



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 05:01 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.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

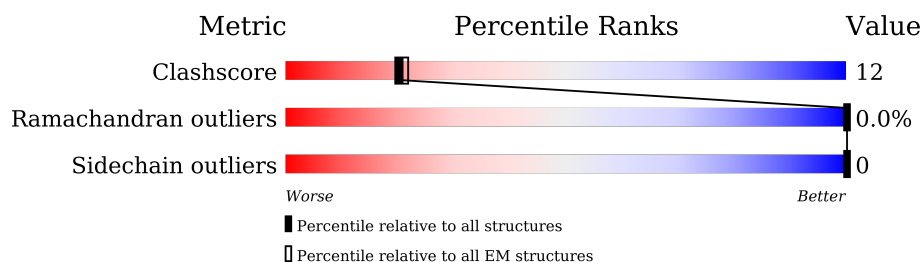
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1261	<div> <div>5%</div> <div>79%</div> <div>5%</div> <div>16%</div> </div>
1	B	1261	<div> <div>10%</div> <div>80%</div> <div>•</div> <div>15%</div> </div>
1	D	1261	<div> <div>7%</div> <div>49%</div> <div>36%</div> <div>15%</div> </div>
2	C	625	<div> <div>29%</div> <div>56%</div> <div>40%</div> <div>•</div> </div>

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
1	D	1068	Total	C	N	O	S	0	0
			8354	5327	1401	1587	39		
1	A	1062	Total	C	N	O	S	0	0
			8310	5300	1394	1578	38		
1	B	1068	Total	C	N	O	S	0	0
			8354	5327	1401	1587	39		

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
2	C	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

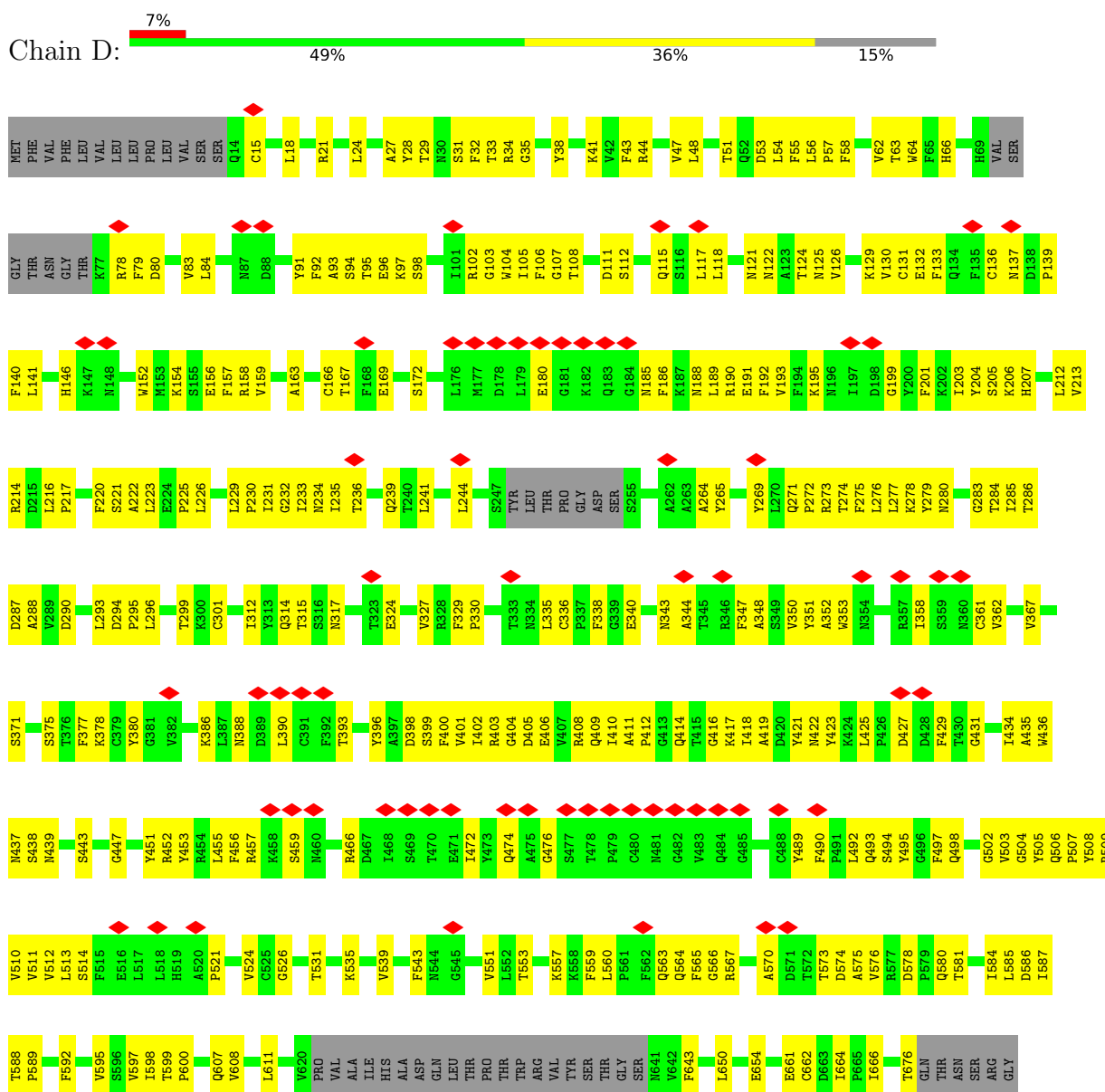
There are 26 discrepancies between the modelled and reference sequences:

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 [i](#)

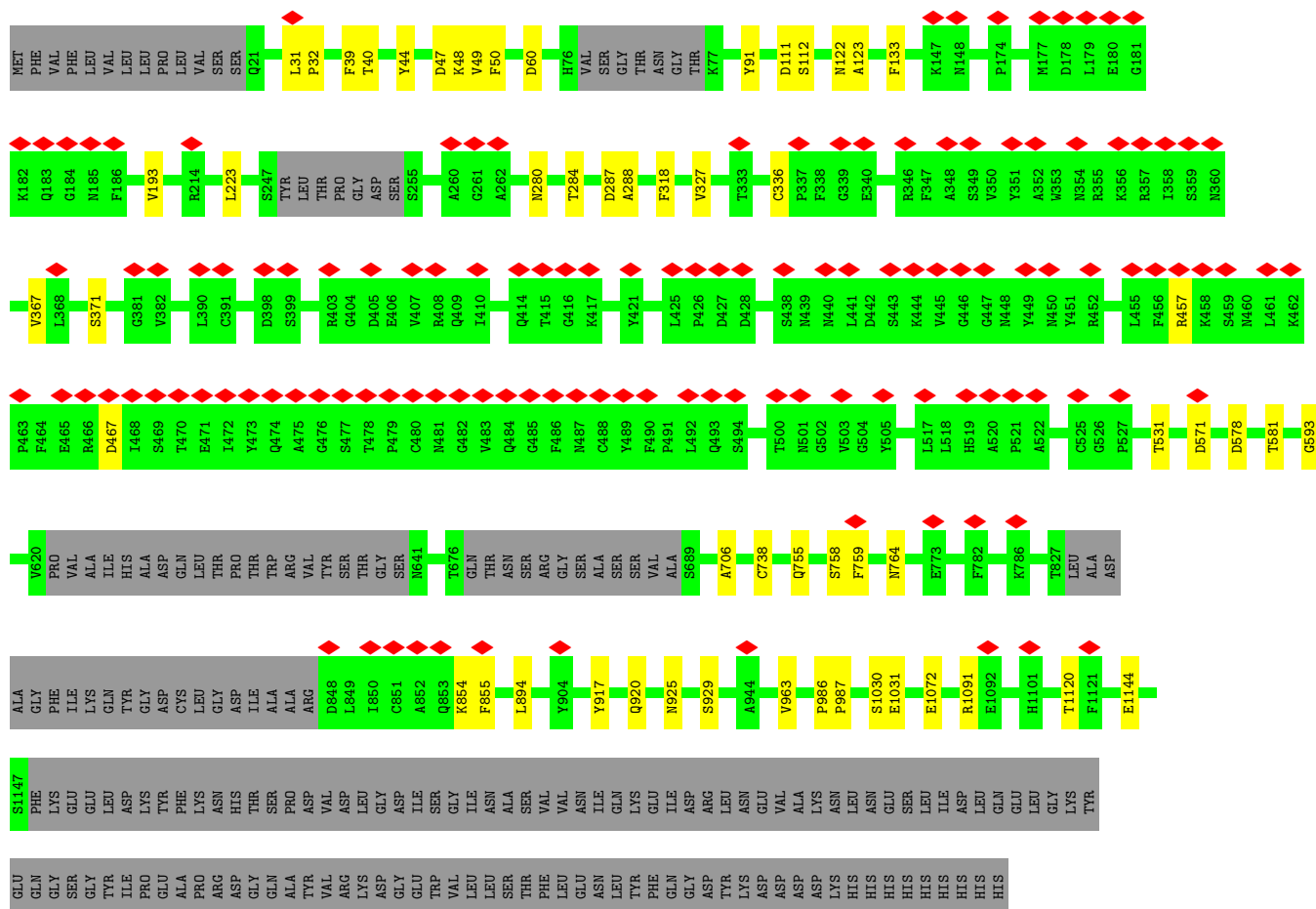
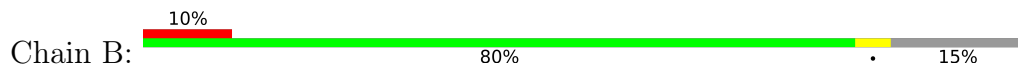
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

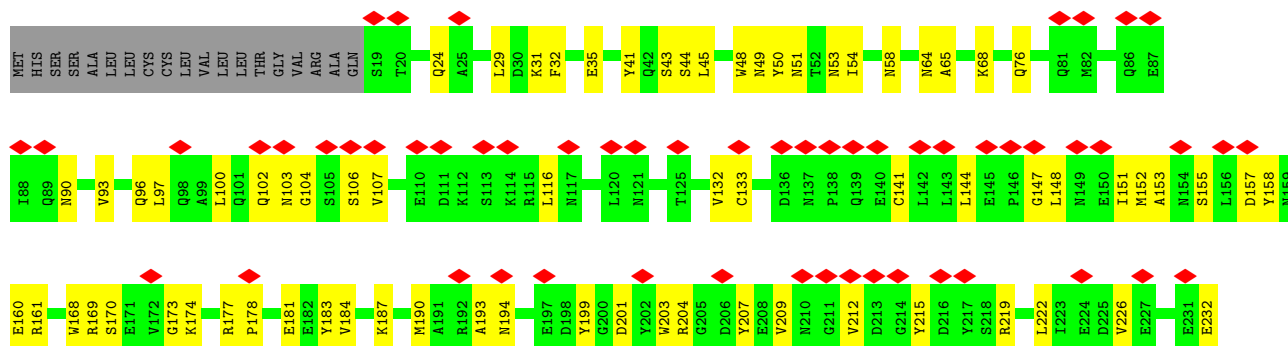


ILE	ASP	GLN	GLU	LEU	GLY	LYS	TYR	GLN	GLY	SER	GLY	TYR	ILE	PRO	GLU	ALA	PRO	ARG	ASP	GLY	GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	GLU	LEU	THR	PHE	LEU	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ASP	LYS	ASP	ASP	ASP	LYS	HIS	HIS	HIS	HIS
HIS	HIS	HIS	HIS																																															

• Molecule 1: Spike glycoprotein



• Molecule 2: Angiotensin-converting enzyme 2



NE86	Q522	L456	A386	W302	I233
Y587	F523	E457	A387	D303	K234
F588	Q524	K458	Q388	A304	P235
E589	F525	W459	P389	G305	L236
P590	Q526		F390	R306	Y237
L591	L529	V463	L391	I307	E238
F592	C530	F464	L392	E310	H239
T593	Q531	K465	R393	K313	
W594	A532	G466	N394	V318	R245
L595	A533	E467	G395	G319	M249
KE96	A534	I468	A396	L320	W250
D597	KE34	P469	N397	H401	A251
QE98	H535	D471	E402	M523	P253
NE99	E536	Q472	E406	T324	S254
K600	G537	W473	A412	Q325	S257
NG01	P538	M474		G326	P258
F602	L539	W477		F327	I259
F603	HE40	W478	P415	W328	G260
V604	K541		K416	E329	C261
G605	S545	K481	H417	M332	L262
W606	N546	E483	I418	L333	P263
S607	S547	I484	K419		A264
T608	A550	V485	S420	P336	H265
D609	G551	G486	G422	G337	L266
W610	Q552	V487	L423	N338	L267
SC11	K553	V488	L424	V339	G268
P612	L554	E489	S425	Q340	D269
Y613	F555		P426	K341	M270
Y613	N556	P492	H427	A342	W271
A614	M557	H493	D427	V343	G272
D615	L558	D494	F428	C344	
HIS	KE59	E495	Q429	H345	W275
HIS	L560	T496	E430		T276
HIS	G561	Y497	D431	Y279	
HIS	K562	C498	M432	L351	S280
HIS	S563	D499	A433	G352	L281
HIS	E564	P500	E433	K353	T282
HIS	P565	A501	T434	G354	V283
HIS	W566	S502	E435	D355	P284
HIS	TE67	L503	I436	F356	F285
	L568	F504	M437	R357	G286
	A569	H505		I358	Q287
	L570	V506	L440	L359	P288
	E571		K441		P289
	NE72	D509	Q442	V364	N290
	VE73	S511	L444	T365	I291
	V574	F512	T445	M366	D292
	G575	I513	I446	H374	V293
	A576	R514	V447		T294
	KE77	Y515			D295
	NE78	Y516	L450	Q380	A296
	W579	T517	P451	Y381	W297
	NE80	R518	T452	D382	V298
	V581	T519	A453	M383	D299
	R582	L520	Y454	A384	Q300
	P583	Y521	M455	Y385	A301
	L584				
	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%)	48	80
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 ⓘ

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

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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 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.

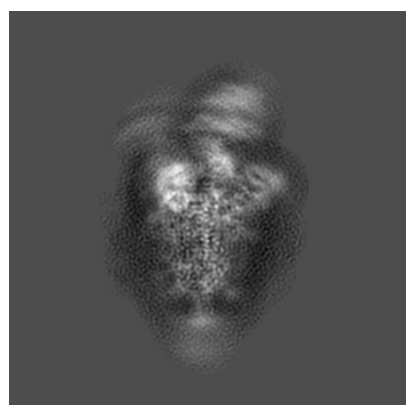
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32174. These allow visual inspection of the internal detail of the map and identification of artifacts.

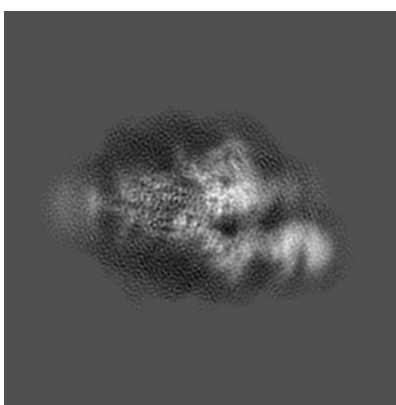
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

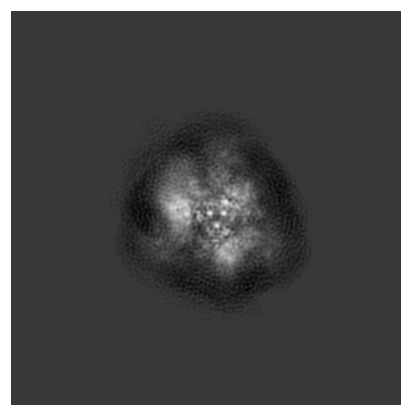
6.1.1 Primary map



X



Y

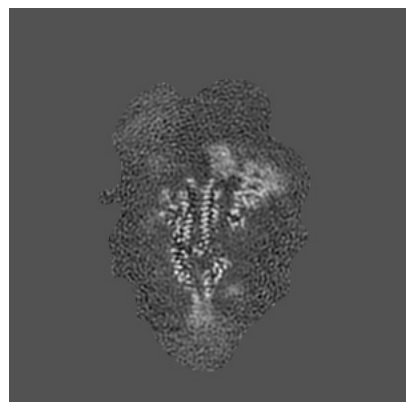


Z

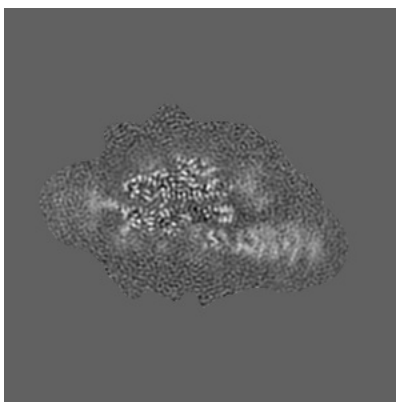
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

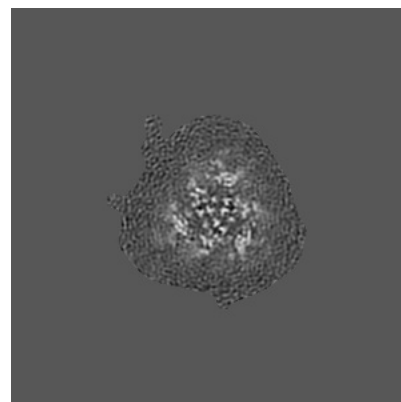
6.2.1 Primary map



X Index: 180



Y Index: 180

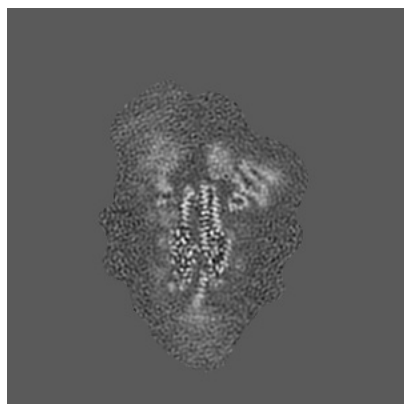


Z Index: 180

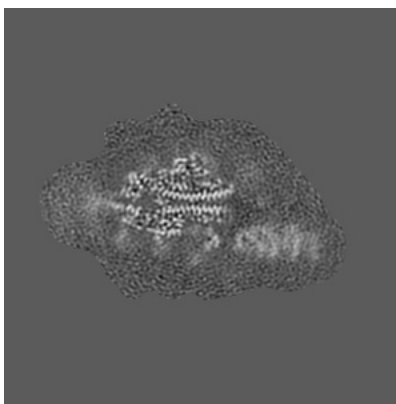
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

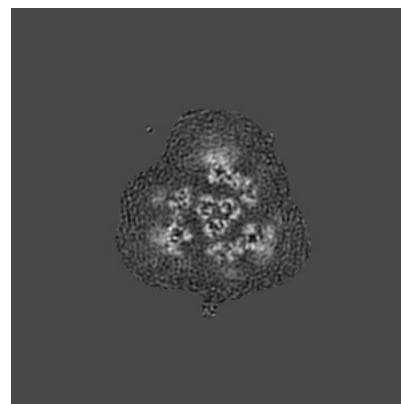
6.3.1 Primary map



X Index: 192



Y Index: 177

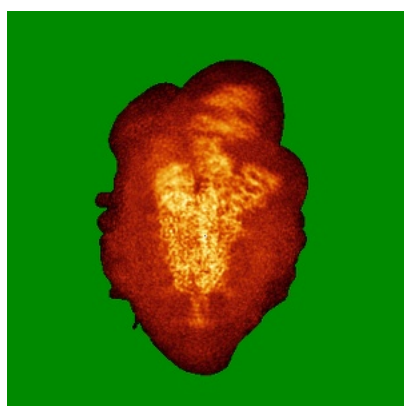


Z Index: 193

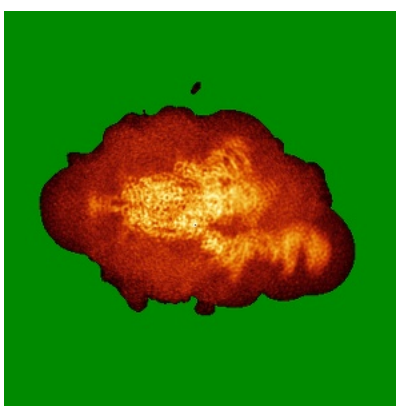
The images above show the largest variance slices of the map in three orthogonal directions.

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

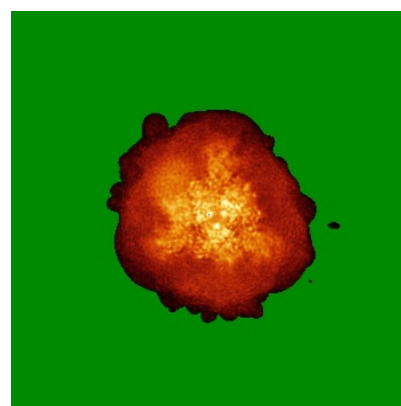
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

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

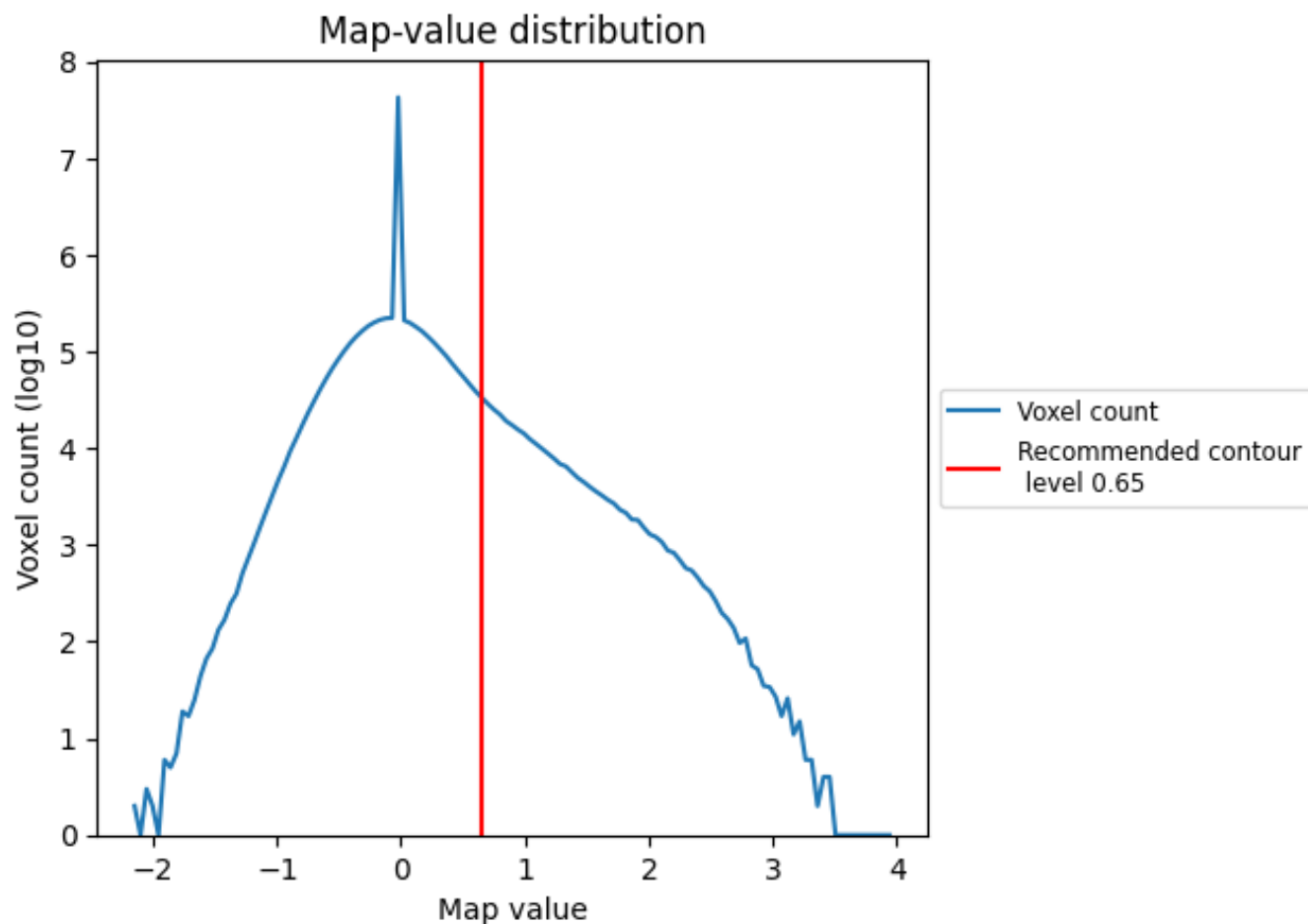
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

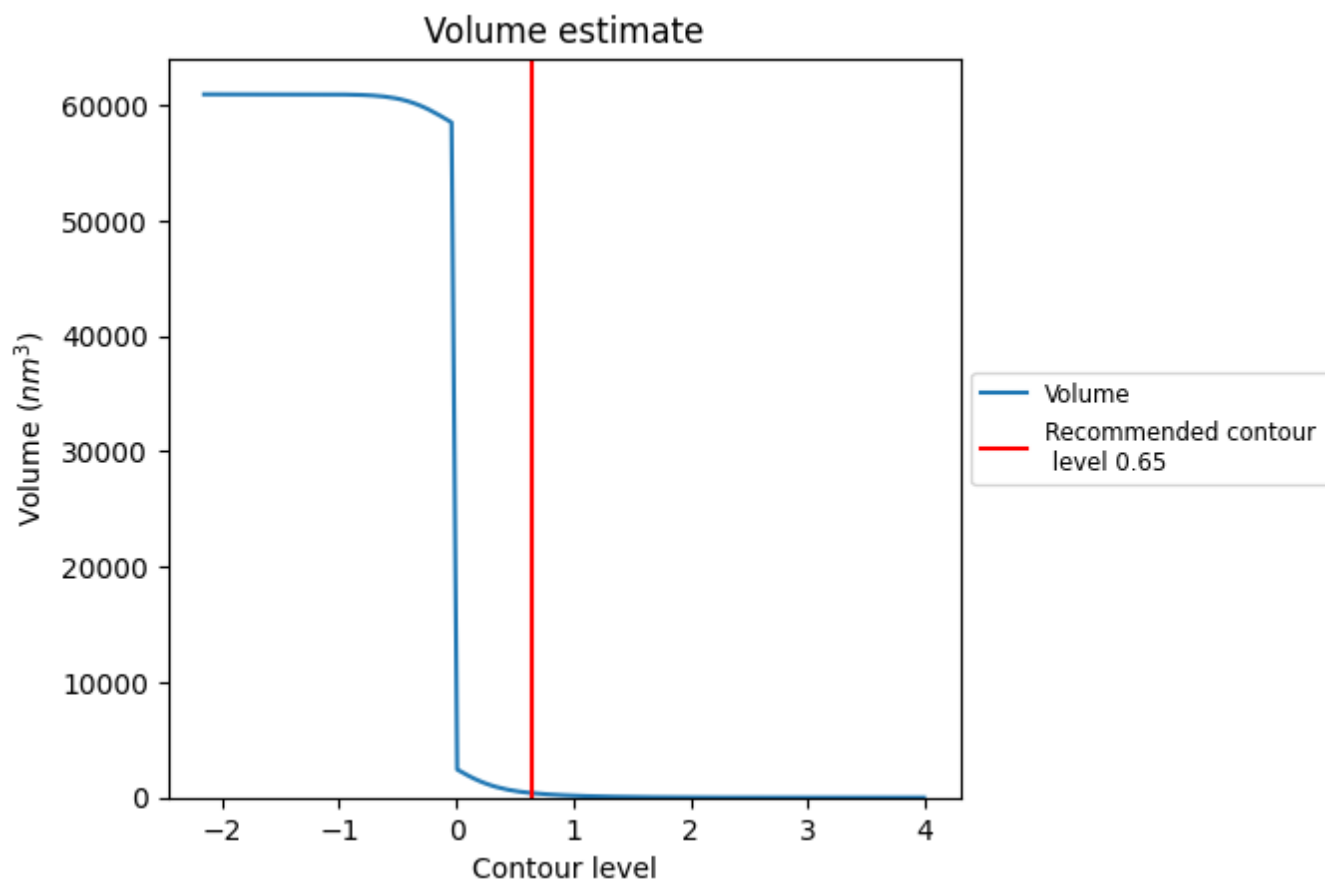
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

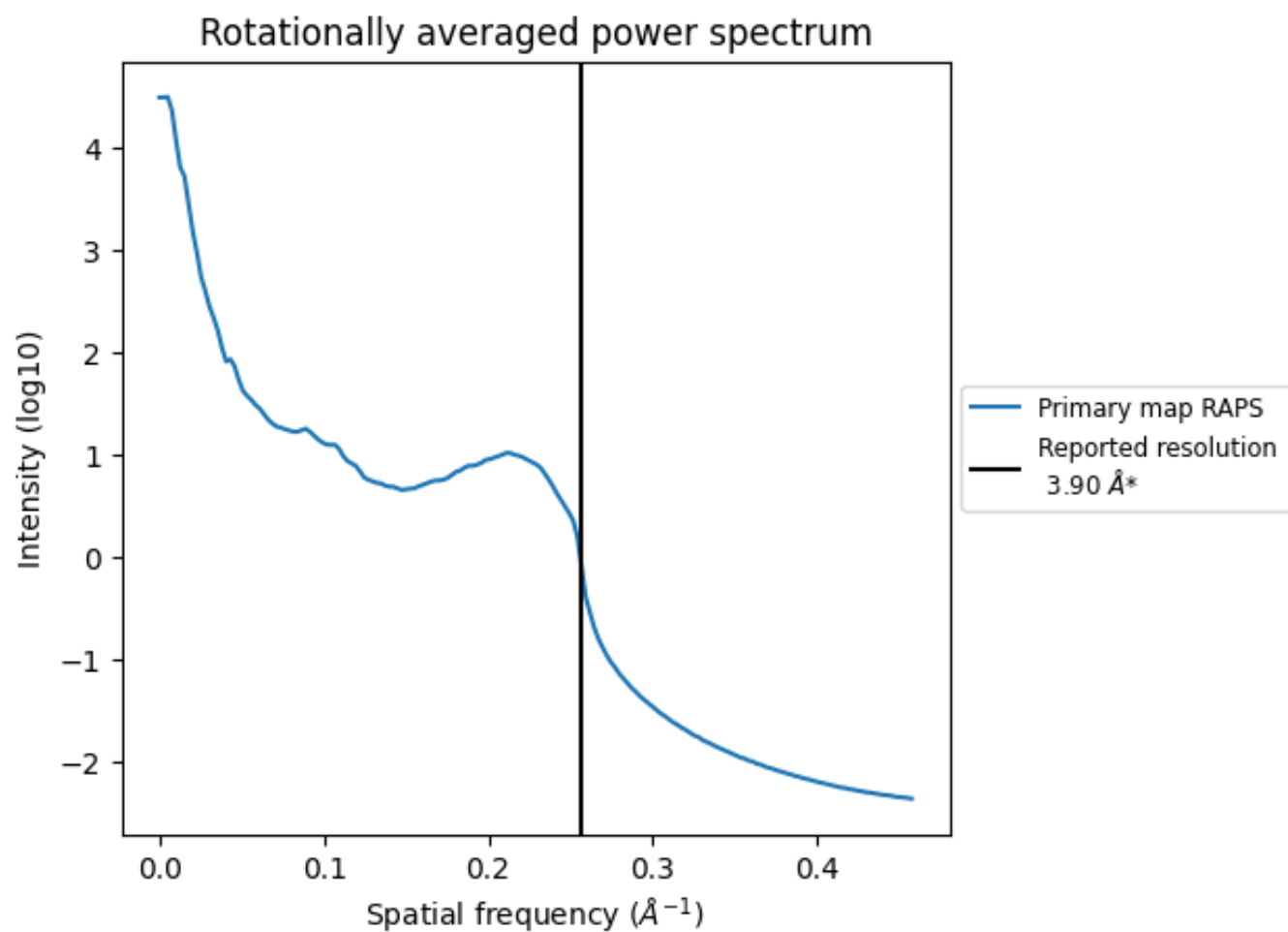
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

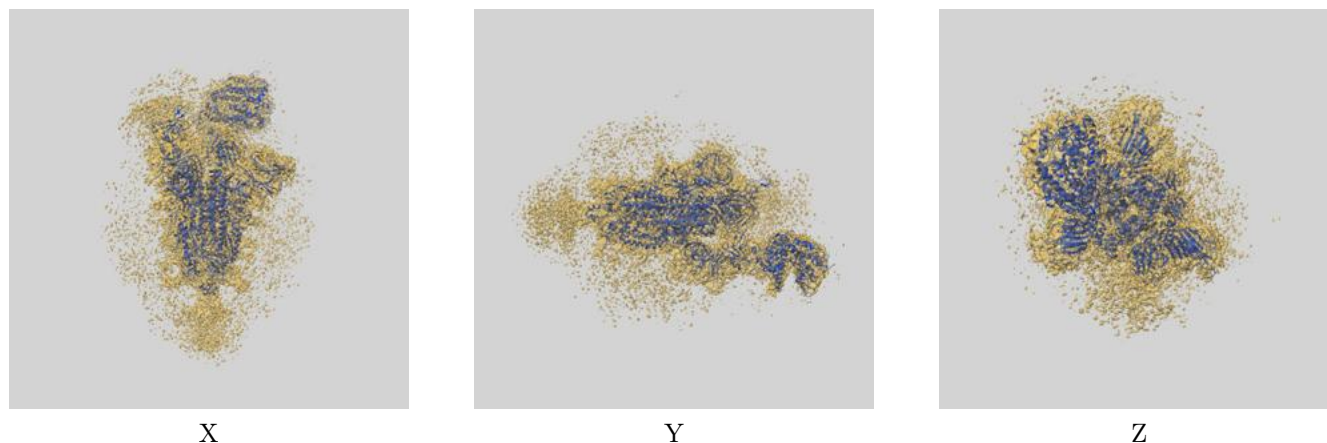
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

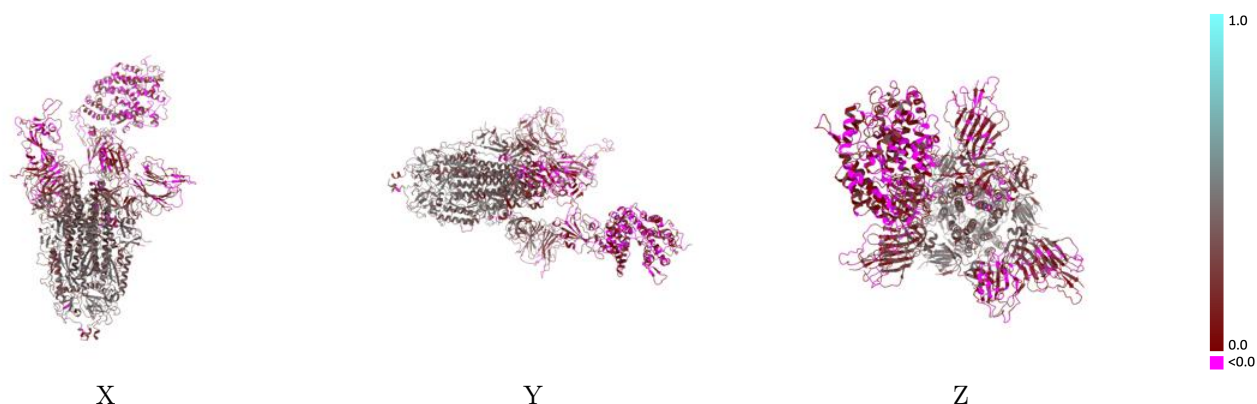
This section contains information regarding the fit between EMDB map EMD-32174 and PDB model 7VXB. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



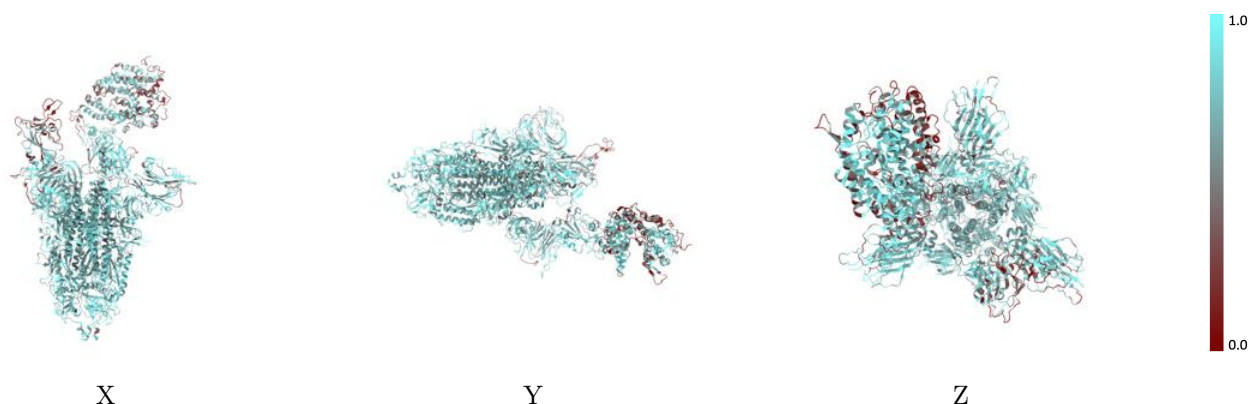
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



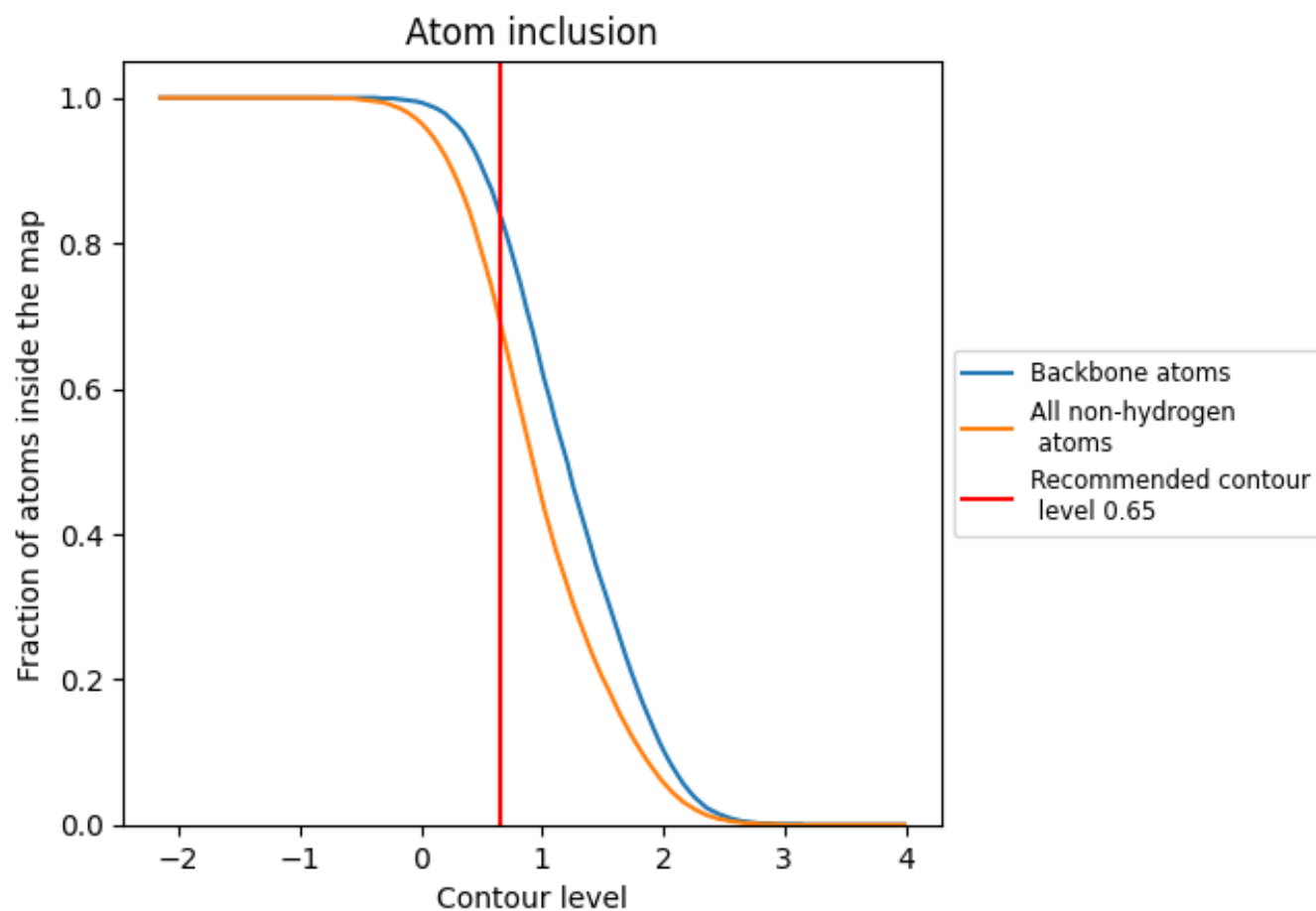
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.6930	<div></div> 0.2220
A	<div></div> 0.7280	<div></div> 0.2640
B	<div></div> 0.6830	<div></div> 0.2640
C	<div></div> 0.5970	<div></div> 0.0460
D	<div></div> 0.7250	<div></div> 0.2430

