DTC2
K	1211	GLY	-	expression tag	UNP P0DTC2
K	1212	TYR	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1255	PHE	-	expression tag	UNP P0DTC2
K	1256	GLU	-	expression tag	UNP P0DTC2
K	1257	LYS	-	expression tag	UNP P0DTC2
K	1258	GLY	-	expression tag	UNP P0DTC2
K	1259	GLY	-	expression tag	UNP P0DTC2
K	1260	GLY	-	expression tag	UNP P0DTC2
K	1261	SER	-	expression tag	UNP P0DTC2
K	1262	GLY	-	expression tag	UNP P0DTC2
K	1263	GLY	-	expression tag	UNP P0DTC2
K	1264	GLY	-	expression tag	UNP P0DTC2
K	1265	SER	-	expression tag	UNP P0DTC2
K	1266	GLY	-	expression tag	UNP P0DTC2
K	1267	GLY	-	expression tag	UNP P0DTC2
K	1268	SER	-	expression tag	UNP P0DTC2
K	1269	ALA	-	expression tag	UNP P0DTC2
K	1270	TRP	-	expression tag	UNP P0DTC2
K	1271	SER	-	expression tag	UNP P0DTC2
K	1272	HIS	-	expression tag	UNP P0DTC2
K	1273	PRO	-	expression tag	UNP P0DTC2
K	1274	GLN	-	expression tag	UNP P0DTC2
K	1275	PHE	-	expression tag	UNP P0DTC2
K	1276	GLU	-	expression tag	UNP P0DTC2
K	1277	LYS	-	expression tag	UNP P0DTC2
K	1278	GLY	-	expression tag	UNP P0DTC2
K	1279	GLY	-	expression tag	UNP P0DTC2
K	1280	SER	-	expression tag	UNP P0DTC2
K	1281	HIS	-	expression tag	UNP P0DTC2
K	1282	HIS	-	expression tag	UNP P0DTC2
K	1283	HIS	-	expression tag	UNP P0DTC2
K	1284	HIS	-	expression tag	UNP P0DTC2
K	1285	HIS	-	expression tag	UNP P0DTC2
K	1286	HIS	-	expression tag	UNP P0DTC2
K	1287	HIS	-	expression tag	UNP P0DTC2
K	1288	HIS	-	expression tag	UNP P0DTC2
L	614	GLY	ASP	variant	UNP P0DTC2
L	682	GLY	ARG	conflict	UNP P0DTC2
L	683	SER	ARG	conflict	UNP P0DTC2
L	685	SER	ARG	conflict	UNP P0DTC2
L	986	PRO	LYS	conflict	UNP P0DTC2
L	987	PRO	VAL	conflict	UNP P0DTC2
L	1209	GLY	-	expression tag	UNP P0DTC2
L	1210	SER	-	expression tag	UNP P0DTC2

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

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

- Molecule 2 is a protein called mAb15 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	225	1704	1077	289	331	7	0	0

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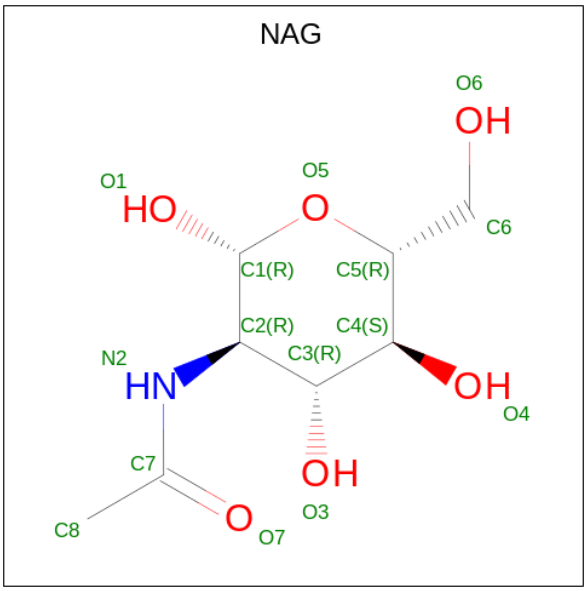
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	225	1704	1077	289	331	7	0	0
2	H	225	1704	1077	289	331	7	0	0
2	M	225	1704	1077	289	331	7	0	0
2	O	225	1704	1077	289	331	7	0	0
2	Q	225	1704	1077	289	331	7	0	0

- Molecule 3 is a protein called mAb15 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	215	1616	999	270	342	5	0	0
3	G	215	1616	999	270	342	5	0	0
3	I	215	1616	999	270	342	5	0	0
3	N	215	1616	999	270	342	5	0	0
3	P	215	1616	999	270	342	5	0	0
3	R	215	1616	999	270	342	5	0	0

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



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

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

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

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

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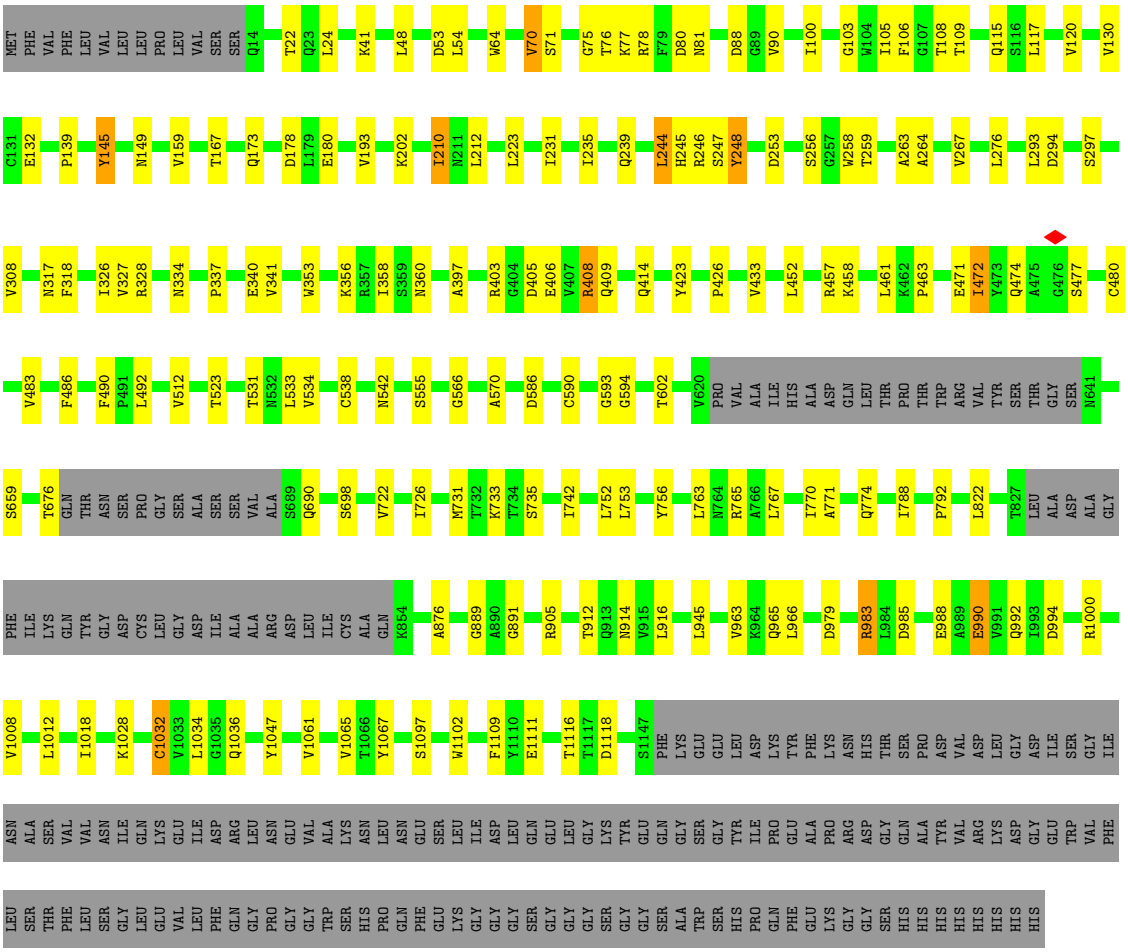
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0
4	L	1	14	8	1	5	0

3 Residue-property plots (i)

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

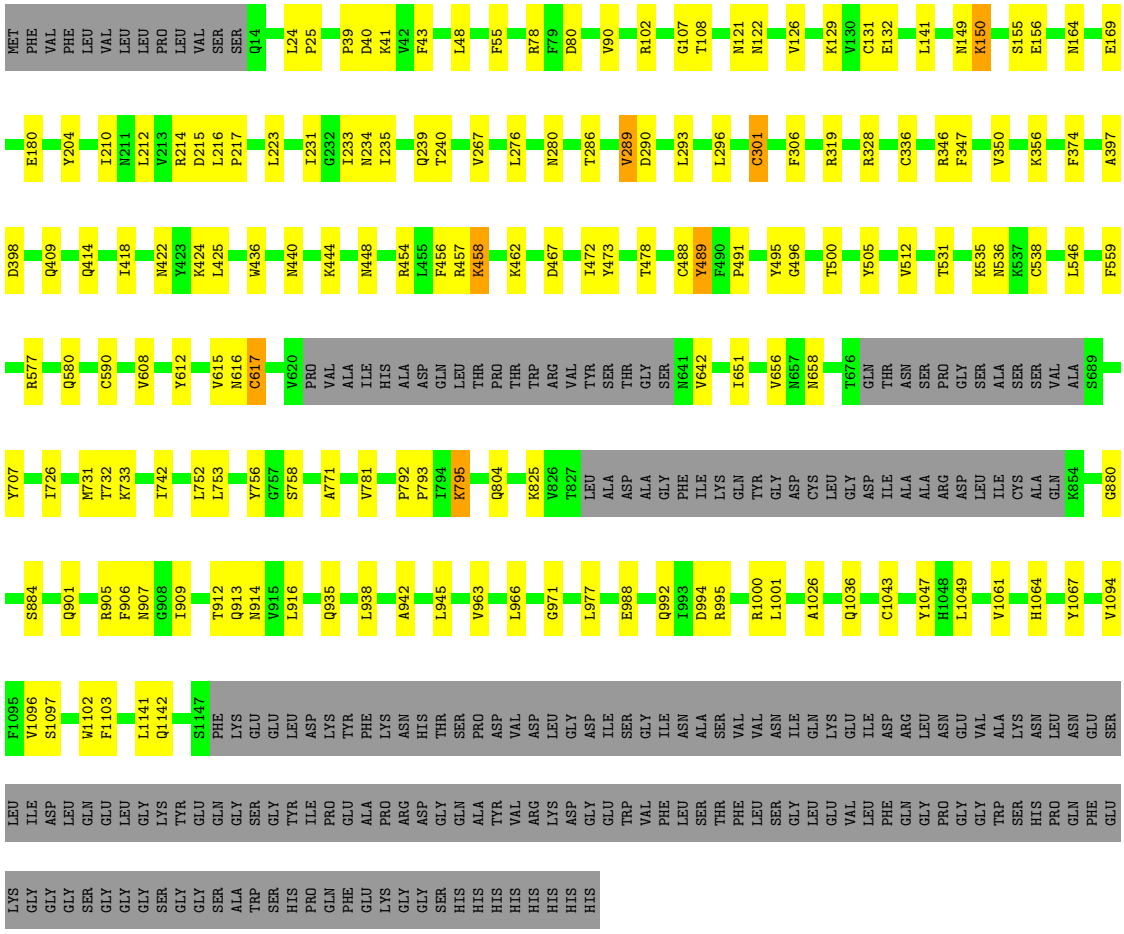
- Molecule 1: Spike glycoprotein

Chain A: 70% 12% • 16%



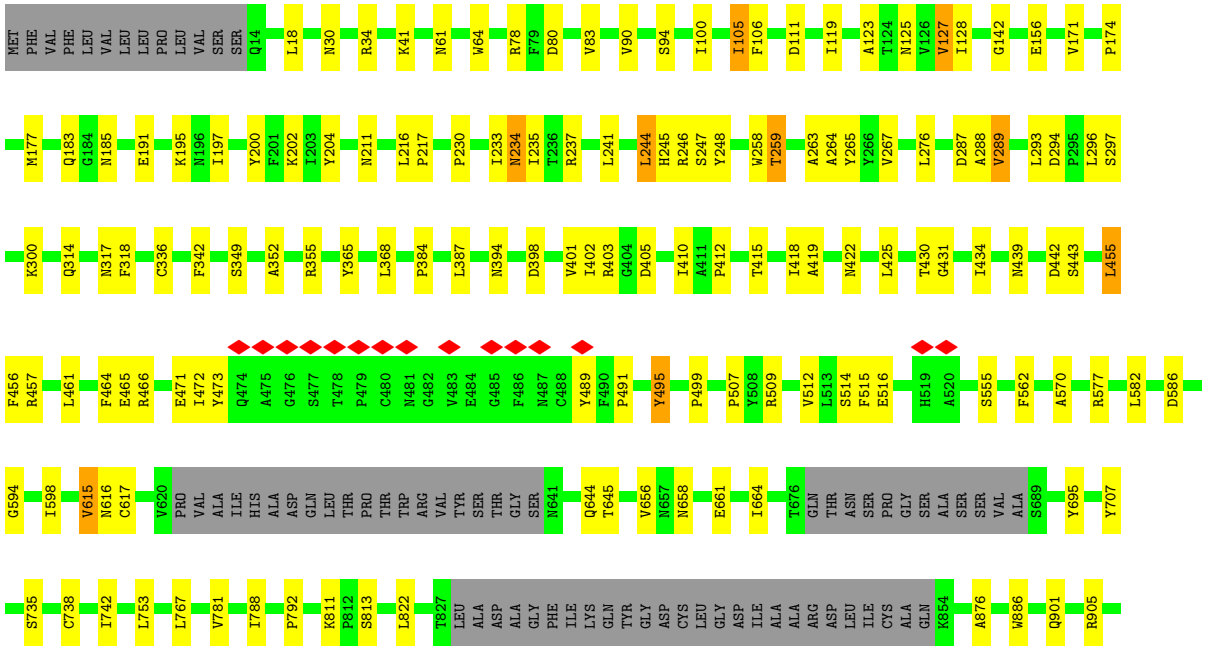
- Molecule 1: Spike glycoprotein

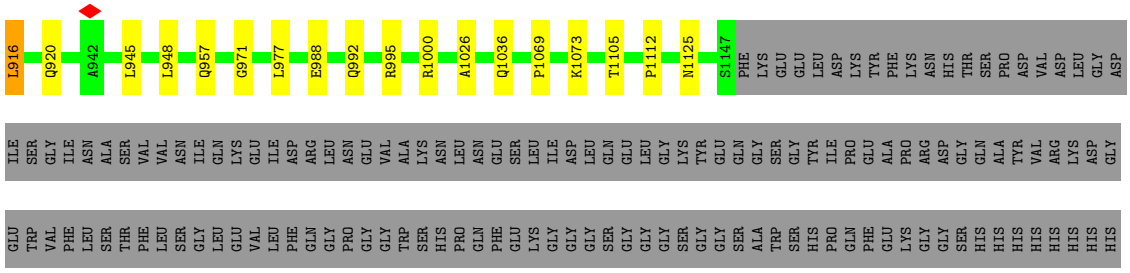
Chain B: 71% 12% • 16%



- Molecule 1: Spike glycoprotein

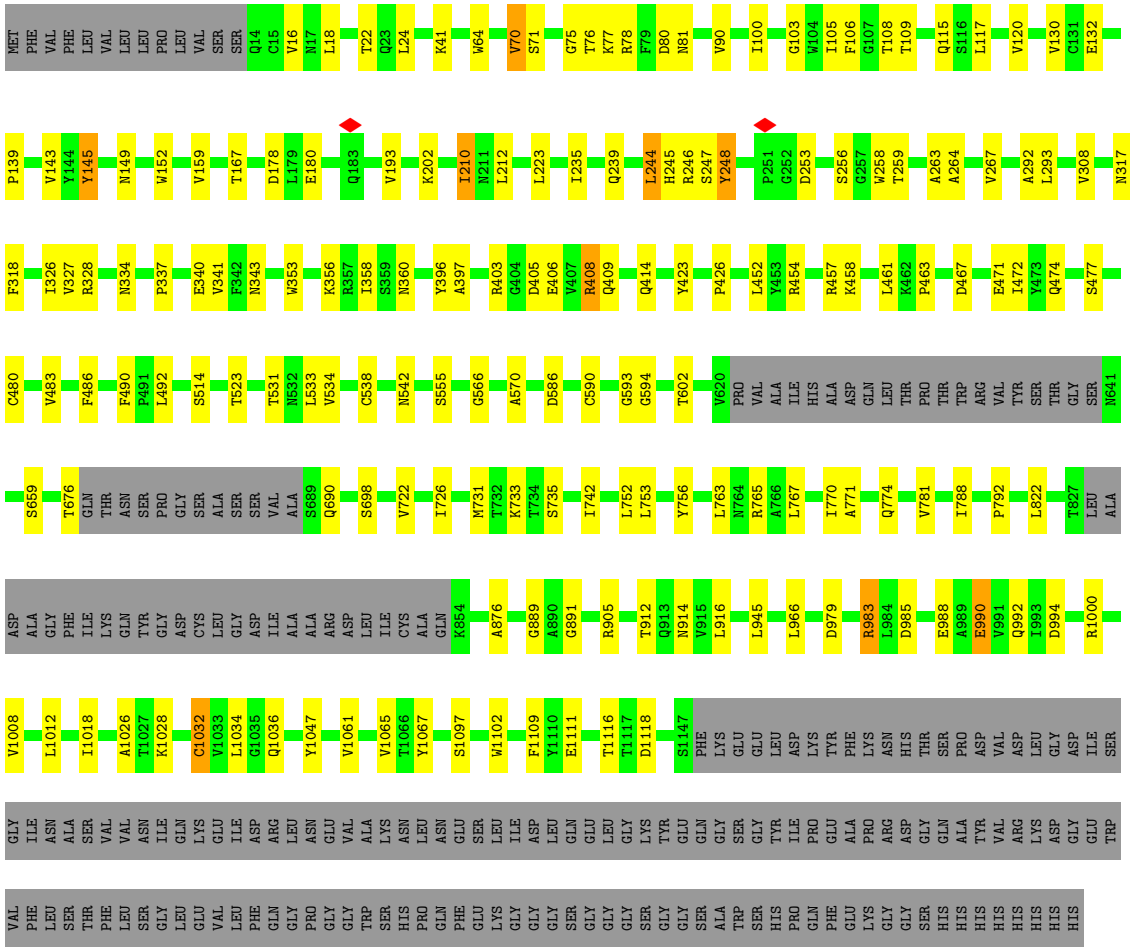
Chain C:





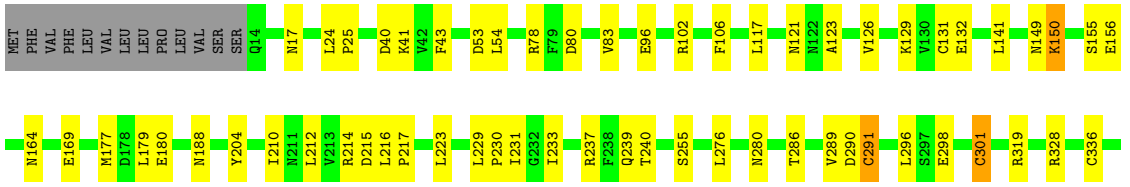
• Molecule 1: Spike glycoprotein

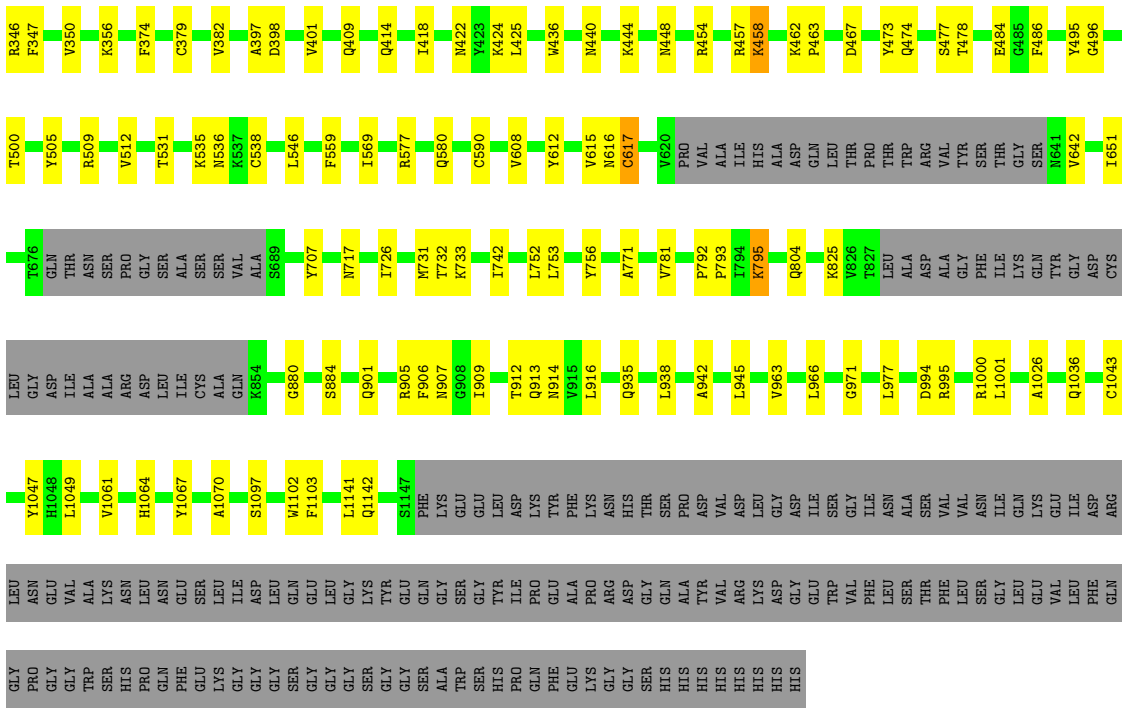
Chain J:



• Molecule 1: Spike glycoprotein

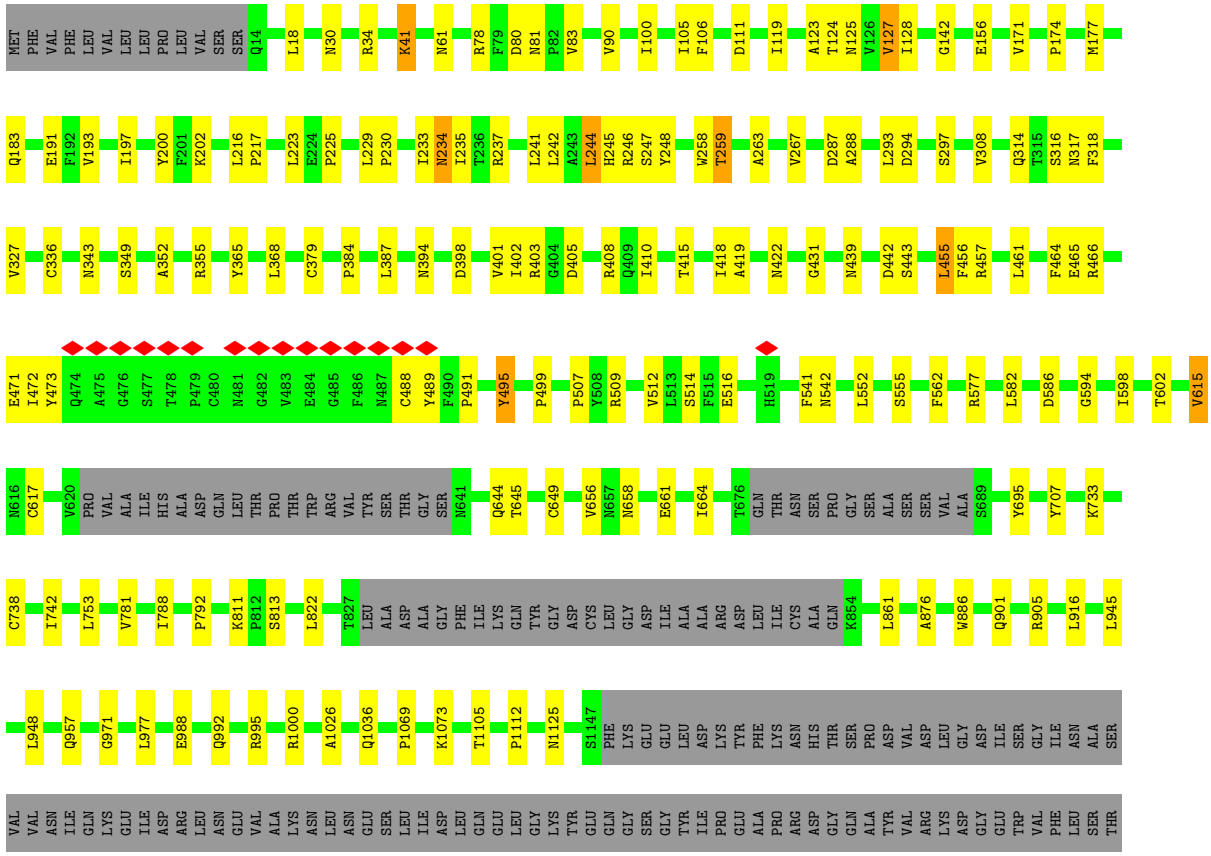
Chain K:





- Molecule 1: Spike glycoprotein

Chain L:



PHE LEU SER GLY LEU GLU VAL LEU PHE GLN GLY PRO GLY GLY TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY SER HIS HIS HIS HIS HIS HIS HIS HIS

- Molecule 2: mAb15 VH

Chain D: 80% 20%

E1 Q6 W33 R38 Q39 A40 K43 N50 Y60 V61 D62 S63 V64 R67 F68 M83 V86 T91 R98 V99 Q111 G112 T116 P125 L130 A131 P132 S133 T137 G145 C146 Y151 F152 P153 E154 P155 S162 L165 V188

T189 V190 P191 N203 H206 K207 P208 T211 P219 K220 S221 C222 D223 K224 T225

- Molecule 2: mAb15 VH

Chain F: 76% 23%

E1 Q6 L11 V12 Q13 P14 A23 T28 F29 S30 W33 A40 K43 W47 N50 I51 K58 R72 K76 N77 S78 M83 V99 Q111 G112 T113 T116 V117 S118 S119 G124 P129 L130 A131 P132 S138 L144 G145 C146

K149 D150 P153 E154 P155 W160 P173 Q177 S178 S179 G180 L181 Y182 S183 T189 V190 P191 S192 S193 G196 T197 I201 V204 N205 H206 K207 P208 D214 K220 S221 C222 D223 K224 T225

- Molecule 2: mAb15 VH

Chain H: 80% 19%

E1 L4 V5 Q6 Q13 R19 F27 W33 A40 K43 W47 N50 I51 N52 Q53 D54 E57 V61 V64 R67 F80 L81 Q82 D90 T91 C96 V99 P105 G110 Q111 T116 S136 A142 C146 P153 E154

P155 V156 T157 S167 L176 Q177 L181 Y182 V190 P191 S192 N205 H206 K207 P208 V213 K220 S221 C222 T225

- Molecule 2: mAb15 VH

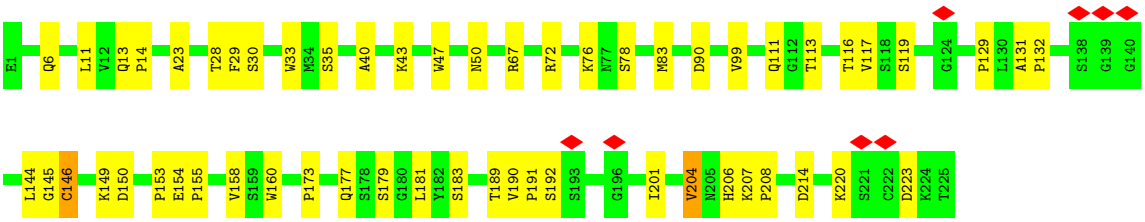
Chain M: 80% 20%

E1 Q6 W33 R38 Q39 A40 K43 N50 Y60 V61 D62 S63 V64 R67 F68 M83 V86 T91 R98 V99 Q111 G112 T116 P125 L130 A131 P132 S133 T137 L144 G145 C146 Y151 F152 P153 E154 P155 S162 L165

V188 T189 V190 P191 N203 H206 K207 P208 T211 K215 P219 K220 S221 C222 D223 K224 T225

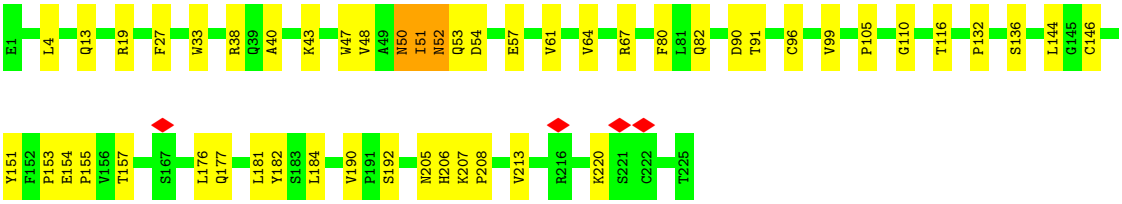
- Molecule 2: mAb15 VH

Chain O: 75% 24%



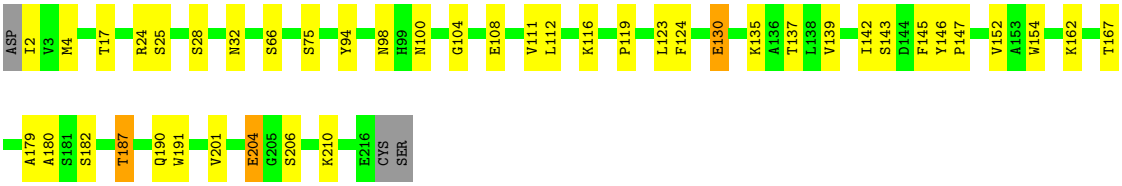
• Molecule 2: mAb15 VH

Chain Q:



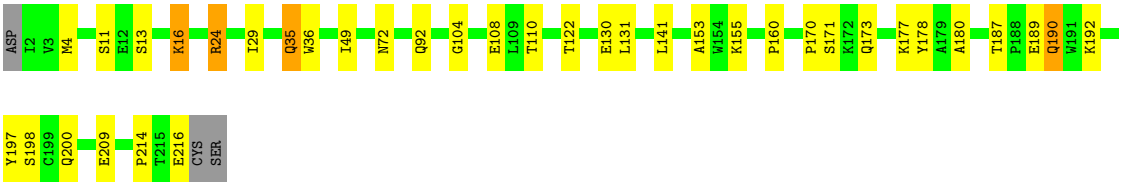
• Molecule 3: mAb15 VL

Chain E:



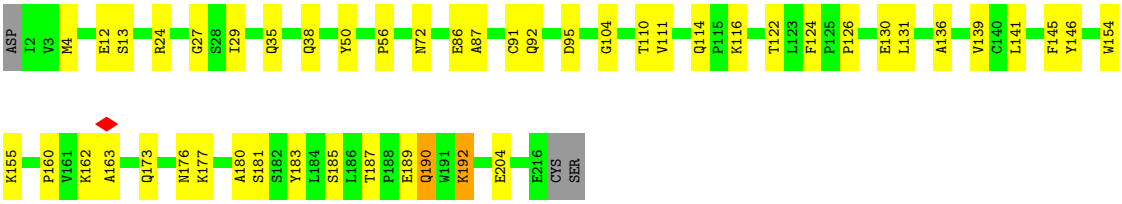
• Molecule 3: mAb15 VL

Chain G:



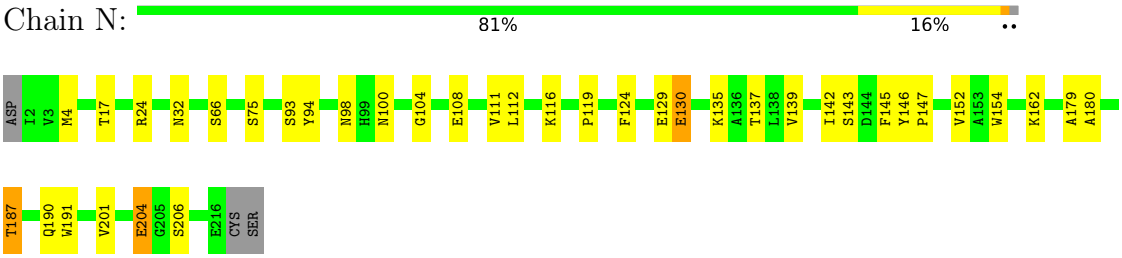
• Molecule 3: mAb15 VL

Chain I:



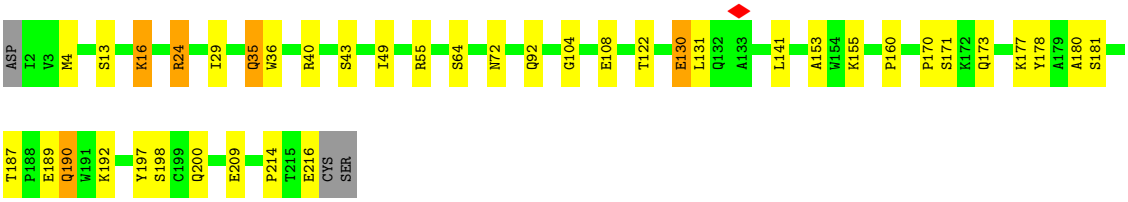
• Molecule 3: mAb15 VL

Chain N:



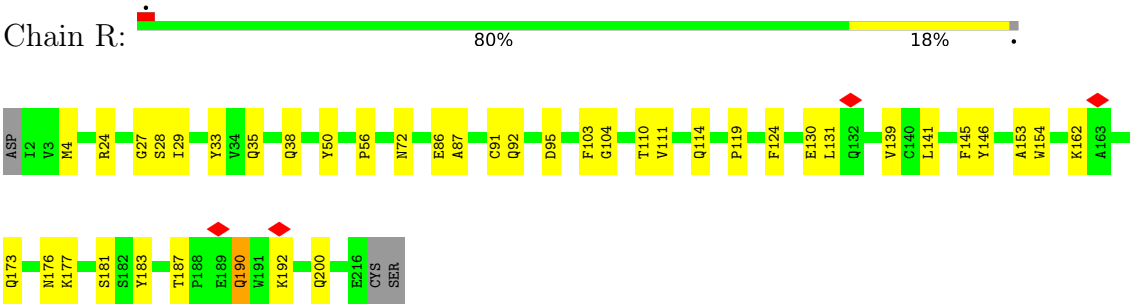
• Molecule 3: mAb15 VL

Chain P:



• Molecule 3: mAb15 VL

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188942	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	61	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.25	0/8534	0.42	0/11626
1	B	0.25	0/8534	0.42	0/11626
1	C	0.25	0/8534	0.42	0/11626
1	J	0.25	0/8534	0.42	0/11626
1	K	0.25	0/8534	0.42	0/11626
1	L	0.25	0/8534	0.42	0/11626
2	D	0.25	0/1748	0.44	0/2379
2	F	0.24	0/1748	0.42	0/2379
2	H	0.24	0/1748	0.42	0/2379
2	M	0.25	0/1748	0.44	0/2379
2	O	0.24	0/1748	0.42	0/2379
2	Q	0.25	0/1748	0.43	0/2379
3	E	0.24	0/1654	0.43	0/2260
3	G	0.24	0/1654	0.42	0/2260
3	I	0.24	0/1654	0.43	0/2260
3	N	0.24	0/1654	0.43	0/2260
3	P	0.24	0/1654	0.42	0/2260
3	R	0.24	0/1654	0.43	0/2260
All	All	0.25	0/71616	0.42	0/97590

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8338	0	8069	93	0
1	B	8338	0	8065	83	0
1	C	8338	0	8065	90	0
1	J	8338	0	8069	91	0
1	K	8338	0	8065	89	0
1	L	8338	0	8065	92	0
2	D	1704	0	1657	24	0
2	F	1704	0	1657	29	0
2	H	1704	0	1657	26	0
2	M	1704	0	1657	26	0
2	O	1704	0	1657	32	0
2	Q	1704	0	1657	30	0
3	E	1616	0	1538	22	0
3	G	1616	0	1538	17	0
3	I	1616	0	1538	26	0
3	N	1616	0	1538	20	0
3	P	1616	0	1538	20	0
3	R	1616	0	1538	23	0
4	A	210	0	195	0	0
4	B	210	0	195	1	0
4	C	210	0	195	4	0
4	J	210	0	195	1	0
4	K	210	0	195	2	0
4	L	210	0	195	5	0
All	All	71208	0	68738	807	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 6.

All (807) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:477:SER:HB2	1:K:486:PHE:CE2	2.17	0.80
2:D:206:HIS:HB3	2:D:211:THR:HB	1.71	0.73
2:M:206:HIS:HB3	2:M:211:THR:HB	1.70	0.73
1:B:356:LYS:HB2	1:B:397:ALA:HB3	1.73	0.71
2:H:52:ASN:HD22	2:H:53:GLN:H	1.38	0.71
2:Q:52:ASN:HD22	2:Q:53:GLN:H	1.39	0.70
2:H:50:ASN:HD22	2:H:51:ILE:H	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:318:PHE:HZ	1:L:615:VAL:HG11	1.56	0.69
1:K:356:LYS:HB2	1:K:397:ALA:HB3	1.73	0.69
1:A:988:GLU:O	1:A:992:GLN:NE2	2.26	0.68
2:M:61:VAL:HG12	2:M:64:VAL:HG22	1.75	0.68
2:D:165:LEU:HD21	2:D:188:VAL:HG21	1.75	0.68
2:M:165:LEU:HD21	2:M:188:VAL:HG21	1.76	0.68
2:D:61:VAL:HG12	2:D:64:VAL:HG22	1.75	0.67
2:F:177:GLN:HB2	2:F:181:LEU:HB2	1.77	0.66
2:O:177:GLN:HB2	2:O:181:LEU:HB2	1.77	0.66
1:J:988:GLU:O	1:J:992:GLN:NE2	2.27	0.66
2:Q:52:ASN:HB2	2:Q:57:GLU:H	1.61	0.66
2:H:52:ASN:HB2	2:H:57:GLU:H	1.61	0.66
2:Q:50:ASN:HD22	2:Q:51:ILE:H	1.42	0.66
2:F:11:LEU:HD13	2:F:116:THR:HG23	1.78	0.66
1:J:742:ILE:O	1:J:1000:ARG:NH1	2.29	0.66
2:Q:190:VAL:HG22	2:Q:192:SER:H	1.60	0.65
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.30	0.65
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.81	0.63
1:J:105:ILE:HD11	1:J:239:GLN:HB3	1.79	0.63
2:O:11:LEU:HD13	2:O:116:THR:HG23	1.79	0.63
1:C:318:PHE:HZ	1:C:615:VAL:HG11	1.64	0.63
1:L:142:GLY:HA3	1:L:156:GLU:HB2	1.80	0.62
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.32	0.62
2:H:105:PRO:HB3	3:I:35:GLN:HG2	1.79	0.62
3:G:13:SER:O	3:G:16:LYS:NZ	2.32	0.62
1:K:474:GLN:NE2	1:K:477:SER:OG	2.32	0.62
3:P:187:THR:HB	3:P:190:GLN:HB2	1.82	0.62
3:E:98:ASN:OD1	3:E:100:ASN:ND2	2.32	0.62
3:P:13:SER:O	3:P:16:LYS:NZ	2.33	0.62
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.64	0.62
1:B:280:ASN:ND2	1:B:286:THR:OG1	2.33	0.62
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.32	0.62
1:K:742:ILE:O	1:K:1000:ARG:NH1	2.33	0.62
3:N:98:ASN:OD1	3:N:100:ASN:ND2	2.32	0.62
1:K:477:SER:HB2	1:K:486:PHE:HE2	1.61	0.61
2:Q:105:PRO:HB3	3:R:35:GLN:HG2	1.80	0.61
1:A:103:GLY:HA3	1:A:120:VAL:HA	1.82	0.61
1:L:742:ILE:O	1:L:1000:ARG:NH1	2.33	0.61
1:K:280:ASN:ND2	1:K:286:THR:OG1	2.34	0.61
2:M:125:PRO:HB3	2:M:151:TYR:HB3	1.83	0.61
3:P:153:ALA:HB3	3:P:200:GLN:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.83	0.61
3:G:187:THR:HB	3:G:190:GLN:HB2	1.82	0.61
1:L:811:LYS:NZ	1:L:813:SER:OG	2.34	0.61
1:J:327:VAL:HG22	1:J:542:ASN:HB3	1.84	0.60
2:O:33:TRP:HB2	2:O:99:VAL:HB	1.83	0.60
1:A:71:SER:HA	1:A:75:GLY:HA2	1.84	0.60
1:C:811:LYS:NZ	1:C:813:SER:OG	2.34	0.60
1:L:106:PHE:HB3	1:L:235:ILE:HD13	1.84	0.60
1:C:276:LEU:HB3	1:C:289:VAL:HG12	1.83	0.60
2:F:201:ILE:HB	2:F:214:ASP:HB3	1.84	0.60
3:G:170:PRO:HB3	3:G:180:ALA:HB2	1.83	0.60
1:J:1047:TYR:HB2	1:J:1067:TYR:HB3	1.82	0.60
3:R:86:GLU:HG3	3:R:110:THR:HA	1.83	0.60
1:B:793:PRO:O	1:B:795:LYS:NZ	2.35	0.60
2:H:190:VAL:HG22	2:H:192:SER:H	1.65	0.60
2:F:190:VAL:HG22	2:F:192:SER:H	1.67	0.60
1:J:64:TRP:HE1	1:J:264:ALA:HB1	1.64	0.59
2:D:152:PHE:HB3	2:D:153:PRO:HD3	1.84	0.59
1:J:115:GLN:HA	1:J:132:GLU:HG2	1.83	0.59
1:C:142:GLY:HA3	1:C:156:GLU:HB2	1.83	0.59
3:I:86:GLU:HG3	3:I:110:THR:HA	1.83	0.59
3:P:170:PRO:HB3	3:P:180:ALA:HB2	1.84	0.59
2:F:33:TRP:HB2	2:F:99:VAL:HB	1.83	0.59
1:A:327:VAL:HG22	1:A:542:ASN:HB3	1.84	0.59
1:L:318:PHE:CZ	1:L:615:VAL:HG11	2.36	0.59
1:A:244:LEU:HD22	1:A:246:ARG:HB2	1.85	0.59
3:G:35:GLN:NE2	3:G:92:GLN:OE1	2.36	0.59
1:J:103:GLY:HA3	1:J:120:VAL:HA	1.85	0.59
1:K:793:PRO:O	1:K:795:LYS:NZ	2.36	0.59
2:D:132:PRO:HD2	2:D:219:PRO:HB3	1.84	0.58
2:M:132:PRO:HD2	2:M:219:PRO:HB3	1.85	0.58
3:P:35:GLN:NE2	3:P:92:GLN:OE1	2.35	0.58
1:A:105:ILE:HD11	1:A:239:GLN:HB3	1.84	0.58
2:D:125:PRO:HB3	2:D:151:TYR:HB3	1.83	0.58
2:F:153:PRO:HG2	2:F:208:PRO:HG2	1.85	0.58
1:J:22:THR:O	1:J:78:ARG:NH1	2.36	0.58
2:M:152:PHE:HB3	2:M:153:PRO:HD3	1.84	0.58
2:F:40:ALA:HB3	2:F:43:LYS:HB2	1.85	0.58
1:A:408:ARG:O	1:A:414:GLN:NE2	2.36	0.58
2:F:29:PHE:O	2:F:72:ARG:NH2	2.37	0.58
3:G:153:ALA:HB3	3:G:200:GLN:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:35:GLN:NE2	3:R:92:GLN:OE1	2.34	0.58
1:C:78:ARG:NH1	1:C:80:ASP:OD1	2.37	0.58
1:C:945:LEU:HD23	1:C:948:LEU:HD12	1.85	0.58
1:L:78:ARG:NH1	1:L:80:ASP:OD1	2.37	0.58
1:L:945:LEU:HD23	1:L:948:LEU:HD12	1.86	0.58
2:O:153:PRO:HG2	2:O:208:PRO:HG2	1.85	0.58
2:Q:177:GLN:HB2	2:Q:181:LEU:HB2	1.86	0.58
1:J:106:PHE:HB3	1:J:235:ILE:HD13	1.85	0.57
2:O:14:PRO:HG3	2:O:117:VAL:HB	1.86	0.57
2:O:28:THR:HG22	2:O:30:SER:H	1.69	0.57
2:O:190:VAL:HG22	2:O:192:SER:H	1.67	0.57
1:K:346:ARG:NH2	1:K:347:PHE:O	2.37	0.57
3:N:119:PRO:HB3	3:N:145:PHE:HB3	1.85	0.57
2:H:177:GLN:HB2	2:H:181:LEU:HB2	1.86	0.57
2:O:29:PHE:O	2:O:72:ARG:NH2	2.37	0.57
1:L:971:GLY:HA3	1:L:995:ARG:HH21	1.69	0.57
1:B:346:ARG:NH2	1:B:347:PHE:O	2.37	0.57
3:I:35:GLN:NE2	3:I:92:GLN:OE1	2.34	0.57
3:I:187:THR:HB	3:I:190:GLN:HE21	1.69	0.57
1:J:408:ARG:O	1:J:414:GLN:NE2	2.37	0.57
3:R:187:THR:HB	3:R:190:GLN:HB2	1.86	0.57
1:J:244:LEU:HD22	1:J:246:ARG:HB2	1.87	0.57
1:J:253:ASP:H	1:J:256:SER:HB3	1.69	0.57
1:K:474:GLN:NE2	1:K:478:THR:O	2.38	0.57
1:L:177:MET:SD	1:L:177:MET:N	2.78	0.57
2:O:201:ILE:HB	2:O:214:ASP:HB3	1.85	0.57
1:C:177:MET:SD	1:C:177:MET:N	2.78	0.57
1:J:24:LEU:O	1:J:78:ARG:NH2	2.38	0.57
2:O:177:GLN:OE1	2:O:183:SER:OG	2.23	0.56
1:C:318:PHE:CZ	1:C:615:VAL:HG11	2.41	0.56
1:C:971:GLY:HA3	1:C:995:ARG:HH21	1.70	0.56
1:A:24:LEU:O	1:A:78:ARG:NH2	2.38	0.56
1:B:121:ASN:HB2	1:B:126:VAL:HG22	1.85	0.56
1:B:150:LYS:NZ	1:B:180:GLU:OE2	2.38	0.56
3:E:119:PRO:HG2	3:E:206:SER:HB3	1.87	0.56
3:E:119:PRO:HB3	3:E:145:PHE:HB3	1.85	0.56
4:L:1315:NAG:H83	4:L:1315:NAG:H3	1.88	0.56
2:F:145:GLY:HA2	2:F:160:TRP:HZ2	1.71	0.56
1:C:349:SER:HB3	1:C:352:ALA:HB3	1.87	0.56
1:K:409:GLN:HA	1:K:414:GLN:HG2	1.88	0.56
2:Q:157:THR:O	2:Q:205:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:HD12	1:A:212:LEU:HD23	1.88	0.56
1:A:474:GLN:NE2	1:A:477:SER:OG	2.39	0.56
1:A:676:THR:OG1	1:A:690:GLN:NE2	2.39	0.56
2:O:145:GLY:HA2	2:O:160:TRP:HZ2	1.70	0.56
1:B:825:LYS:NZ	1:B:938:LEU:O	2.39	0.56
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.87	0.56
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.88	0.56
1:K:409:GLN:HE22	1:K:418:ILE:H	1.54	0.56
1:B:971:GLY:HA3	1:B:995:ARG:HH21	1.71	0.55
4:C:1315:NAG:H3	4:C:1315:NAG:H83	1.88	0.55
1:L:216:LEU:HD12	1:L:217:PRO:HD2	1.88	0.55
1:B:276:LEU:HB3	1:B:289:VAL:HG12	1.88	0.55
2:F:14:PRO:HG3	2:F:117:VAL:HB	1.86	0.55
1:J:763:LEU:HD22	1:J:1008:VAL:HG21	1.88	0.55
1:J:765:ARG:NH2	1:L:957:GLN:OE1	2.39	0.55
1:A:81:ASN:O	1:A:239:GLN:NE2	2.40	0.55
1:C:455:LEU:HD13	1:C:456:PHE:H	1.71	0.55
3:I:187:THR:HB	3:I:190:GLN:HB2	1.88	0.55
3:G:173:GLN:HB2	3:G:177:LYS:HB2	1.89	0.55
2:H:157:THR:O	2:H:205:ASN:ND2	2.39	0.55
1:J:474:GLN:NE2	1:J:477:SER:OG	2.39	0.55
1:K:121:ASN:HB2	1:K:126:VAL:HG22	1.87	0.55
1:K:825:LYS:NZ	1:K:938:LEU:O	2.40	0.55
1:L:401:VAL:HG22	1:L:509:ARG:HG2	1.88	0.55
2:O:40:ALA:HB3	2:O:43:LYS:HB2	1.87	0.55
1:C:439:ASN:HD22	1:C:507:PRO:HD2	1.72	0.55
2:F:28:THR:HG22	2:F:30:SER:H	1.71	0.55
1:A:356:LYS:HB2	1:A:397:ALA:HB3	1.89	0.55
1:C:1105:THR:HG22	1:C:1112:PRO:HA	1.88	0.55
1:J:71:SER:HA	1:J:75:GLY:HA2	1.88	0.55
1:J:676:THR:OG1	1:J:690:GLN:NE2	2.39	0.55
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.89	0.55
1:A:765:ARG:NH2	1:C:957:GLN:OE1	2.40	0.55
1:J:356:LYS:HB2	1:J:397:ALA:HB3	1.87	0.55
1:J:555:SER:HB3	1:J:586:ASP:HB2	1.87	0.55
1:A:253:ASP:H	1:A:256:SER:HB3	1.71	0.55
1:C:105:ILE:HG23	1:C:241:LEU:HD11	1.87	0.55
1:C:431:GLY:HA3	1:C:514:SER:HA	1.89	0.55
3:N:124:PHE:HB2	3:N:139:VAL:HB	1.88	0.55
3:P:24:ARG:HB3	3:P:72:ASN:HB3	1.89	0.55
1:B:328:ARG:NH1	1:B:531:THR:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1073:LYS:HA	4:L:1307:NAG:H82	1.90	0.55
1:B:409:GLN:HA	1:B:414:GLN:HG2	1.88	0.54
1:L:30:ASN:HA	1:L:61:ASN:HA	1.89	0.54
1:J:210:ILE:HD12	1:J:212:LEU:HD23	1.88	0.54
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.06	0.54
3:G:24:ARG:HB3	3:G:72:ASN:HB3	1.90	0.54
1:L:403:ARG:HE	1:L:405:ASP:HB2	1.72	0.54
2:F:177:GLN:OE1	2:F:183:SER:OG	2.24	0.54
1:J:735:SER:HA	1:J:767:LEU:HD13	1.89	0.54
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.89	0.54
1:J:1028:LYS:O	1:J:1032:CYS:HB2	2.07	0.54
3:N:32:ASN:ND2	3:N:94:TYR:O	2.41	0.54
1:A:406:GLU:OE1	1:A:409:GLN:NE2	2.41	0.54
1:A:115:GLN:HA	1:A:132:GLU:HG2	1.90	0.54
1:B:102:ARG:HG3	1:B:141:LEU:HD12	1.90	0.54
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.88	0.54
2:F:131:ALA:HB1	2:F:220:LYS:HE3	1.90	0.54
1:K:102:ARG:HG3	1:K:141:LEU:HD12	1.90	0.54
3:N:119:PRO:HG2	3:N:206:SER:HB3	1.90	0.54
2:Q:47:TRP:HZ2	2:Q:50:ASN:HB2	1.73	0.54
1:J:726:ILE:HG12	1:J:1061:VAL:HG22	1.90	0.54
1:L:105:ILE:HG23	1:L:241:LEU:HD11	1.90	0.54
1:L:455:LEU:HD13	1:L:456:PHE:H	1.73	0.54
3:R:24:ARG:NH2	3:R:95:ASP:OD1	2.36	0.54
1:B:78:ARG:NH1	1:B:80:ASP:OD1	2.41	0.53
2:D:33:TRP:HB2	2:D:99:VAL:HB	1.89	0.53
3:I:50:TYR:HE1	3:I:56:PRO:HB3	1.74	0.53
3:I:116:LYS:NZ	3:I:204:GLU:O	2.40	0.53
1:K:291:CYS:SG	1:K:298:GLU:HA	2.48	0.53
3:P:173:GLN:HB2	3:P:177:LYS:HB2	1.89	0.53
2:Q:19:ARG:HD3	2:Q:80:PHE:HB3	1.90	0.53
1:A:334:ASN:ND2	1:A:360:ASN:O	2.41	0.53
1:K:642:VAL:HA	1:K:651:ILE:HG22	1.91	0.53
1:B:210:ILE:HG12	1:B:212:LEU:H	1.73	0.53
1:C:977:LEU:HD23	1:C:977:LEU:H	1.74	0.53
1:A:245:HIS:HB2	1:A:259:THR:HB	1.90	0.53
1:A:735:SER:HA	1:A:767:LEU:HD13	1.91	0.53
1:C:473:TYR:HB3	1:C:489:TYR:HB2	1.90	0.53
1:L:408:ARG:HG2	3:R:28:SER:HB2	1.89	0.53
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.89	0.53
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:124:PHE:HB2	3:E:139:VAL:HB	1.89	0.53
1:B:214:ARG:NH1	1:B:215:ASP:OD2	2.42	0.53
1:B:642:VAL:HA	1:B:651:ILE:HG22	1.91	0.53
3:R:124:PHE:HB2	3:R:139:VAL:HB	1.91	0.53
1:B:132:GLU:HB2	1:B:164:ASN:HB2	1.91	0.53
2:D:153:PRO:HB2	2:D:155:PRO:HD3	1.91	0.53
1:B:472:ILE:HA	1:B:491:PRO:HD3	1.90	0.53
1:C:317:ASN:HA	1:C:594:GLY:HA2	1.91	0.53
2:H:19:ARG:HD3	2:H:80:PHE:HB3	1.90	0.53
1:J:16:VAL:HA	4:J:1312:NAG:H82	1.90	0.53
1:C:244:LEU:HD13	1:C:246:ARG:HG3	1.91	0.53
1:C:403:ARG:HE	1:C:405:ASP:HB2	1.73	0.53
1:L:457:ARG:HH12	1:L:471:GLU:HB3	1.73	0.53
2:M:133:SER:OG	2:M:223:ASP:OD2	2.27	0.53
1:B:456:PHE:HZ	1:B:489:TYR:HB2	1.74	0.52
1:C:457:ARG:HH12	1:C:471:GLU:HB3	1.73	0.52
3:I:154:TRP:O	3:I:162:LYS:NZ	2.42	0.52
1:L:473:TYR:HB3	1:L:489:TYR:HB2	1.91	0.52
1:A:457:ARG:HH12	1:A:471:GLU:HB3	1.72	0.52
1:B:102:ARG:NH1	1:B:122:ASN:O	2.43	0.52
1:C:394:ASN:HB2	1:C:516:GLU:HB3	1.92	0.52
3:E:152:VAL:HA	3:E:201:VAL:HG22	1.91	0.52
2:M:130:LEU:HB2	2:M:145:GLY:H	1.75	0.52
2:M:153:PRO:HB2	2:M:155:PRO:HD3	1.91	0.52
2:O:132:PRO:HG3	2:O:144:LEU:HB3	1.91	0.52
1:A:752:LEU:HD11	1:A:990:GLU:HG3	1.92	0.52
3:I:24:ARG:NH2	3:I:95:ASP:OD1	2.36	0.52
1:K:132:GLU:HB2	1:K:164:ASN:HB2	1.91	0.52
1:L:83:VAL:HG12	1:L:237:ARG:HG2	1.92	0.52
1:L:349:SER:HB3	1:L:352:ALA:HB3	1.92	0.52
2:H:47:TRP:HZ2	2:H:50:ASN:HB2	1.73	0.52
3:I:111:VAL:O	3:I:146:TYR:OH	2.28	0.52
1:L:457:ARG:NH2	1:L:471:GLU:O	2.43	0.52
3:R:50:TYR:HE1	3:R:56:PRO:HB3	1.74	0.52
1:C:127:VAL:HG12	1:C:171:VAL:HG12	1.92	0.52
1:L:988:GLU:O	1:L:992:GLN:NE2	2.43	0.52
1:C:127:VAL:HG11	4:C:1314:NAG:H62	1.91	0.52
1:C:457:ARG:NH2	1:C:471:GLU:O	2.42	0.52
1:K:707:TYR:HB3	1:L:792:PRO:HG3	1.92	0.52
1:A:360:ASN:ND2	1:A:523:THR:OG1	2.43	0.52
1:C:1073:LYS:HA	4:C:1307:NAG:H82	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:334:ASN:ND2	1:J:360:ASN:O	2.43	0.52
1:J:406:GLU:OE1	1:J:409:GLN:NE2	2.43	0.52
1:K:477:SER:CB	1:K:486:PHE:CE2	2.91	0.52
1:L:127:VAL:HG11	4:L:1314:NAG:H62	1.92	0.52
1:J:457:ARG:HH12	1:J:471:GLU:HB3	1.73	0.52
1:L:355:ARG:HH22	1:L:464:PHE:HB3	1.75	0.52
2:Q:33:TRP:HB2	2:Q:99:VAL:HB	1.91	0.52
1:L:394:ASN:HB2	1:L:516:GLU:HB3	1.92	0.51
1:A:403:ARG:HE	1:A:405:ASP:HB2	1.75	0.51
1:J:193:VAL:HG23	1:J:223:LEU:HD22	1.92	0.51
1:L:244:LEU:HD13	1:L:246:ARG:HG3	1.92	0.51
2:O:153:PRO:HB2	2:O:155:PRO:HD3	1.92	0.51
1:L:317:ASN:HA	1:L:594:GLY:HA2	1.93	0.51
1:L:977:LEU:HD23	1:L:977:LEU:H	1.74	0.51
1:K:276:LEU:HB3	1:K:289:VAL:HG12	1.93	0.51
1:L:34:ARG:NH1	1:L:191:GLU:OE2	2.44	0.51
1:C:901:GLN:O	1:C:905:ARG:HG2	2.10	0.51
1:A:41:LYS:NZ	1:C:562:PHE:O	2.32	0.51
1:C:988:GLU:O	1:C:992:GLN:NE2	2.44	0.51
1:K:328:ARG:NH1	1:K:531:THR:O	2.42	0.51
1:L:901:GLN:O	1:L:905:ARG:HG2	2.10	0.51
2:O:131:ALA:HB1	2:O:220:LYS:HE3	1.93	0.51
3:R:38:GLN:HE21	3:R:87:ALA:HB3	1.75	0.51
3:R:153:ALA:HB3	3:R:200:GLN:HB2	1.93	0.51
1:C:442:ASP:OD2	1:C:509:ARG:NH2	2.44	0.51
2:H:33:TRP:HB2	2:H:99:VAL:HB	1.91	0.51
2:M:153:PRO:HG2	2:M:208:PRO:HG2	1.93	0.51
3:N:187:THR:OG1	3:N:190:GLN:OE1	2.28	0.51
1:C:245:HIS:HB2	1:C:259:THR:HB	1.92	0.50
1:K:129:LYS:HG2	1:K:169:GLU:HG2	1.93	0.50
1:L:431:GLY:HA3	1:L:514:SER:HA	1.92	0.50
1:L:577:ARG:HH21	1:L:582:LEU:HD22	1.74	0.50
1:J:396:TYR:HB2	1:J:514:SER:HB2	1.93	0.50
1:L:1105:THR:HG22	1:L:1112:PRO:HA	1.92	0.50
2:F:153:PRO:HB2	2:F:155:PRO:HD3	1.92	0.50
2:O:47:TRP:NE1	2:O:50:ASN:OD1	2.38	0.50
1:B:909:ILE:HD13	1:B:1049:LEU:HD21	1.94	0.50
1:J:566:GLY:HA2	1:K:43:PHE:H	1.76	0.50
1:K:150:LYS:NZ	1:K:180:GLU:OE2	2.44	0.50
1:L:439:ASN:HD22	1:L:507:PRO:HD2	1.76	0.50
3:N:152:VAL:HA	3:N:201:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:210:ILE:HG12	1:K:212:LEU:H	1.75	0.50
1:B:276:LEU:HD22	1:B:301:CYS:HA	1.93	0.50
2:D:133:SER:OG	2:D:223:ASP:OD2	2.28	0.50
3:E:187:THR:OG1	3:E:190:GLN:OE1	2.28	0.50
3:G:36:TRP:HB2	3:G:49:ILE:HG22	1.94	0.50
1:J:403:ARG:HE	1:J:405:ASP:HB2	1.76	0.50
2:M:33:TRP:HB2	2:M:99:VAL:HB	1.93	0.50
3:P:36:TRP:HB2	3:P:49:ILE:HG22	1.93	0.50
1:B:409:GLN:HE22	1:B:418:ILE:H	1.58	0.50
2:F:132:PRO:HG3	2:F:144:LEU:HB3	1.93	0.50
3:I:141:LEU:HD13	3:I:181:SER:HB2	1.94	0.50
1:J:81:ASN:O	1:J:239:GLN:NE2	2.43	0.50
3:R:111:VAL:O	3:R:146:TYR:OH	2.29	0.50
2:F:220:LYS:HB3	2:F:223:ASP:HB2	1.94	0.50
3:R:154:TRP:O	3:R:162:LYS:NZ	2.45	0.50
1:A:193:VAL:HG23	1:A:223:LEU:HD22	1.94	0.49
3:N:66:SER:OG	3:N:75:SER:OG	2.29	0.49
2:F:47:TRP:NE1	2:F:50:ASN:OD1	2.37	0.49
2:H:4:LEU:HD21	2:H:27:PHE:HE1	1.77	0.49
2:H:206:HIS:CD2	2:H:208:PRO:HD2	2.47	0.49
1:J:1116:THR:HG23	1:J:1118:ASP:H	1.77	0.49
3:N:4:MET:HB2	3:N:104:GLY:HA2	1.94	0.49
1:B:733:LYS:HE3	1:B:771:ALA:HB1	1.94	0.49
3:E:32:ASN:ND2	3:E:94:TYR:O	2.45	0.49
1:J:41:LYS:NZ	1:L:562:PHE:O	2.32	0.49
3:I:38:GLN:HE21	3:I:87:ALA:HB3	1.76	0.49
3:I:114:GLN:HE21	3:I:176:ASN:HB2	1.78	0.49
1:K:971:GLY:HA3	1:K:995:ARG:HH21	1.77	0.49
2:D:130:LEU:HB2	2:D:145:GLY:H	1.77	0.49
3:I:27:GLY:O	3:I:72:ASN:ND2	2.46	0.49
3:R:119:PRO:HB3	3:R:145:PHE:HB3	1.94	0.49
1:B:454:ARG:NH1	1:B:467:ASP:OD2	2.43	0.49
1:C:123:ALA:HB3	4:C:1314:NAG:H82	1.94	0.49
1:A:337:PRO:HD2	1:A:358:ILE:HG12	1.95	0.49
1:K:231:ILE:HD13	1:K:233:ILE:HG12	1.95	0.49
1:K:559:PHE:HB2	1:K:577:ARG:HH21	1.78	0.49
3:I:4:MET:HB2	3:I:104:GLY:HA2	1.95	0.49
1:L:287:ASP:OD1	1:L:288:ALA:N	2.46	0.49
1:L:644:GLN:NE2	1:L:645:THR:O	2.46	0.49
2:Q:206:HIS:CD2	2:Q:208:PRO:HD2	2.48	0.49
1:A:905:ARG:HH11	1:A:1036:GLN:HB2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.95	0.49
2:H:153:PRO:HG2	2:H:208:PRO:HG2	1.95	0.49
1:A:145:TYR:HA	1:A:247:SER:HA	1.95	0.49
1:J:792:PRO:HG3	1:L:707:TYR:HB3	1.95	0.49
3:E:142:ILE:HG23	3:E:180:ALA:HB3	1.96	0.48
1:J:454:ARG:NH1	1:J:467:ASP:O	2.44	0.48
1:K:214:ARG:NH1	1:K:215:ASP:OD2	2.46	0.48
1:A:733:LYS:HE3	1:A:771:ALA:HB1	1.95	0.48
1:J:756:TYR:OH	1:J:994:ASP:OD1	2.24	0.48
1:L:233:ILE:HG22	1:L:234:ASN:H	1.78	0.48
1:L:442:ASP:OD2	1:L:509:ARG:NH2	2.46	0.48
1:C:30:ASN:HA	1:C:61:ASN:HA	1.95	0.48
1:J:210:ILE:HG23	1:J:212:LEU:H	1.77	0.48
1:L:125:ASN:HB3	1:L:174:PRO:HA	1.95	0.48
1:L:822:LEU:HD22	1:L:945:LEU:HD21	1.95	0.48
1:A:1116:THR:HG23	1:A:1118:ASP:H	1.77	0.48
1:J:178:ASP:HB2	1:J:180:GLU:HG2	1.96	0.48
1:B:1103:PHE:HZ	4:B:1302:NAG:H62	1.78	0.48
1:K:96:GLU:O	1:K:188:ASN:ND2	2.46	0.48
1:K:212:LEU:HD13	1:K:217:PRO:HB3	1.96	0.48
1:B:880:GLY:O	1:B:884:SER:OG	2.26	0.48
1:B:977:LEU:HD23	1:B:977:LEU:H	1.79	0.48
2:F:129:PRO:HA	2:F:146:CYS:HA	1.96	0.48
1:K:909:ILE:HD13	1:K:1049:LEU:HD21	1.96	0.48
1:L:781:VAL:HG22	1:L:1026:ALA:HB2	1.96	0.48
2:M:131:ALA:HB1	2:M:219:PRO:HA	1.95	0.48
1:C:125:ASN:HB3	1:C:174:PRO:HA	1.95	0.48
3:E:116:LYS:NZ	3:E:204:GLU:O	2.47	0.48
1:J:317:ASN:HA	1:J:594:GLY:HA2	1.96	0.48
1:A:770:ILE:O	1:A:774:GLN:HG2	2.14	0.48
1:C:233:ILE:HG22	1:C:234:ASN:H	1.79	0.48
3:G:155:LYS:HE2	3:G:160:PRO:HG3	1.96	0.48
1:J:570:ALA:HB1	1:K:963:VAL:HG11	1.96	0.48
1:J:822:LEU:HD22	1:J:945:LEU:HD21	1.96	0.48
1:A:178:ASP:HB2	1:A:180:GLU:HG2	1.95	0.48
1:A:822:LEU:HD22	1:A:945:LEU:HD21	1.96	0.48
1:B:454:ARG:HD3	1:B:457:ARG:HB2	1.96	0.48
1:C:384:PRO:HA	1:C:387:LEU:HG	1.95	0.48
1:C:644:GLN:NE2	1:C:645:THR:O	2.47	0.48
1:J:752:LEU:HD11	1:J:990:GLU:HG3	1.94	0.48
1:J:770:ILE:O	1:J:774:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:374:PHE:HA	1:K:436:TRP:HB3	1.96	0.48
1:K:733:LYS:HE3	1:K:771:ALA:HB1	1.96	0.48
1:L:123:ALA:HB3	4:L:1314:NAG:H82	1.96	0.48
1:J:733:LYS:HE3	1:J:771:ALA:HB1	1.95	0.47
3:R:173:GLN:HB2	3:R:177:LYS:HB2	1.96	0.47
1:J:337:PRO:HD2	1:J:358:ILE:HG12	1.95	0.47
1:J:341:VAL:HG22	1:J:356:LYS:HE3	1.96	0.47
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.24	0.47
2:H:6:GLN:O	2:H:111:GLN:NE2	2.41	0.47
1:K:276:LEU:HD22	1:K:301:CYS:HA	1.96	0.47
3:E:66:SER:OG	3:E:75:SER:OG	2.31	0.47
1:J:115:GLN:OE1	1:J:167:THR:OG1	2.27	0.47
3:G:122:THR:OG1	3:G:141:LEU:O	2.31	0.47
1:L:555:SER:HB3	1:L:586:ASP:HB2	1.96	0.47
2:F:23:ALA:HA	2:F:78:SER:HA	1.97	0.47
2:Q:47:TRP:HB2	3:R:103:PHE:HE1	1.79	0.47
2:F:206:HIS:CD2	2:F:208:PRO:HD2	2.50	0.47
3:I:124:PHE:HB2	3:I:139:VAL:HB	1.97	0.47
1:J:360:ASN:ND2	1:J:523:THR:OG1	2.47	0.47
1:J:659:SER:HB3	1:J:698:SER:HB3	1.96	0.47
1:J:905:ARG:HH11	1:J:1036:GLN:HB2	1.78	0.47
1:K:204:TYR:HB3	1:K:223:LEU:HB3	1.96	0.47
1:K:977:LEU:H	1:K:977:LEU:HD23	1.79	0.47
2:O:149:LYS:NZ	2:O:150:ASP:OD2	2.48	0.47
1:A:108:THR:HG22	1:A:109:THR:HG23	1.95	0.47
1:A:480:CYS:HB3	1:A:486:PHE:H	1.79	0.47
3:G:198:SER:HB2	3:G:209:GLU:HB2	1.97	0.47
1:K:424:LYS:NZ	1:K:425:LEU:O	2.47	0.47
1:L:379:CYS:SG	3:R:33:TYR:OH	2.73	0.47
1:B:129:LYS:HG2	1:B:169:GLU:HG2	1.96	0.47
1:B:756:TYR:OH	1:B:994:ASP:OD1	2.27	0.47
1:K:1103:PHE:HZ	4:K:1302:NAG:H62	1.79	0.47
1:L:127:VAL:HG12	1:L:171:VAL:HG12	1.95	0.47
1:A:979:ASP:HB3	1:A:983:ARG:HH11	1.80	0.47
2:F:119:SER:HG	2:F:179:SER:HG	1.63	0.47
3:I:122:THR:OG1	3:I:141:LEU:O	2.33	0.47
3:I:91:CYS:O	3:I:104:GLY:N	2.46	0.46
3:I:163:ALA:O	3:I:185:SER:OG	2.30	0.46
1:J:245:HIS:HB2	1:J:259:THR:HB	1.97	0.46
1:L:398:ASP:HB2	1:L:512:VAL:HB	1.97	0.46
3:P:197:TYR:HE2	3:P:214:PRO:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:NH2	1:B:580:GLN:OE1	2.48	0.46
3:E:123:LEU:HD22	3:E:210:LYS:HG3	1.97	0.46
1:J:480:CYS:HB3	1:J:486:PHE:H	1.80	0.46
2:M:151:TYR:HE2	2:M:154:GLU:HG2	1.80	0.46
3:P:122:THR:OG1	3:P:141:LEU:O	2.34	0.46
1:A:308:VAL:HG22	1:A:602:THR:HG23	1.97	0.46
1:C:200:TYR:HE1	1:C:230:PRO:HB3	1.81	0.46
1:J:985:ASP:OD1	1:J:985:ASP:N	2.47	0.46
1:L:314:GLN:NE2	1:L:316:SER:O	2.48	0.46
1:L:661:GLU:O	1:L:695:TYR:OH	2.31	0.46
2:O:206:HIS:CD2	2:O:208:PRO:HD2	2.50	0.46
3:P:155:LYS:HE2	3:P:160:PRO:HG3	1.97	0.46
1:A:210:ILE:HG23	1:A:212:LEU:H	1.80	0.46
3:E:154:TRP:O	3:E:162:LYS:NZ	2.41	0.46
1:K:216:LEU:HD12	1:K:217:PRO:HD2	1.98	0.46
2:M:6:GLN:HE22	2:M:111:GLN:H	1.64	0.46
3:N:154:TRP:O	3:N:162:LYS:NZ	2.40	0.46
1:B:107:GLY:H	1:B:235:ILE:HG23	1.79	0.46
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.97	0.46
1:B:559:PHE:HB2	1:B:577:ARG:HH21	1.80	0.46
2:D:151:TYR:HE2	2:D:154:GLU:HG2	1.81	0.46
2:H:54:ASP:OD1	2:H:54:ASP:N	2.49	0.46
1:J:139:PRO:HB3	1:J:159:VAL:HA	1.98	0.46
1:K:942:ALA:HB1	1:K:945:LEU:HD12	1.97	0.46
1:L:402:ILE:HD13	1:L:410:ILE:HD12	1.96	0.46
1:B:901:GLN:O	1:B:905:ARG:HG2	2.15	0.46
1:B:1097:SER:HB3	1:B:1102:TRP:CD2	2.51	0.46
1:C:185:ASN:ND2	1:C:211:ASN:OD1	2.38	0.46
2:F:149:LYS:NZ	2:F:150:ASP:OD2	2.48	0.46
3:I:173:GLN:HB2	3:I:177:LYS:HB2	1.97	0.46
1:J:108:THR:HG22	1:J:109:THR:HG23	1.96	0.46
1:K:454:ARG:HD3	1:K:457:ARG:HB2	1.96	0.46
1:K:901:GLN:O	1:K:905:ARG:HG2	2.15	0.46
2:Q:40:ALA:HB3	2:Q:43:LYS:HB2	1.98	0.46
3:R:27:GLY:O	3:R:72:ASN:ND2	2.48	0.46
1:A:965:GLN:OE1	1:B:758:SER:N	2.46	0.46
1:B:792:PRO:HG2	1:B:795:LYS:HZ2	1.78	0.46
2:F:154:GLU:N	2:F:155:PRO:HD3	2.31	0.46
1:J:979:ASP:HB3	1:J:983:ARG:HH11	1.81	0.46
1:K:78:ARG:NH1	1:K:80:ASP:OD1	2.48	0.46
1:A:100:ILE:HD12	1:A:263:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:LYS:HB3	1:B:462:LYS:HZ2	1.81	0.46
1:B:907:ASN:HD22	1:B:913:GLN:HE21	1.63	0.46
2:F:51:ILE:HG13	2:F:58:LYS:HG2	1.98	0.46
2:M:132:PRO:HG3	2:M:144:LEU:HB3	1.97	0.46
3:N:24:ARG:NH2	3:N:93:SER:OG	2.47	0.46
3:N:142:ILE:HG23	3:N:180:ALA:HB3	1.98	0.46
2:D:6:GLN:HE22	2:D:111:GLN:H	1.63	0.46
3:I:145:PHE:HZ	3:I:180:ALA:H	1.64	0.46
1:B:448:ASN:H	1:B:496:GLY:HA2	1.81	0.46
1:J:145:TYR:HB2	1:J:248:TYR:HB2	1.97	0.46
3:G:4:MET:HB2	3:G:104:GLY:HA2	1.98	0.45
3:G:170:PRO:HB2	3:G:178:TYR:HD2	1.81	0.45
1:L:245:HIS:HB2	1:L:259:THR:HB	1.97	0.45
3:N:116:LYS:NZ	3:N:204:GLU:O	2.50	0.45
2:O:207:LYS:HB2	2:O:208:PRO:HD3	1.98	0.45
3:R:91:CYS:O	3:R:104:GLY:N	2.49	0.45
1:A:78:ARG:NE	1:A:80:ASP:OD2	2.50	0.45
1:A:341:VAL:HG22	1:A:356:LYS:HE3	1.98	0.45
1:K:1097:SER:HB3	1:K:1102:TRP:CD2	2.50	0.45
1:A:566:GLY:HA2	1:B:43:PHE:H	1.80	0.45
1:B:942:ALA:HB1	1:B:945:LEU:HD12	1.98	0.45
2:D:130:LEU:HD23	3:E:124:PHE:HD2	1.81	0.45
2:D:131:ALA:HB1	2:D:219:PRO:HA	1.98	0.45
2:O:220:LYS:HB3	2:O:223:ASP:HB2	1.98	0.45
1:A:77:LYS:HG2	1:A:258:TRP:CH2	2.52	0.45
1:C:119:ILE:HG12	1:C:128:ILE:HG23	1.99	0.45
3:G:197:TYR:HE2	3:G:214:PRO:HB3	1.81	0.45
1:K:880:GLY:O	1:K:884:SER:OG	2.25	0.45
1:A:570:ALA:HB1	1:B:963:VAL:HG11	1.98	0.45
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.98	0.45
1:J:731:MET:SD	1:J:1018:ILE:HG13	2.56	0.45
1:L:905:ARG:HH11	1:L:1036:GLN:HB2	1.80	0.45
1:A:889:GLY:HA3	1:A:1034:LEU:HD23	1.99	0.45
1:C:402:ILE:HD13	1:C:410:ILE:HD12	1.99	0.45
1:K:418:ILE:HA	1:K:422:ASN:HD22	1.82	0.45
1:K:907:ASN:HD22	1:K:913:GLN:HE21	1.65	0.45
3:N:111:VAL:O	3:N:146:TYR:OH	2.31	0.45
2:O:154:GLU:N	2:O:155:PRO:HD3	2.31	0.45
2:O:158:VAL:HA	2:O:204:VAL:HG13	1.99	0.45
1:C:781:VAL:HG22	1:C:1026:ALA:HB2	1.98	0.45
1:K:448:ASN:H	1:K:496:GLY:HA2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:384:PRO:HA	1:L:387:LEU:HG	1.98	0.45
1:L:472:ILE:HA	1:L:491:PRO:HD3	1.99	0.45
2:Q:54:ASP:OD1	2:Q:54:ASP:N	2.49	0.45
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.98	0.45
3:E:143:SER:HA	3:E:179:ALA:HA	1.97	0.45
3:E:146:TYR:HB3	3:E:147:PRO:HD3	1.99	0.45
1:J:145:TYR:HA	1:J:247:SER:HA	1.99	0.45
1:J:722:VAL:HG22	1:J:1065:VAL:HG22	1.99	0.45
1:K:296:LEU:HD13	1:K:608:VAL:HG21	1.99	0.45
3:P:198:SER:HB2	3:P:209:GLU:HB2	1.97	0.45
1:A:115:GLN:OE1	1:A:167:THR:OG1	2.26	0.45
1:A:659:SER:HB3	1:A:698:SER:HB3	1.98	0.45
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.99	0.45
1:C:905:ARG:HH11	1:C:1036:GLN:HB2	1.82	0.45
1:L:343:ASN:OD1	1:L:343:ASN:N	2.48	0.45
2:Q:4:LEU:HD21	2:Q:27:PHE:HE1	1.82	0.45
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.81	0.45
2:D:63:SER:O	2:D:67:ARG:NH2	2.46	0.45
2:F:207:LYS:HB2	2:F:208:PRO:HD3	1.98	0.45
3:N:146:TYR:HB3	3:N:147:PRO:HD3	1.99	0.45
2:O:6:GLN:H	2:O:111:GLN:HE21	1.63	0.45
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.98	0.44
2:D:6:GLN:NE2	2:D:112:GLY:H	2.15	0.44
1:J:70:VAL:HG23	1:J:76:THR:HB	1.99	0.44
3:N:130:GLU:O	3:N:135:LYS:HB2	2.16	0.44
2:Q:153:PRO:HG2	2:Q:208:PRO:HG2	1.99	0.44
1:C:83:VAL:HG12	1:C:237:ARG:HG2	1.99	0.44
1:C:495:TYR:HD1	1:C:495:TYR:HA	1.70	0.44
1:J:117:LEU:HD13	1:J:130:VAL:HG22	1.99	0.44
1:K:123:ALA:HB3	4:K:1314:NAG:H82	1.99	0.44
1:K:398:ASP:HB2	1:K:512:VAL:HB	1.98	0.44
1:K:458:LYS:HE3	1:K:473:TYR:HD1	1.82	0.44
1:L:247:SER:OG	1:L:248:TYR:N	2.50	0.44
1:A:294:ASP:OD1	1:A:297:SER:N	2.43	0.44
1:A:731:MET:SD	1:A:1018:ILE:HG13	2.57	0.44
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.98	0.44
1:C:365:TYR:HA	1:C:368:LEU:HD23	1.99	0.44
1:J:889:GLY:HA3	1:J:1034:LEU:HD23	2.00	0.44
1:K:17:ASN:O	1:K:255:SER:OG	2.32	0.44
2:M:63:SER:O	2:M:67:ARG:NH2	2.47	0.44
2:O:119:SER:HG	2:O:179:SER:HG	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.98	0.44
1:A:458:LYS:NZ	1:A:474:GLN:H	2.16	0.44
1:B:398:ASP:HB2	1:B:512:VAL:HB	2.00	0.44
1:C:457:ARG:HH22	1:C:471:GLU:HB3	1.82	0.44
2:D:154:GLU:N	2:D:155:PRO:HD3	2.33	0.44
1:K:804:GLN:OE1	1:K:935:GLN:NE2	2.42	0.44
1:L:90:VAL:HG13	1:L:267:VAL:HG13	2.00	0.44
1:L:365:TYR:HA	1:L:368:LEU:HD23	1.99	0.44
1:L:398:ASP:O	1:L:512:VAL:N	2.50	0.44
1:K:454:ARG:NH1	1:K:467:ASP:OD2	2.43	0.44
1:L:472:ILE:H	1:L:472:ILE:HG13	1.54	0.44
1:L:656:VAL:HG22	1:L:658:ASN:H	1.83	0.44
2:Q:19:ARG:HE	2:Q:82:GLN:HB2	1.83	0.44
1:A:90:VAL:HG13	1:A:267:VAL:HG13	1.99	0.44
1:B:458:LYS:H	1:B:458:LYS:HD2	1.83	0.44
1:C:287:ASP:OD1	1:C:288:ALA:N	2.51	0.44
3:E:130:GLU:O	3:E:135:LYS:HB2	2.17	0.44
2:H:61:VAL:HG12	2:H:64:VAL:HG22	2.00	0.44
1:K:615:VAL:HG12	1:K:617:CYS:H	1.82	0.44
1:K:1047:TYR:HB2	1:K:1067:TYR:HB3	1.98	0.44
2:O:67:ARG:NH1	2:O:90:ASP:OD2	2.46	0.44
1:C:811:LYS:NZ	1:C:813:SER:O	2.41	0.44
1:K:781:VAL:HG22	1:K:1026:ALA:HB2	2.00	0.44
2:M:6:GLN:NE2	2:M:112:GLY:H	2.15	0.44
2:M:215:LYS:NZ	3:N:129:GLU:OE1	2.41	0.44
2:Q:176:LEU:HD13	2:Q:182:TYR:CZ	2.53	0.44
1:A:327:VAL:H	1:A:531:THR:HB	1.83	0.44
1:B:296:LEU:HD13	1:B:608:VAL:HG21	1.99	0.44
1:J:18:LEU:HD11	1:J:258:TRP:CG	2.53	0.44
1:K:350:VAL:HG12	1:K:422:ASN:HB3	1.98	0.44
1:L:495:TYR:HD1	1:L:495:TYR:HA	1.70	0.44
2:Q:91:THR:HG23	2:Q:116:THR:HA	2.00	0.44
2:Q:207:LYS:HB2	2:Q:208:PRO:HD3	2.00	0.44
3:R:139:VAL:HG22	3:R:183:TYR:HE1	1.83	0.44
1:A:106:PHE:HD2	1:A:235:ILE:HG21	1.83	0.43
1:B:350:VAL:HG12	1:B:422:ASN:HB3	1.99	0.43
1:B:535:LYS:HG3	1:B:536:ASN:HD22	1.83	0.43
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.99	0.43
3:P:4:MET:HB2	3:P:104:GLY:HA2	1.99	0.43
1:A:145:TYR:HB2	1:A:248:TYR:HB2	1.99	0.43
1:A:1109:PHE:HD2	1:A:1111:GLU:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HB3	1:A:276:LEU:HD11	2.00	0.43
1:A:1097:SER:HB3	1:A:1102:TRP:CD2	2.54	0.43
2:D:40:ALA:HB3	2:D:43:LYS:HB2	2.01	0.43
2:F:173:PRO:HD3	3:G:171:SER:HB2	2.01	0.43
3:G:11:SER:HG	3:G:110:THR:HG1	1.66	0.43
1:K:458:LYS:H	1:K:458:LYS:HD2	1.82	0.43
1:K:792:PRO:HG2	1:K:795:LYS:HZ2	1.84	0.43
3:P:170:PRO:HB2	3:P:178:TYR:HD2	1.83	0.43
1:B:48:LEU:HD22	1:B:306:PHE:HE1	1.84	0.43
1:B:781:VAL:HG22	1:B:1026:ALA:HB2	2.00	0.43
1:C:735:SER:HA	1:C:767:LEU:HD13	2.00	0.43
1:L:617:CYS:N	1:L:649:CYS:SG	2.91	0.43
2:M:130:LEU:HD23	3:N:124:PHE:HD2	1.83	0.43
2:D:6:GLN:NE2	2:D:111:GLN:H	2.16	0.43
1:L:200:TYR:HE1	1:L:230:PRO:HB3	1.82	0.43
1:C:443:SER:HB3	1:C:499:PRO:HG3	2.01	0.43
1:C:598:ILE:HG23	1:C:664:ILE:HG21	1.99	0.43
1:C:661:GLU:O	1:C:695:TYR:OH	2.31	0.43
2:H:19:ARG:HE	2:H:82:GLN:HB2	1.83	0.43
2:H:154:GLU:N	2:H:155:PRO:HD3	2.34	0.43
2:Q:38:ARG:HH11	2:Q:48:VAL:HG22	1.84	0.43
2:D:153:PRO:HG2	2:D:208:PRO:HG2	1.99	0.43
2:D:190:VAL:HA	2:D:191:PRO:HD3	1.90	0.43
3:E:2:ILE:HD12	3:E:25:SER:HB3	2.00	0.43
2:H:176:LEU:HD13	2:H:182:TYR:CZ	2.54	0.43
3:I:155:LYS:HE2	3:I:160:PRO:HG3	2.00	0.43
1:J:770:ILE:HD11	1:J:1012:LEU:HD23	2.00	0.43
1:K:535:LYS:HG3	1:K:536:ASN:HD22	1.84	0.43
1:L:733:LYS:O	1:L:861:LEU:N	2.48	0.43
2:O:220:LYS:NZ	3:P:216:GLU:OE1	2.49	0.43
1:A:117:LEU:HD22	1:A:231:ILE:HG21	2.01	0.43
1:A:963:VAL:HG11	1:C:570:ALA:HB1	2.01	0.43
1:B:155:SER:OG	1:B:156:GLU:OE1	2.28	0.43
1:B:212:LEU:HD13	1:B:217:PRO:HB3	2.01	0.43
1:C:656:VAL:HG22	1:C:658:ASN:H	1.83	0.43
2:H:51:ILE:HD13	2:H:52:ASN:H	1.84	0.43
1:J:77:LYS:HG2	1:J:258:TRP:CH2	2.53	0.43
1:J:100:ILE:HD12	1:J:263:ALA:HB2	2.00	0.43
1:J:458:LYS:NZ	1:J:474:GLN:H	2.16	0.43
1:J:912:THR:OG1	1:J:914:ASN:OD1	2.30	0.43
1:J:1097:SER:HB3	1:J:1102:TRP:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:155:SER:OG	1:K:156:GLU:OE1	2.25	0.43
1:L:119:ILE:HG12	1:L:128:ILE:HG23	2.01	0.43
1:L:788:ILE:HG23	1:L:876:ALA:HB2	2.01	0.43
2:M:6:GLN:NE2	2:M:111:GLN:H	2.17	0.43
2:O:23:ALA:HA	2:O:78:SER:HA	2.00	0.43
1:A:70:VAL:HG23	1:A:76:THR:HB	2.01	0.43
1:B:239:GLN:HG2	1:B:240:THR:H	1.84	0.43
1:C:418:ILE:HG23	1:C:422:ASN:HB2	2.01	0.43
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.99	0.43
1:L:418:ILE:HG23	1:L:422:ASN:HB2	2.01	0.43
2:M:154:GLU:N	2:M:155:PRO:HD3	2.33	0.43
2:Q:132:PRO:HG3	2:Q:144:LEU:HB3	2.01	0.43
1:B:149:ASN:OD1	1:B:149:ASN:N	2.52	0.43
1:J:78:ARG:NE	1:J:80:ASP:OD2	2.52	0.43
1:K:53:ASP:OD1	1:K:54:LEU:N	2.49	0.43
1:A:173:GLN:H	1:A:173:GLN:HG3	1.69	0.42
1:A:472:ILE:H	1:A:472:ILE:HG13	1.51	0.42
1:B:24:LEU:HD12	1:B:25:PRO:HD2	2.01	0.42
1:B:1043:CYS:SG	1:B:1064:HIS:ND1	2.91	0.42
1:C:247:SER:OG	1:C:248:TYR:N	2.51	0.42
1:C:472:ILE:HA	1:C:491:PRO:HD3	2.00	0.42
1:C:577:ARG:HH21	1:C:582:LEU:HD22	1.84	0.42
2:H:207:LYS:HB2	2:H:208:PRO:HD3	2.00	0.42
1:J:458:LYS:HZ3	1:J:474:GLN:H	1.66	0.42
1:J:1109:PHE:HD2	1:J:1111:GLU:HG3	1.83	0.42
1:L:18:LEU:HD23	1:L:258:TRP:CE2	2.54	0.42
1:L:100:ILE:HD13	1:L:263:ALA:HB2	2.01	0.42
3:R:24:ARG:HH12	3:R:95:ASP:HB2	1.84	0.42
3:R:114:GLN:HE21	3:R:176:ASN:HB2	1.84	0.42
1:B:108:THR:OG1	1:B:234:ASN:O	2.30	0.42
1:B:612:TYR:HB3	1:B:615:VAL:HG21	2.01	0.42
3:E:111:VAL:O	3:E:146:TYR:OH	2.31	0.42
1:J:781:VAL:HG22	1:J:1026:ALA:HB2	2.02	0.42
1:K:328:ARG:NH2	1:K:580:GLN:OE1	2.52	0.42
1:K:906:PHE:HA	1:K:909:ILE:HG12	2.01	0.42
1:K:912:THR:OG1	1:K:914:ASN:OD1	2.30	0.42
2:Q:19:ARG:HA	2:Q:82:GLN:HA	2.01	0.42
2:Q:96:CYS:O	2:Q:110:GLY:N	2.52	0.42
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.00	0.42
1:C:465:GLU:HG2	1:C:466:ARG:H	1.84	0.42
1:J:788:ILE:HG23	1:J:876:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:905:ARG:HH11	1:K:1036:GLN:HB2	1.84	0.42
1:K:905:ARG:NH1	1:K:1036:GLN:HB2	2.34	0.42
1:L:124:THR:HG23	4:L:1314:NAG:HN2	1.84	0.42
1:L:443:SER:HB3	1:L:499:PRO:HG3	2.01	0.42
1:B:906:PHE:HA	1:B:909:ILE:HG12	2.01	0.42
2:H:96:CYS:O	2:H:110:GLY:N	2.51	0.42
1:K:229:LEU:HA	1:K:230:PRO:HD3	1.93	0.42
1:L:457:ARG:HH22	1:L:471:GLU:HB3	1.83	0.42
2:M:162:SER:HA	2:M:203:ASN:HD22	1.84	0.42
2:Q:61:VAL:HG12	2:Q:64:VAL:HG22	2.01	0.42
3:R:4:MET:HB2	3:R:104:GLY:HA2	2.01	0.42
1:A:912:THR:OG1	1:A:914:ASN:OD1	2.31	0.42
1:B:615:VAL:HG12	1:B:617:CYS:H	1.83	0.42
2:F:6:GLN:HE21	2:F:113:THR:HG23	1.84	0.42
1:J:979:ASP:HB3	1:J:983:ARG:NH1	2.35	0.42
1:K:726:ILE:HG12	1:K:1061:VAL:HG22	2.01	0.42
3:P:40:ARG:HB2	3:P:43:SER:HB2	2.01	0.42
1:B:424:LYS:NZ	1:B:425:LEU:O	2.52	0.42
1:B:458:LYS:HE3	1:B:473:TYR:HD1	1.84	0.42
2:M:190:VAL:HA	2:M:191:PRO:HD3	1.90	0.42
2:O:6:GLN:HE21	2:O:113:THR:HG23	1.84	0.42
2:O:129:PRO:HA	2:O:146:CYS:HA	2.02	0.42
1:A:117:LEU:HD13	1:A:130:VAL:HG22	2.02	0.42
1:B:731:MET:HG2	1:B:732:THR:H	1.84	0.42
1:C:18:LEU:HD23	1:C:258:TRP:CE2	2.54	0.42
1:C:90:VAL:HG13	1:C:267:VAL:HG13	2.00	0.42
2:H:19:ARG:HA	2:H:82:GLN:HA	2.01	0.42
1:J:24:LEU:H	1:J:78:ARG:HH22	1.68	0.42
2:F:220:LYS:NZ	3:G:216:GLU:OE1	2.50	0.42
3:I:12:GLU:HG2	3:I:13:SER:H	1.85	0.42
1:K:731:MET:HG2	1:K:732:THR:H	1.85	0.42
1:K:756:TYR:OH	1:K:994:ASP:OD1	2.27	0.42
1:L:415:THR:HB	1:L:419:ALA:HB2	2.00	0.42
1:A:22:THR:O	1:A:78:ARG:NH1	2.53	0.42
3:I:189:GLU:O	3:I:192:LYS:NZ	2.53	0.42
1:J:891:GLY:HA3	1:L:1069:PRO:HD2	2.02	0.42
3:P:55:ARG:NH2	3:P:64:SER:OG	2.53	0.42
2:Q:154:GLU:N	2:Q:155:PRO:HD3	2.34	0.42
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.55	0.42
1:C:296:LEU:HG	1:C:300:LYS:HE3	2.02	0.42
1:A:318:PHE:N	1:A:593:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:HB3	1:A:492:LEU:HB3	2.01	0.41
1:A:788:ILE:HG23	1:A:876:ALA:HB2	2.00	0.41
1:A:979:ASP:HB3	1:A:983:ARG:NH1	2.35	0.41
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.43	0.41
1:B:905:ARG:HH11	1:B:1036:GLN:HB2	1.85	0.41
1:C:398:ASP:O	1:C:512:VAL:N	2.53	0.41
2:D:64:VAL:HB	2:D:68:PHE:CD1	2.55	0.41
1:J:90:VAL:HG13	1:J:267:VAL:HG13	2.02	0.41
1:L:455:LEU:HD22	1:L:455:LEU:HA	1.89	0.41
2:Q:67:ARG:NH1	2:Q:90:ASP:OD2	2.52	0.41
1:B:231:ILE:HD13	1:B:233:ILE:HG12	2.01	0.41
3:I:139:VAL:HG22	3:I:183:TYR:HE1	1.84	0.41
1:J:143:VAL:HG11	1:J:152:TRP:HB3	2.02	0.41
1:J:318:PHE:N	1:J:593:GLY:O	2.53	0.41
1:A:891:GLY:HA3	1:C:1069:PRO:HD2	2.02	0.41
1:B:90:VAL:HG13	1:B:267:VAL:HG13	2.02	0.41
1:K:1043:CYS:SG	1:K:1064:HIS:ND1	2.93	0.41
1:L:294:ASP:OD1	1:L:297:SER:N	2.43	0.41
3:P:130:GLU:H	3:P:130:GLU:HG3	1.58	0.41
2:Q:51:ILE:HD13	2:Q:52:ASN:H	1.84	0.41
1:A:792:PRO:HG3	1:C:707:TYR:HB3	2.02	0.41
2:D:91:THR:HG23	2:D:116:THR:HA	2.03	0.41
1:J:308:VAL:HG22	1:J:602:THR:HG23	2.01	0.41
1:K:24:LEU:HD12	1:K:25:PRO:HD2	2.02	0.41
1:K:106:PHE:HB2	1:K:117:LEU:HB3	2.01	0.41
1:L:327:VAL:HG22	1:L:542:ASN:HD22	1.86	0.41
1:L:465:GLU:HG2	1:L:466:ARG:H	1.85	0.41
2:M:91:THR:HG23	2:M:116:THR:HA	2.02	0.41
1:B:988:GLU:O	1:B:992:GLN:HG2	2.21	0.41
1:C:355:ARG:HH22	1:C:464:PHE:HB3	1.86	0.41
1:J:426:PRO:HD3	1:J:463:PRO:HB3	2.02	0.41
1:K:612:TYR:HB3	1:K:615:VAL:HG21	2.01	0.41
1:K:1141:LEU:HG	1:K:1142:GLN:H	1.85	0.41
2:O:173:PRO:HD3	3:P:171:SER:HB2	2.01	0.41
1:A:426:PRO:HD3	1:A:463:PRO:HB3	2.02	0.41
1:B:905:ARG:NH1	1:B:1036:GLN:HB2	2.35	0.41
1:C:100:ILE:HD13	1:C:263:ALA:HB2	2.02	0.41
2:F:6:GLN:H	2:F:111:GLN:HE21	1.68	0.41
1:K:149:ASN:N	1:K:149:ASN:OD1	2.54	0.41
1:L:598:ILE:HG23	1:L:664:ILE:HG21	2.02	0.41
1:A:433:VAL:HA	1:A:512:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:HD2	1:C:216:LEU:HD21	2.02	0.41
1:C:94:SER:HA	1:C:265:TYR:HA	2.03	0.41
2:H:91:THR:HG23	2:H:116:THR:HA	2.03	0.41
3:I:126:PRO:HB3	3:I:136:ALA:HB1	2.02	0.41
1:L:308:VAL:HG22	1:L:602:THR:HG23	2.03	0.41
2:M:40:ALA:HB3	2:M:43:LYS:HB2	2.02	0.41
2:Q:19:ARG:NH2	2:Q:82:GLN:OE1	2.44	0.41
1:B:1141:LEU:HG	1:B:1142:GLN:H	1.85	0.41
1:C:195:LYS:HE2	1:C:204:TYR:HE1	1.85	0.41
1:C:788:ILE:HG23	1:C:876:ALA:HB2	2.01	0.41
1:K:569:ILE:H	1:K:569:ILE:HG13	1.55	0.41
2:O:35:SER:HB3	2:O:50:ASN:ND2	2.35	0.41
2:Q:151:TYR:OH	2:Q:184:LEU:HB2	2.20	0.41
3:R:141:LEU:HD13	3:R:181:SER:HB2	2.02	0.41
1:A:985:ASP:OD1	1:A:985:ASP:N	2.47	0.41
1:B:656:VAL:HG22	1:B:658:ASN:H	1.85	0.41
1:B:1094:VAL:HG23	1:B:1096:VAL:HG23	2.03	0.41
1:C:415:THR:HB	1:C:419:ALA:HB2	2.03	0.41
1:C:430:THR:O	1:C:515:PHE:N	2.54	0.41
1:C:616:ASN:OD1	1:C:617:CYS:N	2.53	0.41
2:D:162:SER:HA	2:D:203:ASN:HD22	1.85	0.41
1:J:328:ARG:NH1	1:J:533:LEU:HB2	2.36	0.41
1:K:83:VAL:HG11	1:K:237:ARG:NH2	2.36	0.41
1:K:239:GLN:HG2	1:K:240:THR:H	1.85	0.41
1:K:379:CYS:HB3	1:K:382:VAL:HG22	2.02	0.41
1:L:41:LYS:HE2	1:L:225:PRO:HG2	2.03	0.41
1:L:81:ASN:HB3	1:L:242:LEU:HD13	2.03	0.41
1:L:905:ARG:NH1	1:L:1036:GLN:HB2	2.36	0.41
3:N:98:ASN:O	3:N:100:ASN:ND2	2.54	0.41
1:A:139:PRO:HB3	1:A:159:VAL:HA	2.03	0.41
1:C:314:GLN:HE22	1:C:594:GLY:HA3	1.86	0.41
1:C:342:PHE:HE1	1:C:434:ILE:HG21	1.86	0.41
3:E:24:ARG:NH2	3:E:28:SER:O	2.54	0.41
3:E:167:THR:HA	3:E:182:SER:HA	2.03	0.41
1:J:143:VAL:HG21	1:J:152:TRP:HD1	1.86	0.41
1:J:327:VAL:H	1:J:531:THR:HB	1.86	0.41
1:K:462:LYS:HZ3	1:K:463:PRO:HD2	1.84	0.41
3:N:143:SER:HA	3:N:179:ALA:HA	2.02	0.41
1:A:54:LEU:HD13	1:A:88:ASP:HB3	2.03	0.40
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.53	0.40
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:229:LEU:HA	1:L:230:PRO:HD3	1.95	0.40
1:A:53:ASP:OD1	1:A:54:LEU:N	2.49	0.40
2:H:67:ARG:NH1	2:H:90:ASP:OD2	2.52	0.40
2:M:64:VAL:HB	2:M:68:PHE:CD1	2.56	0.40
1:C:294:ASP:OD1	1:C:297:SER:N	2.43	0.40
1:C:412:PRO:HD3	1:C:425:LEU:HD22	2.01	0.40
1:J:452:LEU:HB3	1:J:492:LEU:HB3	2.03	0.40
1:K:401:VAL:HG22	1:K:509:ARG:HG2	2.04	0.40
1:L:193:VAL:HG23	1:L:223:LEU:HD22	2.03	0.40
3:P:141:LEU:HD13	3:P:181:SER:HB2	2.03	0.40
1:B:912:THR:OG1	1:B:914:ASN:OD1	2.29	0.40
3:E:98:ASN:O	3:E:100:ASN:ND2	2.55	0.40
1:J:490:PHE:CE2	1:J:492:LEU:HB2	2.55	0.40
1:A:328:ARG:NH1	1:A:533:LEU:HB2	2.37	0.40
1:B:39:PRO:HG3	1:B:55:PHE:HZ	1.87	0.40
1:C:916:LEU:O	1:C:920:GLN:HG3	2.21	0.40
3:E:4:MET:HB2	3:E:104:GLY:HA2	2.03	0.40
1:K:177:MET:HE3	1:K:179:LEU:HB2	2.04	0.40
1:K:717:ASN:HB3	1:K:1070:ALA:HB3	2.04	0.40
1:L:541:PHE:HB3	1:L:552:LEU:HD11	2.03	0.40
2:O:190:VAL:HA	2:O:191:PRO:HD3	1.98	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	1068/1288 (83%)	1019 (95%)	49 (5%)	0	100 100
1	B	1068/1288 (83%)	1018 (95%)	50 (5%)	0	100 100
1	C	1068/1288 (83%)	1020 (96%)	48 (4%)	0	100 100
1	J	1068/1288 (83%)	1017 (95%)	50 (5%)	1 (0%)	48 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	1068/1288 (83%)	1022 (96%)	46 (4%)	0	100	100
1	L	1068/1288 (83%)	1017 (95%)	51 (5%)	0	100	100
2	D	223/225 (99%)	202 (91%)	21 (9%)	0	100	100
2	F	223/225 (99%)	195 (87%)	28 (13%)	0	100	100
2	H	223/225 (99%)	199 (89%)	24 (11%)	0	100	100
2	M	223/225 (99%)	202 (91%)	21 (9%)	0	100	100
2	O	223/225 (99%)	195 (87%)	28 (13%)	0	100	100
2	Q	223/225 (99%)	199 (89%)	24 (11%)	0	100	100
3	E	213/218 (98%)	196 (92%)	17 (8%)	0	100	100
3	G	213/218 (98%)	195 (92%)	18 (8%)	0	100	100
3	I	213/218 (98%)	194 (91%)	19 (9%)	0	100	100
3	N	213/218 (98%)	198 (93%)	15 (7%)	0	100	100
3	P	213/218 (98%)	195 (92%)	18 (8%)	0	100	100
3	R	213/218 (98%)	193 (91%)	20 (9%)	0	100	100
All	All	9024/10386 (87%)	8476 (94%)	547 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	292	ALA

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	922/1111 (83%)	897 (97%)	25 (3%)	40	60
1	B	922/1111 (83%)	892 (97%)	30 (3%)	33	54
1	C	922/1111 (83%)	900 (98%)	22 (2%)	44	63
1	J	922/1111 (83%)	896 (97%)	26 (3%)	38	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	922/1111 (83%)	895 (97%)	27 (3%)	37	58
1	L	922/1111 (83%)	901 (98%)	21 (2%)	45	64
2	D	189/189 (100%)	181 (96%)	8 (4%)	25	47
2	F	189/189 (100%)	183 (97%)	6 (3%)	34	55
2	H	189/189 (100%)	181 (96%)	8 (4%)	25	47
2	M	189/189 (100%)	181 (96%)	8 (4%)	25	47
2	O	189/189 (100%)	183 (97%)	6 (3%)	34	55
2	Q	189/189 (100%)	181 (96%)	8 (4%)	25	47
3	E	188/191 (98%)	180 (96%)	8 (4%)	25	47
3	G	188/191 (98%)	178 (95%)	10 (5%)	19	41
3	I	188/191 (98%)	183 (97%)	5 (3%)	40	60
3	N	188/191 (98%)	180 (96%)	8 (4%)	25	47
3	P	188/191 (98%)	178 (95%)	10 (5%)	19	41
3	R	188/191 (98%)	183 (97%)	5 (3%)	40	60
All	All	7794/8946 (87%)	7553 (97%)	241 (3%)	37	55

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	VAL
1	A	145	TYR
1	A	149	ASN
1	A	202	LYS
1	A	210	ILE
1	A	244	LEU
1	A	248	TYR
1	A	293	LEU
1	A	326	ILE
1	A	340	GLU
1	A	353	TRP
1	A	408	ARG
1	A	423	TYR
1	A	461	LEU
1	A	472	ILE
1	A	483	VAL
1	A	534	VAL
1	A	538	CYS

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Mol	Chain	Res	Type
1	A	590	CYS
1	A	753	LEU
1	A	916	LEU
1	A	966	LEU
1	A	983	ARG
1	A	990	GLU
1	A	1032	CYS
1	B	40	ASP
1	B	41	LYS
1	B	131	CYS
1	B	150	LYS
1	B	289	VAL
1	B	290	ASP
1	B	293	LEU
1	B	301	CYS
1	B	319	ARG
1	B	336	CYS
1	B	440	ASN
1	B	444	LYS
1	B	458	LYS
1	B	478	THR
1	B	488	CYS
1	B	489	TYR
1	B	495	TYR
1	B	500	THR
1	B	505	TYR
1	B	538	CYS
1	B	546	LEU
1	B	590	CYS
1	B	616	ASN
1	B	617	CYS
1	B	752	LEU
1	B	753	LEU
1	B	795	LYS
1	B	916	LEU
1	B	966	LEU
1	B	1001	LEU
1	C	41	LYS
1	C	105	ILE
1	C	111	ASP
1	C	127	VAL
1	C	183	GLN

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Mol	Chain	Res	Type
1	C	197	ILE
1	C	202	LYS
1	C	234	ASN
1	C	244	LEU
1	C	259	THR
1	C	289	VAL
1	C	293	LEU
1	C	336	CYS
1	C	455	LEU
1	C	461	LEU
1	C	495	TYR
1	C	615	VAL
1	C	738	CYS
1	C	753	LEU
1	C	886	TRP
1	C	916	LEU
1	C	1125	ASN
2	D	38	ARG
2	D	50	ASN
2	D	60	TYR
2	D	83	MET
2	D	86	VAL
2	D	98	ARG
2	D	137	THR
2	D	146	CYS
3	E	17	THR
3	E	108	GLU
3	E	112	LEU
3	E	130	GLU
3	E	137	THR
3	E	187	THR
3	E	191	TRP
3	E	204	GLU
2	F	13	GLN
2	F	76	LYS
2	F	83	MET
2	F	146	CYS
2	F	189	THR
2	F	204	VAL
3	G	16	LYS
3	G	24	ARG
3	G	29	ILE

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Mol	Chain	Res	Type
3	G	35	GLN
3	G	108	GLU
3	G	130	GLU
3	G	131	LEU
3	G	189	GLU
3	G	190	GLN
3	G	192	LYS
2	H	13	GLN
2	H	50	ASN
2	H	51	ILE
2	H	52	ASN
2	H	136	SER
2	H	146	CYS
2	H	213	VAL
2	H	220	LYS
3	I	29	ILE
3	I	130	GLU
3	I	131	LEU
3	I	190	GLN
3	I	192	LYS
1	J	70	VAL
1	J	145	TYR
1	J	149	ASN
1	J	202	LYS
1	J	210	ILE
1	J	244	LEU
1	J	248	TYR
1	J	293	LEU
1	J	326	ILE
1	J	340	GLU
1	J	343	ASN
1	J	353	TRP
1	J	408	ARG
1	J	423	TYR
1	J	461	LEU
1	J	472	ILE
1	J	483	VAL
1	J	534	VAL
1	J	538	CYS
1	J	590	CYS
1	J	753	LEU
1	J	916	LEU

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Mol	Chain	Res	Type
1	J	966	LEU
1	J	983	ARG
1	J	990	GLU
1	J	1032	CYS
1	K	40	ASP
1	K	41	LYS
1	K	131	CYS
1	K	150	LYS
1	K	290	ASP
1	K	291	CYS
1	K	301	CYS
1	K	319	ARG
1	K	336	CYS
1	K	440	ASN
1	K	444	LYS
1	K	458	LYS
1	K	484	GLU
1	K	495	TYR
1	K	500	THR
1	K	505	TYR
1	K	538	CYS
1	K	546	LEU
1	K	590	CYS
1	K	616	ASN
1	K	617	CYS
1	K	752	LEU
1	K	753	LEU
1	K	795	LYS
1	K	916	LEU
1	K	966	LEU
1	K	1001	LEU
1	L	41	LYS
1	L	111	ASP
1	L	127	VAL
1	L	183	GLN
1	L	197	ILE
1	L	202	LYS
1	L	234	ASN
1	L	244	LEU
1	L	259	THR
1	L	293	LEU
1	L	336	CYS

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Mol	Chain	Res	Type
1	L	455	LEU
1	L	461	LEU
1	L	488	CYS
1	L	495	TYR
1	L	615	VAL
1	L	738	CYS
1	L	753	LEU
1	L	886	TRP
1	L	916	LEU
1	L	1125	ASN
2	M	38	ARG
2	M	50	ASN
2	M	60	TYR
2	M	83	MET
2	M	86	VAL
2	M	98	ARG
2	M	137	THR
2	M	146	CYS
3	N	17	THR
3	N	108	GLU
3	N	112	LEU
3	N	130	GLU
3	N	137	THR
3	N	187	THR
3	N	191	TRP
3	N	204	GLU
2	O	13	GLN
2	O	76	LYS
2	O	83	MET
2	O	146	CYS
2	O	189	THR
2	O	204	VAL
3	P	16	LYS
3	P	24	ARG
3	P	29	ILE
3	P	35	GLN
3	P	108	GLU
3	P	130	GLU
3	P	131	LEU
3	P	189	GLU
3	P	190	GLN
3	P	192	LYS

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Mol	Chain	Res	Type
2	Q	13	GLN
2	Q	50	ASN
2	Q	51	ILE
2	Q	52	ASN
2	Q	136	SER
2	Q	146	CYS
2	Q	213	VAL
2	Q	220	LYS
3	R	29	ILE
3	R	130	GLU
3	R	131	LEU
3	R	190	GLN
3	R	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	23	GLN
1	A	183	GLN
1	A	185	ASN
1	A	354	ASN
1	A	360	ASN
1	A	409	GLN
1	A	414	GLN
1	A	439	ASN
1	A	474	GLN
1	A	493	GLN
1	A	641	ASN
1	A	655	HIS
1	A	690	GLN
1	A	774	GLN
1	A	872	GLN
1	A	907	ASN
1	A	913	GLN
1	A	1002	GLN
1	A	1011	GLN
1	A	1048	HIS
1	A	1101	HIS
1	A	1108	ASN
1	B	23	GLN
1	B	49	HIS

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Mol	Chain	Res	Type
1	B	69	HIS
1	B	115	GLN
1	B	137	ASN
1	B	183	GLN
1	B	218	GLN
1	B	280	ASN
1	B	409	GLN
1	B	414	GLN
1	B	439	ASN
1	B	460	ASN
1	B	493	GLN
1	B	498	GLN
1	B	536	ASN
1	B	907	ASN
1	B	960	ASN
1	B	1011	GLN
1	C	23	GLN
1	C	125	ASN
1	C	183	GLN
1	C	218	GLN
1	C	314	GLN
1	C	409	GLN
1	C	439	ASN
1	C	474	GLN
1	C	493	GLN
1	C	532	ASN
1	C	580	GLN
1	C	613	GLN
1	C	644	GLN
1	C	872	GLN
1	C	914	ASN
1	C	920	GLN
1	C	935	GLN
1	C	954	GLN
1	C	965	GLN
1	C	992	GLN
1	C	1002	GLN
1	C	1011	GLN
1	C	1048	HIS
1	C	1135	ASN
2	D	6	GLN
2	D	203	ASN

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Mol	Chain	Res	Type
3	E	32	ASN
3	E	98	ASN
3	E	100	ASN
3	E	200	GLN
2	F	13	GLN
2	F	77	ASN
2	F	111	GLN
3	G	32	ASN
3	G	35	GLN
3	G	99	HIS
3	G	100	ASN
3	G	190	GLN
3	G	200	GLN
2	H	50	ASN
2	H	52	ASN
2	H	84	ASN
2	H	205	ASN
3	I	38	GLN
3	I	72	ASN
3	I	114	GLN
3	I	190	GLN
3	I	200	GLN
1	J	14	GLN
1	J	23	GLN
1	J	134	GLN
1	J	183	GLN
1	J	185	ASN
1	J	354	ASN
1	J	360	ASN
1	J	409	GLN
1	J	414	GLN
1	J	439	ASN
1	J	474	GLN
1	J	493	GLN
1	J	641	ASN
1	J	655	HIS
1	J	690	GLN
1	J	762	GLN
1	J	774	GLN
1	J	872	GLN
1	J	907	ASN
1	J	913	GLN

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Mol	Chain	Res	Type
1	J	1002	GLN
1	J	1011	GLN
1	J	1048	HIS
1	J	1101	HIS
1	J	1108	ASN
1	K	23	GLN
1	K	49	HIS
1	K	115	GLN
1	K	137	ASN
1	K	183	GLN
1	K	188	ASN
1	K	218	GLN
1	K	280	ASN
1	K	409	GLN
1	K	414	GLN
1	K	439	ASN
1	K	460	ASN
1	K	474	GLN
1	K	493	GLN
1	K	498	GLN
1	K	536	ASN
1	K	907	ASN
1	K	960	ASN
1	K	1011	GLN
1	L	23	GLN
1	L	125	ASN
1	L	183	GLN
1	L	218	GLN
1	L	314	GLN
1	L	409	GLN
1	L	439	ASN
1	L	474	GLN
1	L	493	GLN
1	L	580	GLN
1	L	613	GLN
1	L	644	GLN
1	L	872	GLN
1	L	914	ASN
1	L	920	GLN
1	L	935	GLN
1	L	954	GLN
1	L	965	GLN

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Mol	Chain	Res	Type
1	L	992	GLN
1	L	1002	GLN
1	L	1011	GLN
1	L	1048	HIS
1	L	1135	ASN
2	M	203	ASN
3	N	32	ASN
3	N	98	ASN
3	N	100	ASN
3	N	200	GLN
2	O	13	GLN
2	O	77	ASN
2	O	111	GLN
3	P	32	ASN
3	P	35	GLN
3	P	99	HIS
3	P	100	ASN
3	P	190	GLN
3	P	200	GLN
2	Q	50	ASN
2	Q	52	ASN
2	Q	84	ASN
2	Q	205	ASN
3	R	38	GLN
3	R	72	ASN
3	R	114	GLN
3	R	190	GLN
3	R	200	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

90 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	J	1315	1	14,14,15	0.33	0	17,19,21	0.78	1 (5%)
4	NAG	K	1308	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	L	1303	1	14,14,15	0.25	0	17,19,21	0.53	0
4	NAG	C	1311	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	J	1309	1	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	K	1305	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	C	1302	1	14,14,15	0.23	0	17,19,21	0.37	0
4	NAG	K	1315	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	L	1314	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	B	1301	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	B	1307	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	K	1304	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	J	1301	1	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	C	1305	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	L	1304	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	K	1314	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	A	1310	1	14,14,15	0.24	0	17,19,21	0.53	0
4	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	J	1304	1	14,14,15	0.34	0	17,19,21	0.41	0
4	NAG	A	1315	1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	K	1312	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	K	1301	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	L	1312	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	K	1302	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	J	1310	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	J	1314	1	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	C	1315	1	14,14,15	0.46	0	17,19,21	1.26	1 (5%)
4	NAG	J	1305	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	K	1303	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	A	1311	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	C	1304	1	14,14,15	0.26	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	J	1312	1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	L	1311	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	C	1310	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	A	1307	1	14,14,15	0.34	0	17,19,21	0.40	0
4	NAG	C	1309	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	J	1302	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	B	1315	1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	A	1309	1	14,14,15	0.27	0	17,19,21	0.53	0
4	NAG	C	1313	1	14,14,15	0.42	0	17,19,21	0.38	0
4	NAG	C	1312	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	C	1307	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	L	1313	1	14,14,15	0.42	0	17,19,21	0.38	0
4	NAG	K	1311	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	A	1312	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	K	1307	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	C	1303	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	L	1315	1	14,14,15	0.45	0	17,19,21	1.26	1 (5%)
4	NAG	C	1308	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	B	1313	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	J	1313	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	L	1306	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	C	1306	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	L	1310	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	J	1307	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	L	1307	1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	A	1304	1	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	A	1313	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	L	1301	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	L	1302	1	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	L	1309	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	B	1314	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	A	1301	1	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	A	1306	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	K	1309	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	A	1314	1	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	A	1303	1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	B	1311	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1310	1	14,14,15	0.43	0	17,19,21	1.25	1 (5%)
4	NAG	J	1306	1	14,14,15	0.33	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	A	1305	1	14,14,15	0.34	0	17,19,21	0.41	0
4	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1312	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	K	1306	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1309	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	K	1310	1	14,14,15	0.43	0	17,19,21	1.25	1 (5%)
4	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	J	1308	1	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	J	1311	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	J	1303	1	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	A	1308	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	K	1313	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	L	1308	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	C	1314	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	L	1305	1	14,14,15	0.21	0	17,19,21	0.42	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	J	1315	1	-	0/6/23/26	0/1/1/1
4	NAG	K	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	L	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	J	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	K	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	K	1315	1	-	0/6/23/26	0/1/1/1
4	NAG	L	1314	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	K	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	J	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	L	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	K	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	J	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1315	1	-	2/6/23/26	0/1/1/1
4	NAG	K	1312	1	-	1/6/23/26	0/1/1/1
4	NAG	K	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	L	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	K	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	J	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	J	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1315	1	-	3/6/23/26	0/1/1/1
4	NAG	J	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	K	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	J	1312	1	-	0/6/23/26	0/1/1/1
4	NAG	L	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	J	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1315	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	L	1313	1	-	2/6/23/26	0/1/1/1
4	NAG	K	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	K	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	L	1315	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	4/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1310	NAG	C1-O5-C5	4.74	118.61	112.19
4	K	1310	NAG	C1-O5-C5	4.73	118.61	112.19
4	L	1315	NAG	C2-N2-C7	4.31	129.04	122.90
4	C	1315	NAG	C2-N2-C7	4.31	129.04	122.90
4	J	1315	NAG	O5-C5-C6	2.04	110.39	107.20

There are no chirality outliers.

All (141) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1307	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	J	1302	NAG	O5-C5-C6-O6
4	L	1305	NAG	O5-C5-C6-O6
4	L	1312	NAG	C4-C5-C6-O6
4	L	1307	NAG	O5-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	L	1302	NAG	C4-C5-C6-O6
4	L	1305	NAG	C4-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	B	1311	NAG	O5-C5-C6-O6
4	B	1313	NAG	O5-C5-C6-O6
4	K	1311	NAG	O5-C5-C6-O6
4	L	1311	NAG	O5-C5-C6-O6
4	L	1312	NAG	O5-C5-C6-O6
4	K	1314	NAG	O5-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	B	1314	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	C	1311	NAG	O5-C5-C6-O6
4	C	1313	NAG	O5-C5-C6-O6
4	B	1314	NAG	O5-C5-C6-O6
4	B	1313	NAG	C4-C5-C6-O6
4	K	1311	NAG	C4-C5-C6-O6
4	J	1311	NAG	O5-C5-C6-O6
4	K	1305	NAG	O5-C5-C6-O6
4	L	1302	NAG	O5-C5-C6-O6
4	L	1313	NAG	O5-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	C	1312	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	J	1302	NAG	C4-C5-C6-O6
4	K	1314	NAG	C4-C5-C6-O6
4	A	1312	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	J	1301	NAG	O5-C5-C6-O6
4	B	1311	NAG	C4-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	J	1307	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	A	1312	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	L	1313	NAG	C4-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	C	1311	NAG	C4-C5-C6-O6
4	J	1301	NAG	C4-C5-C6-O6
4	J	1311	NAG	C4-C5-C6-O6
4	L	1307	NAG	C4-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	C	1313	NAG	C4-C5-C6-O6
4	A	1315	NAG	C8-C7-N2-C2
4	A	1315	NAG	O7-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1310	NAG	C8-C7-N2-C2
4	B	1310	NAG	O7-C7-N2-C2
4	B	1313	NAG	C8-C7-N2-C2
4	B	1313	NAG	O7-C7-N2-C2
4	C	1301	NAG	C8-C7-N2-C2
4	C	1301	NAG	O7-C7-N2-C2
4	C	1315	NAG	C8-C7-N2-C2
4	C	1315	NAG	O7-C7-N2-C2
4	J	1314	NAG	C8-C7-N2-C2
4	J	1314	NAG	O7-C7-N2-C2
4	K	1304	NAG	C8-C7-N2-C2
4	K	1304	NAG	O7-C7-N2-C2
4	K	1310	NAG	C8-C7-N2-C2
4	K	1310	NAG	O7-C7-N2-C2
4	K	1313	NAG	C8-C7-N2-C2
4	K	1313	NAG	O7-C7-N2-C2
4	L	1301	NAG	C8-C7-N2-C2
4	L	1301	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	L	1315	NAG	C8-C7-N2-C2
4	L	1315	NAG	O7-C7-N2-C2
4	K	1308	NAG	O5-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	J	1307	NAG	C4-C5-C6-O6
4	K	1305	NAG	C4-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	L	1308	NAG	O5-C5-C6-O6
4	L	1311	NAG	C4-C5-C6-O6
4	J	1304	NAG	C4-C5-C6-O6
4	L	1304	NAG	C4-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	K	1307	NAG	C4-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	L	1308	NAG	C4-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	B	1312	NAG	O5-C5-C6-O6
4	K	1303	NAG	O5-C5-C6-O6
4	K	1313	NAG	O5-C5-C6-O6
4	K	1308	NAG	C4-C5-C6-O6
4	L	1315	NAG	O5-C5-C6-O6
4	C	1312	NAG	O5-C5-C6-O6
4	L	1315	NAG	C4-C5-C6-O6
4	K	1312	NAG	O5-C5-C6-O6
4	J	1308	NAG	O5-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	J	1308	NAG	C4-C5-C6-O6
4	L	1304	NAG	O5-C5-C6-O6
4	A	1309	NAG	C4-C5-C6-O6
4	J	1304	NAG	O5-C5-C6-O6
4	B	1309	NAG	C4-C5-C6-O6
4	C	1309	NAG	C4-C5-C6-O6
4	A	1309	NAG	O5-C5-C6-O6
4	K	1307	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	J	1309	NAG	O5-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	K	1309	NAG	C4-C5-C6-O6
4	K	1309	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	L	1306	NAG	C4-C5-C6-O6
4	J	1310	NAG	C4-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	L	1309	NAG	C4-C5-C6-O6
4	K	1313	NAG	C4-C5-C6-O6
4	A	1304	NAG	C3-C2-N2-C7
4	A	1309	NAG	C3-C2-N2-C7
4	A	1310	NAG	C3-C2-N2-C7
4	C	1303	NAG	C3-C2-N2-C7
4	C	1304	NAG	C3-C2-N2-C7
4	J	1303	NAG	C3-C2-N2-C7
4	J	1308	NAG	C3-C2-N2-C7
4	J	1309	NAG	C3-C2-N2-C7
4	L	1303	NAG	C3-C2-N2-C7
4	L	1304	NAG	C3-C2-N2-C7
4	J	1310	NAG	O5-C5-C6-O6
4	L	1309	NAG	O5-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	L	1303	NAG	C4-C5-C6-O6
4	L	1306	NAG	O5-C5-C6-O6
4	C	1315	NAG	C3-C2-N2-C7
4	L	1315	NAG	C3-C2-N2-C7
4	L	1301	NAG	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1314	NAG	3	0
4	K	1314	NAG	1	0
4	B	1302	NAG	1	0
4	K	1302	NAG	1	0
4	C	1315	NAG	1	0
4	J	1312	NAG	1	0
4	C	1307	NAG	1	0
4	L	1315	NAG	1	0
4	L	1307	NAG	1	0
4	C	1314	NAG	2	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.

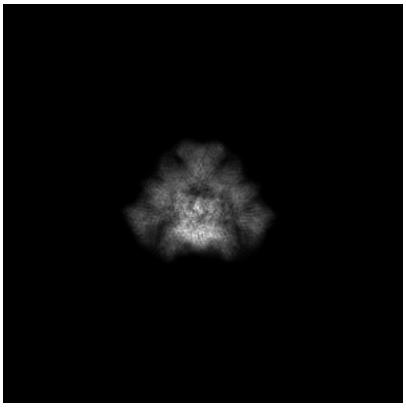
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32638. These allow visual inspection of the internal detail of the map and identification of artifacts.

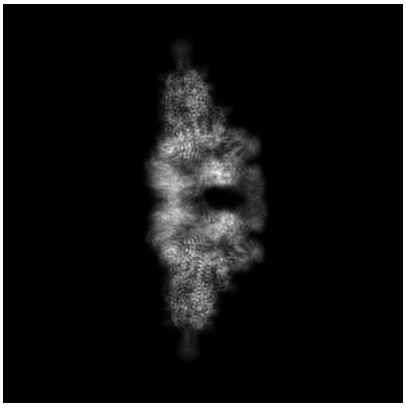
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

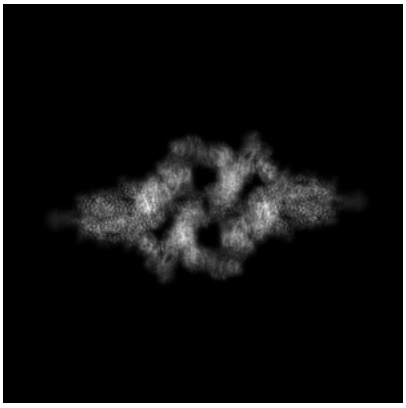
6.1.1 Primary map



X



Y



Z

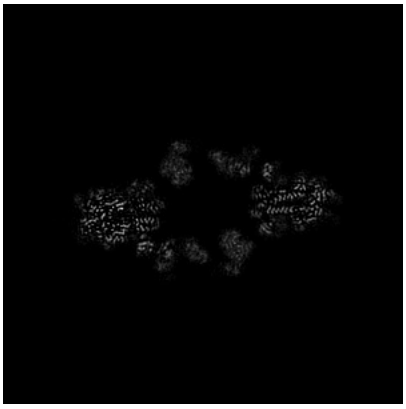
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

X Index: 240

Y Index: 240

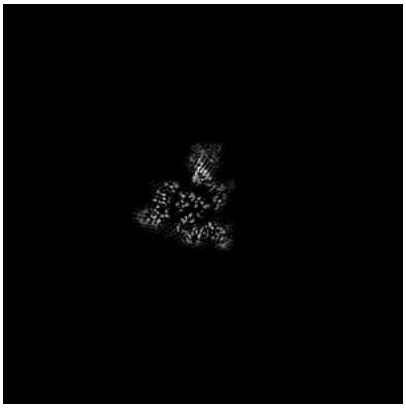


Z Index: 240

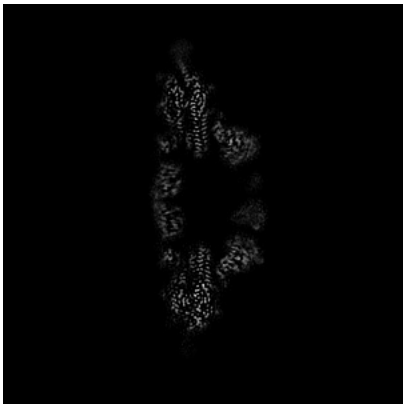
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

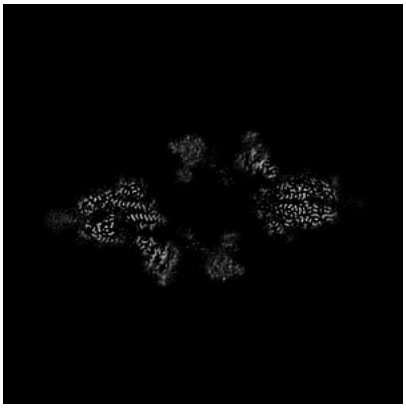
6.3.1 Primary map



X Index: 174



Y Index: 234

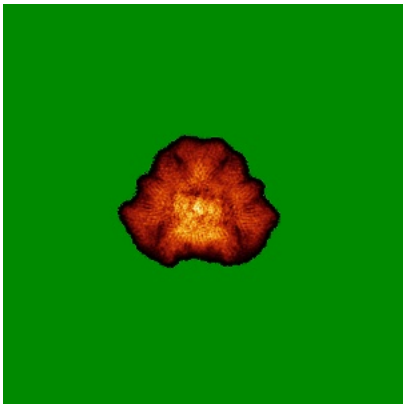


Z Index: 228

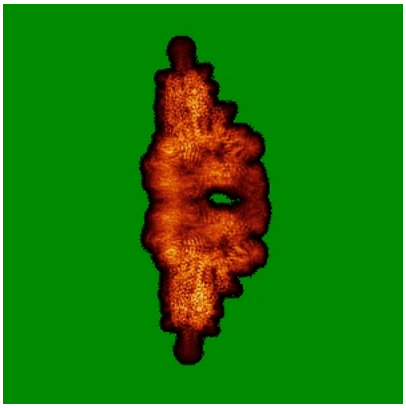
The images above show the largest variance slices of the map in three orthogonal directions.

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

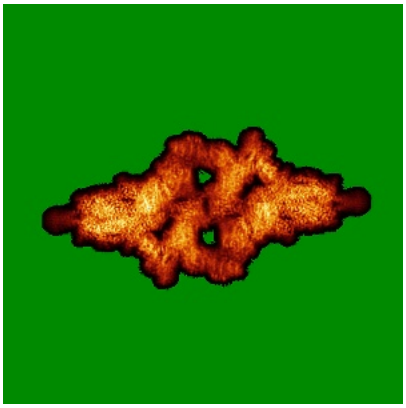
6.4.1 Primary map



X



Y

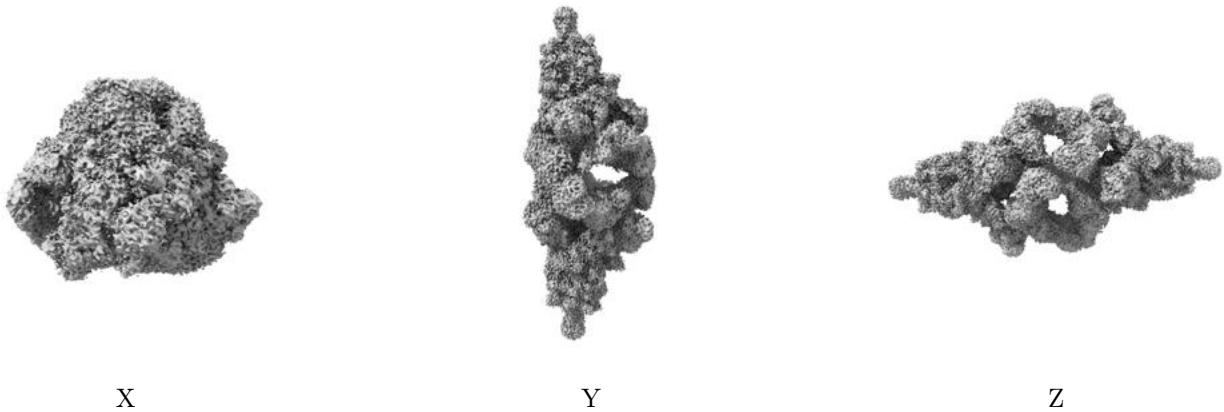


Z

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

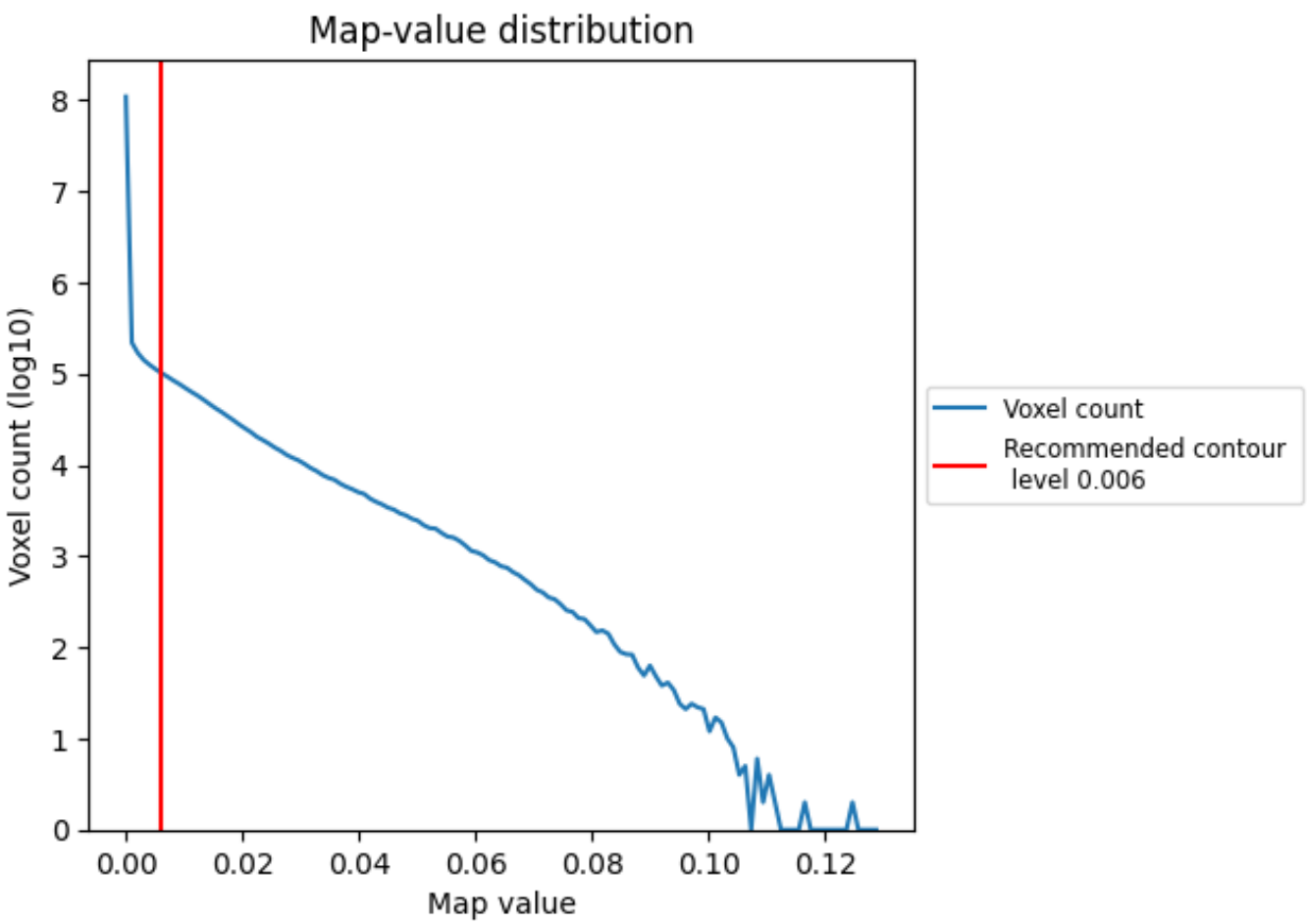
6.6 Mask visualisation (i)

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

7 Map analysis (i)

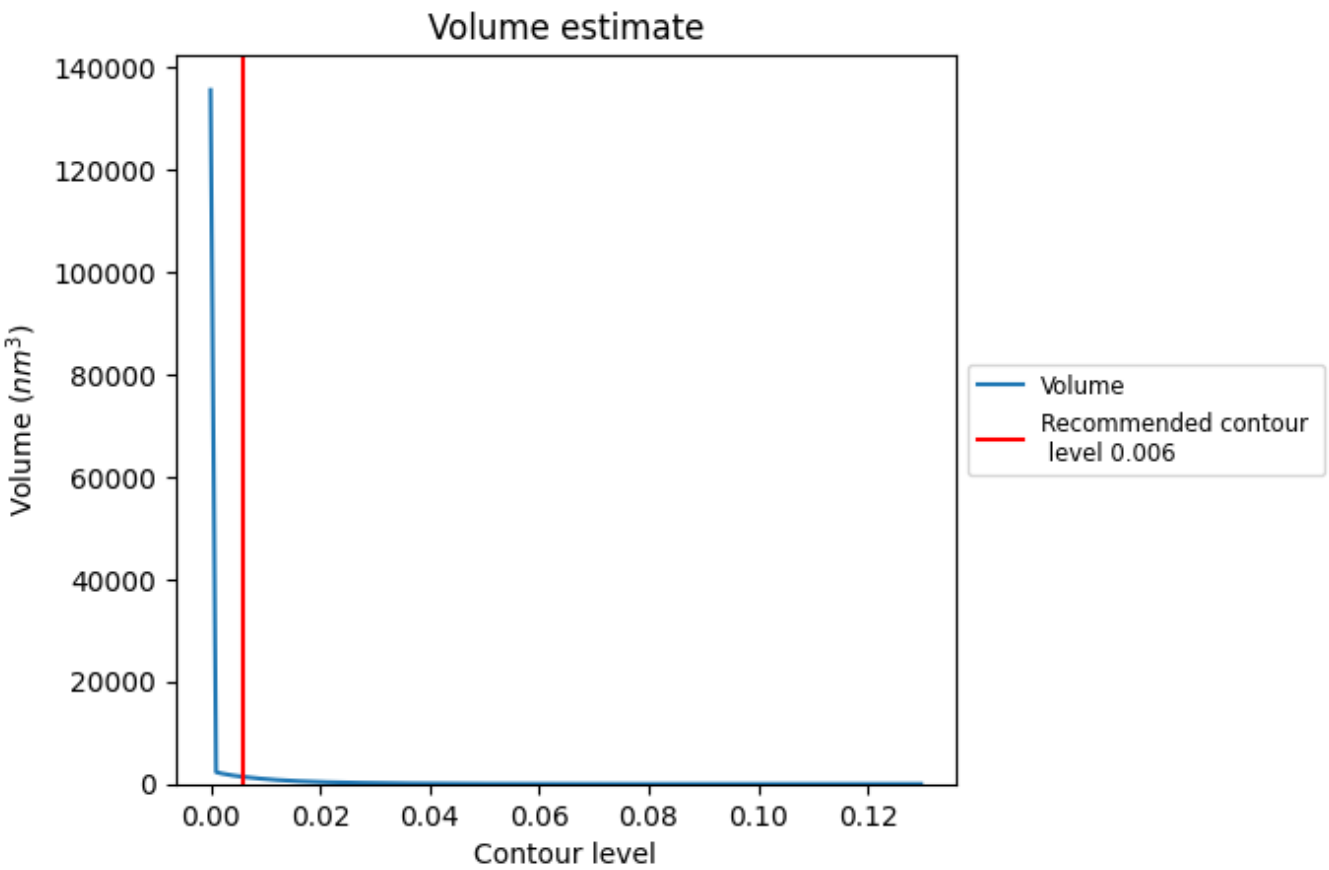
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

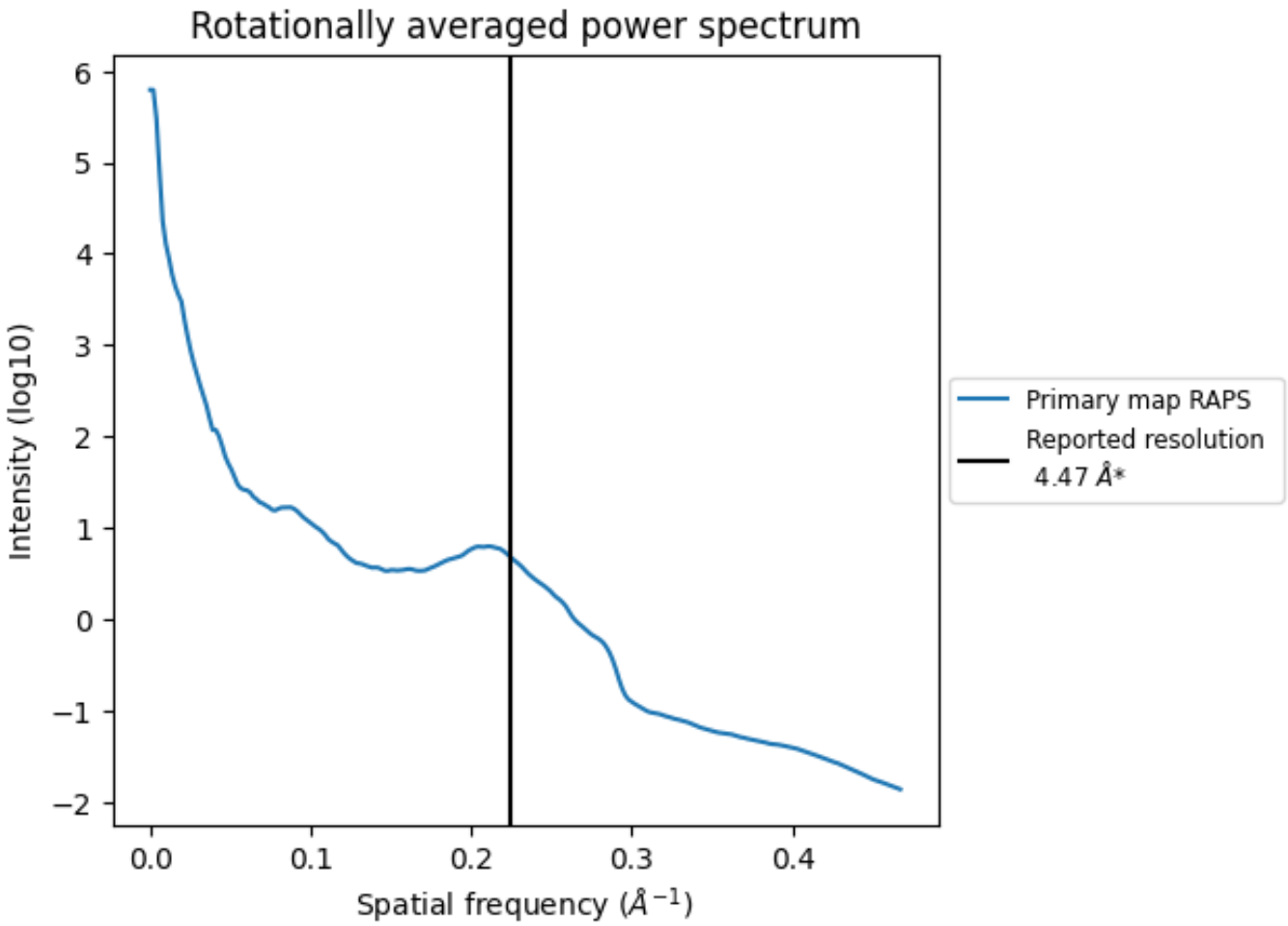
7.2 Volume estimate (i)



The volume at the recommended contour level is 1388 nm^3; this corresponds to an approximate mass of 1254 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 0.224 Å^{-1}

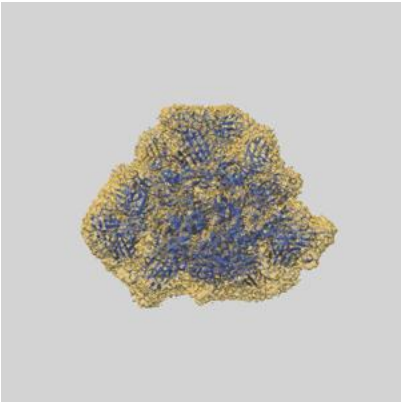
8 Fourier-Shell correlation (i)

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

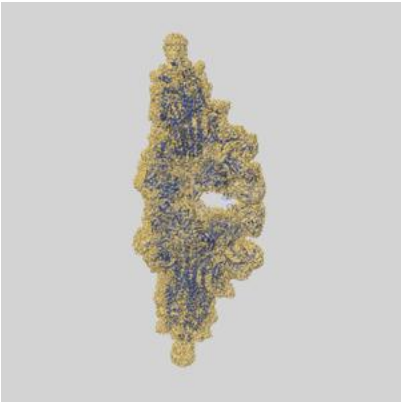
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32638 and PDB model 7WO4. Per-residue inclusion information can be found in section 3 on page 23.

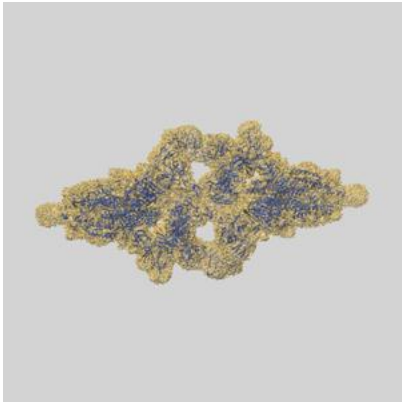
9.1 Map-model overlay (i)



X



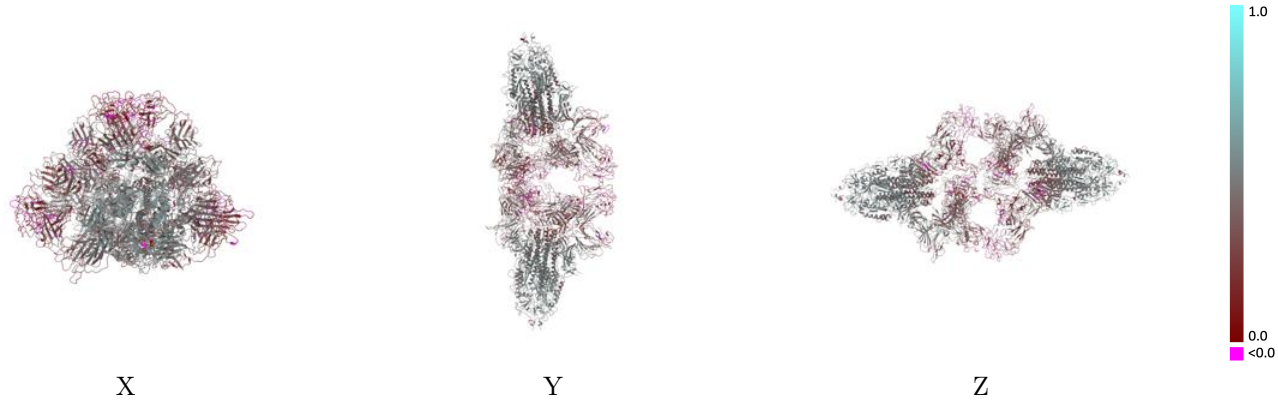
Y



Z

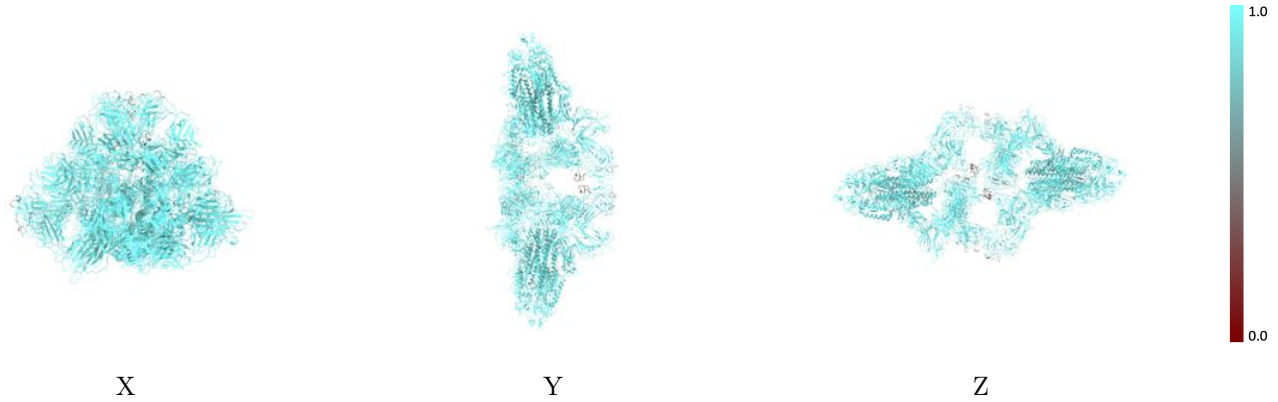
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



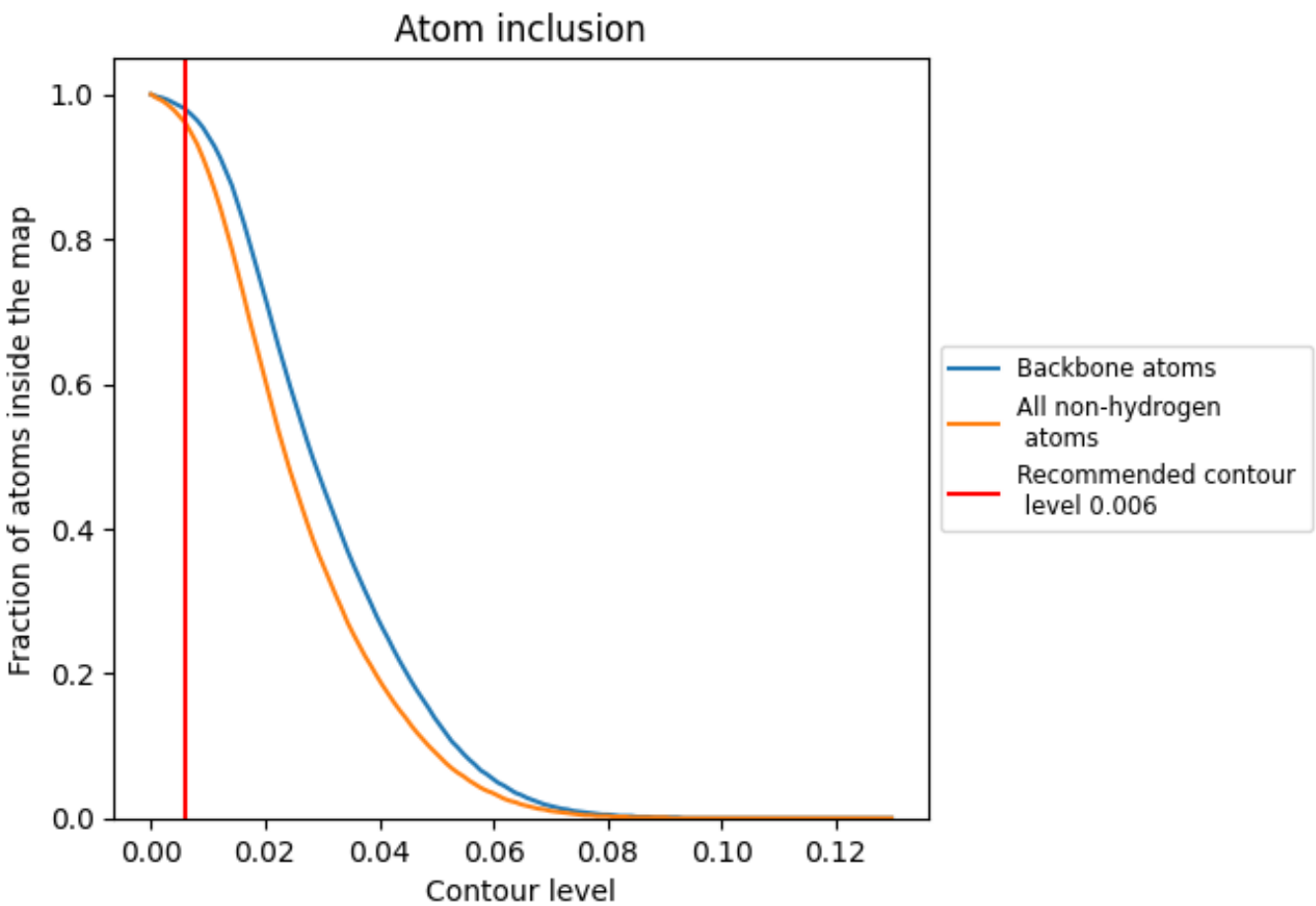
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.3760
A	0.9710	0.4270
B	0.9690	0.4360
C	0.9580	0.4100
D	0.9430	0.3080
E	0.9590	0.3050
F	0.9240	0.2840
G	0.9720	0.2940
H	0.9600	0.2710
I	0.9440	0.2310
J	0.9690	0.3980
K	0.9650	0.4100
L	0.9570	0.3940
M	0.9430	0.3090
N	0.9500	0.3090
O	0.9430	0.2900
P	0.9770	0.2910
Q	0.9490	0.2580
R	0.9420	0.2120