



## Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 07:21 PM JST

PDB ID : 7VXC  
EMDB ID : EMD-32175  
Title : SARS-CoV-2 Kappa variant spike protein in C3 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

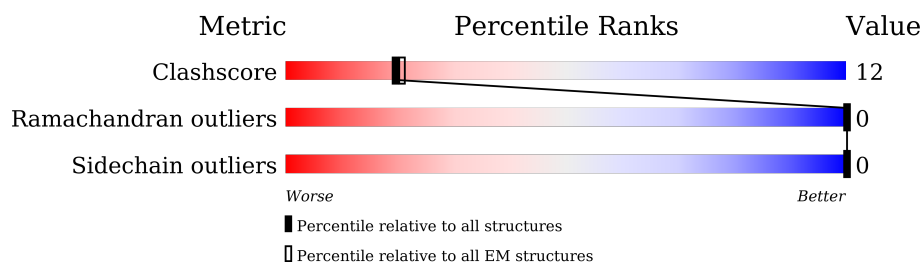
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1261	<div> <div>8%</div> <div>81%</div> <div>15%</div> </div>
1	B	1261	<div> <div>8%</div> <div>80%</div> <div>15%</div> </div>
1	D	1261	<div> <div>6%</div> <div>48%</div> <div>37%</div> <div>15%</div> </div>
2	C	625	<div> <div>25%</div> <div>57%</div> <div>39%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 46264 atoms, of which 16332 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	1068	Total	C	H	N	O	S	0	0
			16520	5327	8166	1401	1587	39		
1	B	1068	Total	C	H	N	O	S	0	0
			16520	5327	8166	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

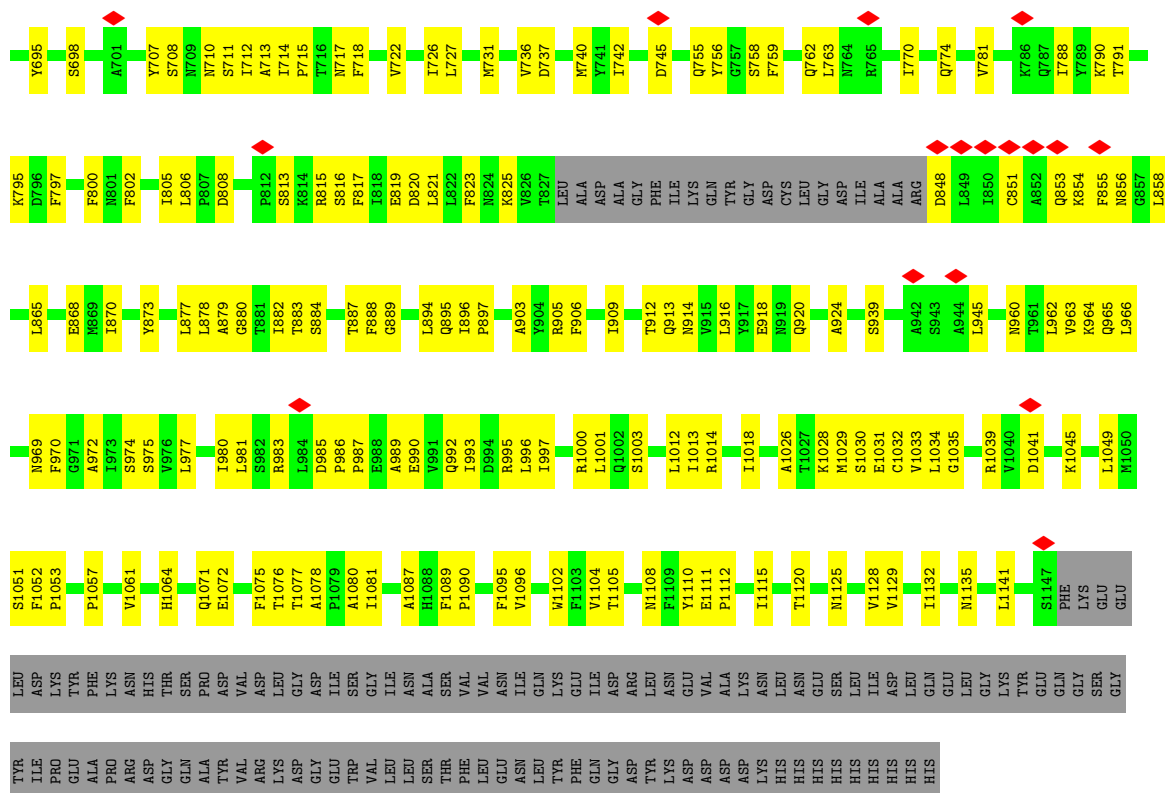


### 3 Residue-property plots

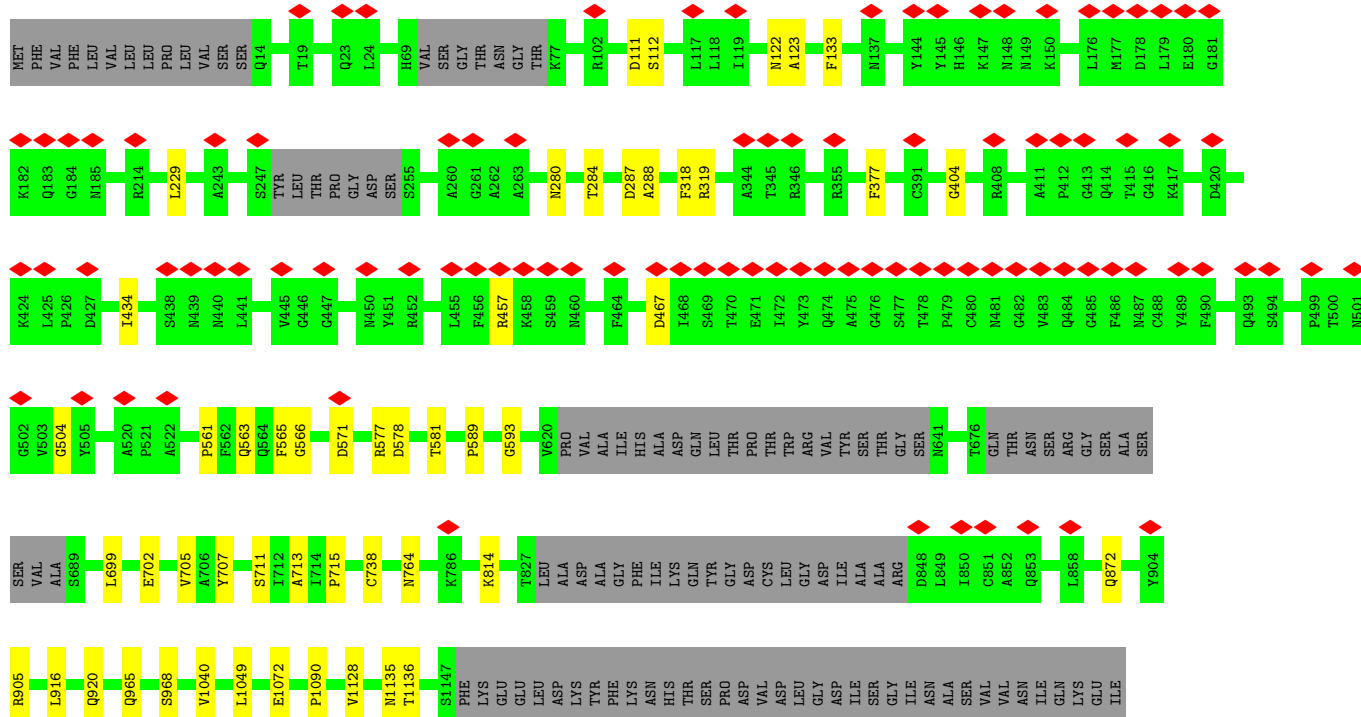
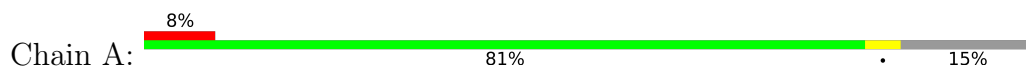
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





K234	P235	L236	Y237	E238	H239	K240	P241	L242	Y243	E244	H245	K246	P247	L248	Y249	E250	H251	K252	P253	L254	Y255	E256	H257	K258	P259	L260	Y261	E262	H263	K264	P265	L266	Y267	E268	H269	K270	P271	L272	Y273	E274	H275	K276	P277	L278	Y279	E280	H281	K282	P283	L284	Y285	E286	H287	K288	P289	L290	Y291	E292	H293	K294	P295	L296	Y297	E298	H299	K300	P301	L302	Y303	E304	H305	K306	P307	L308	Y309	E310	H311	K312	P313	L314	Y315	E316	H317	K318	P319	L320	Y321	E322	H323	K324	P325	L326	Y327	E328	H329	K330	P331	L332	Y333	E334	H335	K336	P337	L338	Y339	E340	H341	K342	P343	L344	Y345	E346	H347	K348	P349	L350	Y351	E352	H353	K354	P355	L356	Y357	E358	H359	K360	P361	L362	Y363	E364	H365	K366	P367	L368	Y369	E370	H371	K372	P373	L374	Y375	E376	H377	K378	P379	L380	Y381	E382	H383	K384	P385	L386	Y387	E388	H389	K390	P391	L392	Y393	E394	H395	K396	P397	L398	Y399	E400	H401	K402	P403	L404	Y405	E406	H407	K408	P409	L410	Y411	E412	H413	K414	P415	L416	Y417	E418	H419	K420	P421	L422	Y423	E424	H425	K426	P427	L428	Y429	E430	H431	K432	P433	L434	Y435	E436	H437	K438	P439	L440	Y441	E442	H443	K444	P445	L446	Y447	E448	H449	K450	P451	L452	Y453	E454	H455	K456	P457	L458	Y459	E460	H461	K462	P463	L464	Y465	E466	H467	K468	P469	L470	Y471	E472	H473	K474	P475	L476	Y477	E478	H479	K480	P481	L482	Y483	E484	H485	K486	P487	L488	Y489	E490	H491	K492	P493	L494	Y495	E496	H497	K498	P499	L500	Y501	E502	H503	K504	P505	L506	Y507	E508	H509	K510	P511	L512	Y513	E514	H515	K516	P517	L518	Y519	E520	H521	K522	P523	L524	Y525	E526	H527	K528	P529	L530	Y531	E532	H533	K534	P535	L536	Y537	E538	H539	K540	P541	L542	Y543	E544	H545	K546	P547	L548	Y549	E550	H551	K552	P553	L554	Y555	E556	H557	K558	P559	L560	Y561	E562	H563	K564	P565	L566	Y567	E568	H569	K570	P571	L572	Y573	E574	H575	K576	P577	L578	Y579	E580	H581	K582	P583	L584	Y585	E586	H587	K588	P589	L590	Y591	E592	H593	K594	P595	L596	Y597	E598	H599	K600	P601	L602	Y603	E604	H605	K606	P607	L608	Y609	E610	H611	K612	P613	L614	Y615	E616	H617	K618	P619	L620	Y621	E622	H623	K624	P625	L626	Y627	E628	H629	K630	P631	L632	Y633	E634	H635	K636	P637	L638	Y639	E640	H641	K642	P643	L644	Y645	E646	H647	K648	P649	L650	Y651	E652	H653	K654	P655	L656	Y657	E658	H659	K660	P661	L662	Y663	E664	H665	K666	P667	L668	Y669	E670	H671	K672	P673	L674	Y675	E676	H677	K678	P679	L680	Y681	E682	H683	K684	P685	L686	Y687	E688	H689	K690	P691	L692	Y693	E694	H695	K696	P697	L698	Y699	E700	H701	K702	P703	L704	Y705	E706	H707	K708	P709	L710	Y711	E712	H713	K714	P715	L716	Y717	E718	H719	K720	P721	L722	Y723	E724	H725	K726	P727	L728	Y729	E730	H731	K732	P733	L734	Y735	E736	H737	K738	P739	L740	Y741	E742	H743	K744	P745	L746	Y747	E748	H749	K750	P751	L752	Y753	E754	H755	K756	P757	L758	Y759	E760	H761	K762	P763	L764	Y765	E766	H767	K768	P769	L770	Y771	E772	H773	K774	P775	L776	Y777	E778	H779	K780	P781	L782	Y783	E784	H785	K786	P787	L788	Y789	E790	H791	K792	P793	L794	Y795	E796	H797	K798	P799	L800	Y801	E802	H803	K804	P805	L806	Y807	E808	H809	K810	P811	L812	Y813	E814	H815	K816	P817	L818	Y819	E820	H821	K822	P823	L824	Y825	E826	H827	K828	P829	L830	Y831	E832	H833	K834	P835	L836	Y837	E838	H839	K840	P841	L842	Y843	E844	H845	K846	P847	L848	Y849	E850	H851	K852	P853	L854	Y855	E856	H857	K858	P859	L860	Y861	E862	H863	K864	P865	L866	Y867	E868	H869	K870	P871	L872	Y873	E874	H875	K876	P877	L878	Y879	E880	H881	K882	P883	L884	Y885	E886	H887	K888	P889	L890	Y891	E892	H893	K894	P895	L896	Y897	E898	H899	K900	P901	L902	Y903	E904	H905	K906	P907	L908	Y909	E910	H911	K912	P913	L914	Y915	E916	H917	K918	P919	L920	Y921	E922	H923	K924	P925	L926	Y927	E928	H929	K930	P931	L932	Y933	E934	H935	K936	P937	L938	Y939	E940	H941	K942	P943	L944	Y945	E946	H947	K948	P949	L950	Y951	E952	H953	K954	P955	L956	Y957	E958	H959	K960	P961	L962	Y963	E964	H965	K966	P967	L968	Y969	E970	H971	K972	P973	L974	Y975	E976	H977	K978	P979	L980	Y981	E982	H983	K984	P985	L986	Y987	E988	H989	K990	P991	L992	Y993	E994	H995	K996	P997	L998	Y999	E1000	H1001	K1002	P1003	L1004	Y1005	E1006	H1007	K1008	P1009	L1010	Y1011	E1012	H1013	K1014	P1015	L1016	Y1017	E1018	H1019	K1020	P1021	L1022	Y1023	E1024	H1025	K1026	P1027	L1028	Y1029	E1030	H1031	K1032	P1033	L1034	Y1035	E1036	H1037	K1038	P1039	L1040	Y1041	E1042	H1043	K1044	P1045	L1046	Y1047	E1048	H1049	K1050	P1051	L1052	Y1053	E1054	H1055	K1056	P1057	L1058	Y1059	E1060	H1061	K1062	P1063	L1064	Y1065	E1066	H1067	K1068	P1069	L1070	Y1071	E1072	H1073	K1074	P1075	L1076	Y1077	E1078	H1079	K1080	P1081	L1082	Y1083	E1084	H1085	K1086	P1087	L1088	Y1089	E1090	H1091	K1092	P1093	L1094	Y1095	E1096	H1097	K1098	P1099	L1100	Y1101	E1102	H1103	K1104	P1105	L1106	Y1107	E1108	H1109	K1110	P1111	L1112	Y1113	E1114	H1115	K1116	P1117	L1118	Y1119	E1120	H1121	K1122	P1123	L1124	Y1125	E1126	H1127	K1128	P1129	L1130	Y1131	E1132	H1133	K1134	P1135	L1136	Y1137	E1138	H1139	K1140	P1141	L1142	Y1143	E1144	H1145	K1146	P1147	L1148	Y1149	E1150	H1151	K1152	P1153	L1154	Y1155	E1156	H1157	K1158	P1159	L1160	Y1161	E1162	H1163	K1164	P1165	L1166	Y1167	E1168	H1169	K1170	P1171	L1172	Y1173	E1174	H1175	K1176	P1177	L1178	Y1179	E1180	H1181	K1182	P1183	L1184	Y1185	E1186	H1187	K1188	P1189	L1190	Y1191	E1192	H1193	K1194	P1195	L1196	Y1197	E1198	H1199	K1200	P1201	L1202	Y1203	E1204	H1205	K1206	P1207	L1208	Y1209	E1210	H1211	K1212	P1213	L1214	Y1215	E1216	H1217	K1218	P1219	L1220	Y1221	E1222	H1223	K1224	P1225	L1226	Y1227	E1228	H1229	K1230	P1231	L1232	Y1233	E1234	H1235	K1236	P1237	L1238	Y1239	E1240	H1241	K1242	P1243	L1244	Y1245	E1246	H1247	K1248	P1249	L1250	Y1251	E1252	H1253	K1254	P1255	L1256	Y1257	E1258	H1259	K1260	P1261	L1262	Y1263	E1264	H1265	K1266	P1267	L1268	Y1269	E1270	H1271	K1272	P1273	L1274	Y1275	E1276	H1277	K1278	P1279	L1280	Y1281	E1282	H1283	K1284	P1285	L1286	Y1287	E1288	H1289	K1290	P1291	L1292	Y1293	E1294	H1295	K1296	P1297	L1298	Y1299	E1300	H1301	K1302	P1303	L1304	Y1305	E1306	H1307	K1308	P1309	L1310	Y1311	E1312	H1313	K1314	P1315	L1316	Y1317	E1318	H1319	K1320	P1321	L1322	Y1323	E1324	H1325	K1326	P1327	L1328	Y1329	E1330	H1331	K1332	P1333	L1334	Y1335	E1336	H1337	K1338	P1339	L1340	Y1341	E1342	H1343	K1344	P1345	L1346	Y1347	E1348	H1349	K1350	P1351	L1352	Y1353	E1354	H1355	K1356	P1357	L1358	Y1359	E1360	H1361	K1362	P1363	L1364	Y1365	E1366	H1367	K1368	P1369	L1370	Y1371	E1372	H1373	K1374	P1375	L1376	Y1377	E1378	H1379	K1380	P1381	L1382	Y1383	E1384	H1385	K1386	P1387	L1388	Y1389	E1390	H1391	K1392	P1393	L1394	Y1395	E1396	H1397	K1398	P1399	L1400	Y1401	E1402	H1403	K1404	P1405	L1406	Y1407	E1408	H1409	K1410	P1411	L1412	Y1413	E1414	H1415	K1416	P1417	L1418	Y1419	E1420	H1421	K1422	P1423	L1424	Y1425	E1426	H1427	K1428	P1429	L1430	Y1431	E1432	H1433	K1434	P1435	L1436	Y1437	E1438	H1439	K1440	P1441	L1442	Y1443	E1444	H1445	K1446	P1447	L1448	Y1449	E1450	H1451	K1452	P1453	L1454	Y1455	E1456	H1457	K1458	P1459	L1460	Y1461	E1462	H1463	K1464	P1465	L1466	Y1467	E1468	H1469	K1470	P1471	L1472	Y1473	E1474	H1475	K1476	P1477	L1478	Y1479	E1480	H1481	K1482	P1483	L1484	Y1485	E1486	H1487	K1488	P1489	L1490	Y1491	E1492	H1493	K1494	P1495	L1496	Y1497	E1498	H1499	K1500	P1501	L1502	Y1503	E1504	H1505	K1506	P1507	L1508	Y1509	E1510	H1511	K1512	P1513	L1514	Y1515	E1516	H1517	K1518	P1519	L1520	Y1521	E1522	H1523	K1524	P1525	L1526	Y1527	E1528	H1529	K1530	P1531	L1532	Y1533	E1534	H1535	K1536	P1537	L1538	Y1539	E1540	H1541	K1542	P1543	L1544	Y1545	E1546	H1547	K1548	P1549	L1550	Y1551	E1552	H1553	K1554	P1555	L1556	Y1557	E1558	H1559	K1560	P1561	L1562	Y1563	E1564	H1565	K1566	P1567	L1568	Y1569	E1570	H1571	K1572	P1573	L1574	Y1575	E1576	H1577	K1578	P1579	L1580	Y1581	E1582	H1583	K1584	P1585	L1586	Y1587	E1588	H1589	K1590	P1591	L1592	Y1593	E1594	H1595	K1596	P1597	L1598	Y1599	E1600	H1601	K1602	P1603	L1604	Y1605	E1606	H1607	K1608	P1609	L1610	Y1611	E1612	H1613	K1614	P1615	L1616	Y1617	E1618	H1619	K1620	P1621	L1622	Y1623	E1624	H1625	K1626	P1627	L1628	Y1629	E1630	H1631	K1632	P1633	L1634	Y1635	E1636	H1637	K1638	P1639	L1640	Y1641	E1642	H1643	K1644	P1645	L1646	Y1647	E1648	H1649	K1650	P1651	L1652
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88957	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	3.711	Depositor
Minimum map value	-2.180	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.116	Depositor
Recommended contour level	0.65	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	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	0.26	1/8546 (0.0%)	0.41	0/11625
1	B	0.28	2/8546 (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	0.26	3/30645 (0.0%)	0.40	0/41678

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	CYS	C-N	9.34	1.51	1.34
1	B	229	LEU	C-N	6.56	1.46	1.34
1	A	229	LEU	C-N	5.22	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	8354	8166	8159	42	0
1	B	8354	8166	8159	37	0
1	D	8354	0	8159	459	0
2	C	4870	0	4643	232	0
All	All	29932	16332	29120	727	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 (727) 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	1.44	1.00
2:C:503:LEU:HD23	2:C:506:VAL:HG23	1.42	0.98
2:C:539:LEU:HD23	2:C:587:TYR:HB2	1.44	0.97
1:D:129:LYS:HG2	1:D:169:GLU:HA	1.46	0.97
1:D:296:LEU:HB2	1:D:608:VAL:HG21	1.44	0.96
2:C:538:PRO:HD2	2:C:541:LYS:HD2	1.48	0.95
1:D:1030:SER:HA	1:D:1034:LEU:HB3	1.52	0.92
1:D:212:LEU:HD22	1:D:217:PRO:HD3	1.51	0.91
2:C:144:LEU:HD12	2:C:148:LEU:HB2	1.54	0.88
1:D:33:THR:HG21	1:D:220:PHE:HA	1.54	0.86
2:C:144:LEU:HA	2:C:148:LEU:HB2	1.55	0.86
1:D:418:ILE:HA	1:D:422:ASN:HD22	1.42	0.84
1:D:344:ALA:HB3	1:D:347:PHE:HE1	1.43	0.84
1:D:884:SER:HB2	1:D:888:PHE:HB3	1.56	0.84
1:D:398:ASP:HB3	1:D:512:VAL:HB	1.61	0.82
1:D:32:PHE:CD2	1:D:33:THR:HG23	2.15	0.81
2:C:457:GLU:HG2	2:C:513:ILE:HD13	1.62	0.81
1:D:1089:PHE:HZ	1:D:1129:VAL:HG21	1.45	0.80
1:D:44:ARG:NH2	1:A:571:ASP:OD1	2.14	0.80
1:D:781:VAL:HG22	1:D:1026:ALA:HB2	1.63	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	1.64	0.79
1:D:106:PHE:HB2	1:D:117:LEU:HB3	1.65	0.78
1:D:712:ILE:HG21	1:D:1077:THR:HB	1.66	0.78
1:D:1035:GLY:HA3	1:A:1040:VAL:HG21	1.66	0.77
2:C:152:MET:O	2:C:161:ARG:NH1	2.16	0.77
1:D:278:LYS:O	1:D:286:THR:N	2.13	0.77
1:D:1031:GLU:OE1	1:D:1039:ARG:NH2	2.19	0.76
2:C:389:PRO:HG2	2:C:392:LEU:HD12	1.67	0.76
1:D:742:ILE:O	1:D:1000:ARG:NH1	2.18	0.75
1:D:905:ARG:NH1	1:D:1049:LEU:O	2.19	0.75
1:D:879:ALA:O	1:D:883:THR:N	2.18	0.75
2:C:301:ALA:O	2:C:306:ARG:NH2	2.19	0.75
2:C:446:ILE:HD13	2:C:523:PHE:HZ	1.52	0.75
1:D:758:SER:OG	1:A:965:GLN:NE2	2.19	0.74
2:C:157:ASP:HB3	2:C:160:GLU:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:LEU:HD21	2:C:271:TRP:HH2	1.52	0.74
1:D:437:ASN:ND2	1:D:506:GLN:OE1	2.21	0.74
1:D:102:ARG:HH12	1:D:154:LYS:HE2	1.53	0.74
1:D:43:PHE:CE1	1:D:283:GLY:HA3	2.23	0.74
1:D:157:PHE:CZ	1:D:159:VAL:HB	2.22	0.74
1:D:490:PHE:CE2	1:D:492:LEU:HB2	2.24	0.73
2:C:394:ASN:OD1	2:C:395:GLY:N	2.22	0.73
1:D:338:PHE:HE1	1:D:358:ILE:HG21	1.52	0.73
1:D:95:THR:OG1	1:D:188:ASN:O	2.02	0.73
2:C:524:GLN:HB3	2:C:574:VAL:HG11	1.68	0.73
1:D:329:PHE:HB3	1:D:330:PRO:HD2	1.70	0.73
1:D:813:SER:OG	1:D:868:GLU:OE1	2.05	0.73
1:D:476:GLY:HA3	2:C:24:GLN:HE21	1.53	0.72
1:D:883:THR:HG23	1:A:707:TYR:HE2	1.55	0.72
2:C:190:MET:O	2:C:194:ASN:ND2	2.22	0.72
2:C:451:PRO:HB2	2:C:485:VAL:HG12	1.72	0.72
1:D:417:LYS:HD2	1:D:455:LEU:HD12	1.70	0.72
1:D:437:ASN:HA	1:D:508:TYR:HD1	1.52	0.72
2:C:263:PRO:HG2	2:C:266:LEU:HD12	1.71	0.71
1:D:106:PHE:HD2	1:D:117:LEU:HD23	1.54	0.71
1:D:726:ILE:HG12	1:D:1061:VAL:HG22	1.72	0.71
1:D:102:ARG:HB3	1:D:241:LEU:HB3	1.72	0.71
1:D:121:ASN:O	1:D:154:LYS:NZ	2.23	0.71
1:D:889:GLY:HA3	1:D:1034:LEU:HD11	1.73	0.71
2:C:132:VAL:HG23	2:C:168:TRP:HE3	1.55	0.71
1:D:95:THR:HG23	1:D:186:PHE:HD2	1.54	0.71
1:D:44:ARG:HB2	1:D:279:TYR:CD2	2.26	0.71
1:D:599:THR:OG1	1:D:607:GLN:O	2.07	0.71
2:C:276:THR:OG1	2:C:445:THR:OG1	2.09	0.70
2:C:144:LEU:HA	2:C:148:LEU:CB	2.21	0.70
1:D:745:ASP:OD1	1:A:319:ARG:NH2	2.25	0.69
2:C:450:LEU:HB2	2:C:451:PRO:HD3	1.74	0.69
1:D:802:PHE:CD2	1:D:882:ILE:HD13	2.28	0.69
1:D:447:GLY:HA2	1:D:497:PHE:O	1.92	0.69
1:D:578:ASP:OD2	1:D:581:THR:N	2.26	0.69
1:D:131:CYS:HB2	1:D:133:PHE:CE1	2.27	0.69
1:D:865:LEU:HD21	1:D:873:TYR:HE2	1.58	0.69
1:D:204:TYR:HD1	1:D:225:PRO:HA	1.55	0.69
1:D:848:ASP:HB2	1:D:851:CYS:HB2	1.75	0.68
1:D:105:ILE:HG12	1:D:118:LEU:HD13	1.75	0.68
1:D:1129:VAL:HG22	1:B:917:TYR:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1033:VAL:HA	1:D:1051:SER:HB3	1.74	0.68
2:C:204:ARG:HG2	2:C:222:LEU:HD23	1.76	0.68
2:C:396:ALA:HB3	2:C:400:PHE:CD2	2.29	0.68
1:D:108:THR:HA	1:D:236:THR:H	1.58	0.68
1:D:788:ILE:HD11	1:A:699:LEU:HB2	1.77	0.67
1:A:578:ASP:OD2	1:A:581:THR:OG1	2.08	0.67
1:D:437:ASN:HA	1:D:508:TYR:CD1	2.29	0.67
1:D:43:PHE:HB3	1:A:566:GLY:HA2	1.75	0.67
1:D:855:PHE:HB3	1:A:589:PRO:HG2	1.77	0.67
1:D:335:LEU:CD2	1:D:362:VAL:HB	2.24	0.67
1:D:338:PHE:CE1	1:D:358:ILE:HG21	2.29	0.67
1:D:708:SER:HB3	1:D:711:SER:CB	2.24	0.67
1:D:884:SER:CB	1:D:888:PHE:HB3	2.23	0.67
1:D:290:ASP:HB3	1:D:293:LEU:HB2	1.76	0.67
2:C:389:PRO:O	2:C:393:ARG:HG3	1.96	0.66
1:D:758:SER:O	1:D:762:GLN:N	2.21	0.66
2:C:304:ALA:HB1	2:C:333:LEU:HD22	1.76	0.66
1:D:918:GLU:HG2	1:A:1128:VAL:HG11	1.78	0.66
1:D:44:ARG:HB3	1:D:47:VAL:CG2	2.26	0.66
1:D:1089:PHE:CZ	1:D:1129:VAL:HG21	2.31	0.66
1:D:35:GLY:HA3	1:D:56:LEU:HB3	1.77	0.65
2:C:235:PRO:O	2:C:239:HIS:ND1	2.24	0.65
1:D:102:ARG:HB3	1:D:241:LEU:CB	2.26	0.65
1:D:756:TYR:HB3	1:D:759:PHE:CD2	2.32	0.65
2:C:29:LEU:HD13	2:C:96:GLN:OE1	1.97	0.65
2:C:595:LEU:O	2:C:599:ASN:ND2	2.28	0.65
1:D:15:CYS:HA	1:D:137:ASN:HB2	1.79	0.65
1:D:24:LEU:HD21	1:D:80:ASP:OD2	1.97	0.65
1:D:347:PHE:CE2	1:D:509:ARG:HD3	2.32	0.65
1:D:551:VAL:N	1:D:588:THR:O	2.24	0.64
1:D:712:ILE:O	1:D:1075:PHE:N	2.29	0.64
1:D:713:ALA:HB3	1:B:894:LEU:CD1	2.27	0.64
2:C:100:LEU:HD11	2:C:391:LEU:HD11	1.80	0.64
2:C:554:LEU:O	2:C:558:LEU:HG	1.97	0.64
1:D:502:GLY:O	1:D:506:GLN:HG3	1.98	0.64
1:D:80:ASP:O	1:D:265:TYR:OH	2.16	0.64
2:C:302:TRP:HA	2:C:306:ARG:HH21	1.61	0.64
1:D:912:THR:HG22	1:D:914:ASN:H	1.62	0.63
1:D:27:ALA:HB3	1:D:64:TRP:HB3	1.79	0.63
1:D:204:TYR:CD1	1:D:225:PRO:HA	2.34	0.63
1:D:277:LEU:HD22	1:D:285:ILE:HD13	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:LEU:HD11	1:D:301:CYS:HA	1.81	0.63
1:D:102:ARG:NH1	1:D:154:LYS:HE2	2.12	0.63
1:D:350:VAL:HG22	1:D:422:ASN:HB3	1.81	0.63
1:D:853:GLN:NE2	1:D:960:ASN:OD1	2.30	0.63
2:C:267:LEU:CD1	2:C:272:GLY:HA3	2.28	0.63
2:C:469:PRO:HD2	2:C:472:GLN:OE1	1.99	0.63
1:D:96:GLU:O	1:D:188:ASN:HB2	1.99	0.63
2:C:144:LEU:O	2:C:148:LEU:N	2.32	0.63
2:C:158:TYR:HB2	2:C:252:TYR:CE2	2.34	0.63
2:C:396:ALA:HB1	2:C:566:TRP:HB3	1.81	0.63
1:D:329:PHE:O	1:D:580:GLN:HB2	1.98	0.63
2:C:155:SER:O	2:C:161:ARG:HD2	1.99	0.63
1:D:38:TYR:HE1	1:D:285:ILE:HG13	1.64	0.63
1:D:717:ASN:OD1	1:D:718:PHE:N	2.32	0.63
1:B:756:TYR:OH	1:B:994:ASP:OD1	2.14	0.63
1:D:31:SER:HB3	1:D:34:ARG:HB2	1.81	0.62
1:D:412:PRO:HB3	1:D:427:ASP:HA	1.80	0.62
2:C:382:ASP:HA	2:C:385:TYR:CE2	2.34	0.62
1:D:755:GLN:O	1:A:968:SER:OG	2.17	0.62
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.32	0.62
1:B:112:SER:N	1:B:133:PHE:O	2.32	0.62
1:D:33:THR:CG2	1:D:220:PHE:HA	2.28	0.62
1:D:122:ASN:HA	1:D:154:LYS:HZ3	1.65	0.62
2:C:453:THR:CG2	2:C:516:TYR:HB2	2.30	0.62
1:D:32:PHE:HD2	1:D:33:THR:HG23	1.61	0.62
1:D:378:LYS:HE2	1:D:380:TYR:HE1	1.65	0.61
1:D:895:GLN:HG2	1:A:713:ALA:HB2	1.80	0.61
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.32	0.61
1:D:713:ALA:HB3	1:B:894:LEU:HD11	1.81	0.61
1:D:965:GLN:NE2	1:B:758:SER:OG	2.32	0.61
1:D:106:PHE:O	1:D:117:LEU:N	2.34	0.61
1:D:212:LEU:CD2	1:D:217:PRO:HD3	2.28	0.61
1:D:1030:SER:HA	1:D:1034:LEU:CB	2.29	0.61
2:C:382:ASP:OD1	2:C:385:TYR:OH	2.15	0.61
2:C:389:PRO:CG	2:C:392:LEU:HD12	2.30	0.61
1:D:708:SER:HB3	1:D:711:SER:HB2	1.81	0.61
1:D:770:ILE:HD11	1:D:1012:LEU:HD23	1.82	0.61
1:D:880:GLY:HA2	1:D:883:THR:HB	1.83	0.61
1:D:403:ARG:HB2	1:D:406:GLU:HG2	1.82	0.61
1:D:600:PRO:HD2	1:D:607:GLN:O	2.01	0.61
1:D:206:LYS:HD2	1:D:222:ALA:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:PHE:HD1	1:D:434:ILE:HG12	1.66	0.61
1:D:439:ASN:O	1:D:443:SER:OG	2.18	0.61
1:D:553:THR:O	1:D:586:ASP:N	2.34	0.61
1:D:661:GLU:O	1:D:695:TYR:OH	2.16	0.61
2:C:144:LEU:HA	2:C:148:LEU:CG	2.31	0.61
1:D:95:THR:HG23	1:D:186:PHE:CD2	2.34	0.60
2:C:144:LEU:HD21	2:C:271:TRP:CH2	2.36	0.60
1:D:856:ASN:HD22	1:D:963:VAL:HG22	1.66	0.60
1:D:231:ILE:HG22	1:D:233:ILE:HG23	1.82	0.60
2:C:396:ALA:HB3	2:C:400:PHE:CE2	2.37	0.60
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.34	0.60
2:C:482:ARG:O	2:C:606:TRP:NE1	2.31	0.60
1:D:883:THR:HG23	1:A:707:TYR:CE2	2.36	0.60
2:C:421:ILE:HD11	2:C:423:LEU:CD1	2.31	0.60
1:D:107:GLY:H	1:D:235:ILE:HG23	1.66	0.60
1:D:108:THR:OG1	1:D:234:ASN:O	2.20	0.60
1:D:361:CYS:O	1:D:524:VAL:HA	2.02	0.60
2:C:44:SER:CB	2:C:351:LEU:HG	2.31	0.60
1:D:118:LEU:HB2	1:D:133:PHE:HE2	1.66	0.60
1:D:896:ILE:HG23	1:D:897:PRO:HD2	1.84	0.60
2:C:374:HIS:CE1	2:C:402:GLU:HG3	2.37	0.60
2:C:406:GLU:HG3	2:C:518:ARG:HH11	1.67	0.60
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.33	0.60
1:D:83:VAL:HG22	1:D:239:GLN:HG2	1.82	0.59
1:D:190:ARG:HH11	1:D:192:PHE:HZ	1.50	0.59
1:D:351:TYR:HE2	1:D:452:ARG:HB2	1.67	0.59
2:C:103:ASN:HB3	2:C:106:SER:HB2	1.84	0.59
1:D:140:PHE:O	1:D:158:ARG:HB2	2.03	0.59
1:D:29:THR:O	1:D:62:VAL:HG22	2.03	0.59
1:D:140:PHE:CE1	1:D:244:LEU:HD12	2.37	0.59
1:D:714:ILE:HB	1:D:1075:PHE:HE2	1.67	0.59
1:D:897:PRO:HD3	1:A:711:SER:O	2.02	0.59
1:D:418:ILE:O	1:D:422:ASN:HB2	2.02	0.59
1:B:287:ASP:OD1	1:B:288:ALA:N	2.35	0.59
1:D:205:SER:HB2	1:D:226:LEU:HD22	1.85	0.59
2:C:389:PRO:HD2	2:C:392:LEU:HD12	1.84	0.59
1:D:344:ALA:HB3	1:D:347:PHE:CE1	2.32	0.59
2:C:294:THR:O	2:C:298:VAL:HG23	2.03	0.59
1:A:287:ASP:OD1	1:A:288:ALA:N	2.36	0.59
1:D:419:ALA:HA	1:D:423:TYR:O	2.03	0.59
1:D:659:SER:OG	1:D:698:SER:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:517:THR:HB	2:C:521:TYR:CE2	2.38	0.59
1:D:34:ARG:HH22	1:D:217:PRO:HD2	1.67	0.58
2:C:144:LEU:HD12	2:C:148:LEU:CB	2.29	0.58
2:C:394:ASN:HB3	2:C:562:LYS:HD3	1.85	0.58
1:D:854:LYS:HA	1:D:858:LEU:O	2.02	0.58
1:D:1125:ASN:OD1	1:D:1128:VAL:HG23	2.03	0.58
2:C:245:ARG:HG3	2:C:262:LEU:HD21	1.85	0.58
2:C:499:ASP:HB3	2:C:500:PRO:HD3	1.84	0.58
1:D:578:ASP:HB3	1:D:581:THR:O	2.04	0.58
2:C:456:LEU:HB3	2:C:512:PHE:CE2	2.39	0.58
1:D:94:SER:HB2	1:D:264:ALA:O	2.04	0.58
1:D:727:LEU:HD11	1:D:1028:LYS:NZ	2.18	0.58
1:D:797:PHE:CE2	1:D:802:PHE:HB2	2.39	0.58
2:C:267:LEU:HD13	2:C:272:GLY:HA3	1.86	0.57
1:D:94:SER:HB3	1:D:265:TYR:HA	1.87	0.57
2:C:303:ASP:O	2:C:307:ILE:HG13	2.04	0.57
1:B:578:ASP:OD2	1:B:581:THR:OG1	2.20	0.57
1:D:43:PHE:HB3	1:A:565:PHE:O	2.04	0.57
1:D:287:ASP:OD1	1:D:288:ALA:N	2.35	0.57
2:C:453:THR:HA	2:C:512:PHE:CE2	2.40	0.57
1:D:790:LYS:HD2	1:A:702:GLU:OE2	2.03	0.57
2:C:419:LYS:HE3	2:C:424:LEU:HD23	1.87	0.57
1:D:136:CYS:O	1:D:139:PRO:HD3	2.04	0.57
1:D:756:TYR:HB3	1:D:759:PHE:HD2	1.70	0.57
2:C:455:MET:SD	2:C:481:LYS:HG3	2.44	0.57
2:C:184:VAL:HG22	2:C:464:PHE:HE1	1.69	0.57
1:D:1141:LEU:HD23	1:B:1144:GLU:OE1	2.05	0.57
2:C:446:ILE:HD13	2:C:523:PHE:CZ	2.36	0.56
2:C:539:LEU:HD23	2:C:587:TYR:CB	2.28	0.56
2:C:470:LYS:HA	2:C:473:TRP:CE2	2.41	0.56
1:B:457:ARG:NH1	1:B:459:SER:OG	2.38	0.56
1:D:708:SER:HB3	1:D:711:SER:HB3	1.87	0.56
2:C:470:LYS:HA	2:C:473:TRP:NE1	2.20	0.56
1:D:44:ARG:HD3	1:D:47:VAL:HG23	1.86	0.56
2:C:222:LEU:O	2:C:226:VAL:HG22	2.05	0.56
2:C:451:PRO:CB	2:C:485:VAL:HG12	2.35	0.56
2:C:237:TYR:CE1	2:C:451:PRO:HG2	2.41	0.56
1:D:405:ASP:O	1:D:408:ARG:HG2	2.06	0.56
1:D:97:LYS:HE2	1:D:186:PHE:CE1	2.40	0.56
2:C:29:LEU:HD21	2:C:97:LEU:CD2	2.35	0.55
2:C:450:LEU:HD21	2:C:519:THR:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:LEU:HD11	1:D:276:LEU:HB3	1.87	0.55
1:D:279:TYR:HE1	1:D:285:ILE:HG12	1.69	0.55
1:D:451:TYR:HD2	1:D:497:PHE:HE2	1.54	0.55
2:C:457:GLU:HG2	2:C:513:ILE:CD1	2.35	0.55
1:D:124:THR:HG22	1:D:125:ASN:ND2	2.20	0.55
1:A:112:SER:N	1:A:133:PHE:O	2.39	0.55
1:D:404:GLY:HA2	1:D:508:TYR:CD2	2.42	0.55
1:D:410:ILE:HG23	1:D:425:LEU:HD11	1.88	0.55
1:D:474:GLN:HG2	1:D:476:GLY:O	2.07	0.55
1:D:121:ASN:OD1	1:D:126:VAL:HG22	2.07	0.55
1:D:756:TYR:HE2	1:D:997:ILE:HG21	1.71	0.55
2:C:233:ILE:HG12	2:C:584:LEU:CD2	2.36	0.55
1:D:93:ALA:CB	1:D:191:GLU:HG2	2.36	0.55
1:D:386:LYS:HE2	1:D:390:LEU:HD11	1.87	0.55
2:C:455:MET:SD	2:C:481:LYS:HA	2.46	0.55
1:D:1090:PRO:HA	1:D:1120:THR:HG22	1.88	0.55
2:C:332:MET:HE3	2:C:336:PRO:HD3	1.88	0.55
1:D:34:ARG:NH2	1:D:216:LEU:HB3	2.22	0.55
2:C:181:GLU:HG2	2:C:473:TRP:HH2	1.72	0.55
2:C:589:GLU:HB3	2:C:590:PRO:HD3	1.88	0.55
1:D:335:LEU:HD22	1:D:362:VAL:O	2.07	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:412:ALA:HA	2:C:417:HIS:CD2	2.42	0.55
2:C:402:GLU:O	2:C:406:GLU:HG2	2.07	0.54
1:D:1013:ILE:HD13	1:B:1012:LEU:HB3	1.88	0.54
2:C:394:ASN:HB3	2:C:562:LYS:CD	2.36	0.54
1:D:557:LYS:O	1:D:584:ILE:HG21	2.07	0.54
2:C:168:TRP:HE1	2:C:502:SER:HB2	1.72	0.54
2:C:212:VAL:HG11	2:C:215:TYR:HD2	1.73	0.54
2:C:389:PRO:CD	2:C:392:LEU:HD12	2.37	0.54
1:D:411:ALA:HB3	1:D:414:GLN:CG	2.38	0.54
1:D:870:ILE:HA	1:D:873:TYR:CD2	2.42	0.54
1:D:972:ALA:HA	1:D:992:GLN:OE1	2.06	0.54
1:D:1090:PRO:HD3	1:D:1095:PHE:CZ	2.43	0.54
1:D:111:ASP:OD1	1:D:112:SER:N	2.37	0.54
1:D:805:ILE:HB	1:D:878:LEU:HD11	1.90	0.54
2:C:44:SER:HB3	2:C:351:LEU:HG	1.88	0.54
1:D:453:TYR:O	1:D:492:LEU:HA	2.08	0.54
1:D:965:GLN:HB3	1:D:970:PHE:HZ	1.73	0.54
1:D:1028:LYS:O	1:D:1032:CYS:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:187:LYS:HB3	2:C:199:TYR:CD1	2.42	0.54
1:D:560:LEU:HD12	1:D:563:GLN:CD	2.27	0.54
1:D:1033:VAL:CG1	1:D:1053:PRO:HD3	2.38	0.54
1:D:815:ARG:NH2	1:D:820:ASP:OD1	2.38	0.54
1:D:396:TYR:HB2	1:D:514:SER:HB3	1.90	0.54
1:D:472:ILE:HG23	1:D:489:TYR:O	2.07	0.54
2:C:356:PHE:HE2	2:C:383:MET:HG2	1.72	0.54
1:D:126:VAL:HB	1:D:172:SER:HB3	1.89	0.54
1:D:1110:TYR:CZ	1:D:1112:PRO:HG3	2.43	0.54
2:C:144:LEU:HD22	2:C:168:TRP:CZ2	2.43	0.54
1:D:327:VAL:HB	1:D:531:THR:OG1	2.07	0.53
1:D:567:ARG:HD2	1:B:42:VAL:HG11	1.89	0.53
1:D:805:ILE:HD12	1:D:878:LEU:HD21	1.89	0.53
1:D:997:ILE:O	1:D:1001:LEU:HG	2.08	0.53
2:C:203:TRP:CZ3	2:C:511:SER:HB2	2.43	0.53
1:D:802:PHE:CE2	1:D:882:ILE:HD13	2.42	0.53
1:D:1033:VAL:CA	1:D:1051:SER:HB3	2.37	0.53
2:C:236:LEU:HD21	2:C:588:PHE:HD2	1.73	0.53
1:D:93:ALA:HA	1:D:191:GLU:HG2	1.91	0.53
1:D:731:MET:N	1:D:774:GLN:OE1	2.24	0.53
1:D:906:PHE:CE2	1:D:916:LEU:HD13	2.43	0.53
1:D:1081:ILE:HG23	1:D:1135:ASN:HB3	1.89	0.53
2:C:32:PHE:HE2	2:C:391:LEU:HD21	1.74	0.53
2:C:402:GLU:HB3	2:C:518:ARG:HD3	1.90	0.53
1:A:377:PHE:CD1	1:A:434:ILE:HG22	2.42	0.53
2:C:520:LEU:O	2:C:524:GLN:HG3	2.08	0.53
1:D:199:GLY:HA2	1:D:232:GLY:HA2	1.91	0.53
2:C:170:SER:HA	2:C:497:TYR:HE1	1.73	0.53
2:C:263:PRO:CG	2:C:266:LEU:HD12	2.37	0.53
1:D:94:SER:CB	1:D:265:TYR:HA	2.38	0.53
1:D:576:VAL:HG13	1:D:587:ILE:HD11	1.89	0.53
1:D:43:PHE:HE1	1:D:283:GLY:HA3	1.69	0.53
2:C:302:TRP:CZ3	2:C:423:LEU:HD21	2.43	0.53
2:C:381:TYR:HD1	2:C:558:LEU:HD22	1.74	0.53
2:C:389:PRO:HD2	2:C:392:LEU:HB2	1.91	0.53
1:A:738:CYS:SG	1:A:764:ASN:ND2	2.82	0.53
1:D:296:LEU:HB2	1:D:608:VAL:CG2	2.29	0.52
1:D:643:PHE:HE2	1:D:654:GLU:HA	1.74	0.52
1:D:375:SER:OG	1:D:436:TRP:HA	2.09	0.52
1:D:410:ILE:HG23	1:D:425:LEU:CD1	2.39	0.52
1:D:974:SER:OG	1:D:983:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:343:VAL:HG12	2:C:345:HIS:H	1.75	0.52
1:D:453:TYR:CZ	1:D:493:GLN:HB2	2.44	0.52
1:D:54:LEU:HA	1:D:271:GLN:O	2.10	0.52
1:D:398:ASP:O	1:D:511:VAL:HA	2.09	0.52
1:D:503:VAL:HA	1:D:506:GLN:CD	2.29	0.52
1:D:575:ALA:HB2	1:D:586:ASP:HA	1.92	0.52
2:C:144:LEU:HA	2:C:148:LEU:HD12	1.91	0.52
2:C:232:GLU:OE1	2:C:581:VAL:HB	2.09	0.52
1:A:280:ASN:OD1	1:A:284:THR:N	2.42	0.52
1:D:438:SER:HB3	1:D:509:ARG:HG3	1.90	0.52
1:D:805:ILE:HD12	1:D:878:LEU:HD11	1.90	0.52
2:C:318:VAL:O	2:C:551:GLY:HA3	2.10	0.52
1:D:103:GLY:N	1:D:241:LEU:HB2	2.25	0.52
1:D:378:LYS:HE2	1:D:380:TYR:CE1	2.45	0.52
2:C:453:THR:HG21	2:C:516:TYR:HB2	1.92	0.52
2:C:611:SER:HB3	2:C:614:ALA:HB3	1.91	0.52
1:D:192:PHE:HE1	1:D:205:SER:HG	1.57	0.52
1:D:388:ASN:O	1:D:526:GLY:HA3	2.10	0.52
1:D:455:LEU:HG	1:D:456:PHE:CE1	2.44	0.52
1:D:714:ILE:HG13	1:D:1096:VAL:HG11	1.92	0.52
1:D:1087:ALA:HB1	1:D:1089:PHE:CE1	2.44	0.52
1:D:1041:ASP:OD1	1:D:1045:LYS:HA	2.10	0.51
1:B:1072:GLU:N	1:B:1072:GLU:OE1	2.43	0.51
2:C:526:GLN:HG3	2:C:539:LEU:HD11	1.92	0.51
1:D:1030:SER:CA	1:D:1034:LEU:HB3	2.33	0.51
2:C:494:ASP:OD1	2:C:496:THR:OG1	2.27	0.51
1:D:986:PRO:N	1:D:987:PRO:HD2	2.25	0.51
2:C:597:ASP:HA	2:C:600:LYS:HE3	1.91	0.51
2:C:284:PRO:HD3	2:C:440:LEU:HD23	1.93	0.51
2:C:236:LEU:HD21	2:C:588:PHE:CD2	2.44	0.51
1:D:574:ASP:O	1:D:587:ILE:N	2.26	0.51
1:D:816:SER:OG	1:D:819:GLU:HG3	2.11	0.51
2:C:158:TYR:HB2	2:C:252:TYR:HE2	1.74	0.51
2:C:488:VAL:HG11	2:C:612:PRO:HD3	1.91	0.51
1:D:505:TYR:CD2	2:C:353:LYS:HA	2.45	0.51
2:C:177:ARG:HD3	2:C:496:THR:O	2.11	0.51
2:C:215:TYR:CE2	2:C:568:LEU:HD12	2.46	0.51
2:C:293:VAL:CG2	2:C:366:MET:HA	2.41	0.51
2:C:116:LEU:HD11	2:C:187:LYS:HD3	1.93	0.50
2:C:170:SER:O	2:C:174:LYS:HB2	2.10	0.50
1:D:156:GLU:HB3	1:D:158:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:ILE:HD12	1:D:598:ILE:HD11	1.92	0.50
1:D:589:PRO:HG2	1:B:855:PHE:HB3	1.92	0.50
1:D:894:LEU:HD21	1:A:715:PRO:HG3	1.92	0.50
2:C:181:GLU:HG2	2:C:473:TRP:CH2	2.45	0.50
1:D:1081:ILE:CG2	1:D:1135:ASN:HB3	2.41	0.50
1:D:497:PHE:CE1	1:D:507:PRO:HB3	2.45	0.50
2:C:402:GLU:HG2	2:C:518:ARG:HD2	1.92	0.50
2:C:474:MET:HG3	2:C:494:ASP:O	2.12	0.50
1:D:130:VAL:O	1:D:166:CYS:HA	2.11	0.50
1:D:589:PRO:HG2	1:B:855:PHE:CB	2.41	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	2.47	0.50
1:D:95:THR:CG2	1:D:186:PHE:HD2	2.25	0.50
2:C:170:SER:HA	2:C:497:TYR:CE1	2.47	0.50
1:D:34:ARG:HB3	1:D:91:TYR:CE2	2.47	0.50
1:D:43:PHE:HB2	1:A:563:GLN:HG2	1.93	0.50
1:D:598:ILE:HD11	1:D:666:ILE:HG12	1.94	0.50
1:D:906:PHE:HA	1:D:909:ILE:HG12	1.94	0.50
1:D:1029:MET:O	1:D:1033:VAL:HB	2.12	0.50
1:D:409:GLN:NE2	1:D:416:GLY:HA3	2.26	0.49
1:D:452:ARG:HG2	1:D:494:SER:OG	2.12	0.49
1:D:598:ILE:HG23	1:D:664:ILE:HG21	1.94	0.49
1:D:566:GLY:O	1:D:573:THR:HG23	2.11	0.49
1:D:802:PHE:O	1:D:806:LEU:HG	2.10	0.49
1:D:43:PHE:HA	1:A:563:GLN:NE2	2.27	0.49
1:D:564:GLN:HG2	1:D:565:PHE:CE1	2.47	0.49
2:C:48:TRP:CZ3	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:233:ILE:HG12	2:C:584:LEU:HD23	1.93	0.49
1:B:912:THR:HG22	1:B:1109:PHE:CZ	2.47	0.49
1:D:201:PHE:HB3	1:D:229:LEU:O	2.12	0.49
1:D:986:PRO:O	1:D:990:GLU:HG3	2.13	0.49
1:D:1080:ALA:HB3	1:D:1132:ILE:HG13	1.95	0.49
1:D:34:ARG:CZ	1:D:216:LEU:HB3	2.43	0.49
1:D:808:ASP:HB2	1:D:817:PHE:CE1	2.47	0.49
1:D:380:TYR:CD2	1:D:412:PRO:HD3	2.47	0.49
1:D:611:LEU:HD13	1:D:650:LEU:HD13	1.93	0.49
2:C:396:ALA:HB3	2:C:400:PHE:HD2	1.76	0.49
1:D:55:PHE:HB3	1:D:275:PHE:CE2	2.48	0.49
1:D:129:LYS:HD3	1:D:169:GLU:HG2	1.95	0.49
1:D:279:TYR:CE1	1:D:285:ILE:HG12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1014:ARG:O	1:D:1018:ILE:HG12	2.12	0.49
2:C:174:LYS:HD2	2:C:497:TYR:CZ	2.47	0.49
2:C:201:ASP:OD2	2:C:219:ARG:NE	2.46	0.49
2:C:279:TYR:HA	2:C:282:THR:OG1	2.12	0.49
2:C:393:ARG:O	2:C:394:ASN:HB2	2.12	0.49
1:D:53:ASP:OD1	1:D:54:LEU:N	2.39	0.49
1:D:329:PHE:HB3	1:D:330:PRO:CD	2.42	0.49
2:C:275:TRP:HB2	2:C:444:LEU:HB3	1.93	0.49
1:D:877:LEU:HD13	1:D:1029:MET:SD	2.53	0.49
2:C:44:SER:HB2	2:C:351:LEU:HG	1.94	0.49
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.44	0.49
1:D:104:TRP:HA	1:D:239:GLN:O	2.13	0.49
1:D:825:LYS:HE3	1:D:939:SER:HA	1.95	0.49
1:D:906:PHE:HE2	1:D:916:LEU:HD13	1.78	0.49
2:C:237:TYR:CD1	2:C:451:PRO:HG2	2.47	0.49
2:C:478:TRP:CD2	2:C:489:GLU:HB3	2.48	0.49
2:C:450:LEU:HD21	2:C:519:THR:HB	1.95	0.48
2:C:50:TYR:O	2:C:54:ILE:HD13	2.13	0.48
1:D:34:ARG:NH2	1:D:217:PRO:HD2	2.28	0.48
1:D:453:TYR:HB3	1:D:495:TYR:CZ	2.48	0.48
2:C:279:TYR:O	2:C:283:VAL:HG23	2.13	0.48
1:D:51:THR:O	1:D:274:THR:HG23	2.13	0.48
1:D:411:ALA:O	1:D:414:GLN:HG2	2.13	0.48
1:D:916:LEU:O	1:D:920:GLN:HB3	2.13	0.48
2:C:443:ALA:O	2:C:447:VAL:N	2.46	0.48
1:D:188:ASN:HB3	1:D:207:HIS:HE1	1.78	0.48
1:D:903:ALA:HB1	1:D:913:GLN:HB2	1.94	0.48
2:C:48:TRP:CH2	2:C:359:LEU:HB2	2.48	0.48
2:C:406:GLU:HG3	2:C:518:ARG:NH1	2.28	0.48
1:D:393:THR:HG23	1:D:521:PRO:O	2.13	0.48
1:D:48:LEU:HD12	1:D:277:LEU:O	2.13	0.48
2:C:279:TYR:CE1	2:C:441:LYS:HB2	2.49	0.48
2:C:453:THR:HA	2:C:512:PHE:CZ	2.48	0.48
1:D:353:TRP:CZ2	1:D:466:ARG:HB2	2.49	0.48
1:D:44:ARG:HD2	1:D:279:TYR:CE2	2.49	0.48
1:D:731:MET:HB3	1:D:774:GLN:NE2	2.28	0.48
1:D:980:ILE:HD12	1:D:996:LEU:HD11	1.96	0.48
2:C:103:ASN:HB2	2:C:107:VAL:HG13	1.95	0.48
1:A:318:PHE:N	1:A:593:GLY:O	2.44	0.48
1:D:106:PHE:N	1:D:117:LEU:O	2.34	0.48
2:C:581:VAL:HG12	2:C:581:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:LEU:HB2	1:D:133:PHE:CE2	2.48	0.47
1:D:1104:VAL:HG23	1:D:1115:ILE:HG12	1.94	0.47
1:D:58:PHE:HB2	1:D:293:LEU:HD22	1.94	0.47
1:D:435:ALA:HB2	1:D:510:VAL:HG22	1.96	0.47
2:C:170:SER:O	2:C:174:LYS:HD3	2.15	0.47
2:C:234:LYS:O	2:C:238:GLU:HG3	2.15	0.47
2:C:293:VAL:HG11	2:C:423:LEU:HD13	1.96	0.47
1:D:887:THR:OG1	1:D:894:LEU:HB2	2.15	0.47
2:C:470:LYS:HG2	2:C:473:TRP:CZ2	2.50	0.47
1:D:275:PHE:CD1	1:D:290:ASP:HA	2.50	0.47
1:D:770:ILE:O	1:D:774:GLN:HG2	2.14	0.47
1:D:909:ILE:O	1:D:1108:ASN:ND2	2.47	0.47
2:C:489:GLU:O	2:C:489:GLU:HG2	2.14	0.47
2:C:209:VAL:HG13	2:C:565:PRO:HB3	1.97	0.47
2:C:327:PHE:CE1	2:C:379:ILE:HG21	2.50	0.47
2:C:453:THR:HG22	2:C:516:TYR:HB2	1.97	0.47
1:D:56:LEU:HD22	1:D:91:TYR:CD2	2.50	0.47
1:D:396:TYR:O	1:D:513:LEU:HA	2.15	0.47
1:D:543:PHE:CD2	1:D:576:VAL:HG21	2.50	0.47
1:D:714:ILE:HG21	1:D:1110:TYR:HA	1.97	0.47
2:C:157:ASP:OD1	2:C:158:TYR:N	2.47	0.47
2:C:424:LEU:HD21	2:C:428:PHE:CD2	2.49	0.47
1:D:34:ARG:CZ	1:D:216:LEU:HD13	2.44	0.47
1:D:57:PRO:HG3	1:D:273:ARG:HG3	1.96	0.47
1:D:314:GLN:HG3	1:D:595:VAL:O	2.14	0.47
1:D:335:LEU:HD23	1:D:362:VAL:HB	1.97	0.47
1:D:455:LEU:HG	1:D:456:PHE:CD1	2.50	0.47
1:D:576:VAL:HG13	1:D:587:ILE:CD1	2.45	0.47
2:C:45:LEU:HA	2:C:351:LEU:HD21	1.97	0.47
1:D:107:GLY:N	1:D:235:ILE:HG23	2.29	0.47
1:D:213:VAL:HG12	1:D:214:ARG:HG2	1.97	0.47
1:D:821:LEU:O	1:D:825:LYS:HG2	2.15	0.47
1:D:1030:SER:O	1:D:1035:GLY:N	2.34	0.47
2:C:102:GLN:HG2	2:C:104:GLY:H	1.79	0.47
1:D:294:ASP:HB3	1:D:295:PRO:HD2	1.96	0.47
1:D:505:TYR:HD2	2:C:353:LYS:HA	1.80	0.47
2:C:203:TRP:CE3	2:C:511:SER:HB2	2.50	0.47
1:D:589:PRO:HD2	1:B:855:PHE:CD1	2.50	0.46
2:C:459:TRP:CZ2	2:C:463:VAL:HG21	2.50	0.46
1:D:93:ALA:HB1	1:D:191:GLU:HG2	1.98	0.46
1:D:94:SER:O	1:D:189:LEU:HD12	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:ILE:HA	1:D:422:ASN:ND2	2.21	0.46
1:D:398:ASP:N	1:D:512:VAL:O	2.23	0.46
2:C:51:ASN:O	2:C:342:ALA:HA	2.15	0.46
1:D:894:LEU:HD23	1:A:1072:GLU:OE1	2.15	0.46
1:D:1003:SER:HB3	1:B:759:PHE:HE1	1.80	0.46
1:D:1077:THR:OG1	1:D:1095:PHE:O	2.26	0.46
2:C:233:ILE:HD13	2:C:450:LEU:HD13	1.97	0.46
1:D:421:TYR:CD1	1:D:457:ARG:HB3	2.50	0.46
1:D:592:PHE:HZ	1:B:854:LYS:O	1.99	0.46
2:C:304:ALA:HA	2:C:307:ILE:HD12	1.96	0.46
1:A:561:PRO:O	1:A:577:ARG:NH1	2.43	0.46
1:B:453:TYR:HE1	1:B:455:LEU:HD12	1.81	0.46
2:C:184:VAL:HG22	2:C:464:PHE:CE1	2.51	0.46
1:D:63:THR:HG21	1:D:84:LEU:HD21	1.97	0.46
1:D:132:GLU:O	1:D:163:ALA:HA	2.16	0.46
1:D:972:ALA:HB3	1:D:996:LEU:HD21	1.98	0.46
1:D:1072:GLU:N	1:D:1072:GLU:OE1	2.49	0.46
1:D:129:LYS:HG2	1:D:169:GLU:CA	2.33	0.46
1:D:398:ASP:OD1	1:D:399:SER:N	2.48	0.46
1:D:28:TYR:HA	1:D:62:VAL:O	2.16	0.46
1:D:33:THR:HG21	1:D:220:PHE:CA	2.35	0.46
1:D:126:VAL:HB	1:D:172:SER:CB	2.45	0.46
1:D:401:VAL:HG22	1:D:509:ARG:HG2	1.98	0.46
1:D:535:LYS:HE2	1:D:585:LEU:CD2	2.46	0.46
1:D:714:ILE:CG1	1:D:1096:VAL:HG11	2.46	0.46
1:D:985:ASP:HB3	1:D:987:PRO:HD2	1.97	0.46
1:D:44:ARG:HB3	1:D:47:VAL:HG22	1.97	0.46
1:D:350:VAL:O	1:D:353:TRP:HD1	1.99	0.46
1:D:367:VAL:O	1:D:371:SER:HB3	2.15	0.45
1:D:503:VAL:HA	1:D:506:GLN:HG3	1.97	0.45
2:C:306:ARG:O	2:C:310:GLU:HG2	2.15	0.45
2:C:446:ILE:HG21	2:C:523:PHE:HZ	1.81	0.45
1:D:21:ARG:HG3	1:D:79:PHE:HB3	1.98	0.45
1:D:97:LYS:HE2	1:D:186:PHE:CD1	2.51	0.45
1:D:98:SER:OG	1:D:180:GLU:O	2.13	0.45
1:D:280:ASN:HD21	1:D:284:THR:HB	1.81	0.45
1:D:350:VAL:HG12	1:D:452:ARG:O	2.15	0.45
1:D:131:CYS:HB3	1:D:163:ALA:HB1	1.98	0.45
2:C:32:PHE:CE1	2:C:76:GLN:HG3	2.52	0.45
2:C:64:ASN:O	2:C:68:LYS:HG3	2.15	0.45
2:C:478:TRP:CE3	2:C:489:GLU:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:TYR:CE2	1:D:93:ALA:HB2	2.51	0.45
1:D:457:ARG:NH1	1:D:459:SER:OG	2.49	0.45
1:D:1051:SER:HG	1:D:1064:HIS:CE1	2.34	0.45
1:D:1095:PHE:CD1	1:D:1104:VAL:HG22	2.50	0.45
2:C:581:VAL:HG13	2:C:584:LEU:HD23	1.98	0.45
1:D:271:GLN:HB3	1:D:272:PRO:HD2	1.99	0.45
2:C:302:TRP:HA	2:C:306:ARG:NH2	2.31	0.45
1:D:193:VAL:HG23	1:D:223:LEU:HD13	1.99	0.45
1:D:400:PHE:CD1	1:D:402:ILE:HG23	2.52	0.45
2:C:257:SER:OG	2:C:258:PRO:HD2	2.17	0.45
2:C:446:ILE:HG21	2:C:523:PHE:CZ	2.51	0.45
1:D:400:PHE:HD1	1:D:402:ILE:HG23	1.81	0.45
2:C:32:PHE:CE2	2:C:391:LEU:HD21	2.52	0.45
1:D:429:PHE:CZ	1:D:431:GLY:HA3	2.52	0.45
2:C:533:ALA:HB3	2:C:535:HIS:CD2	2.52	0.45
1:D:597:VAL:HG13	1:D:608:VAL:HG13	1.99	0.45
1:D:611:LEU:CD2	1:D:666:ILE:HG23	2.47	0.45
2:C:431:ASP:OD1	2:C:434:THR:HG23	2.17	0.45
1:D:44:ARG:HD2	1:D:279:TYR:HE2	1.82	0.44
1:D:895:GLN:HB3	1:A:705:VAL:HG11	1.99	0.44
2:C:279:TYR:HA	2:C:282:THR:HG1	1.82	0.44
1:D:340:GLU:HA	1:D:343:ASN:HB3	1.98	0.44
1:D:676:THR:HA	1:D:690:GLN:HG2	1.99	0.44
1:D:758:SER:H	1:A:965:GLN:HE22	1.63	0.44
2:C:521:TYR:CE1	2:C:579:MET:HG2	2.52	0.44
1:D:201:PHE:HE2	1:D:203:ILE:HB	1.82	0.44
1:D:1105:THR:HG22	1:D:1111:GLU:O	2.17	0.44
2:C:261:CYS:HB3	2:C:486:GLY:O	2.18	0.44
1:B:40:ASP:OD1	1:B:41:LYS:N	2.45	0.44
1:D:348:ALA:HB1	1:D:352:ALA:O	2.18	0.44
1:D:1095:PHE:CE1	1:D:1104:VAL:HG22	2.53	0.44
1:D:107:GLY:O	1:D:235:ILE:HG23	2.18	0.44
1:B:122:ASN:O	1:B:123:ALA:HB3	2.18	0.44
1:D:597:VAL:HG13	1:D:608:VAL:CG1	2.48	0.44
2:C:43:SER:HA	2:C:65:ALA:HB1	2.00	0.44
2:C:263:PRO:HG2	2:C:266:LEU:CD1	2.43	0.44
2:C:478:TRP:CE3	2:C:481:LYS:HD2	2.52	0.44
2:C:503:LEU:HD23	2:C:506:VAL:CG2	2.29	0.44
2:C:556:ASN:O	2:C:560:LEU:HG	2.17	0.44
1:D:201:PHE:CE2	1:D:203:ILE:HB	2.53	0.44
1:D:18:LEU:HB2	1:D:21:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:GLY:O	1:D:241:LEU:N	2.37	0.44
1:D:336:CYS:SG	1:D:358:ILE:HG23	2.57	0.44
1:D:564:GLN:HG2	1:D:565:PHE:CD1	2.52	0.44
1:D:865:LEU:HG	1:D:870:ILE:HG13	2.00	0.44
1:A:122:ASN:O	1:A:123:ALA:HB3	2.18	0.44
1:B:193:VAL:HG23	1:B:223:LEU:HD22	2.00	0.44
2:C:267:LEU:HD12	2:C:272:GLY:HA3	1.99	0.43
1:A:404:GLY:N	1:A:504:GLY:O	2.50	0.43
1:D:314:GLN:HA	1:D:595:VAL:O	2.18	0.43
1:D:418:ILE:HD13	1:D:422:ASN:ND2	2.33	0.43
1:D:714:ILE:HB	1:D:1075:PHE:CE2	2.51	0.43
1:D:759:PHE:O	1:D:763:LEU:HG	2.17	0.43
1:D:913:GLN:HE22	1:A:1090:PRO:HG2	1.83	0.43
1:B:318:PHE:N	1:B:593:GLY:O	2.46	0.43
1:D:895:GLN:HB3	1:A:705:VAL:CG1	2.49	0.43
1:D:977:LEU:O	1:D:981:LEU:HG	2.19	0.43
2:C:31:LYS:HE2	2:C:35:GLU:OE2	2.18	0.43
2:C:132:VAL:HG23	2:C:168:TRP:CE3	2.44	0.43
1:B:280:ASN:OD1	1:B:284:THR:N	2.51	0.43
1:D:102:ARG:CZ	1:D:141:LEU:HB3	2.48	0.43
1:D:788:ILE:HD11	1:A:699:LEU:CB	2.46	0.43
2:C:292:ASP:HA	2:C:366:MET:SD	2.58	0.43
1:B:738:CYS:SG	1:B:764:ASN:ND2	2.91	0.43
2:C:245:ARG:HG3	2:C:262:LEU:CD2	2.47	0.43
1:D:66:HIS:CE1	1:D:78:ARG:HE	2.36	0.43
2:C:49:ASN:O	2:C:58:ASN:ND2	2.51	0.43
2:C:144:LEU:CA	2:C:148:LEU:HB2	2.38	0.43
2:C:358:ILE:HD11	2:C:379:ILE:HG13	2.01	0.43
1:A:814:LYS:NZ	1:A:872:GLN:OE1	2.32	0.43
1:D:598:ILE:CD1	1:D:666:ILE:HG12	2.49	0.43
1:D:714:ILE:HG22	1:D:1110:TYR:HB2	1.99	0.43
1:D:823:PHE:CD1	1:D:1057:PRO:HD3	2.54	0.43
2:C:435:GLU:OE2	2:C:541:LYS:HE2	2.18	0.43
1:D:883:THR:HG22	1:A:707:TYR:OH	2.19	0.43
1:D:1033:VAL:HG13	1:D:1053:PRO:HD3	2.01	0.43
1:D:185:ASN:OD1	1:D:213:VAL:HG22	2.19	0.43
1:D:707:TYR:HB3	1:B:792:PRO:HG3	2.00	0.43
1:D:1080:ALA:CB	1:D:1089:PHE:HE1	2.32	0.43
1:D:1105:THR:HG22	1:D:1111:GLU:C	2.40	0.43
1:B:553:THR:O	1:B:586:ASP:N	2.47	0.43
1:D:570:ALA:HB1	1:B:963:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:32:PHE:HE1	2:C:76:GLN:HG3	1.84	0.43
1:B:327:VAL:O	1:B:531:THR:N	2.52	0.43
1:D:129:LYS:HE2	1:D:169:GLU:HB3	2.01	0.42
1:D:411:ALA:HB3	1:D:414:GLN:NE2	2.33	0.42
1:D:452:ARG:HA	1:D:494:SER:HA	2.01	0.42
2:C:401:HIS:HB2	2:C:514:ARG:NH2	2.34	0.42
2:C:478:TRP:CE2	2:C:489:GLU:HB3	2.54	0.42
1:D:960:ASN:O	1:D:964:LYS:HG3	2.18	0.42
2:C:90:ASN:ND2	2:C:93:VAL:HG23	2.34	0.42
2:C:488:VAL:CG1	2:C:612:PRO:HD3	2.49	0.42
1:A:111:ASP:OD1	1:A:112:SER:N	2.47	0.42
1:D:559:PHE:HZ	1:D:575:ALA:HB3	1.83	0.42
1:D:966:LEU:O	1:D:975:SER:HB2	2.19	0.42
1:D:1078:ALA:HB2	1:D:1102:TRP:CH2	2.55	0.42
2:C:374:HIS:HE1	2:C:402:GLU:HG3	1.84	0.42
1:B:916:LEU:O	1:B:920:GLN:N	2.52	0.42
1:D:44:ARG:NE	1:D:49:HIS:HB2	2.34	0.42
1:D:324:GLU:O	1:D:539:VAL:HB	2.20	0.42
2:C:594:TRP:CE3	2:C:595:LEU:HD23	2.54	0.42
2:C:269:ASP:OD1	2:C:272:GLY:HA2	2.19	0.42
1:D:129:LYS:CD	1:D:169:GLU:HG2	2.49	0.42
2:C:234:LYS:N	2:C:235:PRO:HD2	2.33	0.42
2:C:518:ARG:O	2:C:522:GLN:HG2	2.20	0.42
1:D:102:ARG:NH2	1:D:141:LEU:HD22	2.35	0.42
1:D:503:VAL:HA	1:D:506:GLN:CG	2.50	0.42
1:B:453:TYR:CE1	1:B:455:LEU:HD12	2.54	0.42
1:D:206:LYS:HE2	1:D:221:SER:HB3	2.01	0.42
1:D:278:LYS:CG	1:D:286:THR:HB	2.50	0.42
1:D:410:ILE:O	1:D:411:ALA:HB2	2.20	0.42
1:D:146:HIS:HE1	1:D:152:TRP:HA	1.85	0.42
1:D:858:LEU:HD21	1:D:962:LEU:HD23	2.01	0.42
1:D:986:PRO:CD	1:D:987:PRO:HD2	2.49	0.42
2:C:144:LEU:HA	2:C:148:LEU:CD1	2.48	0.42
2:C:207:TYR:CE1	2:C:397:ASN:HB2	2.54	0.42
1:D:970:PHE:O	1:D:995:ARG:HB3	2.19	0.42
1:D:996:LEU:O	1:D:1000:ARG:HG3	2.20	0.42
2:C:177:ARG:O	2:C:181:GLU:HG3	2.19	0.42
1:D:476:GLY:HA3	2:C:24:GLN:NE2	2.27	0.41
1:D:710:ASN:HB3	1:D:1076:THR:HG23	2.01	0.41
1:D:808:ASP:HB2	1:D:817:PHE:HE1	1.84	0.41
2:C:29:LEU:HD21	2:C:97:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:432:ASN:O	2:C:436:ILE:HG13	2.20	0.41
1:A:916:LEU:O	1:A:920:GLN:N	2.53	0.41
1:D:95:THR:HG21	1:D:212:LEU:HD23	2.02	0.41
1:D:343:ASN:O	1:D:343:ASN:OD1	2.38	0.41
1:D:404:GLY:HA3	1:D:504:GLY:O	2.19	0.41
1:D:737:ASP:OD2	1:D:740:MET:HG2	2.20	0.41
1:D:34:ARG:NH2	1:D:216:LEU:HD22	2.35	0.41
2:C:107:VAL:HB	2:C:193:ALA:HB1	2.03	0.41
2:C:284:PRO:HD3	2:C:440:LEU:CD2	2.50	0.41
1:D:451:TYR:HD2	1:D:497:PHE:CE2	2.37	0.41
1:D:726:ILE:HD13	1:D:945:LEU:HD23	2.02	0.41
2:C:571:GLU:O	2:C:575:GLY:HA2	2.21	0.41
1:D:280:ASN:OD1	1:D:283:GLY:N	2.53	0.41
1:D:351:TYR:CE2	1:D:452:ARG:HB2	2.50	0.41
1:D:916:LEU:O	1:D:920:GLN:N	2.52	0.41
1:D:1033:VAL:HG22	1:D:1051:SER:OG	2.21	0.41
2:C:144:LEU:HB2	2:C:168:TRP:CH2	2.55	0.41
2:C:293:VAL:HG22	2:C:366:MET:HG3	2.02	0.41
2:C:455:MET:HB2	2:C:484:ILE:HG21	2.03	0.41
1:D:105:ILE:HG12	1:D:118:LEU:CD1	2.49	0.41
1:D:714:ILE:HG12	1:D:1075:PHE:HD2	1.86	0.41
1:D:715:PRO:HA	1:D:1071:GLN:O	2.21	0.41
1:D:965:GLN:HG3	1:D:1003:SER:HB2	2.03	0.41
1:B:367:VAL:O	1:B:371:SER:N	2.53	0.41
1:D:722:VAL:HA	1:D:1064:HIS:O	2.21	0.41
1:D:865:LEU:HD21	1:D:873:TYR:CE2	2.45	0.41
1:D:986:PRO:HD2	1:D:987:PRO:HD2	2.02	0.41
2:C:582:ARG:N	2:C:583:PRO:HD2	2.36	0.41
1:D:453:TYR:N	1:D:493:GLN:O	2.54	0.41
2:C:144:LEU:CA	2:C:148:LEU:HD12	2.51	0.41
1:D:93:ALA:CA	1:D:191:GLU:HG2	2.50	0.41
1:D:190:ARG:HD3	1:D:192:PHE:CZ	2.56	0.41
1:D:434:ILE:O	1:D:510:VAL:HA	2.21	0.41
1:D:791:THR:CB	1:D:795:LYS:HE2	2.51	0.41
1:D:805:ILE:HD13	1:D:1052:PHE:CD2	2.56	0.41
2:C:177:ARG:N	2:C:178:PRO:HD2	2.36	0.41
2:C:500:PRO:O	2:C:506:VAL:HB	2.20	0.41
1:A:377:PHE:HD1	1:A:434:ILE:HG22	1.84	0.41
1:D:216:LEU:HD11	1:D:266:TYR:HD2	1.86	0.41
1:D:974:SER:CB	1:D:983:ARG:HH22	2.33	0.41
1:D:1033:VAL:HG11	1:D:1053:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:GLY:O	2:C:151:ILE:HG12	2.21	0.41
1:B:986:PRO:N	1:B:987:PRO:HD2	2.36	0.41
1:D:65:PHE:CZ	1:D:82:PRO:HG3	2.56	0.40
1:D:989:ALA:O	1:D:993:ILE:HG13	2.22	0.40
2:C:187:LYS:HB3	2:C:199:TYR:CE1	2.56	0.40
2:C:594:TRP:CZ3	2:C:595:LEU:HD23	2.56	0.40
1:D:83:VAL:CG2	1:D:239:GLN:HE21	2.34	0.40
1:D:612:TYR:O	1:D:648:GLY:HA3	2.21	0.40
2:C:53:ASN:OD1	2:C:340:GLN:HB3	2.21	0.40
2:C:133:CYS:HA	2:C:141:CYS:HA	2.03	0.40
2:C:182:GLU:O	2:C:186:LEU:HG	2.20	0.40
2:C:284:PRO:HD2	2:C:437:ASN:OD1	2.21	0.40
1:D:33:THR:HG21	1:D:220:PHE:CD1	2.57	0.40
1:D:102:ARG:NE	1:D:141:LEU:HB3	2.36	0.40
1:D:800:PHE:CE1	1:D:924:ALA:HA	2.56	0.40
1:D:906:PHE:CE2	1:D:916:LEU:HB2	2.55	0.40
1:D:216:LEU:HD21	1:D:266:TYR:CD2	2.57	0.40
1:D:269:TYR:HD1	1:D:271:GLN:HE21	1.69	0.40
1:D:403:ARG:HB2	1:D:406:GLU:CG	2.50	0.40
1:D:575:ALA:CB	1:D:586:ASP:HA	2.51	0.40
1:D:879:ALA:O	1:D:883:THR:CB	2.69	0.40
2:C:169:ARG:HA	2:C:173:GLY:H	1.87	0.40
2:C:500:PRO:CB	2:C:506:VAL:HG11	2.51	0.40
1:B:111:ASP:OD1	1:B:112:SER:N	2.46	0.40
1:D:24:LEU:HD12	1:D:24:LEU:C	2.42	0.40
1:D:185:ASN:HB3	1:D:212:LEU:O	2.21	0.40
1:D:299:THR:HA	1:D:315:THR:HG22	2.04	0.40
1:D:318:PHE:N	1:D:593:GLY:O	2.55	0.40
1:D:419:ALA:O	1:D:424:LYS:HB2	2.22	0.40
1:D:611:LEU:HD21	1:D:666:ILE:HG23	2.03	0.40
1:D:1105:THR:HG22	1:D:1112:PRO:HA	2.03	0.40
2:C:108:LEU:HD21	2:C:190:MET:N	2.36	0.40
2:C:245:ARG:CB	2:C:262:LEU:HD21	2.51	0.40
2:C:477:TRP:NE1	2:C:499:ASP:OD2	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1056/1261 (84%)	1007 (95%)	49 (5%)	0	100	100
1	B	1056/1261 (84%)	1007 (95%)	49 (5%)	0	100	100
1	D	1056/1261 (84%)	1004 (95%)	52 (5%)	0	100	100
2	C	595/625 (95%)	587 (99%)	8 (1%)	0	100	100
All	All	3763/4408 (85%)	3605 (96%)	158 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	933/1099 (85%)	933 (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	3326/3849 (86%)	3326 (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 (23) 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	913	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
2	C	524	GLN
2	C	526	GLN
1	A	965	GLN
1	B	895	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

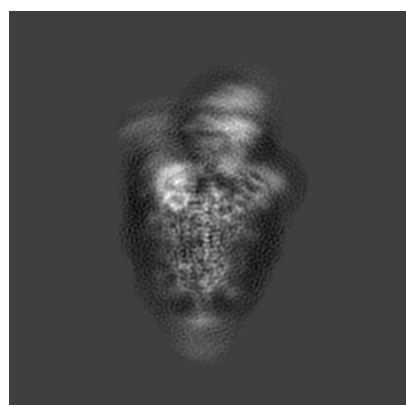
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32175. These allow visual inspection of the internal detail of the map and identification of artifacts.

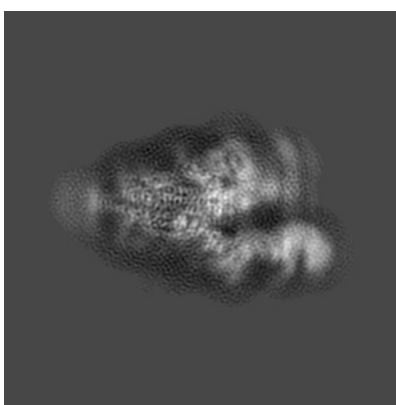
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

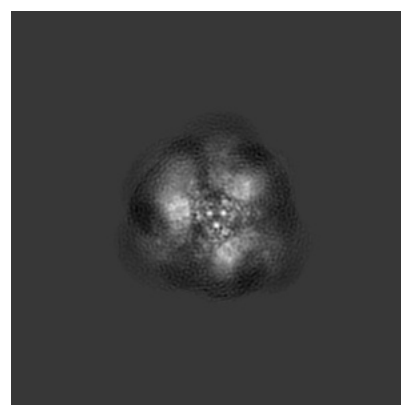
#### 6.1.1 Primary map



X



Y

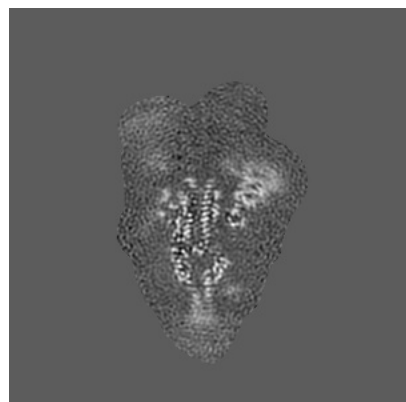


Z

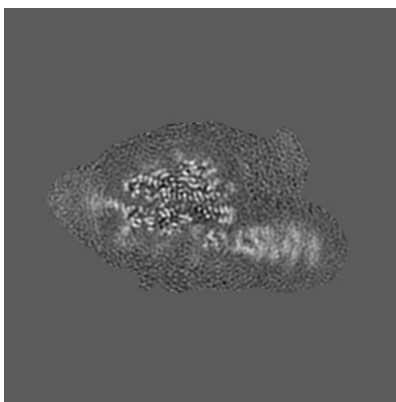
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

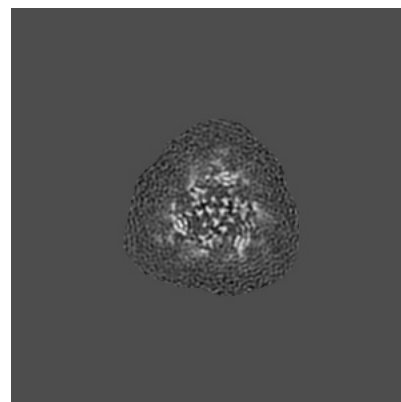
#### 6.2.1 Primary map



X Index: 180



Y Index: 180



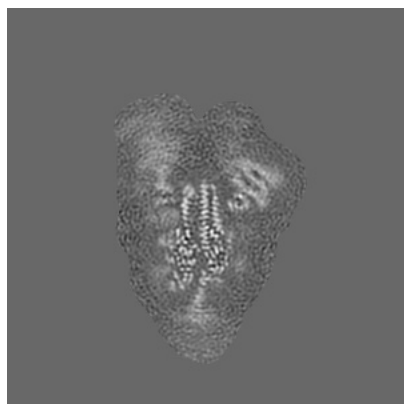
Z Index: 180



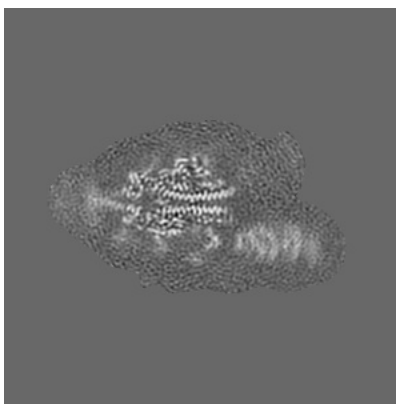
The images above show central slices of the map in three orthogonal directions.

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

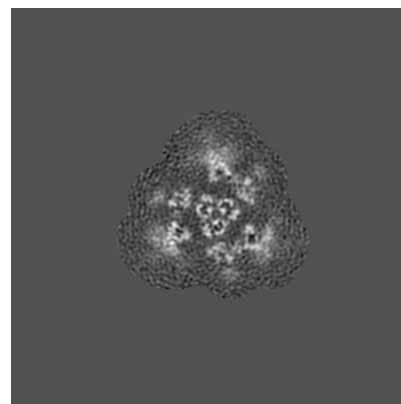
### 6.3.1 Primary map



X Index: 191



Y Index: 177

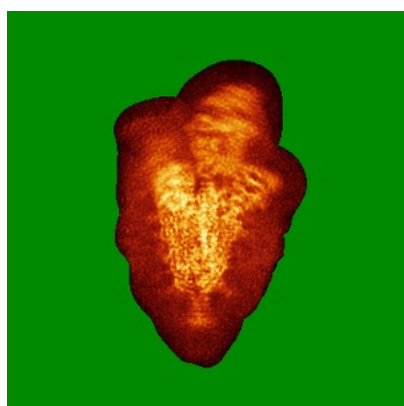


Z Index: 194

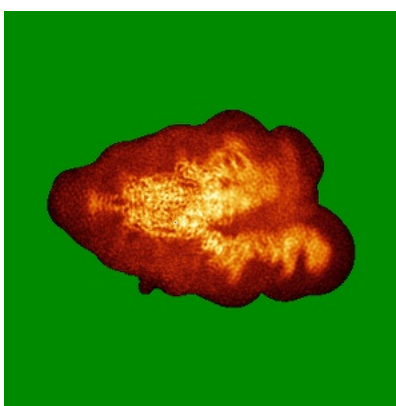
The images above show the largest variance slices of the map in three orthogonal directions.

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

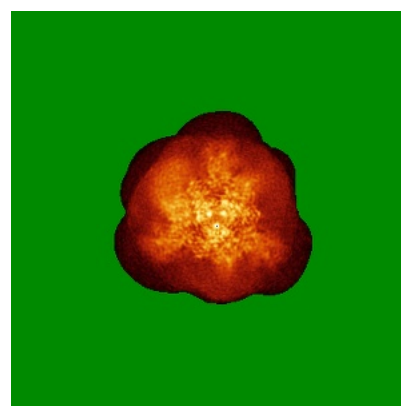
### 6.4.1 Primary map



X



Y

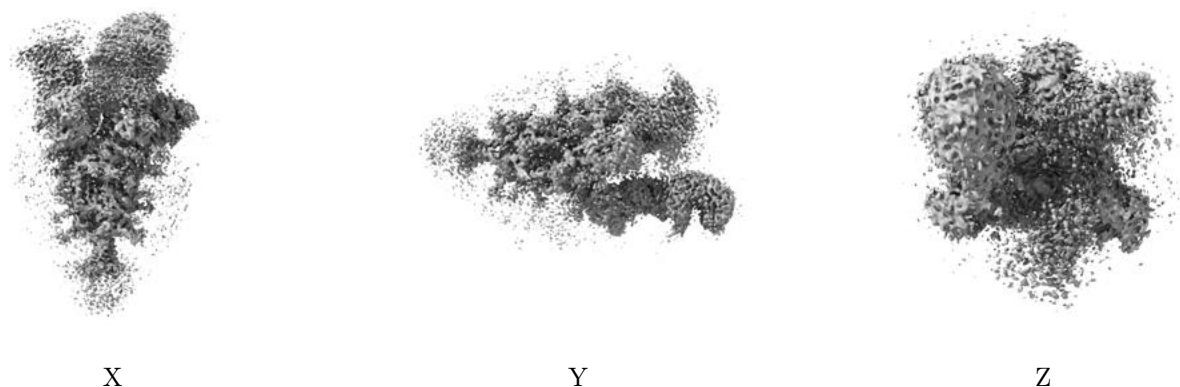


Z

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

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

### 6.5.1 Primary map



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

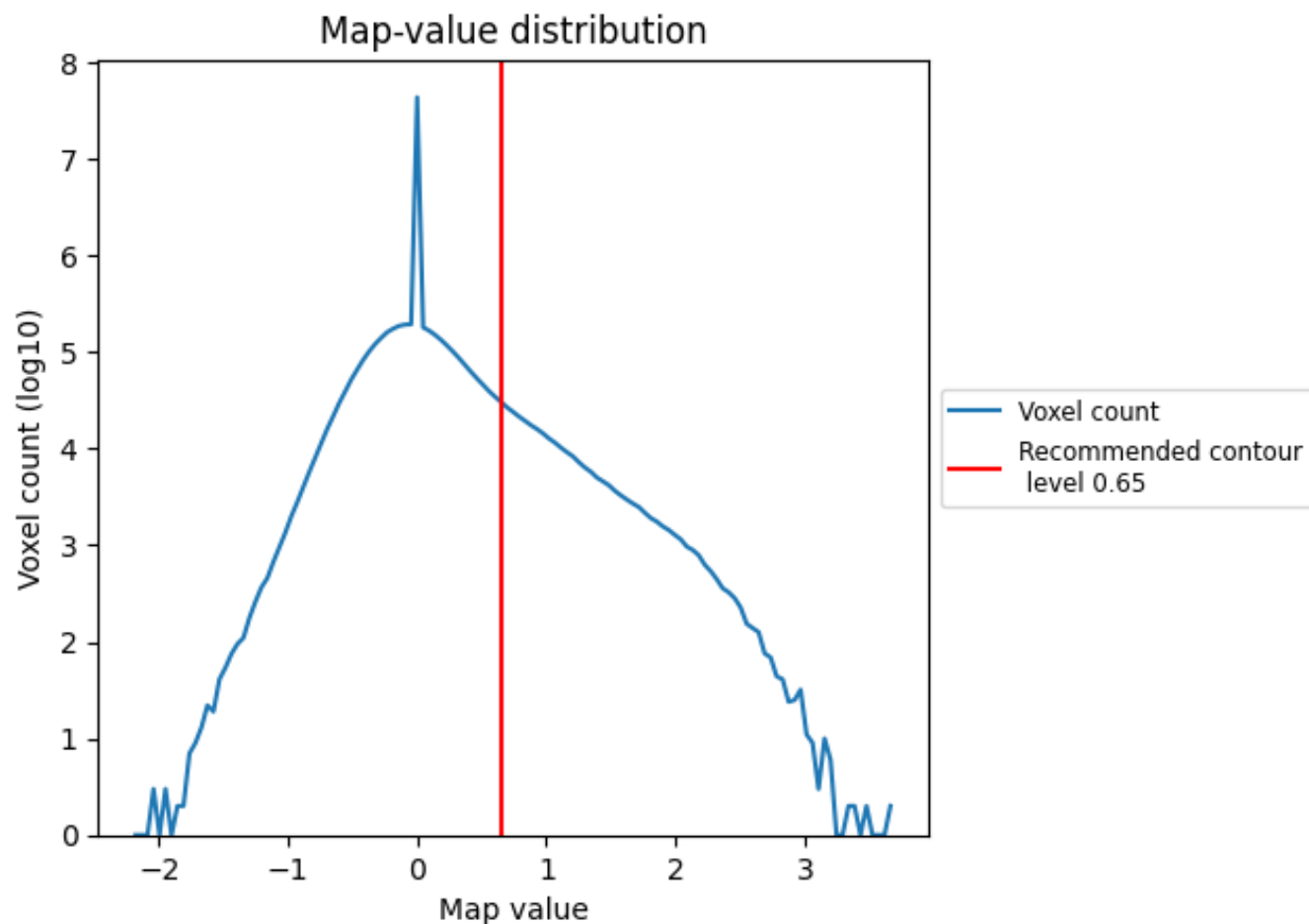
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

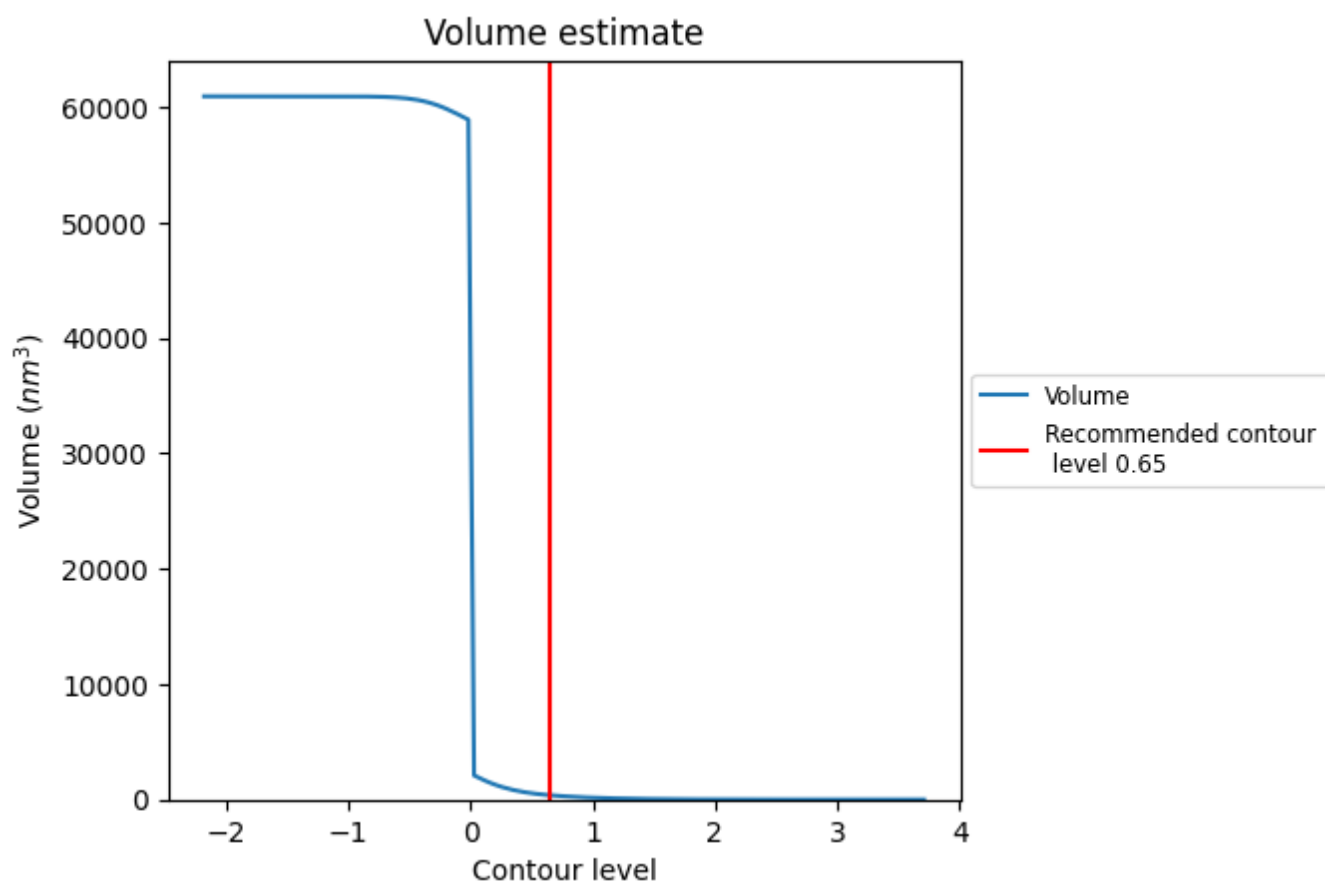
This section contains the results of statistical analysis of the map.

### 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.

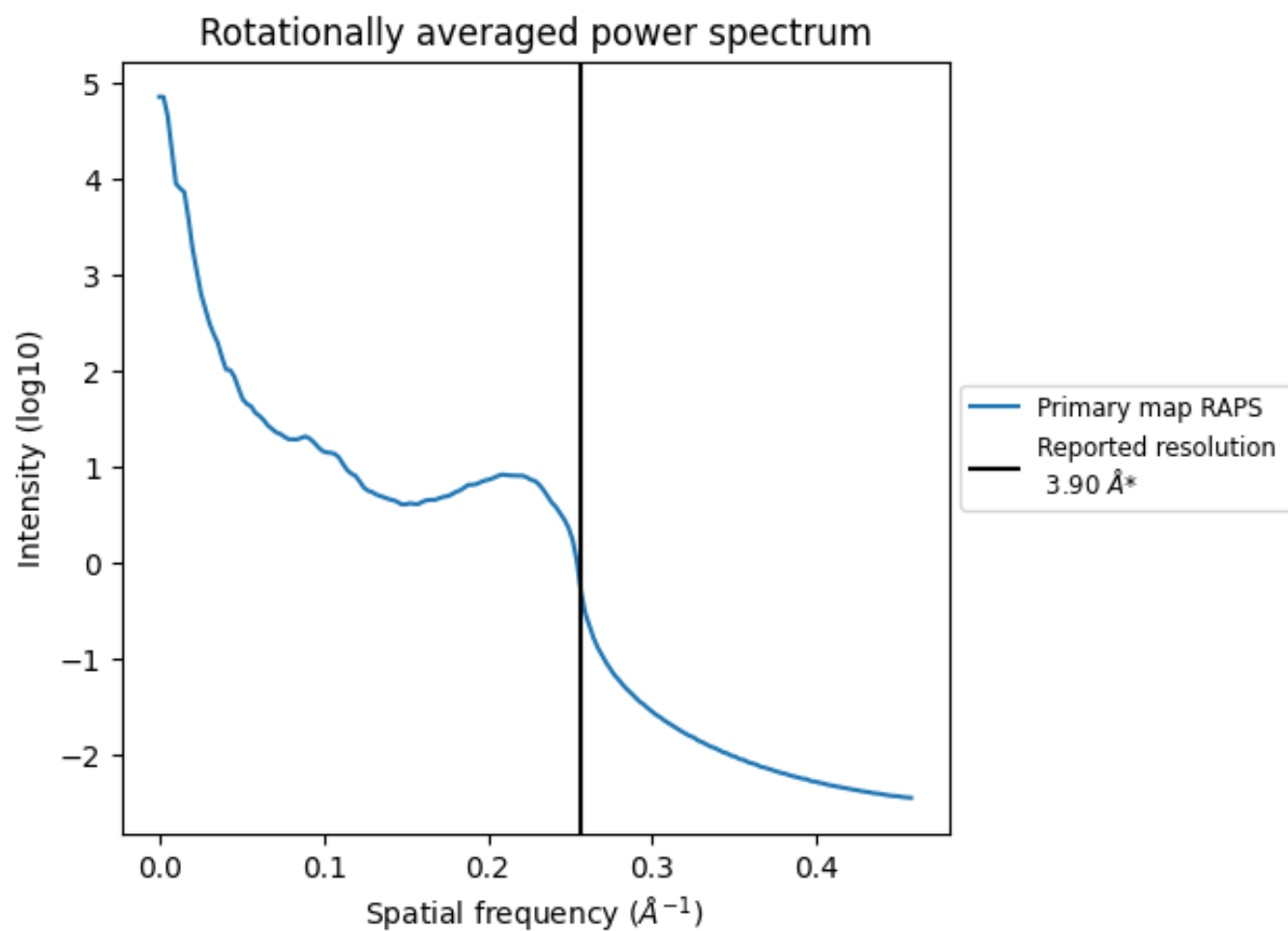
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 376 nm<sup>3</sup>; this corresponds to an approximate mass of 340 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  $\text{\AA}^{-1}$

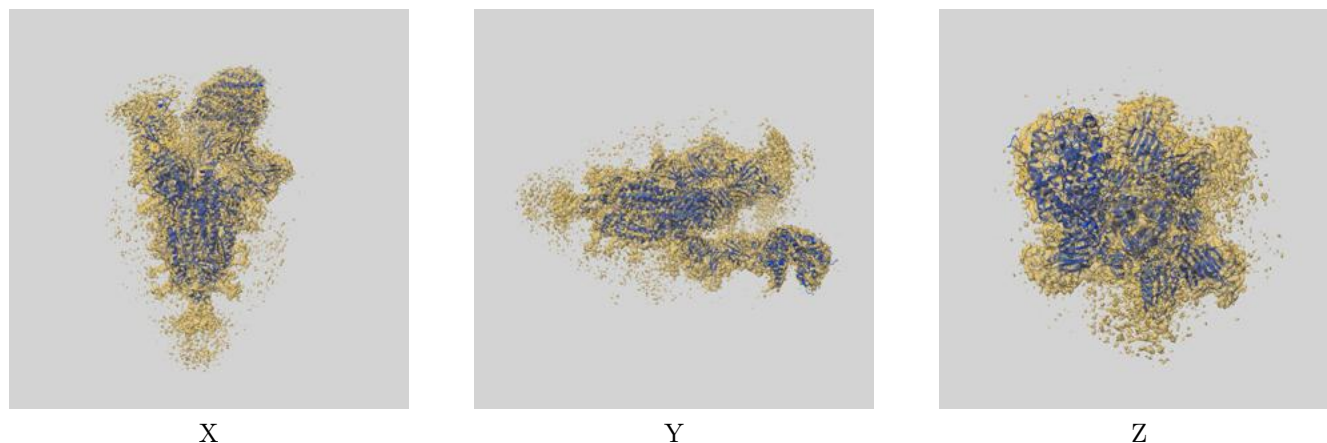
## 8 Fourier-Shell correlation

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

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

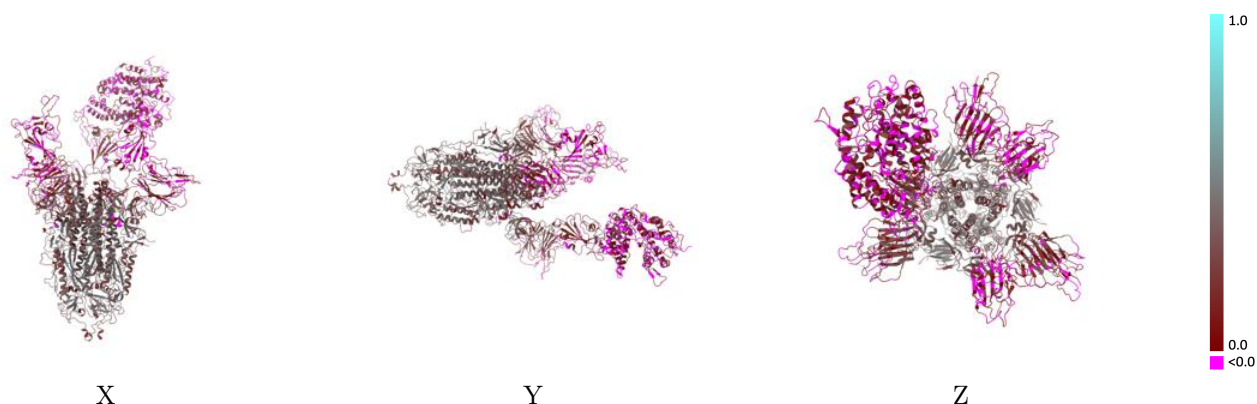
This section contains information regarding the fit between EMDB map EMD-32175 and PDB model 7VXC. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



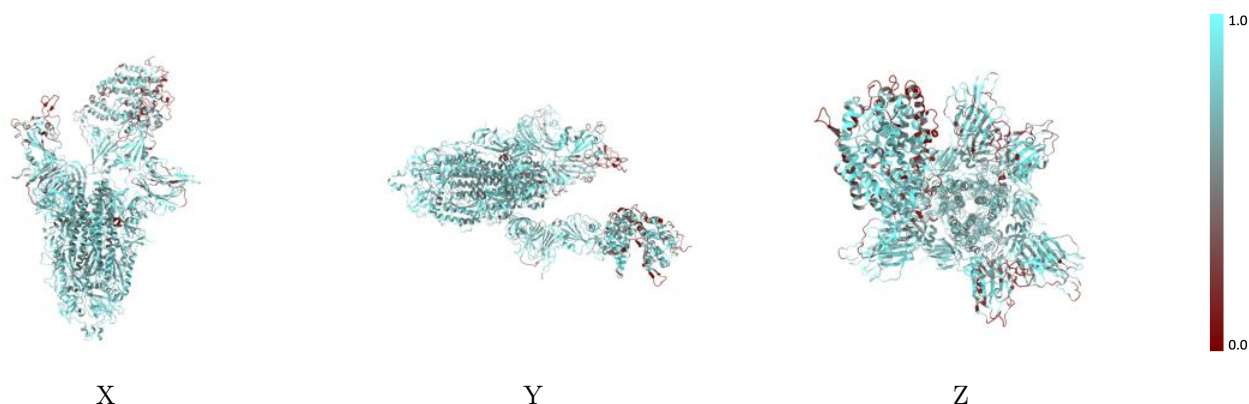
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

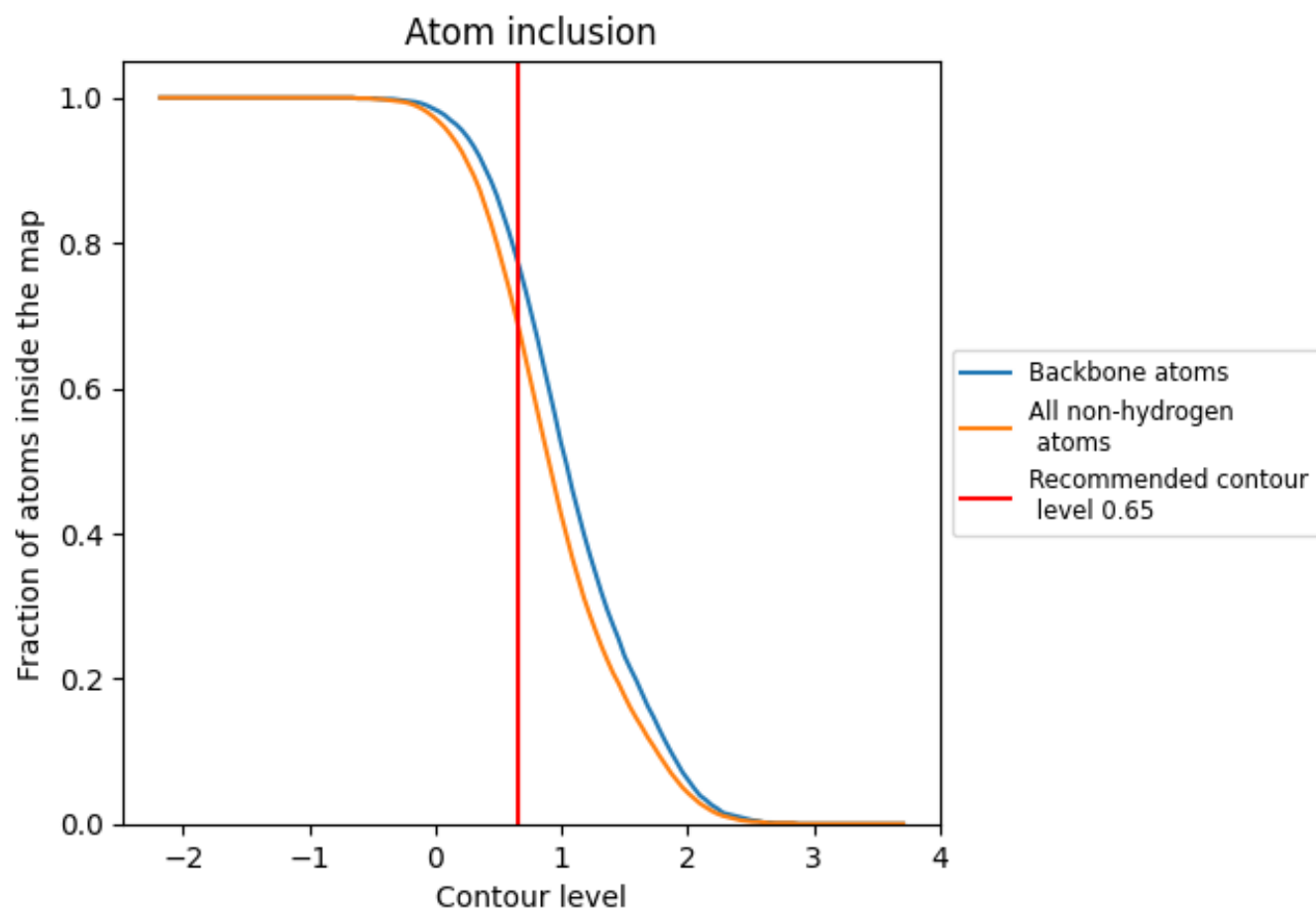
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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, 78% 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> 0.6910	<div></div> 0.2210
A	<div></div> 0.7050	<div></div> 0.2500
B	<div></div> 0.7030	<div></div> 0.2620
C	<div></div> 0.6230	<div></div> 0.0460
D	<div></div> 0.7260	<div></div> 0.2520

