



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 09:15 AM EDT

PDB ID : 8TAZ  
EMDB ID : EMD-41143  
Title : Cryo-EM structure of mink variant Y453F trimeric spike protein bound to one mink ACE2 receptors  
Authors : Ahn, H.M.; Calderon, B.; Fan, X.; Gao, Y.; Horgan, N.; Liang, B.  
Deposited on : 2023-06-28  
Resolution : 3.75 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
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

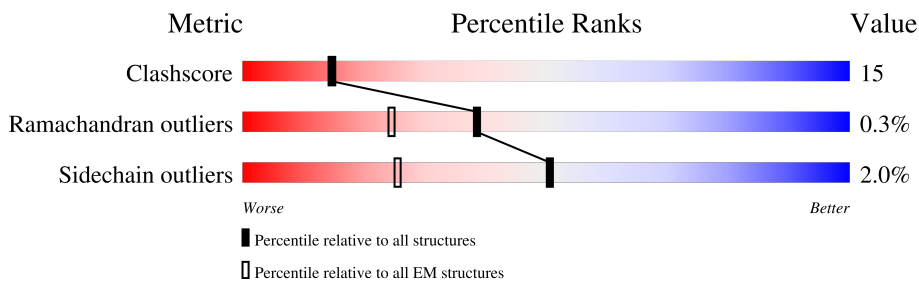
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.75 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  $\geq 3$ , 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	1269	
1	B	1269	
1	C	1269	
2	D	771	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28269 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1062	Total	C	N	O	S	0	0
			8291	5293	1382	1578	38		
1	B	1065	Total	C	N	O	S	0	0
			8312	5305	1388	1581	38		
1	C	868	Total	C	N	O	S	0	0
			6755	4306	1126	1293	30		

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	453	PHE	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	engineered mutation	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	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	SER	-	expression tag	UNP P0DTC2
A	1217	GLY	-	expression tag	UNP P0DTC2
A	1218	TYR	-	expression tag	UNP P0DTC2
A	1219	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	GLU	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	ARG	-	expression tag	UNP P0DTC2
A	1225	ASP	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	GLN	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	TYR	-	expression tag	UNP P0DTC2
A	1230	VAL	-	expression tag	UNP P0DTC2
A	1231	ARG	-	expression tag	UNP P0DTC2
A	1232	LYS	-	expression tag	UNP P0DTC2
A	1233	ASP	-	expression tag	UNP P0DTC2
A	1234	GLY	-	expression tag	UNP P0DTC2
A	1235	GLU	-	expression tag	UNP P0DTC2
A	1236	TRP	-	expression tag	UNP P0DTC2
A	1237	VAL	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	SER	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	SER	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
A	1258	LEU	-	expression tag	UNP P0DTC2
A	1259	ASN	-	expression tag	UNP P0DTC2
A	1260	ASP	-	expression tag	UNP P0DTC2
A	1261	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1262	PHE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	ALA	-	expression tag	UNP P0DTC2
A	1265	GLN	-	expression tag	UNP P0DTC2
A	1266	LYS	-	expression tag	UNP P0DTC2
A	1267	ILE	-	expression tag	UNP P0DTC2
A	1268	GLU	-	expression tag	UNP P0DTC2
A	1269	TRP	-	expression tag	UNP P0DTC2
A	1270	HIS	-	expression tag	UNP P0DTC2
A	1271	GLU	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	453	PHE	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	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	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	SER	-	expression tag	UNP P0DTC2
B	1217	GLY	-	expression tag	UNP P0DTC2
B	1218	TYR	-	expression tag	UNP P0DTC2
B	1219	ILE	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	GLU	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	ARG	-	expression tag	UNP P0DTC2
B	1225	ASP	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	GLN	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1270	HIS	-	expression tag	UNP P0DTC2
B	1271	GLU	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	453	PHE	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	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	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	SER	-	expression tag	UNP P0DTC2
C	1217	GLY	-	expression tag	UNP P0DTC2
C	1218	TYR	-	expression tag	UNP P0DTC2
C	1219	ILE	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	GLU	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	ARG	-	expression tag	UNP P0DTC2
C	1225	ASP	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	GLN	-	expression tag	UNP P0DTC2
C	1228	ALA	-	expression tag	UNP P0DTC2
C	1229	TYR	-	expression tag	UNP P0DTC2
C	1230	VAL	-	expression tag	UNP P0DTC2
C	1231	ARG	-	expression tag	UNP P0DTC2
C	1232	LYS	-	expression tag	UNP P0DTC2
C	1233	ASP	-	expression tag	UNP P0DTC2
C	1234	GLY	-	expression tag	UNP P0DTC2
C	1235	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1236	TRP	-	expression tag	UNP P0DTC2
C	1237	VAL	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	THR	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	SER	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	SER	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	GLY	-	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
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	GLY	-	expression tag	UNP P0DTC2
C	1258	LEU	-	expression tag	UNP P0DTC2
C	1259	ASN	-	expression tag	UNP P0DTC2
C	1260	ASP	-	expression tag	UNP P0DTC2
C	1261	ILE	-	expression tag	UNP P0DTC2
C	1262	PHE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	ALA	-	expression tag	UNP P0DTC2
C	1265	GLN	-	expression tag	UNP P0DTC2
C	1266	LYS	-	expression tag	UNP P0DTC2
C	1267	ILE	-	expression tag	UNP P0DTC2
C	1268	GLU	-	expression tag	UNP P0DTC2
C	1269	TRP	-	expression tag	UNP P0DTC2
C	1270	HIS	-	expression tag	UNP P0DTC2
C	1271	GLU	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	596	Total	C	N	O	S	1	0
			4911	3138	826	918	29		



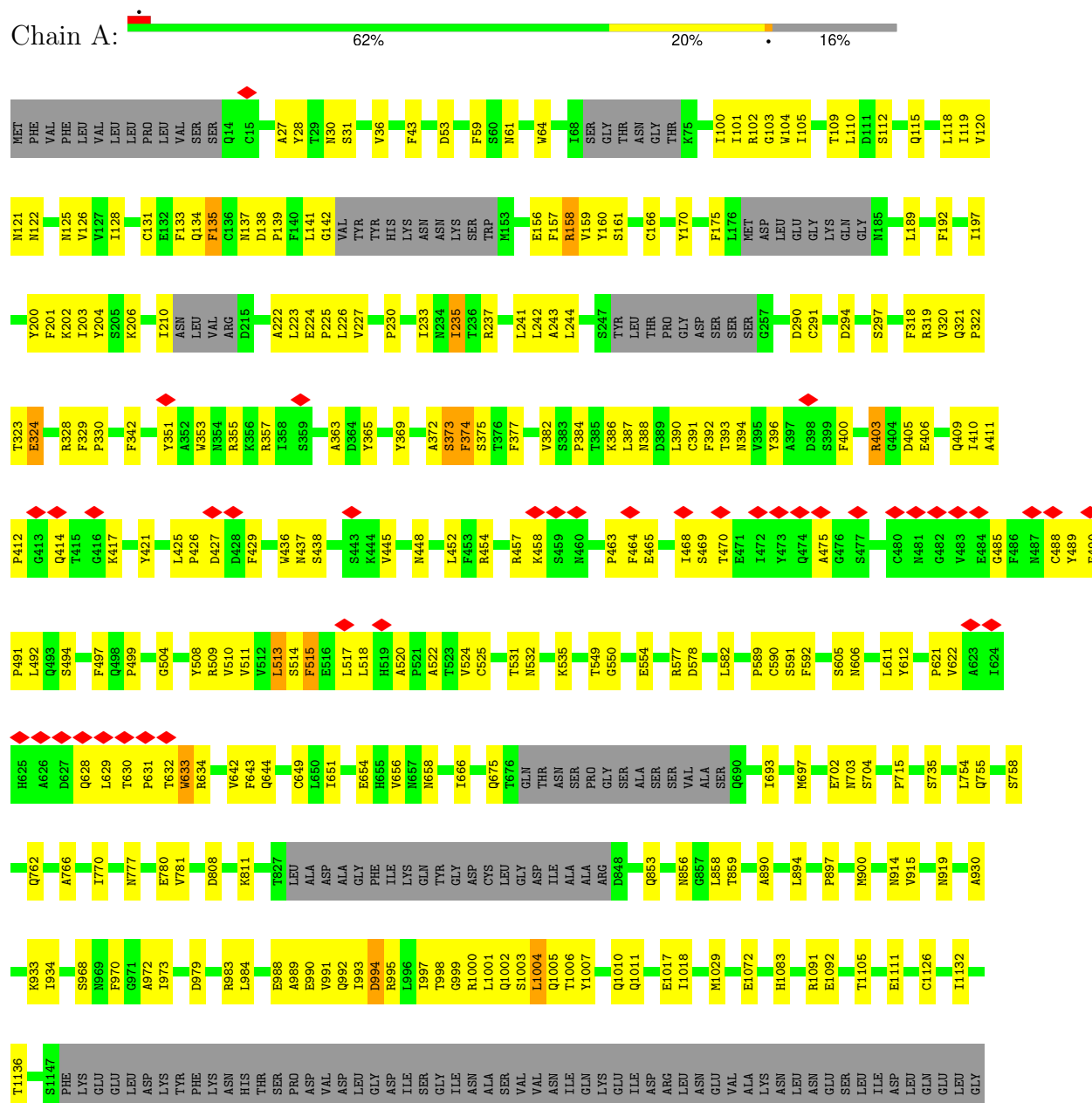
There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	740	GLY	-	expression tag	UNP A0A7T0Q2W2
D	741	SER	-	expression tag	UNP A0A7T0Q2W2
D	742	GLY	-	expression tag	UNP A0A7T0Q2W2
D	743	SER	-	expression tag	UNP A0A7T0Q2W2
D	744	GLY	-	expression tag	UNP A0A7T0Q2W2
D	745	SER	-	expression tag	UNP A0A7T0Q2W2
D	746	GLY	-	expression tag	UNP A0A7T0Q2W2
D	747	HIS	-	expression tag	UNP A0A7T0Q2W2
D	748	HIS	-	expression tag	UNP A0A7T0Q2W2
D	749	HIS	-	expression tag	UNP A0A7T0Q2W2
D	750	HIS	-	expression tag	UNP A0A7T0Q2W2
D	751	HIS	-	expression tag	UNP A0A7T0Q2W2
D	752	HIS	-	expression tag	UNP A0A7T0Q2W2
D	753	GLY	-	expression tag	UNP A0A7T0Q2W2
D	754	SER	-	expression tag	UNP A0A7T0Q2W2
D	755	GLY	-	expression tag	UNP A0A7T0Q2W2
D	756	SER	-	expression tag	UNP A0A7T0Q2W2
D	757	GLY	-	expression tag	UNP A0A7T0Q2W2
D	758	LEU	-	expression tag	UNP A0A7T0Q2W2
D	759	ASN	-	expression tag	UNP A0A7T0Q2W2
D	760	ASP	-	expression tag	UNP A0A7T0Q2W2
D	761	ILE	-	expression tag	UNP A0A7T0Q2W2
D	762	PHE	-	expression tag	UNP A0A7T0Q2W2
D	763	GLU	-	expression tag	UNP A0A7T0Q2W2
D	764	ALA	-	expression tag	UNP A0A7T0Q2W2
D	765	GLN	-	expression tag	UNP A0A7T0Q2W2
D	766	LYS	-	expression tag	UNP A0A7T0Q2W2
D	767	ILE	-	expression tag	UNP A0A7T0Q2W2
D	768	GLU	-	expression tag	UNP A0A7T0Q2W2
D	769	TRP	-	expression tag	UNP A0A7T0Q2W2
D	770	HIS	-	expression tag	UNP A0A7T0Q2W2
D	771	GLU	-	expression tag	UNP A0A7T0Q2W2

### 3 Residue-property plots

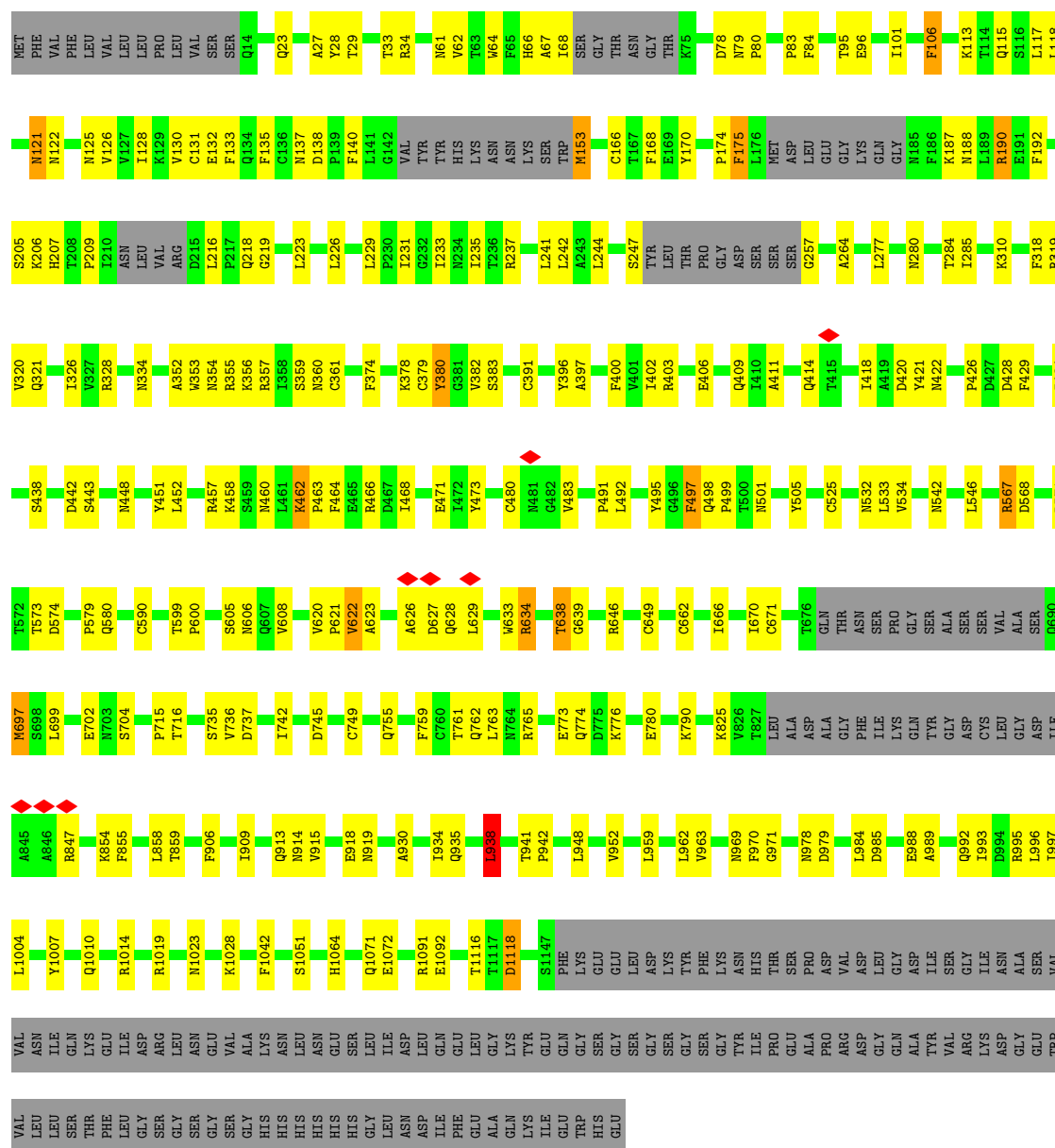
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



- Molecule 1: Spike glycoprotein

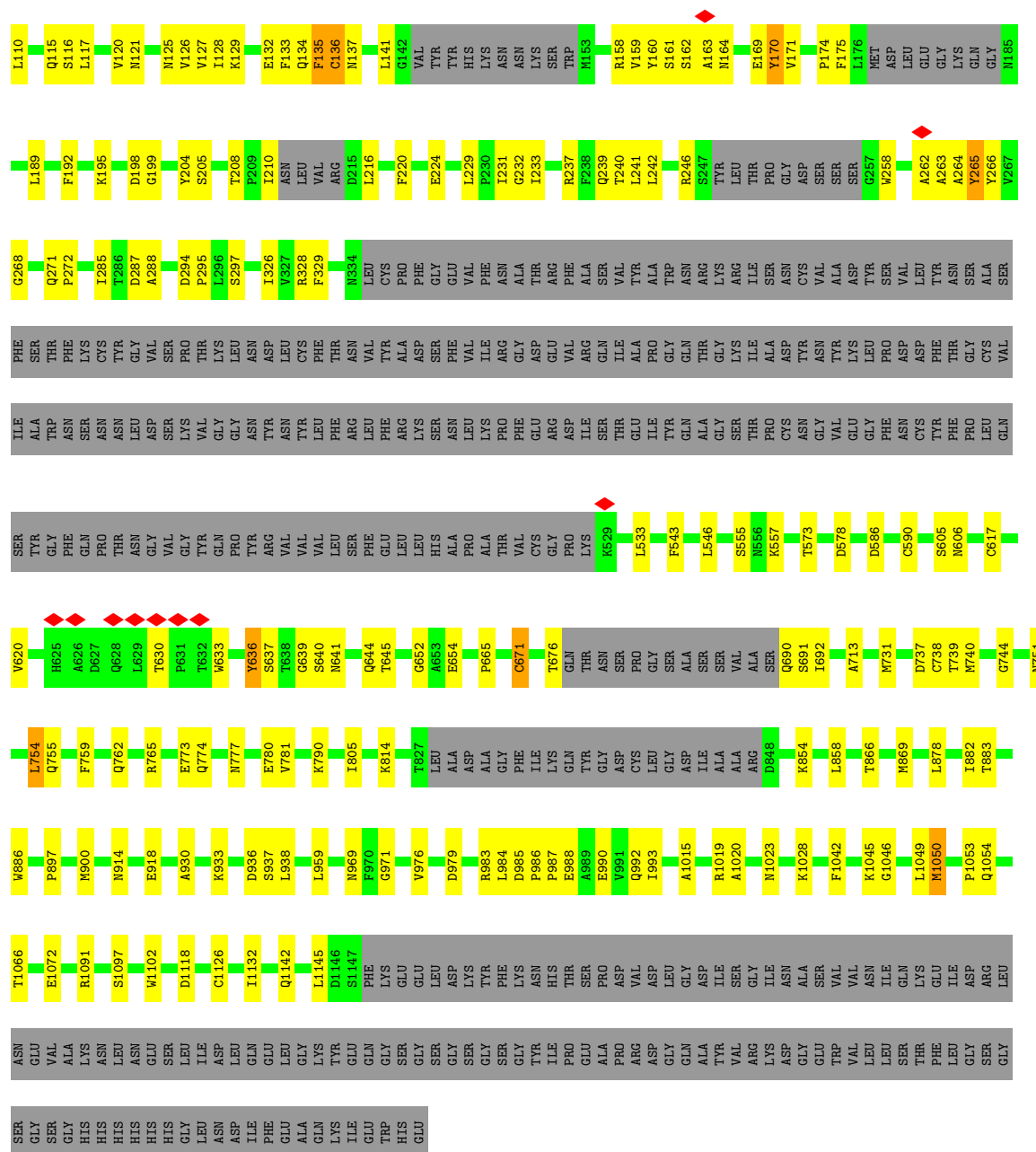
Chain B:  64% 19% 16%



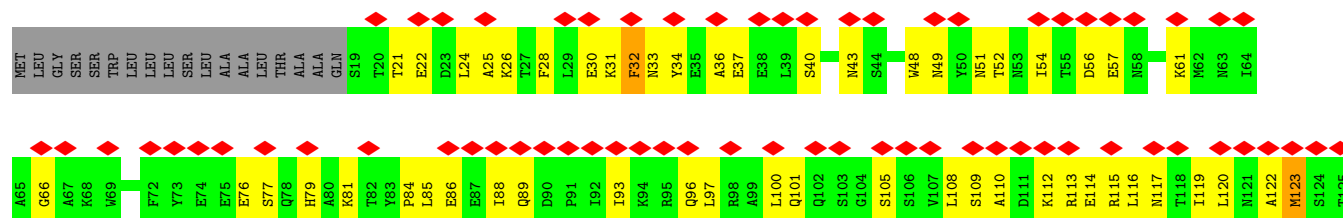
- Molecule 1: Spike glycoprotein

Chain C:  53% 15% 32%





### • Molecule 2: Angiotensin-converting enzyme



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130988	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 ( $e^-/\text{\AA}^2$ )	49.98	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.229	Depositor
Minimum map value	-0.834	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.211	Depositor
Map size (Å)	568.32, 568.32, 568.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.27	0/8484	0.53	1/11552 (0.0%)
1	B	0.28	0/8505	0.53	2/11580 (0.0%)
1	C	0.27	0/6902	0.52	0/9397
2	D	2.13	18/5058 (0.4%)	0.84	16/6869 (0.2%)
All	All	0.93	18/28949 (0.1%)	0.59	19/39398 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	D	0	1
All	All	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	245	ARG	CB-CG	69.69	3.40	1.52
2	D	279	TYR	CD1-CE1	63.52	2.34	1.39
2	D	279	TYR	CD2-CE2	62.47	2.33	1.39
2	D	279	TYR	CE1-CZ	43.98	1.95	1.38
2	D	279	TYR	CE2-CZ	42.24	1.93	1.38
2	D	606	TRP	CE3-CZ3	33.58	1.95	1.38
2	D	279	TYR	CG-CD1	33.36	1.82	1.39
2	D	279	TYR	CG-CD2	32.66	1.81	1.39
2	D	444	LEU	CB-CG	26.66	2.29	1.52
2	D	590	PRO	CG-CD	-21.57	0.79	1.50
2	D	606	TRP	CZ3-CH2	21.46	1.74	1.40
2	D	606	TRP	CE2-CZ2	18.51	1.71	1.39
2	D	606	TRP	CD2-CE2	16.47	1.61	1.41
2	D	606	TRP	CD2-CE3	11.38	1.57	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	590	PRO	N-CD	11.21	1.63	1.47
2	D	606	TRP	CZ2-CH2	10.73	1.57	1.37
2	D	590	PRO	CB-CG	6.76	1.83	1.50
2	D	590	PRO	N-CA	-5.17	1.38	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	444	LEU	CA-CB-CG	20.11	161.55	115.30
2	D	590	PRO	N-CD-CG	-14.14	81.98	103.20
2	D	590	PRO	CA-N-CD	-13.93	91.99	111.50
2	D	444	LEU	CB-CG-CD2	13.01	133.12	111.00
2	D	444	LEU	CB-CG-CD1	12.12	131.61	111.00
2	D	469	PRO	CA-N-CD	-9.84	97.73	111.50
2	D	245	ARG	CA-CB-CG	9.06	133.32	113.40
2	D	590	PRO	CA-CB-CG	-8.75	87.38	104.00
2	D	590	PRO	N-CA-CB	-8.71	92.85	103.30
2	D	179	LEU	CA-CB-CG	8.19	134.13	115.30
2	D	245	ARG	CB-CG-CD	7.48	131.05	111.60
2	D	305	ARG	CA-CB-CG	6.81	128.39	113.40
2	D	148	LEU	CA-CB-CG	6.47	130.18	115.30
2	D	444	LEU	CD1-CG-CD2	-6.17	91.99	110.50
2	D	176	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	994	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	985	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	938	LEU	CA-CB-CG	5.31	127.51	115.30
2	D	279	TYR	CB-CG-CD2	-5.06	117.96	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	PHE	Peptide
2	D	497	TYR	Peptide

## 5.2 Too-close contacts

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	8291	0	8094	197	0
1	B	8312	0	8117	171	0
1	C	6755	0	6632	152	0
2	D	4911	0	4674	342	0
All	All	28269	0	27517	837	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 15.

All (837) 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:D:279:TYR:CD2	2:D:279:TYR:CG	1.81	1.62
2:D:279:TYR:CG	2:D:279:TYR:CD1	1.82	1.61
2:D:279:TYR:CZ	2:D:279:TYR:CE2	1.93	1.56
2:D:606:TRP:CZ3	2:D:606:TRP:CE3	1.95	1.55
2:D:279:TYR:CD2	2:D:444:LEU:HB3	1.42	1.54
2:D:279:TYR:CZ	2:D:279:TYR:CE1	1.95	1.51
2:D:590:PRO:CG	2:D:590:PRO:CB	1.83	1.51
2:D:590:PRO:CG	2:D:590:PRO:N	1.71	1.48
2:D:279:TYR:CE2	2:D:444:LEU:HB2	1.49	1.46
2:D:279:TYR:CZ	2:D:444:LEU:HG	1.56	1.38
2:D:279:TYR:CE1	2:D:444:LEU:HG	1.61	1.33
2:D:279:TYR:CD2	2:D:444:LEU:CB	2.17	1.28
2:D:279:TYR:CZ	2:D:444:LEU:HB2	1.69	1.28
2:D:279:TYR:CE2	2:D:444:LEU:CB	2.17	1.27
2:D:279:TYR:CZ	2:D:444:LEU:CB	2.21	1.24
2:D:279:TYR:CE1	2:D:444:LEU:CB	2.23	1.22
2:D:279:TYR:CG	2:D:444:LEU:HB3	1.73	1.22
2:D:279:TYR:CD1	2:D:444:LEU:CB	2.22	1.20
2:D:583:PRO:O	2:D:587:TYR:HB3	1.38	1.20
2:D:279:TYR:CD2	2:D:279:TYR:CE2	2.33	1.17
2:D:444:LEU:HG	2:D:444:LEU:CB	1.74	1.17
2:D:279:TYR:CG	2:D:444:LEU:CB	2.28	1.16
2:D:245:ARG:CB	2:D:606:TRP:CZ3	2.31	1.14
2:D:279:TYR:CD1	2:D:279:TYR:CE1	2.34	1.14
2:D:245:ARG:CG	2:D:606:TRP:CE2	2.32	1.13
2:D:245:ARG:CB	2:D:606:TRP:CE3	2.32	1.12
2:D:444:LEU:CB	2:D:444:LEU:CG	2.29	1.10
2:D:245:ARG:CG	2:D:606:TRP:CD2	2.35	1.09
2:D:245:ARG:CG	2:D:606:TRP:CE3	2.37	1.07
2:D:590:PRO:CG	2:D:590:PRO:CA	2.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:ARG:CB	2:D:606:TRP:CD2	2.41	1.04
2:D:279:TYR:CZ	2:D:444:LEU:CG	2.41	1.03
2:D:279:TYR:CE1	2:D:444:LEU:CG	2.40	1.03
2:D:590:PRO:CG	2:D:590:PRO:HD3	1.50	1.02
2:D:245:ARG:CB	2:D:606:TRP:CH2	2.44	1.00
2:D:245:ARG:CG	2:D:606:TRP:CZ3	2.44	1.00
2:D:590:PRO:CG	2:D:590:PRO:HD2	1.50	1.00
2:D:245:ARG:CB	2:D:606:TRP:CE2	2.44	1.00
2:D:245:ARG:CG	2:D:606:TRP:CZ2	2.45	0.99
2:D:590:PRO:CD	2:D:590:PRO:HG3	1.47	0.98
2:D:33:ASN:O	2:D:37:GLU:HB3	1.64	0.98
2:D:590:PRO:CD	2:D:590:PRO:HG2	1.47	0.96
2:D:279:TYR:CE2	2:D:444:LEU:CG	2.48	0.96
2:D:245:ARG:HB3	2:D:606:TRP:CE3	2.01	0.95
2:D:245:ARG:CB	2:D:606:TRP:CZ2	2.50	0.95
2:D:279:TYR:CD1	2:D:444:LEU:CG	2.51	0.94
2:D:245:ARG:CG	2:D:606:TRP:CH2	2.49	0.93
2:D:279:TYR:CD2	2:D:444:LEU:CG	2.52	0.92
1:A:319:ARG:H	1:A:629:LEU:HB2	1.34	0.92
2:D:245:ARG:HG2	2:D:606:TRP:CD2	2.03	0.92
2:D:81:LYS:HA	2:D:101:GLN:HG2	1.52	0.92
2:D:264:ALA:HA	2:D:487:VAL:HG13	1.52	0.91
2:D:169:ARG:HD2	2:D:501:ALA:H	1.33	0.90
2:D:233:ILE:HG22	2:D:237:TYR:HB2	1.51	0.90
2:D:590:PRO:N	2:D:590:PRO:HG3	1.57	0.88
2:D:245:ARG:HB2	2:D:606:TRP:CH2	2.11	0.86
2:D:279:TYR:CG	2:D:444:LEU:CG	2.59	0.85
2:D:245:ARG:HG3	2:D:606:TRP:CZ2	2.09	0.85
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.60	0.82
1:A:197:ILE:O	1:A:202:LYS:NZ	2.13	0.82
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.62	0.82
2:D:588:PHE:O	2:D:592:PHE:N	2.12	0.81
2:D:358:ILE:HD11	2:D:379:ILE:HD11	1.63	0.80
2:D:590:PRO:CG	2:D:590:PRO:CD	0.79	0.79
2:D:279:TYR:CE2	2:D:444:LEU:HG	2.18	0.79
1:A:121:ASN:HA	1:A:126:VAL:HG12	1.65	0.78
2:D:176:LEU:HB2	2:D:179:LEU:HD22	1.64	0.78
1:A:353:TRP:HB3	1:A:400:PHE:HB3	1.66	0.78
1:A:351:TYR:HB3	1:A:454:ARG:HE	1.49	0.77
1:C:229:LEU:HD12	1:C:231:ILE:HD11	1.64	0.77
2:D:233:ILE:O	2:D:237:TYR:N	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:PRO:HD2	1:B:847:ARG:HH22	1.50	0.76
1:A:403:ARG:NH1	1:A:406:GLU:OE1	2.20	0.75
1:A:135:PHE:HA	1:A:160:TYR:HA	1.67	0.75
2:D:457:GLU:O	2:D:460:ARG:HG2	1.87	0.75
2:D:245:ARG:HB2	2:D:606:TRP:CZ3	2.18	0.74
2:D:593:THR:O	2:D:597:GLU:N	2.17	0.74
1:A:328:ARG:NH1	1:A:531:THR:O	2.21	0.74
2:D:328:TRP:HA	2:D:331:SER:HB3	1.69	0.73
1:B:418:ILE:HA	1:B:422:ASN:HB2	1.70	0.73
2:D:462:MET:O	2:D:466:GLY:N	2.22	0.73
2:D:115:ARG:O	2:D:119:ILE:HG12	1.88	0.73
1:A:897:PRO:HB2	1:A:900:MET:HG3	1.71	0.72
2:D:279:TYR:CD1	2:D:444:LEU:CD2	2.72	0.72
2:D:259:THR:HA	2:D:607:ASN:HB2	1.69	0.72
1:B:443:SER:HB3	1:B:499:PRO:HB3	1.70	0.72
1:B:128:ILE:HD13	1:B:170:TYR:HB3	1.72	0.71
2:D:261:CYS:HB3	2:D:488:VAL:HG11	1.73	0.71
1:A:1001:LEU:O	1:A:1005:GLN:HB2	1.91	0.71
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.73	0.71
2:D:305:ARG:HH22	2:D:309:LYS:CG	2.04	0.70
2:D:539:LEU:HD13	2:D:587:TYR:HB2	1.73	0.70
1:A:611:LEU:HD22	1:A:666:ILE:HD11	1.72	0.70
1:B:353:TRP:HB3	1:B:400:PHE:HB3	1.73	0.70
1:C:67:ALA:HB1	1:C:258:TRP:HH2	1.57	0.70
1:A:642:VAL:HG22	1:A:651:ILE:HG12	1.72	0.70
2:D:119:ILE:HG23	2:D:179:LEU:HG	1.73	0.70
1:A:319:ARG:NH2	1:B:737:ASP:OD2	2.26	0.69
2:D:133:CYS:HB2	2:D:141:CYS:HA	1.73	0.69
1:A:452:LEU:HA	1:A:494:SER:HA	1.74	0.69
1:A:105:ILE:HG22	1:A:118:LEU:HA	1.74	0.69
1:C:110:LEU:HG	1:C:237:ARG:HH22	1.57	0.69
1:C:773:GLU:OE1	1:C:774:GLN:NE2	2.25	0.69
2:D:61:LYS:O	2:D:66:GLY:N	2.26	0.69
1:C:676:THR:HB	1:C:690:GLN:HB2	1.74	0.68
1:A:393:THR:HG22	1:A:520:ALA:HB2	1.75	0.68
2:D:169:ARG:HD2	2:D:501:ALA:N	2.07	0.68
1:B:188:ASN:OD1	1:B:207:HIS:NE2	2.26	0.68
2:D:279:TYR:CE2	2:D:444:LEU:CD1	2.77	0.68
1:A:535:LYS:NZ	1:A:554:GLU:OE2	2.28	0.67
1:B:1019:ARG:HH11	1:B:1023:ASN:HD21	1.43	0.67
1:C:546:LEU:HD21	1:C:573:THR:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:PRO:HB2	1:C:900:MET:HG2	1.76	0.67
2:D:234:LYS:HA	2:D:237:TYR:HB3	1.77	0.67
2:D:260:GLY:HA3	2:D:610:TRP:HE3	1.59	0.67
1:A:319:ARG:HB2	1:A:629:LEU:HD12	1.78	0.66
1:A:382:VAL:HG21	1:A:387:LEU:HD13	1.78	0.66
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.77	0.66
1:B:971:GLY:H	1:C:755:GLN:HE22	1.42	0.66
2:D:25:ALA:HB3	2:D:93:ILE:HD13	1.77	0.66
2:D:304:ALA:HA	2:D:307:ILE:HG12	1.78	0.66
2:D:270:MET:SD	2:D:270:MET:N	2.69	0.66
1:A:412:PRO:HB3	1:A:427:ASP:HA	1.78	0.65
1:C:644:GLN:NE2	1:C:645:THR:O	2.29	0.65
1:A:128:ILE:HD13	1:A:170:TYR:HB3	1.76	0.65
1:A:465:GLU:OE2	1:A:465:GLU:N	2.30	0.65
2:D:169:ARG:NH1	2:D:500:PRO:HG2	2.12	0.65
1:B:352:ALA:HA	1:B:468:ILE:HG22	1.79	0.65
1:B:546:LEU:HD11	1:B:573:THR:HG21	1.79	0.65
1:C:31:SER:HA	1:C:216:LEU:HD21	1.77	0.65
1:B:451:TYR:HB2	1:B:495:TYR:HE2	1.61	0.64
2:D:263:PRO:HB3	2:D:490:PRO:HG3	1.79	0.64
1:B:457:ARG:HG2	1:B:458:LYS:H	1.62	0.64
1:A:226:LEU:HD23	1:A:227:VAL:HG23	1.80	0.64
2:D:245:ARG:HG3	2:D:606:TRP:CE2	2.29	0.64
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.80	0.64
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.81	0.63
2:D:119:ILE:O	2:D:123:MET:HG2	1.98	0.63
2:D:233:ILE:HD11	2:D:516:TYR:CZ	2.33	0.63
1:B:374:PHE:HB3	1:B:434:ILE:HG23	1.80	0.63
2:D:208:GLU:OE2	2:D:208:GLU:N	2.31	0.63
1:A:134:GLN:O	1:A:161:SER:N	2.31	0.63
2:D:517:THR:O	2:D:521:TYR:HB2	1.99	0.63
2:D:76:GLU:HA	2:D:79:HIS:HB2	1.80	0.63
1:A:192:PHE:HD2	1:A:203:ILE:HD11	1.64	0.63
1:A:206:LYS:HB2	1:A:223:LEU:HB2	1.81	0.63
2:D:49:ASN:HA	2:D:52:THR:HG22	1.81	0.63
1:A:134:GLN:H	1:A:160:TYR:HB2	1.63	0.62
1:A:1092:GLU:N	1:A:1092:GLU:OE1	2.32	0.62
1:B:969:ASN:HB2	1:C:755:GLN:HE21	1.64	0.62
2:D:227:GLU:O	2:D:231:THR:N	2.29	0.62
1:B:735:SER:OG	1:B:859:THR:OG1	2.18	0.62
1:B:126:VAL:HG13	1:B:174:PRO:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:983:ARG:NE	1:C:983:ARG:O	2.32	0.62
2:D:239:HIS:CE1	2:D:595:LEU:HB3	2.34	0.62
1:A:454:ARG:NH1	1:A:469:SER:O	2.33	0.62
1:B:33:THR:OG1	1:B:219:GLY:O	2.15	0.62
1:C:985:ASP:HB3	1:C:987:PRO:HD2	1.81	0.61
1:A:104:TRP:HD1	1:A:241:LEU:H	1.48	0.61
2:D:113:ARG:HE	2:D:116:LEU:HD12	1.64	0.61
2:D:265:HIS:H	2:D:265:HIS:CD2	2.17	0.61
1:B:382:VAL:HG23	1:C:983:ARG:NH1	2.15	0.61
2:D:456:LEU:O	2:D:460:ARG:HB3	2.00	0.61
1:B:1010:GLN:HB3	1:B:1014:ARG:HH12	1.66	0.61
2:D:200:GLY:HA3	2:D:464:PHE:CZ	2.36	0.61
2:D:269:ASP:HB2	2:D:273:ARG:H	1.64	0.61
2:D:381:TYR:HA	2:D:558:LEU:HD13	1.83	0.61
2:D:455:MET:HG3	2:D:477:TRP:CZ3	2.36	0.61
1:B:131:CYS:HA	1:B:166:CYS:HB3	1.83	0.61
2:D:456:LEU:HD23	2:D:512:PHE:HD1	1.66	0.61
1:B:319:ARG:HG2	1:B:629:LEU:HB2	1.82	0.60
1:C:127:VAL:HG12	1:C:171:VAL:HG22	1.83	0.60
2:D:480:MET:HG2	2:D:484:ILE:HD11	1.83	0.60
1:C:988:GLU:OE2	1:C:988:GLU:N	2.31	0.60
2:D:315:PHE:HB3	2:D:320:LEU:HB2	1.83	0.60
1:A:755:GLN:HE22	1:C:971:GLY:H	1.48	0.60
1:A:915:VAL:O	1:A:919:ASN:ND2	2.27	0.60
1:B:621:PRO:O	1:B:623:ALA:N	2.34	0.60
2:D:530:CYS:O	2:D:535:HIS:N	2.31	0.60
1:A:103:GLY:HA3	1:A:120:VAL:HA	1.83	0.60
1:A:475:ALA:HB1	2:D:24:LEU:HD22	1.83	0.60
1:C:900:MET:SD	1:C:900:MET:N	2.74	0.60
1:A:457:ARG:HG2	1:A:458:LYS:H	1.67	0.60
1:C:134:GLN:O	1:C:161:SER:OG	2.19	0.60
2:D:590:PRO:HD2	2:D:591:LEU:H	1.66	0.60
2:D:294:THR:HA	2:D:297:MET:HG3	1.83	0.59
1:A:485:GLY:H	1:A:488:CYS:HB2	1.65	0.59
1:C:271:GLN:HG2	1:C:272:PRO:HD2	1.84	0.59
1:C:543:PHE:HE2	1:C:578:ASP:HA	1.67	0.59
2:D:377:GLY:O	2:D:381:TYR:HB3	2.02	0.59
2:D:591:LEU:HG	2:D:595:LEU:HD23	1.82	0.59
1:B:428:ASP:OD1	1:B:428:ASP:N	2.34	0.59
2:D:237:TYR:O	2:D:241:HIS:N	2.19	0.59
1:B:498:GLN:N	1:B:505:TYR:OH	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:ASN:ND2	1:C:654:GLU:OE1	2.36	0.59
2:D:113:ARG:HA	2:D:113:ARG:NE	2.17	0.59
1:A:654:GLU:OE2	1:A:654:GLU:N	2.35	0.59
1:C:773:GLU:OE2	1:C:777:ASN:ND2	2.36	0.59
2:D:590:PRO:HD2	2:D:591:LEU:N	2.18	0.59
1:A:100:ILE:O	1:A:243:ALA:N	2.31	0.59
1:A:997:ILE:O	1:A:1001:LEU:HG	2.02	0.59
1:C:294:ASP:OD1	1:C:297:SER:OG	2.19	0.59
2:D:200:GLY:HA3	2:D:464:PHE:CE2	2.38	0.59
1:A:122:ASN:N	1:A:125:ASN:O	2.35	0.58
1:A:550:GLY:HA2	1:A:589:PRO:HA	1.84	0.58
2:D:28:PHE:HZ	2:D:76:GLU:HB3	1.68	0.58
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.36	0.58
2:D:110:ALA:O	2:D:114:GLU:HB2	2.02	0.58
2:D:330:ASN:HD22	2:D:357:ARG:HD3	1.67	0.58
1:B:854:LYS:HA	1:B:858:LEU:O	2.02	0.58
2:D:478:TRP:CZ2	2:D:489:GLU:HG2	2.38	0.58
1:B:638:THR:OG1	1:B:639:GLY:N	2.36	0.58
1:C:295:PRO:HG3	1:C:633:TRP:CE3	2.38	0.58
1:C:136:CYS:SG	1:C:137:ASN:N	2.76	0.58
2:D:105:SER:OG	2:D:113:ARG:NH1	2.36	0.58
1:A:452:LEU:HD13	1:A:492:LEU:HD22	1.86	0.58
1:B:620:VAL:HG13	1:B:622:VAL:HG23	1.86	0.58
1:B:34:ARG:NH2	1:B:218:GLN:O	2.36	0.58
2:D:97:LEU:O	2:D:101:GLN:N	2.28	0.58
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.37	0.58
1:A:578:ASP:OD1	1:A:578:ASP:N	2.37	0.57
1:A:589:PRO:HG2	1:B:855:PHE:CD1	2.39	0.57
1:A:808:ASP:OD2	1:A:811:LYS:NZ	2.36	0.57
1:C:328:ARG:HE	1:C:533:LEU:HD12	1.69	0.57
2:D:230:PHE:O	2:D:234:LYS:N	2.35	0.57
1:C:132:GLU:HB2	1:C:164:ASN:HB2	1.87	0.57
2:D:451:PRO:HB3	2:D:484:ILE:HG22	1.86	0.57
2:D:553:LYS:O	2:D:557:MET:N	2.32	0.57
1:A:630:THR:O	1:A:632:THR:N	2.34	0.57
2:D:156:LYS:HZ3	2:D:281:LEU:HD12	1.68	0.57
1:A:735:SER:OG	1:A:859:THR:OG1	2.22	0.57
2:D:271:TRP:HB3	2:D:452:PHE:CE2	2.39	0.57
1:A:577:ARG:HD3	1:A:582:LEU:HD12	1.85	0.57
1:B:378:LYS:HD2	1:B:380:TYR:OH	2.04	0.57
1:B:755:GLN:N	1:B:755:GLN:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:109:SER:OG	2:D:112:LYS:HG3	2.05	0.57
1:A:994:ASP:O	1:A:998:THR:HG23	2.04	0.57
1:B:79:ASN:HD21	1:B:242:LEU:HD13	1.70	0.57
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.86	0.57
1:A:702:GLU:HG3	1:B:790:LYS:HZ2	1.70	0.57
1:B:153:MET:SD	1:B:153:MET:N	2.78	0.56
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.39	0.56
1:C:665:PRO:HA	1:C:671:CYS:HB3	1.87	0.56
2:D:596:LYS:NZ	2:D:604:VAL:HG21	2.20	0.56
1:A:621:PRO:HG2	1:A:628:GLN:HG3	1.87	0.56
2:D:243:TYR:O	2:D:247:LYS:N	2.38	0.56
1:A:391:CYS:HB3	1:A:522:ALA:HB3	1.88	0.56
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.88	0.56
1:A:984:LEU:HD11	1:A:988:GLU:HB3	1.87	0.56
1:B:187:LYS:HA	1:B:209:PRO:HA	1.88	0.56
2:D:305:ARG:HH22	2:D:309:LYS:HG2	1.69	0.56
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.88	0.56
2:D:40:SER:HA	2:D:43:ASN:HB2	1.87	0.56
1:C:878:LEU:O	1:C:882:ILE:HG22	2.06	0.56
2:D:271:TRP:CZ2	2:D:501:ALA:HA	2.41	0.56
1:A:28:TYR:CD1	1:A:61:ASN:HB3	2.41	0.56
1:C:605:SER:OG	1:C:606:ASN:N	2.39	0.56
2:D:122:ALA:O	2:D:126:ILE:HG12	2.06	0.56
2:D:236:LEU:O	2:D:240:LEU:N	2.29	0.56
2:D:279:TYR:OH	2:D:440:LEU:O	2.24	0.55
1:C:751:ASN:HA	1:C:754:LEU:HG	1.87	0.55
2:D:115:ARG:HG2	2:D:115:ARG:HH11	1.70	0.55
1:A:531:THR:OG1	1:A:532:ASN:N	2.39	0.55
2:D:481:LYS:HE2	2:D:487:VAL:HB	1.88	0.55
1:A:644:GLN:HA	1:A:649:CYS:HB2	1.88	0.55
2:D:156:LYS:NZ	2:D:281:LEU:HB2	2.22	0.55
2:D:264:ALA:H	2:D:490:PRO:HD3	1.71	0.55
2:D:365:THR:HG22	2:D:367:ASP:H	1.72	0.55
1:B:379:CYS:HB3	1:B:382:VAL:HG13	1.88	0.55
1:B:383:SER:O	1:C:983:ARG:NH2	2.40	0.55
1:B:599:THR:HB	1:B:608:VAL:HG12	1.88	0.55
1:C:328:ARG:HE	1:C:533:LEU:HB2	1.72	0.55
2:D:480:MET:O	2:D:483:ASP:N	2.40	0.55
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.88	0.55
1:B:318:PHE:HA	1:B:629:LEU:HB3	1.87	0.55
1:C:777:ASN:O	1:C:781:VAL:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ARG:HH22	1:A:470:THR:HG22	1.71	0.55
2:D:349:TRP:CZ2	2:D:359:LYS:HD2	2.42	0.55
1:B:745:ASP:OD1	1:B:745:ASP:N	2.34	0.55
1:C:116:SER:OG	1:C:117:LEU:N	2.40	0.55
2:D:245:ARG:CD	2:D:606:TRP:CZ3	2.89	0.55
1:B:34:ARG:HG3	1:B:216:LEU:HD22	1.88	0.54
1:B:978:ASN:OD1	1:B:979:ASP:N	2.40	0.54
2:D:539:LEU:HB2	2:D:587:TYR:CD1	2.42	0.54
1:C:930:ALA:HA	1:C:933:LYS:HD2	1.89	0.54
1:B:96:GLU:OE2	1:B:101:ILE:N	2.33	0.54
1:B:915:VAL:O	1:B:919:ASN:ND2	2.39	0.54
2:D:56:ASP:OD2	2:D:57:GLU:N	2.40	0.54
2:D:481:LYS:CE	2:D:487:VAL:HB	2.38	0.54
1:B:762:GLN:H	1:B:762:GLN:CD	2.10	0.54
2:D:372:ALA:O	2:D:376:MET:HG2	2.07	0.54
1:A:489:TYR:CZ	1:A:491:PRO:HA	2.42	0.54
2:D:108:LEU:HD11	2:D:193:ALA:HB3	1.89	0.54
2:D:481:LYS:HA	2:D:484:ILE:HG12	1.88	0.54
2:D:547:SER:O	2:D:551:GLY:N	2.41	0.54
1:C:263:ALA:HB1	1:C:265:TYR:CZ	2.42	0.54
2:D:192:ARG:HG2	2:D:197:GLU:O	2.07	0.54
1:A:363:ALA:HB1	1:A:365:TYR:CZ	2.42	0.54
1:C:328:ARG:NE	1:C:533:LEU:HB2	2.23	0.54
2:D:245:ARG:CA	2:D:606:TRP:CE2	2.90	0.54
2:D:588:PHE:HB3	2:D:592:PHE:HB2	1.90	0.54
1:B:971:GLY:N	1:C:755:GLN:HE22	2.05	0.54
2:D:169:ARG:HE	2:D:173:GLY:HA3	1.72	0.54
1:B:78:ASP:OD1	1:B:78:ASP:N	2.40	0.54
2:D:231:THR:HA	2:D:234:LYS:HB2	1.90	0.54
2:D:234:LYS:O	2:D:238:GLU:N	2.31	0.54
1:A:972:ALA:HB2	1:A:992:GLN:HB3	1.90	0.53
1:B:131:CYS:N	1:B:166:CYS:SG	2.81	0.53
1:A:200:TYR:HB2	1:A:202:LYS:HZ2	1.73	0.53
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.90	0.53
2:D:265:HIS:NE2	2:D:490:PRO:HG2	2.24	0.53
1:B:218:GLN:N	1:B:218:GLN:OE1	2.42	0.53
2:D:293:VAL:HG22	2:D:296:ALA:HB3	1.89	0.53
1:A:437:ASN:HB3	1:A:508:TYR:CE1	2.43	0.53
1:B:567:ARG:HD2	1:B:571:ASP:HA	1.90	0.53
1:B:67:ALA:HB3	1:B:264:ALA:HA	1.89	0.53
2:D:242:ALA:HA	2:D:606:TRP:CZ3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:GLU:HA	2:D:33:ASN:HD22	1.73	0.53
2:D:590:PRO:CD	2:D:591:LEU:H	2.21	0.53
1:C:287:ASP:OD1	1:C:288:ALA:N	2.42	0.53
1:C:936:ASP:OD1	1:C:937:SER:N	2.42	0.53
2:D:169:ARG:NE	2:D:498:CYS:SG	2.82	0.53
2:D:279:TYR:CD1	2:D:444:LEU:CA	2.92	0.53
2:D:144:LEU:HD12	2:D:149:ASP:OD2	2.09	0.53
1:B:354:ASN:OD1	1:B:355:ARG:N	2.42	0.52
2:D:402:GLU:O	2:D:518:ARG:HB2	2.09	0.52
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.92	0.52
2:D:338:ASP:OD1	2:D:339:ASN:N	2.41	0.52
2:D:396:ALA:HB2	2:D:560:LEU:HD22	1.92	0.52
1:A:319:ARG:N	1:A:629:LEU:HB2	2.16	0.52
2:D:330:ASN:HD22	2:D:357:ARG:HH11	1.56	0.52
1:C:76:ARG:O	1:C:258:TRP:N	2.39	0.52
2:D:404:VAL:HG11	2:D:558:LEU:HD21	1.92	0.52
1:A:1004:LEU:HA	1:A:1007:TYR:HB3	1.91	0.52
1:B:84:PHE:H	1:B:237:ARG:HA	1.75	0.52
2:D:33:ASN:O	2:D:37:GLU:CB	2.47	0.52
1:B:113:LYS:HE3	1:B:113:LYS:HA	1.92	0.52
1:B:1116:THR:OG1	1:B:1118:ASP:OD1	2.19	0.52
1:C:189:LEU:N	1:C:208:THR:O	2.33	0.52
2:D:279:TYR:O	2:D:444:LEU:HD22	2.09	0.52
2:D:314:PHE:O	2:D:317:SER:OG	2.21	0.52
1:C:159:VAL:HG23	1:C:160:TYR:CD2	2.44	0.52
1:B:1051:SER:OG	1:B:1064:HIS:ND1	2.31	0.52
2:D:474:MET:SD	2:D:474:MET:N	2.82	0.52
1:A:233:ILE:HG13	1:A:235:ILE:HG13	1.91	0.52
1:A:999:GLY:O	1:A:1003:SER:OG	2.24	0.52
1:C:220:PHE:HE2	1:C:285:ILE:HG22	1.75	0.52
2:D:142:LEU:HD12	2:D:146:PRO:HD2	1.92	0.52
2:D:196:TYR:HD2	2:D:202:TYR:HA	1.75	0.52
2:D:363:LYS:HD3	2:D:364:VAL:N	2.25	0.52
1:A:204:TYR:HA	1:A:225:PRO:HA	1.91	0.52
1:C:16:VAL:HG21	1:C:246:ARG:HH21	1.75	0.52
2:D:32:PHE:O	2:D:36:ALA:HB3	2.10	0.52
1:A:323:THR:O	1:A:324:GLU:HG3	2.10	0.51
1:B:277:LEU:HD23	1:B:285:ILE:HD13	1.91	0.51
1:C:988:GLU:O	1:C:992:GLN:HG2	2.11	0.51
1:A:101:ILE:HA	1:A:242:LEU:HA	1.91	0.51
2:D:270:MET:CE	2:D:503:LEU:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:479:GLU:O	2:D:482:ARG:HG2	2.10	0.51
1:A:43:PHE:HE2	1:C:557:LYS:HD2	1.75	0.51
1:A:197:ILE:H	1:A:202:LYS:NZ	2.08	0.51
1:A:777:ASN:HA	1:A:780:GLU:OE2	2.11	0.51
1:C:326:ILE:HD12	1:C:328:ARG:HD3	1.93	0.51
1:C:637:SER:O	1:C:639:GLY:N	2.42	0.51
2:D:169:ARG:CD	2:D:501:ALA:H	2.14	0.51
1:A:406:GLU:HB2	1:A:409:GLN:HG3	1.91	0.51
1:B:382:VAL:HG23	1:C:983:ARG:CZ	2.40	0.51
1:B:776:LYS:O	1:B:780:GLU:HG2	2.11	0.51
1:B:970:PHE:C	1:B:995:ARG:HH12	2.13	0.51
1:A:135:PHE:HD1	1:A:159:VAL:O	1.94	0.51
1:A:290:ASP:OD1	1:A:291:CYS:N	2.44	0.51
1:B:378:LYS:O	1:B:378:LYS:HG3	2.10	0.51
1:B:736:VAL:HG22	1:B:858:LEU:HD12	1.93	0.51
2:D:590:PRO:CD	2:D:591:LEU:N	2.73	0.51
1:A:755:GLN:NE2	1:C:969:ASN:HB2	2.25	0.51
1:C:159:VAL:HG23	1:C:160:TYR:HD2	1.76	0.51
1:C:1019:ARG:O	1:C:1023:ASN:ND2	2.44	0.51
1:A:990:GLU:HA	1:A:993:ILE:HG12	1.92	0.51
2:D:270:MET:HB3	2:D:502:ALA:HB3	1.93	0.51
2:D:174:LYS:HD3	2:D:496:THR:O	2.10	0.51
1:A:103:GLY:O	1:A:241:LEU:HB2	2.11	0.50
1:A:656:VAL:HG23	1:A:658:ASN:H	1.77	0.50
1:A:1000:ARG:O	1:A:1004:LEU:HG	2.11	0.50
1:B:140:PHE:CD2	1:B:244:LEU:HB2	2.45	0.50
1:C:231:ILE:HG22	1:C:233:ILE:HG12	1.92	0.50
2:D:460:ARG:O	2:D:464:PHE:CG	2.64	0.50
2:D:596:LYS:O	2:D:600:ARG:N	2.44	0.50
1:A:373:SER:O	1:A:375:SER:N	2.45	0.50
2:D:388:GLN:NE2	2:D:389:PRO:HD2	2.26	0.50
1:B:402:ILE:HD12	1:B:406:GLU:HB2	1.92	0.50
1:B:622:VAL:O	1:B:634:ARG:HG3	2.10	0.50
2:D:261:CYS:HB3	2:D:488:VAL:CG1	2.40	0.50
1:A:139:PRO:HB3	1:A:159:VAL:HA	1.92	0.50
2:D:550:ALA:HB1	2:D:553:LYS:HE2	1.93	0.50
1:B:452:LEU:HD13	1:B:492:LEU:HB3	1.94	0.50
1:C:189:LEU:HD11	1:C:210:ILE:HD13	1.93	0.50
2:D:213:ASP:N	2:D:213:ASP:OD1	2.45	0.50
2:D:241:HIS:O	2:D:245:ARG:HB2	2.12	0.50
2:D:264:ALA:HB2	2:D:489:GLU:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PHE:HD1	1:A:330:PRO:HD2	1.77	0.50
1:C:14:GLN:N	1:C:160:TYR:O	2.44	0.50
1:C:640:SER:HB3	1:C:652:GLY:HA2	1.94	0.50
1:B:206:LYS:HB2	1:B:223:LEU:HA	1.92	0.50
2:D:279:TYR:CE2	2:D:444:LEU:HD12	2.46	0.50
1:B:29:THR:O	1:B:62:VAL:HG22	2.11	0.50
1:C:100:ILE:HG22	1:C:242:LEU:HD12	1.92	0.50
2:D:239:HIS:HA	2:D:242:ALA:HB3	1.94	0.50
2:D:279:TYR:CD1	2:D:444:LEU:HG	2.42	0.50
2:D:381:TYR:OH	2:D:401:HIS:HA	2.12	0.50
2:D:550:ALA:O	2:D:554:LEU:N	2.38	0.50
1:A:622:VAL:HA	1:A:634:ARG:NE	2.27	0.50
1:B:501:ASN:HB2	1:B:505:TYR:CE1	2.47	0.50
1:C:740:MET:SD	1:C:740:MET:N	2.84	0.50
2:D:133:CYS:HB2	2:D:141:CYS:CA	2.42	0.50
2:D:433:GLU:O	2:D:436:ILE:HG22	2.11	0.50
2:D:85:LEU:HA	2:D:88:ILE:HD11	1.94	0.49
1:A:643:PHE:O	1:A:649:CYS:HB2	2.12	0.49
1:B:992:GLN:O	1:B:995:ARG:HG2	2.12	0.49
2:D:271:TRP:CE3	2:D:503:LEU:HD23	2.47	0.49
2:D:532:ILE:HB	2:D:553:LYS:HZ2	1.76	0.49
1:A:351:TYR:HB2	1:A:468:ILE:HA	1.94	0.49
1:C:882:ILE:HG23	1:C:883:THR:HG23	1.93	0.49
1:C:1049:LEU:HB3	1:C:1050:MET:SD	2.53	0.49
2:D:458:LYS:O	2:D:462:MET:HG2	2.11	0.49
1:B:247:SER:N	1:B:257:GLY:O	2.41	0.49
2:D:88:ILE:HG22	2:D:89:GLN:O	2.12	0.49
1:B:115:GLN:HG2	1:B:130:VAL:O	2.12	0.49
1:B:205:SER:OG	1:B:226:LEU:HD12	2.13	0.49
1:C:141:LEU:HD23	1:C:158:ARG:H	1.77	0.49
2:D:145:GLU:HB3	2:D:146:PRO:HD3	1.94	0.49
1:B:356:LYS:O	1:B:397:ALA:N	2.43	0.49
1:C:691:SER:OG	1:C:692:ILE:N	2.45	0.49
1:A:438:SER:OG	1:A:509:ARG:NE	2.42	0.49
1:A:766:ALA:O	1:A:770:ILE:HG23	2.13	0.49
1:B:326:ILE:HD11	1:B:534:VAL:HG12	1.94	0.49
1:C:990:GLU:O	1:C:993:ILE:HG12	2.13	0.49
2:D:77:SER:HA	2:D:100:LEU:O	2.13	0.49
2:D:403:ALA:O	2:D:407:ILE:HG23	2.12	0.49
1:A:914:ASN:OD1	1:A:914:ASN:N	2.45	0.49
1:B:420:ASP:O	1:B:460:ASN:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:LEU:HD22	2:D:168:TRP:CE2	2.47	0.49
2:D:229:THR:O	2:D:233:ILE:HG13	2.13	0.49
2:D:52:THR:HB	2:D:359:LYS:NZ	2.28	0.49
2:D:478:TRP:HA	2:D:478:TRP:CE3	2.47	0.49
1:B:568:ASP:HB3	1:B:574:ASP:HB2	1.94	0.49
2:D:162:LEU:O	2:D:166:GLU:HG2	2.13	0.49
2:D:270:MET:HE3	2:D:503:LEU:HB2	1.94	0.49
2:D:480:MET:C	2:D:484:ILE:HG12	2.33	0.49
1:A:393:THR:OG1	1:A:518:LEU:HB2	2.13	0.48
1:A:853:GLN:HB3	1:A:858:LEU:HB2	1.95	0.48
1:B:190:ARG:HB3	1:B:192:PHE:CZ	2.48	0.48
1:C:976:VAL:HG13	1:C:979:ASP:HB3	1.93	0.48
2:D:169:ARG:HH11	2:D:500:PRO:HG2	1.77	0.48
2:D:176:LEU:CB	2:D:179:LEU:HD22	2.38	0.48
2:D:453:THR:HG23	2:D:512:PHE:HD2	1.77	0.48
2:D:521:TYR:HB3	2:D:525:PHE:CE2	2.47	0.48
1:A:318:PHE:HB2	1:A:630:THR:HG22	1.94	0.48
1:B:27:ALA:HB3	1:B:64:TRP:HB3	1.94	0.48
1:C:630:THR:HB	1:C:633:TRP:CZ2	2.48	0.48
1:C:984:LEU:HD12	1:C:988:GLU:HG3	1.95	0.48
2:D:148:LEU:HD21	2:D:160:GLU:O	2.12	0.48
2:D:233:ILE:HD11	2:D:516:TYR:CE2	2.49	0.48
2:D:543:ASP:OD1	2:D:544:ILE:N	2.44	0.48
1:A:36:VAL:HG23	1:A:222:ALA:HA	1.96	0.48
1:A:157:PHE:O	1:A:157:PHE:CD2	2.66	0.48
1:A:989:ALA:O	1:A:993:ILE:HG23	2.14	0.48
1:C:106:PHE:CD2	1:C:117:LEU:HD22	2.48	0.48
2:D:255:ARG:HG3	2:D:256:ILE:HD12	1.95	0.48
1:B:121:ASN:HA	1:B:126:VAL:HG12	1.95	0.48
1:B:406:GLU:HB3	1:B:409:GLN:HB2	1.95	0.48
2:D:184:VAL:HG11	2:D:470:LYS:HE3	1.96	0.48
1:A:30:ASN:ND2	1:A:59:PHE:HD2	2.11	0.48
1:B:742:ILE:HD11	1:B:997:ILE:HA	1.96	0.48
1:C:866:THR:H	1:C:869:MET:CE	2.26	0.48
2:D:194:ASN:O	2:D:195:ASN:HB3	2.13	0.48
1:B:318:PHE:HD2	1:B:628:GLN:HG3	1.77	0.48
1:B:704:SER:HB2	1:C:790:LYS:HZ1	1.79	0.48
2:D:54:ILE:HG13	2:D:341:LYS:NZ	2.28	0.48
2:D:225:ASP:OD1	2:D:226:VAL:N	2.46	0.48
1:A:437:ASN:HA	1:A:508:TYR:HA	1.96	0.48
1:A:973:ILE:HD12	1:A:983:ARG:HH21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:THR:OG1	1:C:262:ALA:O	2.22	0.48
2:D:245:ARG:HA	2:D:606:TRP:CE2	2.48	0.48
2:D:480:MET:O	2:D:484:ILE:HG12	2.13	0.48
1:A:353:TRP:HZ3	1:A:355:ARG:HB2	1.78	0.48
1:B:133:PHE:HB2	1:B:135:PHE:CZ	2.49	0.48
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.43	0.48
1:A:697:MET:N	1:A:697:MET:SD	2.87	0.48
1:B:321:GLN:HB2	1:B:626:ALA:O	2.14	0.48
1:A:755:GLN:NE2	1:C:971:GLY:H	2.11	0.48
1:B:666:ILE:HD12	1:B:670:ILE:HG22	1.96	0.48
2:D:460:ARG:HB2	2:D:464:PHE:CZ	2.49	0.48
1:A:485:GLY:N	1:A:488:CYS:HB2	2.29	0.47
1:C:81:VAL:HG11	1:C:237:ARG:HH11	1.78	0.47
1:C:85:ASN:OD1	1:C:85:ASN:N	2.46	0.47
2:D:279:TYR:OH	2:D:441:LYS:HA	2.14	0.47
1:B:231:ILE:HG22	1:B:233:ILE:HG23	1.95	0.47
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.96	0.47
2:D:34:TYR:O	2:D:37:GLU:HG2	2.14	0.47
2:D:180:TYR:OH	2:D:509:ASP:OD1	2.32	0.47
1:A:405:ASP:N	1:A:504:GLY:O	2.47	0.47
1:A:513:LEU:HD12	1:A:513:LEU:H	1.79	0.47
1:B:229:LEU:HG	1:B:231:ILE:HG13	1.96	0.47
1:B:471:GLU:O	1:B:491:PRO:HG3	2.14	0.47
1:C:1091:ARG:NE	1:C:1118:ASP:O	2.45	0.47
2:D:143:LEU:O	2:D:144:LEU:HB3	2.13	0.47
2:D:200:GLY:HA3	2:D:464:PHE:CE1	2.49	0.47
2:D:271:TRP:HE3	2:D:503:LEU:HD23	1.78	0.47
2:D:355:ASP:OD2	2:D:357:ARG:NH2	2.47	0.47
1:B:334:ASN:HB3	1:B:361:CYS:HA	1.95	0.47
1:C:1045:LYS:O	1:C:1066:THR:HG21	2.14	0.47
2:D:327:PHE:HA	2:D:356:PHE:O	2.15	0.47
2:D:412:ALA:HA	2:D:417:HIS:HB3	1.96	0.47
1:C:115:GLN:HA	1:C:132:GLU:HG3	1.96	0.47
1:A:322:PRO:HG3	1:A:549:THR:HG21	1.95	0.47
2:D:201:ASP:HA	2:D:204:ARG:HB2	1.97	0.47
1:A:27:ALA:HB3	1:A:64:TRP:HB3	1.96	0.47
1:A:612:TYR:HE2	1:A:651:ILE:HD12	1.80	0.47
2:D:115:ARG:NH2	2:D:186:LEU:HB3	2.29	0.47
2:D:169:ARG:O	2:D:173:GLY:N	2.43	0.47
2:D:458:LYS:HD2	2:D:462:MET:HE1	1.97	0.47
2:D:460:ARG:NE	2:D:464:PHE:HE2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:PHE:HD1	1:A:517:LEU:HA	1.79	0.47
1:A:930:ALA:O	1:A:934:ILE:HG22	2.15	0.47
1:B:914:ASN:O	1:B:918:GLU:HG3	2.15	0.47
1:B:970:PHE:O	1:B:995:ARG:NH1	2.44	0.47
1:C:866:THR:H	1:C:869:MET:HE2	1.79	0.47
2:D:22:GLU:HG2	2:D:93:ILE:HD12	1.96	0.47
2:D:379:ILE:O	2:D:383:MET:HB2	2.15	0.47
1:A:141:LEU:HD23	1:A:142:GLY:N	2.30	0.47
1:B:906:PHE:HA	1:B:909:ILE:HG22	1.97	0.47
1:B:935:GLN:O	1:B:938:LEU:HD12	2.15	0.47
1:C:160:TYR:CE1	1:C:163:ALA:HB2	2.50	0.47
1:C:1020:ALA:HA	1:C:1023:ASN:HD22	1.79	0.47
2:D:21:THR:HA	2:D:24:LEU:HG	1.97	0.47
2:D:307:ILE:HD12	2:D:369:PHE:HD1	1.78	0.47
2:D:569:ALA:O	2:D:573:VAL:HG22	2.14	0.47
1:B:984:LEU:HD13	1:B:988:GLU:OE1	2.15	0.46
1:C:126:VAL:HG11	1:C:175:PHE:CZ	2.50	0.46
1:C:636:TYR:CG	1:C:637:SER:N	2.83	0.46
1:A:189:LEU:HB2	1:A:210:ILE:HB	1.97	0.46
1:A:342:PHE:HE1	1:A:511:VAL:HG11	1.79	0.46
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.97	0.46
1:B:451:TYR:HB2	1:B:495:TYR:CE2	2.46	0.46
1:C:115:GLN:NE2	1:C:132:GLU:OE2	2.48	0.46
1:C:129:LYS:HD3	1:C:169:GLU:HG2	1.96	0.46
2:D:262:LEU:HD21	2:D:266:LEU:HB2	1.97	0.46
1:B:702:GLU:OE2	1:C:790:LYS:NZ	2.48	0.46
1:C:328:ARG:HH21	1:C:533:LEU:HD12	1.80	0.46
1:A:110:LEU:HD23	1:A:237:ARG:HG3	1.98	0.46
1:A:141:LEU:HD23	1:A:142:GLY:H	1.79	0.46
1:A:387:LEU:HD21	1:A:515:PHE:CE1	2.51	0.46
1:C:126:VAL:HB	1:C:174:PRO:HA	1.97	0.46
2:D:148:LEU:CD1	2:D:160:GLU:HG3	2.46	0.46
1:B:438:SER:OG	1:B:442:ASP:OD2	2.26	0.46
1:B:1092:GLU:N	1:B:1092:GLU:OE2	2.49	0.46
1:C:328:ARG:HB3	1:C:543:PHE:CE1	2.49	0.46
2:D:303:ASP:O	2:D:307:ILE:HG23	2.14	0.46
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.97	0.46
1:C:765:ARG:HA	1:C:765:ARG:NE	2.30	0.46
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.45	0.46
2:D:439:LEU:HD13	2:D:594:TRP:CZ3	2.50	0.46
1:A:631:PRO:HG2	1:A:633:TRP:NE1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:ARG:HE	1:C:42:VAL:HG11	1.79	0.46
1:C:93:ALA:HB3	1:C:266:TYR:CD1	2.51	0.46
1:C:983:ARG:HG3	1:C:984:LEU:HD22	1.96	0.46
2:D:191:ALA:HA	2:D:194:ASN:HB2	1.97	0.46
1:A:363:ALA:HB2	1:A:524:VAL:HG22	1.98	0.46
1:B:28:TYR:HD1	1:B:61:ASN:HB3	1.80	0.46
2:D:116:LEU:O	2:D:120:LEU:HG	2.15	0.46
1:B:23:GLN:N	1:B:23:GLN:OE1	2.49	0.46
1:B:699:LEU:HD21	1:C:869:MET:HB3	1.98	0.46
2:D:236:LEU:HA	2:D:592:PHE:CE1	2.51	0.46
2:D:265:HIS:O	2:D:266:LEU:HD13	2.15	0.46
1:A:426:PRO:HB3	1:A:463:PRO:HB3	1.98	0.46
1:A:1010:GLN:HE22	1:A:1011:GLN:HE21	1.64	0.46
1:B:357:ARG:HG3	1:B:396:TYR:CE1	2.51	0.46
1:B:462:LYS:HD2	1:B:463:PRO:O	2.16	0.46
1:B:934:ILE:O	1:B:938:LEU:HG	2.16	0.46
1:C:64:TRP:CE3	1:C:266:TYR:HE2	2.34	0.46
2:D:384:ALA:HB2	2:D:558:LEU:HB3	1.98	0.46
2:D:456:LEU:HD23	2:D:512:PHE:CD1	2.50	0.46
1:C:739:THR:O	1:C:744:GLY:N	2.46	0.45
2:D:245:ARG:HB3	2:D:606:TRP:CZ3	2.42	0.45
1:A:550:GLY:CA	1:A:589:PRO:HA	2.46	0.45
1:B:1118:ASP:OD1	1:B:1118:ASP:N	2.38	0.45
2:D:48:TRP:CD2	2:D:359:LYS:HE3	2.51	0.45
2:D:112:LYS:HA	2:D:115:ARG:HD3	1.99	0.45
2:D:305:ARG:NH2	2:D:309:LYS:HB2	2.32	0.45
2:D:320:LEU:HD13	2:D:380:GLN:HG2	1.98	0.45
1:C:239:GLN:HG2	1:C:240:THR:H	1.81	0.45
2:D:158:TYR:CE1	2:D:265:HIS:CE1	3.03	0.45
2:D:520:ILE:HD13	2:D:581:VAL:HG12	1.98	0.45
1:A:631:PRO:HG2	1:A:633:TRP:HE1	1.80	0.45
1:A:993:ILE:O	1:A:997:ILE:HG13	2.16	0.45
1:C:869:MET:SD	1:C:869:MET:N	2.87	0.45
2:D:115:ARG:CZ	2:D:186:LEU:HD13	2.47	0.45
2:D:262:LEU:HB3	2:D:486:GLY:O	2.17	0.45
2:D:479:GLU:HA	2:D:482:ARG:CD	2.47	0.45
1:A:590:CYS:O	1:B:855:PHE:HE1	2.00	0.45
1:B:319:ARG:H	1:B:629:LEU:CB	2.30	0.45
1:B:532:ASN:OD1	1:B:533:LEU:N	2.48	0.45
1:B:761:THR:HB	1:B:765:ARG:HH21	1.81	0.45
1:A:758:SER:O	1:A:762:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:ASP:OD1	1:A:979:ASP:N	2.50	0.45
1:B:357:ARG:HH22	1:B:359:SER:HB3	1.82	0.45
1:B:359:SER:OG	1:B:360:ASN:N	2.50	0.45
1:C:133:PHE:HB2	1:C:135:PHE:CE2	2.51	0.45
2:D:142:LEU:HD21	2:D:148:LEU:H	1.81	0.45
2:D:230:PHE:HA	2:D:233:ILE:HD12	1.97	0.45
2:D:271:TRP:CZ3	2:D:506:VAL:HB	2.52	0.45
1:A:141:LEU:HA	1:A:156:GLU:HB2	1.99	0.45
1:A:1091:ARG:HB3	1:A:1092:GLU:OE1	2.16	0.45
1:B:930:ALA:O	1:B:934:ILE:HG22	2.17	0.45
1:B:320:VAL:HB	1:B:627:ASP:OD1	2.17	0.45
1:B:825:LYS:NZ	1:B:942:PRO:HA	2.32	0.45
2:D:148:LEU:CD2	2:D:164:ALA:HB2	2.46	0.45
2:D:279:TYR:CE1	2:D:444:LEU:CA	2.97	0.45
1:B:480:CYS:HB3	1:B:483:VAL:O	2.17	0.45
2:D:157:ASP:HB3	2:D:160:GLU:HB2	1.98	0.45
1:B:101:ILE:HG23	1:B:241:LEU:O	2.17	0.44
1:B:913:GLN:H	1:B:913:GLN:HG2	1.60	0.44
2:D:169:ARG:CZ	2:D:498:CYS:SG	3.04	0.44
2:D:232:GLN:OE1	2:D:581:VAL:HG21	2.17	0.44
2:D:245:ARG:HG2	2:D:606:TRP:O	2.17	0.44
1:A:139:PRO:HB3	1:A:159:VAL:HG22	1.98	0.44
1:A:375:SER:HG	1:A:377:PHE:HE2	1.63	0.44
1:B:326:ILE:O	1:B:542:ASN:N	2.49	0.44
1:A:109:THR:HA	1:A:237:ARG:HD3	2.00	0.44
1:A:115:GLN:HA	1:A:131:CYS:O	2.17	0.44
1:A:133:PHE:HD2	1:A:160:TYR:CG	2.35	0.44
1:A:890:ALA:HB1	1:C:1046:GLY:HA2	1.98	0.44
1:B:137:ASN:OD1	1:B:138:ASP:N	2.50	0.44
1:B:662:CYS:HB2	1:B:671:CYS:HB2	1.49	0.44
2:D:173:GLY:HA3	2:D:498:CYS:SG	2.58	0.44
2:D:308:PHE:HZ	2:D:323:MET:SD	2.41	0.44
1:A:970:PHE:HD1	1:A:995:ARG:HE	1.65	0.44
1:C:160:TYR:HE1	1:C:163:ALA:HB2	1.82	0.44
2:D:324:THR:HG1	2:D:327:PHE:HD2	1.65	0.44
1:A:31:SER:O	1:A:59:PHE:N	2.38	0.44
1:A:156:GLU:O	1:A:158:ARG:N	2.47	0.44
1:A:294:ASP:OD2	1:A:297:SER:N	2.31	0.44
1:A:933:LYS:HA	1:A:933:LYS:HD2	1.71	0.44
1:A:202:LYS:HB2	1:A:202:LYS:HE2	1.73	0.44
1:A:386:LYS:HZ2	1:A:390:LEU:HG	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ILE:HD11	1:A:510:VAL:HG11	1.99	0.44
1:C:328:ARG:HD2	1:C:328:ARG:HA	1.75	0.44
2:D:148:LEU:HD23	2:D:164:ALA:HB2	2.00	0.44
1:A:675:GLN:HB2	1:A:693:ILE:HD11	2.00	0.44
1:B:773:GLU:OE2	1:B:774:GLN:NE2	2.45	0.44
1:C:65:PHE:CE2	1:C:67:ALA:HB2	2.53	0.44
1:C:110:LEU:HD22	1:C:135:PHE:CE1	2.53	0.44
2:D:28:PHE:CZ	2:D:76:GLU:HB3	2.51	0.44
2:D:513:ILE:N	2:D:513:ILE:HD12	2.32	0.44
1:A:102:ARG:O	1:A:121:ASN:HB2	2.18	0.43
1:A:644:GLN:HA	1:A:649:CYS:CB	2.48	0.43
1:B:66:HIS:CD2	1:B:68:ILE:HB	2.53	0.43
1:C:731:MET:HE1	1:C:1015:ALA:HA	2.00	0.43
2:D:245:ARG:HG2	2:D:606:TRP:CE2	2.33	0.43
2:D:478:TRP:HA	2:D:478:TRP:HE3	1.83	0.43
1:A:605:SER:OG	1:A:606:ASN:N	2.50	0.43
1:C:16:VAL:HG21	1:C:246:ARG:NH2	2.33	0.43
2:D:187:LYS:HA	2:D:190:MET:HG3	2.00	0.43
1:A:702:GLU:HG3	1:B:790:LYS:NZ	2.31	0.43
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.17	0.43
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.51	0.43
1:B:356:LYS:HB3	1:B:397:ALA:HB3	1.99	0.43
1:C:224:GLU:N	1:C:224:GLU:OE1	2.51	0.43
1:A:363:ALA:HB3	1:A:525:CYS:C	2.38	0.43
1:A:994:ASP:HA	1:A:997:ILE:HD12	1.99	0.43
1:B:83:PRO:HA	1:B:237:ARG:HG3	2.01	0.43
1:C:240:THR:OG1	1:C:241:LEU:N	2.52	0.43
2:D:478:TRP:HZ2	2:D:489:GLU:HG2	1.81	0.43
1:A:629:LEU:HD23	1:A:629:LEU:HA	1.86	0.43
1:B:95:THR:OG1	1:B:264:ALA:O	2.21	0.43
1:B:280:ASN:CG	1:B:284:THR:HG22	2.39	0.43
1:B:948:LEU:O	1:B:952:VAL:HG23	2.18	0.43
1:B:989:ALA:O	1:B:993:ILE:HG12	2.18	0.43
1:C:192:PHE:HE1	1:C:205:SER:HG	1.64	0.43
2:D:22:GLU:HG3	2:D:89:GLN:O	2.18	0.43
1:B:122:ASN:N	1:B:125:ASN:O	2.51	0.43
1:B:355:ARG:HB2	1:B:466:ARG:HH22	1.84	0.43
1:C:30:ASN:HD21	1:C:59:PHE:HD1	1.67	0.43
1:A:119:ILE:HD12	1:A:119:ILE:H	1.83	0.43
1:A:133:PHE:HD2	1:A:160:TYR:CD1	2.36	0.43
1:A:206:LYS:HD3	1:A:224:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ALA:HB3	1:C:64:TRP:CD1	2.53	0.43
1:C:65:PHE:O	1:C:264:ALA:HA	2.18	0.43
2:D:84:PRO:HB2	2:D:86:GLU:OE1	2.19	0.43
1:A:138:ASP:HA	1:A:139:PRO:HD3	1.89	0.43
1:C:66:HIS:HD2	1:C:68:ILE:HD11	1.84	0.43
2:D:540:TYR:C	2:D:541:LYS:HD3	2.39	0.43
2:D:547:SER:OG	2:D:550:ALA:HB3	2.19	0.43
1:C:854:LYS:HA	1:C:858:LEU:O	2.19	0.43
2:D:477:TRP:HZ3	2:D:484:ILE:HG13	1.83	0.43
1:A:244:LEU:H	1:A:244:LEU:HD23	1.84	0.43
1:A:1029:MET:HE2	1:A:1029:MET:HA	2.01	0.43
1:B:763:LEU:HD13	1:B:1004:LEU:HD22	2.00	0.43
2:D:105:SER:OG	2:D:113:ARG:HD3	2.19	0.43
2:D:349:TRP:N	2:D:349:TRP:CD1	2.86	0.43
1:B:359:SER:OG	1:B:360:ASN:OD1	2.31	0.42
1:C:88:VAL:HA	1:C:268:GLY:O	2.18	0.42
1:C:914:ASN:O	1:C:918:GLU:HG3	2.19	0.42
1:C:1142:GLN:O	1:C:1145:LEU:HG	2.19	0.42
2:D:237:TYR:CZ	2:D:454:TYR:HE2	2.37	0.42
2:D:458:LYS:HD3	2:D:458:LYS:HA	1.67	0.42
1:A:630:THR:HB	1:A:633:TRP:CZ2	2.54	0.42
1:A:1083:HIS:ND1	1:A:1136:THR:HA	2.35	0.42
1:B:959:LEU:O	1:B:963:VAL:HG12	2.19	0.42
1:C:133:PHE:HD2	1:C:162:SER:O	2.02	0.42
2:D:469:PRO:O	2:D:469:PRO:HD2	2.18	0.42
1:B:411:ALA:HB3	1:B:414:GLN:HG3	2.00	0.42
1:A:396:TYR:O	1:A:514:SER:HB3	2.20	0.42
1:A:436:TRP:O	1:A:509:ARG:N	2.51	0.42
1:B:457:ARG:HG2	1:B:458:LYS:N	2.33	0.42
1:B:1010:GLN:HB3	1:B:1014:ARG:NH1	2.32	0.42
2:D:96:GLN:O	2:D:100:LEU:N	2.52	0.42
2:D:252:TYR:HD2	2:D:256:ILE:HD13	1.84	0.42
2:D:541:LYS:HD3	2:D:541:LYS:N	2.35	0.42
1:A:197:ILE:H	1:A:202:LYS:HZ3	1.67	0.42
1:A:755:GLN:HE21	1:C:969:ASN:HB2	1.84	0.42
1:C:233:ILE:HD13	1:C:233:ILE:HA	1.86	0.42
2:D:307:ILE:HB	2:D:369:PHE:CD1	2.55	0.42
2:D:315:PHE:CD1	2:D:320:LEU:HD12	2.54	0.42
2:D:590:PRO:HB2	2:D:594:TRP:CZ3	2.55	0.42
1:A:386:LYS:NZ	1:A:390:LEU:HG	2.34	0.42
1:B:646:ARG:O	1:B:646:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:HD3	1:C:98:SER:H	1.84	0.42
1:C:120:VAL:O	1:C:126:VAL:HA	2.20	0.42
2:D:81:LYS:HA	2:D:101:GLN:CG	2.36	0.42
2:D:112:LYS:O	2:D:115:ARG:NH1	2.53	0.42
2:D:117:ASN:HA	2:D:120:LEU:HG	2.00	0.42
1:A:372:ALA:O	1:A:373:SER:O	2.37	0.42
1:A:703:ASN:OD1	1:A:704:SER:N	2.53	0.42
1:A:990:GLU:OE1	1:A:990:GLU:N	2.53	0.42
1:B:357:ARG:HH12	1:B:359:SER:CB	2.33	0.42
1:B:402:ILE:HG13	1:B:403:ARG:O	2.20	0.42
1:C:170:TYR:CD1	1:C:229:LEU:HD21	2.55	0.42
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.86	0.42
1:A:351:TYR:CE1	1:A:452:LEU:HD11	2.55	0.42
2:D:115:ARG:NE	2:D:186:LEU:HD13	2.35	0.42
2:D:160:GLU:HA	2:D:163:TRP:CE3	2.55	0.42
2:D:271:TRP:CH2	2:D:506:VAL:HB	2.54	0.42
2:D:30:GLU:HA	2:D:33:ASN:ND2	2.35	0.42
2:D:455:MET:HG3	2:D:477:TRP:CH2	2.54	0.42
2:D:593:THR:O	2:D:596:LYS:N	2.52	0.42
1:A:320:VAL:HG23	1:A:591:SER:O	2.20	0.42
1:A:426:PRO:HG3	1:A:464:PHE:CE2	2.55	0.42
1:A:1001:LEU:O	1:A:1004:LEU:HD12	2.20	0.42
1:B:130:VAL:HB	1:B:166:CYS:HB2	2.02	0.42
1:B:605:SER:OG	1:B:606:ASN:N	2.53	0.42
1:C:199:GLY:HA2	1:C:232:GLY:HA2	2.02	0.42
1:C:759:PHE:HA	1:C:762:GLN:OE1	2.20	0.42
2:D:52:THR:HB	2:D:359:LYS:HZ3	1.84	0.42
2:D:158:TYR:OH	2:D:266:LEU:HD21	2.19	0.42
2:D:388:GLN:CD	2:D:389:PRO:HD2	2.40	0.42
1:B:328:ARG:HE	1:B:579:PRO:HD2	1.84	0.41
1:C:15:CYS:HB2	1:C:136:CYS:HB3	1.90	0.41
2:D:51:ASN:ND2	2:D:349:TRP:HH2	2.17	0.41
2:D:200:GLY:HA3	2:D:464:PHE:CD2	2.54	0.41
2:D:212:ALA:HB3	2:D:565:PRO:HG2	2.02	0.41
2:D:249:MET:HG3	2:D:250:ASP:N	2.35	0.41
1:A:777:ASN:O	1:A:781:VAL:HG12	2.21	0.41
1:A:968:SER:HB2	1:A:970:PHE:CE2	2.55	0.41
1:B:106:PHE:HB3	1:B:235:ILE:HD11	2.02	0.41
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.86	0.41
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.83	0.41
1:A:445:VAL:HA	1:A:499:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.55	0.41
2:D:279:TYR:CD1	2:D:444:LEU:HA	2.55	0.41
1:B:328:ARG:NH2	1:B:580:GLN:HB2	2.35	0.41
1:B:497:PHE:HD1	1:B:497:PHE:HA	1.77	0.41
1:C:15:CYS:SG	1:C:16:VAL:N	2.93	0.41
2:D:241:HIS:CD2	2:D:606:TRP:HH2	2.39	0.41
2:D:248:LEU:HD22	2:D:278:LEU:HD22	2.02	0.41
2:D:351:LEU:HD13	2:D:357:ARG:HD2	2.02	0.41
2:D:379:ILE:HD13	2:D:379:ILE:HA	1.97	0.41
2:D:464:PHE:N	2:D:464:PHE:CD1	2.87	0.41
2:D:588:PHE:O	2:D:591:LEU:N	2.54	0.41
1:A:318:PHE:O	1:A:592:PHE:HB2	2.19	0.41
1:C:65:PHE:CD2	1:C:67:ALA:HB2	2.55	0.41
1:C:106:PHE:HD2	1:C:117:LEU:HD22	1.85	0.41
2:D:271:TRP:HB3	2:D:452:PHE:CZ	2.56	0.41
2:D:279:TYR:CD2	2:D:444:LEU:CD1	3.03	0.41
1:A:490:PHE:HE1	1:A:492:LEU:HB2	1.85	0.41
1:C:30:ASN:OD1	1:C:59:PHE:HA	2.20	0.41
1:A:417:LYS:O	1:A:421:TYR:HB2	2.20	0.41
1:A:990:GLU:OE2	1:A:991:VAL:HG23	2.20	0.41
1:A:1017:GLU:OE2	1:A:1018:ILE:HG12	2.21	0.41
1:C:1049:LEU:HD23	1:C:1049:LEU:HA	1.89	0.41
2:D:279:TYR:CD2	2:D:279:TYR:CB	2.84	0.41
2:D:457:GLU:HG2	2:D:513:ILE:HG13	2.01	0.41
2:D:586:ASN:HA	2:D:589:GLU:HB2	2.02	0.41
1:A:200:TYR:HA	1:A:230:PRO:HA	2.03	0.41
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	2.03	0.41
1:B:115:GLN:HA	1:B:132:GLU:HG2	2.01	0.41
1:B:241:LEU:O	1:B:242:LEU:HD12	2.21	0.41
1:A:201:PHE:CE2	1:A:203:ILE:HB	2.56	0.41
1:A:369:TYR:OH	1:A:384:PRO:O	2.23	0.41
1:A:489:TYR:OH	2:D:31:LYS:HD3	2.21	0.41
1:B:126:VAL:HG11	1:B:175:PHE:CD1	2.56	0.41
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.54	0.41
1:C:105:ILE:HD11	1:C:239:GLN:HB3	2.02	0.41
1:C:195:LYS:HE2	1:C:204:TYR:CE1	2.55	0.41
1:C:543:PHE:CE2	1:C:578:ASP:HA	2.53	0.41
1:C:805:ILE:HD12	1:C:805:ILE:HA	1.88	0.41
1:C:938:LEU:HD23	1:C:938:LEU:HA	1.91	0.41
1:B:117:LEU:O	1:B:118:LEU:HD23	2.21	0.41
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:962:LEU:HD22	1:B:1007:TYR:CG	2.56	0.41
2:D:319:GLY:HA3	2:D:548:ARG:HH21	1.85	0.41
2:D:326:GLY:HA2	2:D:329:GLN:HE21	1.85	0.41
2:D:454:TYR:OH	2:D:484:ILE:HD12	2.20	0.41
2:D:597:GLU:HA	2:D:600:ARG:HG3	2.03	0.41
1:A:112:SER:OG	1:A:134:GLN:HG3	2.20	0.40
1:C:814:LYS:HE2	1:C:814:LYS:HB2	1.87	0.40
2:D:187:LYS:HB3	2:D:199:TYR:HB3	2.02	0.40
2:D:460:ARG:HB2	2:D:464:PHE:CE2	2.56	0.40
1:A:522:ALA:O	1:A:525:CYS:SG	2.79	0.40
1:B:473:TYR:HB2	1:B:491:PRO:HB3	2.03	0.40
1:B:662:CYS:HB3	1:B:697:MET:HB3	2.03	0.40
1:C:617:CYS:HA	1:C:620:VAL:HB	2.02	0.40
1:C:737:ASP:OD1	1:C:738:CYS:N	2.54	0.40
1:A:1001:LEU:O	1:A:1005:GLN:CB	2.64	0.40
1:C:14:GLN:HB2	1:C:158:ARG:HD3	2.02	0.40
1:C:986:PRO:O	1:C:990:GLU:HG2	2.21	0.40
1:B:567:ARG:NH1	1:B:568:ASP:O	2.54	0.40
1:B:716:THR:OG1	1:B:1071:GLN:O	2.36	0.40
1:B:790:LYS:HE2	1:B:790:LYS:HB2	1.84	0.40
1:B:941:THR:HA	1:B:942:PRO:HD3	1.94	0.40
2:D:54:ILE:HG13	2:D:341:LYS:HZ1	1.87	0.40
2:D:349:TRP:HB2	2:D:357:ARG:O	2.21	0.40
2:D:407:ILE:HG13	2:D:408:MET:H	1.85	0.40
2:D:442:GLN:HG3	2:D:446:ILE:HD12	2.03	0.40
1:A:357:ARG:HG3	1:A:394:ASN:HB3	2.03	0.40
1:A:1105:THR:OG1	1:A:1111:GLU:OE1	2.32	0.40
2:D:532:ILE:HB	2:D:553:LYS:NZ	2.37	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	1046/1269 (82%)	969 (93%)	72 (7%)	5 (0%)	25	58
1	B	1049/1269 (83%)	982 (94%)	65 (6%)	2 (0%)	44	73
1	C	850/1269 (67%)	790 (93%)	60 (7%)	0	100	100
2	D	595/771 (77%)	531 (89%)	62 (10%)	2 (0%)	37	68
All	All	3540/4578 (77%)	3272 (92%)	259 (7%)	9 (0%)	38	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	SER
1	A	388	ASN
2	D	403	ALA
1	A	324	GLU
1	A	235	ILE
2	D	500	PRO
1	A	374	PHE
1	B	638	THR
1	B	622	VAL

### 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	929/1101 (84%)	916 (99%)	13 (1%)	62	77
1	B	930/1101 (84%)	910 (98%)	20 (2%)	47	66
1	C	762/1101 (69%)	746 (98%)	16 (2%)	48	68
2	D	525/676 (78%)	510 (97%)	15 (3%)	37	60
All	All	3146/3979 (79%)	3082 (98%)	64 (2%)	50	69

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	137	ASN

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Mol	Chain	Res	Type
1	A	158	ARG
1	A	175	PHE
1	A	321	GLN
1	A	374	PHE
1	A	403	ARG
1	A	513	LEU
1	A	515	PHE
1	A	633	TRP
1	A	754	LEU
1	A	856	ASN
1	A	1004	LEU
1	B	80	PRO
1	B	106	PHE
1	B	121	ASN
1	B	153	MET
1	B	175	PHE
1	B	190	ARG
1	B	380	TYR
1	B	462	LYS
1	B	464	PHE
1	B	497	PHE
1	B	567	ARG
1	B	590	CYS
1	B	633	TRP
1	B	634	ARG
1	B	649	CYS
1	B	697	MET
1	B	749	CYS
1	B	759	PHE
1	B	938	LEU
1	B	1118	ASP
1	C	15	CYS
1	C	79	ASN
1	C	121	ASN
1	C	135	PHE
1	C	136	CYS
1	C	170	TYR
1	C	198	ASP
1	C	265	TYR
1	C	329	PHE
1	C	590	CYS
1	C	636	TYR

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Mol	Chain	Res	Type
1	C	671	CYS
1	C	754	LEU
1	C	780	GLU
1	C	886	TRP
1	C	1050	MET
2	D	26	LYS
2	D	32	PHE
2	D	123	MET
2	D	128	SER
2	D	159	ASN
2	D	176	LEU
2	D	190	MET
2	D	331	SER
2	D	381	TYR
2	D	494	ASP
2	D	497	TYR
2	D	512	PHE
2	D	568	PHE
2	D	582	ARG
2	D	609	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1011	GLN
1	B	644	GLN
1	C	755	GLN
1	C	774	GLN
1	C	1023	ASN
2	D	33	ASN
2	D	265	HIS
2	D	330	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

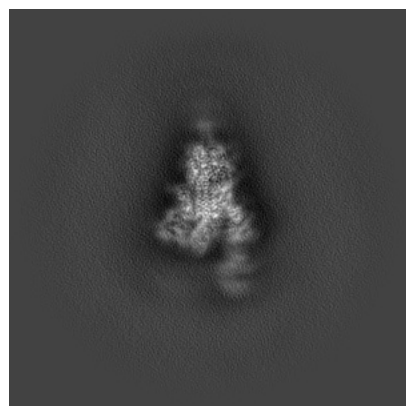
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41143. These allow visual inspection of the internal detail of the map and identification of artifacts.

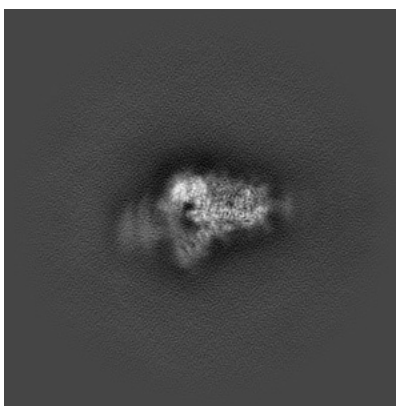
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

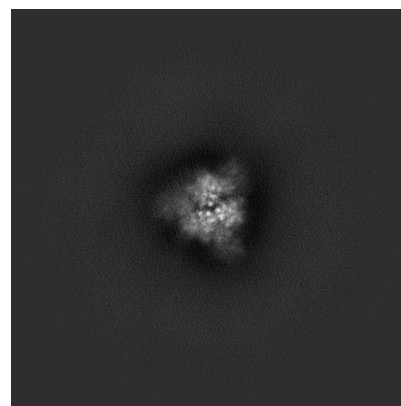
#### 6.1.1 Primary map



X

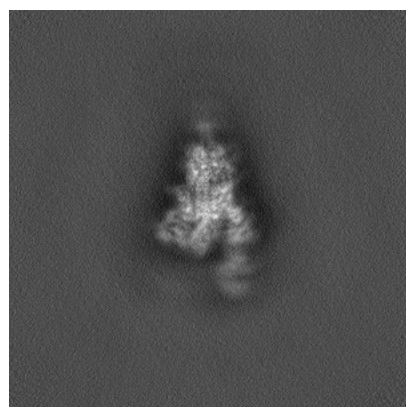


Y

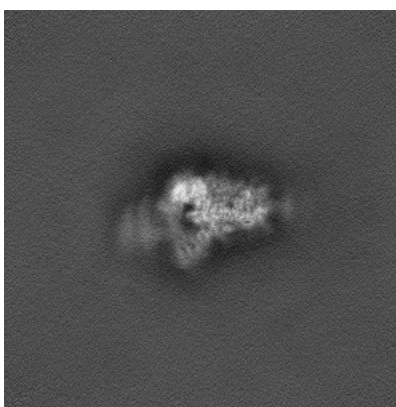


Z

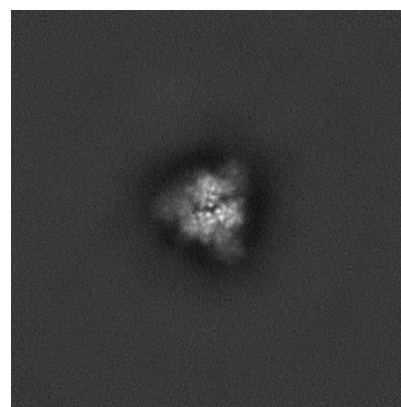
#### 6.1.2 Raw map



X



Y

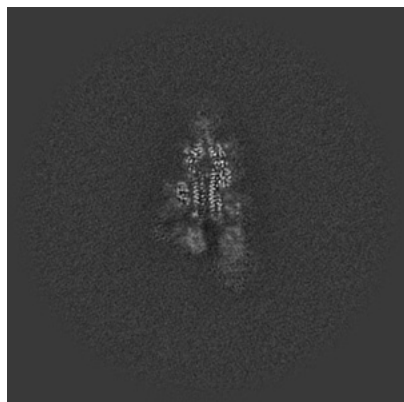


Z

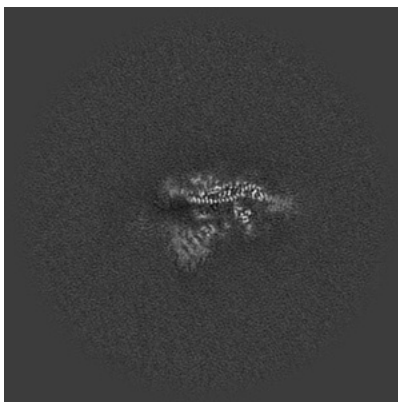
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

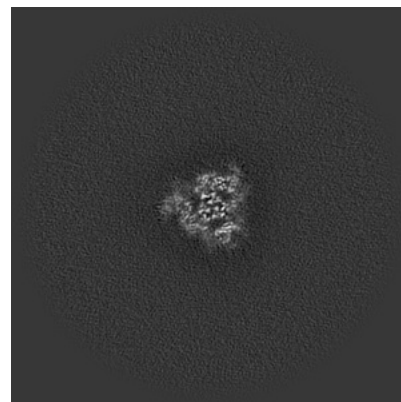
### 6.2.1 Primary map



X Index: 256



Y Index: 256

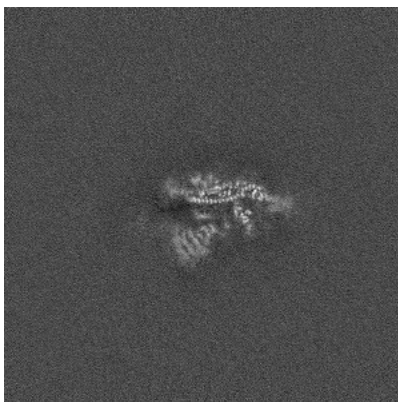


Z Index: 256

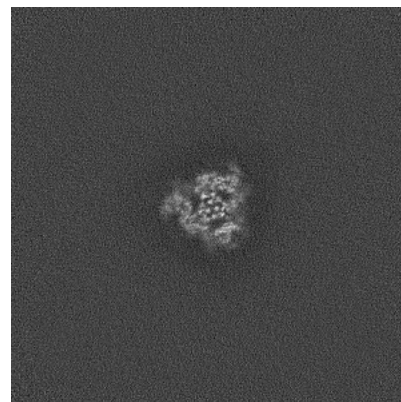
### 6.2.2 Raw map



X Index: 256



Y Index: 256



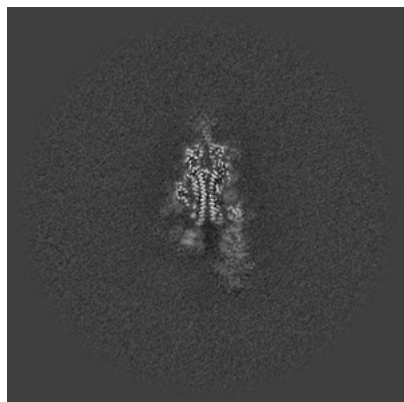
Z Index: 256

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



## 6.3 Largest variance slices [i](#)

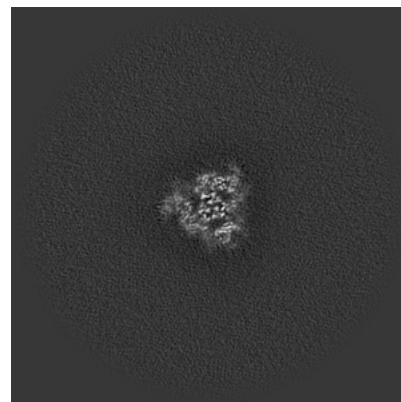
### 6.3.1 Primary map



X Index: 253

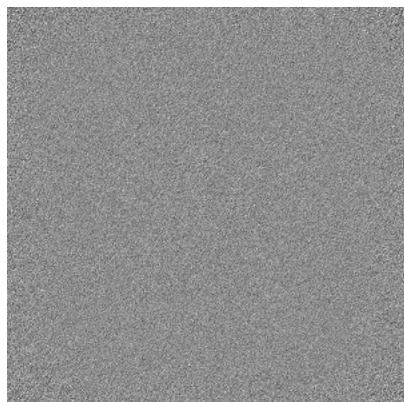


Y Index: 248

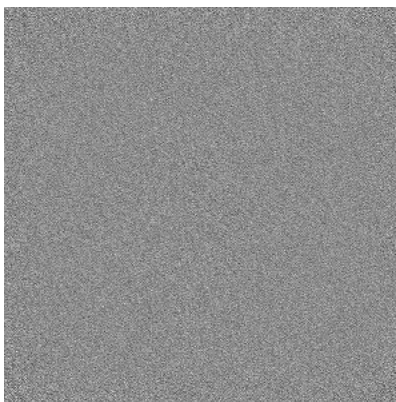


Z Index: 256

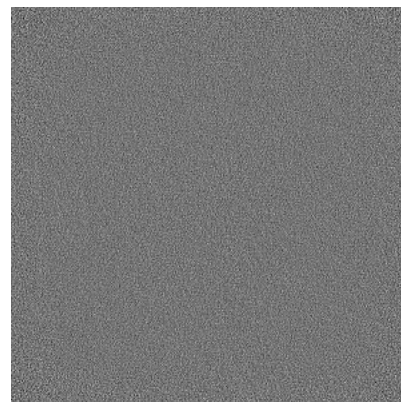
### 6.3.2 Raw map



X Index: 0



Y Index: 0

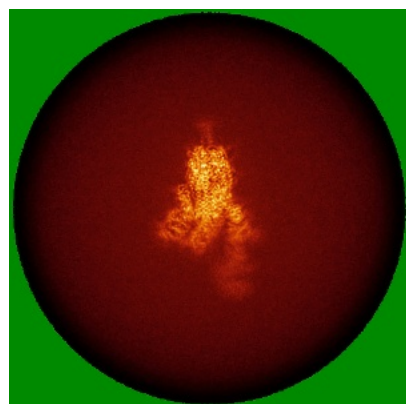


Z Index: 0

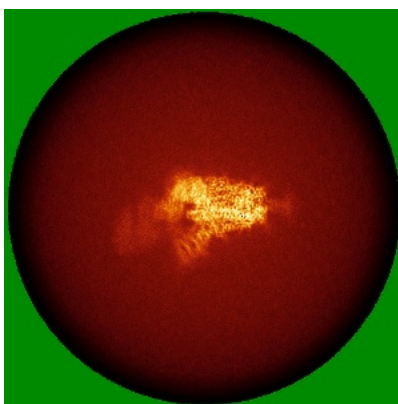
The images above show the largest variance slices of the map in three orthogonal directions.

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

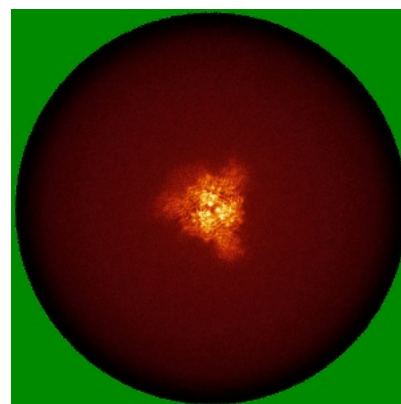
### 6.4.1 Primary map



X

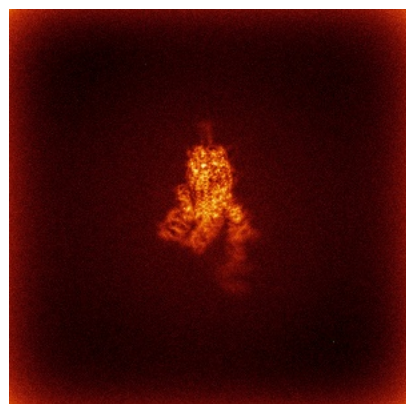


Y

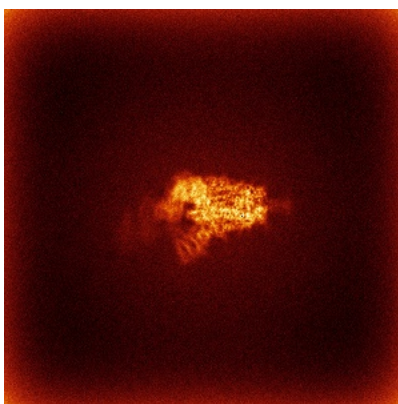


Z

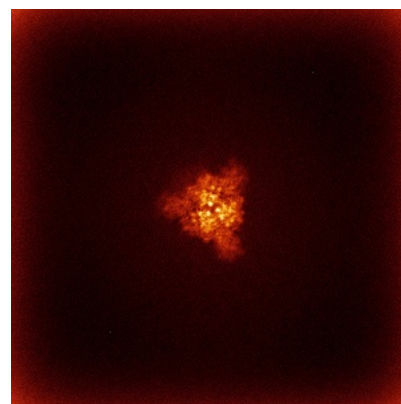
### 6.4.2 Raw map



X



Y

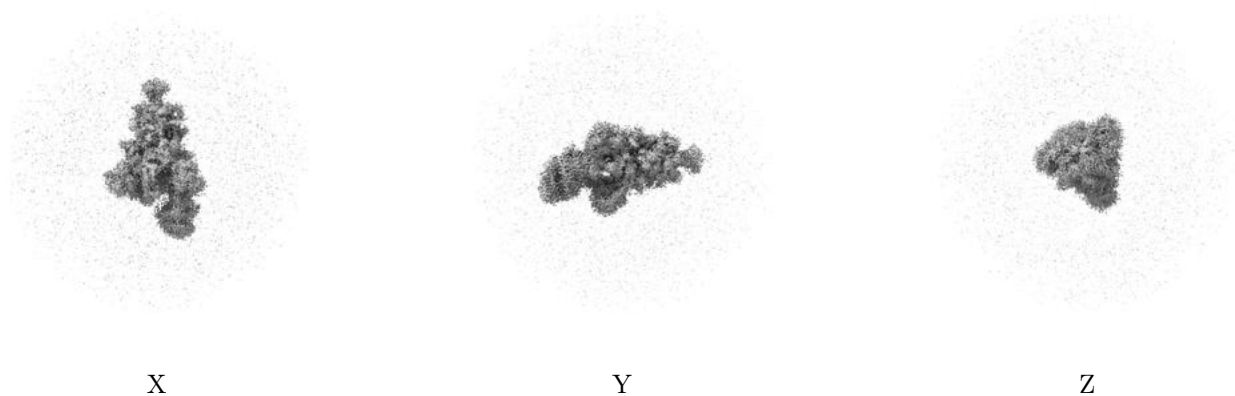


Z

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.

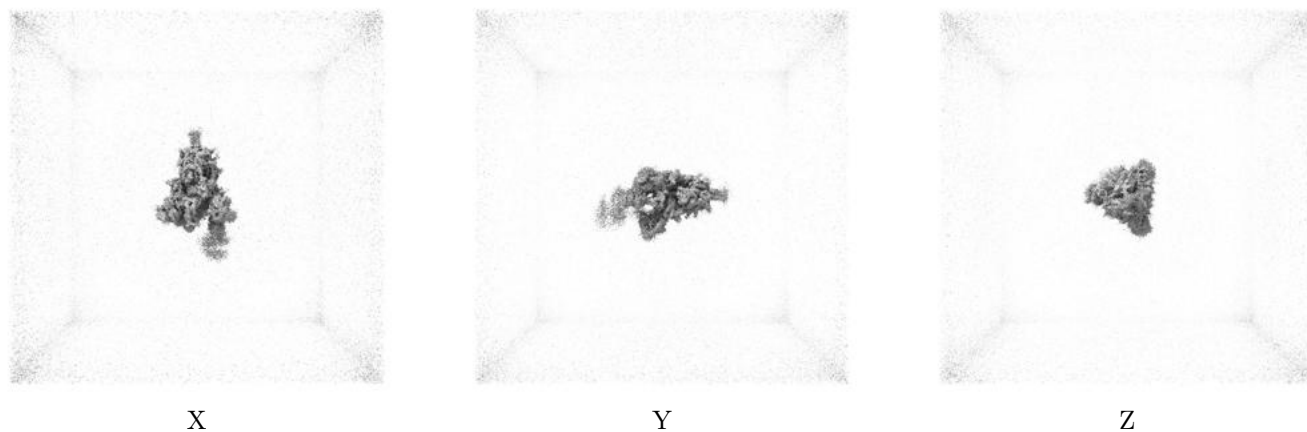
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.211. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

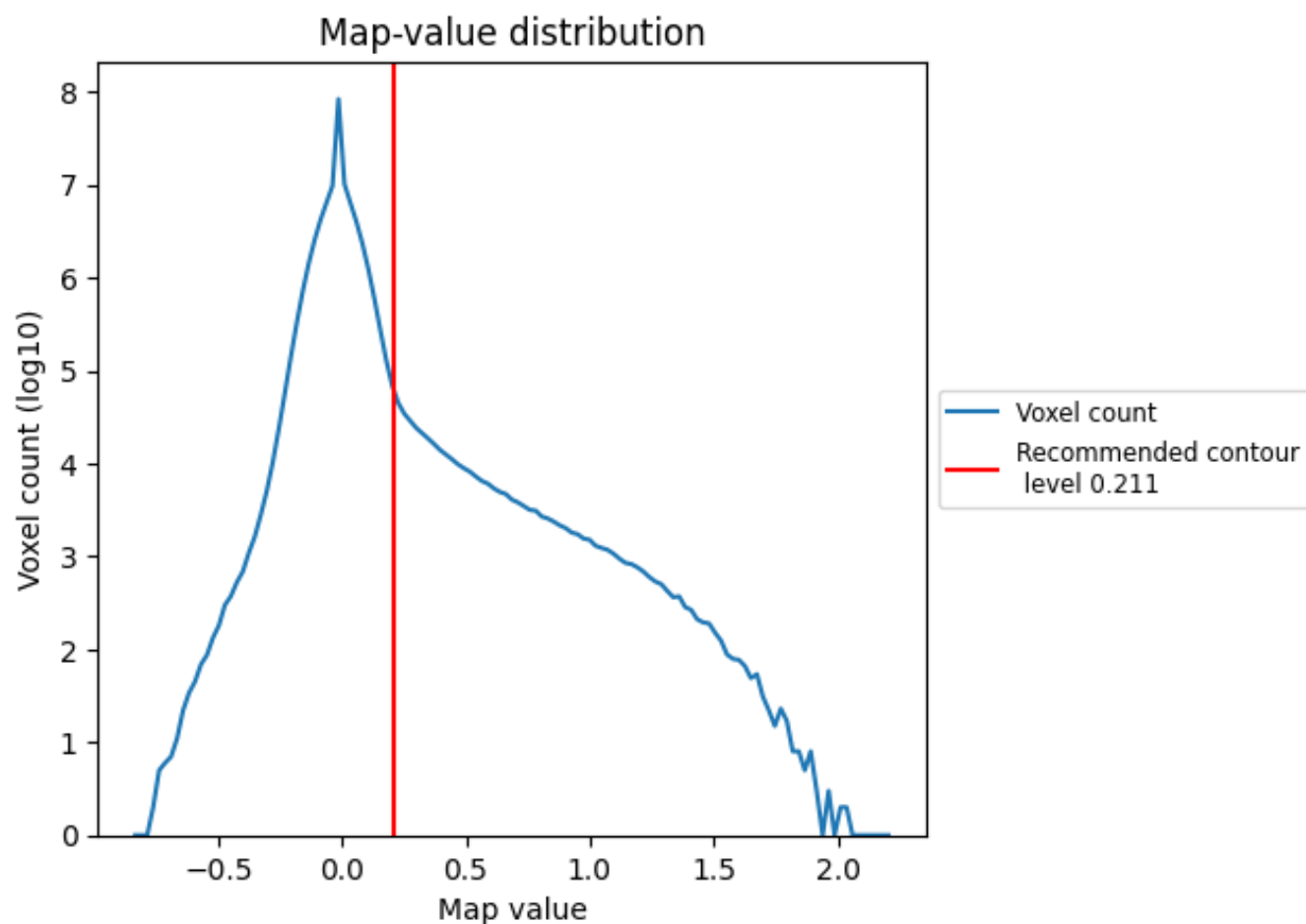
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

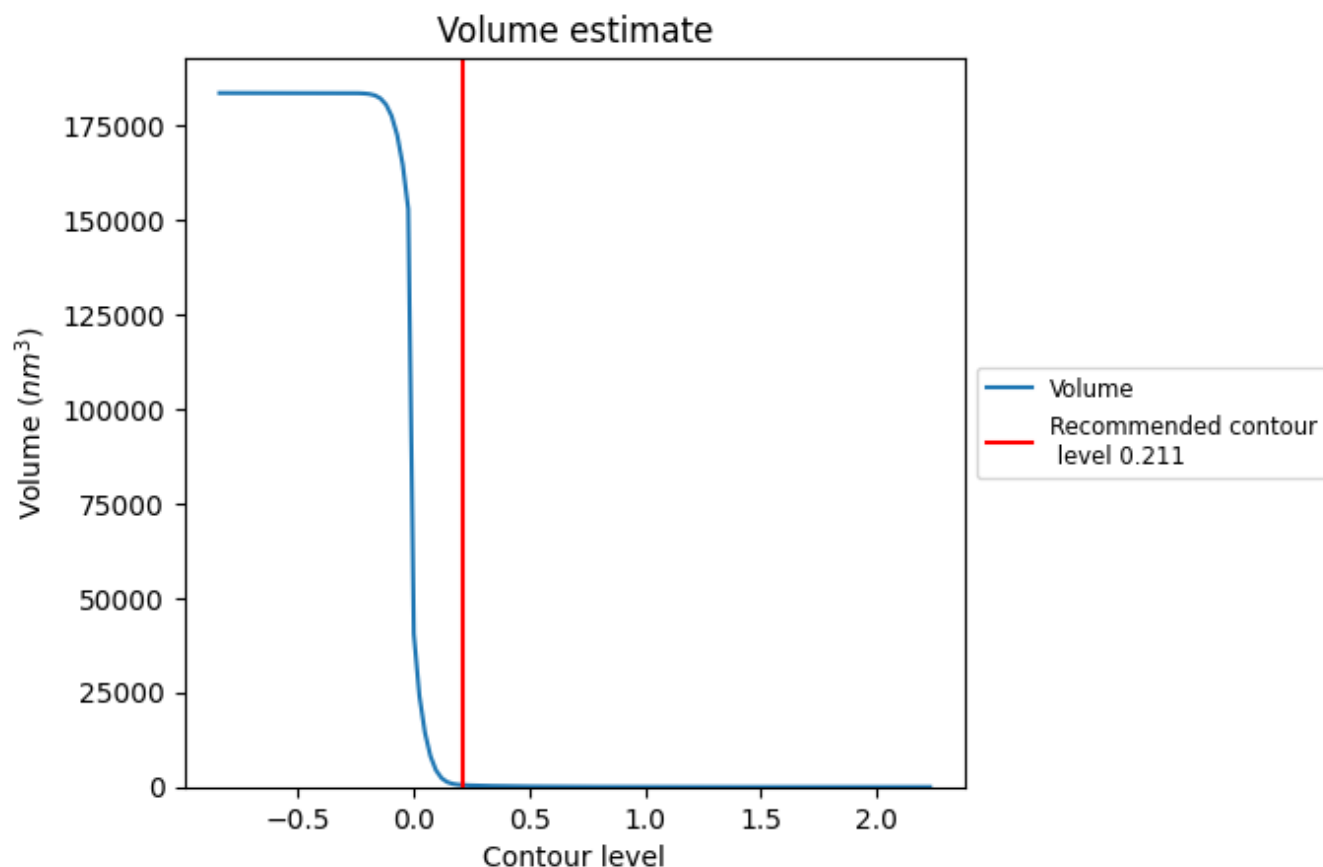
This section contains the results of statistical analysis of the map.

### 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.

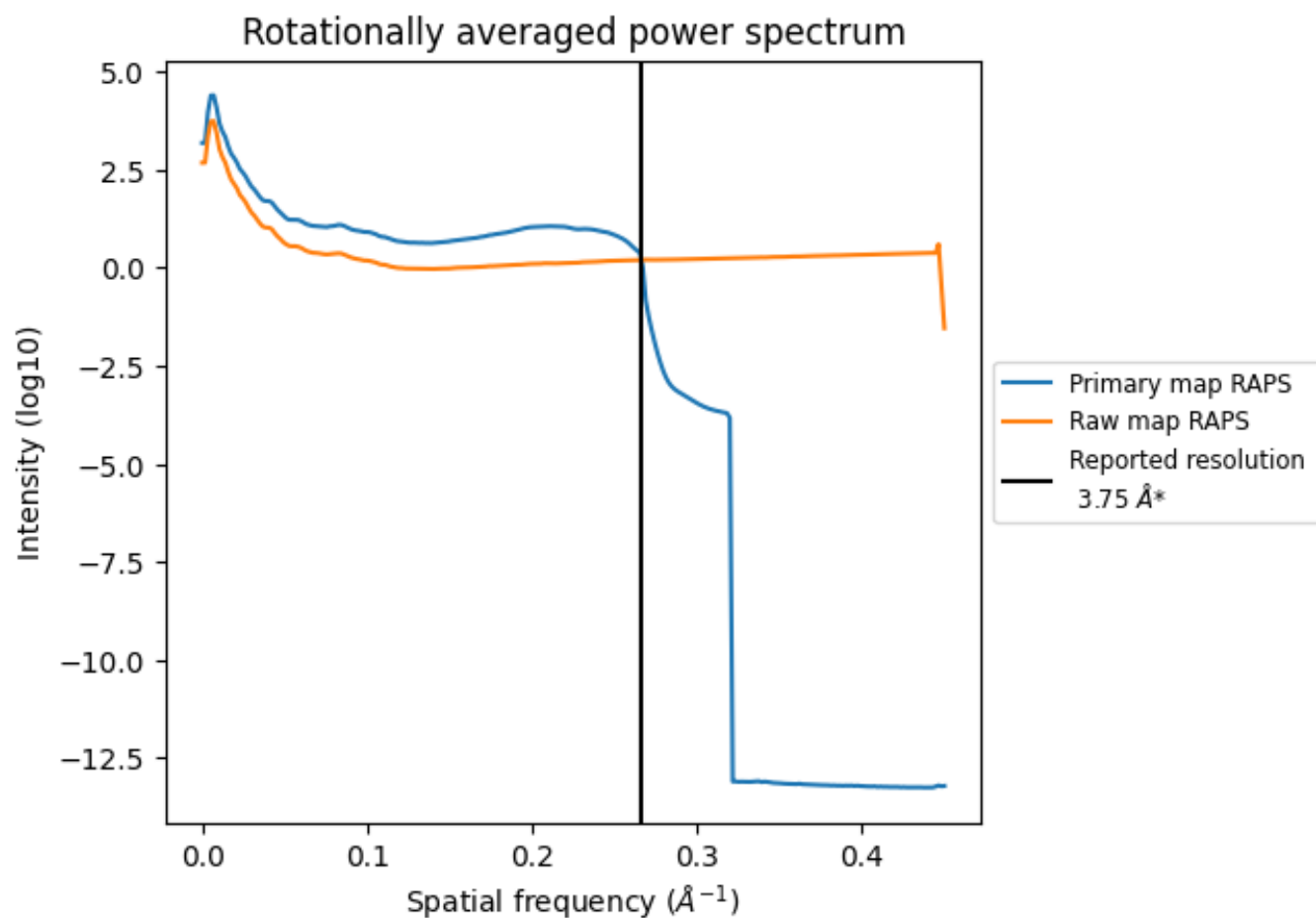
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 526 nm<sup>3</sup>; this corresponds to an approximate mass of 475 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 ⓘ

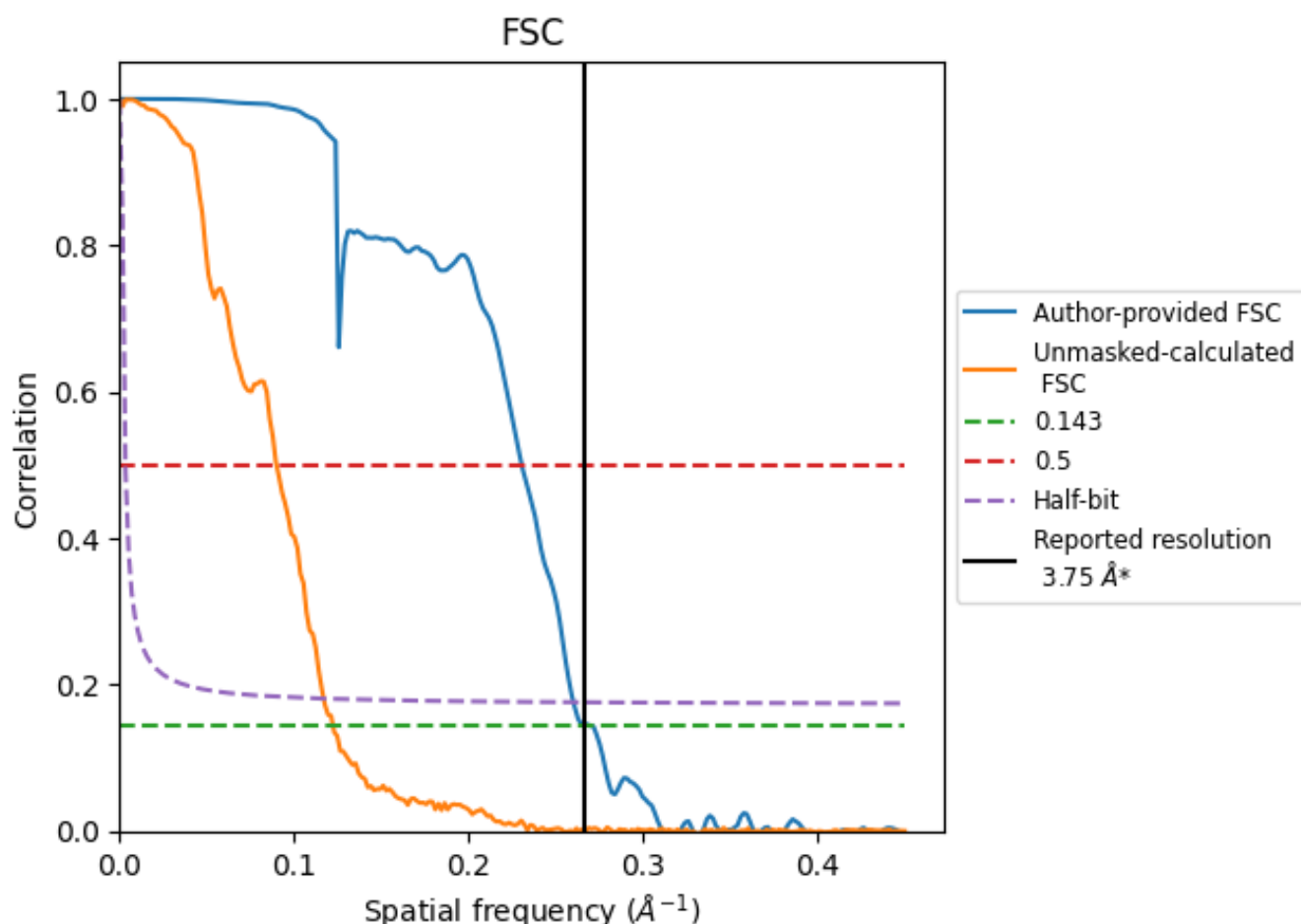


\*Reported resolution corresponds to spatial frequency of 0.267 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.267 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

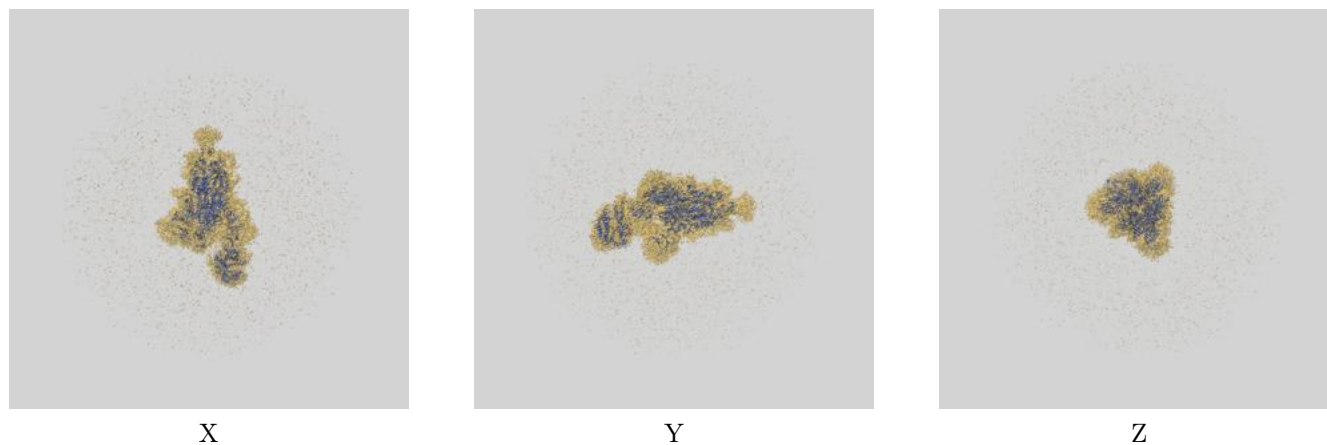
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.75	4.33	3.84
Unmasked-calculated*	8.16	11.10	8.53

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.16 differs from the reported value 3.75 by more than 10 %

## 9 Map-model fit [i](#)

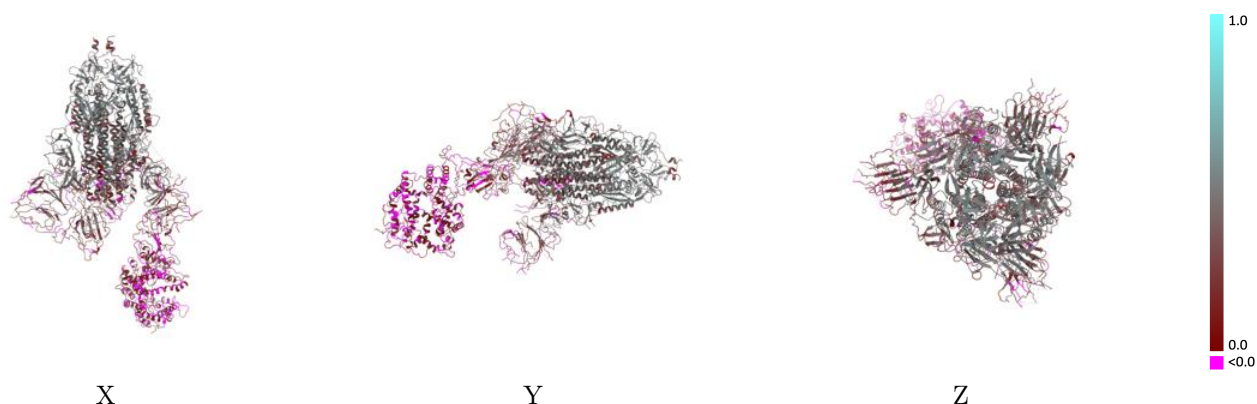
This section contains information regarding the fit between EMDB map EMD-41143 and PDB model 8TAZ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

### 9.1 Map-model overlay [i](#)



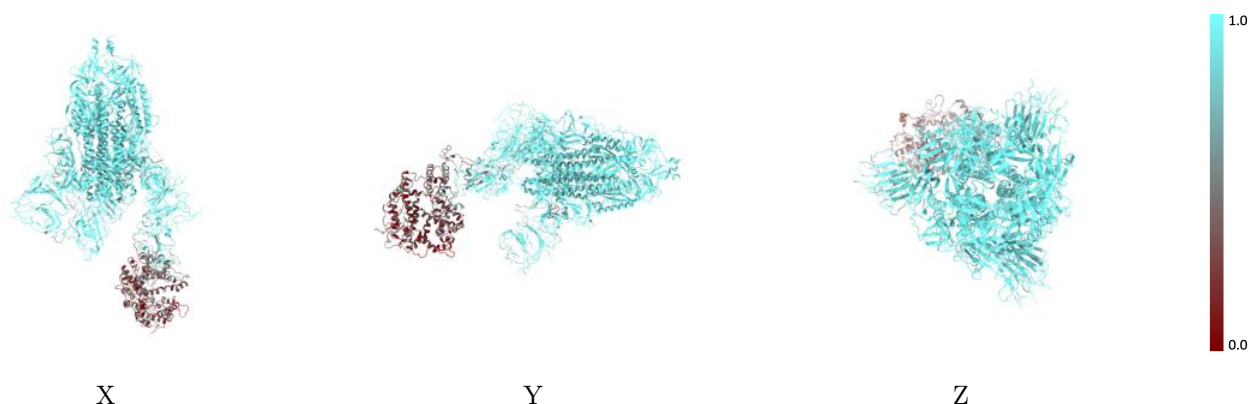
The images above show the 3D surface view of the map at the recommended contour level 0.211 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



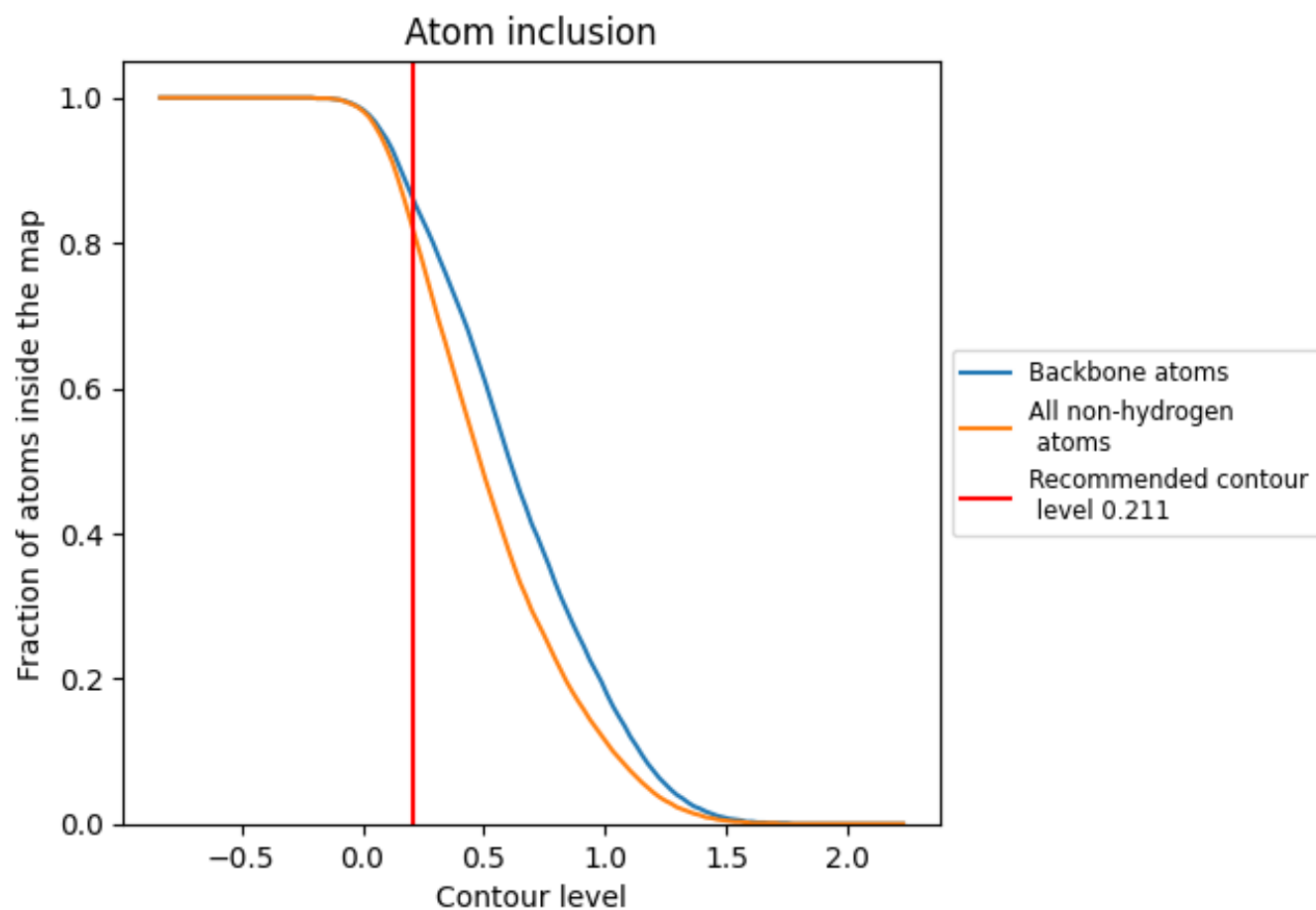
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.211).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.211) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8160	<div></div> 0.3000
A	<div></div> 0.8990	<div></div> 0.3110
B	<div></div> 0.9380	<div></div> 0.3530
C	<div></div> 0.9470	<div></div> 0.3750
D	<div></div> 0.2850	<div></div> 0.0880

