



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 05:17 AM JST

PDB ID : 7VXB
EMDB ID : EMD-32174
Title : SARS-CoV-2 Kappa variant spike protein in C2b state
Authors : Xu, C.; Cong, Y.
Deposited on : 2021-11-12
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

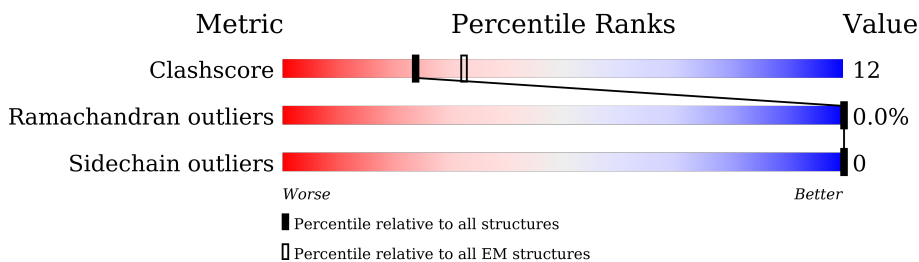
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1261	 5% 79% 5% 16%
1	B	1261	 10% 80% 5% 15%
1	D	1261	 7% 49% 36% 15%
2	C	625	 29% 56% 40% 15%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 29888 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	1068	8354	5327	1401	1587	39	0	0
1	A	1062	8310	5300	1394	1578	38	0	0
1	B	1068	8354	5327	1401	1587	39	0	0

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	142	ASP	GLY	variant	UNP P0DTC2
D	154	LYS	GLU	variant	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	484	GLN	GLU	variant	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	681	ARG	PRO	variant	UNP P0DTC2
D	682	GLY	ARG	variant	UNP P0DTC2
D	683	SER	ARG	variant	UNP P0DTC2
D	685	SER	ARG	variant	UNP P0DTC2
D	986	PRO	LYS	variant	UNP P0DTC2
D	987	PRO	VAL	variant	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	SER	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2
D	1212	TYR	-	expression tag	UNP P0DTC2
D	1213	ILE	-	expression tag	UNP P0DTC2
D	1214	PRO	-	expression tag	UNP P0DTC2
D	1215	GLU	-	expression tag	UNP P0DTC2
D	1216	ALA	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	ARG	-	expression tag	UNP P0DTC2
D	1219	ASP	-	expression tag	UNP P0DTC2
D	1220	GLY	-	expression tag	UNP P0DTC2
D	1221	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1222	ALA	-	expression tag	UNP P0DTC2
D	1223	TYR	-	expression tag	UNP P0DTC2
D	1224	VAL	-	expression tag	UNP P0DTC2
D	1225	ARG	-	expression tag	UNP P0DTC2
D	1226	LYS	-	expression tag	UNP P0DTC2
D	1227	ASP	-	expression tag	UNP P0DTC2
D	1228	GLY	-	expression tag	UNP P0DTC2
D	1229	GLU	-	expression tag	UNP P0DTC2
D	1230	TRP	-	expression tag	UNP P0DTC2
D	1231	VAL	-	expression tag	UNP P0DTC2
D	1232	LEU	-	expression tag	UNP P0DTC2
D	1233	LEU	-	expression tag	UNP P0DTC2
D	1234	SER	-	expression tag	UNP P0DTC2
D	1235	THR	-	expression tag	UNP P0DTC2
D	1236	PHE	-	expression tag	UNP P0DTC2
D	1237	LEU	-	expression tag	UNP P0DTC2
D	1238	GLU	-	expression tag	UNP P0DTC2
D	1239	ASN	-	expression tag	UNP P0DTC2
D	1240	LEU	-	expression tag	UNP P0DTC2
D	1241	TYR	-	expression tag	UNP P0DTC2
D	1242	PHE	-	expression tag	UNP P0DTC2
D	1243	GLN	-	expression tag	UNP P0DTC2
D	1244	GLY	-	expression tag	UNP P0DTC2
D	1245	ASP	-	expression tag	UNP P0DTC2
D	1246	TYR	-	expression tag	UNP P0DTC2
D	1247	LYS	-	expression tag	UNP P0DTC2
D	1248	ASP	-	expression tag	UNP P0DTC2
D	1249	ASP	-	expression tag	UNP P0DTC2
D	1250	ASP	-	expression tag	UNP P0DTC2
D	1251	ASP	-	expression tag	UNP P0DTC2
D	1252	LYS	-	expression tag	UNP P0DTC2
D	1253	HIS	-	expression tag	UNP P0DTC2
D	1254	HIS	-	expression tag	UNP P0DTC2
D	1255	HIS	-	expression tag	UNP P0DTC2
D	1256	HIS	-	expression tag	UNP P0DTC2
D	1257	HIS	-	expression tag	UNP P0DTC2
D	1258	HIS	-	expression tag	UNP P0DTC2
D	1259	HIS	-	expression tag	UNP P0DTC2
D	1260	HIS	-	expression tag	UNP P0DTC2
D	1261	HIS	-	expression tag	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	154	LYS	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	452	ARG	LEU	variant	UNP P0DTC2
A	484	GLN	GLU	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
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	GLU	-	expression tag	UNP P0DTC2
A	1239	ASN	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	TYR	-	expression tag	UNP P0DTC2
A	1247	LYS	-	expression tag	UNP P0DTC2
A	1248	ASP	-	expression tag	UNP P0DTC2
A	1249	ASP	-	expression tag	UNP P0DTC2
A	1250	ASP	-	expression tag	UNP P0DTC2
A	1251	ASP	-	expression tag	UNP P0DTC2
A	1252	LYS	-	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	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	154	LYS	GLU	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	484	GLN	GLU	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	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	GLU	-	expression tag	UNP P0DTC2
B	1239	ASN	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	TYR	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	TYR	-	expression tag	UNP P0DTC2
B	1247	LYS	-	expression tag	UNP P0DTC2
B	1248	ASP	-	expression tag	UNP P0DTC2
B	1249	ASP	-	expression tag	UNP P0DTC2
B	1250	ASP	-	expression tag	UNP P0DTC2
B	1251	ASP	-	expression tag	UNP P0DTC2
B	1252	LYS	-	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	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	597	4870	3115	806	920	29	0	0

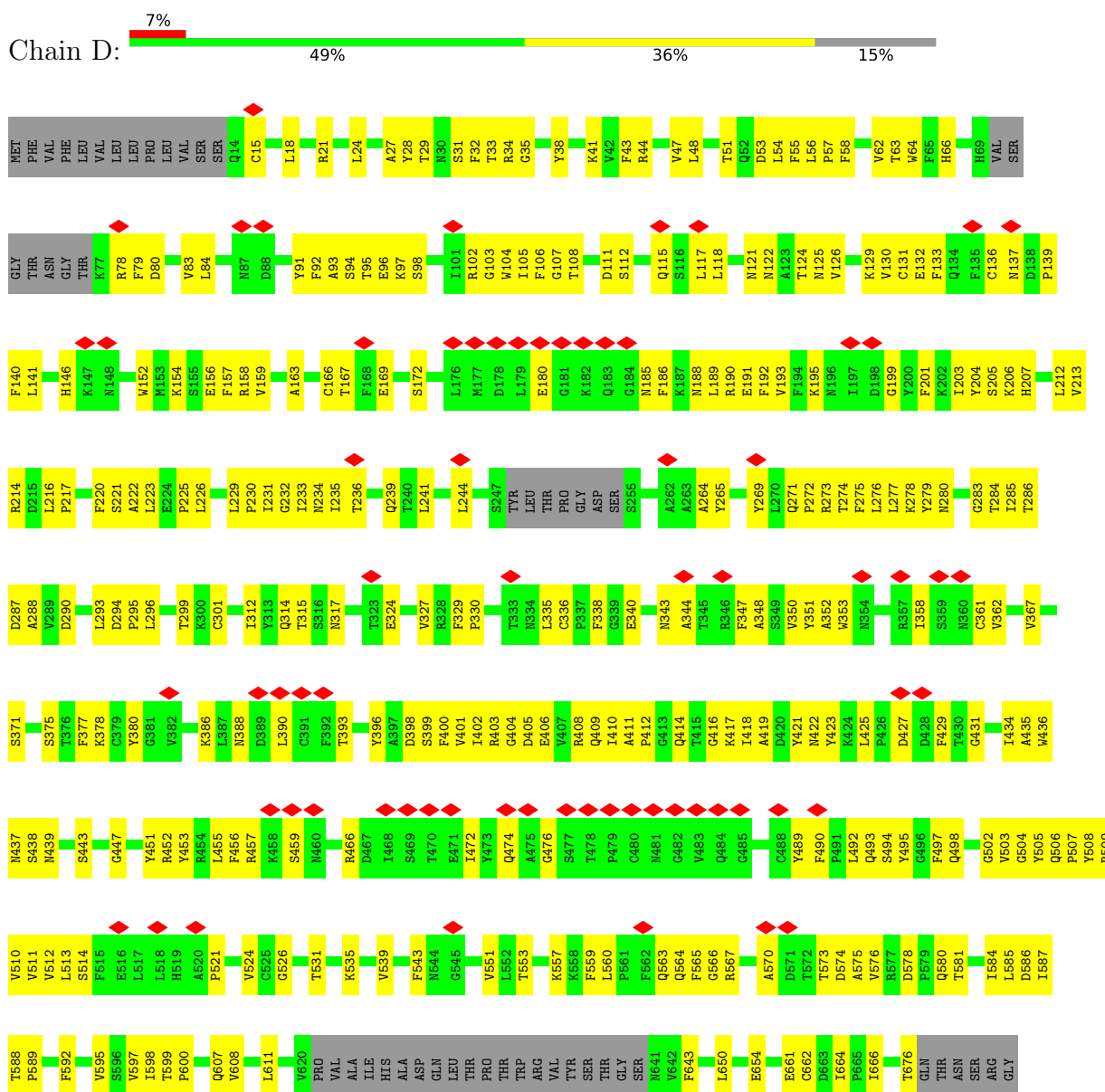
There are 26 discrepancies between the modelled and reference sequences:

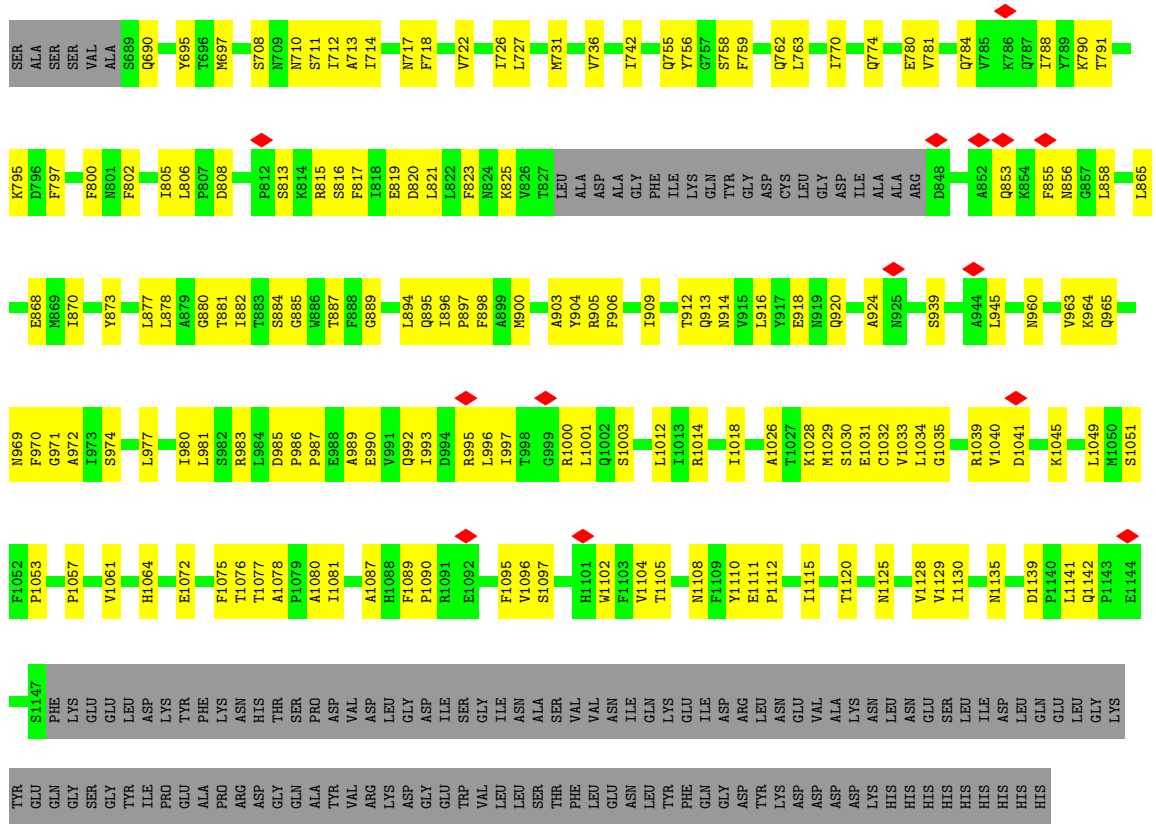
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP Q9BYF1
C	1	HIS	-	expression tag	UNP Q9BYF1
C	2	SER	-	expression tag	UNP Q9BYF1
C	3	SER	-	expression tag	UNP Q9BYF1
C	4	ALA	-	expression tag	UNP Q9BYF1
C	5	LEU	-	expression tag	UNP Q9BYF1
C	6	LEU	-	expression tag	UNP Q9BYF1
C	7	CYS	-	expression tag	UNP Q9BYF1
C	8	CYS	-	expression tag	UNP Q9BYF1
C	9	LEU	-	expression tag	UNP Q9BYF1
C	10	VAL	-	expression tag	UNP Q9BYF1
C	11	LEU	-	expression tag	UNP Q9BYF1
C	12	LEU	-	expression tag	UNP Q9BYF1
C	13	THR	-	expression tag	UNP Q9BYF1
C	14	GLY	-	expression tag	UNP Q9BYF1
C	15	VAL	-	expression tag	UNP Q9BYF1
C	16	ARG	-	expression tag	UNP Q9BYF1
C	616	HIS	-	expression tag	UNP Q9BYF1
C	617	HIS	-	expression tag	UNP Q9BYF1
C	618	HIS	-	expression tag	UNP Q9BYF1
C	619	HIS	-	expression tag	UNP Q9BYF1
C	620	HIS	-	expression tag	UNP Q9BYF1
C	621	HIS	-	expression tag	UNP Q9BYF1
C	622	HIS	-	expression tag	UNP Q9BYF1
C	623	HIS	-	expression tag	UNP Q9BYF1
C	624	HIS	-	expression tag	UNP Q9BYF1

3 Residue-property plots

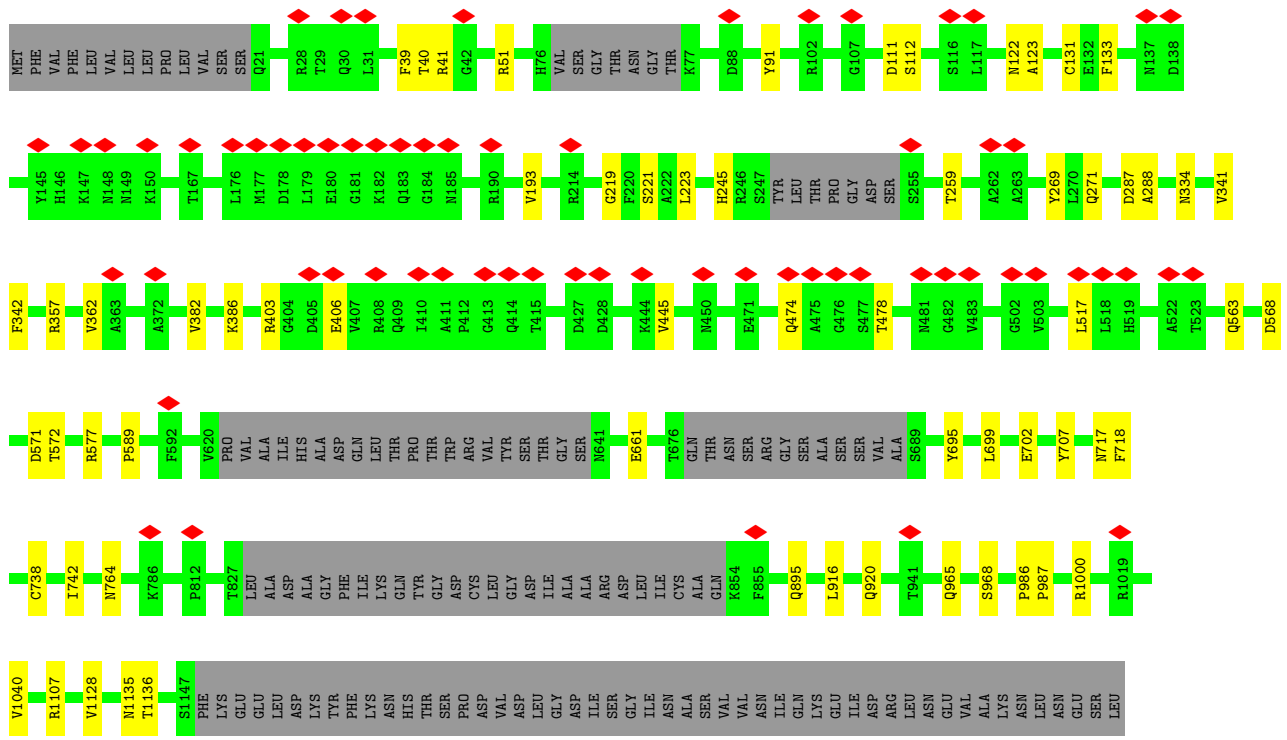
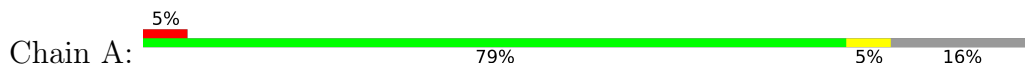
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



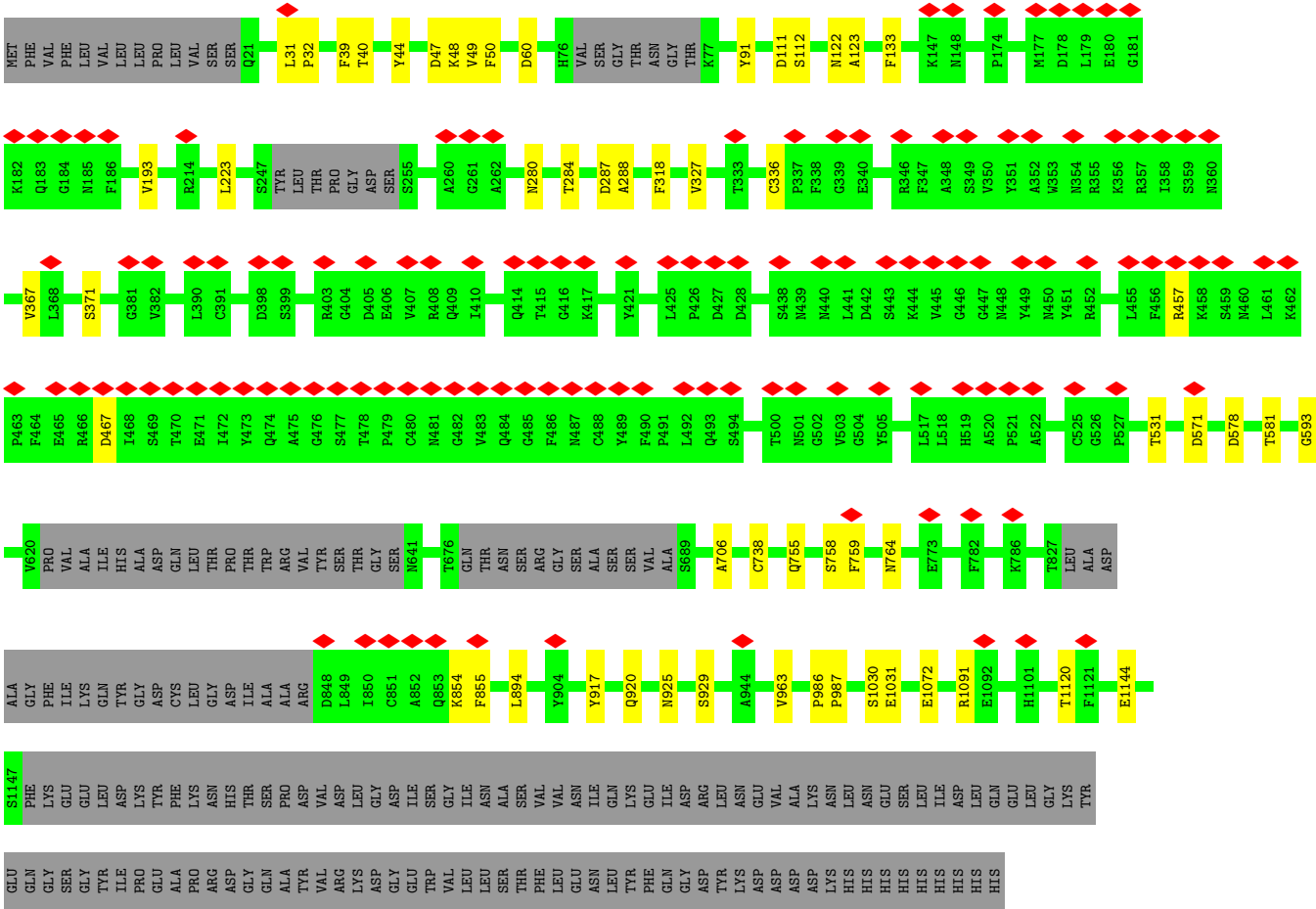
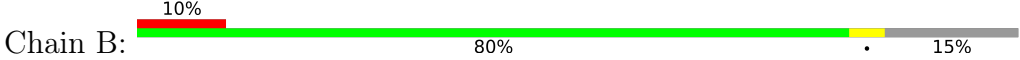


• Molecule 1: Spike glycoprotein

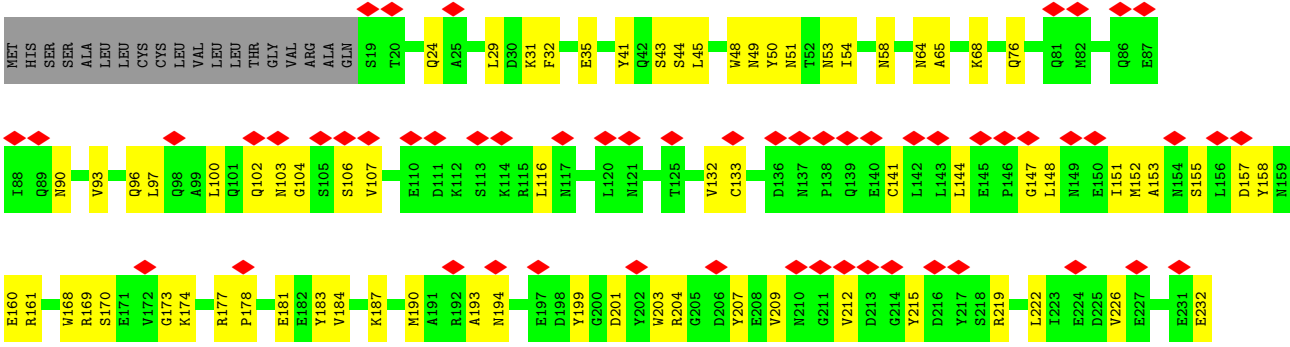


ILE	ASP	LEU	GLN	GLU	LEU	GLY	LYS	TYR	GLU	GLN	GLY	SER	GLY	TYR	ILE	LEU	PRO	PRO	ALA	PRO	ARG	ASP	GLY	LYS	ASP	VAL	VAL	ARG	LYS	GLY	GLU	TRP	VAL	GLY	LEU	LEU	SER	THR	PHE	LEU	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ASP	ASP	LYS	LYS	ASP	HIS	HIS	HIS	HIS	HIS	
HIS	HIS	HIS	HIS	HIS																																																						

● Molecule 1: Spike glycoprotein



● Molecule 2: Angiotensin-converting enzyme 2



M686	L233	A866	W802	I333	L456	Q522	W607	L886	HIS
Y687	K234	A387	D303	K234	E457	F623	L481	HIS	HIS
F688	P235	Q388	A304	P235	K458	Q524	R482	HIS	HIS
E589	L236	P389	G305	L236	W459	F525	E483	HIS	HIS
P590	Y237	E390	R306	Y237	V463	Q526	V485	HIS	HIS
L591	E238	L391	I307	E238	F464	L529	A486	HIS	HIS
F592	H239	L392	E310	H239	K465	C530	G487	HIS	HIS
T593	R245	R393	K313	R245	G466	Q531	V488	HIS	HIS
W594	M249	N394	V318	M249	E467	A532	E489	HIS	HIS
L595	N250	G395	G319	N250	I468	A533	P492	HIS	HIS
K596	A251	A396	G320	A251	P469	K534	H493	HIS	HIS
D597	Y252	A396	L320	Y252	K470	H535	D494	HIS	HIS
Q598	P253	A396	M523	P253	D471	E536	E495	HIS	HIS
N599	S254	A396	T324	S254	Q472	G537	L496	HIS	HIS
K600	S257	A396	Q325	S257	W473	P538	M557	HIS	HIS
N601	P258	A396	G326	P258	M474	L539	L558	HIS	HIS
S602	I259	A396	F327	I259	W477	H540	L560	HIS	HIS
F603	C261	A396	W328	C261	W478	K541	L561	HIS	HIS
V604	L262	A396	E329	L262	K481	S545	L562	HIS	HIS
W606	P263	A396	M332	P263	R482	N546	G561	HIS	HIS
S607	A264	A396	L333	A264	E483	S547	K562	HIS	HIS
T608	H265	A396	P336	H265	V485	A550	E564	HIS	HIS
D609	L266	A396	I421	L266	G486	G551	P565	HIS	HIS
M610	L267	A396	G337	M610	V487	Q552	N566	HIS	HIS
S611	G268	A396	M338	S611	W488	K553	M567	HIS	HIS
P612	D269	A396	V339	P612	E489	L554	L568	HIS	HIS
V613	M270	A396	Q340	V613	P492	F555	L569	HIS	HIS
A614	W271	A396	K341	A614	H493	N556	L570	HIS	HIS
D615	G272	A396	A342	D615	D494	M557	E571	HIS	HIS
HIS	W275	A396	C344	HIS	E495	L558	N572	HIS	HIS
HIS	T276	A396	H345	HIS	T496	L559	V573	HIS	HIS
HIS	Y279	A396	L351	HIS	Y497	L560	G575	HIS	HIS
HIS	S280	A396	G352	HIS	C498	L561	A576	HIS	HIS
HIS	L281	A396	K353	HIS	D499	G562	K577	HIS	HIS
HIS	T282	A396	G354	HIS	P500	S563	N578	HIS	HIS
HIS	V283	A396	D355	HIS	A501	E564	M579	HIS	HIS
HIS	P284	A396	F356	HIS	S502	P565	N580	HIS	HIS
HIS	F285	A396	R357	HIS	L503	W566	V581	HIS	HIS
HIS	G286	A396	I358	HIS	F504	T567	R582	HIS	HIS
HIS	Q287	A396	L359	HIS	H505	L568	L584	HIS	HIS
HIS	K288	A396	L359	HIS	D509	L570	L585	HIS	HIS
HIS	P289	A396	V364	HIS	E510	E571			
HIS	N290	A396	T365	HIS	N572	N572			
HIS	I291	A396	M366	HIS	F512	V573			
HIS	D292	A396	H374	HIS	V574	V574			
HIS	V293	A396	I379	HIS	G575	G575			
HIS	T294	A396	Q380	HIS	A576	A576			
HIS	D295	A396	Y381	HIS	K577	K577			
HIS	A296	A396	D382	HIS	N578	N578			
HIS	M297	A396	M383	HIS	M579	M579			
HIS	V298	A396	M383	HIS	N580	N580			
HIS	D299	A396	A384	HIS	V581	V581			
HIS	Q300	A396	Y385	HIS	R582	R582			
HIS	A301	A396		HIS	P583	P583			
HIS					L584	L584			
HIS					L585	L585			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67543	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 (6k x 4k)	Depositor
Maximum map value	3.992	Depositor
Minimum map value	-2.150	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.126	Depositor
Recommended contour level	0.65	Depositor
Map size (\AA)	393.48, 393.48, 393.48	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.093, 1.093, 1.093	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/8502	0.41	0/11565
1	B	0.25	1/8546 (0.0%)	0.41	0/11625
1	D	0.25	0/8546	0.40	0/11625
2	C	0.23	0/5007	0.35	0/6803
All	All	0.24	1/30601 (0.0%)	0.40	0/41618

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	CYS	C-N	5.38	1.44	1.34

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	8310	0	8117	48	0
1	B	8354	0	8159	45	0
1	D	8354	0	8159	436	0
2	C	4870	0	4643	231	0
All	All	29888	0	29078	714	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 12.

All (714) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:PHE:HB3	1:D:235:ILE:HD13	1.41	1.02
1:D:736:VAL:HG22	1:D:858:LEU:HG	1.45	0.98
2:C:503:LEU:HD23	2:C:506:VAL:HG23	1.43	0.97
2:C:539:LEU:HD23	2:C:587:TYR:HB2	1.44	0.97
1:D:129:LYS:HG2	1:D:169:GLU:HA	1.47	0.96
1:D:296:LEU:HB2	1:D:608:VAL:HG21	1.44	0.95
1:A:269:TYR:HE1	1:A:271:GLN:NE2	1.64	0.94
2:C:538:PRO:HD2	2:C:541:LYS:HD2	1.49	0.94
1:D:212:LEU:HD22	1:D:217:PRO:HD3	1.51	0.90
1:D:805:ILE:HD12	1:D:878:LEU:HD11	1.52	0.90
1:D:33:THR:HG21	1:D:220:PHE:HA	1.53	0.89
1:D:1030:SER:HA	1:D:1034:LEU:HB3	1.56	0.88
2:C:144:LEU:HA	2:C:148:LEU:HB2	1.55	0.87
2:C:144:LEU:HD12	2:C:148:LEU:HB2	1.55	0.87
1:D:344:ALA:HB3	1:D:347:PHE:HE1	1.40	0.86
1:D:418:ILE:HA	1:D:422:ASN:HD22	1.42	0.84
2:C:457:GLU:HG2	2:C:513:ILE:HD13	1.60	0.83
1:D:398:ASP:HB3	1:D:512:VAL:HB	1.61	0.82
1:D:32:PHE:CD2	1:D:33:THR:HG23	2.16	0.80
1:D:314:GLN:NE2	1:D:317:ASN:OD1	2.16	0.79
1:D:24:LEU:HB3	1:D:78:ARG:HD2	1.65	0.79
1:D:712:ILE:HG21	1:D:1077:THR:HB	1.65	0.79
1:D:781:VAL:HG22	1:D:1026:ALA:HB2	1.65	0.78
1:D:106:PHE:HB2	1:D:117:LEU:HB3	1.65	0.78
2:C:152:MET:O	2:C:161:ARG:NH1	2.15	0.78
1:D:758:SER:OG	1:A:965:GLN:NE2	2.18	0.77
2:C:389:PRO:HG2	2:C:392:LEU:HD12	1.66	0.77
2:C:301:ALA:O	2:C:306:ARG:NH2	2.18	0.76
1:D:1035:GLY:HA3	1:A:1040:VAL:HG21	1.66	0.76
2:C:446:ILE:HD13	2:C:523:PHE:HZ	1.52	0.75
1:A:403:ARG:NH2	1:A:406:GLU:OE2	2.20	0.75
1:D:277:LEU:HD22	1:D:285:ILE:HD13	1.67	0.75
2:C:144:LEU:HD21	2:C:271:TRP:HH2	1.53	0.74
1:D:490:PHE:CE2	1:D:492:LEU:HB2	2.23	0.74
1:D:813:SER:OG	1:D:868:GLU:OE1	2.04	0.74
1:A:269:TYR:CE1	1:A:271:GLN:NE2	2.47	0.74
1:D:157:PHE:CZ	1:D:159:VAL:HB	2.22	0.74
1:D:742:ILE:O	1:D:1000:ARG:NH1	2.20	0.74
2:C:157:ASP:HB3	2:C:160:GLU:HB3	1.70	0.74
2:C:524:GLN:HB3	2:C:574:VAL:HG11	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:ASN:HA	1:D:508:TYR:HD1	1.50	0.73
1:D:770:ILE:HD11	1:D:1012:LEU:HD23	1.70	0.73
1:D:887:THR:HG21	1:D:894:LEU:HD12	1.68	0.73
1:D:1031:GLU:OE1	1:D:1039:ARG:NH2	2.21	0.73
2:C:394:ASN:OD1	2:C:395:GLY:N	2.22	0.73
1:D:981:LEU:O	1:A:386:LYS:NZ	2.22	0.73
1:D:278:LYS:O	1:D:286:THR:N	2.13	0.73
1:D:476:GLY:HA3	2:C:24:GLN:HE21	1.53	0.73
2:C:263:PRO:HG2	2:C:266:LEU:HD12	1.70	0.73
1:D:102:ARG:HH12	1:D:154:LYS:HE2	1.54	0.73
1:D:338:PHE:HE1	1:D:358:ILE:HG21	1.52	0.73
1:D:437:ASN:ND2	1:D:506:GLN:OE1	2.22	0.73
2:C:451:PRO:HB2	2:C:485:VAL:HG12	1.71	0.72
1:D:329:PHE:HB3	1:D:330:PRO:HD2	1.70	0.72
1:D:726:ILE:HG12	1:D:1061:VAL:HG22	1.72	0.72
2:C:132:VAL:HG23	2:C:168:TRP:HE3	1.55	0.72
2:C:190:MET:O	2:C:194:ASN:ND2	2.22	0.72
1:D:102:ARG:HB3	1:D:241:LEU:HB3	1.71	0.72
1:D:121:ASN:O	1:D:154:LYS:NZ	2.23	0.71
1:D:106:PHE:HD2	1:D:117:LEU:HD23	1.54	0.71
1:D:417:LYS:HD2	1:D:455:LEU:HD12	1.71	0.71
1:D:599:THR:OG1	1:D:607:GLN:O	2.07	0.71
1:D:1039:ARG:HD3	1:B:1031:GLU:OE2	1.91	0.70
1:D:1129:VAL:HG22	1:B:917:TYR:HB3	1.73	0.70
2:C:276:THR:OG1	2:C:445:THR:OG1	2.09	0.70
2:C:450:LEU:HB2	2:C:451:PRO:HD3	1.73	0.70
1:D:204:TYR:HD1	1:D:225:PRO:HA	1.53	0.70
2:C:144:LEU:HA	2:C:148:LEU:CB	2.21	0.70
1:D:43:PHE:HB2	1:A:563:GLN:CD	2.12	0.69
1:D:437:ASN:HA	1:D:508:TYR:CD1	2.27	0.69
1:D:1033:VAL:HA	1:D:1051:SER:HB3	1.73	0.69
1:D:131:CYS:HB2	1:D:133:PHE:CE1	2.27	0.69
1:D:578:ASP:OD2	1:D:581:THR:N	2.25	0.69
1:D:44:ARG:HB3	1:D:47:VAL:CG2	2.23	0.68
2:C:204:ARG:HG2	2:C:222:LEU:HD23	1.75	0.68
1:D:788:ILE:HD11	1:A:699:LEU:HB2	1.76	0.68
1:A:40:THR:OG1	1:A:219:GLY:O	2.10	0.68
1:D:447:GLY:HA2	1:D:497:PHE:O	1.93	0.68
1:D:108:THR:HA	1:D:236:THR:H	1.58	0.68
1:D:335:LEU:CD2	1:D:362:VAL:HB	2.24	0.68
1:D:758:SER:O	1:D:762:GLN:N	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:396:ALA:HB3	2:C:400:PHE:CD2	2.30	0.67
1:D:338:PHE:CE1	1:D:358:ILE:HG21	2.29	0.67
1:D:865:LEU:HD21	1:D:873:TYR:HE2	1.60	0.66
2:C:29:LEU:HD13	2:C:96:GLN:OE1	1.95	0.66
1:D:35:GLY:HA3	1:D:56:LEU:HB3	1.76	0.66
2:C:304:ALA:HB1	2:C:333:LEU:HD22	1.76	0.66
1:D:713:ALA:HB3	1:B:894:LEU:CD1	2.25	0.66
2:C:235:PRO:O	2:C:239:HIS:ND1	2.24	0.66
1:D:105:ILE:HG12	1:D:118:LEU:HD13	1.77	0.66
1:A:717:ASN:OD1	1:A:718:PHE:N	2.29	0.66
1:D:102:ARG:HB3	1:D:241:LEU:CB	2.26	0.66
2:C:389:PRO:O	2:C:393:ARG:HG3	1.96	0.66
1:D:48:LEU:HD11	1:D:276:LEU:HB3	1.77	0.65
1:D:290:ASP:HB3	1:D:293:LEU:HB2	1.78	0.65
1:A:563:GLN:O	1:A:577:ARG:NH1	2.29	0.65
1:D:347:PHE:CE2	1:D:509:ARG:HD3	2.32	0.65
1:D:31:SER:HB3	1:D:34:ARG:HB2	1.79	0.65
1:D:204:TYR:CD1	1:D:225:PRO:HA	2.32	0.65
1:D:15:CYS:HA	1:D:137:ASN:HB2	1.79	0.64
1:D:24:LEU:HD21	1:D:80:ASP:OD2	1.97	0.64
1:D:95:THR:HG22	1:D:189:LEU:HD13	1.79	0.64
2:C:100:LEU:HD11	2:C:391:LEU:HD11	1.80	0.64
1:D:912:THR:HG22	1:D:914:ASN:H	1.60	0.64
1:D:502:GLY:O	1:D:506:GLN:HG3	1.98	0.64
2:C:595:LEU:O	2:C:599:ASN:ND2	2.29	0.64
2:C:554:LEU:O	2:C:558:LEU:HG	1.97	0.64
1:D:712:ILE:O	1:D:1075:PHE:N	2.29	0.64
2:C:469:PRO:HD2	2:C:472:GLN:OE1	1.98	0.64
1:D:350:VAL:HG22	1:D:422:ASN:HB3	1.80	0.64
1:D:96:GLU:O	1:D:188:ASN:HB2	1.98	0.63
2:C:302:TRP:HA	2:C:306:ARG:HH21	1.62	0.63
1:A:895:GLN:NE2	1:B:706:ALA:O	2.31	0.63
2:C:267:LEU:CD1	2:C:272:GLY:HA3	2.28	0.63
1:D:80:ASP:O	1:D:265:TYR:OH	2.16	0.63
2:C:158:TYR:HB2	2:C:252:TYR:CE2	2.33	0.63
1:D:717:ASN:OD1	1:D:718:PHE:N	2.32	0.63
2:C:155:SER:O	2:C:161:ARG:HD2	1.99	0.63
2:C:396:ALA:HB1	2:C:566:TRP:HB3	1.81	0.63
2:C:144:LEU:O	2:C:148:LEU:N	2.32	0.63
1:D:106:PHE:O	1:D:117:LEU:N	2.33	0.62
1:D:756:TYR:HB3	1:D:759:PHE:CD2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:965:GLN:NE2	1:B:758:SER:OG	2.33	0.62
1:D:329:PHE:O	1:D:580:GLN:HB2	1.99	0.62
2:C:382:ASP:HA	2:C:385:TYR:CE2	2.34	0.62
1:D:231:ILE:HG22	1:D:233:ILE:HG23	1.80	0.62
1:D:33:THR:CG2	1:D:220:PHE:HA	2.27	0.62
1:D:412:PRO:HB3	1:D:427:ASP:HA	1.80	0.62
2:C:382:ASP:OD1	2:C:385:TYR:OH	2.14	0.62
1:D:27:ALA:HB3	1:D:64:TRP:HB3	1.81	0.62
1:D:439:ASN:O	1:D:443:SER:OG	2.17	0.62
1:D:661:GLU:O	1:D:695:TYR:OH	2.15	0.62
1:D:856:ASN:HD22	1:D:963:VAL:HG22	1.65	0.62
2:C:453:THR:CG2	2:C:516:TYR:HB2	2.30	0.61
1:D:102:ARG:NH1	1:D:154:LYS:HE2	2.14	0.61
2:C:389:PRO:CG	2:C:392:LEU:HD12	2.29	0.61
1:D:378:LYS:HE2	1:D:380:TYR:HE1	1.66	0.61
1:D:206:LYS:HD2	1:D:222:ALA:O	2.01	0.61
1:D:1089:PHE:HZ	1:D:1129:VAL:HG21	1.65	0.61
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.32	0.61
2:C:144:LEU:HD12	2:C:148:LEU:CB	2.29	0.61
1:A:245:HIS:O	1:A:259:THR:OG1	2.17	0.61
1:D:344:ALA:HB3	1:D:347:PHE:CE1	2.30	0.61
1:D:212:LEU:CD2	1:D:217:PRO:HD3	2.29	0.61
1:D:600:PRO:HD2	1:D:607:GLN:O	2.01	0.61
2:C:144:LEU:HA	2:C:148:LEU:CG	2.31	0.61
2:C:406:GLU:HG3	2:C:518:ARG:HH11	1.66	0.61
1:D:34:ARG:HH22	1:D:217:PRO:HD2	1.65	0.60
1:D:118:LEU:HB2	1:D:133:PHE:HE2	1.66	0.60
1:D:884:SER:HA	1:D:894:LEU:O	2.01	0.60
1:D:44:ARG:HB2	1:D:279:TYR:CD2	2.36	0.60
2:C:44:SER:CB	2:C:351:LEU:HG	2.30	0.60
1:D:122:ASN:HA	1:D:154:LYS:HZ3	1.66	0.60
1:D:43:PHE:HB2	1:A:563:GLN:OE1	2.01	0.60
1:D:905:ARG:NH1	1:D:1049:LEU:O	2.35	0.60
1:D:32:PHE:HD2	1:D:33:THR:HG23	1.63	0.60
1:D:190:ARG:HH11	1:D:192:PHE:HZ	1.50	0.60
1:D:377:PHE:HD1	1:D:434:ILE:HG12	1.67	0.60
1:D:403:ARG:HB2	1:D:406:GLU:HG2	1.83	0.60
1:D:708:SER:HB3	1:D:711:SER:CB	2.32	0.60
1:D:790:LYS:HD2	1:A:702:GLU:OE2	2.01	0.60
1:D:918:GLU:HG2	1:A:1128:VAL:HG11	1.84	0.60
1:D:108:THR:OG1	1:D:234:ASN:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:LEU:HD21	2:C:271:TRP:CH2	2.36	0.60
2:C:396:ALA:HB3	2:C:400:PHE:CE2	2.37	0.60
2:C:421:ILE:HD11	2:C:423:LEU:CD1	2.31	0.60
1:D:140:PHE:O	1:D:158:ARG:HB2	2.02	0.60
1:D:140:PHE:CE1	1:D:244:LEU:HD12	2.37	0.60
1:D:83:VAL:HG22	1:D:239:GLN:HG2	1.82	0.60
2:C:482:ARG:O	2:C:606:TRP:NE1	2.32	0.60
1:D:205:SER:HB2	1:D:226:LEU:HD22	1.84	0.59
1:B:287:ASP:OD1	1:B:288:ALA:N	2.35	0.59
1:D:95:THR:HG22	1:D:189:LEU:CD1	2.32	0.59
1:D:351:TYR:HE2	1:D:452:ARG:HB2	1.67	0.59
1:D:896:ILE:HG23	1:D:897:PRO:HD2	1.84	0.59
1:D:361:CYS:O	1:D:524:VAL:HA	2.02	0.59
2:C:103:ASN:HB3	2:C:106:SER:HB2	1.84	0.59
2:C:374:HIS:CE1	2:C:402:GLU:HG3	2.37	0.59
1:D:889:GLY:HA3	1:D:1034:LEU:HD11	1.85	0.59
2:C:517:THR:HB	2:C:521:TYR:CE2	2.38	0.59
1:D:974:SER:OG	1:D:983:ARG:NH2	2.35	0.59
1:D:29:THR:O	1:D:62:VAL:HG22	2.03	0.59
1:D:797:PHE:CE2	1:D:802:PHE:HB2	2.38	0.59
1:D:1125:ASN:OD1	1:D:1128:VAL:HG23	2.03	0.59
1:B:112:SER:N	1:B:133:PHE:O	2.36	0.59
1:D:418:ILE:O	1:D:422:ASN:HB2	2.03	0.59
1:D:714:ILE:HB	1:D:1075:PHE:HE2	1.68	0.59
1:A:287:ASP:OD1	1:A:288:ALA:N	2.36	0.59
2:C:394:ASN:HB3	2:C:562:LYS:HD3	1.85	0.59
2:C:499:ASP:HB3	2:C:500:PRO:HD3	1.84	0.59
1:D:107:GLY:H	1:D:235:ILE:HG23	1.67	0.58
1:D:965:GLN:HB3	1:D:970:PHE:HZ	1.68	0.58
1:D:287:ASP:OD1	1:D:288:ALA:N	2.34	0.58
1:D:419:ALA:HA	1:D:423:TYR:O	2.03	0.58
2:C:267:LEU:HD13	2:C:272:GLY:HA3	1.85	0.58
2:C:332:MET:HE3	2:C:336:PRO:HD3	1.84	0.58
1:D:276:LEU:HD11	1:D:301:CYS:HA	1.86	0.58
2:C:303:ASP:O	2:C:307:ILE:HG13	2.03	0.58
1:D:756:TYR:HE2	1:D:997:ILE:HG21	1.68	0.58
1:D:1030:SER:HA	1:D:1034:LEU:CB	2.32	0.58
2:C:389:PRO:HD2	2:C:392:LEU:HD12	1.85	0.58
2:C:470:LYS:HA	2:C:473:TRP:NE1	2.18	0.58
1:D:870:ILE:HA	1:D:873:TYR:CD2	2.38	0.58
1:D:553:THR:O	1:D:586:ASP:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:294:THR:O	2:C:298:VAL:HG23	2.04	0.57
1:D:565:PHE:O	1:B:50:PHE:N	2.32	0.57
1:D:578:ASP:HB3	1:D:581:THR:O	2.05	0.57
2:C:446:ILE:HD13	2:C:523:PHE:CZ	2.36	0.57
2:C:457:GLU:HG2	2:C:513:ILE:CD1	2.34	0.57
2:C:455:MET:SD	2:C:481:LYS:HG3	2.44	0.57
2:C:470:LYS:HA	2:C:473:TRP:CE2	2.40	0.57
2:C:245:ARG:HG3	2:C:262:LEU:HD21	1.86	0.57
2:C:419:LYS:HE3	2:C:424:LEU:HD23	1.87	0.57
2:C:453:THR:HA	2:C:512:PHE:CE2	2.40	0.57
2:C:456:LEU:HB3	2:C:512:PHE:CE2	2.40	0.57
1:D:136:CYS:O	1:D:139:PRO:HD3	2.04	0.57
1:A:41:ARG:NH1	1:A:221:SER:OG	2.38	0.57
2:C:184:VAL:HG22	2:C:464:PHE:HE1	1.69	0.57
1:D:94:SER:HB2	1:D:264:ALA:O	2.05	0.57
1:D:97:LYS:HE2	1:D:186:PHE:CE1	2.39	0.57
1:D:404:GLY:HA2	1:D:508:TYR:CD2	2.40	0.56
1:D:94:SER:HB3	1:D:265:TYR:HA	1.88	0.56
1:A:334:ASN:O	1:A:362:VAL:N	2.38	0.56
1:D:1040:VAL:O	1:B:1030:SER:OG	2.24	0.56
2:C:451:PRO:CB	2:C:485:VAL:HG12	2.35	0.56
1:D:44:ARG:NH2	1:A:571:ASP:OD1	2.32	0.56
1:D:1130:ILE:HD12	1:B:920:GLN:NE2	2.21	0.56
1:D:335:LEU:HD22	1:D:362:VAL:O	2.06	0.56
1:D:405:ASP:O	1:D:408:ARG:HG2	2.06	0.56
2:C:222:LEU:O	2:C:226:VAL:HG22	2.06	0.56
1:B:39:PHE:CD2	1:B:40:THR:HG23	2.41	0.56
1:D:1090:PRO:HA	1:D:1120:THR:HG22	1.87	0.56
2:C:539:LEU:HD23	2:C:587:TYR:CB	2.28	0.56
1:D:34:ARG:NH2	1:D:216:LEU:HB3	2.21	0.55
1:D:93:ALA:CB	1:D:191:GLU:HG2	2.36	0.55
1:D:121:ASN:OD1	1:D:126:VAL:HG22	2.07	0.55
1:D:897:PRO:HA	1:A:707:TYR:CE1	2.41	0.55
1:D:111:ASP:OD1	1:D:112:SER:N	2.36	0.55
1:D:474:GLN:HG2	1:D:476:GLY:O	2.07	0.55
1:D:708:SER:HB3	1:D:711:SER:HB2	1.88	0.55
1:D:727:LEU:HD11	1:D:1028:LYS:NZ	2.21	0.55
1:D:972:ALA:HA	1:D:992:GLN:OE1	2.05	0.55
2:C:237:TYR:CE1	2:C:451:PRO:HG2	2.41	0.55
1:A:112:SER:N	1:A:133:PHE:O	2.39	0.55
1:A:661:GLU:O	1:A:695:TYR:OH	2.17	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:LYS:HE2	1:D:390:LEU:HD11	1.87	0.55
1:D:453:TYR:HB3	1:D:495:TYR:CE2	2.42	0.55
1:D:969:ASN:HB3	1:D:972:ALA:O	2.07	0.55
2:C:455:MET:SD	2:C:481:LYS:HA	2.46	0.55
1:D:1033:VAL:CG1	1:D:1053:PRO:HD3	2.37	0.55
1:D:714:ILE:HG13	1:D:1096:VAL:HG11	1.89	0.55
2:C:450:LEU:HD21	2:C:519:THR:CB	2.37	0.55
1:D:124:THR:HG22	1:D:125:ASN:ND2	2.21	0.55
1:D:567:ARG:HD2	1:B:49:VAL:HG11	1.89	0.55
1:D:983:ARG:HG2	1:A:382:VAL:HG12	1.89	0.55
2:C:203:TRP:CZ3	2:C:511:SER:HB2	2.42	0.55
2:C:212:VAL:HG11	2:C:215:TYR:HD2	1.72	0.55
2:C:589:GLU:HB3	2:C:590:PRO:HD3	1.88	0.55
1:D:451:TYR:HD2	1:D:497:PHE:HE2	1.55	0.55
2:C:233:ILE:HG12	2:C:584:LEU:CD2	2.36	0.55
2:C:394:ASN:HB3	2:C:562:LYS:CD	2.35	0.55
2:C:412:ALA:HA	2:C:417:HIS:CD2	2.42	0.55
1:D:855:PHE:HB3	1:A:589:PRO:HG2	1.89	0.54
1:D:1033:VAL:CA	1:D:1051:SER:HB3	2.36	0.54
1:D:1089:PHE:CZ	1:D:1129:VAL:HG21	2.43	0.54
2:C:181:GLU:HG2	2:C:473:TRP:HH2	1.72	0.54
2:C:236:LEU:HD21	2:C:588:PHE:HD2	1.72	0.54
2:C:402:GLU:O	2:C:406:GLU:HG2	2.07	0.54
1:D:411:ALA:HB3	1:D:414:GLN:CG	2.38	0.54
2:C:44:SER:HB3	2:C:351:LEU:HG	1.88	0.54
1:D:662:CYS:HB2	1:D:697:MET:HG3	1.88	0.54
2:C:29:LEU:HD21	2:C:97:LEU:CD2	2.36	0.54
1:D:44:ARG:HB2	1:D:279:TYR:CE2	2.43	0.54
1:D:731:MET:N	1:D:774:GLN:OE1	2.23	0.54
2:C:168:TRP:HE1	2:C:502:SER:HB2	1.72	0.54
2:C:170:SER:HA	2:C:497:TYR:HE1	1.72	0.54
1:D:756:TYR:HB3	1:D:759:PHE:HD2	1.73	0.54
1:D:126:VAL:HB	1:D:172:SER:HB3	1.89	0.54
1:D:472:ILE:HG23	1:D:489:TYR:O	2.07	0.54
1:D:1110:TYR:CZ	1:D:1112:PRO:HG3	2.43	0.54
1:D:38:TYR:HE1	1:D:285:ILE:HG13	1.73	0.54
1:D:199:GLY:HA2	1:D:232:GLY:HA2	1.90	0.54
1:D:815:ARG:NH2	1:D:820:ASP:OD1	2.37	0.54
1:D:327:VAL:HB	1:D:531:THR:OG1	2.07	0.54
1:D:453:TYR:O	1:D:492:LEU:HA	2.08	0.54
1:D:557:LYS:O	1:D:584:ILE:HG21	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:356:PHE:HE2	2:C:383:MET:HG2	1.72	0.54
2:C:389:PRO:CD	2:C:392:LEU:HD12	2.38	0.54
1:D:559:PHE:HZ	1:D:575:ALA:HB3	1.73	0.54
1:D:396:TYR:HB2	1:D:514:SER:HB3	1.90	0.53
1:D:410:ILE:HG23	1:D:425:LEU:HD11	1.90	0.53
2:C:187:LYS:HB3	2:C:199:TYR:CD1	2.43	0.53
1:D:93:ALA:HA	1:D:191:GLU:HG2	1.91	0.53
1:D:906:PHE:CE2	1:D:916:LEU:HD13	2.43	0.53
2:C:144:LEU:HD22	2:C:168:TRP:CZ2	2.44	0.53
2:C:263:PRO:CG	2:C:266:LEU:HD12	2.37	0.53
2:C:302:TRP:CZ3	2:C:423:LEU:HD21	2.43	0.53
1:D:1081:ILE:HG23	1:D:1135:ASN:HB3	1.90	0.53
2:C:402:GLU:HB3	2:C:518:ARG:HD3	1.90	0.53
2:C:343:VAL:HG12	2:C:345:HIS:H	1.74	0.53
2:C:520:LEU:O	2:C:524:GLN:HG3	2.08	0.53
1:D:54:LEU:HA	1:D:271:GLN:O	2.09	0.53
2:C:32:PHE:HE2	2:C:391:LEU:HD21	1.74	0.53
1:B:280:ASN:OD1	1:B:284:THR:N	2.41	0.53
2:C:381:TYR:HD1	2:C:558:LEU:HD22	1.74	0.53
1:D:887:THR:OG1	1:D:894:LEU:HB2	2.10	0.52
1:D:903:ALA:HB1	1:D:913:GLN:HB2	1.91	0.52
1:D:1081:ILE:CG2	1:D:1135:ASN:HB3	2.38	0.52
1:D:438:SER:HB3	1:D:509:ARG:HG3	1.90	0.52
1:D:455:LEU:HG	1:D:456:PHE:CE1	2.44	0.52
1:D:643:PHE:HE2	1:D:654:GLU:HA	1.74	0.52
1:D:94:SER:CB	1:D:265:TYR:HA	2.39	0.52
1:D:997:ILE:O	1:D:1001:LEU:HG	2.09	0.52
2:C:144:LEU:HA	2:C:148:LEU:HD12	1.91	0.52
2:C:494:ASP:OD1	2:C:496:THR:OG1	2.26	0.52
1:D:95:THR:CG2	1:D:189:LEU:HD13	2.38	0.52
1:D:398:ASP:O	1:D:511:VAL:HA	2.09	0.52
1:D:453:TYR:CZ	1:D:493:GLN:HB2	2.45	0.52
1:D:503:VAL:HA	1:D:506:GLN:CD	2.29	0.52
2:C:318:VAL:O	2:C:551:GLY:HA3	2.10	0.52
2:C:611:SER:HB3	2:C:614:ALA:HB3	1.91	0.52
1:D:103:GLY:N	1:D:241:LEU:HB2	2.25	0.52
2:C:389:PRO:HD2	2:C:392:LEU:HB2	1.92	0.52
1:D:279:TYR:HE1	1:D:285:ILE:HG12	1.75	0.52
2:C:526:GLN:HG3	2:C:539:LEU:HD11	1.92	0.52
1:D:201:PHE:HB3	1:D:229:LEU:O	2.09	0.52
1:D:410:ILE:HG23	1:D:425:LEU:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1028:LYS:O	1:D:1032:CYS:HB2	2.09	0.52
2:C:284:PRO:HD3	2:C:440:LEU:HD23	1.92	0.52
1:D:296:LEU:HB2	1:D:608:VAL:CG2	2.29	0.51
1:D:378:LYS:HE2	1:D:380:TYR:CE1	2.46	0.51
2:C:232:GLU:OE1	2:C:581:VAL:HB	2.10	0.51
1:D:802:PHE:O	1:D:806:LEU:HG	2.09	0.51
1:D:887:THR:CG2	1:D:894:LEU:HD12	2.38	0.51
1:D:986:PRO:O	1:D:990:GLU:HG3	2.10	0.51
2:C:453:THR:HG21	2:C:516:TYR:HB2	1.92	0.51
1:D:1003:SER:HB3	1:B:759:PHE:CE1	2.45	0.51
1:D:34:ARG:CZ	1:D:216:LEU:HB3	2.41	0.51
1:D:280:ASN:HD21	1:D:284:THR:HB	1.75	0.51
1:D:574:ASP:O	1:D:587:ILE:N	2.27	0.51
1:D:980:ILE:HD12	1:D:996:LEU:HD11	1.93	0.51
1:D:1041:ASP:OD1	1:D:1045:LYS:HA	2.10	0.51
2:C:48:TRP:CZ3	2:C:359:LEU:HB2	2.45	0.51
2:C:597:ASP:HA	2:C:600:LYS:HE3	1.91	0.51
1:D:192:PHE:HE1	1:D:205:SER:HG	1.58	0.51
1:A:916:LEU:O	1:A:920:GLN:N	2.44	0.51
1:D:375:SER:OG	1:D:436:TRP:HA	2.10	0.51
2:C:170:SER:HA	2:C:497:TYR:CE1	2.46	0.51
1:D:986:PRO:N	1:D:987:PRO:HD2	2.25	0.51
2:C:215:TYR:CE2	2:C:568:LEU:HD12	2.46	0.51
1:D:409:GLN:NE2	1:D:416:GLY:HA3	2.25	0.51
1:D:816:SER:OG	1:D:819:GLU:HG3	2.11	0.51
1:D:1029:MET:O	1:D:1033:VAL:HB	2.11	0.51
2:C:116:LEU:HD11	2:C:187:LYS:HD3	1.93	0.51
2:C:236:LEU:HD21	2:C:588:PHE:CD2	2.44	0.51
2:C:474:MET:HG3	2:C:494:ASP:O	2.11	0.51
1:D:34:ARG:NH2	1:D:217:PRO:HD2	2.26	0.50
2:C:158:TYR:HB2	2:C:252:TYR:HE2	1.74	0.50
2:C:177:ARG:HD3	2:C:496:THR:O	2.11	0.50
2:C:293:VAL:CG2	2:C:366:MET:HA	2.42	0.50
1:D:44:ARG:HB3	1:D:47:VAL:HG21	1.92	0.50
1:D:576:VAL:HG13	1:D:587:ILE:HD11	1.91	0.50
2:C:402:GLU:HG2	2:C:518:ARG:HD2	1.92	0.50
1:D:312:ILE:HD12	1:D:598:ILE:HD11	1.92	0.50
1:D:505:TYR:CD2	2:C:353:LYS:HA	2.46	0.50
1:D:897:PRO:HG2	1:D:900:MET:HB2	1.93	0.50
1:D:388:ASN:O	1:D:526:GLY:HA3	2.12	0.50
1:D:551:VAL:N	1:D:588:THR:O	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:181:GLU:HG2	2:C:473:TRP:CH2	2.45	0.50
1:D:130:VAL:O	1:D:166:CYS:HA	2.12	0.50
1:D:156:GLU:HB3	1:D:158:ARG:NH1	2.27	0.50
1:D:1130:ILE:HD12	1:B:920:GLN:HE22	1.77	0.50
2:C:233:ILE:HG12	2:C:584:LEU:HD23	1.93	0.50
2:C:488:VAL:HG11	2:C:612:PRO:HD3	1.92	0.50
1:D:589:PRO:HD2	1:B:855:PHE:CD1	2.47	0.50
1:D:881:THR:HA	1:D:885:GLY:O	2.12	0.50
1:D:53:ASP:OD1	1:D:54:LEU:N	2.38	0.50
1:D:335:LEU:HD23	1:D:362:VAL:HB	1.94	0.50
1:D:708:SER:HB3	1:D:711:SER:HB3	1.94	0.50
1:D:713:ALA:HB3	1:B:894:LEU:HD11	1.94	0.50
2:C:170:SER:O	2:C:174:LYS:HB2	2.11	0.50
2:C:545:SER:O	2:C:546:ASN:HB2	2.12	0.50
1:D:92:PHE:CE1	1:D:265:TYR:HB2	2.48	0.49
2:C:44:SER:HB2	2:C:351:LEU:HG	1.93	0.49
1:D:566:GLY:O	1:D:573:THR:HG23	2.11	0.49
1:D:598:ILE:HD11	1:D:666:ILE:HG12	1.94	0.49
2:C:453:THR:HA	2:C:512:PHE:CZ	2.47	0.49
1:D:452:ARG:HG2	1:D:494:SER:OG	2.13	0.49
1:D:589:PRO:HG2	1:B:855:PHE:CB	2.42	0.49
2:C:406:GLU:HG3	2:C:518:ARG:NH1	2.27	0.49
1:B:1072:GLU:N	1:B:1072:GLU:OE1	2.45	0.49
1:D:564:GLN:HG2	1:D:565:PHE:CE1	2.47	0.49
1:D:808:ASP:HB2	1:D:817:PHE:CE1	2.48	0.49
2:C:48:TRP:CH2	2:C:359:LEU:HB2	2.47	0.49
2:C:183:TYR:O	2:C:187:LYS:HG2	2.12	0.49
2:C:396:ALA:HB3	2:C:400:PHE:HD2	1.76	0.49
1:D:43:PHE:CE1	1:D:283:GLY:HA3	2.48	0.49
1:D:598:ILE:HG23	1:D:664:ILE:HG21	1.94	0.49
1:D:611:LEU:HD13	1:D:650:LEU:HD13	1.94	0.49
1:D:916:LEU:O	1:D:920:GLN:HB3	2.13	0.49
2:C:279:TYR:HA	2:C:282:THR:OG1	2.12	0.49
2:C:478:TRP:CD2	2:C:489:GLU:HB3	2.48	0.49
1:D:380:TYR:CD2	1:D:412:PRO:HD3	2.48	0.49
1:D:714:ILE:CG1	1:D:1096:VAL:HG11	2.43	0.49
2:C:174:LYS:HD2	2:C:497:TYR:CZ	2.47	0.49
2:C:393:ARG:O	2:C:394:ASN:HB2	2.12	0.49
1:A:193:VAL:HG23	1:A:223:LEU:HD22	1.94	0.49
1:A:341:VAL:HG23	1:A:342:PHE:N	2.28	0.49
1:D:55:PHE:HB3	1:D:275:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LYS:HD3	1:D:169:GLU:HG2	1.95	0.49
1:D:104:TRP:HA	1:D:239:GLN:O	2.13	0.48
1:D:453:TYR:HB3	1:D:495:TYR:CZ	2.47	0.48
1:D:825:LYS:HE3	1:D:939:SER:HA	1.95	0.48
2:C:50:TYR:O	2:C:54:ILE:HD13	2.13	0.48
1:D:118:LEU:HB2	1:D:133:PHE:CE2	2.47	0.48
1:D:353:TRP:CZ2	1:D:466:ARG:HB2	2.48	0.48
2:C:275:TRP:HB2	2:C:444:LEU:HB3	1.94	0.48
2:C:450:LEU:HD21	2:C:519:THR:HB	1.95	0.48
2:C:470:LYS:HG2	2:C:473:TRP:CZ2	2.49	0.48
1:D:909:ILE:O	1:D:1108:ASN:ND2	2.46	0.48
1:D:34:ARG:HB3	1:D:91:TYR:CE2	2.48	0.48
1:D:329:PHE:HB3	1:D:330:PRO:CD	2.43	0.48
1:D:564:GLN:H	1:B:48:LYS:HB3	1.77	0.48
1:D:33:THR:HG21	1:D:220:PHE:CA	2.34	0.48
1:D:393:THR:HG23	1:D:521:PRO:O	2.13	0.48
1:D:710:ASN:HB3	1:D:1076:THR:HG23	1.93	0.48
1:D:714:ILE:HG21	1:D:1110:TYR:HA	1.96	0.48
2:C:237:TYR:CD1	2:C:451:PRO:HG2	2.48	0.48
2:C:279:TYR:CE1	2:C:441:LYS:HB2	2.49	0.48
1:A:341:VAL:HG23	1:A:342:PHE:H	1.77	0.48
1:D:106:PHE:N	1:D:117:LEU:O	2.35	0.48
2:C:279:TYR:O	2:C:283:VAL:HG23	2.13	0.48
2:C:443:ALA:O	2:C:447:VAL:N	2.46	0.48
1:D:731:MET:HB3	1:D:774:GLN:NE2	2.28	0.48
2:C:103:ASN:HB2	2:C:107:VAL:HG13	1.95	0.48
2:C:234:LYS:O	2:C:238:GLU:HG3	2.14	0.48
1:D:58:PHE:HB2	1:D:293:LEU:HD22	1.94	0.48
1:D:188:ASN:HB3	1:D:207:HIS:HE1	1.78	0.48
1:D:455:LEU:HG	1:D:456:PHE:CD1	2.49	0.48
1:D:497:PHE:CE1	1:D:507:PRO:HB3	2.48	0.48
1:D:575:ALA:HB2	1:D:586:ASP:HA	1.96	0.48
1:D:906:PHE:HE2	1:D:916:LEU:HD13	1.79	0.47
1:D:279:TYR:CE1	1:D:285:ILE:HG12	2.49	0.47
1:D:1014:ARG:O	1:D:1018:ILE:HG12	2.13	0.47
2:C:293:VAL:HG11	2:C:423:LEU:HD13	1.95	0.47
1:D:103:GLY:O	1:D:241:LEU:N	2.38	0.47
1:D:1030:SER:CA	1:D:1034:LEU:HB3	2.37	0.47
2:C:157:ASP:OD1	2:C:158:TYR:N	2.47	0.47
2:C:170:SER:O	2:C:174:LYS:HD3	2.15	0.47
2:C:203:TRP:CE3	2:C:511:SER:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:233:ILE:HD13	2:C:450:LEU:HD13	1.96	0.47
1:D:41:LYS:O	1:A:563:GLN:NE2	2.47	0.47
1:D:294:ASP:HB3	1:D:295:PRO:HD2	1.96	0.47
2:C:489:GLU:O	2:C:489:GLU:HG2	2.14	0.47
1:D:411:ALA:O	1:D:414:GLN:HG2	2.15	0.47
1:D:755:GLN:O	1:A:968:SER:OG	2.31	0.47
2:C:327:PHE:CE1	2:C:379:ILE:HG21	2.50	0.47
1:D:56:LEU:HD22	1:D:91:TYR:CD2	2.50	0.47
1:D:213:VAL:HG12	1:D:214:ARG:HG2	1.97	0.47
1:D:770:ILE:O	1:D:774:GLN:HG2	2.14	0.47
2:C:424:LEU:HD21	2:C:428:PHE:CD2	2.49	0.47
2:C:453:THR:HG22	2:C:516:TYR:HB2	1.97	0.47
2:C:581:VAL:HG12	2:C:581:VAL:O	2.13	0.47
2:C:209:VAL:HG13	2:C:565:PRO:HB3	1.97	0.47
1:D:94:SER:O	1:D:189:LEU:HD12	2.14	0.47
1:D:543:PHE:CD2	1:D:576:VAL:HG21	2.50	0.47
1:D:821:LEU:O	1:D:825:LYS:HG2	2.15	0.47
1:D:972:ALA:HB3	1:D:996:LEU:HD21	1.97	0.47
1:D:107:GLY:N	1:D:235:ILE:HG23	2.29	0.47
1:D:396:TYR:O	1:D:513:LEU:HA	2.15	0.47
2:C:45:LEU:HA	2:C:351:LEU:HD21	1.97	0.47
1:D:63:THR:HG21	1:D:84:LEU:HD21	1.97	0.46
1:D:983:ARG:HD3	1:A:517:LEU:CD2	2.45	0.46
1:D:1104:VAL:HG23	1:D:1115:ILE:HG12	1.95	0.46
2:C:102:GLN:HG2	2:C:104:GLY:H	1.79	0.46
1:D:93:ALA:HB1	1:D:191:GLU:HG2	1.98	0.46
1:D:97:LYS:HE2	1:D:186:PHE:CD1	2.50	0.46
1:D:314:GLN:HG3	1:D:595:VAL:O	2.14	0.46
1:D:398:ASP:OD1	1:D:399:SER:N	2.48	0.46
1:D:421:TYR:CD1	1:D:457:ARG:HB3	2.49	0.46
1:B:578:ASP:OD2	1:B:581:THR:OG1	2.26	0.46
1:D:34:ARG:CZ	1:D:216:LEU:HD13	2.44	0.46
2:C:459:TRP:CZ2	2:C:463:VAL:HG21	2.51	0.46
1:D:28:TYR:HA	1:D:62:VAL:O	2.15	0.46
1:D:350:VAL:O	1:D:353:TRP:HD1	1.98	0.46
1:D:865:LEU:HG	1:D:870:ILE:HG13	1.98	0.46
1:D:906:PHE:HA	1:D:909:ILE:HG12	1.98	0.46
2:C:51:ASN:O	2:C:342:ALA:HA	2.15	0.46
1:D:132:GLU:O	1:D:163:ALA:HA	2.16	0.46
1:D:780:GLU:O	1:D:784:GLN:NE2	2.45	0.46
2:C:184:VAL:HG22	2:C:464:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:THR:O	1:D:274:THR:HG23	2.16	0.46
1:D:57:PRO:HG3	1:D:273:ARG:HG3	1.97	0.46
1:D:126:VAL:HB	1:D:172:SER:CB	2.45	0.46
1:D:576:VAL:HG13	1:D:587:ILE:CD1	2.46	0.46
1:D:853:GLN:NE2	1:D:960:ASN:OD1	2.49	0.46
2:C:201:ASP:OD2	2:C:219:ARG:NE	2.46	0.46
1:D:457:ARG:NH1	1:D:459:SER:OG	2.49	0.46
1:D:505:TYR:HD2	2:C:353:LYS:HA	1.81	0.46
1:D:971:GLY:H	1:B:755:GLN:HB3	1.81	0.46
1:D:1090:PRO:HD3	1:D:1095:PHE:CZ	2.51	0.46
2:C:64:ASN:O	2:C:68:LYS:HG3	2.15	0.46
1:B:122:ASN:O	1:B:123:ALA:HB3	2.16	0.46
1:D:131:CYS:HB3	1:D:163:ALA:HB1	1.97	0.45
1:D:535:LYS:HE2	1:D:585:LEU:CD2	2.46	0.45
2:C:446:ILE:HG21	2:C:523:PHE:HZ	1.81	0.45
1:D:401:VAL:HG22	1:D:509:ARG:HG2	1.98	0.45
1:D:1087:ALA:HB1	1:D:1089:PHE:CE1	2.51	0.45
2:C:304:ALA:HA	2:C:307:ILE:HD12	1.97	0.45
2:C:306:ARG:O	2:C:310:GLU:HG2	2.16	0.45
2:C:478:TRP:CE3	2:C:489:GLU:HB3	2.51	0.45
1:D:418:ILE:HA	1:D:422:ASN:ND2	2.21	0.45
1:D:985:ASP:HB3	1:D:987:PRO:HD2	1.98	0.45
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.41	0.45
2:C:32:PHE:CE1	2:C:76:GLN:HG3	2.52	0.45
2:C:263:PRO:HG2	2:C:266:LEU:CD1	2.42	0.45
1:A:474:GLN:NE2	1:A:478:THR:O	2.49	0.45
1:D:21:ARG:HG3	1:D:79:PHE:HB3	1.99	0.45
1:D:367:VAL:O	1:D:371:SER:HB3	2.15	0.45
1:D:503:VAL:HA	1:D:506:GLN:HG3	1.98	0.45
1:D:788:ILE:HD11	1:A:699:LEU:CB	2.44	0.45
1:D:970:PHE:O	1:D:995:ARG:HB3	2.15	0.45
1:D:1051:SER:HG	1:D:1064:HIS:CE1	2.33	0.45
2:C:302:TRP:HA	2:C:306:ARG:NH2	2.31	0.45
1:D:91:TYR:CE2	1:D:93:ALA:HB2	2.51	0.45
1:D:193:VAL:HG23	1:D:223:LEU:HD13	1.99	0.45
1:D:271:GLN:HB3	1:D:272:PRO:HD2	1.99	0.45
1:D:971:GLY:HA2	1:B:755:GLN:OE1	2.16	0.45
1:D:340:GLU:HA	1:D:343:ASN:HB3	1.97	0.45
1:D:398:ASP:N	1:D:512:VAL:O	2.23	0.45
1:D:400:PHE:CD1	1:D:402:ILE:HG23	2.52	0.45
2:C:446:ILE:HG21	2:C:523:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:VAL:HG12	1:D:452:ARG:O	2.16	0.45
1:D:1072:GLU:N	1:D:1072:GLU:OE1	2.50	0.45
1:D:400:PHE:HD1	1:D:402:ILE:HG23	1.81	0.45
1:D:887:THR:CB	1:D:894:LEU:HD12	2.46	0.45
1:D:1030:SER:O	1:D:1035:GLY:N	2.36	0.45
2:C:32:PHE:CE2	2:C:391:LEU:HD21	2.52	0.45
2:C:257:SER:OG	2:C:258:PRO:HD2	2.17	0.45
2:C:279:TYR:HA	2:C:282:THR:HG1	1.81	0.45
1:D:275:PHE:CD1	1:D:290:ASP:HA	2.52	0.45
1:D:560:LEU:HD12	1:D:563:GLN:CD	2.36	0.45
1:D:759:PHE:O	1:D:763:LEU:HG	2.16	0.45
2:C:533:ALA:HB3	2:C:535:HIS:CD2	2.52	0.45
1:D:336:CYS:SG	1:D:358:ILE:HG23	2.56	0.44
1:D:597:VAL:HG13	1:D:608:VAL:HG13	1.99	0.44
1:D:611:LEU:CD2	1:D:666:ILE:HG23	2.47	0.44
1:D:880:GLY:O	1:D:884:SER:HB2	2.17	0.44
1:D:98:SER:OG	1:D:180:GLU:O	2.13	0.44
1:D:1033:VAL:HG13	1:D:1053:PRO:HD3	1.99	0.44
1:D:1105:THR:HG22	1:D:1111:GLU:O	2.18	0.44
1:B:44:TYR:OH	1:B:60:ASP:OD2	2.35	0.44
1:D:452:ARG:HA	1:D:494:SER:HA	2.00	0.44
1:D:564:GLN:HG2	1:D:565:PHE:CD1	2.52	0.44
2:C:431:ASP:OD1	2:C:434:THR:HG23	2.18	0.44
1:A:568:ASP:OD2	1:A:572:THR:OG1	2.36	0.44
2:C:132:VAL:HG23	2:C:168:TRP:CE3	2.44	0.44
1:D:429:PHE:CZ	1:D:431:GLY:HA3	2.52	0.44
1:D:597:VAL:HG13	1:D:608:VAL:CG1	2.48	0.44
1:D:676:THR:HA	1:D:690:GLN:HG2	1.99	0.44
1:D:974:SER:CB	1:D:983:ARG:HH22	2.31	0.44
1:D:996:LEU:O	1:D:1000:ARG:HG3	2.18	0.44
2:C:521:TYR:CE1	2:C:579:MET:HG2	2.53	0.44
1:D:18:LEU:HB2	1:D:21:ARG:HB2	2.00	0.44
1:D:107:GLY:O	1:D:235:ILE:HG23	2.18	0.44
1:B:39:PHE:CE2	1:B:40:THR:HG23	2.52	0.44
1:D:800:PHE:CE1	1:D:924:ALA:HA	2.52	0.44
1:D:904:TYR:HB2	1:A:1107:ARG:HH22	1.83	0.44
2:C:43:SER:HA	2:C:65:ALA:HB1	2.00	0.44
2:C:503:LEU:HD23	2:C:506:VAL:CG2	2.29	0.44
2:C:581:VAL:HG13	2:C:584:LEU:HD23	2.00	0.44
2:C:261:CYS:HB3	2:C:486:GLY:O	2.18	0.44
1:B:738:CYS:SG	1:B:764:ASN:ND2	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ALA:HB1	1:D:352:ALA:O	2.18	0.43
1:D:435:ALA:HB2	1:D:510:VAL:HG22	2.00	0.43
1:D:1080:ALA:HB2	1:D:1089:PHE:HE1	1.82	0.43
2:C:144:LEU:CA	2:C:148:LEU:HB2	2.38	0.43
2:C:478:TRP:CE3	2:C:481:LYS:HD2	2.52	0.43
1:D:185:ASN:OD1	1:D:213:VAL:HG22	2.18	0.43
2:C:49:ASN:O	2:C:58:ASN:ND2	2.51	0.43
1:A:39:PHE:CD2	1:A:40:THR:HG23	2.53	0.43
1:D:230:PRO:HG2	1:A:357:ARG:HH12	1.83	0.43
1:D:592:PHE:HZ	1:B:854:LYS:O	2.01	0.43
1:D:714:ILE:HB	1:D:1075:PHE:CE2	2.52	0.43
2:C:556:ASN:O	2:C:560:LEU:HG	2.18	0.43
1:A:269:TYR:HE1	1:A:271:GLN:HE21	0.78	0.43
1:D:102:ARG:NH2	1:D:141:LEU:HD22	2.34	0.43
1:D:324:GLU:O	1:D:539:VAL:HB	2.19	0.43
2:C:292:ASP:HA	2:C:366:MET:SD	2.58	0.43
2:C:435:GLU:OE2	2:C:541:LYS:HE2	2.18	0.43
1:D:314:GLN:HA	1:D:595:VAL:O	2.18	0.43
1:D:589:PRO:HG2	1:B:855:PHE:HB3	2.00	0.43
1:D:800:PHE:CD2	1:D:898:PHE:HE2	2.37	0.43
1:D:977:LEU:O	1:D:981:LEU:HG	2.18	0.43
2:C:267:LEU:HD12	2:C:272:GLY:HA3	1.99	0.43
1:D:102:ARG:CZ	1:D:141:LEU:HB3	2.49	0.43
1:D:201:PHE:HE2	1:D:203:ILE:HB	1.83	0.43
1:D:906:PHE:CE2	1:D:916:LEU:HB2	2.53	0.43
1:D:960:ASN:O	1:D:964:LYS:HG3	2.19	0.43
2:C:234:LYS:N	2:C:235:PRO:HD2	2.33	0.43
2:C:478:TRP:CE2	2:C:489:GLU:HB3	2.54	0.43
1:D:598:ILE:CD1	1:D:666:ILE:HG12	2.49	0.43
1:D:1105:THR:HG22	1:D:1111:GLU:C	2.40	0.43
2:C:32:PHE:HE1	2:C:76:GLN:HG3	1.84	0.43
1:A:122:ASN:O	1:A:123:ALA:HB3	2.18	0.43
1:D:895:GLN:O	1:D:895:GLN:HG3	2.19	0.43
2:C:31:LYS:HE2	2:C:35:GLU:OE2	2.19	0.43
1:D:66:HIS:CE1	1:D:78:ARG:HE	2.36	0.42
1:D:418:ILE:HD13	1:D:422:ASN:ND2	2.34	0.42
1:D:201:PHE:CE2	1:D:203:ILE:HB	2.54	0.42
1:D:570:ALA:HB1	1:B:963:VAL:HG11	2.01	0.42
1:D:714:ILE:HG12	1:D:1075:PHE:HD2	1.84	0.42
1:A:738:CYS:SG	1:A:764:ASN:ND2	2.93	0.42
1:B:457:ARG:NH1	1:B:467:ASP:OD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:245:ARG:HG3	2:C:262:LEU:CD2	2.48	0.42
2:C:401:HIS:HB2	2:C:514:ARG:NH2	2.34	0.42
1:A:131:CYS:HB2	1:A:133:PHE:CE1	2.54	0.42
1:B:31:LEU:HB2	1:B:32:PRO:HD2	2.01	0.42
1:B:193:VAL:HG23	1:B:223:LEU:HD13	2.00	0.42
1:D:714:ILE:HG22	1:D:1110:TYR:HB2	2.00	0.42
2:C:269:ASP:OD1	2:C:272:GLY:HA2	2.19	0.42
1:D:802:PHE:CD2	1:D:882:ILE:HD13	2.54	0.42
1:D:453:TYR:N	1:D:493:GLN:O	2.53	0.42
2:C:90:ASN:ND2	2:C:93:VAL:HG23	2.34	0.42
1:D:713:ALA:O	1:B:894:LEU:HD11	2.20	0.42
2:C:488:VAL:CG1	2:C:612:PRO:HD3	2.49	0.42
1:B:318:PHE:N	1:B:593:GLY:O	2.52	0.42
1:D:146:HIS:HE1	1:D:152:TRP:HA	1.85	0.42
1:D:411:ALA:HB3	1:D:414:GLN:NE2	2.34	0.42
2:C:284:PRO:HD3	2:C:440:LEU:CD2	2.49	0.42
2:C:374:HIS:HE1	2:C:402:GLU:HG3	1.84	0.42
1:D:410:ILE:O	1:D:411:ALA:HB2	2.20	0.42
1:D:503:VAL:HA	1:D:506:GLN:CG	2.50	0.42
1:D:91:TYR:HE1	1:D:223:LEU:HD11	1.85	0.42
1:D:1078:ALA:HB2	1:D:1102:TRP:CH2	2.55	0.42
2:C:500:PRO:O	2:C:506:VAL:HB	2.19	0.42
1:B:327:VAL:O	1:B:531:THR:N	2.53	0.42
1:D:129:LYS:CD	1:D:169:GLU:HG2	2.49	0.41
1:D:190:ARG:HD3	1:D:192:PHE:CZ	2.55	0.41
1:D:989:ALA:O	1:D:993:ILE:HG13	2.20	0.41
2:C:144:LEU:HA	2:C:148:LEU:CD1	2.48	0.41
2:C:358:ILE:HD11	2:C:379:ILE:HG13	2.02	0.41
2:C:594:TRP:CE3	2:C:595:LEU:HD23	2.55	0.41
1:A:51:ARG:NH2	1:B:571:ASP:OD1	2.53	0.41
1:D:34:ARG:NH2	1:D:216:LEU:HD22	2.35	0.41
1:D:476:GLY:HA3	2:C:24:GLN:NE2	2.27	0.41
1:D:726:ILE:HD13	1:D:945:LEU:HD23	2.01	0.41
1:D:877:LEU:HD13	1:D:1029:MET:SD	2.60	0.41
2:C:207:TYR:CE1	2:C:397:ASN:HB2	2.54	0.41
2:C:518:ARG:O	2:C:522:GLN:HG2	2.20	0.41
2:C:107:VAL:HB	2:C:193:ALA:HB1	2.03	0.41
2:C:293:VAL:HG22	2:C:366:MET:HG3	2.02	0.41
2:C:432:ASN:O	2:C:436:ILE:HG13	2.20	0.41
1:D:498:GLN:OE1	2:C:41:TYR:HE2	2.03	0.41
1:D:1033:VAL:HG22	1:D:1051:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1095:PHE:CD1	1:D:1104:VAL:HG22	2.54	0.41
2:C:571:GLU:O	2:C:575:GLY:HA2	2.21	0.41
1:D:129:LYS:HE2	1:D:169:GLU:HB3	2.03	0.41
2:C:177:ARG:N	2:C:178:PRO:HD2	2.36	0.41
2:C:582:ARG:N	2:C:583:PRO:HD2	2.35	0.41
1:B:91:TYR:HD1	1:B:193:VAL:HG22	1.85	0.41
1:B:111:ASP:OD1	1:B:112:SER:N	2.45	0.41
1:D:83:VAL:CG2	1:D:239:GLN:HE21	2.34	0.41
1:D:93:ALA:CA	1:D:191:GLU:HG2	2.49	0.41
1:D:206:LYS:HE2	1:D:221:SER:HB3	2.02	0.41
2:C:144:LEU:HB2	2:C:168:TRP:CH2	2.55	0.41
1:A:986:PRO:N	1:A:987:PRO:HD2	2.36	0.41
1:B:1091:ARG:NE	1:B:1120:THR:O	2.54	0.41
1:D:53:ASP:OD2	1:D:195:LYS:NZ	2.54	0.41
1:D:102:ARG:NE	1:D:141:LEU:HB3	2.36	0.41
1:D:269:TYR:HD1	1:D:271:GLN:HE21	1.69	0.41
1:D:404:GLY:HA3	1:D:504:GLY:O	2.20	0.41
2:C:144:LEU:CA	2:C:148:LEU:HD12	2.51	0.41
2:C:169:ARG:HA	2:C:173:GLY:H	1.86	0.41
1:B:47:ASP:OD1	1:B:48:LYS:N	2.45	0.41
1:D:33:THR:HG21	1:D:220:PHE:CD1	2.56	0.41
1:D:1033:VAL:HG11	1:D:1053:PRO:HD3	2.01	0.41
1:A:111:ASP:OD1	1:A:112:SER:N	2.46	0.41
1:D:451:TYR:HD2	1:D:497:PHE:CE2	2.37	0.41
1:D:712:ILE:CG2	1:D:1077:THR:HB	2.44	0.41
1:D:791:THR:CB	1:D:795:LYS:HE2	2.51	0.41
1:D:808:ASP:HB2	1:D:817:PHE:HE1	1.86	0.41
1:D:823:PHE:CD1	1:D:1057:PRO:HD3	2.56	0.41
1:D:1141:LEU:HD23	1:B:1144:GLU:OE1	2.21	0.41
2:C:53:ASN:OD1	2:C:340:GLN:HB3	2.21	0.41
2:C:147:GLY:O	2:C:151:ILE:HG12	2.21	0.41
2:C:161:ARG:NH2	2:C:265:HIS:O	2.53	0.41
2:C:455:MET:HB2	2:C:484:ILE:HG21	2.03	0.41
2:C:477:TRP:NE1	2:C:499:ASP:OD2	2.54	0.41
2:C:555:PHE:HA	2:C:558:LEU:HD12	2.02	0.41
1:D:351:TYR:CE2	1:D:452:ARG:HB2	2.51	0.41
1:D:986:PRO:CD	1:D:987:PRO:HD2	2.50	0.41
1:D:1097:SER:HB2	1:D:1102:TRP:CE3	2.56	0.41
2:C:133:CYS:HA	2:C:141:CYS:HA	2.03	0.41
1:D:434:ILE:O	1:D:510:VAL:HA	2.21	0.40
1:D:986:PRO:HD2	1:D:987:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:ARG:O	2:C:181:GLU:HG3	2.20	0.40
1:A:91:TYR:HD1	1:A:193:VAL:HG22	1.86	0.40
1:B:925:ASN:O	1:B:929:SER:OG	2.33	0.40
1:D:129:LYS:HG2	1:D:169:GLU:CA	2.34	0.40
1:D:896:ILE:CG2	1:D:897:PRO:HD2	2.51	0.40
2:C:498:CYS:SG	2:C:501:ALA:HB2	2.61	0.40
1:B:986:PRO:N	1:B:987:PRO:HD2	2.37	0.40
1:D:115:GLN:HE22	1:D:167:THR:HG21	1.85	0.40
1:D:643:PHE:CE2	1:D:654:GLU:HA	2.54	0.40
1:D:865:LEU:HD11	1:D:873:TYR:CE2	2.57	0.40
1:D:1139:ASP:HB3	1:D:1142:GLN:HG3	2.03	0.40
2:C:153:ALA:HA	2:C:268:GLY:O	2.21	0.40
2:C:594:TRP:CZ3	2:C:595:LEU:HD23	2.56	0.40
1:B:367:VAL:O	1:B:371:SER:N	2.54	0.40
1:D:299:THR:HA	1:D:315:THR:HG22	2.04	0.40
1:D:535:LYS:HE2	1:D:585:LEU:HD21	2.03	0.40
1:D:722:VAL:HA	1:D:1064:HIS:O	2.22	0.40
2:C:284:PRO:HD2	2:C:437:ASN:OD1	2.22	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	1050/1261 (83%)	1001 (95%)	48 (5%)	1 (0%)	51	84
1	B	1056/1261 (84%)	1008 (96%)	48 (4%)	0	100	100
1	D	1056/1261 (84%)	1005 (95%)	51 (5%)	0	100	100
2	C	595/625 (95%)	587 (99%)	8 (1%)	0	100	100
All	All	3757/4408 (85%)	3601 (96%)	155 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	928/1099 (84%)	928 (100%)	0	100	100
1	B	933/1099 (85%)	933 (100%)	0	100	100
1	D	933/1099 (85%)	933 (100%)	0	100	100
2	C	527/552 (96%)	527 (100%)	0	100	100
All	All	3321/3849 (86%)	3321 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	115	GLN
1	D	137	ASN
1	D	207	HIS
1	D	239	GLN
1	D	343	ASN
1	D	394	ASN
1	D	414	GLN
1	D	422	ASN
1	D	853	GLN
1	D	895	GLN
1	D	965	GLN
1	D	1101	HIS
1	D	1106	GLN
2	C	24	GLN
2	C	210	ASN
2	C	380	GLN
2	C	401	HIS
2	C	417	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	524	GLN
2	C	526	GLN
1	A	965	GLN
1	B	99	ASN
1	B	895	GLN
1	B	920	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

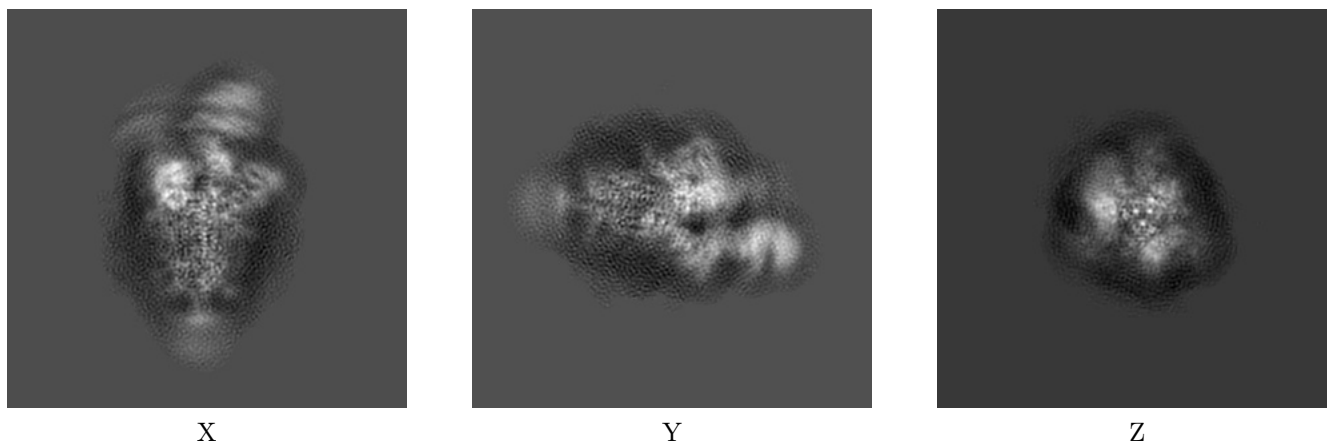
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32174. 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](#)

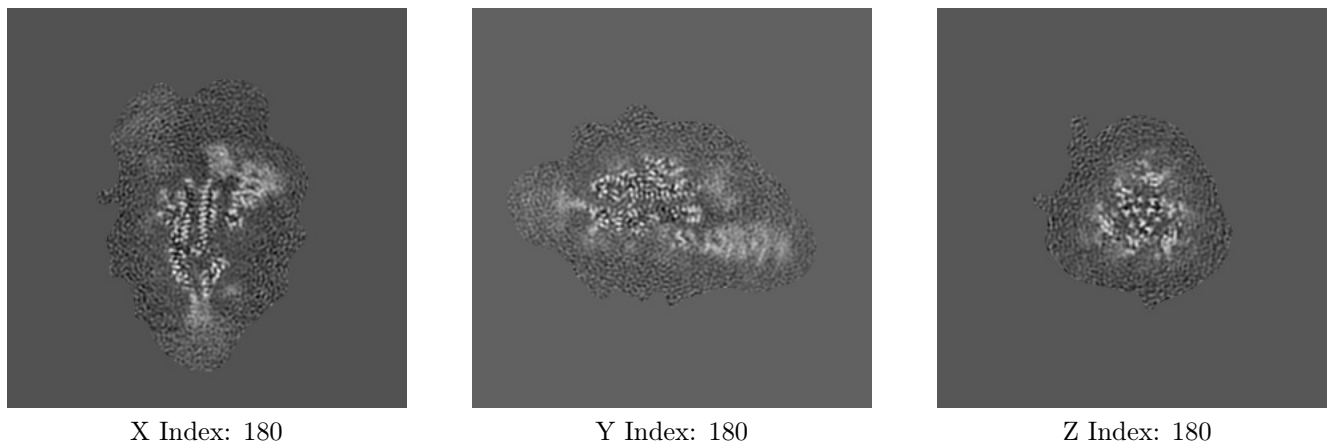
6.1.1 Primary map



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

6.2 Central slices [i](#)

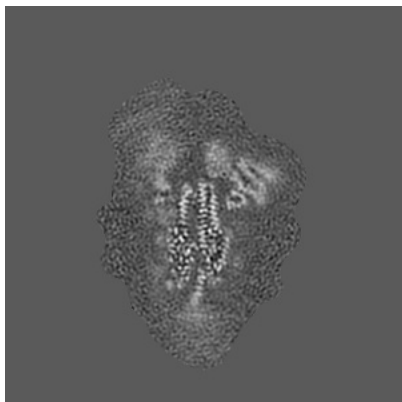
6.2.1 Primary map



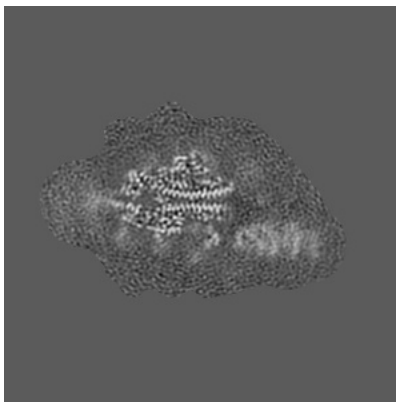
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

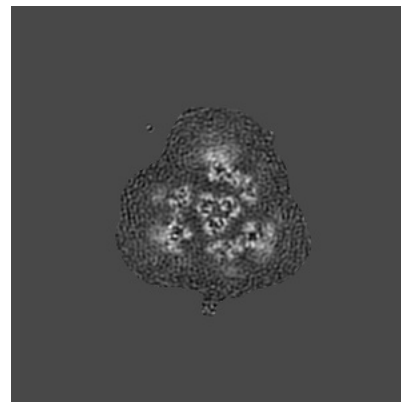
6.3.1 Primary map



X Index: 192



Y Index: 177



Z Index: 193

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

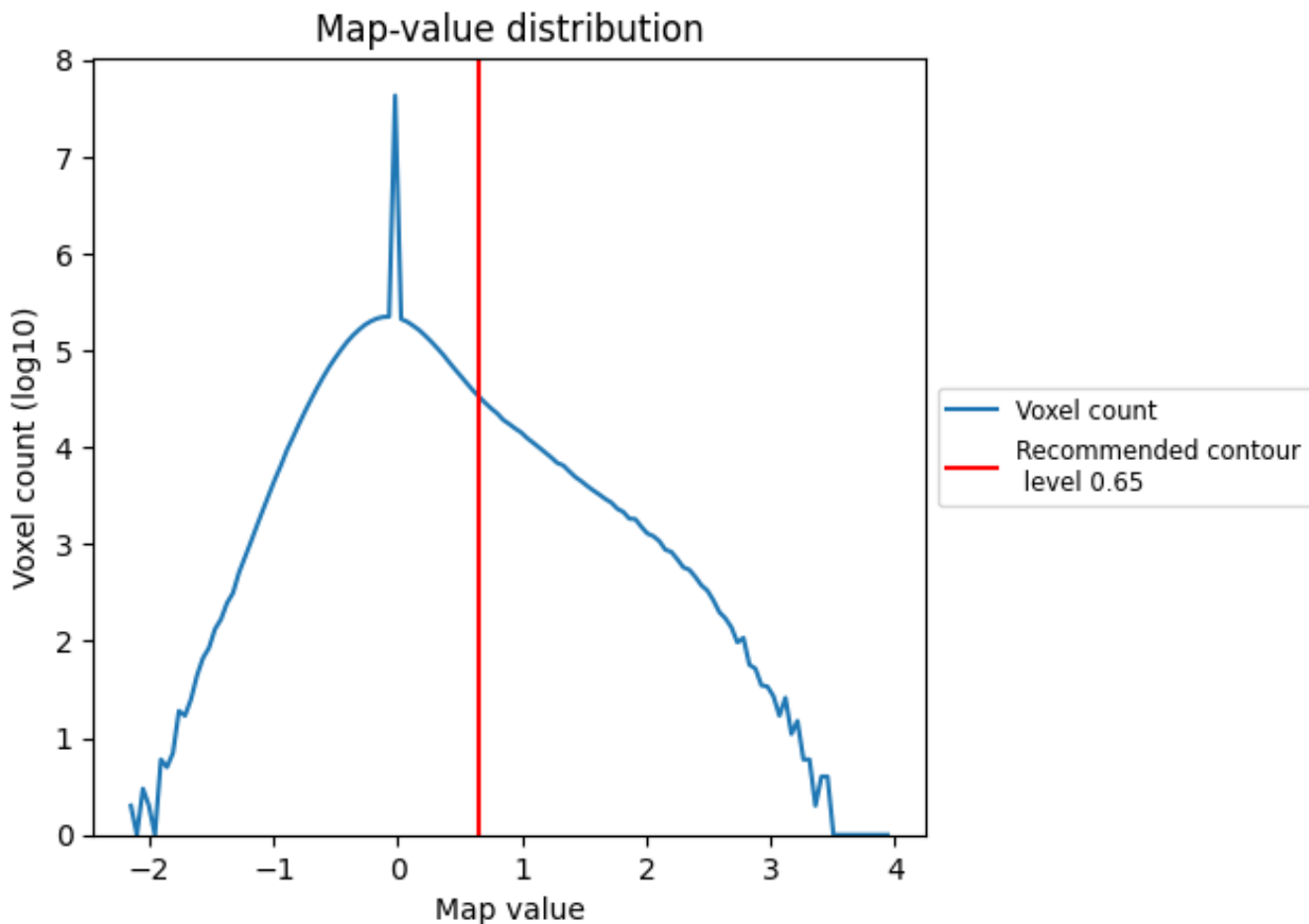
6.5 Mask visualisation

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

7 Map analysis [i](#)

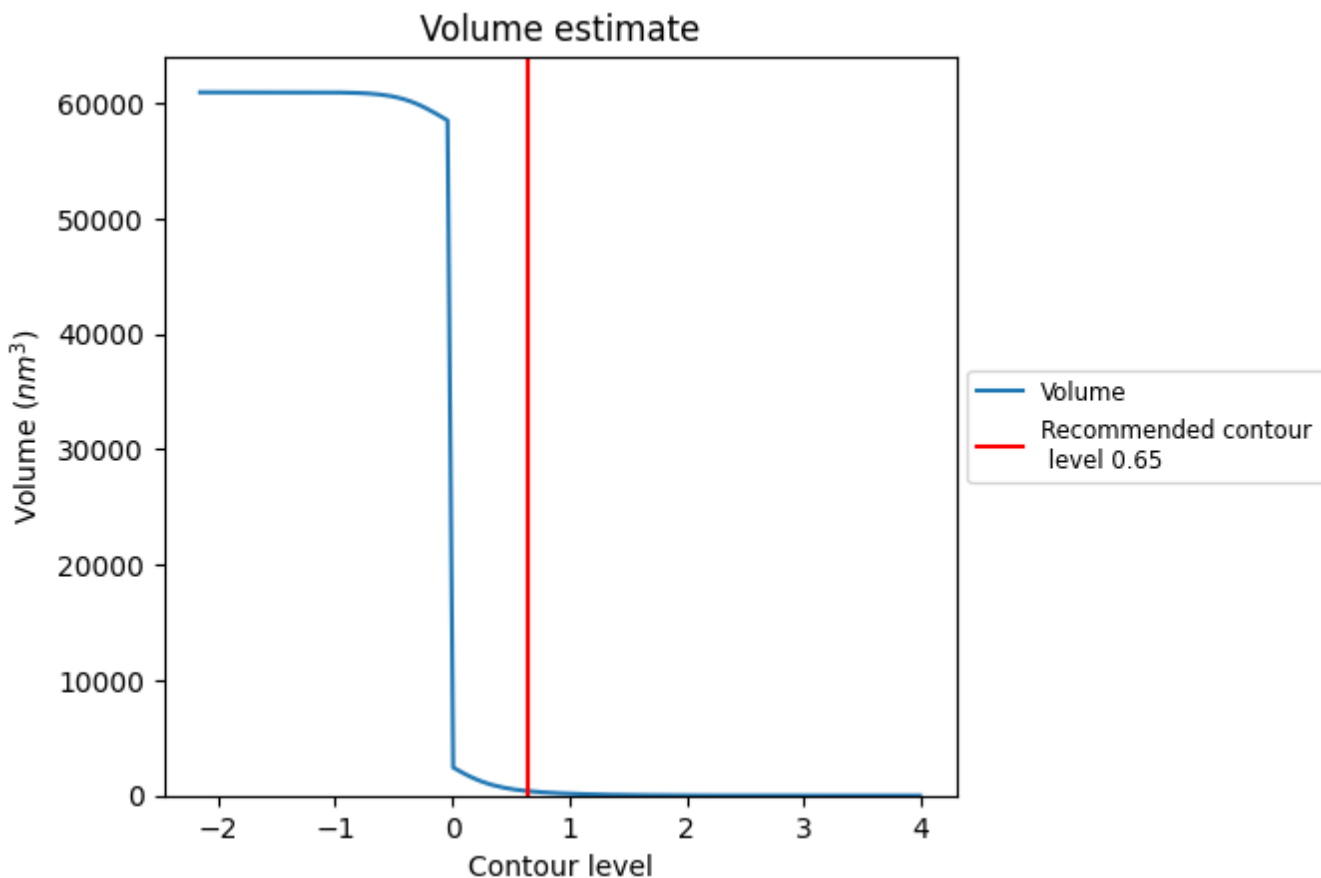
This section contains the results of statistical analysis of the map.

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.

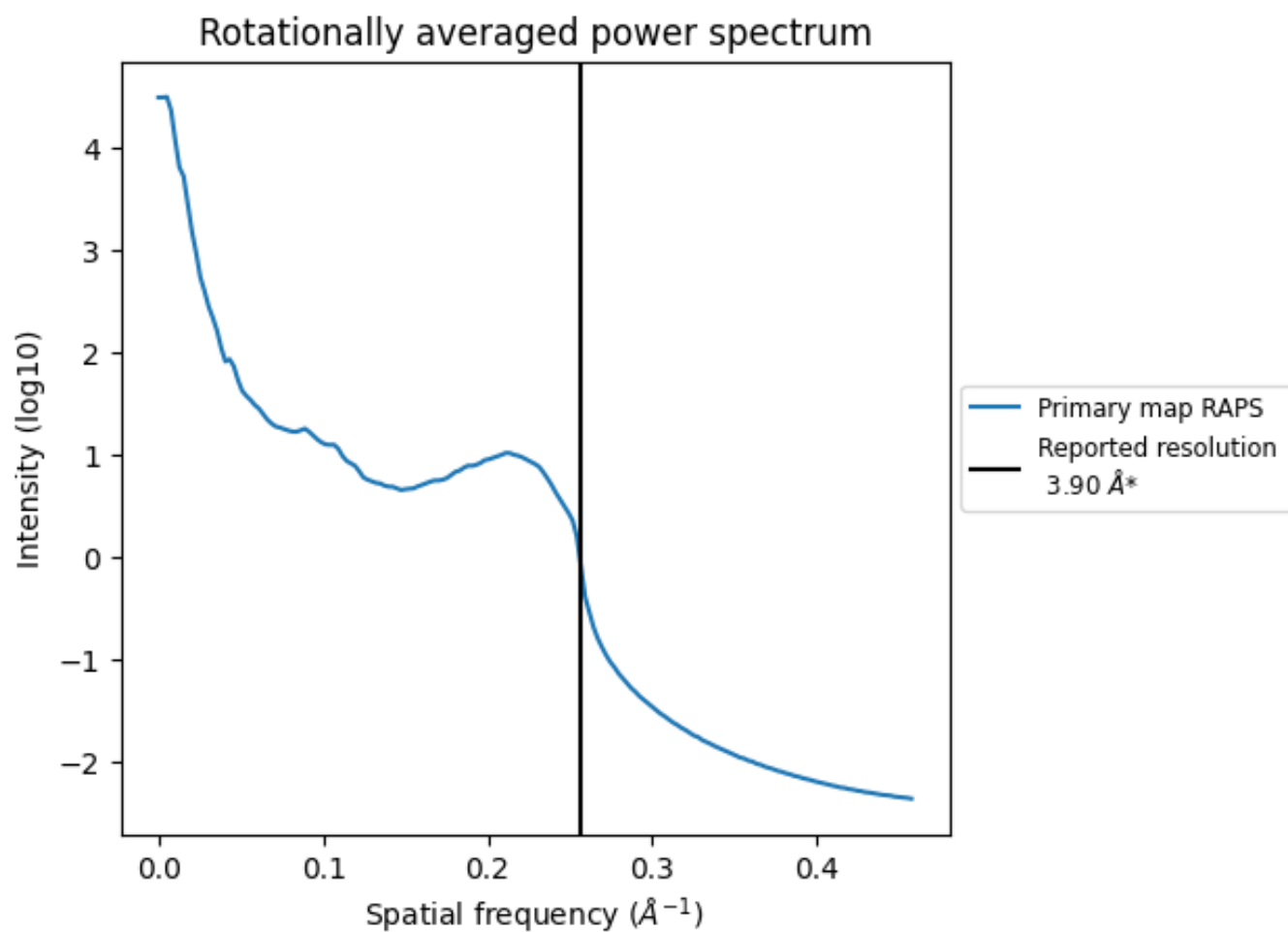
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 385 nm³; this corresponds to an approximate mass of 348 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.256\AA^{-1}

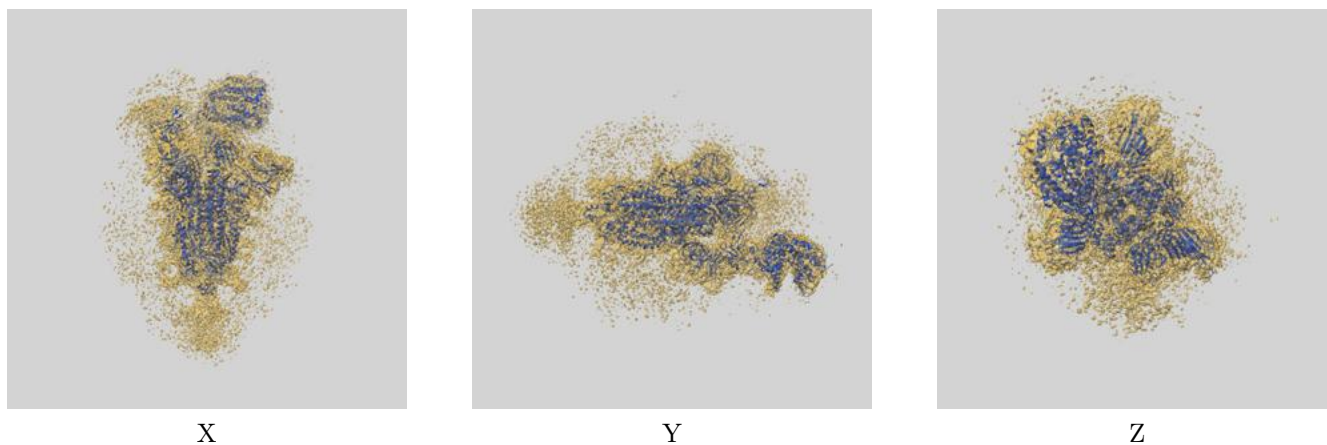
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

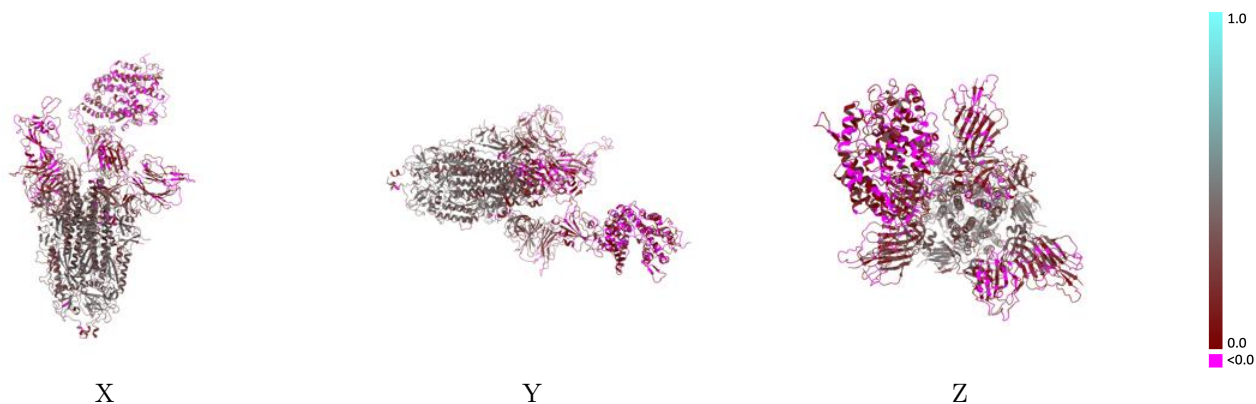
This section contains information regarding the fit between EMDB map EMD-32174 and PDB model 7VXB. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



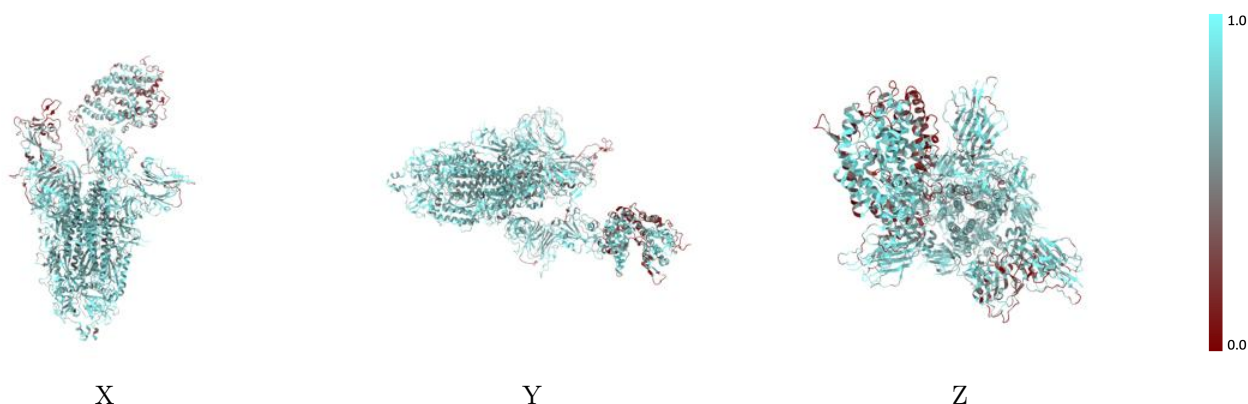
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



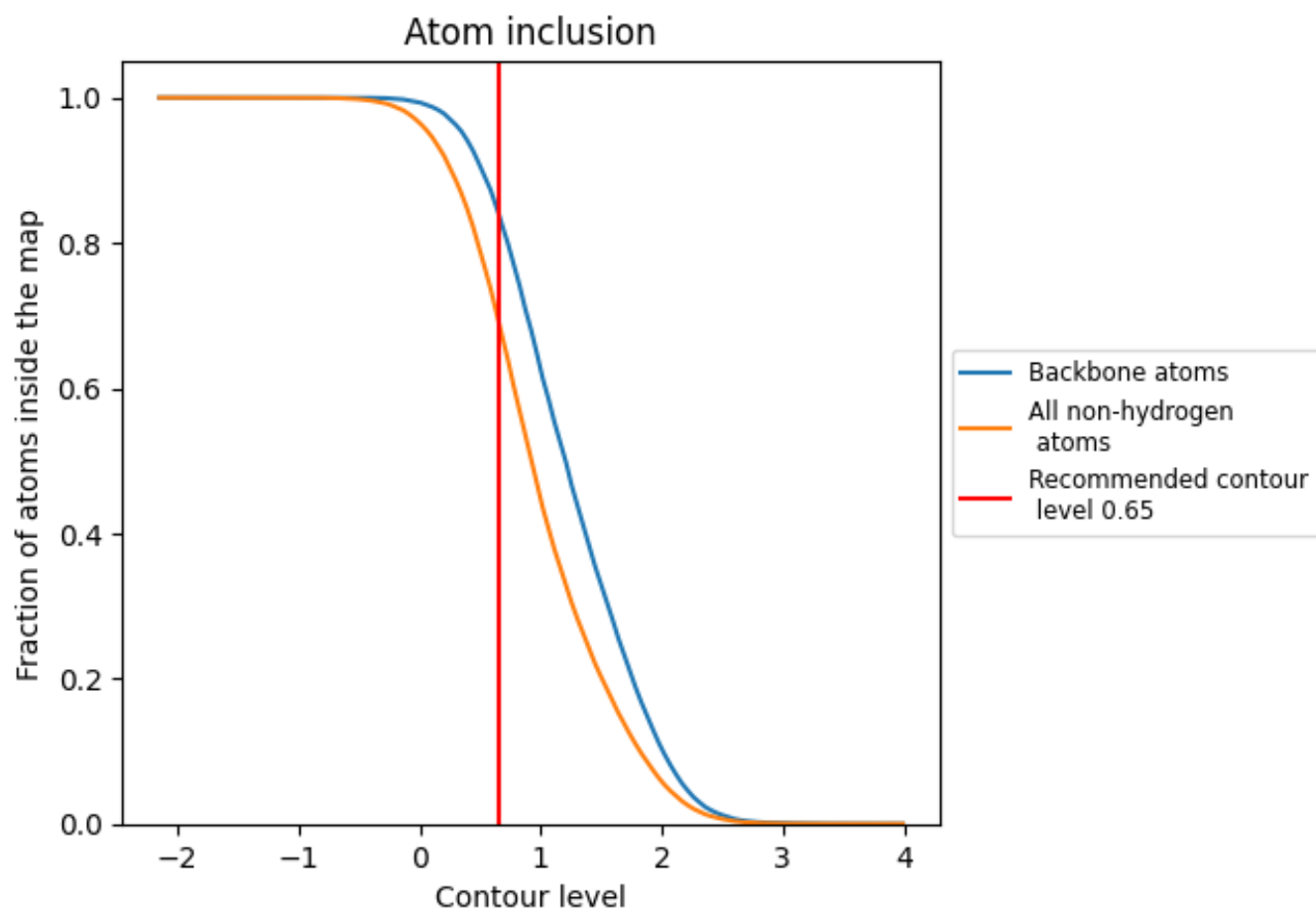
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.65).








9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 69% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6931	 0.2220
A	 0.7282	 0.2640
B	 0.6828	 0.2640
C	 0.5965	 0.0460
D	 0.7248	 0.2430

