



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 03:51 PM JST

PDB ID : 7E9Q
EMDB ID : EMD-31036
Title : Cryo-EM structure of the SARS-CoV-2 S-6P in complex with 35B5 Fab(1 out RBD, state3)
Authors : Wang, X.F.; Zhu, Y.Q.
Deposited on : 2021-03-04
Resolution : 3.65 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

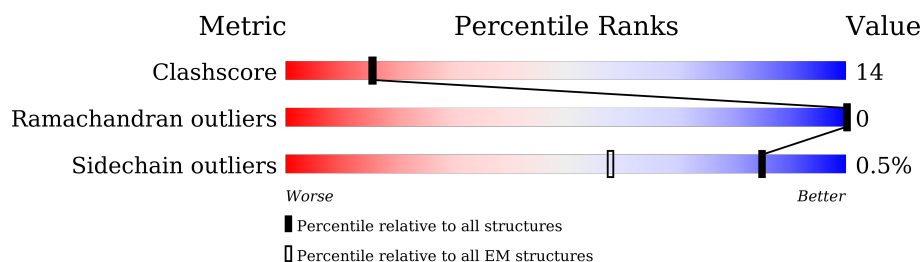
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1288	
1	B	1288	
1	C	1288	
2	E	219	
2	L	219	
2	X	219	
3	F	237	
3	H	237	

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Mol	Chain	Length	Quality of chain
3	Y	237	<div> <div>52%</div> <div>55%</div> <div>40%</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33876 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1002	Total	C	N	O	S	0	0
			7825	4998	1300	1492	35		
1	A	1002	Total	C	N	O	S	0	0
			7825	4998	1300	1492	35		
1	C	1002	Total	C	N	O	S	0	0
			7825	4998	1300	1492	35		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	LEU	-	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	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
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	LEU	-	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	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
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	LEU	-	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	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2

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

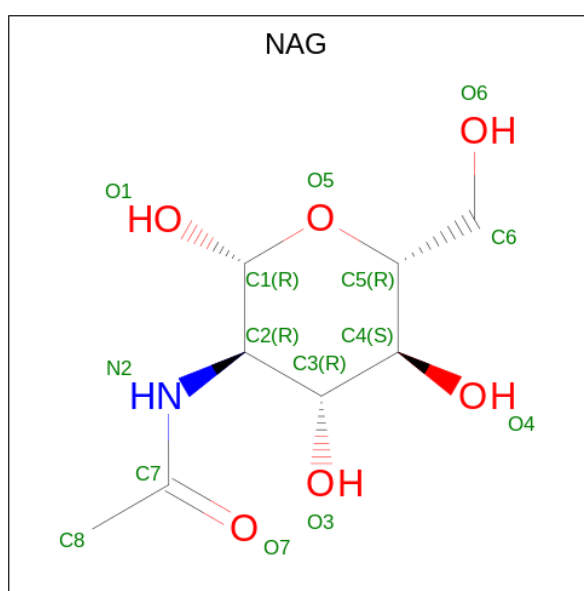
- Molecule 2 is a protein called Light chain of 35B5 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	218	Total	C	N	O	S	0	0
			1673	1050	280	337	6		
2	X	218	Total	C	N	O	S	0	0
			1673	1050	280	337	6		
2	E	218	Total	C	N	O	S	0	0
			1673	1050	280	337	6		

- Molecule 3 is a protein called Heavy chain of 35B5 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	226	Total	C	N	O	S	0	0
			1668	1048	285	327	8		
3	Y	226	Total	C	N	O	S	0	0
			1668	1048	285	327	8		
3	F	226	Total	C	N	O	S	0	0
			1668	1048	285	327	8		

- 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
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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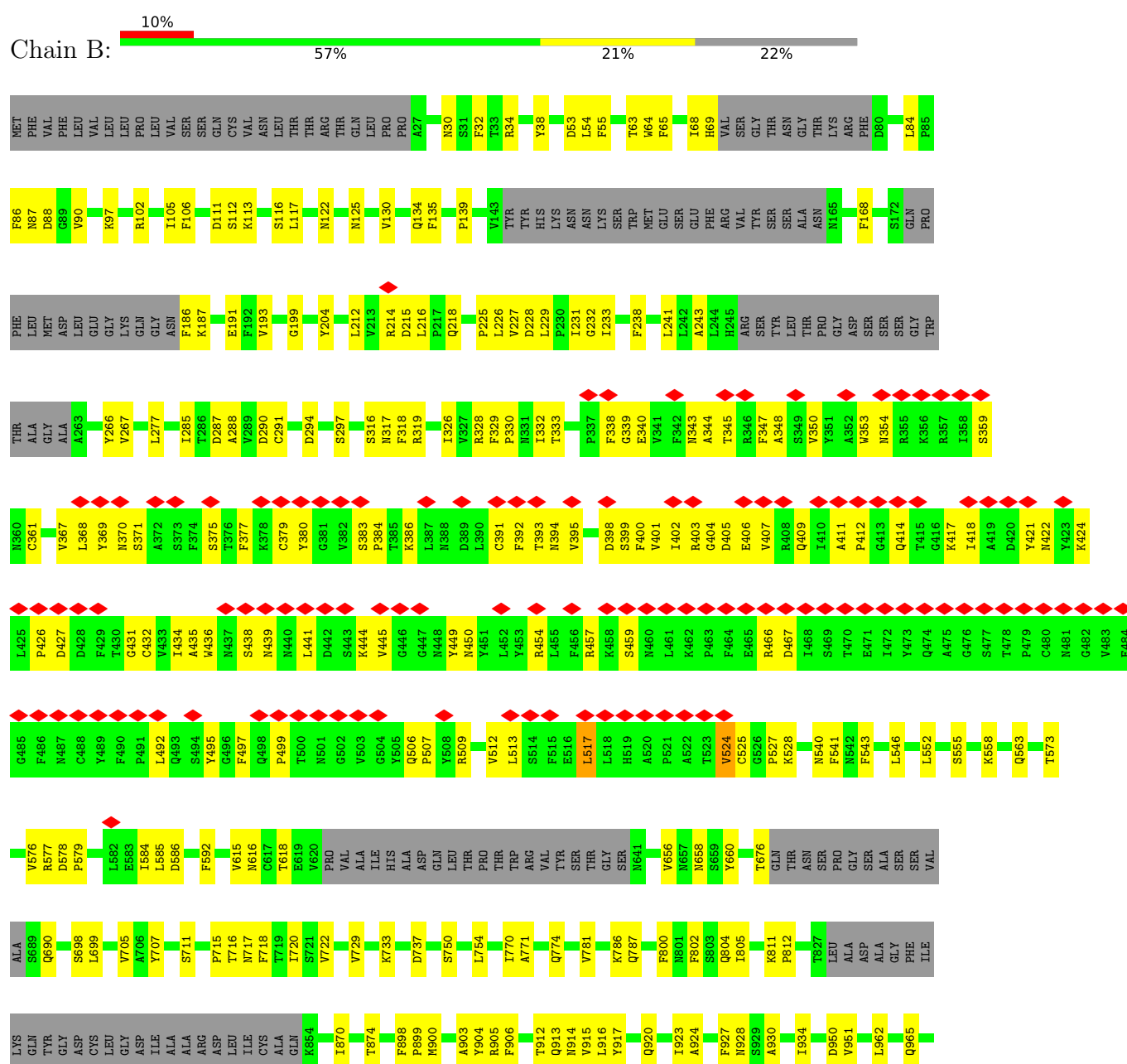
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C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

3 Residue-property plots

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

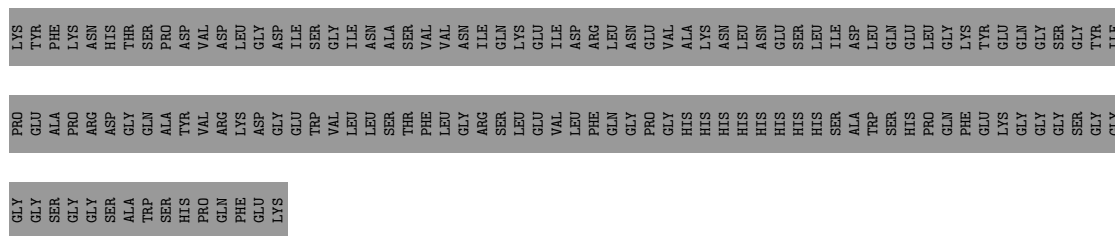


GLY		GLN		PHE	
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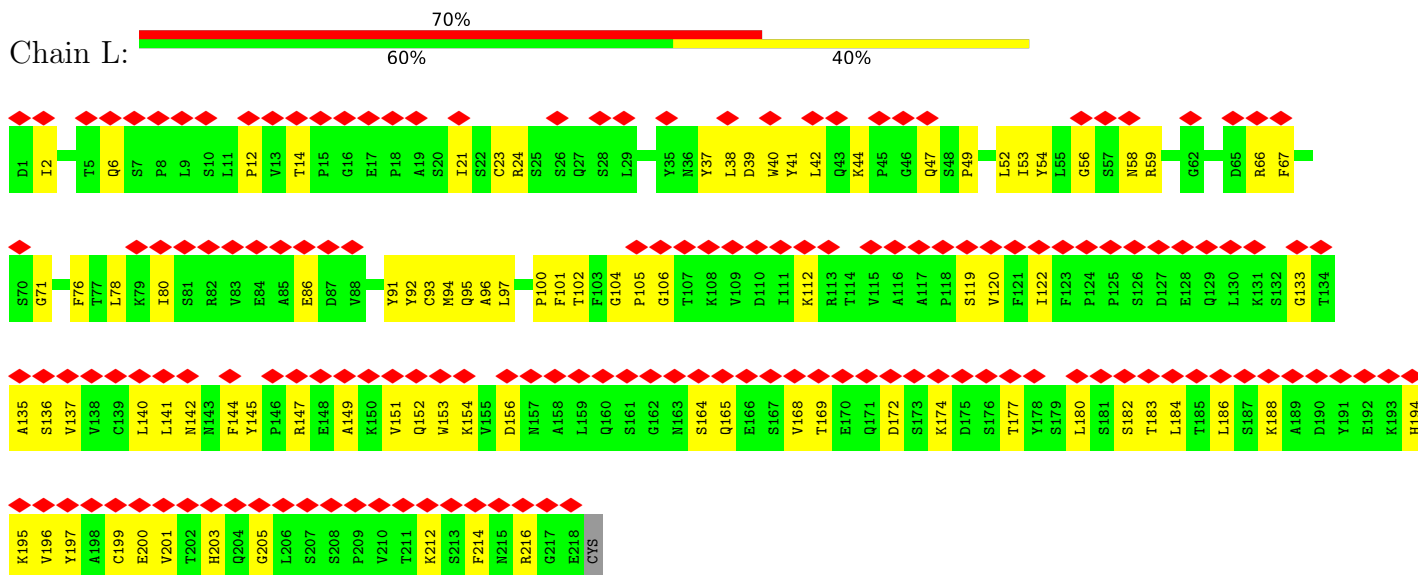
• Molecule 1: Spike glycoprotein

Chain A:  58% 20% 22%

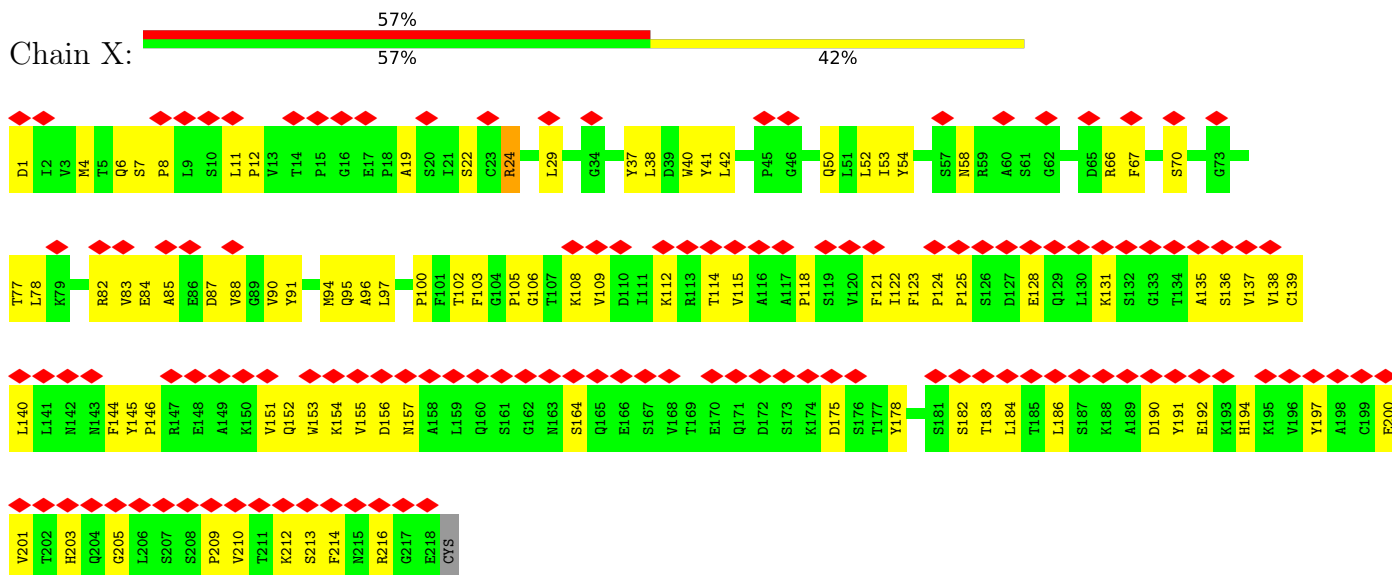
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A93	S94	K97	I100	G103	N122	N125	C131	E132	G141	G142	V143	TYR	HIS	LYS	ASN	ASN	LYS	SER	TRP	MET	GLU	SER	GLY	PHE	ARG	VAL	SER	SER	SER	ALA	ASN	N165	S172	GLN	PRO	PHE	SER	LEU	LEU	MET	THR	ASP	GLY	THR	GLY	GLN	GLY	ASN	F186	R190	E191	
F192	K195	N196	F201	K202	I203	K206	N211	L212	P217	F220	S221	L223	L226	V227	D228	L229	F230	F238	Q239	L240	L241	L242	H245	ARG	SER	SER	TYR	LEU	THR	THR	THR	PRO	GLY	ASP	SER	SER	SER	GLY	TRP	ALA	ALA	A263	G268	R273	L276							
L277	N280	T284	I285	V289	D290	C291	D294	P295	T299	E309	N317	F318	V320	R328	F329	T345	R346	F347	A348	S349	V350	Y351	A352	W353	N354	I358	S366	Y369	N370	S371	A372	T376	C379	Y380	P384	T385	K386	L387	N388	D389	L390	C391										
V395	V401	I402	R403	G404	D405	E406	V407	R408	Q409	I410	A411	P412	G413	T415	G416	K417	Y421	N422	Y423	K424	L425	P426	D427	D428	C432	N437	S438	N439	N440	K444	V445	N448	Y449	N450	L452	R454	F456	R457	K458	S459	N460	L461	K462	P463	F464	E465	R466	D467	I468			
S469	T470	E471	I472	V473	Q474	A475	G476	S477	T478	P479	C480	M481	G482	V483	E484	G485	F486	M487	C488	F489	F490	Q493	F497	Q498	F499	T500	N501	G502	Y505	Y508	R509	H519	A520	C525	N532	L533	C538	Y539	N540	N542	F543	N544	V551	L560	Q563	D568						
I569	P579	Q580	I587	C590	G593	G594	V597	Y612	V620	PRO	VAL	ALA	ILE	HIS	ALA	ASP	GLN	LEU	THR	PRO	THR	TRP	ARG	VAL	TYR	SER	THR	GLY	SER	H641	T645	G648	C649	L650	A653	I664	P665	I666	T670	C671	Y674	G675	T676	GLN	THR	ASN						
SER	PRO	GLY	SER	SER	SER	ALA	VAL	ALA	Q690	I712	I713	I714	N717	F718	V722	E725	I726	S730	V736	D737	C738	T739	C743	E748	C749	F759	N777	T778	Q779	V781	K786	Q787	P792	F802	I805	S816	E819	B820	L821	T827												
LEU	ALA	ASP	GLY	PHE	ILE	LYS	GLN	TYR	ASP	CYS	LEU	GLY	ILE	ALA	ALA	ARG	ASP	ILE	ALA	CYS	GLN	K854	F855	E988	L858	L865	I870	R995	T874	G880	S884	P897	F898	P899	M900	G901	N902	R905	F906	T912	Q913	N914	Y915	L916	Q920	R921	L922					
I923	Q926	A930	I934	Q935	A944	L945	L948	L962	V963	L966	S967	S968	L977	I980	D985	P986	P987	E988	A989	E990	I993	D994	R995	L996	I997	R1000	L1001	Y1007	K1028	C1032	L1049	M1050	P1063	Q1064	H1068	V1061	H1064	V1065														



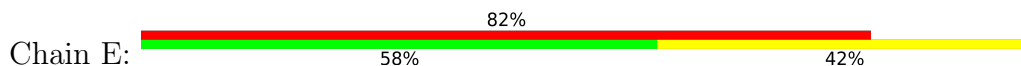
- Molecule 2: Light chain of 35B5 Fab



- Molecule 2: Light chain of 35B5 Fab

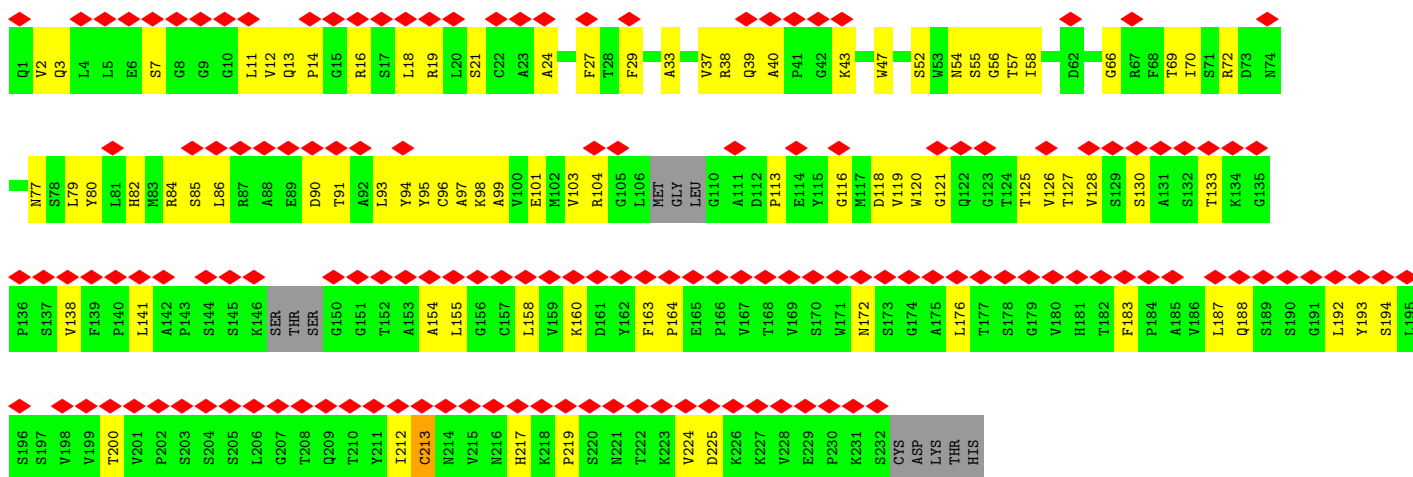


- Molecule 2: Light chain of 35B5 Fab

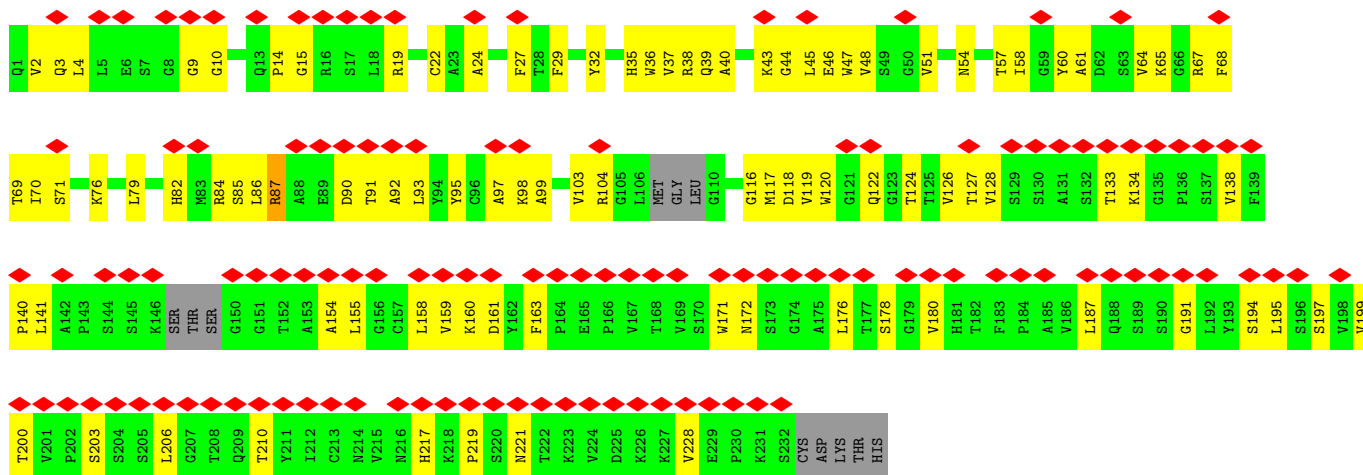




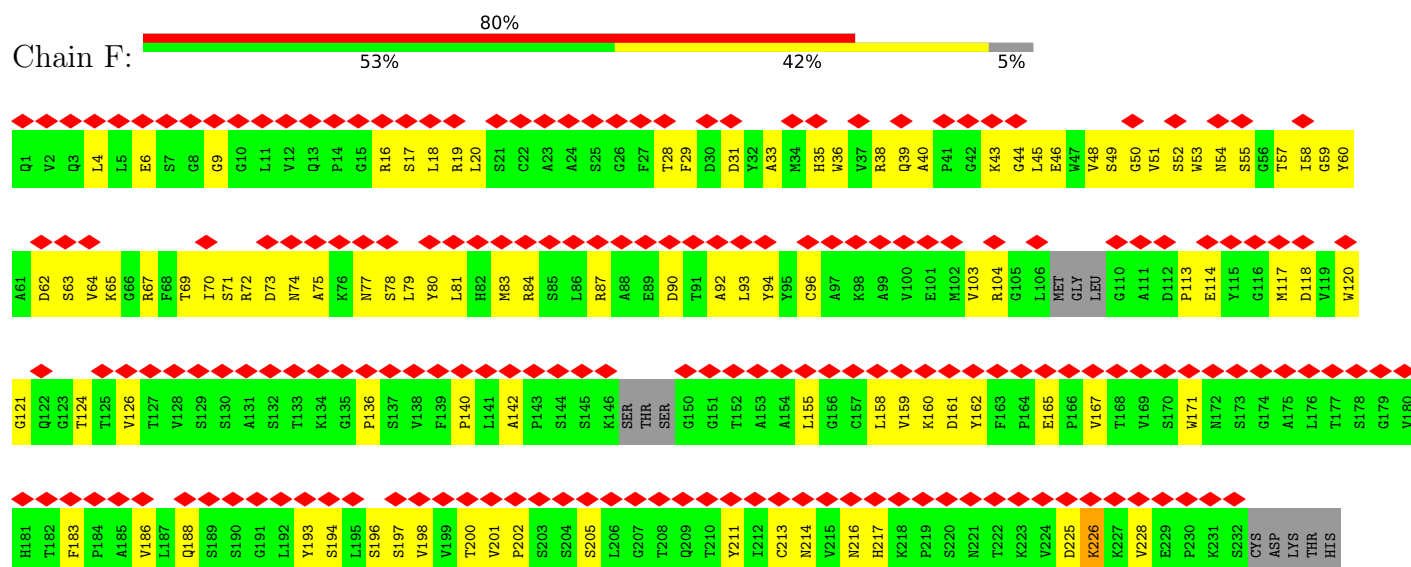
• Molecule 3: Heavy chain of 35B5 Fab



• Molecule 3: Heavy chain of 35B5 Fab



● Molecule 3: Heavy chain of 35B5 Fab



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75721	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	41.752	Depositor
Minimum map value	-24.647	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (Å)	361.35, 361.35, 361.35	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	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	0.32	0/8004	0.54	0/10896
1	B	0.33	0/8004	0.55	0/10896
1	C	0.32	0/8004	0.53	0/10896
2	E	0.29	0/1711	0.50	0/2326
2	L	0.27	0/1711	0.50	0/2326
2	X	0.28	0/1711	0.51	0/2326
3	F	0.28	0/1706	0.49	0/2323
3	H	0.30	0/1706	0.51	0/2323
3	Y	0.32	0/1706	0.55	0/2323
All	All	0.32	0/34263	0.53	0/46635

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	7825	0	7635	175	0
1	B	7825	0	7637	197	0
1	C	7825	0	7637	184	0
2	E	1673	0	1628	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1673	0	1628	75	0
2	X	1673	0	1628	87	0
3	F	1668	0	1609	83	0
3	H	1668	0	1609	64	0
3	Y	1668	0	1609	79	0
4	A	126	0	117	0	0
4	B	126	0	117	1	0
4	C	126	0	117	3	0
All	All	33876	0	32971	967	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (967) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:141:LEU:O	2:E:179:SER:HA	1.62	0.98
2:X:201:VAL:O	2:X:209:PRO:HA	1.64	0.96
3:F:17:SER:HA	3:F:83:MET:O	1.67	0.93
3:Y:171:TRP:HE1	3:Y:197:SER:HG	1.18	0.88
1:B:439:ASN:HA	1:B:507:PRO:HG2	1.57	0.87
1:B:441:LEU:HB3	1:B:509:ARG:HH21	1.42	0.84
3:Y:86:LEU:HD23	3:Y:128:VAL:HG22	1.59	0.83
1:B:353:TRP:HE1	1:B:467:ASP:H	1.24	0.82
2:E:140:LEU:HA	2:E:180:LEU:O	1.79	0.82
2:X:12:PRO:HB2	2:X:112:LYS:HB2	1.62	0.81
2:X:91:TYR:O	2:X:106:GLY:HA2	1.81	0.80
2:E:141:LEU:HD11	2:E:201:VAL:HG11	1.63	0.80
1:B:449:TYR:HB2	3:F:65:LYS:HG2	1.63	0.79
3:Y:160:LYS:HD3	3:Y:194:SER:HB2	1.65	0.78
1:C:662:CYS:HB2	1:C:697:MET:HG2	1.65	0.78
1:B:417:LYS:O	1:B:421:TYR:HB2	1.83	0.78
1:C:226:LEU:HG	1:C:227:VAL:HG23	1.65	0.77
1:B:361:CYS:H	1:B:524:VAL:HB	1.50	0.77
1:C:1032:CYS:SG	1:C:1048:HIS:NE2	2.58	0.76
3:Y:103:VAL:HG12	3:Y:104:ARG:HG3	1.67	0.76
1:B:86:PHE:HB2	1:B:238:PHE:HD1	1.50	0.75
1:C:729:VAL:HG11	1:C:781:VAL:HG11	1.69	0.75
2:E:119:SER:HB2	2:E:142:ASN:O	1.87	0.75
1:B:555:SER:HB2	1:B:584:ILE:HG23	1.68	0.74
1:B:438:SER:HB2	1:B:441:LEU:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:147:ARG:HH22	2:E:180:LEU:HB2	1.52	0.73
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.70	0.73
1:A:317:ASN:HD22	1:A:593:GLY:H	1.36	0.72
1:C:912:THR:HG22	1:C:913:GLN:H	1.54	0.72
2:E:53:ILE:HG12	2:E:59:ARG:HA	1.71	0.72
1:B:215:ASP:CG	1:B:216:LEU:H	1.91	0.72
1:A:912:THR:HG22	1:A:913:GLN:H	1.54	0.71
2:L:38:LEU:HA	2:L:94:MET:O	1.91	0.71
3:F:103:VAL:HG12	3:F:104:ARG:HG2	1.73	0.71
1:C:193:VAL:HG22	1:C:204:TYR:HB2	1.73	0.71
2:E:17:GLU:HG2	2:E:18:PRO:HD2	1.73	0.70
1:B:950:ASP:OD1	1:B:951:VAL:N	2.24	0.70
1:A:97:LYS:HB3	1:A:186:PHE:HA	1.73	0.70
2:E:142:ASN:ND2	3:F:200:THR:OG1	2.25	0.70
1:B:193:VAL:HG22	1:B:204:TYR:HB2	1.73	0.70
1:A:476:GLY:H	1:A:487:ASN:HB3	1.56	0.70
3:H:19:ARG:HH11	3:H:80:TYR:HB2	1.56	0.70
2:E:120:VAL:HG11	2:E:210:VAL:HG11	1.74	0.70
1:B:924:ALA:O	1:B:928:ASN:ND2	2.24	0.70
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.71	0.70
2:L:137:VAL:HB	2:L:184:LEU:HB3	1.74	0.70
1:C:476:GLY:HA3	1:C:487:ASN:HB3	1.72	0.70
2:L:39:ASP:HB2	2:L:94:MET:HB3	1.71	0.70
2:X:42:LEU:HB2	2:X:52:LEU:HD11	1.74	0.69
1:B:406:GLU:HB2	1:B:418:ILE:HD12	1.74	0.69
3:F:60:TYR:HB2	3:F:65:LYS:HA	1.74	0.69
3:Y:180:VAL:HG22	3:Y:199:VAL:HG22	1.73	0.69
1:B:424:LYS:HG2	1:B:426:PRO:HD3	1.75	0.69
1:B:804:GLN:NE2	4:B:1305:NAG:O6	2.26	0.69
3:Y:36:TRP:HE1	3:Y:79:LEU:HD21	1.57	0.69
2:E:39:ASP:OD1	2:E:55:LEU:N	2.24	0.69
1:B:450:ASN:HB2	3:F:59:GLY:HA2	1.75	0.69
2:L:91:TYR:O	2:L:106:GLY:HA2	1.92	0.69
2:X:67:PHE:HB3	2:X:78:LEU:HD11	1.75	0.69
2:E:4:MET:HA	2:E:24:ARG:O	1.93	0.69
1:B:344:ALA:HB1	3:F:54:ASN:HD22	1.57	0.69
1:B:729:VAL:HG11	1:B:781:VAL:HG11	1.73	0.69
1:A:345:THR:HG23	1:A:346:ARG:HG2	1.74	0.69
1:B:1141:LEU:HG	1:B:1145:LEU:HD23	1.74	0.68
1:B:112:SER:HB3	1:B:134:GLN:HA	1.74	0.68
3:F:40:ALA:HB3	3:F:43:LYS:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:158:LEU:HA	3:F:196:SER:HB2	1.76	0.68
2:X:7:SER:OG	2:X:24:ARG:NH2	2.26	0.68
3:Y:70:ILE:HD11	3:Y:79:LEU:HD21	1.76	0.68
2:X:191:TYR:O	2:X:216:ARG:NH2	2.27	0.68
1:B:720:ILE:HG13	1:B:923:ILE:HG23	1.75	0.67
3:F:4:LEU:HB2	3:F:121:GLY:HA3	1.75	0.67
3:F:205:SER:HA	3:F:211:TYR:HE2	1.59	0.67
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.28	0.67
2:X:66:ARG:NH1	2:X:82:ARG:O	2.27	0.67
1:C:105:ILE:HG22	1:C:110:LEU:HD22	1.77	0.67
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.25	0.67
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.77	0.67
3:F:33:ALA:HA	3:F:51:VAL:O	1.95	0.67
3:Y:155:LEU:HD13	3:Y:228:VAL:HG11	1.76	0.66
2:E:138:VAL:HG22	2:E:183:THR:HG22	1.75	0.66
1:B:811:LYS:HD3	1:B:812:PRO:HD2	1.77	0.66
2:X:151:VAL:HG22	2:X:201:VAL:HG22	1.76	0.66
1:B:186:PHE:N	1:B:212:LEU:O	2.29	0.66
1:B:392:PHE:O	1:B:524:VAL:HG13	1.95	0.66
1:A:650:LEU:HD13	1:A:653:ALA:HB3	1.78	0.66
3:H:52:SER:O	3:H:72:ARG:NH1	2.28	0.66
1:B:418:ILE:HA	1:B:422:ASN:HB2	1.76	0.66
1:A:354:ASN:ND2	3:H:54:ASN:O	2.28	0.66
2:X:8:PRO:HG2	2:X:11:LEU:HB3	1.77	0.66
1:C:412:PRO:HG3	1:C:429:PHE:HD2	1.61	0.66
2:X:186:LEU:HB3	2:X:190:ASP:HB3	1.77	0.66
1:C:437:ASN:ND2	1:C:506:GLN:OE1	2.27	0.66
2:E:91:TYR:HB2	2:E:107:THR:HB	1.76	0.66
1:A:231:ILE:HG13	1:A:232:GLY:H	1.61	0.66
2:X:144:PHE:O	2:X:178:TYR:N	2.26	0.66
1:B:228:ASP:OD1	1:B:229:LEU:N	2.29	0.65
1:A:328:ARG:HD2	1:A:580:GLN:HG2	1.79	0.65
3:F:214:ASN:ND2	3:F:225:ASP:OD1	2.25	0.65
1:C:390:LEU:HD23	1:C:392:PHE:HE2	1.62	0.65
1:C:720:ILE:HG13	1:C:923:ILE:HG23	1.76	0.65
1:B:1043:CYS:HB3	1:B:1048:HIS:CD2	2.32	0.65
3:H:2:VAL:HG11	3:H:119:VAL:HG11	1.78	0.65
1:B:737:ASP:OD1	1:C:317:ASN:ND2	2.30	0.65
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.30	0.65
3:F:38:ARG:HB2	3:F:92:ALA:HB3	1.79	0.65
1:B:214:ARG:HD2	1:B:215:ASP:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:THR:HG23	3:F:104:ARG:HH12	1.62	0.64
3:Y:40:ALA:HA	3:Y:92:ALA:HA	1.80	0.64
1:A:738:CYS:SG	1:A:739:THR:N	2.70	0.64
1:A:352:ALA:HB1	1:A:466:ARG:HH21	1.63	0.64
1:C:722:VAL:HG12	1:C:930:ALA:HB1	1.79	0.64
1:B:347:PHE:H	1:B:509:ARG:HH12	1.46	0.63
1:A:391:CYS:HB2	1:A:525:CYS:HA	1.80	0.63
1:C:354:ASN:ND2	3:Y:54:ASN:O	2.31	0.63
3:H:133:THR:HA	3:H:163:PHE:CD2	2.34	0.63
2:X:137:VAL:HB	2:X:184:LEU:HB3	1.79	0.63
1:B:402:ILE:HD11	1:B:407:VAL:HG22	1.80	0.63
2:L:37:TYR:HB3	2:L:96:ALA:HB3	1.81	0.63
3:F:87:ARG:H	3:F:90:ASP:HB2	1.63	0.63
1:C:909:ILE:HD11	1:C:1047:TYR:HB3	1.80	0.63
3:Y:38:ARG:HG3	3:Y:46:GLU:HB2	1.81	0.63
3:F:38:ARG:HH22	3:F:64:VAL:HG11	1.64	0.63
2:E:8:PRO:HG2	2:E:11:LEU:HD22	1.81	0.63
2:X:40:TRP:HB2	2:X:53:ILE:HB	1.80	0.63
2:L:66:ARG:HB3	2:L:80:ILE:HG23	1.79	0.62
1:B:436:TRP:HE1	1:B:509:ARG:HD2	1.64	0.62
2:L:195:LYS:HA	2:L:216:ARG:HE	1.64	0.62
3:H:14:PRO:HD2	3:H:130:SER:HB2	1.80	0.62
2:L:42:LEU:HB2	2:L:52:LEU:HD11	1.82	0.62
2:L:120:VAL:HG12	2:L:141:LEU:HG	1.80	0.62
1:B:379:CYS:HB3	1:B:432:CYS:HA	1.80	0.62
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.26	0.62
3:H:13:GLN:HE21	3:H:16:ARG:HG3	1.65	0.62
2:X:186:LEU:HD12	2:X:191:TYR:HD1	1.65	0.62
3:Y:36:TRP:HE1	3:Y:79:LEU:CD2	2.13	0.62
3:H:118:ASP:OD2	3:H:119:VAL:N	2.32	0.62
1:A:203:ILE:HB	1:A:227:VAL:HB	1.80	0.62
1:A:280:ASN:ND2	1:A:284:THR:OG1	2.32	0.62
1:A:329:PHE:O	1:A:580:GLN:NE2	2.32	0.62
1:C:656:VAL:HG12	1:C:658:ASN:H	1.65	0.62
2:L:195:LYS:HG3	2:L:196:VAL:HG23	1.81	0.62
3:H:141:LEU:HD21	3:H:158:LEU:HB2	1.81	0.61
3:Y:67:ARG:O	3:Y:84:ARG:NH2	2.33	0.61
2:E:51:LEU:HD23	3:F:118:ASP:HB3	1.82	0.61
1:A:100:ILE:HG22	1:A:242:LEU:HD22	1.83	0.61
1:A:532:ASN:OD1	1:A:533:LEU:N	2.28	0.61
3:H:172:ASN:HD22	3:H:176:LEU:HB3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:115:VAL:HG22	2:X:146:PRO:HD3	1.81	0.61
1:B:404:GLY:HA3	1:B:506:GLN:HB2	1.81	0.61
1:C:452:LEU:HB3	1:C:492:LEU:HB3	1.82	0.61
1:C:578:ASP:OD2	1:C:581:THR:N	2.33	0.61
1:B:370:ASN:OD1	1:B:371:SER:N	2.33	0.61
1:B:552:LEU:HD13	1:B:585:LEU:HD13	1.83	0.61
1:C:976:VAL:HG23	1:C:979:ASP:HB3	1.82	0.61
3:Y:140:PRO:HB3	3:Y:228:VAL:HG22	1.82	0.61
1:A:290:ASP:OD1	1:A:291:CYS:N	2.34	0.60
3:H:133:THR:HA	3:H:163:PHE:HD2	1.65	0.60
1:B:563:GLN:O	1:B:577:ARG:NH2	2.34	0.60
1:C:64:TRP:HD1	1:C:65:PHE:H	1.49	0.60
3:F:19:ARG:NH1	3:F:71:SER:OG	2.34	0.60
1:B:402:ILE:HB	1:B:418:ILE:HD13	1.82	0.60
2:L:95:GLN:NE2	2:L:100:PRO:O	2.35	0.60
3:Y:217:HIS:O	3:Y:221:ASN:N	2.35	0.60
1:B:353:TRP:HE1	1:B:467:ASP:N	1.99	0.60
1:C:726:ILE:HG23	1:C:1061:VAL:HG12	1.84	0.60
2:L:6:GLN:HB3	2:L:21:ILE:HD11	1.82	0.60
2:E:151:VAL:O	2:E:152:GLN:NE2	2.34	0.60
1:B:403:ARG:HD3	1:B:405:ASP:HB3	1.82	0.59
1:C:417:LYS:O	1:C:421:TYR:HB2	2.01	0.59
1:C:760:CYS:HA	1:C:763:LEU:HD12	1.84	0.59
3:Y:48:VAL:HA	3:Y:61:ALA:HB2	1.85	0.59
3:Y:160:LYS:NZ	3:Y:161:ASP:OD1	2.31	0.59
1:C:1087:ALA:O	1:C:1088:HIS:ND1	2.35	0.59
2:L:38:LEU:O	2:L:56:GLY:N	2.35	0.59
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.84	0.59
1:A:1087:ALA:O	1:A:1088:HIS:ND1	2.35	0.59
1:C:868:GLU:OE1	1:C:872:GLN:NE2	2.31	0.59
1:B:353:TRP:HB2	1:B:400:PHE:CD1	2.37	0.59
1:C:470:THR:H	3:Y:19:ARG:HH12	1.47	0.59
1:A:726:ILE:HD13	1:A:945:LEU:HD13	1.85	0.59
2:L:14:THR:HG23	2:L:112:LYS:HB3	1.84	0.59
2:L:37:TYR:HD2	2:L:97:LEU:HA	1.66	0.59
2:X:197:TYR:HH	2:X:216:ARG:HH21	1.50	0.59
2:X:194:HIS:O	2:X:216:ARG:NH2	2.34	0.59
3:Y:118:ASP:OD1	3:Y:119:VAL:N	2.36	0.59
3:F:171:TRP:HH2	3:F:228:VAL:HG11	1.66	0.59
1:C:354:ASN:HB2	1:C:399:SER:HB2	1.85	0.59
1:C:64:TRP:HD1	1:C:65:PHE:N	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:ARG:HB2	3:Y:54:ASN:HD21	1.67	0.58
2:L:172:ASP:N	2:L:177:THR:O	2.35	0.58
2:L:133:GLY:HA2	2:L:188:LYS:HB2	1.86	0.58
3:H:11:LEU:HD23	3:H:127:THR:HB	1.85	0.58
2:X:7:SER:N	2:X:24:ARG:HH12	2.01	0.58
2:E:147:ARG:NH2	2:E:180:LEU:HB2	2.19	0.58
1:A:328:ARG:HG3	1:A:579:PRO:HG2	1.84	0.58
1:C:133:PHE:HB3	1:C:135:PHE:HD2	1.67	0.58
3:Y:36:TRP:NE1	3:Y:70:ILE:HD11	2.17	0.58
1:A:53:ASP:OD1	1:A:54:LEU:N	2.30	0.58
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.67	0.58
2:E:134:THR:HG21	3:F:160:LYS:HZ1	1.68	0.58
1:C:189:LEU:HB2	1:C:210:ILE:HD13	1.86	0.58
1:A:403:ARG:HH22	1:A:406:GLU:HG2	1.69	0.58
1:A:722:VAL:HG22	1:A:930:ALA:HB1	1.85	0.58
3:F:38:ARG:N	3:F:46:GLU:O	2.36	0.58
1:B:231:ILE:HG22	1:B:233:ILE:HG12	1.86	0.58
1:A:64:TRP:HD1	1:A:65:PHE:H	1.52	0.57
1:C:661:GLU:O	1:C:695:TYR:OH	2.21	0.57
3:F:213:CYS:SG	3:F:226:LYS:HE3	2.44	0.57
1:B:215:ASP:CG	1:B:216:LEU:N	2.57	0.57
3:H:103:VAL:HG22	3:H:104:ARG:HG2	1.85	0.57
1:B:906:PHE:CD1	1:B:1049:LEU:HD11	2.39	0.57
1:C:34:ARG:NH1	1:C:219:GLY:O	2.38	0.57
3:H:101:GLU:HG3	3:H:113:PRO:HB2	1.86	0.57
2:E:42:LEU:HB3	2:E:50:GLN:HB2	1.86	0.57
1:C:204:TYR:CD1	1:C:225:PRO:HA	2.39	0.57
2:X:66:ARG:NH1	2:X:87:ASP:OD2	2.37	0.57
3:Y:4:LEU:HD13	3:Y:24:ALA:HB2	1.85	0.57
1:B:411:ALA:HB3	1:B:414:GLN:HB2	1.86	0.57
2:X:123:PHE:HE2	2:X:140:LEU:HD12	1.70	0.57
1:A:821:LEU:HD11	1:A:935:GLN:HE21	1.70	0.57
1:C:411:ALA:HB3	1:C:414:GLN:HB2	1.85	0.57
1:C:454:ARG:HG3	1:C:491:PRO:HB2	1.86	0.57
2:X:115:VAL:HG13	2:X:145:TYR:O	2.05	0.57
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.69	0.57
1:A:34:ARG:NH2	1:A:217:PRO:O	2.37	0.57
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.36	0.57
1:A:897:PRO:HG2	1:A:900:MET:HE3	1.87	0.56
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.40	0.56
1:C:298:GLU:O	1:C:302:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:125:PRO:HD3	2:E:137:VAL:HG22	1.87	0.56
2:E:136:SER:HA	2:E:184:LEU:O	2.04	0.56
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.31	0.56
2:X:22:SER:OG	2:X:24:ARG:NH1	2.37	0.56
3:Y:38:ARG:N	3:Y:46:GLU:O	2.38	0.56
1:B:403:ARG:HB3	1:B:418:ILE:HD11	1.87	0.56
1:B:656:VAL:HG12	1:B:658:ASN:H	1.70	0.56
1:A:722:VAL:HA	1:A:1064:HIS:O	2.04	0.56
1:C:355:ARG:HH11	1:C:355:ARG:HG2	1.70	0.56
2:L:147:ARG:O	2:L:147:ARG:NH1	2.38	0.56
2:L:172:ASP:OD1	2:L:174:LYS:NZ	2.38	0.56
2:X:164:SER:HB2	2:X:184:LEU:HA	1.86	0.56
3:Y:15:GLY:HA2	3:Y:85:SER:HA	1.87	0.56
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.87	0.56
1:B:998:THR:O	1:B:1002:GLN:HG2	2.05	0.56
3:Y:171:TRP:HB3	3:Y:176:LEU:HB3	1.88	0.56
1:B:353:TRP:HA	1:B:400:PHE:HB3	1.87	0.56
2:X:152:GLN:NE2	2:X:200:GLU:OE1	2.39	0.56
3:F:9:GLY:HA3	3:F:126:VAL:HG22	1.86	0.56
1:B:111:ASP:O	1:B:112:SER:OG	2.23	0.56
1:C:727:LEU:HD12	1:C:728:PRO:HD2	1.88	0.56
1:B:802:PHE:HD2	1:B:805:ILE:HD11	1.70	0.56
3:H:70:ILE:HD11	3:H:79:LEU:HD21	1.86	0.56
1:A:37:TYR:HB3	1:A:223:LEU:HD23	1.88	0.56
1:B:1043:CYS:HB3	1:B:1048:HIS:HD2	1.71	0.55
1:B:65:PHE:HE2	1:B:84:LEU:HD11	1.70	0.55
1:A:353:TRP:CD1	1:A:423:TYR:HB2	2.41	0.55
1:C:739:THR:HG22	1:C:753:LEU:HD21	1.87	0.55
1:B:406:GLU:O	1:B:409:GLN:HB2	2.06	0.55
1:A:448:ASN:H	1:A:497:PHE:H	1.53	0.55
2:L:40:TRP:HB2	2:L:53:ILE:HB	1.87	0.55
2:L:142:ASN:HD22	3:H:200:THR:HG21	1.71	0.55
3:F:72:ARG:HG3	3:F:79:LEU:HD13	1.87	0.55
1:A:568:ASP:OD1	1:A:569:ILE:N	2.34	0.55
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.39	0.55
2:L:93:CYS:O	2:L:104:GLY:N	2.39	0.55
3:H:164:PRO:HD2	3:H:217:HIS:CE1	2.41	0.55
2:E:12:PRO:HB2	2:E:112:LYS:HD3	1.89	0.55
1:B:900:MET:HG2	1:B:917:TYR:OH	2.07	0.55
3:Y:37:VAL:HG11	3:Y:45:LEU:HB2	1.88	0.55
2:E:137:VAL:HG21	2:E:214:PHE:HZ	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ARG:HH12	3:F:75:ALA:H	1.54	0.55
1:C:456:PHE:HD2	1:C:491:PRO:HA	1.71	0.55
1:C:665:PRO:HA	1:C:671:CYS:HB2	1.88	0.55
1:C:880:GLY:O	1:C:884:SER:OG	2.22	0.55
3:F:48:VAL:O	3:F:60:TYR:HA	2.06	0.55
1:C:87:ASN:OD1	1:C:88:ASP:N	2.39	0.55
1:C:99:ASN:O	1:C:102:ARG:NH2	2.40	0.55
1:C:122:ASN:OD1	1:C:125:ASN:HB3	2.07	0.55
1:C:358:ILE:HB	1:C:395:VAL:HG13	1.89	0.55
2:L:152:GLN:HE22	2:L:154:LYS:HE3	1.72	0.55
1:B:130:VAL:HG11	1:B:231:ILE:HD12	1.89	0.55
1:B:350:VAL:HB	1:B:402:ILE:HG22	1.89	0.55
1:A:320:VAL:HB	1:A:590:CYS:HB3	1.89	0.55
1:A:458:LYS:HZ2	1:A:473:TYR:HA	1.72	0.55
2:X:156:ASP:OD2	2:X:194:HIS:ND1	2.31	0.55
1:A:968:SER:OG	1:C:755:GLN:O	2.24	0.55
1:C:1106:GLN:OE1	1:C:1111:GLU:HB2	2.07	0.55
2:L:203:HIS:CD2	2:L:205:GLY:H	2.25	0.55
2:E:2:ILE:HG23	2:E:26:SER:HB3	1.88	0.54
3:F:67:ARG:HB2	3:F:84:ARG:HB2	1.88	0.54
1:C:106:PHE:CE1	1:C:238:PHE:HB2	2.42	0.54
3:F:70:ILE:HD11	3:F:79:LEU:HD11	1.89	0.54
1:B:377:PHE:HE2	1:B:384:PRO:HB3	1.71	0.54
2:X:12:PRO:HB2	2:X:112:LYS:CB	2.35	0.54
2:X:22:SER:O	2:X:24:ARG:NH1	2.41	0.54
1:B:347:PHE:HB2	1:B:401:VAL:HG23	1.88	0.54
1:A:354:ASN:HD21	3:H:55:SER:HB3	1.71	0.54
1:A:712:ILE:HG21	1:A:1096:VAL:HG12	1.90	0.54
1:C:334:ASN:HD21	1:C:361:CYS:HA	1.72	0.54
1:B:398:ASP:HB2	1:B:512:VAL:HB	1.90	0.54
3:Y:217:HIS:CD2	3:Y:219:PRO:HD2	2.43	0.54
1:C:906:PHE:CD1	1:C:1049:LEU:HD11	2.42	0.54
2:L:141:LEU:HB2	2:L:180:LEU:HB3	1.89	0.54
2:E:145:TYR:CG	2:E:146:PRO:HA	2.42	0.54
1:B:229:LEU:HB3	1:B:231:ILE:HG12	1.90	0.54
1:B:354:ASN:HB3	1:B:399:SER:O	2.08	0.54
1:C:748:GLU:N	1:C:748:GLU:OE1	2.41	0.54
1:A:349:SER:HB3	1:A:351:TYR:CE1	2.42	0.54
1:B:722:VAL:HG12	1:B:930:ALA:HB1	1.90	0.54
1:B:380:TYR:CE2	1:B:412:PRO:HD3	2.43	0.54
1:A:231:ILE:HG13	1:A:232:GLY:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:44:LYS:HB2	2:L:47:GLN:HB2	1.90	0.54
2:X:118:PRO:HB3	2:X:144:PHE:HB3	1.90	0.54
1:B:445:VAL:HA	1:B:499:PRO:HD3	1.89	0.53
1:B:979:ASP:OD2	1:B:983:ARG:NH2	2.41	0.53
1:A:922:LEU:O	1:A:926:GLN:HG3	2.07	0.53
1:C:214:ARG:NH1	1:C:215:ASP:HB3	2.23	0.53
1:C:666:ILE:HD12	1:C:671:CYS:HA	1.89	0.53
3:Y:36:TRP:HE1	3:Y:70:ILE:HD11	1.73	0.53
1:B:707:TYR:HB3	1:A:792:PRO:HG3	1.89	0.53
1:A:86:PHE:HB2	1:A:238:PHE:HD1	1.72	0.53
1:B:30:ASN:HB3	1:B:32:PHE:HE2	1.74	0.53
1:C:822:LEU:HD23	1:C:1056:ALA:HB2	1.91	0.53
1:A:722:VAL:HG12	1:A:1065:VAL:HG22	1.90	0.53
3:F:186:VAL:HG22	3:F:194:SER:HB3	1.89	0.53
1:A:406:GLU:O	1:A:410:ILE:HG12	2.08	0.53
3:H:19:ARG:HE	3:H:80:TYR:HB3	1.74	0.53
2:E:41:TYR:CZ	2:E:51:LEU:HD13	2.43	0.53
2:X:103:PHE:HE2	3:Y:47:TRP:N	2.06	0.53
3:Y:60:TYR:H	3:Y:65:LYS:HE2	1.74	0.53
2:L:14:THR:HG23	2:L:112:LYS:HE2	1.89	0.53
1:C:406:GLU:HA	1:C:409:GLN:HB2	1.90	0.53
2:X:153:TRP:CD2	2:X:184:LEU:HB2	2.43	0.53
1:A:438:SER:HB3	1:A:509:ARG:HG3	1.91	0.53
1:C:328:ARG:NH1	1:C:578:ASP:OD1	2.42	0.53
2:X:37:TYR:HB3	2:X:96:ALA:HB3	1.89	0.53
3:Y:172:ASN:ND2	3:Y:210:THR:O	2.41	0.53
3:F:38:ARG:NH2	3:F:64:VAL:HG11	2.24	0.53
1:B:870:ILE:O	1:B:874:THR:HG23	2.09	0.52
1:A:995:ARG:NH2	1:C:994:ASP:OD1	2.42	0.52
1:C:403:ARG:HD2	1:C:505:TYR:HA	1.91	0.52
1:C:756:TYR:OH	1:C:994:ASP:OD2	2.27	0.52
2:X:155:VAL:HG22	2:X:184:LEU:HD21	1.89	0.52
3:F:52:SER:OG	3:F:54:ASN:OD1	2.27	0.52
2:E:22:SER:HB2	2:E:24:ARG:HH22	1.74	0.52
1:B:431:GLY:HA3	1:B:513:LEU:O	2.09	0.52
3:Y:98:LYS:HD2	3:Y:99:ALA:O	2.09	0.52
1:B:903:ALA:HB1	1:B:913:GLN:HB2	1.91	0.52
1:A:717:ASN:OD1	1:A:718:PHE:N	2.41	0.52
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.09	0.52
3:H:39:GLN:NE2	3:H:43:LYS:O	2.40	0.52
3:Y:43:LYS:HD3	3:Y:44:GLY:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:167:VAL:HG12	3:F:217:HIS:HA	1.91	0.52
1:B:332:ILE:HG13	1:B:333:THR:H	1.75	0.52
1:B:930:ALA:O	1:B:934:ILE:HG12	2.09	0.52
1:B:977:LEU:HA	1:B:980:ILE:HD12	1.90	0.52
1:A:64:TRP:HD1	1:A:65:PHE:N	2.06	0.52
3:H:163:PHE:HD1	3:H:192:LEU:HD13	1.74	0.52
1:B:277:LEU:HD11	1:B:285:ILE:HD13	1.91	0.52
1:A:405:ASP:O	1:A:408:ARG:NH1	2.42	0.52
1:A:777:ASN:O	1:A:781:VAL:HG23	2.09	0.52
2:L:169:THR:HG22	3:H:183:PHE:HA	1.92	0.52
2:X:194:HIS:O	2:X:197:TYR:OH	2.27	0.52
1:B:290:ASP:OD1	1:B:291:CYS:N	2.42	0.52
1:B:338:PHE:O	1:B:343:ASN:N	2.40	0.52
1:C:360:ASN:H	1:C:523:THR:HG23	1.74	0.52
2:E:2:ILE:HD12	2:E:101:PHE:HA	1.91	0.52
2:E:88:VAL:HB	2:E:109:VAL:HG12	1.92	0.52
2:E:137:VAL:HG21	2:E:214:PHE:CZ	2.45	0.52
1:A:542:ASN:OD1	1:A:543:PHE:N	2.43	0.52
2:X:153:TRP:NE1	2:X:182:SER:OG	2.42	0.52
1:A:103:GLY:HA3	1:A:241:LEU:HB2	1.92	0.52
1:C:502:GLY:O	1:C:506:GLN:HG3	2.09	0.52
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.45	0.52
2:E:2:ILE:HG21	2:E:95:GLN:HE22	1.75	0.52
2:E:145:TYR:CD2	2:E:146:PRO:HA	2.44	0.52
1:B:87:ASN:OD1	1:B:88:ASP:N	2.42	0.51
1:B:319:ARG:CZ	1:B:592:PHE:HB3	2.40	0.51
1:A:986:PRO:O	1:A:990:GLU:HG3	2.10	0.51
2:L:95:GLN:HE21	2:L:102:THR:H	1.59	0.51
3:Y:97:ALA:HB1	3:Y:117:MET:HB3	1.93	0.51
3:Y:133:THR:HG23	3:Y:163:PHE:O	2.11	0.51
2:E:94:MET:HG2	2:E:103:PHE:CZ	2.45	0.51
1:B:786:LYS:HG3	1:B:787:GLN:HG3	1.92	0.51
1:A:277:LEU:HD23	1:A:285:ILE:HD13	1.93	0.51
1:A:802:PHE:HD2	1:A:805:ILE:HD11	1.74	0.51
2:E:145:TYR:O	2:E:203:HIS:NE2	2.41	0.51
1:B:135:PHE:HD1	1:B:139:PRO:HG2	1.75	0.51
1:C:46:SER:HA	1:C:279:TYR:O	2.10	0.51
1:C:950:ASP:OD1	1:C:951:VAL:N	2.41	0.51
1:B:328:ARG:NH2	1:B:578:ASP:OD2	2.44	0.51
1:A:317:ASN:OD1	1:A:318:PHE:N	2.44	0.51
3:F:28:THR:HG23	3:F:31:ASP:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:161:ASP:OD1	3:F:188:GLN:NE2	2.44	0.51
3:F:205:SER:HA	3:F:211:TYR:CE2	2.43	0.51
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.93	0.51
1:A:1028:LYS:O	1:A:1032:CYS:CB	2.59	0.51
1:C:958:ALA:O	1:C:961:THR:OG1	2.22	0.51
2:L:153:TRP:NE1	2:L:182:SER:OG	2.40	0.51
2:L:195:LYS:HB3	2:L:216:ARG:HH21	1.75	0.51
1:C:287:ASP:OD1	1:C:288:ALA:N	2.44	0.51
1:C:403:ARG:HB3	1:C:406:GLU:HG2	1.91	0.51
1:C:909:ILE:HD11	1:C:1047:TYR:CB	2.41	0.51
2:X:123:PHE:HB2	3:Y:141:LEU:HD11	1.92	0.51
3:Y:160:LYS:HD2	3:Y:161:ASP:H	1.76	0.51
3:F:73:ASP:HB3	3:F:78:SER:HB2	1.93	0.51
1:B:53:ASP:OD1	1:B:54:LEU:N	2.37	0.51
1:A:388:ASN:OD1	1:A:389:ASP:N	2.41	0.51
1:A:540:ASN:OD1	1:A:541:PHE:N	2.44	0.51
1:C:358:ILE:HB	1:C:395:VAL:CG1	2.41	0.51
3:H:188:GLN:HE21	3:H:192:LEU:C	2.14	0.51
1:B:905:ARG:HH12	1:B:1050:MET:HG3	1.76	0.50
2:L:38:LEU:HD11	2:L:93:CYS:HB2	1.93	0.50
2:E:22:SER:HB2	2:E:24:ARG:NH2	2.26	0.50
1:B:403:ARG:HG2	1:B:405:ASP:H	1.76	0.50
1:A:676:THR:HA	1:A:690:GLN:HA	1.93	0.50
2:X:52:LEU:HD22	2:X:67:PHE:CZ	2.46	0.50
2:E:124:PRO:HB2	2:E:217:GLY:HA2	1.93	0.50
2:L:153:TRP:CE2	2:L:184:LEU:HB2	2.46	0.50
1:B:495:TYR:HB2	1:B:497:PHE:CE1	2.46	0.50
1:A:912:THR:HG22	1:A:913:GLN:N	2.24	0.50
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.46	0.50
1:B:316:SER:OG	1:B:317:ASN:N	2.41	0.50
1:A:444:LYS:HD2	1:A:448:ASN:HA	1.93	0.50
1:C:233:ILE:HG22	1:C:234:ASN:N	2.27	0.50
1:C:280:ASN:ND2	1:C:284:THR:OG1	2.45	0.50
1:C:619:GLU:OE1	1:C:619:GLU:N	2.41	0.50
2:L:49:PRO:HG2	3:H:120:TRP:CE2	2.46	0.50
1:A:538:CYS:HB3	1:A:551:VAL:CG2	2.41	0.50
2:E:42:LEU:N	2:E:50:GLN:O	2.32	0.50
2:E:143:ASN:ND2	2:E:175:ASP:OD2	2.44	0.50
1:B:102:ARG:HD2	1:B:243:ALA:HB2	1.94	0.50
1:B:368:LEU:HD22	1:B:434:ILE:HG12	1.94	0.50
1:A:985:ASP:HB3	1:A:987:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:ALA:O	1:A:993:ILE:HG12	2.12	0.50
3:F:38:ARG:O	3:F:46:GLU:N	2.38	0.50
1:B:676:THR:HG22	1:B:690:GLN:HG2	1.93	0.50
1:A:280:ASN:OD1	1:A:284:THR:N	2.39	0.50
2:X:123:PHE:CZ	3:Y:154:ALA:HB3	2.47	0.50
2:X:125:PRO:HB3	2:X:136:SER:H	1.77	0.50
1:A:930:ALA:O	1:A:934:ILE:HG12	2.12	0.50
1:C:906:PHE:O	1:C:909:ILE:N	2.44	0.50
2:X:122:ILE:HG12	2:X:214:PHE:HE1	1.77	0.50
2:X:192:GLU:HA	2:X:216:ARG:HH22	1.76	0.50
1:C:484:GLU:OE1	1:C:490:PHE:HB2	2.13	0.49
2:E:154:LYS:HB3	2:E:198:ALA:HB3	1.94	0.49
2:X:1:ASP:N	2:X:100:PRO:O	2.45	0.49
2:E:42:LEU:HB2	2:E:52:LEU:HD21	1.93	0.49
2:E:123:PHE:HA	3:F:142:ALA:O	2.12	0.49
3:F:6:GLU:OE1	3:F:124:THR:N	2.45	0.49
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.94	0.49
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.94	0.49
1:C:353:TRP:O	1:C:466:ARG:NE	2.43	0.49
1:C:387:LEU:HD12	1:C:390:LEU:HD22	1.93	0.49
1:C:877:LEU:O	1:C:881:THR:HG23	2.12	0.49
2:L:120:VAL:HA	2:L:140:LEU:O	2.12	0.49
2:E:127:ASP:OD2	2:E:127:ASP:N	2.45	0.49
3:F:31:ASP:HA	3:F:53:TRP:HB3	1.94	0.49
1:B:287:ASP:OD1	1:B:288:ALA:N	2.45	0.49
1:C:86:PHE:HD1	1:C:90:VAL:HG23	1.77	0.49
1:C:449:TYR:HB3	3:Y:65:LYS:HD2	1.93	0.49
2:L:38:LEU:HD23	2:L:76:PHE:HB2	1.94	0.49
3:Y:38:ARG:O	3:Y:46:GLU:N	2.39	0.49
3:F:183:PHE:HD2	3:F:196:SER:HB3	1.77	0.49
1:A:369:TYR:OH	1:A:384:PRO:O	2.21	0.49
2:L:135:ALA:HB3	2:L:186:LEU:HB2	1.94	0.49
3:H:91:THR:HB	3:H:127:THR:HG23	1.95	0.49
3:Y:37:VAL:HG11	3:Y:45:LEU:HD12	1.93	0.49
3:F:171:TRP:HZ3	3:F:211:TYR:HB3	1.78	0.49
2:L:54:TYR:O	2:L:58:ASN:N	2.43	0.49
2:L:152:GLN:NE2	2:L:200:GLU:OE1	2.44	0.49
3:H:33:ALA:H	3:H:99:ALA:HB3	1.77	0.49
3:H:66:GLY:O	3:H:84:ARG:NH1	2.45	0.49
3:Y:138:VAL:HG22	3:Y:159:VAL:HG22	1.94	0.49
1:A:786:LYS:HG3	1:A:787:GLN:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:GLN:HG2	2:L:23:CYS:SG	2.52	0.49
3:H:96:CYS:O	3:H:121:GLY:N	2.46	0.49
2:X:154:LYS:HB3	2:X:157:ASN:HA	1.95	0.49
1:B:393:THR:HB	1:B:517:LEU:HA	1.93	0.49
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.93	0.49
2:E:29:LEU:HD21	2:E:95:GLN:HB2	1.94	0.49
1:B:347:PHE:HD2	1:B:509:ARG:HH11	1.61	0.49
1:A:897:PRO:CG	1:A:900:MET:HE3	2.43	0.49
1:A:920:GLN:O	1:A:923:ILE:HG22	2.13	0.49
3:Y:2:VAL:HG21	3:Y:98:LYS:HE2	1.95	0.49
3:Y:71:SER:O	3:Y:79:LEU:HG	2.13	0.49
1:A:358:ILE:HB	1:A:395:VAL:HB	1.95	0.49
1:C:870:ILE:O	1:C:874:THR:HG23	2.12	0.49
1:B:122:ASN:OD1	1:B:125:ASN:HB2	2.13	0.48
1:B:199:GLY:HA2	1:B:232:GLY:HA2	1.95	0.48
1:A:437:ASN:HD21	1:A:439:ASN:HB2	1.78	0.48
1:A:1094:VAL:HG23	1:A:1096:VAL:HG13	1.95	0.48
2:L:67:PHE:HD1	2:L:78:LEU:HD11	1.78	0.48
2:L:147:ARG:NE	2:L:168:VAL:HG21	2.28	0.48
2:L:147:ARG:HD3	2:L:168:VAL:HG11	1.95	0.48
3:Y:178:SER:OG	3:Y:200:THR:O	2.22	0.48
3:F:64:VAL:HG23	3:F:67:ARG:HD2	1.95	0.48
1:B:540:ASN:OD1	1:B:541:PHE:N	2.46	0.48
1:C:930:ALA:O	1:C:934:ILE:HG12	2.13	0.48
3:H:18:LEU:HG	3:H:19:ARG:H	1.78	0.48
2:E:153:TRP:HZ3	2:E:197:TYR:HB3	1.78	0.48
1:B:348:ALA:HB2	3:F:55:SER:O	2.13	0.48
1:A:722:VAL:HG23	1:A:934:ILE:HG13	1.95	0.48
1:C:490:PHE:CE2	3:Y:69:THR:HG21	2.48	0.48
1:C:717:ASN:OD1	1:C:718:PHE:N	2.46	0.48
2:X:38:LEU:HA	2:X:94:MET:O	2.14	0.48
2:X:94:MET:HG2	2:X:103:PHE:CE1	2.48	0.48
2:X:200:GLU:HA	2:X:210:VAL:O	2.13	0.48
1:B:130:VAL:HG22	1:B:168:PHE:HB3	1.95	0.48
1:B:350:VAL:N	1:B:401:VAL:O	2.46	0.48
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.43	0.48
1:C:906:PHE:CE2	1:C:916:LEU:HD12	2.48	0.48
1:C:973:ILE:HD12	1:C:983:ARG:HH11	1.79	0.48
2:L:2:ILE:HG23	2:L:95:GLN:HG2	1.96	0.48
2:L:156:ASP:OD1	2:L:195:LYS:N	2.43	0.48
3:Y:87:ARG:HB2	3:Y:90:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:95:TYR:OH	3:Y:122:GLN:OE1	2.31	0.48
3:F:201:VAL:HB	3:F:202:PRO:HD2	1.96	0.48
1:B:340:GLU:HA	3:F:53:TRP:CZ3	2.48	0.48
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.95	0.48
3:Y:27:PHE:CE2	3:Y:29:PHE:HA	2.49	0.48
2:E:113:ARG:HD2	2:E:176:SER:HB2	1.96	0.48
2:E:165:GLN:NE2	2:E:166:GLU:O	2.47	0.48
1:B:1054:GLN:HB2	1:B:1061:VAL:HG13	1.95	0.48
1:A:645:THR:HG21	1:A:670:ILE:HG21	1.94	0.48
1:C:64:TRP:CD1	1:C:65:PHE:N	2.81	0.48
2:L:153:TRP:CD2	2:L:184:LEU:HB2	2.49	0.48
1:A:299:THR:HG21	1:A:597:VAL:HG11	1.95	0.48
1:A:945:LEU:HD12	1:A:948:LEU:HD12	1.95	0.48
1:B:216:LEU:N	1:B:266:TYR:OH	2.47	0.48
1:A:460:ASN:OD1	1:A:461:LEU:N	2.46	0.48
2:L:71:GLY:HA3	2:L:76:PHE:HA	1.95	0.48
2:E:6:GLN:NE2	2:E:23:CYS:SG	2.87	0.48
1:A:402:ILE:HD12	1:A:406:GLU:HB2	1.96	0.47
1:C:393:THR:HA	1:C:522:ALA:HA	1.95	0.47
2:L:165:GLN:NE2	3:H:187:LEU:O	2.47	0.47
1:A:294:ASP:OD1	1:A:294:ASP:N	2.48	0.47
1:A:421:TYR:HB3	1:A:454:ARG:HG2	1.96	0.47
1:A:538:CYS:HB3	1:A:551:VAL:HG22	1.96	0.47
1:A:403:ARG:NH2	1:A:406:GLU:HG2	2.29	0.47
2:X:153:TRP:CE2	2:X:184:LEU:HB2	2.49	0.47
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.96	0.47
1:B:369:TYR:CZ	1:B:377:PHE:HB3	2.48	0.47
1:A:962:LEU:HD11	1:A:1007:TYR:CD2	2.50	0.47
1:A:1093:GLY:H	1:A:1107:ARG:NH1	2.12	0.47
1:C:417:LYS:HZ1	1:C:453:TYR:HE2	1.63	0.47
1:C:746:SER:HB3	1:C:749:CYS:SG	2.55	0.47
3:F:39:GLN:HB2	3:F:45:LEU:HG	1.95	0.47
1:A:141:LEU:HD23	1:A:245:HIS:HA	1.96	0.47
1:A:816:SER:OG	1:A:819:GLU:HG3	2.14	0.47
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.94	0.47
1:A:870:ILE:O	1:A:874:THR:HG23	2.14	0.47
1:A:880:GLY:O	1:A:884:SER:OG	2.22	0.47
1:C:96:GLU:HG3	1:C:98:SER:H	1.80	0.47
1:C:111:ASP:N	1:C:111:ASP:OD1	2.47	0.47
1:C:532:ASN:OD1	1:C:533:LEU:N	2.41	0.47
2:X:90:VAL:HG22	2:X:108:LYS:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:160:LYS:HG3	3:F:194:SER:HB2	1.95	0.47
1:B:204:TYR:CE1	1:B:225:PRO:HB3	2.50	0.47
1:B:436:TRP:NE1	1:B:509:ARG:HD2	2.26	0.47
1:A:422:ASN:HD21	1:A:454:ARG:H	1.61	0.47
2:L:136:SER:HB3	2:L:183:THR:HG23	1.97	0.47
2:L:197:TYR:HB2	2:L:214:PHE:CE1	2.50	0.47
3:H:69:THR:OG1	3:H:82:HIS:HB3	2.14	0.47
2:X:139:CYS:HB3	2:X:182:SER:HB3	1.97	0.47
2:X:153:TRP:HB3	2:X:184:LEU:HD13	1.96	0.47
3:F:35:HIS:O	3:F:96:CYS:HA	2.15	0.47
2:E:67:PHE:CD1	2:E:80:ILE:HG12	2.50	0.47
1:B:435:ALA:HA	1:B:509:ARG:O	2.15	0.47
1:B:716:THR:HG21	1:B:1073:LYS:HE3	1.97	0.47
1:A:206:LYS:HE2	1:A:221:SER:HB2	1.97	0.47
3:Y:158:LEU:HD12	3:Y:195:LEU:O	2.14	0.47
2:E:95:GLN:HG3	2:E:101:PHE:CD1	2.49	0.47
1:B:38:TYR:CE2	1:B:285:ILE:HG13	2.50	0.47
1:C:722:VAL:HA	1:C:1064:HIS:O	2.15	0.47
2:X:192:GLU:N	2:X:192:GLU:OE1	2.48	0.47
3:Y:51:VAL:HA	3:Y:57:THR:HA	1.97	0.47
1:B:912:THR:O	1:B:915:VAL:HG22	2.15	0.46
1:C:135:PHE:HB3	1:C:139:PRO:HG3	1.96	0.46
2:L:119:SER:HB2	2:L:142:ASN:HB3	1.97	0.46
3:H:39:GLN:NE2	3:H:40:ALA:O	2.48	0.46
3:Y:35:HIS:HE1	3:Y:58:ILE:HD11	1.79	0.46
3:Y:37:VAL:CG1	3:Y:45:LEU:HB2	2.45	0.46
1:B:906:PHE:HD1	1:B:1049:LEU:HD11	1.80	0.46
1:C:36:VAL:HG21	1:C:220:PHE:CZ	2.50	0.46
1:C:351:TYR:HE1	1:C:452:LEU:O	1.98	0.46
1:C:530:SER:OG	1:C:531:THR:N	2.48	0.46
1:C:906:PHE:HD1	1:C:1049:LEU:HD11	1.79	0.46
2:X:41:TYR:HE1	3:Y:120:TRP:HZ2	1.63	0.46
1:A:905:ARG:NH1	1:A:1050:MET:HG2	2.30	0.46
1:C:290:ASP:OD1	1:C:291:CYS:N	2.48	0.46
2:X:37:TYR:HD2	2:X:97:LEU:HA	1.80	0.46
2:E:111:ILE:HB	2:E:171:GLN:HE22	1.81	0.46
1:B:367:VAL:HA	1:B:371:SER:HB3	1.97	0.46
1:B:404:GLY:HA2	1:B:407:VAL:HG23	1.97	0.46
1:B:993:ILE:O	1:B:997:ILE:HG23	2.15	0.46
1:A:81:ASN:O	1:A:239:GLN:NE2	2.47	0.46
2:X:41:TYR:OH	3:Y:117:MET:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:29:PHE:CD2	3:F:77:ASN:HA	2.50	0.46
3:F:155:LEU:O	3:F:198:VAL:HA	2.15	0.46
1:B:546:LEU:HD21	1:B:573:THR:HG21	1.97	0.46
1:B:750:SER:O	1:B:754:LEU:HG	2.15	0.46
1:C:273:ARG:HD2	1:C:292:ALA:HB3	1.98	0.46
1:C:580:GLN:O	4:C:1303:NAG:H62	2.15	0.46
1:A:317:ASN:HB2	1:A:594:GLY:HA2	1.97	0.46
1:A:1093:GLY:H	1:A:1107:ARG:CZ	2.28	0.46
3:H:38:ARG:NH2	3:H:94:TYR:OH	2.36	0.46
1:B:318:PHE:HE2	1:B:615:VAL:HG11	1.80	0.46
1:B:375:SER:HB3	1:B:436:TRP:HA	1.97	0.46
1:C:326:ILE:HD11	1:C:534:VAL:HG12	1.98	0.46
1:B:291:CYS:HA	1:B:297:SER:OG	2.16	0.46
1:C:490:PHE:HE2	1:C:492:LEU:HD12	1.81	0.46
3:H:138:VAL:HB	3:H:224:VAL:HG11	1.97	0.46
1:A:501:ASN:HB3	1:A:505:TYR:HD2	1.79	0.46
1:A:898:PHE:N	1:A:899:PRO:HD2	2.31	0.46
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.98	0.46
1:A:195:LYS:HG3	1:A:202:LYS:HB2	1.97	0.46
2:L:151:VAL:HG22	2:L:201:VAL:HG22	1.98	0.46
3:H:18:LEU:HG	3:H:19:ARG:N	2.31	0.46
1:B:105:ILE:HG13	1:B:241:LEU:HD23	1.98	0.45
1:B:116:SER:OG	1:B:117:LEU:N	2.49	0.45
1:B:226:LEU:HB3	1:B:227:VAL:HG23	1.98	0.45
1:B:912:THR:HG22	1:B:914:ASN:H	1.82	0.45
1:B:968:SER:OG	1:B:969:ASN:N	2.49	0.45
1:A:122:ASN:HB2	1:A:125:ASN:HB2	1.97	0.45
1:A:376:THR:HG21	1:A:407:VAL:HG11	1.96	0.45
1:A:454:ARG:HD3	1:A:457:ARG:HB2	1.97	0.45
1:C:673:SER:HG	1:C:695:TYR:HE2	1.63	0.45
2:L:6:GLN:HG3	2:L:105:PRO:HG2	1.98	0.45
2:X:103:PHE:HE2	3:Y:47:TRP:H	1.64	0.45
3:F:159:VAL:O	3:F:194:SER:HA	2.16	0.45
1:B:616:ASN:OD1	1:B:618:THR:HG23	2.16	0.45
1:A:212:LEU:HD12	1:A:217:PRO:HG3	1.98	0.45
1:C:979:ASP:O	1:C:983:ARG:HG2	2.16	0.45
1:A:276:LEU:HB3	1:A:289:VAL:HG12	1.98	0.45
1:A:347:PHE:HB2	1:A:401:VAL:HG23	1.97	0.45
4:C:1304:NAG:O7	4:C:1304:NAG:O4	2.32	0.45
2:E:125:PRO:HB2	2:E:129:GLN:HB3	1.98	0.45
1:C:37:TYR:OH	1:C:195:LYS:NZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ASN:OD1	1:C:126:VAL:N	2.49	0.45
1:C:130:VAL:HG22	1:C:168:PHE:HB3	1.98	0.45
2:X:29:LEU:HA	2:X:97:LEU:HD22	1.98	0.45
2:X:136:SER:HB3	2:X:183:THR:HG23	1.98	0.45
3:Y:10:GLY:H	3:Y:126:VAL:HG22	1.81	0.45
1:B:368:LEU:HD22	1:B:434:ILE:HG21	1.99	0.45
1:C:453:TYR:CE2	1:C:455:LEU:HB3	2.51	0.45
2:L:122:ILE:HB	2:L:212:LYS:HG3	1.97	0.45
3:H:52:SER:N	3:H:56:GLY:O	2.40	0.45
3:H:90:ASP:HB2	3:H:128:VAL:HG21	1.99	0.45
2:X:70:SER:OG	2:X:77:THR:OG1	2.21	0.45
3:F:117:MET:O	3:F:120:TRP:NE1	2.50	0.45
1:A:568:ASP:OD1	1:A:569:ILE:HG12	2.16	0.45
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.49	0.45
2:L:140:LEU:HD21	2:L:142:ASN:HB2	1.99	0.45
3:Y:24:ALA:HB1	3:Y:27:PHE:HE1	1.81	0.45
3:Y:187:LEU:HD11	3:Y:191:GLY:HA2	1.98	0.45
2:E:67:PHE:HB3	2:E:78:LEU:HD11	1.97	0.45
1:C:355:ARG:HG2	1:C:355:ARG:NH1	2.31	0.45
1:C:912:THR:HG22	1:C:913:GLN:N	2.25	0.45
3:H:7:SER:OG	3:H:21:SER:HB3	2.16	0.45
1:B:294:ASP:N	1:B:294:ASP:OD1	2.49	0.45
1:A:366:SER:HA	1:A:369:TYR:HD2	1.81	0.45
3:H:212:ILE:HD13	3:H:212:ILE:HA	1.83	0.45
2:X:203:HIS:CD2	2:X:205:GLY:H	2.35	0.45
3:Y:171:TRP:NE1	3:Y:197:SER:OG	2.29	0.45
3:F:94:TYR:HB2	3:F:124:THR:HG22	1.99	0.45
1:B:394:ASN:OD1	1:B:395:VAL:N	2.50	0.45
1:A:97:LYS:HD3	1:A:186:PHE:N	2.32	0.45
1:A:1028:LYS:O	1:A:1032:CYS:HB3	2.17	0.45
1:C:1029:MET:HA	1:C:1033:VAL:HG23	1.98	0.45
2:X:19:ALA:HB2	2:X:83:VAL:HG21	1.97	0.45
1:B:86:PHE:O	1:B:86:PHE:CG	2.70	0.45
1:B:395:VAL:HG21	1:B:513:LEU:HB3	1.98	0.45
1:A:437:ASN:HA	1:A:508:TYR:CD1	2.52	0.45
1:C:44:ARG:HD3	1:C:47:VAL:HG11	1.99	0.45
1:C:109:THR:HG21	1:C:113:LYS:HD2	1.99	0.45
2:L:67:PHE:CE1	2:L:80:ILE:HD11	2.52	0.44
2:L:67:PHE:CD1	2:L:80:ILE:HD11	2.51	0.44
2:X:42:LEU:O	2:X:50:GLN:N	2.50	0.44
2:X:54:TYR:CE1	3:Y:116:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:91:THR:HA	3:Y:127:THR:HA	1.99	0.44
3:F:196:SER:OG	3:F:197:SER:N	2.50	0.44
1:B:68:ILE:HG22	1:B:69:HIS:ND1	2.32	0.44
1:B:904:TYR:OH	1:C:1094:VAL:HG22	2.17	0.44
1:A:131:CYS:SG	1:A:132:GLU:N	2.90	0.44
1:C:40:ASP:N	1:C:40:ASP:OD1	2.49	0.44
1:C:108:THR:HG22	1:C:236:THR:HG23	1.98	0.44
1:C:202:LYS:HD2	1:C:204:TYR:OH	2.16	0.44
1:C:405:ASP:O	1:C:408:ARG:HG3	2.17	0.44
2:X:85:ALA:HA	2:X:88:VAL:HG23	2.00	0.44
3:Y:3:GLN:O	3:Y:24:ALA:HA	2.17	0.44
3:F:29:PHE:HD2	3:F:74:ASN:HA	1.83	0.44
1:B:403:ARG:HB2	1:B:495:TYR:CE1	2.52	0.44
1:B:492:LEU:HD22	3:F:69:THR:HG21	2.00	0.44
1:C:818:ILE:O	1:C:821:LEU:N	2.50	0.44
1:C:1002:GLN:O	1:C:1006:THR:HG23	2.17	0.44
3:H:3:GLN:O	3:H:24:ALA:HA	2.17	0.44
1:A:854:LYS:HG2	1:A:855:PHE:CE1	2.52	0.44
2:X:66:ARG:NH2	2:X:84:GLU:OE2	2.32	0.44
2:E:85:ALA:HA	2:E:88:VAL:HG22	1.99	0.44
1:C:337:PRO:O	1:C:340:GLU:HG2	2.18	0.44
3:H:37:VAL:HG12	3:H:47:TRP:CD1	2.53	0.44
1:B:63:THR:HB	1:B:267:VAL:HG22	1.98	0.44
1:B:353:TRP:HB2	1:B:400:PHE:CG	2.52	0.44
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.66	0.44
1:A:196:ASN:HB3	1:A:201:PHE:CD1	2.53	0.44
1:A:453:TYR:CE1	1:A:493:GLN:HB3	2.52	0.44
1:C:426:PRO:HB3	1:C:463:PRO:HB3	2.00	0.44
2:X:94:MET:HG2	2:X:103:PHE:CD1	2.53	0.44
3:F:140:PRO:HB2	3:F:228:VAL:HG13	1.99	0.44
1:B:229:LEU:HD12	1:B:231:ILE:HD11	2.00	0.44
1:B:332:ILE:HG22	1:B:527:PRO:CG	2.48	0.44
1:B:412:PRO:HB3	1:B:427:ASP:HA	1.99	0.44
1:A:30:ASN:OD1	1:A:31:SER:N	2.50	0.44
1:C:424:LYS:HB2	1:C:461:LEU:HB2	1.99	0.44
1:C:1009:THR:O	1:C:1013:ILE:HG12	2.17	0.44
1:B:543:PHE:HD2	1:B:576:VAL:HG21	1.83	0.44
1:A:730:SER:O	1:A:1058:HIS:HB3	2.18	0.44
1:A:906:PHE:CE1	1:A:1049:LEU:HD11	2.52	0.44
1:C:119:ILE:HD12	1:C:128:ILE:HD12	1.99	0.44
2:L:94:MET:CE	2:L:101:PHE:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:133:THR:HA	3:Y:163:PHE:HB3	1.98	0.44
1:B:330:PRO:HD3	1:B:579:PRO:HB2	2.00	0.44
1:C:387:LEU:HA	1:C:390:LEU:HD13	1.98	0.44
2:X:1:ASP:HB3	2:X:100:PRO:HD2	2.00	0.44
3:F:39:GLN:HG3	3:F:45:LEU:HD12	1.99	0.44
1:B:30:ASN:HB3	1:B:32:PHE:CE2	2.52	0.43
1:B:348:ALA:HA	3:F:57:THR:HG22	1.99	0.43
1:A:1089:PHE:HE1	1:C:917:TYR:HD1	1.65	0.43
1:A:64:TRP:CD1	1:A:65:PHE:N	2.85	0.43
1:C:273:ARG:HD3	1:C:273:ARG:HA	1.80	0.43
1:C:1052:PHE:HD1	1:C:1063:LEU:HD11	1.83	0.43
3:H:154:ALA:HB2	3:H:200:THR:HG22	1.99	0.43
3:H:217:HIS:CE1	3:H:219:PRO:HD2	2.54	0.43
2:X:175:ASP:OD1	2:X:175:ASP:N	2.48	0.43
3:F:39:GLN:O	3:F:93:LEU:HB2	2.18	0.43
1:B:319:ARG:NH1	1:B:592:PHE:HB3	2.33	0.43
1:B:717:ASN:OD1	1:B:718:PHE:N	2.51	0.43
1:A:563:GLN:NE2	1:C:43:PHE:HA	2.33	0.43
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.73	0.43
1:A:996:LEU:HD21	1:A:1000:ARG:CZ	2.48	0.43
1:C:901:GLN:O	1:C:901:GLN:HG2	2.17	0.43
1:C:1082:CYS:HB2	1:C:1126:CYS:HB2	1.92	0.43
2:X:123:PHE:HZ	3:Y:154:ALA:HB3	1.82	0.43
3:F:58:ILE:HG13	3:F:59:GLY:N	2.32	0.43
1:B:457:ARG:HH11	1:B:459:SER:H	1.65	0.43
1:B:698:SER:OG	1:B:699:LEU:N	2.52	0.43
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.50	0.43
1:B:86:PHE:HB2	1:B:238:PHE:CD1	2.42	0.43
1:A:920:GLN:HA	1:A:923:ILE:HG22	2.00	0.43
1:C:34:ARG:NH2	1:C:218:GLN:O	2.48	0.43
1:C:364:ASP:OD1	1:C:365:TYR:N	2.51	0.43
1:C:616:ASN:OD1	4:C:1304:NAG:H62	2.19	0.43
2:L:164:SER:HB2	2:L:184:LEU:HA	1.99	0.43
3:H:37:VAL:HG12	3:H:47:TRP:HD1	1.83	0.43
2:E:94:MET:HE1	3:F:120:TRP:HH2	1.83	0.43
1:B:64:TRP:CD1	1:B:266:TYR:CE1	3.06	0.43
1:B:1094:VAL:HG23	1:B:1096:VAL:HG13	2.01	0.43
1:A:295:PRO:O	1:A:299:THR:HG23	2.18	0.43
1:A:714:ILE:HD11	1:A:1094:VAL:HG21	2.00	0.43
1:C:976:VAL:O	1:C:980:ILE:HG12	2.19	0.43
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ALA:HB3	1:A:414:GLN:HB2	2.01	0.43
1:C:962:LEU:HD11	1:C:1007:TYR:CD2	2.54	0.43
2:X:54:TYR:HB2	2:X:58:ASN:HB2	2.00	0.43
2:X:122:ILE:HG12	2:X:214:PHE:CE1	2.53	0.43
1:B:444:LYS:NZ	2:E:99:THR:H	2.17	0.43
1:B:552:LEU:HA	1:B:586:ASP:O	2.19	0.43
1:A:408:ARG:H	1:A:408:ARG:HD3	1.84	0.43
1:C:83:VAL:CG1	1:C:237:ARG:HE	2.32	0.43
1:C:421:TYR:HB3	1:C:454:ARG:O	2.19	0.43
1:C:790:LYS:HD2	1:C:790:LYS:HA	1.84	0.43
3:H:97:ALA:HA	3:H:119:VAL:O	2.18	0.43
1:A:226:LEU:HD23	1:A:227:VAL:HG23	2.01	0.43
1:A:317:ASN:ND2	1:A:593:GLY:H	2.10	0.43
1:A:664:ILE:O	1:A:671:CYS:HB2	2.19	0.43
2:L:38:LEU:HD12	2:L:94:MET:O	2.18	0.43
3:Y:9:GLY:HA3	3:Y:124:THR:OG1	2.19	0.43
3:Y:70:ILE:HD12	3:Y:70:ILE:HA	1.85	0.43
2:E:91:TYR:O	2:E:106:GLY:HA2	2.18	0.43
1:B:350:VAL:HG23	1:B:400:PHE:CE2	2.54	0.42
1:A:228:ASP:OD1	1:A:229:LEU:N	2.52	0.42
1:A:450:ASN:ND2	3:H:57:THR:O	2.51	0.42
1:A:944:ALA:O	1:A:945:LEU:HB2	2.19	0.42
1:C:422:ASN:ND2	1:C:454:ARG:O	2.52	0.42
2:L:41:TYR:HB2	2:L:92:TYR:HB2	2.01	0.42
3:H:12:VAL:HG21	3:H:126:VAL:HG13	2.01	0.42
3:H:40:ALA:HB1	3:H:43:LYS:HE3	2.01	0.42
3:H:99:ALA:HA	3:H:116:GLY:O	2.18	0.42
2:E:119:SER:HB3	2:E:121:PHE:HE2	1.84	0.42
3:F:71:SER:O	3:F:79:LEU:HD12	2.19	0.42
1:B:53:ASP:HB3	1:B:55:PHE:HE1	1.84	0.42
2:X:197:TYR:O	2:X:213:SER:HA	2.17	0.42
1:B:86:PHE:HD1	1:B:90:VAL:HG23	1.84	0.42
1:A:92:PHE:HE2	1:A:94:SER:HB2	1.84	0.42
1:A:779:GLN:OE1	1:A:865:LEU:HD21	2.19	0.42
3:H:155:LEU:HD23	3:H:155:LEU:H	1.84	0.42
1:A:541:PHE:CZ	1:A:587:ILE:HD13	2.54	0.42
1:C:455:LEU:HD23	1:C:455:LEU:H	1.84	0.42
3:Y:32:TYR:HB3	3:Y:98:LYS:HG2	2.01	0.42
2:E:148:GLU:O	2:E:204:GLN:NE2	2.37	0.42
3:F:16:ARG:NH2	3:F:18:LEU:HD21	2.34	0.42
3:F:49:SER:OG	3:F:50:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:62:ASP:OD1	3:F:63:SER:N	2.46	0.42
1:A:66:HIS:O	1:A:80:ASP:HB3	2.19	0.42
1:C:568:ASP:OD1	1:C:569:ILE:N	2.44	0.42
2:L:144:PHE:HE1	2:L:147:ARG:HA	1.83	0.42
2:L:164:SER:HB2	2:L:183:THR:O	2.19	0.42
2:X:197:TYR:OH	2:X:216:ARG:NH2	2.30	0.42
3:Y:79:LEU:C	3:Y:79:LEU:HD23	2.40	0.42
1:A:455:LEU:HD22	1:A:493:GLN:HB2	2.00	0.42
3:F:36:TRP:CE3	3:F:94:TYR:HB3	2.55	0.42
1:C:375:SER:H	1:C:436:TRP:HA	1.84	0.42
1:C:490:PHE:HE2	3:Y:69:THR:HG21	1.83	0.42
1:B:329:PHE:HB2	1:B:528:LYS:HB2	2.02	0.42
1:A:458:LYS:NZ	1:A:473:TYR:HA	2.33	0.42
3:H:192:LEU:HG	3:H:193:TYR:H	1.85	0.42
2:X:121:PHE:HB3	2:X:123:PHE:CZ	2.54	0.42
2:X:124:PRO:HB3	2:X:214:PHE:HE2	1.85	0.42
3:F:58:ILE:HD13	3:F:114:GLU:OE1	2.20	0.42
1:B:97:LYS:HG2	1:B:187:LYS:H	1.85	0.42
1:B:1028:LYS:O	1:B:1032:CYS:HB3	2.20	0.42
1:A:329:PHE:HE2	1:A:544:ASN:HA	1.85	0.42
1:C:102:ARG:HA	1:C:102:ARG:HD3	1.75	0.42
1:C:119:ILE:HG23	1:C:128:ILE:CD1	2.49	0.42
1:C:328:ARG:NH2	1:C:533:LEU:HB2	2.35	0.42
1:C:403:ARG:HG3	1:C:404:GLY:N	2.35	0.42
2:L:42:LEU:HD21	2:L:44:LYS:HE3	2.02	0.42
2:X:125:PRO:HG3	2:X:135:ALA:HB1	2.01	0.42
2:E:67:PHE:HB3	2:E:78:LEU:HD21	2.01	0.42
1:B:962:LEU:O	1:B:965:GLN:HB2	2.19	0.42
1:A:612:TYR:O	1:A:648:GLY:HA3	2.20	0.42
1:A:759:PHE:CD2	1:A:1001:LEU:HD21	2.55	0.42
1:C:922:LEU:O	1:C:926:GLN:HG3	2.20	0.42
2:L:44:LYS:NZ	2:L:86:GLU:O	2.26	0.42
1:A:666:ILE:HB	1:A:670:ILE:O	2.20	0.41
1:C:111:ASP:O	1:C:113:LYS:HG3	2.20	0.41
1:C:369:TYR:OH	1:C:387:LEU:HB3	2.20	0.41
1:C:643:PHE:CZ	1:C:655:HIS:HD2	2.37	0.41
1:C:898:PHE:N	1:C:899:PRO:HD2	2.34	0.41
2:L:6:GLN:NE2	2:L:106:GLY:H	2.18	0.41
2:L:112:LYS:HA	2:L:145:TYR:CE1	2.55	0.41
3:Y:14:PRO:HA	3:Y:86:LEU:HB2	2.01	0.41
2:E:155:VAL:O	2:E:158:ALA:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:VAL:HG11	1:C:237:ARG:HE	1.86	0.41
2:L:156:ASP:OD2	2:L:194:HIS:ND1	2.54	0.41
2:X:139:CYS:HB2	2:X:153:TRP:CH2	2.55	0.41
2:E:13:VAL:C	2:E:112:LYS:HB3	2.40	0.41
2:E:142:ASN:OD1	2:E:143:ASN:N	2.53	0.41
3:F:20:LEU:O	3:F:80:TYR:HA	2.19	0.41
1:B:111:ASP:O	1:B:113:LYS:HD2	2.20	0.41
1:B:326:ILE:HD13	1:B:326:ILE:HA	1.97	0.41
1:B:339:GLY:HA2	1:B:343:ASN:O	2.19	0.41
1:B:811:LYS:CD	1:B:812:PRO:HD2	2.47	0.41
1:B:1088:HIS:CE1	1:B:1122:VAL:HG22	2.55	0.41
1:A:560:LEU:HD23	1:A:560:LEU:HA	1.87	0.41
1:A:748:GLU:H	1:A:748:GLU:CD	2.22	0.41
1:A:977:LEU:HA	1:A:980:ILE:HD13	2.02	0.41
1:C:382:VAL:HG22	1:C:383:SER:H	1.85	0.41
1:C:401:VAL:HG22	1:C:509:ARG:HA	2.02	0.41
1:C:416:GLY:N	1:C:419:ALA:HB3	2.35	0.41
1:C:868:GLU:O	1:C:872:GLN:HG3	2.21	0.41
3:F:136:PRO:HB3	3:F:162:TYR:HB2	2.01	0.41
3:F:167:VAL:HA	3:F:216:ASN:O	2.19	0.41
1:B:347:PHE:HD2	1:B:509:ARG:HD3	1.84	0.41
1:B:898:PHE:N	1:B:899:PRO:HD2	2.35	0.41
1:C:906:PHE:O	1:C:909:ILE:HG22	2.20	0.41
3:H:213:CYS:O	3:H:225:ASP:HA	2.19	0.41
2:E:36:ASN:HB3	2:E:76:PHE:CE2	2.54	0.41
2:E:110:ASP:N	2:E:110:ASP:OD1	2.53	0.41
3:F:165:GLU:HB2	3:F:193:TYR:HD2	1.85	0.41
1:B:705:VAL:O	1:B:707:TYR:N	2.51	0.41
1:A:1094:VAL:HG13	1:A:1107:ARG:HG2	2.02	0.41
3:Y:38:ARG:HG2	3:Y:48:VAL:HB	2.01	0.41
2:E:92:TYR:CE2	3:F:44:GLY:HA3	2.55	0.41
3:F:51:VAL:HG11	3:F:79:LEU:HD13	2.02	0.41
1:A:190:ARG:HB3	1:A:192:PHE:CZ	2.56	0.41
1:A:309:GLU:OE2	1:A:309:GLU:N	2.53	0.41
1:A:963:VAL:O	1:A:966:LEU:HB2	2.19	0.41
1:C:538:CYS:HB2	1:C:590:CYS:HB3	1.67	0.41
2:L:59:ARG:NE	2:L:67:PHE:O	2.52	0.41
2:L:149:ALA:HB2	2:L:203:HIS:ND1	2.36	0.41
2:L:169:THR:HG23	3:H:183:PHE:CD1	2.55	0.41
2:X:97:LEU:HA	2:X:97:LEU:HD12	1.92	0.41
3:Y:4:LEU:HD11	3:Y:22:CYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:60:TYR:N	3:Y:65:LYS:HE2	2.35	0.41
3:Y:64:VAL:HG21	3:Y:68:PHE:CE1	2.56	0.41
3:F:57:THR:OG1	3:F:70:ILE:HG21	2.20	0.41
1:B:130:VAL:CG2	1:B:168:PHE:HB3	2.51	0.41
1:B:733:LYS:HE3	1:B:771:ALA:HB1	2.01	0.41
1:A:380:TYR:CE2	1:A:412:PRO:HD3	2.56	0.41
1:C:879:ALA:O	1:C:883:THR:OG1	2.32	0.41
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	2.02	0.41
3:H:86:LEU:HB3	3:H:128:VAL:HG11	2.02	0.41
2:X:6:GLN:HB2	2:X:105:PRO:HG2	2.02	0.41
2:E:124:PRO:HB2	2:E:218:GLU:H	1.86	0.41
3:F:48:VAL:HG11	3:F:81:LEU:HD21	2.02	0.41
3:F:159:VAL:HG21	3:F:167:VAL:HG21	2.02	0.41
1:B:97:LYS:HD3	1:B:186:PHE:HA	2.01	0.41
1:A:328:ARG:NH1	1:A:580:GLN:HB2	2.36	0.41
1:C:212:LEU:HD12	1:C:213:VAL:H	1.85	0.41
1:C:377:PHE:HD1	1:C:434:ILE:HG12	1.86	0.41
1:C:443:SER:OG	1:C:497:PHE:HB3	2.21	0.41
2:L:39:ASP:O	2:L:93:CYS:HA	2.21	0.41
2:X:122:ILE:HG22	2:X:212:LYS:HE3	2.02	0.41
2:E:49:PRO:HG3	3:F:45:LEU:HD21	2.02	0.41
1:B:347:PHE:H	1:B:509:ARG:NH1	2.16	0.41
1:B:359:SER:HA	1:B:524:VAL:HG11	2.03	0.41
1:B:454:ARG:HH21	1:B:492:LEU:HD21	1.86	0.41
1:A:36:VAL:HG21	1:A:220:PHE:CZ	2.56	0.41
1:A:195:LYS:HE3	1:A:202:LYS:HD2	2.02	0.41
1:C:458:LYS:HG2	1:C:473:TYR:OH	2.21	0.41
2:L:141:LEU:HD11	2:L:201:VAL:HG21	2.03	0.41
3:H:27:PHE:CD2	3:H:98:LYS:HE3	2.55	0.41
2:X:12:PRO:C	2:X:112:LYS:HB2	2.41	0.41
2:X:128:GLU:HG2	2:X:131:LYS:HE2	2.02	0.41
3:Y:203:SER:O	3:Y:206:LEU:HG	2.21	0.41
2:E:107:THR:HG22	2:E:109:VAL:HG23	2.02	0.41
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.54	0.41
1:B:319:ARG:NH2	1:B:592:PHE:HB3	2.36	0.41
1:B:770:ILE:O	1:B:774:GLN:HG2	2.20	0.41
1:A:498:GLN:N	1:A:501:ASN:OD1	2.52	0.41
1:A:674:TYR:CE1	1:A:690:GLN:HG2	2.56	0.41
1:A:914:ASN:OD1	1:A:915:VAL:N	2.54	0.41
2:L:12:PRO:HB2	2:L:112:LYS:HD3	2.03	0.41
2:L:199:CYS:O	2:L:212:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:ALA:HB3	3:H:99:ALA:HB2	2.03	0.41
3:H:93:LEU:HG	3:H:125:THR:HA	2.03	0.41
3:H:160:LYS:HG2	3:H:194:SER:HB2	2.03	0.41
3:Y:69:THR:OG1	3:Y:82:HIS:HB3	2.21	0.41
3:F:53:TRP:HE1	3:F:113:PRO:HD2	1.85	0.41
1:B:403:ARG:CZ	1:B:417:LYS:HE2	2.52	0.40
1:C:216:LEU:HA	1:C:217:PRO:HD3	1.91	0.40
1:C:866:THR:O	1:C:870:ILE:HG12	2.21	0.40
2:X:4:MET:HA	2:X:24:ARG:O	2.21	0.40
1:B:32:PHE:CD1	1:B:218:GLN:HB2	2.56	0.40
1:B:383:SER:H	1:B:386:LYS:HD3	1.87	0.40
1:B:711:SER:O	1:A:897:PRO:HD3	2.21	0.40
1:A:379:CYS:HA	1:A:432:CYS:HA	2.03	0.40
3:H:85:SER:O	3:H:85:SER:OG	2.35	0.40
2:X:95:GLN:HE21	2:X:102:THR:H	1.70	0.40
3:Y:39:GLN:O	3:Y:93:LEU:N	2.52	0.40
2:E:95:GLN:HG3	2:E:101:PHE:HD1	1.85	0.40
3:F:36:TRP:CE2	3:F:81:LEU:HB2	2.56	0.40
1:B:193:VAL:CG2	1:B:204:TYR:HB2	2.46	0.40
1:B:899:PRO:HB3	1:B:920:GLN:NE2	2.36	0.40
1:B:1129:VAL:HG23	1:B:1132:ILE:HB	2.03	0.40
1:A:736:VAL:HG23	1:A:858:LEU:HG	2.02	0.40
1:C:674:TYR:HD1	1:C:692:ILE:HG12	1.86	0.40
3:H:37:VAL:HG23	3:H:95:TYR:HB2	2.03	0.40
3:H:91:THR:HG22	3:H:128:VAL:H	1.86	0.40
2:X:138:VAL:HG12	2:X:140:LEU:HG	2.03	0.40
2:X:152:GLN:CG	2:X:200:GLU:HB2	2.51	0.40
2:E:84:GLU:O	2:E:88:VAL:HG13	2.21	0.40
1:C:484:GLU:HB2	1:C:488:CYS:O	2.21	0.40
3:H:29:PHE:CD2	3:H:77:ASN:HA	2.57	0.40
3:H:58:ILE:H	3:H:58:ILE:HD12	1.86	0.40
2:X:91:TYR:HE2	2:X:109:VAL:HB	1.86	0.40
2:X:123:PHE:CE2	2:X:140:LEU:HD12	2.52	0.40
3:Y:76:LYS:HD3	3:Y:76:LYS:O	2.21	0.40
1:B:318:PHE:CE2	1:B:615:VAL:HG11	2.57	0.40
1:B:917:TYR:HD1	1:C:1089:PHE:HE2	1.69	0.40
1:A:440:ASN:OD1	1:A:440:ASN:N	2.51	0.40
1:A:993:ILE:O	1:A:997:ILE:HG12	2.22	0.40
1:C:672:ALA:HA	1:C:694:ALA:HA	2.03	0.40
3:F:20:LEU:HD13	3:F:124:THR:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	986/1288 (77%)	938 (95%)	48 (5%)	0	100	100
1	B	986/1288 (77%)	912 (92%)	74 (8%)	0	100	100
1	C	986/1288 (77%)	925 (94%)	61 (6%)	0	100	100
2	E	216/219 (99%)	206 (95%)	10 (5%)	0	100	100
2	L	216/219 (99%)	200 (93%)	16 (7%)	0	100	100
2	X	216/219 (99%)	201 (93%)	15 (7%)	0	100	100
3	F	220/237 (93%)	193 (88%)	27 (12%)	0	100	100
3	H	220/237 (93%)	212 (96%)	8 (4%)	0	100	100
3	Y	220/237 (93%)	206 (94%)	14 (6%)	0	100	100
All	All	4266/5232 (82%)	3993 (94%)	273 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	879/1116 (79%)	877 (100%)	2 (0%)	92	96
1	B	879/1116 (79%)	874 (99%)	5 (1%)	84	90
1	C	879/1116 (79%)	877 (100%)	2 (0%)	92	96
2	E	192/193 (100%)	191 (100%)	1 (0%)	86	92
2	L	192/193 (100%)	191 (100%)	1 (0%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	192/193 (100%)	190 (99%)	2 (1%)	73	82
3	F	181/195 (93%)	180 (99%)	1 (1%)	84	90
3	H	181/195 (93%)	180 (99%)	1 (1%)	84	90
3	Y	181/195 (93%)	179 (99%)	2 (1%)	70	81
All	All	3756/4512 (83%)	3739 (100%)	17 (0%)	85	92

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	517	LEU
1	B	524	VAL
1	B	558	LYS
1	B	660	TYR
1	B	1106	GLN
1	A	408	ARG
1	A	902	MET
1	C	338	PHE
1	C	902	MET
2	L	24	ARG
3	H	213	CYS
2	X	24	ARG
2	X	114	THR
3	Y	87	ARG
3	Y	134	LYS
2	E	195	LYS
3	F	226	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	804	GLN
1	B	1048	HIS
1	C	655	HIS
3	H	13	GLN
2	E	152	GLN

5.3.3 RNA ⓘ

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](#)

27 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	B	1307	1	14,14,15	1.86	4 (28%)	17,19,21	1.20	2 (11%)
4	NAG	B	1303	1	14,14,15	1.88	3 (21%)	17,19,21	1.17	2 (11%)
4	NAG	B	1309	1	14,14,15	1.91	4 (28%)	17,19,21	1.19	1 (5%)
4	NAG	C	1301	1	14,14,15	1.87	4 (28%)	17,19,21	1.20	2 (11%)
4	NAG	C	1308	1	14,14,15	1.99	4 (28%)	17,19,21	1.30	3 (17%)
4	NAG	C	1307	1	14,14,15	1.94	4 (28%)	17,19,21	1.79	6 (35%)
4	NAG	C	1303	1	14,14,15	1.91	4 (28%)	17,19,21	1.29	2 (11%)
4	NAG	B	1306	1	14,14,15	1.88	4 (28%)	17,19,21	1.29	3 (17%)
4	NAG	A	1301	1	14,14,15	1.94	4 (28%)	17,19,21	1.23	2 (11%)
4	NAG	C	1302	1	14,14,15	1.93	4 (28%)	17,19,21	1.13	1 (5%)
4	NAG	C	1304	1	14,14,15	2.09	4 (28%)	17,19,21	2.13	4 (23%)
4	NAG	A	1303	1	14,14,15	1.94	4 (28%)	17,19,21	1.18	3 (17%)
4	NAG	A	1304	1	14,14,15	2.04	4 (28%)	17,19,21	1.16	1 (5%)
4	NAG	B	1308	1	14,14,15	1.91	4 (28%)	17,19,21	1.10	1 (5%)
4	NAG	A	1302	1	14,14,15	1.98	4 (28%)	17,19,21	1.13	1 (5%)
4	NAG	A	1305	1	14,14,15	1.98	4 (28%)	17,19,21	1.93	5 (29%)
4	NAG	A	1307	1	14,14,15	1.86	3 (21%)	17,19,21	1.15	2 (11%)
4	NAG	C	1306	1	14,14,15	1.89	4 (28%)	17,19,21	1.13	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1304	1	14,14,15	1.97	4 (28%)	17,19,21	1.13	1 (5%)
4	NAG	B	1305	1	14,14,15	1.89	4 (28%)	17,19,21	1.25	2 (11%)
4	NAG	A	1306	1	14,14,15	1.92	4 (28%)	17,19,21	1.25	3 (17%)
4	NAG	C	1305	1	14,14,15	1.89	4 (28%)	17,19,21	1.11	2 (11%)
4	NAG	A	1308	1	14,14,15	1.89	4 (28%)	17,19,21	1.12	2 (11%)
4	NAG	C	1309	1	14,14,15	2.05	4 (28%)	17,19,21	1.70	3 (17%)
4	NAG	A	1309	1	14,14,15	1.90	4 (28%)	17,19,21	1.41	3 (17%)
4	NAG	B	1302	1	14,14,15	1.97	4 (28%)	17,19,21	1.49	4 (23%)
4	NAG	B	1301	1	14,14,15	1.92	4 (28%)	17,19,21	1.17	1 (5%)

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	B	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	3/6/23/26	0/1/1/1

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1304	NAG	O5-C1	5.02	1.51	1.43
4	C	1308	NAG	O5-C1	4.76	1.51	1.43
4	A	1304	NAG	O5-C1	4.73	1.51	1.43
4	C	1309	NAG	O5-C1	4.72	1.51	1.43
4	C	1307	NAG	O5-C1	4.72	1.51	1.43
4	A	1302	NAG	O5-C1	4.66	1.51	1.43
4	A	1301	NAG	O5-C1	4.65	1.51	1.43
4	B	1302	NAG	O5-C1	4.57	1.51	1.43
4	C	1302	NAG	O5-C1	4.51	1.50	1.43
4	A	1303	NAG	O5-C1	4.51	1.50	1.43
4	A	1306	NAG	O5-C1	4.49	1.50	1.43
4	B	1309	NAG	O5-C1	4.48	1.50	1.43
4	B	1308	NAG	O5-C1	4.47	1.50	1.43
4	B	1305	NAG	O5-C1	4.45	1.50	1.43
4	C	1303	NAG	O5-C1	4.42	1.50	1.43
4	B	1303	NAG	O5-C1	4.42	1.50	1.43
4	C	1305	NAG	O5-C1	4.42	1.50	1.43
4	A	1308	NAG	O5-C1	4.39	1.50	1.43
4	C	1306	NAG	O5-C1	4.38	1.50	1.43
4	C	1301	NAG	O5-C1	4.34	1.50	1.43
4	A	1307	NAG	O5-C1	4.32	1.50	1.43
4	B	1304	NAG	O5-C1	4.32	1.50	1.43
4	B	1307	NAG	O5-C1	4.31	1.50	1.43
4	B	1301	NAG	O5-C1	4.29	1.50	1.43
4	A	1305	NAG	O5-C1	4.28	1.50	1.43
4	B	1306	NAG	O5-C1	4.26	1.50	1.43
4	A	1309	NAG	O5-C1	4.23	1.50	1.43
4	A	1305	NAG	C7-N2	3.53	1.46	1.34
4	C	1304	NAG	C7-N2	3.42	1.46	1.34
4	A	1304	NAG	C7-N2	3.41	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1304	NAG	C7-N2	3.40	1.46	1.34
4	B	1301	NAG	C7-N2	3.40	1.46	1.34
4	C	1309	NAG	C7-N2	3.38	1.46	1.34
4	A	1302	NAG	C7-N2	3.38	1.46	1.34
4	A	1303	NAG	C7-N2	3.33	1.45	1.34
4	C	1303	NAG	C7-N2	3.31	1.45	1.34
4	B	1306	NAG	C7-N2	3.30	1.45	1.34
4	A	1309	NAG	C7-N2	3.30	1.45	1.34
4	C	1302	NAG	C7-N2	3.29	1.45	1.34
4	C	1308	NAG	C7-N2	3.29	1.45	1.34
4	C	1301	NAG	C7-N2	3.28	1.45	1.34
4	A	1308	NAG	C7-N2	3.28	1.45	1.34
4	B	1308	NAG	C7-N2	3.28	1.45	1.34
4	B	1307	NAG	C7-N2	3.28	1.45	1.34
4	B	1309	NAG	C7-N2	3.28	1.45	1.34
4	C	1305	NAG	C7-N2	3.26	1.45	1.34
4	C	1307	NAG	C7-N2	3.26	1.45	1.34
4	B	1302	NAG	C7-N2	3.26	1.45	1.34
4	B	1305	NAG	C7-N2	3.26	1.45	1.34
4	A	1306	NAG	C7-N2	3.26	1.45	1.34
4	A	1301	NAG	C7-N2	3.25	1.45	1.34
4	C	1306	NAG	C7-N2	3.25	1.45	1.34
4	A	1307	NAG	C7-N2	3.23	1.45	1.34
4	B	1303	NAG	C7-N2	3.21	1.45	1.34
4	C	1309	NAG	O5-C5	2.72	1.49	1.43
4	A	1305	NAG	C2-N2	2.70	1.50	1.46
4	C	1304	NAG	C2-N2	2.68	1.50	1.46
4	B	1302	NAG	O5-C5	2.65	1.48	1.43
4	A	1304	NAG	C2-N2	2.54	1.50	1.46
4	B	1304	NAG	O5-C5	2.49	1.48	1.43
4	C	1308	NAG	O5-C5	2.48	1.48	1.43
4	A	1304	NAG	O5-C5	2.47	1.48	1.43
4	C	1309	NAG	C2-N2	2.46	1.50	1.46
4	B	1304	NAG	C2-N2	2.44	1.50	1.46
4	B	1301	NAG	C2-N2	2.42	1.50	1.46
4	A	1309	NAG	O5-C5	2.40	1.48	1.43
4	A	1305	NAG	O5-C5	2.33	1.48	1.43
4	B	1301	NAG	O5-C5	2.32	1.48	1.43
4	C	1304	NAG	O5-C5	2.32	1.48	1.43
4	C	1303	NAG	C2-N2	2.27	1.50	1.46
4	B	1306	NAG	O5-C5	2.24	1.48	1.43
4	B	1309	NAG	O5-C5	2.24	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1302	NAG	C2-N2	2.23	1.50	1.46
4	A	1303	NAG	C2-N2	2.23	1.50	1.46
4	C	1306	NAG	O5-C5	2.21	1.47	1.43
4	A	1302	NAG	O5-C5	2.21	1.47	1.43
4	B	1308	NAG	O5-C5	2.20	1.47	1.43
4	C	1302	NAG	O5-C5	2.19	1.47	1.43
4	C	1307	NAG	C2-N2	2.19	1.50	1.46
4	A	1303	NAG	O5-C5	2.19	1.47	1.43
4	C	1305	NAG	O5-C5	2.18	1.47	1.43
4	A	1301	NAG	O5-C5	2.16	1.47	1.43
4	C	1308	NAG	C2-N2	2.15	1.50	1.46
4	A	1308	NAG	O5-C5	2.13	1.47	1.43
4	A	1306	NAG	O5-C5	2.13	1.47	1.43
4	C	1302	NAG	C2-N2	2.12	1.49	1.46
4	C	1301	NAG	O5-C5	2.12	1.47	1.43
4	B	1303	NAG	O5-C5	2.11	1.47	1.43
4	A	1307	NAG	O5-C5	2.11	1.47	1.43
4	B	1307	NAG	C2-N2	2.11	1.49	1.46
4	A	1306	NAG	C2-N2	2.11	1.49	1.46
4	C	1307	NAG	O5-C5	2.09	1.47	1.43
4	B	1302	NAG	C2-N2	2.09	1.49	1.46
4	A	1301	NAG	C2-N2	2.08	1.49	1.46
4	B	1308	NAG	C2-N2	2.08	1.49	1.46
4	B	1305	NAG	C2-N2	2.07	1.49	1.46
4	C	1303	NAG	O5-C5	2.06	1.47	1.43
4	B	1306	NAG	C2-N2	2.06	1.49	1.46
4	A	1308	NAG	C2-N2	2.06	1.49	1.46
4	B	1307	NAG	O5-C5	2.06	1.47	1.43
4	C	1301	NAG	C2-N2	2.05	1.49	1.46
4	C	1305	NAG	C2-N2	2.05	1.49	1.46
4	A	1309	NAG	C2-N2	2.05	1.49	1.46
4	B	1309	NAG	C2-N2	2.04	1.49	1.46
4	C	1306	NAG	C2-N2	2.02	1.49	1.46
4	B	1305	NAG	O5-C5	2.01	1.47	1.43

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1305	NAG	C8-C7-N2	4.97	124.51	116.10
4	C	1304	NAG	C1-O5-C5	4.92	118.86	112.19
4	C	1309	NAG	C1-O5-C5	4.61	118.44	112.19
4	A	1305	NAG	C2-N2-C7	3.90	128.46	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1304	NAG	C4-C3-C2	3.81	116.61	111.02
4	C	1304	NAG	O5-C1-C2	3.80	117.30	111.29
4	C	1307	NAG	C4-C3-C2	3.14	115.61	111.02
4	A	1302	NAG	C8-C7-N2	3.04	121.25	116.10
4	A	1309	NAG	C2-N2-C7	-2.96	118.69	122.90
4	B	1302	NAG	C1-O5-C5	2.89	116.11	112.19
4	C	1307	NAG	O5-C1-C2	2.87	115.82	111.29
4	C	1307	NAG	C2-N2-C7	-2.85	118.84	122.90
4	A	1304	NAG	C1-O5-C5	2.80	115.98	112.19
4	C	1309	NAG	C3-C4-C5	2.75	115.14	110.24
4	C	1304	NAG	C3-C4-C5	2.74	115.12	110.24
4	C	1308	NAG	C1-O5-C5	2.69	115.84	112.19
4	A	1307	NAG	C2-N2-C7	-2.66	119.11	122.90
4	B	1309	NAG	C8-C7-N2	2.63	120.55	116.10
4	C	1306	NAG	C2-N2-C7	-2.59	119.22	122.90
4	A	1306	NAG	C2-N2-C7	-2.58	119.22	122.90
4	B	1306	NAG	C2-N2-C7	-2.53	119.30	122.90
4	C	1307	NAG	C3-C4-C5	2.52	114.74	110.24
4	A	1303	NAG	C8-C7-N2	2.49	120.31	116.10
4	B	1302	NAG	C3-C4-C5	2.46	114.62	110.24
4	A	1301	NAG	C8-C7-N2	2.44	120.23	116.10
4	C	1302	NAG	C8-C7-N2	2.44	120.23	116.10
4	C	1305	NAG	C2-N2-C7	-2.44	119.43	122.90
4	A	1309	NAG	C8-C7-N2	2.43	120.22	116.10
4	C	1306	NAG	C8-C7-N2	2.43	120.22	116.10
4	A	1306	NAG	C8-C7-N2	2.43	120.22	116.10
4	C	1308	NAG	O5-C5-C6	2.40	110.97	107.20
4	A	1308	NAG	C2-N2-C7	-2.40	119.49	122.90
4	B	1308	NAG	C8-C7-N2	2.39	120.15	116.10
4	C	1307	NAG	C8-C7-N2	2.38	120.14	116.10
4	B	1303	NAG	C2-N2-C7	-2.38	119.51	122.90
4	A	1305	NAG	O7-C7-N2	-2.37	117.60	121.95
4	C	1309	NAG	O5-C5-C4	2.36	116.57	110.83
4	A	1308	NAG	C8-C7-N2	2.36	120.09	116.10
4	B	1307	NAG	C8-C7-N2	2.35	120.09	116.10
4	C	1301	NAG	C2-N2-C7	-2.34	119.57	122.90
4	C	1305	NAG	C8-C7-N2	2.32	120.03	116.10
4	C	1301	NAG	C8-C7-N2	2.32	120.02	116.10
4	B	1302	NAG	C8-C7-N2	2.31	120.01	116.10
4	C	1307	NAG	C1-O5-C5	2.31	115.32	112.19
4	B	1306	NAG	C8-C7-N2	2.28	119.95	116.10
4	A	1303	NAG	C2-N2-C7	-2.27	119.67	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1303	NAG	C8-C7-N2	2.27	119.94	116.10
4	A	1305	NAG	O7-C7-C8	-2.24	117.89	122.06
4	B	1303	NAG	C8-C7-N2	2.23	119.87	116.10
4	A	1307	NAG	C8-C7-N2	2.22	119.85	116.10
4	C	1303	NAG	O5-C5-C6	2.21	110.67	107.20
4	B	1305	NAG	C8-C7-N2	2.21	119.84	116.10
4	B	1301	NAG	C3-C4-C5	2.19	114.15	110.24
4	B	1304	NAG	C6-C5-C4	-2.13	108.00	113.00
4	A	1309	NAG	C3-C4-C5	2.12	114.02	110.24
4	B	1307	NAG	C2-N2-C7	-2.12	119.89	122.90
4	B	1302	NAG	C2-N2-C7	-2.10	119.91	122.90
4	C	1308	NAG	C8-C7-N2	2.08	119.62	116.10
4	A	1301	NAG	C6-C5-C4	-2.08	108.14	113.00
4	B	1305	NAG	C6-C5-C4	-2.07	108.15	113.00
4	B	1306	NAG	C6-C5-C4	-2.05	108.20	113.00
4	A	1306	NAG	C6-C5-C4	-2.01	108.29	113.00
4	A	1305	NAG	C6-C5-C4	-2.00	108.31	113.00
4	A	1303	NAG	C6-C5-C4	-2.00	108.32	113.00

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1309	NAG	C4-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1307	NAG	C4-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	B	1306	NAG	C8-C7-N2-C2
4	B	1306	NAG	O7-C7-N2-C2
4	B	1307	NAG	C8-C7-N2-C2
4	B	1307	NAG	O7-C7-N2-C2
4	B	1308	NAG	C8-C7-N2-C2
4	B	1308	NAG	O7-C7-N2-C2
4	B	1309	NAG	C8-C7-N2-C2
4	B	1309	NAG	O7-C7-N2-C2
4	A	1301	NAG	C8-C7-N2-C2
4	A	1301	NAG	O7-C7-N2-C2
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	A	1305	NAG	C8-C7-N2-C2
4	A	1305	NAG	O7-C7-N2-C2
4	C	1302	NAG	C8-C7-N2-C2
4	C	1302	NAG	O7-C7-N2-C2
4	A	1306	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	A	1309	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	A	1305	NAG	C3-C2-N2-C7
4	C	1309	NAG	C3-C2-N2-C7
4	A	1302	NAG	C4-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	B	1301	NAG	C3-C2-N2-C7
4	B	1304	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	A	1304	NAG	C3-C2-N2-C7
4	C	1308	NAG	C4-C5-C6-O6
4	B	1301	NAG	C1-C2-N2-C7
4	B	1304	NAG	C1-C2-N2-C7
4	C	1304	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1303	NAG	1	0
4	C	1304	NAG	2	0
4	B	1305	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

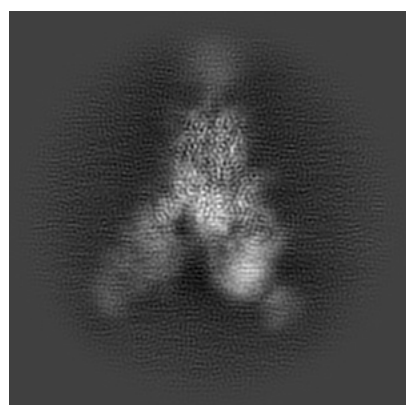
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31036. These allow visual inspection of the internal detail of the map and identification of artifacts.

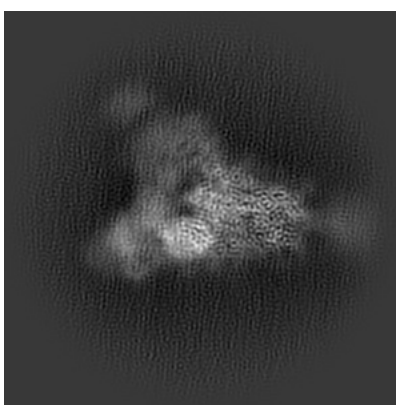
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

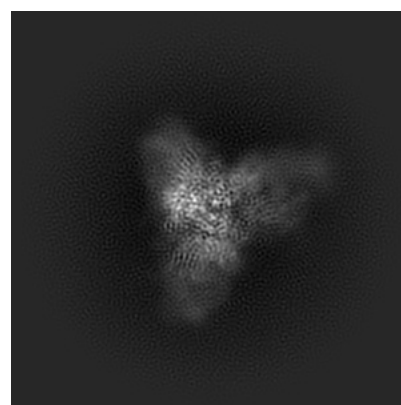
6.1.1 Primary map



X



Y

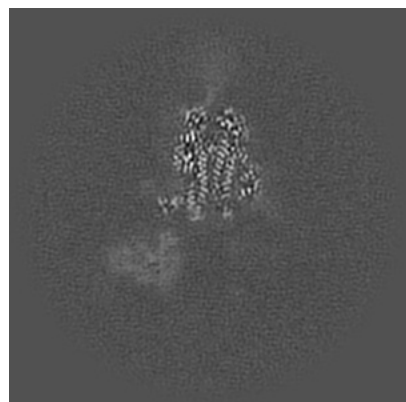


Z

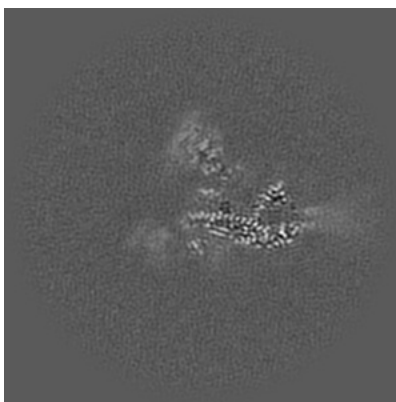
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

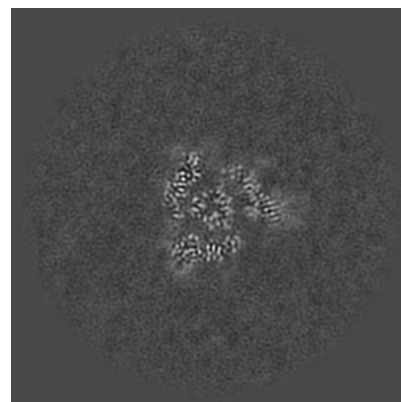
6.2.1 Primary map



X Index: 165



Y Index: 165

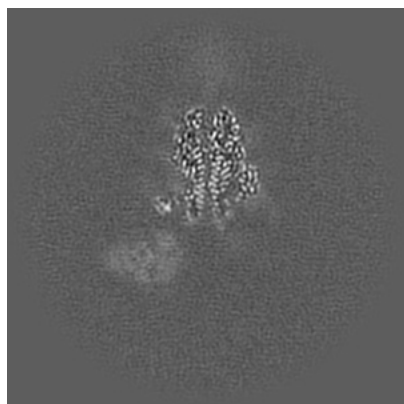


Z Index: 165

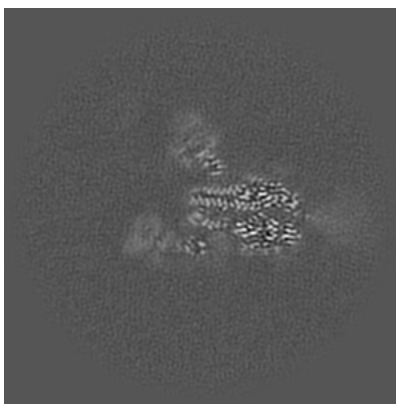
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

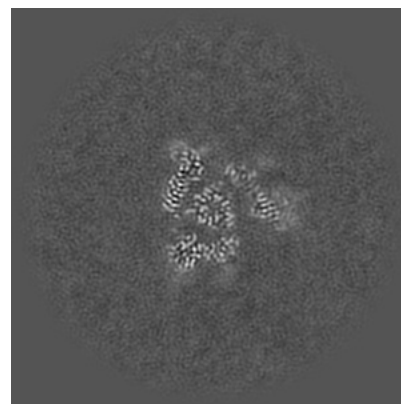
6.3.1 Primary map



X Index: 167



Y Index: 172

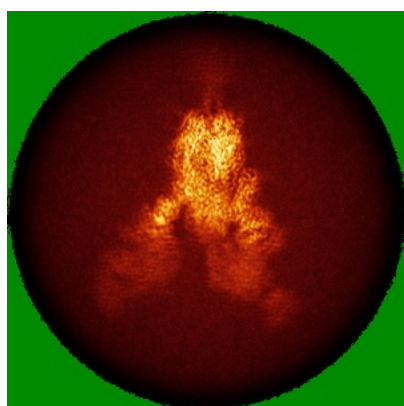


Z Index: 162

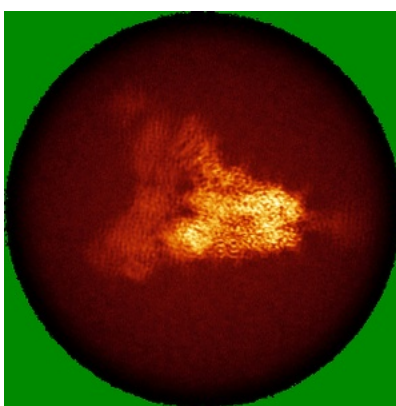
The images above show the largest variance slices of the map in three orthogonal directions.

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

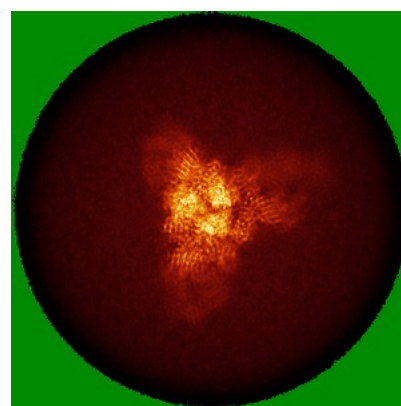
6.4.1 Primary map



X



Y

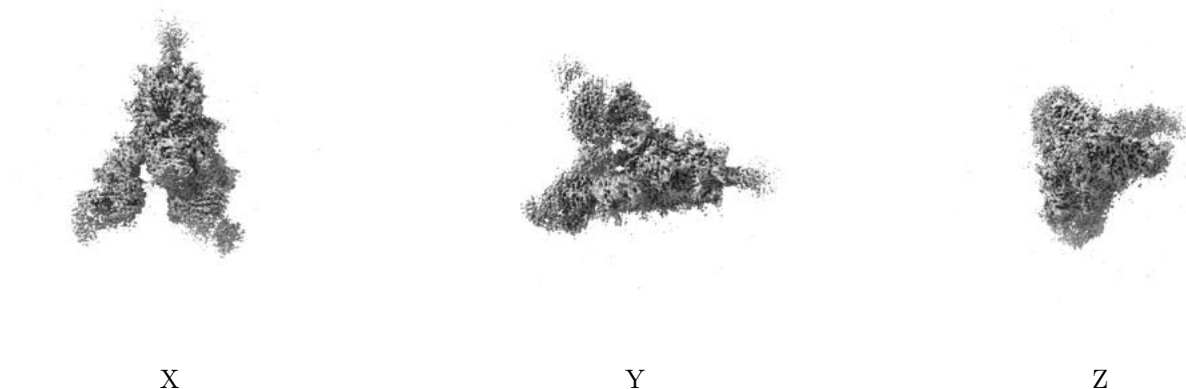


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

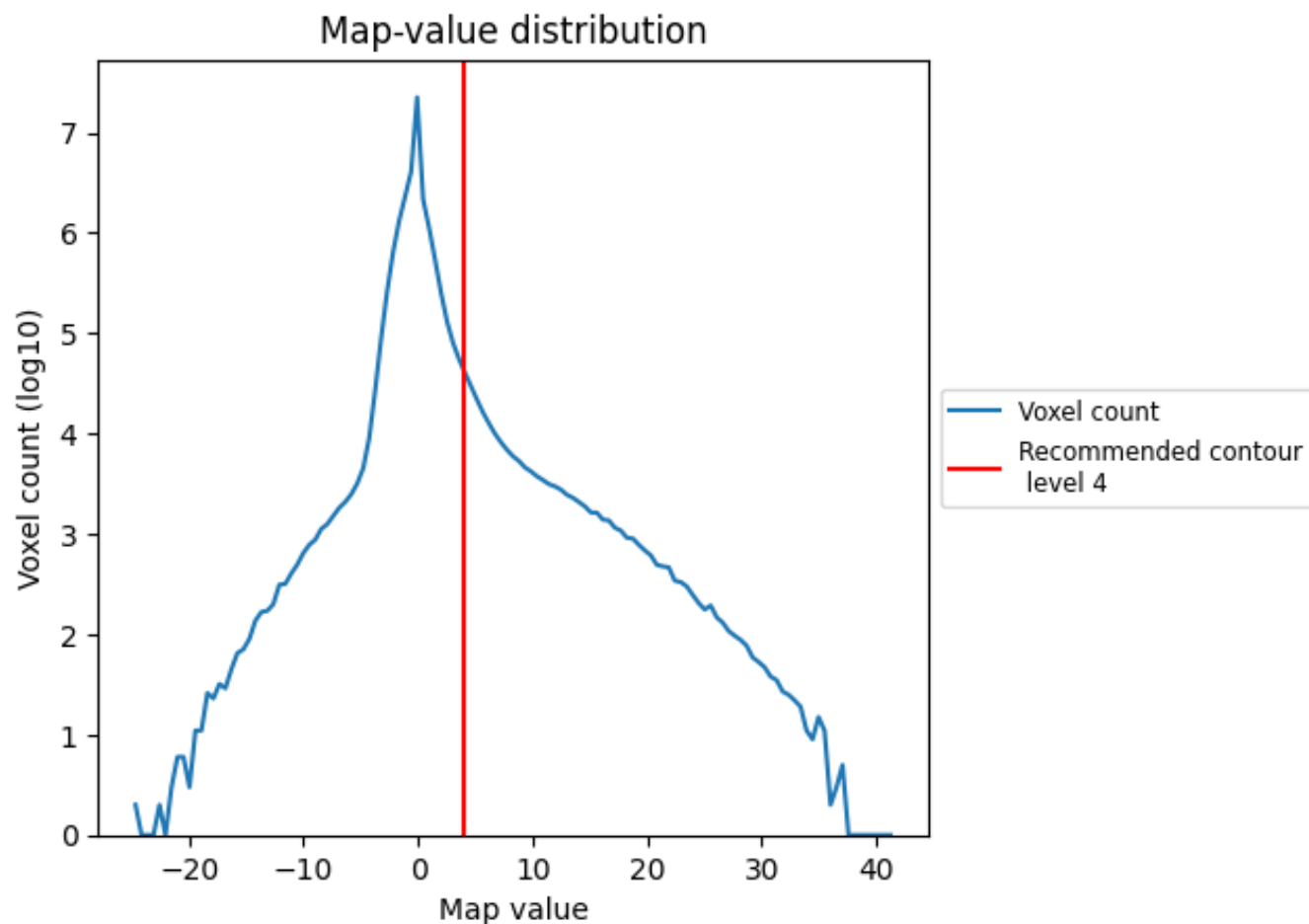
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

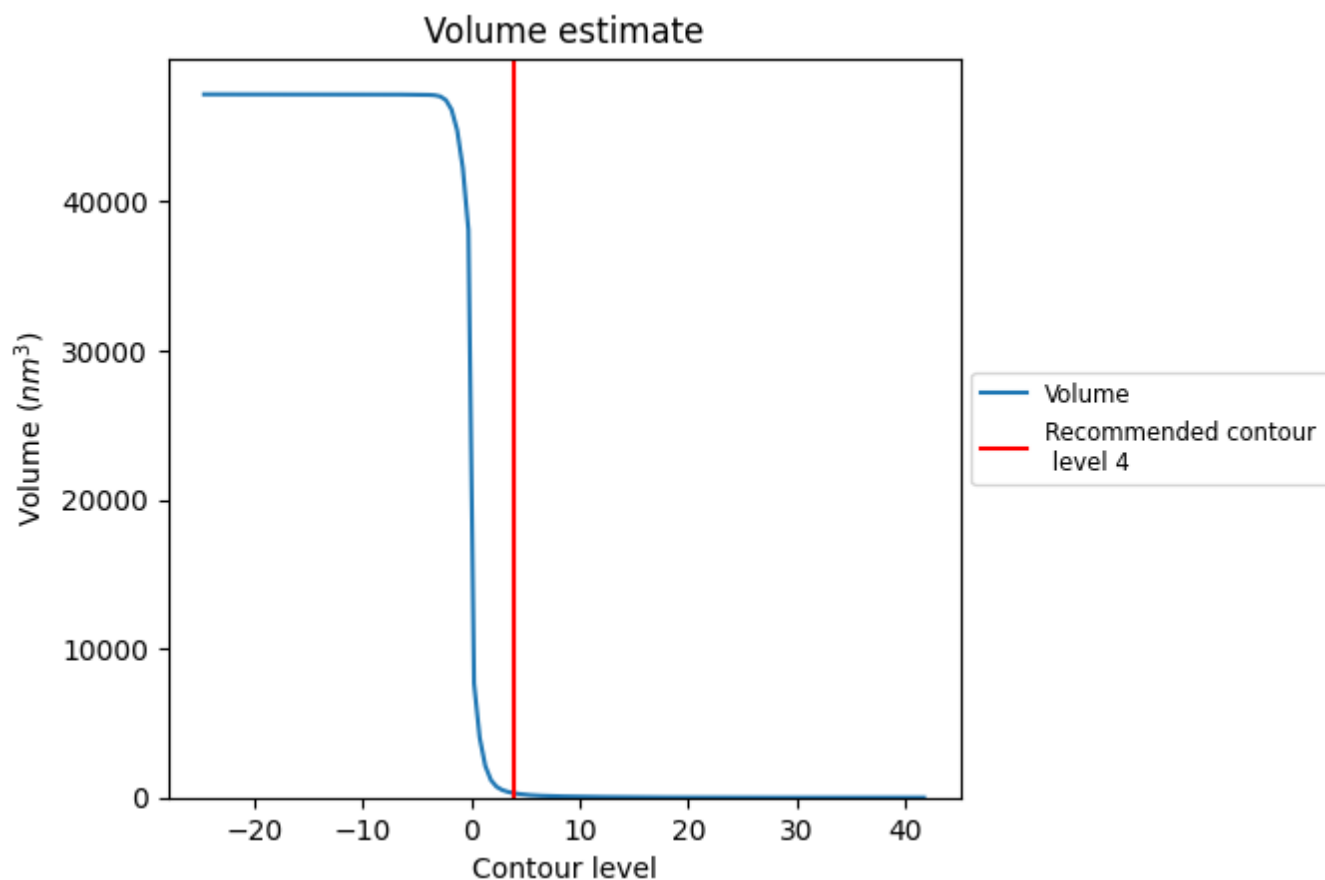
This section contains the results of statistical analysis of the map.

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.

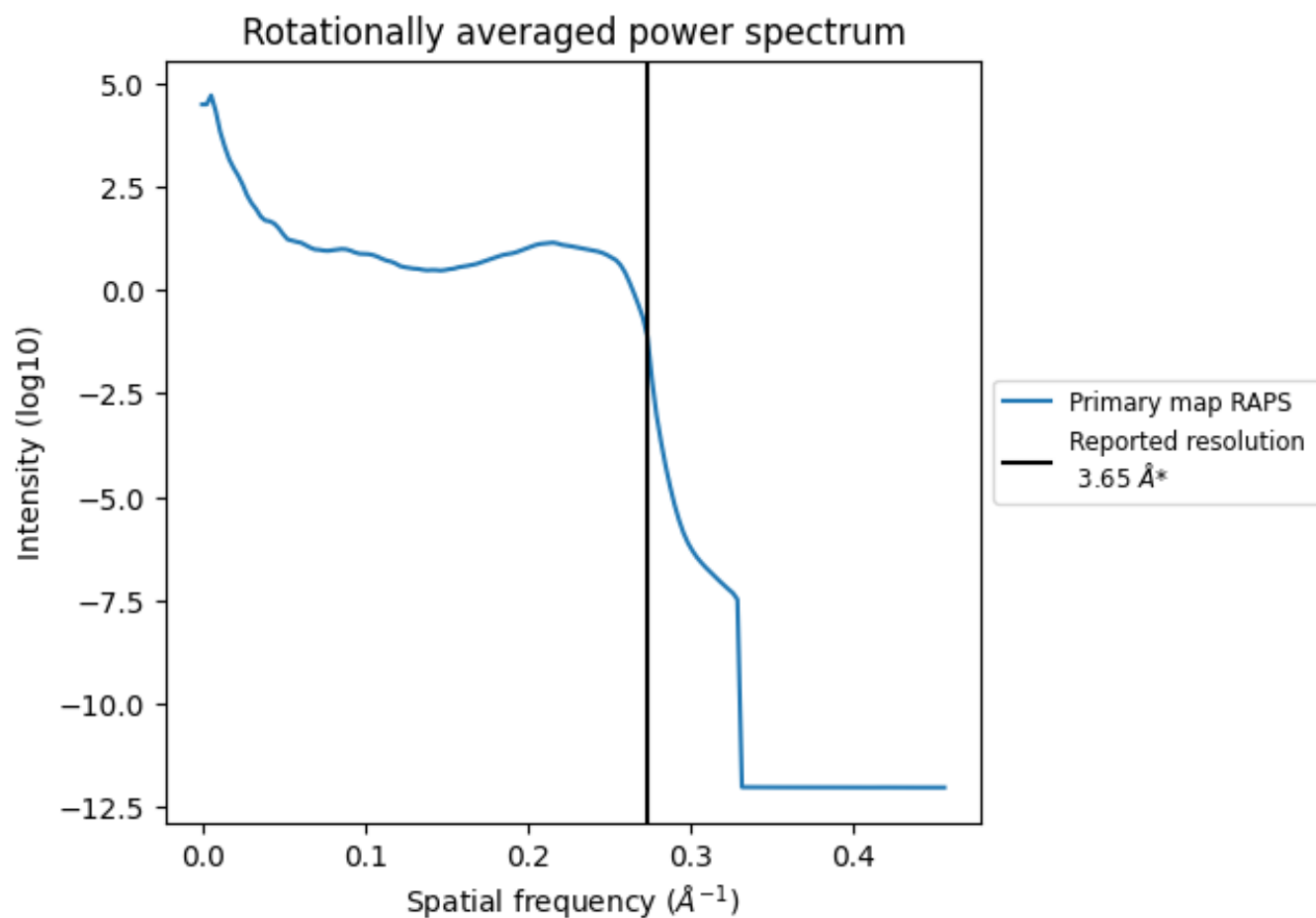
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 287 nm³; this corresponds to an approximate mass of 259 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.274 Å⁻¹

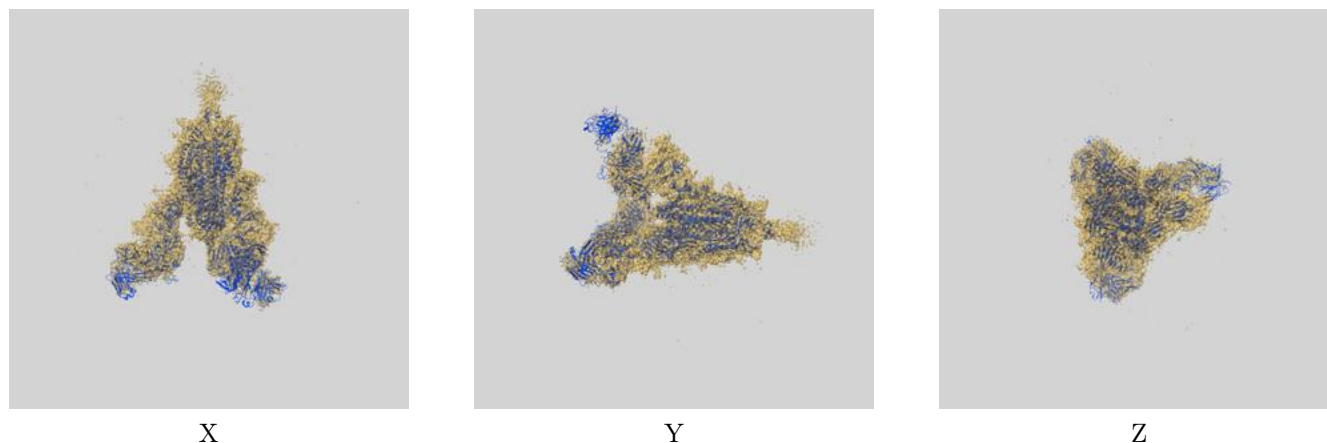
8 Fourier-Shell correlation ⓘ

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-31036 and PDB model 7E9Q. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



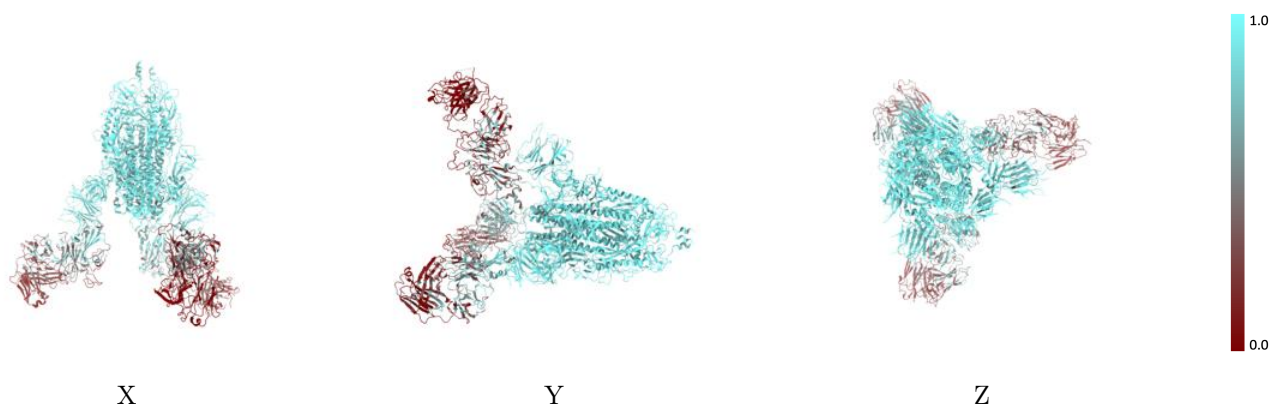
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



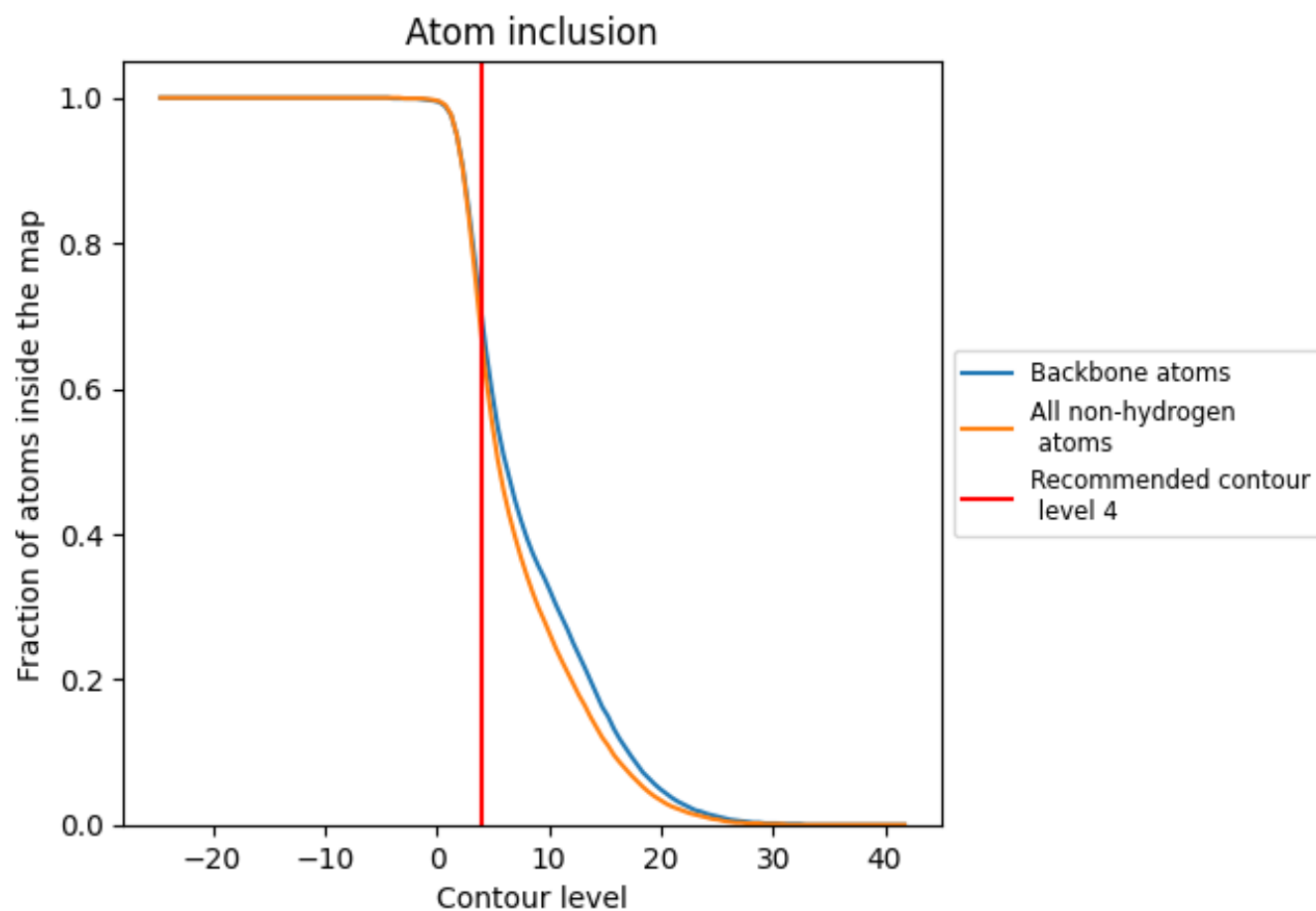
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6700	<div></div> 0.3600
A	<div></div> 0.8390	<div></div> 0.4200
B	<div></div> 0.7980	<div></div> 0.4160
C	<div></div> 0.8560	<div></div> 0.4310
E	<div></div> 0.1760	<div></div> 0.2050
F	<div></div> 0.1760	<div></div> 0.1930
H	<div></div> 0.3140	<div></div> 0.2360
L	<div></div> 0.2730	<div></div> 0.2100
X	<div></div> 0.3720	<div></div> 0.1990
Y	<div></div> 0.4150	<div></div> 0.2370

1.0

0.0

<0.0