



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:37 PM UTC

PDB ID : 8YZ5 / pdb_00008yz5
EMDB ID : EMD-39685
Title : SARS-CoV-2 Delta Spike in complex with Fab of JE-5C
Authors : Chen, X.; Wu, Y.-M.
Deposited on : 2024-04-06
Resolution : 3.93 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:

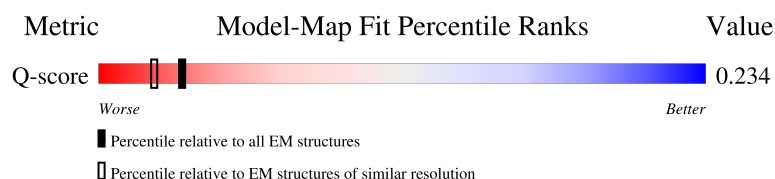
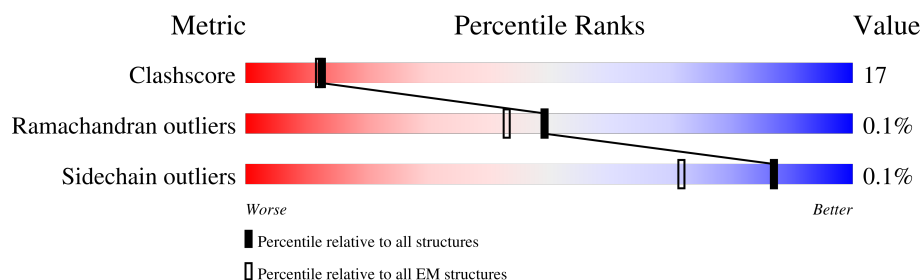
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

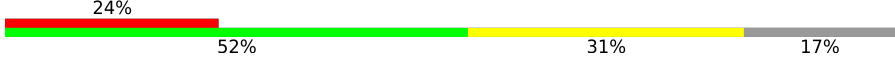
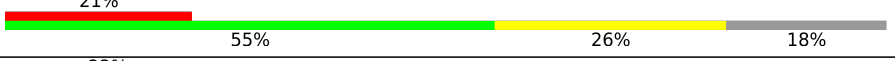
The reported resolution of this entry is 3.93 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7811 (3.43 - 4.43)

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	1259	
1	C	1259	
1	D	1259	
2	G	119	

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Mol	Chain	Length	Quality of chain
2	I	119	82% 60%39%
3	J	107	68% 65%35%
3	K	107	77% 78%21%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 27677 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	C	1027	Total	C	N	O	S	0	0
			8023	5124	1339	1526	34		
1	A	1042	Total	C	N	O	S	0	0
			8138	5190	1366	1546	36		
1	D	1037	Total	C	N	O	S	0	0
			8102	5173	1353	1540	36		

There are 243 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	MET	-	expression tag	UNP P0DTC2
C	-4	LYS	-	expression tag	UNP P0DTC2
C	-3	VAL	-	expression tag	UNP P0DTC2
C	-2	LYS	-	expression tag	UNP P0DTC2
C	-1	LEU	-	expression tag	UNP P0DTC2
C	0	LEU	-	expression tag	UNP P0DTC2
C	1	VAL	-	expression tag	UNP P0DTC2
C	2	LEU	-	expression tag	UNP P0DTC2
C	3	LEU	-	expression tag	UNP P0DTC2
C	4	CYS	-	expression tag	UNP P0DTC2
C	5	THR	-	expression tag	UNP P0DTC2
C	6	PHE	-	expression tag	UNP P0DTC2
C	7	THR	-	expression tag	UNP P0DTC2
C	8	ALA	-	expression tag	UNP P0DTC2
C	9	THR	-	expression tag	UNP P0DTC2
C	10	TYR	-	expression tag	UNP P0DTC2
C	11	ALA	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	19	ARG	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	GLU	deletion	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	158	GLY	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	452	ARG	LEU	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	GLY	ARG	variant	UNP P0DTC2
C	950	ASN	ASP	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	ASP	-	expression tag	UNP P0DTC2
C	1210	ILE	-	expression tag	UNP P0DTC2
C	1211	ARG	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	LEU	-	expression tag	UNP P0DTC2
C	1214	VAL	-	expression tag	UNP P0DTC2
C	1215	PRO	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	GLY	-	expression tag	UNP P0DTC2
C	1218	SER	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	SER	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	ILE	-	expression tag	UNP P0DTC2
C	1225	PRO	-	expression tag	UNP P0DTC2
C	1226	GLU	-	expression tag	UNP P0DTC2
C	1227	ALA	-	expression tag	UNP P0DTC2
C	1228	PRO	-	expression tag	UNP P0DTC2
C	1229	ARG	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLN	-	expression tag	UNP P0DTC2
C	1233	ALA	-	expression tag	UNP P0DTC2
C	1234	TYR	-	expression tag	UNP P0DTC2
C	1235	VAL	-	expression tag	UNP P0DTC2
C	1236	ARG	-	expression tag	UNP P0DTC2
C	1237	LYS	-	expression tag	UNP P0DTC2
C	1238	ASP	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1241	TRP	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	SER	-	expression tag	UNP P0DTC2
C	1246	THR	-	expression tag	UNP P0DTC2
C	1247	PHE	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
A	-5	MET	-	expression tag	UNP P0DTC2
A	-4	LYS	-	expression tag	UNP P0DTC2
A	-3	VAL	-	expression tag	UNP P0DTC2
A	-2	LYS	-	expression tag	UNP P0DTC2
A	-1	LEU	-	expression tag	UNP P0DTC2
A	0	LEU	-	expression tag	UNP P0DTC2
A	1	VAL	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	3	LEU	-	expression tag	UNP P0DTC2
A	4	CYS	-	expression tag	UNP P0DTC2
A	5	THR	-	expression tag	UNP P0DTC2
A	6	PHE	-	expression tag	UNP P0DTC2
A	7	THR	-	expression tag	UNP P0DTC2
A	8	ALA	-	expression tag	UNP P0DTC2
A	9	THR	-	expression tag	UNP P0DTC2
A	10	TYR	-	expression tag	UNP P0DTC2
A	11	ALA	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	19	ARG	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	GLU	deletion	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	158	GLY	ARG	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	681	ARG	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	GLY	ARG	variant	UNP P0DTC2
A	950	ASN	ASP	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	ASP	-	expression tag	UNP P0DTC2
A	1210	ILE	-	expression tag	UNP P0DTC2
A	1211	ARG	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	LEU	-	expression tag	UNP P0DTC2
A	1214	VAL	-	expression tag	UNP P0DTC2
A	1215	PRO	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	GLY	-	expression tag	UNP P0DTC2
A	1218	SER	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	SER	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	ILE	-	expression tag	UNP P0DTC2
A	1225	PRO	-	expression tag	UNP P0DTC2
A	1226	GLU	-	expression tag	UNP P0DTC2
A	1227	ALA	-	expression tag	UNP P0DTC2
A	1228	PRO	-	expression tag	UNP P0DTC2
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLN	-	expression tag	UNP P0DTC2
A	1233	ALA	-	expression tag	UNP P0DTC2
A	1234	TYR	-	expression tag	UNP P0DTC2
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	ARG	-	expression tag	UNP P0DTC2
A	1237	LYS	-	expression tag	UNP P0DTC2
A	1238	ASP	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	GLU	-	expression tag	UNP P0DTC2
A	1241	TRP	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	SER	-	expression tag	UNP P0DTC2
A	1246	THR	-	expression tag	UNP P0DTC2
A	1247	PHE	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
D	-5	MET	-	expression tag	UNP P0DTC2
D	-4	LYS	-	expression tag	UNP P0DTC2
D	-3	VAL	-	expression tag	UNP P0DTC2
D	-2	LYS	-	expression tag	UNP P0DTC2
D	-1	LEU	-	expression tag	UNP P0DTC2
D	0	LEU	-	expression tag	UNP P0DTC2
D	1	VAL	-	expression tag	UNP P0DTC2
D	2	LEU	-	expression tag	UNP P0DTC2
D	3	LEU	-	expression tag	UNP P0DTC2
D	4	CYS	-	expression tag	UNP P0DTC2
D	5	THR	-	expression tag	UNP P0DTC2
D	6	PHE	-	expression tag	UNP P0DTC2
D	7	THR	-	expression tag	UNP P0DTC2
D	8	ALA	-	expression tag	UNP P0DTC2
D	9	THR	-	expression tag	UNP P0DTC2
D	10	TYR	-	expression tag	UNP P0DTC2
D	11	ALA	-	expression tag	UNP P0DTC2
D	12	GLY	-	expression tag	UNP P0DTC2
D	13	THR	-	expression tag	UNP P0DTC2
D	19	ARG	THR	variant	UNP P0DTC2
D	142	ASP	GLY	variant	UNP P0DTC2
D	?	-	GLU	deletion	UNP P0DTC2
D	?	-	PHE	deletion	UNP P0DTC2
D	158	GLY	ARG	variant	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	478	LYS	THR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	685	GLY	ARG	variant	UNP P0DTC2
D	950	ASN	ASP	variant	UNP P0DTC2
D	986	PRO	LYS	variant	UNP P0DTC2
D	987	PRO	VAL	variant	UNP P0DTC2
D	1209	ASP	-	expression tag	UNP P0DTC2
D	1210	ILE	-	expression tag	UNP P0DTC2
D	1211	ARG	-	expression tag	UNP P0DTC2
D	1212	SER	-	expression tag	UNP P0DTC2
D	1213	LEU	-	expression tag	UNP P0DTC2
D	1214	VAL	-	expression tag	UNP P0DTC2
D	1215	PRO	-	expression tag	UNP P0DTC2
D	1216	ARG	-	expression tag	UNP P0DTC2
D	1217	GLY	-	expression tag	UNP P0DTC2
D	1218	SER	-	expression tag	UNP P0DTC2
D	1219	PRO	-	expression tag	UNP P0DTC2
D	1220	GLY	-	expression tag	UNP P0DTC2
D	1221	SER	-	expression tag	UNP P0DTC2
D	1222	GLY	-	expression tag	UNP P0DTC2
D	1223	TYR	-	expression tag	UNP P0DTC2
D	1224	ILE	-	expression tag	UNP P0DTC2
D	1225	PRO	-	expression tag	UNP P0DTC2
D	1226	GLU	-	expression tag	UNP P0DTC2
D	1227	ALA	-	expression tag	UNP P0DTC2
D	1228	PRO	-	expression tag	UNP P0DTC2
D	1229	ARG	-	expression tag	UNP P0DTC2
D	1230	ASP	-	expression tag	UNP P0DTC2
D	1231	GLY	-	expression tag	UNP P0DTC2
D	1232	GLN	-	expression tag	UNP P0DTC2
D	1233	ALA	-	expression tag	UNP P0DTC2
D	1234	TYR	-	expression tag	UNP P0DTC2
D	1235	VAL	-	expression tag	UNP P0DTC2
D	1236	ARG	-	expression tag	UNP P0DTC2
D	1237	LYS	-	expression tag	UNP P0DTC2
D	1238	ASP	-	expression tag	UNP P0DTC2
D	1239	GLY	-	expression tag	UNP P0DTC2
D	1240	GLU	-	expression tag	UNP P0DTC2
D	1241	TRP	-	expression tag	UNP P0DTC2
D	1242	VAL	-	expression tag	UNP P0DTC2
D	1243	LEU	-	expression tag	UNP P0DTC2
D	1244	LEU	-	expression tag	UNP P0DTC2
D	1245	SER	-	expression tag	UNP P0DTC2
D	1246	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1247	PHE	-	expression tag	UNP P0DTC2
D	1248	LEU	-	expression tag	UNP P0DTC2
D	1249	GLY	-	expression tag	UNP P0DTC2
D	1250	HIS	-	expression tag	UNP P0DTC2
D	1251	HIS	-	expression tag	UNP P0DTC2
D	1252	HIS	-	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

- Molecule 2 is a protein called Fab heavy chain of JE-5C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	119	Total	C	N	O	S	0	0
			889	551	156	177	5		
2	I	118	Total	C	N	O	S	0	0
			884	548	155	176	5		

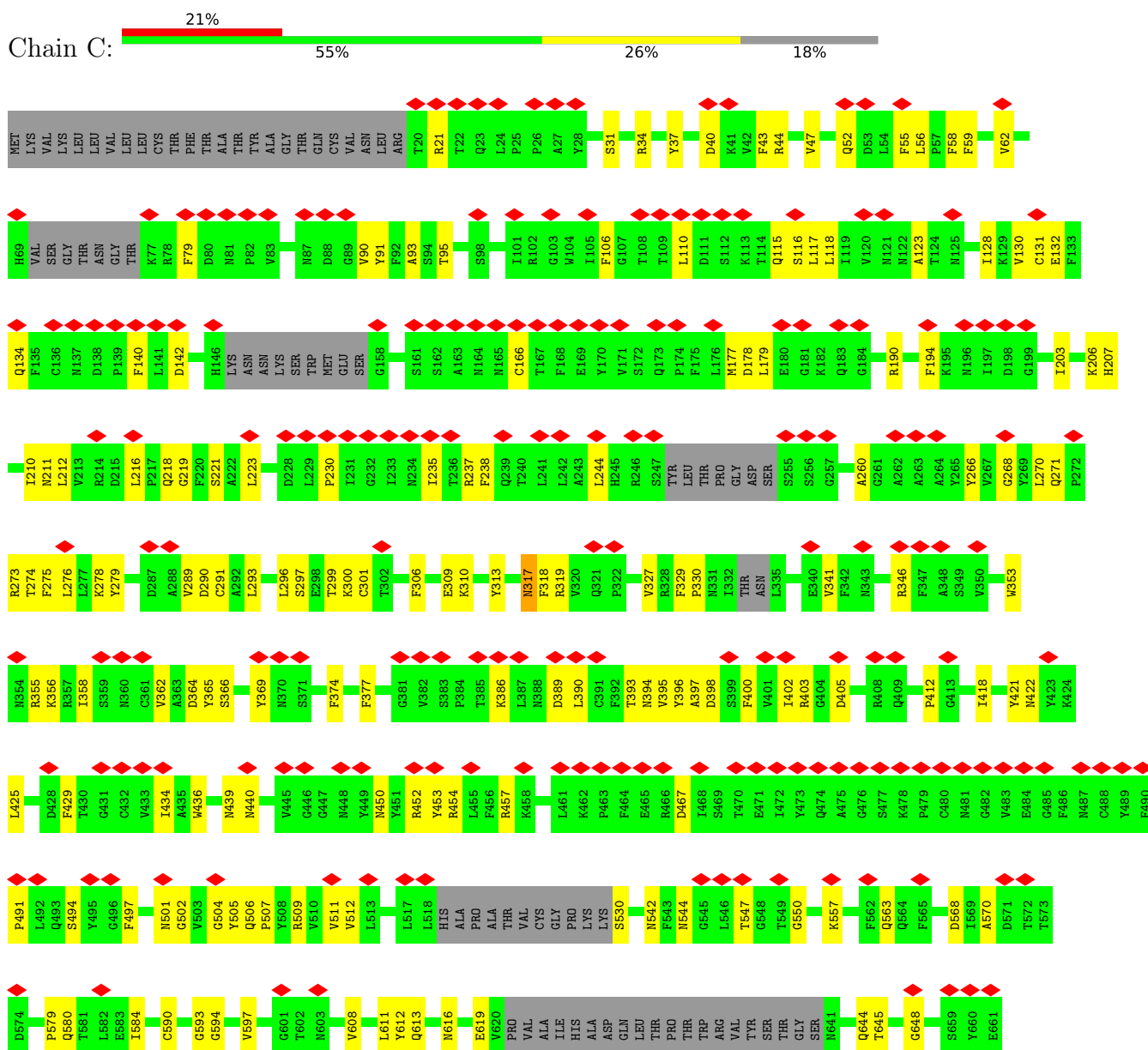
- Molecule 3 is a protein called Fab light chain of JE-5C.

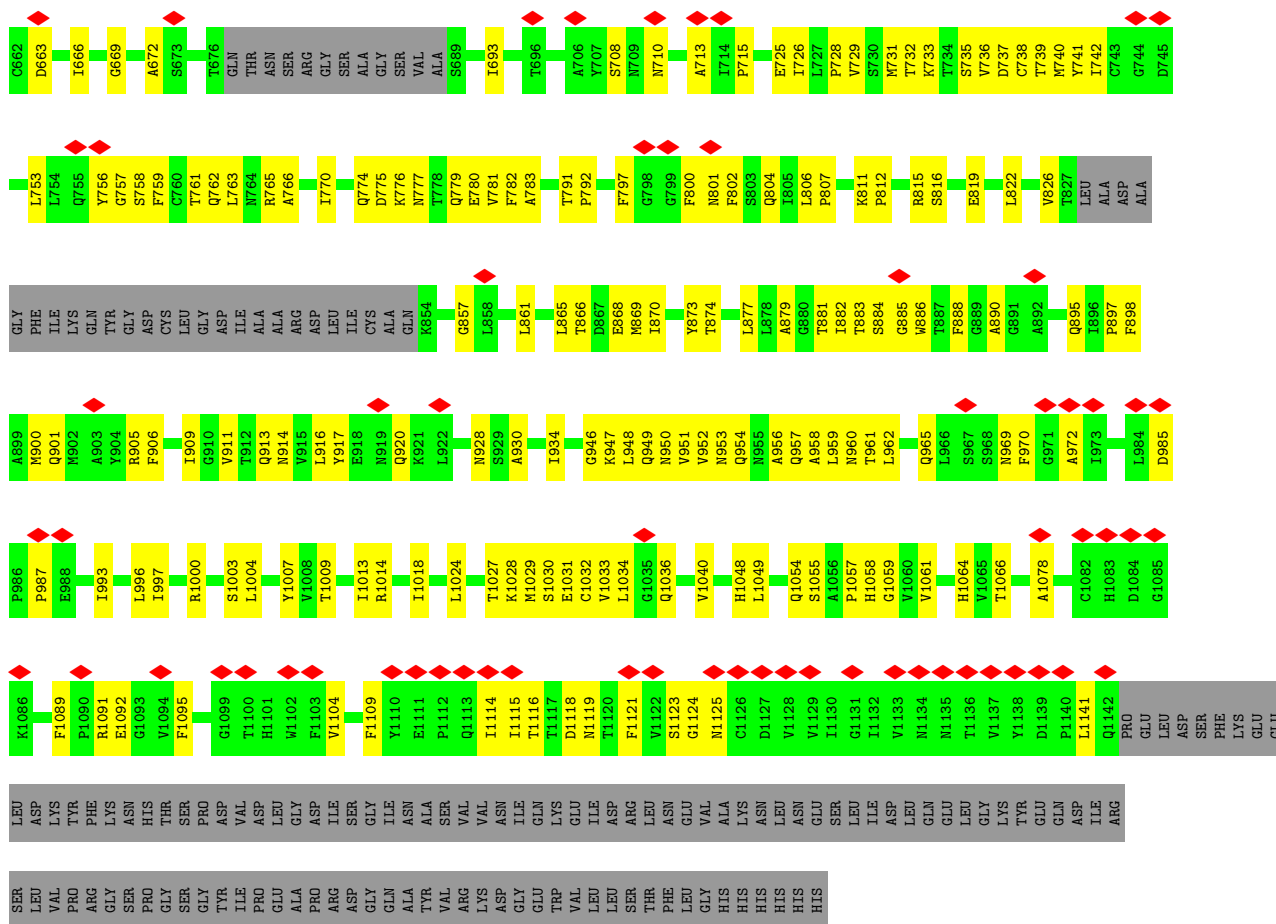
Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	106	Total	C	N	O	S	0	0
			815	514	131	167	3		
3	J	107	Total	C	N	O	S	0	0
			826	520	135	168	3		

3 Residue-property plots

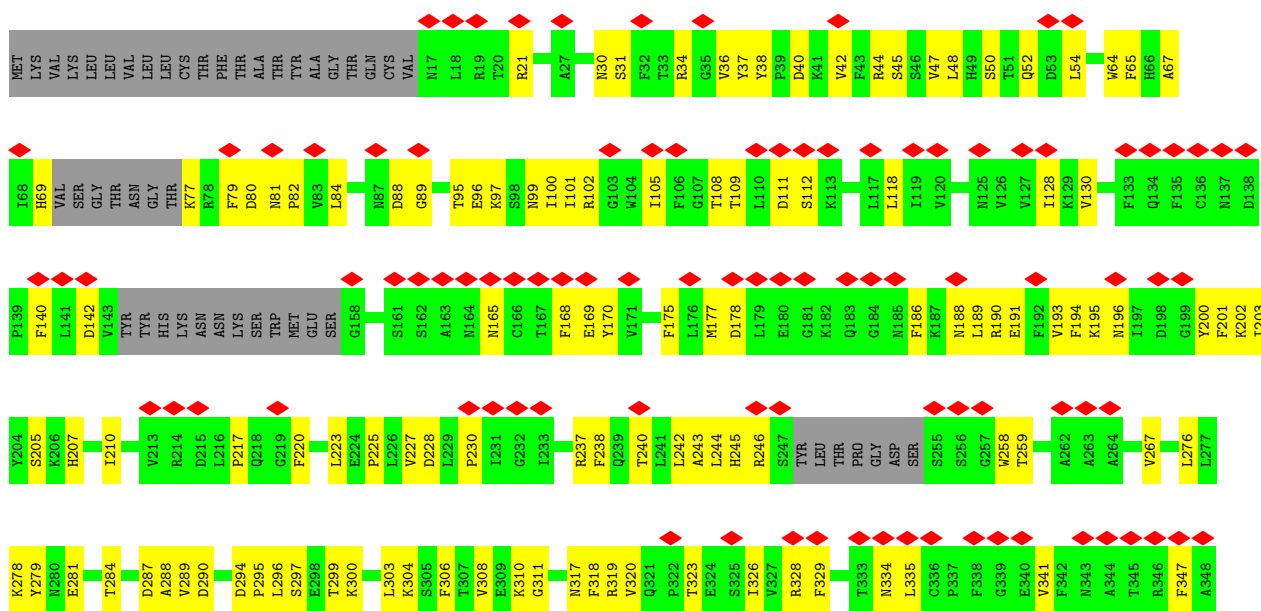
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



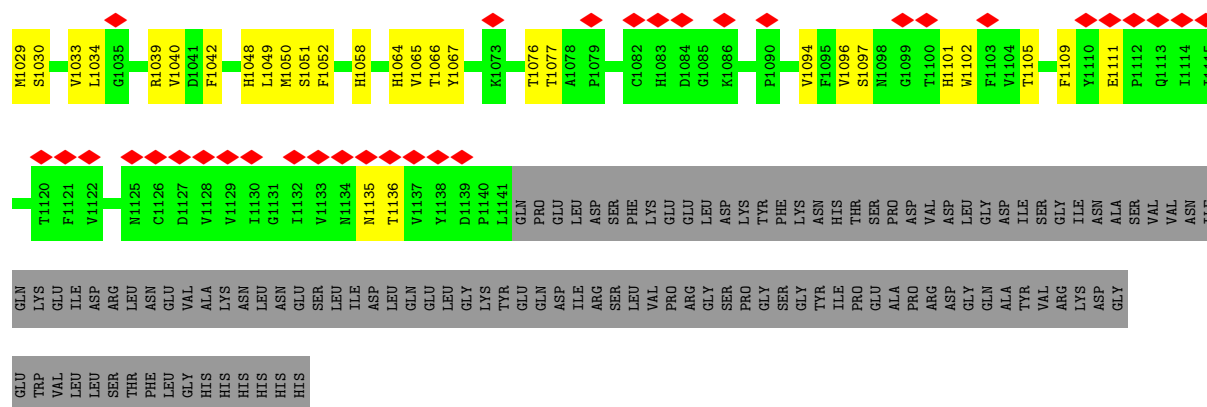


• Molecule 1: Spike glycoprotein

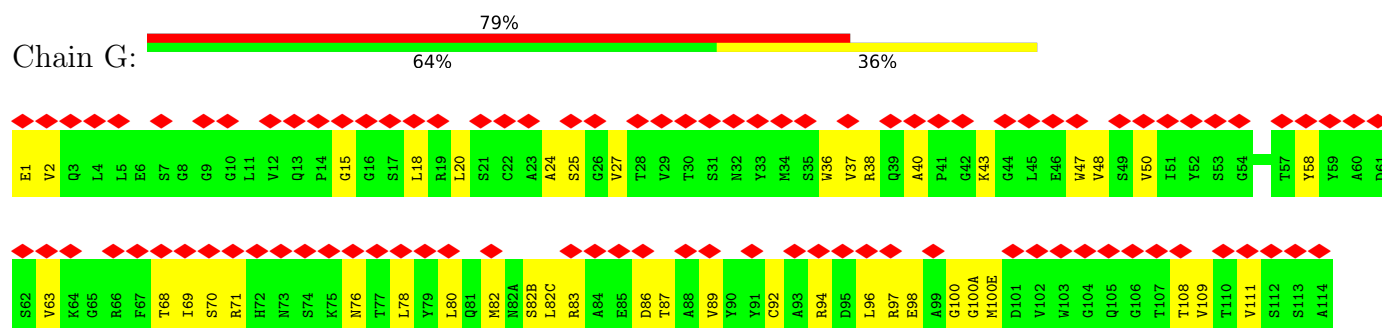




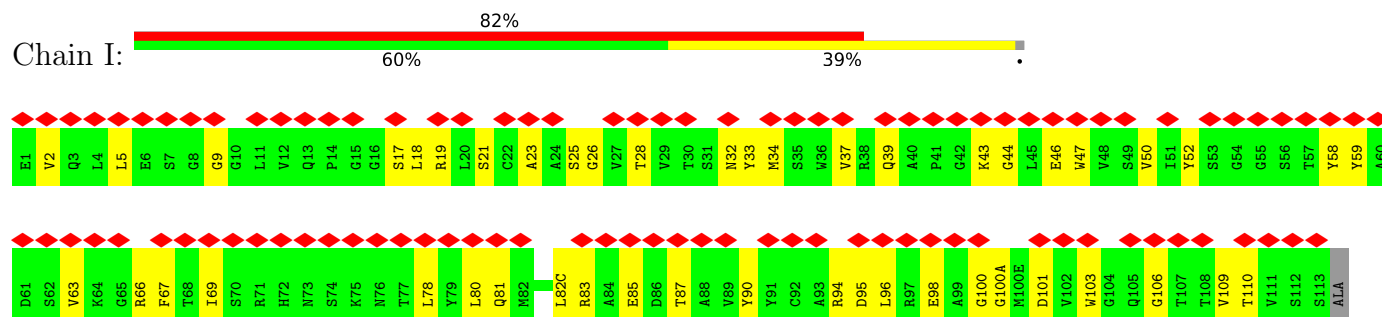
Y952	A879	K811	P728	SER	H641	S555	F491	Y421	E340	V267	G199	Q134	A67	MET
N953	G880	R815	M731	H641	S555	L492	L492	N422	E340	V267	G199	Q134	A67	LYS
N954	I881	S816	T732	F643	L560	Q493	Q493	Y423	T345	Y269	Y200	F135	I68	VAL
N955	I882	F817	K733	F643	F561	S494	S494	Q431	A348	R273	K201	C136	H69	LYS
Q957	S864	F818	T734	F643	F562	Y495	Y495	C432	S349	T274	I203	N137	SER	LEU
A958	G885	F819				Q496	Q496	C433	V350	F275	Y204	D138	GLY	LEU
L959	F888	L822	C738	H655	F565	Q498	Q498	C434	V351	L277	K206	F140	THR	VAL
N960	A893	K825	T739	H656	R567	F497	F497	C435	A352	K278	H207	L141	GLY	LEU
L962	L894	T826	W740	D568	N567	T500	T500	N436	W353			L142	THR	LEU
N963	Q895	T827	W741	I569	A570	N501	N501	N437	S359	E281	I210	Y143	CYS	CYS
Q965	I896	D663	C743	D663	D571	G502	G502	S438	S359			Y144	THR	PHE
L966	F897	P665	W745	P665	D571	G503	G503	N439	N360	D287	L216	Y145	THR	THR
S967	F898	I666	D745	I666	A575	G504	G504	N440	C361	A288	Q217	H146	ALA	ALA
N968	Q901	L670	E748	L670	A575	G505	G505	K444	A363	V289	G219	K147	TYR	TYR
F970	M902	C671	L752	C671	L582	G506	G506	V445	D364	D290	F220	N148	GLY	GLY
Q971	A903	S673	L753	S673	F583	G507	G507	G446	V367	C291		N149	THR	THR
N972	Y904	Y674	L754	Y674	I584	G508	G508	G447	L368	A292	L226	K150	GLN	GLN
L973	R905	Q675	Q755	Q675	T588	G509	G509	G447	Y369	L293	V227	S151	VAL	VAL
N977	F906	T676	W756	T676	P589	G510	G510	N448	N370	P295	D228	W152	ASN	ASN
Q978	G908	Q676	F759	Q676	C590	G511	G511	Y449	Y369	D294	V227	E154	VAL	VAL
N979	L909	Q677	C760	Q677	C590	G512	G512	N450	S371	S297	P230	E154	LEU	LEU
Q980	G910	Q678	T761	Q678	F592	G513	G513	Y451	A372	T299	I231	S155	ARG	ARG
N981	V911	Q679	Q762	Q679	F592	G514	G514	R452	S373	E298	G232	GLY	T20	T20
Q982	T912	Q680	L763	Q680	T599	G515	G515	Y453	F374	L303	I233	VAL	R21	R21
N983	Q913	Q681	M764	Q681	P600	G516	G516	R454	Y380	F306	N234	SER	Q22	Q22
L984	N914	Q682	R765	Q682	G601	G517	G517	L455	Y380	T307	T236	SER	L24	L24
N985	Q915	Q683	R766	Q683	G601	G518	G518	L456	K386	V308	G237	ALA	P25	P25
P986	L916	Q684	G769	Q684	V608	G519	G519	R457	L390	E309	F238	ASN	Q26	Q26
N987	Q917	Q685	W770	Q685	L611	G520	G520	K458	C391	K310	Q239	C166	A27	A27
Q988	E918	Q686	A771	Q686	V615	G521	G521	N459	F392	Y313	T240	I167	Y28	Y28
N989	N919	Q687	E772	Q687	N616	G522	G522	N460	T393	Q314	L241	F168	T29	T29
Q992	Q920	Q688	W773	Q688	N616	G523	G523	N460	A397	N317	L242	E169	G35	G35
N994	A924	Q689	D775	Q689	C617	G524	G524	N460	D398	F318	L242	E169	V36	V36
L995	N928	Q690	K776	Q690	T618	G525	G525	N460	R466	R319	A243	Y170	D40	D40
N996	S929	Q691	T778	Q691	E619	G526	G526	N460	S399	V320	L244	V171	K41	K41
Q998	A930	Q692	Q779	Q692	V620	G527	G527	N460	F400	Q321	H245	S172	V42	V42
L1000	I934	Q693	W780	Q693	PRO	G528	G528	N460	V401	P322	R246	Q173	F43	F43
N1004	L338	Q694	A783	Q694	VAL	G529	G529	N460	I402	T323	S247	L176	R44	R44
Q1005	S939	Q695	W789	Q695	ALA	G530	G530	N460	G404	G325	THR	M177	S46	S46
N1006	E868	Q696	T789	Q696	ALA	G531	G531	N460	D405	I326	THR	D178	V47	V47
Y1007	M869	Q697	G798	Q697	ASP	G532	G532	N460	E406	V327	GLY	L179	S50	S50
V1008	T941	Q698	G798	Q698	GLN	G533	G533	N460	V407	R328	ASP	E180	T51	T51
N1014	Q942	Q699	A713	Q699	THR	G534	G534	N460	Q408	P330	SER	G181	Q52	Q52
L1018	S943	Q700	W714	Q700	THR	G535	G535	N460	Q409	N331	S255	K182	D53	D53
N1019	R873	Q701	T715	Q701	THR	G536	G536	N460	I410	I332	S256	Q183	L54	L54
L945	T875	Q702	F718	Q702	TRP	G537	G537	N460	A411	T333	G257	G184	F55	F55
Q946	R876	Q703	F718	Q703	ARG	G538	G538	N460	P412	C336	W258	N125	L56	L56
N947	S877	Q704	E725	Q704	VAL	G539	G539	N460	Q413	P337	T259	N126	P57	P57
L948	A876	Q705	I726	Q705	TYR	G540	G540	N460	Q414		G261	V127	L57	L57
N949	L877	Q706	L727	Q706	SER	G541	G541	N460	T415		E191	K129	N61	N61
Q950	D808	Q707		Q707	THR	G542	G542	N460	G416		A262	F192	H66	H66
N951	V951	Q708		Q708	GLY	G543	G543	N460	K417		A263	V193		
		Q709		Q709		G544	G544	N460	E484		A264	F194		
		Q710		Q710		G545	G545	N460	I418		Y265	K195		
		Q711		Q711		G546	G546	N460	A419		Y266	I197		
		Q712		Q712		G547	G547	N460	D420			D198		



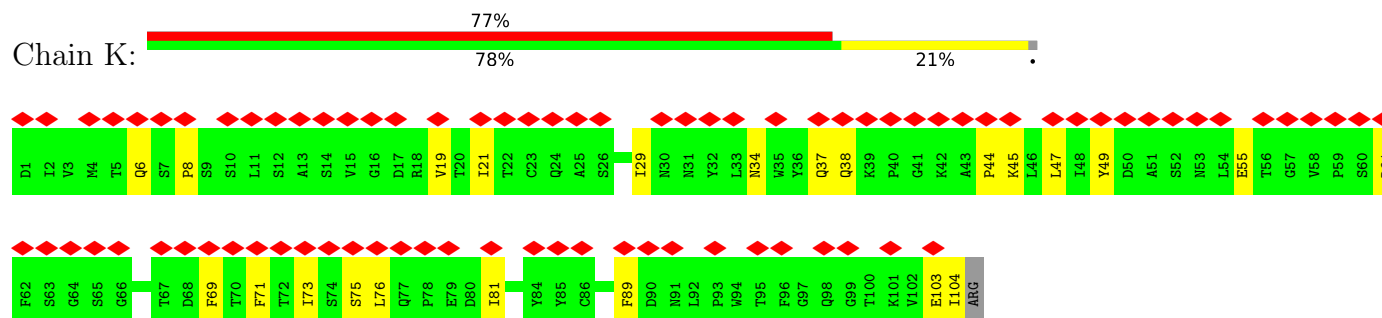
• Molecule 2: Fab heavy chain of JE-5C



• Molecule 2: Fab heavy chain of JE-5C

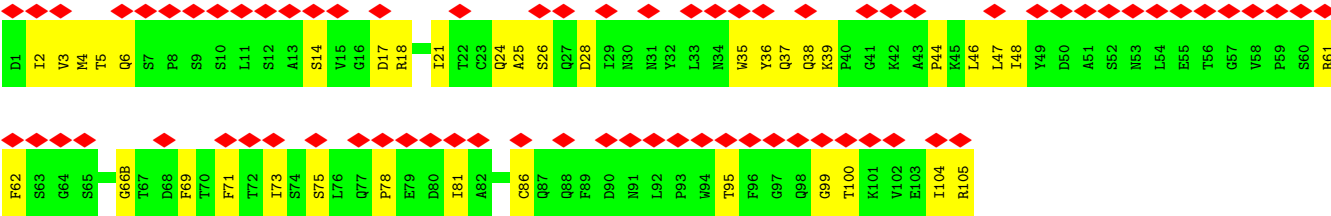


• Molecule 3: Fab light chain of JE-5C



• Molecule 3: Fab light chain of JE-5C





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180312	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 ($e^-/\text{\AA}^2$)	1.1	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0034	Depositor
Map size (Å)	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	0.15	0/8323	0.37	0/11321
1	C	0.15	0/8205	0.37	0/11160
1	D	0.17	0/8287	0.39	0/11271
2	G	0.13	0/905	0.37	0/1228
2	I	0.12	0/900	0.36	0/1221
3	J	0.10	0/845	0.34	0/1151
3	K	0.12	0/834	0.38	0/1137
All	All	0.15	0/28299	0.38	0/38489

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8138	0	7957	304	0
1	C	8023	0	7814	265	0
1	D	8102	0	7896	297	0
2	G	889	0	857	36	0
2	I	884	0	852	40	0
3	J	826	0	787	28	0
3	K	815	0	774	17	0
All	All	27677	0	26937	918	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 17.

All (918) 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:A:593:GLY:HA3	1:A:613:GLN:O	1.37	1.24
1:A:142:ASP:HB2	1:A:258:TRP:CZ3	1.86	1.09
1:D:332:ILE:HG22	1:D:333:THR:H	1.13	1.07
1:A:142:ASP:OD2	1:A:258:TRP:CZ2	2.12	1.02
1:C:140:PHE:CE1	1:C:142:ASP:HB3	1.96	1.00
1:A:142:ASP:HB2	1:A:258:TRP:CE3	2.01	0.95
1:D:332:ILE:HG22	1:D:333:THR:N	1.78	0.93
1:A:190:ARG:HH11	1:A:207:HIS:HB2	1.39	0.87
1:C:779:GLN:HA	1:C:783:ALA:HB3	1.55	0.87
1:C:140:PHE:HE1	1:C:142:ASP:HB3	1.35	0.86
1:D:725:GLU:OE2	1:D:1028:LYS:NZ	2.09	0.84
2:I:90:TYR:O	2:I:106:GLY:HA2	1.77	0.84
1:A:951:VAL:O	1:A:955:ASN:ND2	2.10	0.83
1:A:954:GLN:O	1:A:958:ALA:N	2.12	0.83
1:C:319:ARG:HH21	1:D:740:MET:HB2	1.43	0.82
1:D:763:LEU:HD22	1:D:1008:VAL:HG11	1.61	0.82
1:C:389:ASP:OD2	1:C:542:ASN:ND2	2.15	0.80
1:A:95:THR:HG22	1:A:186:PHE:HB2	1.63	0.79
2:G:87:THR:HA	2:G:109:VAL:O	1.82	0.79
1:D:332:ILE:CG2	1:D:333:THR:H	1.93	0.79
1:D:903:ALA:HB2	1:D:916:LEU:HD11	1.64	0.79
2:G:2:VAL:HA	2:G:25:SER:O	1.84	0.77
1:D:44:ARG:HG3	1:D:47:VAL:HG21	1.66	0.77
1:D:725:GLU:OE1	1:D:1064:HIS:NE2	2.17	0.77
1:D:957:GLN:HA	1:D:960:ASN:HB3	1.66	0.77
1:D:865:LEU:HD13	1:D:873:TYR:HE2	1.51	0.77
1:D:731:MET:H	1:D:774:GLN:HG2	1.50	0.76
1:D:965:GLN:HG2	1:D:970:PHE:HZ	1.50	0.76
2:I:2:VAL:HA	2:I:25:SER:O	1.84	0.76
1:D:777:ASN:O	1:D:781:VAL:N	2.16	0.75
1:D:779:GLN:HA	1:D:783:ALA:HB3	1.68	0.75
1:A:575:ALA:HB1	1:A:584:ILE:HD11	1.69	0.74
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.20	0.74
1:C:713:ALA:HB3	1:D:895:GLN:H	1.52	0.74
1:C:412:PRO:HB3	1:C:429:PHE:HB3	1.70	0.74
1:A:953:ASN:O	1:A:956:ALA:HB3	1.87	0.74
1:A:919:ASN:HB3	1:A:922:LEU:HD13	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ALA:HB1	1:D:177:MET:HB2	1.68	0.74
1:A:726:ILE:HG22	1:A:948:LEU:HD13	1.70	0.73
1:D:924:ALA:O	1:D:928:ASN:ND2	2.21	0.73
1:D:880:GLY:O	1:D:885:GLY:N	2.20	0.73
1:A:97:LYS:HB3	1:A:186:PHE:HA	1.70	0.72
1:C:879:ALA:O	1:C:883:THR:OG1	2.05	0.72
1:A:358:ILE:HB	1:A:395:VAL:HB	1.71	0.72
1:D:393:THR:HG21	1:D:518:LEU:H	1.54	0.72
3:J:38:GLN:HG3	3:J:44:PRO:HG3	1.72	0.71
1:D:295:PRO:HB2	1:D:608:VAL:HG11	1.71	0.71
1:C:140:PHE:CD1	1:C:142:ASP:HB3	2.26	0.71
1:C:389:ASP:HB2	1:C:547:THR:HG22	1.72	0.71
1:A:48:LEU:O	1:A:304:LYS:NZ	2.23	0.71
1:D:951:VAL:HA	1:D:954:GLN:HG2	1.73	0.71
3:K:76:LEU:HD21	3:K:104:ILE:HG12	1.73	0.71
1:D:130:VAL:HB	1:D:168:PHE:HB3	1.73	0.70
1:D:496:GLY:O	1:D:501:ASN:ND2	2.22	0.70
1:C:770:ILE:HG22	1:C:774:GLN:HE22	1.56	0.70
1:C:1027:THR:O	1:C:1031:GLU:HB2	1.90	0.70
2:I:19:ARG:NH2	2:I:21:SER:OG	2.23	0.70
1:A:950:ASN:O	1:A:954:GLN:N	2.22	0.70
1:C:952:VAL:O	1:C:956:ALA:N	2.19	0.70
1:A:897:PRO:HB3	1:D:709:ASN:HA	1.71	0.70
1:C:770:ILE:O	1:C:774:GLN:NE2	2.25	0.69
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.21	0.69
1:D:454:ARG:NH1	1:D:469:SER:O	2.26	0.69
3:K:19:VAL:HB	3:K:73:ILE:HB	1.72	0.69
1:A:244:LEU:HD23	1:A:258:TRP:HB2	1.74	0.69
2:I:37:VAL:HG22	2:I:47:TRP:HA	1.73	0.69
1:A:965:GLN:HA	1:A:968:SER:HB2	1.73	0.69
1:C:454:ARG:NH1	1:C:467:ASP:O	2.27	0.68
1:C:728:PRO:HG3	1:C:951:VAL:HG21	1.74	0.68
1:A:189:LEU:HD12	1:A:210:ILE:HD13	1.75	0.68
1:A:341:VAL:HG21	1:A:358:ILE:HD11	1.75	0.68
1:A:788:ILE:HG13	1:D:699:LEU:HB2	1.75	0.68
1:D:712:ILE:HB	1:D:1077:THR:HB	1.75	0.68
1:D:905:ARG:NH2	1:D:1050:MET:SD	2.67	0.68
3:J:37:GLN:HG3	3:J:47:LEU:HD22	1.74	0.68
1:C:742:ILE:HD11	1:C:1004:LEU:HD22	1.74	0.67
1:A:500:THR:HG22	2:I:82(C):LEU:HA	1.76	0.67
1:A:949:GLN:O	1:A:953:ASN:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:ALA:O	1:A:770:ILE:HD12	1.95	0.66
1:C:140:PHE:HE1	1:C:142:ASP:CB	2.07	0.66
1:C:362:VAL:HA	1:C:544:ASN:HB2	1.76	0.66
1:C:946:GLY:HA2	1:C:949:GLN:HB2	1.76	0.66
1:C:1030:SER:OG	1:A:1040:VAL:O	2.14	0.66
1:C:811:LYS:HE3	1:C:812:PRO:HD2	1.78	0.66
1:A:498:GLN:HA	2:I:83:ARG:HH21	1.60	0.66
1:C:330:PRO:HA	1:C:580:GLN:HA	1.77	0.66
1:A:798:GLY:O	1:A:920:GLN:NE2	2.29	0.66
1:D:726:ILE:O	1:D:947:LYS:HD2	1.96	0.66
1:D:950:ASN:O	1:D:954:GLN:N	2.18	0.65
1:C:341:VAL:HG21	1:C:356:LYS:HE3	1.77	0.65
1:A:825:LYS:HE2	1:A:938:LEU:HD12	1.79	0.65
1:D:106:PHE:HD2	1:D:235:ILE:HG21	1.61	0.65
1:D:129:LYS:HE2	1:D:169:GLU:HG3	1.77	0.65
1:C:244:LEU:HA	1:C:260:ALA:HB2	1.78	0.65
1:C:756:TYR:HA	1:A:970:PHE:HA	1.77	0.65
2:I:94:ARG:NH1	2:I:95:ASP:O	2.30	0.65
1:D:575:ALA:HB1	1:D:584:ILE:HD11	1.78	0.65
1:A:1020:ALA:O	1:A:1024:LEU:HB2	1.97	0.65
1:C:1009:THR:O	1:C:1013:ILE:HG13	1.97	0.65
1:A:855:PHE:HB3	1:D:589:PRO:HG3	1.79	0.65
1:D:955:ASN:O	1:D:958:ALA:HB3	1.97	0.65
1:C:106:PHE:HB3	1:C:235:ILE:HG21	1.77	0.64
1:C:358:ILE:HB	1:C:395:VAL:HB	1.79	0.64
1:C:44:ARG:NH2	1:C:279:TYR:OH	2.30	0.64
1:D:551:VAL:HG23	1:D:590:CYS:HB3	1.79	0.64
1:C:726:ILE:HB	1:C:947:LYS:HB3	1.80	0.64
1:A:614:GLY:N	1:A:647:ALA:O	2.22	0.64
1:D:67:ALA:O	1:D:262:ALA:HA	1.96	0.64
1:C:791:THR:HG21	1:C:806:LEU:HD22	1.78	0.64
1:A:598:ILE:HG21	1:A:672:ALA:HB3	1.78	0.63
3:J:5:THR:O	3:J:24:GLN:NE2	2.30	0.63
1:D:769:GLY:O	1:D:773:GLU:HG2	1.99	0.63
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.81	0.63
1:C:884:SER:HA	1:A:707:TYR:HE2	1.62	0.63
3:J:38:GLN:HA	3:J:44:PRO:HA	1.81	0.63
1:A:130:VAL:HG22	1:A:168:PHE:HB3	1.80	0.63
1:A:972:ALA:HA	1:A:995:ARG:HH21	1.64	0.63
1:C:801:ASN:O	1:C:928:ASN:ND2	2.31	0.63
2:I:32:ASN:OD1	2:I:94:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.81	0.62
1:A:318:PHE:H	1:A:594:GLY:HA2	1.62	0.62
2:I:66:ARG:HH11	2:I:67:PHE:HE1	1.45	0.62
1:A:237:ARG:NH1	1:A:237:ARG:HA	2.14	0.62
1:C:969:ASN:HB3	1:C:972:ALA:HB3	1.81	0.62
1:C:758:SER:HG	1:C:762:GLN:HE22	1.44	0.62
2:I:87:THR:HA	2:I:109:VAL:O	1.99	0.62
1:C:31:SER:O	1:C:59:PHE:HA	2.00	0.62
2:G:37:VAL:HG11	2:G:100(E):MET:HE1	1.82	0.62
1:D:437:ASN:HD21	1:D:506:GLN:HB3	1.63	0.61
3:J:3:VAL:O	3:J:26:SER:OG	2.18	0.61
1:A:900:MET:HE1	1:D:1094:VAL:HG11	1.80	0.61
1:C:364:ASP:OD1	1:C:530:SER:N	2.33	0.61
1:C:563:GLN:HA	1:D:41:LYS:HB3	1.81	0.61
1:D:327:VAL:H	1:D:531:THR:HG22	1.65	0.61
1:C:290:ASP:OD1	1:C:291:CYS:N	2.34	0.61
1:A:100:ILE:HG22	1:A:242:LEU:HD12	1.81	0.61
2:I:28:THR:O	2:I:32:ASN:ND2	2.26	0.61
1:D:980:ILE:HD12	1:D:996:LEU:HD11	1.82	0.61
2:G:100:GLY:HA2	3:K:34:ASN:HD21	1.63	0.61
1:A:89:GLY:HA2	1:A:194:PHE:O	1.99	0.61
3:J:6:GLN:NE2	3:J:86:CYS:SG	2.69	0.61
1:C:758:SER:O	1:C:761:THR:OG1	2.17	0.61
1:C:1116:THR:HG23	1:C:1118:ASP:H	1.66	0.61
1:C:1141:LEU:HD21	1:A:1141:LEU:HD21	1.82	0.61
1:C:742:ILE:HG21	1:C:997:ILE:HG23	1.81	0.60
1:C:792:PRO:HG3	1:A:706:ALA:HB2	1.83	0.60
1:C:758:SER:OG	1:C:762:GLN:NE2	2.25	0.60
1:D:819:GLU:HA	1:D:822:LEU:HD12	1.82	0.60
3:J:21:ILE:HG12	3:J:100:THR:HG21	1.81	0.60
1:D:1004:LEU:O	1:D:1008:VAL:HG12	2.01	0.60
3:J:14:SER:HA	3:J:105:ARG:H	1.66	0.60
1:C:296:LEU:HB2	1:C:608:VAL:HG21	1.83	0.60
1:C:374:PHE:HD1	1:C:436:TRP:HB3	1.67	0.60
2:I:59:TYR:HB3	2:I:63:VAL:HG23	1.84	0.60
2:G:69:ILE:HD11	2:G:78:LEU:HD21	1.84	0.60
2:I:2:VAL:HG12	2:I:26:GLY:HA3	1.83	0.60
1:D:290:ASP:OD1	1:D:291:CYS:N	2.33	0.60
1:D:336:CYS:HA	1:D:361:CYS:HB2	1.84	0.60
1:D:332:ILE:CG2	1:D:333:THR:N	2.53	0.59
1:D:374:PHE:HA	1:D:436:TRP:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:PHE:CE1	1:C:142:ASP:CB	2.80	0.59
1:A:902:MET:HE1	1:A:920:GLN:HG3	1.84	0.59
1:D:487:ASN:OD1	2:G:94:ARG:NH2	2.34	0.59
1:C:616:ASN:HA	1:C:644:GLN:HE22	1.67	0.59
1:C:736:VAL:HG11	1:C:1004:LEU:HD11	1.85	0.59
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.84	0.59
1:A:1014:ARG:O	1:A:1018:ILE:HG12	2.02	0.59
1:D:865:LEU:HD13	1:D:873:TYR:CE2	2.36	0.59
1:C:740:MET:SD	1:A:319:ARG:HD2	2.43	0.59
1:C:895:GLN:HA	1:A:707:TYR:CE2	2.37	0.59
1:A:697:MET:HE2	1:A:699:LEU:HA	1.85	0.59
1:D:309:GLU:O	1:D:313:TYR:OH	2.17	0.59
1:A:726:ILE:HG12	1:A:945:LEU:HA	1.85	0.59
1:A:726:ILE:CG2	1:A:948:LEU:HD13	2.32	0.59
1:D:877:LEU:O	1:D:881:THR:HG23	2.02	0.59
2:G:27:VAL:O	2:G:76:ASN:ND2	2.36	0.59
1:A:424:LYS:HE2	1:A:460:ASN:HB3	1.84	0.59
1:A:310:LYS:HE2	1:A:664:ILE:HD11	1.84	0.59
1:D:527:PRO:O	1:D:530:SER:N	2.36	0.59
1:D:728:PRO:HG3	1:D:951:VAL:HG21	1.84	0.59
1:A:976:VAL:HG22	1:A:978:ASN:H	1.67	0.58
1:D:866:THR:HG22	1:D:868:GLU:H	1.69	0.58
3:K:37:GLN:HE21	3:K:45:LYS:HD3	1.67	0.58
1:A:44:ARG:CZ	1:D:567:ARG:HH21	2.16	0.58
1:D:738:CYS:HB2	1:D:753:LEU:HD21	1.84	0.58
3:J:18:ARG:HA	3:J:73:ILE:O	2.02	0.58
1:D:950:ASN:OD1	1:D:951:VAL:N	2.36	0.58
1:D:457:ARG:NH1	1:D:459:SER:O	2.36	0.58
1:A:101:ILE:HA	1:A:242:LEU:HD13	1.85	0.58
1:A:1089:PHE:HB2	1:A:1121:PHE:HB2	1.85	0.58
1:A:669:GLY:O	1:A:697:MET:N	2.23	0.58
1:A:108:THR:HG23	1:A:109:THR:HG23	1.86	0.58
1:C:62:VAL:HG12	1:C:268:GLY:HA2	1.86	0.57
1:A:869:MET:HE2	1:D:699:LEU:HD21	1.86	0.57
1:A:969:ASN:HB3	1:A:972:ALA:H	1.68	0.57
1:D:905:ARG:NH1	1:D:1049:LEU:O	2.37	0.57
1:A:592:PHE:HB2	1:A:615:VAL:HA	1.86	0.57
1:A:758:SER:O	1:A:761:THR:HG22	2.04	0.57
1:A:865:LEU:HD13	1:A:873:TYR:CE2	2.38	0.57
1:C:1104:VAL:HG11	1:C:1119:ASN:HB3	1.87	0.57
1:C:278:LYS:HB2	1:C:306:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:881:THR:HG23	1:C:882:ILE:HD12	1.84	0.57
1:A:769:GLY:O	1:A:773:GLU:HG3	2.05	0.57
1:A:858:LEU:HD13	1:A:959:LEU:HD23	1.85	0.57
1:A:964:LYS:O	1:A:968:SER:N	2.32	0.57
1:D:202:LYS:HD2	1:D:228:ASP:HB2	1.85	0.57
1:D:916:LEU:O	1:D:920:GLN:HG3	2.05	0.57
1:A:1094:VAL:O	1:A:1104:VAL:HA	2.04	0.57
1:A:142:ASP:HB2	1:A:258:TRP:CH2	2.36	0.57
1:C:271:GLN:HB3	1:C:273:ARG:HE	1.69	0.57
1:C:318:PHE:HZ	1:C:619:GLU:HB2	1.69	0.56
1:C:731:MET:HG2	1:C:732:THR:H	1.70	0.56
1:C:961:THR:O	1:C:965:GLN:N	2.38	0.56
1:C:1030:SER:OG	1:A:1040:VAL:HG13	2.05	0.56
1:A:102:ARG:HG3	1:A:243:ALA:HB2	1.85	0.56
1:A:659:SER:HB3	1:A:698:SER:HB2	1.86	0.56
1:D:804:GLN:HG3	1:D:817:PHE:HD2	1.70	0.56
1:D:1024:LEU:HG	1:D:1028:LYS:HE3	1.87	0.56
1:C:132:GLU:O	1:C:134:GLN:NE2	2.39	0.56
1:D:477:SER:HB3	2:G:1:GLU:HB3	1.87	0.56
2:G:98:GLU:O	2:G:98:GLU:HG3	2.05	0.56
1:D:204:TYR:HA	1:D:225:PRO:HA	1.87	0.56
1:C:56:LEU:HB2	1:C:91:TYR:CE1	2.40	0.56
1:C:327:VAL:HB	1:C:530:SER:HA	1.86	0.56
1:A:165:ASN:ND2	1:D:464:PHE:O	2.39	0.56
1:D:770:ILE:HG23	1:D:774:GLN:HE22	1.69	0.56
1:C:731:MET:H	1:C:774:GLN:HG2	1.71	0.56
1:C:874:THR:OG1	1:C:1055:SER:OG	2.23	0.56
1:C:1124:GLY:N	1:D:914:ASN:OD1	2.38	0.56
1:C:742:ILE:HG22	1:C:997:ILE:HD12	1.85	0.56
1:D:454:ARG:HH12	1:D:470:THR:HA	1.71	0.56
1:D:993:ILE:O	1:D:997:ILE:HG13	2.06	0.56
1:A:818:ILE:O	1:A:822:LEU:HG	2.06	0.56
1:D:734:THR:HB	1:D:858:LEU:HD11	1.87	0.56
1:C:885:GLY:HA2	1:C:901:GLN:NE2	2.21	0.56
1:C:877:LEU:HD22	1:C:1029:MET:HE2	1.88	0.56
1:C:1024:LEU:HG	1:C:1028:LYS:HE2	1.88	0.56
1:A:328:ARG:HB2	1:A:579:PRO:HD2	1.88	0.56
1:D:742:ILE:HG21	1:D:997:ILE:HG23	1.88	0.56
1:C:1114:ILE:O	1:C:1119:ASN:ND2	2.37	0.55
1:A:642:VAL:HG22	1:A:651:ILE:HG22	1.88	0.55
1:A:741:TYR:HD2	1:A:742:ILE:HG13	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:741:TYR:HD2	1:D:742:ILE:HG13	1.71	0.55
1:C:317:ASN:HD22	1:C:317:ASN:C	2.14	0.55
1:A:54:LEU:HD13	1:A:88:ASP:HB2	1.87	0.55
1:D:81:ASN:OD1	1:D:239:GLN:NE2	2.39	0.55
1:D:1039:ARG:HD3	1:D:1042:PHE:CG	2.41	0.55
1:C:21:ARG:HH21	1:C:79:PHE:HE2	1.54	0.55
1:D:104:TRP:CD1	1:D:240:THR:HG22	2.42	0.55
1:C:959:LEU:HD23	1:C:962:LEU:HD12	1.88	0.55
1:D:102:ARG:NH1	1:D:141:LEU:O	2.40	0.55
2:I:100(A):GLY:O	3:J:36:TYR:OH	2.21	0.55
1:C:317:ASN:O	1:C:317:ASN:ND2	2.36	0.55
1:C:355:ARG:HD3	1:C:356:LYS:N	2.21	0.55
1:C:453:TYR:HE1	2:I:98:GLU:HG3	1.72	0.55
1:A:736:VAL:HG11	1:A:1004:LEU:HD21	1.89	0.55
1:C:882:ILE:HG23	1:C:898:PHE:CD1	2.42	0.55
1:C:895:GLN:HB3	1:A:713:ALA:HB2	1.88	0.55
1:A:971:GLY:O	1:A:995:ARG:NH2	2.39	0.55
1:A:47:VAL:H	1:A:279:TYR:HB2	1.72	0.55
1:A:499:PRO:HD2	2:I:83:ARG:HE	1.72	0.55
1:C:502:GLY:H	3:J:28:ASP:HB3	1.72	0.55
1:A:590:CYS:SG	1:A:591:SER:N	2.79	0.55
1:D:775:ASP:O	1:D:778:THR:OG1	2.23	0.55
3:J:21:ILE:HD12	3:J:71:PHE:HD2	1.72	0.55
1:A:377:PHE:HD1	1:A:434:ILE:HG12	1.71	0.54
1:A:961:THR:HA	1:A:964:LYS:HB2	1.88	0.54
1:D:815:ARG:HD3	1:D:819:GLU:OE2	2.06	0.54
1:A:366:SER:H	1:A:388:ASN:HD21	1.56	0.54
1:A:909:ILE:HD12	1:A:1049:LEU:HD22	1.90	0.54
1:A:1032:CYS:HB3	1:A:1048:HIS:CE1	2.42	0.54
2:G:15:GLY:HA2	2:G:82(B):SER:HA	1.90	0.54
1:D:776:LYS:O	1:D:780:GLU:N	2.41	0.54
1:C:802:PHE:HD1	1:C:928:ASN:HD21	1.56	0.54
1:D:543:PHE:HB2	1:D:546:LEU:HB2	1.88	0.54
1:C:276:LEU:HD11	1:C:301:CYS:HA	1.90	0.54
1:C:612:TYR:O	1:C:648:GLY:HA3	2.08	0.54
1:A:1083:HIS:CE1	1:A:1137:VAL:H	2.26	0.54
1:D:811:LYS:NZ	1:D:815:ARG:O	2.40	0.54
3:K:81:ILE:HG23	3:K:103:GLU:HA	1.88	0.54
2:I:17:SER:HB2	2:I:81:GLN:NE2	2.23	0.54
1:A:105:ILE:HG12	1:A:118:LEU:HG	1.90	0.54
1:A:142:ASP:CG	1:A:258:TRP:CH2	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:GLN:HG2	1:C:274:THR:OG1	2.08	0.53
1:D:323:THR:HG22	1:D:324:GLU:HG3	1.90	0.53
1:C:58:PHE:HB2	1:C:293:LEU:HD22	1.90	0.53
1:A:612:TYR:O	1:A:648:GLY:HA3	2.09	0.53
1:A:725:GLU:HG2	1:A:727:LEU:HG	1.90	0.53
1:D:854:LYS:HD3	1:D:860:VAL:HG12	1.90	0.53
2:G:18:LEU:HB3	2:G:82:MET:HE3	1.89	0.53
1:A:295:PRO:HB2	1:A:608:VAL:HG11	1.91	0.53
1:D:190:ARG:HG2	1:D:207:HIS:CD2	2.44	0.53
1:D:326:ILE:HD12	1:D:539:VAL:HG21	1.91	0.53
1:D:642:VAL:HG22	1:D:651:ILE:HG22	1.91	0.53
2:G:86:ASP:HB2	2:G:111:VAL:HG21	1.90	0.53
1:C:913:GLN:NE2	1:C:917:TYR:OH	2.41	0.53
1:C:1032:CYS:HB3	1:C:1048:HIS:CE1	2.44	0.53
1:A:95:THR:HG23	1:A:210:ILE:HD11	1.91	0.53
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.42	0.53
2:I:101:ASP:HA	3:J:46:LEU:HB3	1.90	0.53
1:D:759:PHE:O	1:D:763:LEU:HG	2.08	0.53
1:C:309:GLU:O	1:C:313:TYR:OH	2.23	0.53
1:D:44:ARG:CG	1:D:47:VAL:HG21	2.39	0.53
1:D:599:THR:HB	1:D:608:VAL:HG22	1.91	0.53
1:C:1029:MET:O	1:C:1033:VAL:HB	2.09	0.52
1:A:50:SER:H	1:A:304:LYS:HE2	1.73	0.52
1:A:191:GLU:O	1:A:205:SER:HA	2.09	0.52
1:A:196:ASN:HD22	1:A:201:PHE:HD1	1.57	0.52
1:A:326:ILE:HB	1:A:541:PHE:HA	1.89	0.52
1:A:950:ASN:HA	1:A:953:ASN:HB2	1.91	0.52
1:C:1024:LEU:O	1:C:1028:LYS:HG3	2.09	0.52
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.90	0.52
1:A:522:ALA:O	1:A:544:ASN:ND2	2.43	0.52
1:A:985:ASP:O	1:A:989:ALA:N	2.33	0.52
1:D:431:GLY:HA2	1:D:515:PHE:HD1	1.73	0.52
1:D:671:CYS:SG	1:D:697:MET:HB3	2.49	0.52
1:D:877:LEU:HD23	1:D:888:PHE:HE2	1.74	0.52
1:A:1024:LEU:HG	1:A:1028:LYS:HZ2	1.74	0.52
1:D:275:PHE:CD1	1:D:290:ASP:HA	2.45	0.52
1:C:230:PRO:HB2	1:A:396:TYR:OH	2.10	0.52
1:C:729:VAL:H	1:C:1059:GLY:HA2	1.74	0.52
1:A:290:ASP:O	1:A:297:SER:HB2	2.10	0.52
1:A:319:ARG:NH2	1:A:591:SER:O	2.42	0.52
1:D:1105:THR:OG1	1:D:1111:GLU:N	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:66(B):GLY:H	3:J:69:PHE:HE1	1.57	0.52
1:C:275:PHE:CD1	1:C:290:ASP:HA	2.45	0.52
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.92	0.52
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.45	0.52
1:A:303:LEU:HD12	1:A:308:VAL:HG12	1.92	0.52
1:A:957:GLN:HA	1:A:960:ASN:HB2	1.91	0.52
1:D:107:GLY:O	1:D:237:ARG:HG3	2.10	0.52
1:C:616:ASN:OD1	1:C:644:GLN:NE2	2.43	0.52
1:D:776:LYS:HA	1:D:779:GLN:HB2	1.92	0.52
1:C:110:LEU:HD11	1:C:237:ARG:HH12	1.74	0.52
1:A:329:PHE:O	1:A:580:GLN:NE2	2.43	0.52
1:A:945:LEU:HB2	1:A:949:GLN:HE22	1.74	0.52
1:C:725:GLU:OE2	1:C:1064:HIS:NE2	2.42	0.52
1:A:551:VAL:HG22	1:A:588:THR:HB	1.92	0.52
1:A:873:TYR:OH	1:D:699:LEU:HD22	2.10	0.52
1:C:115:GLN:HB3	1:C:130:VAL:HG12	1.92	0.51
1:C:550:GLY:HA2	1:C:590:CYS:H	1.75	0.51
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.91	0.51
1:A:741:TYR:CE1	1:A:966:LEU:HD21	2.44	0.51
1:A:1073:LYS:NZ	1:A:1075:PHE:HE1	2.08	0.51
1:C:398:ASP:O	1:C:511:VAL:HA	2.10	0.51
1:A:142:ASP:OD2	1:A:258:TRP:CE2	2.60	0.51
1:C:454:ARG:NH2	1:C:457:ARG:HG3	2.25	0.51
1:C:708:SER:OG	1:C:710:ASN:OD1	2.28	0.51
1:A:434:ILE:O	1:A:510:VAL:HA	2.10	0.51
1:C:866:THR:O	1:C:870:ILE:N	2.33	0.51
1:A:84:LEU:HD13	1:A:267:VAL:HG11	1.91	0.51
1:D:45:SER:HB2	1:D:281:GLU:HA	1.93	0.51
1:D:380:TYR:OH	1:D:410:ILE:O	2.24	0.51
3:J:81:ILE:HD11	3:J:104:ILE:HG12	1.92	0.51
1:C:1000:ARG:O	1:C:1003:SER:OG	2.24	0.51
1:A:203:ILE:HB	1:A:227:VAL:HG23	1.92	0.51
1:C:758:SER:O	1:C:761:THR:N	2.41	0.51
1:A:300:LYS:NZ	1:A:306:PHE:O	2.40	0.51
1:A:959:LEU:HA	1:A:962:LEU:HB3	1.91	0.51
1:D:995:ARG:HG3	1:D:995:ARG:HH11	1.75	0.51
1:C:950:ASN:OD1	1:C:951:VAL:N	2.44	0.51
1:A:38:TYR:HB2	1:A:225:PRO:HD3	1.92	0.51
1:C:55:PHE:O	1:C:270:LEU:HA	2.10	0.51
1:C:1091:ARG:HD2	1:C:1121:PHE:HB2	1.92	0.51
1:A:756:TYR:HD1	1:D:970:PHE:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ILE:HG13	1:D:197:ILE:O	2.11	0.51
1:C:947:LYS:HA	1:C:950:ASN:HD21	1.76	0.51
1:A:142:ASP:CG	1:A:258:TRP:CZ2	2.88	0.51
1:D:1014:ARG:O	1:D:1018:ILE:HG13	2.10	0.51
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.91	0.50
1:A:69:HIS:O	1:A:77:LYS:N	2.44	0.50
1:D:290:ASP:C	1:D:297:SER:HB3	2.35	0.50
1:A:972:ALA:HA	1:A:995:ARG:NH2	2.26	0.50
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.92	0.50
1:D:273:ARG:NH2	1:D:291:CYS:HB2	2.26	0.50
1:C:993:ILE:O	1:C:997:ILE:HG12	2.11	0.50
1:A:67:ALA:HB2	1:A:80:ASP:HB2	1.93	0.50
1:A:442:ASP:O	1:A:448:ASN:ND2	2.45	0.50
1:C:816:SER:OG	1:C:1054:GLN:OE1	2.29	0.50
1:A:808:ASP:O	1:A:811:LYS:HG2	2.12	0.50
1:D:329:PHE:HB3	1:D:331:ASN:HD21	1.76	0.50
1:C:454:ARG:HH21	1:C:457:ARG:HA	1.76	0.50
1:D:29:THR:HG21	1:D:266:TYR:HE2	1.76	0.50
1:A:21:ARG:HA	1:A:79:PHE:HB3	1.94	0.50
1:A:353:TRP:CD1	1:A:398:ASP:HB3	2.46	0.50
1:D:618:THR:OG1	1:D:619:GLU:OE1	2.23	0.50
1:C:330:PRO:HD3	1:C:579:PRO:HB2	1.93	0.50
1:A:105:ILE:O	1:A:238:PHE:HA	2.12	0.50
1:D:299:THR:HG23	1:D:313:TYR:HD2	1.77	0.50
1:D:666:ILE:HB	1:D:670:ILE:O	2.12	0.50
1:C:131:CYS:HA	1:C:166:CYS:HB3	1.94	0.50
1:D:189:LEU:HD22	1:D:210:ILE:HD13	1.92	0.50
1:D:741:TYR:CE2	1:D:1004:LEU:HD21	2.47	0.50
1:D:866:THR:O	1:D:870:ILE:N	2.34	0.50
1:C:290:ASP:O	1:C:297:SER:HB3	2.12	0.49
1:C:914:ASN:HA	1:C:917:TYR:CD2	2.48	0.49
1:A:310:LYS:HD2	1:A:601:GLY:H	1.77	0.49
1:A:472:ILE:HD12	1:A:491:PRO:HD3	1.93	0.49
2:G:36:TRP:CE2	2:G:92:CYS:HB3	2.46	0.49
2:G:100(A):GLY:H	3:K:34:ASN:ND2	2.10	0.49
3:K:6:GLN:HG2	3:K:8:PRO:HD2	1.94	0.49
1:D:93:ALA:HB3	1:D:266:TYR:HB2	1.94	0.49
1:D:108:THR:HG22	1:D:236:THR:HG23	1.94	0.49
1:D:216:LEU:O	1:D:218:GLN:NE2	2.45	0.49
1:D:1050:MET:HE3	1:D:1051:SER:H	1.76	0.49
1:C:43:PHE:C	1:C:44:ARG:HD3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1125:ASN:ND2	1:D:918:GLU:OE2	2.45	0.49
1:C:394:ASN:OD1	1:C:395:VAL:N	2.45	0.49
1:A:407:VAL:HG11	1:A:435:ALA:HB2	1.92	0.49
1:A:431:GLY:HA3	1:A:513:LEU:O	2.12	0.49
1:D:756:TYR:HH	1:D:998:THR:HG1	1.50	0.49
1:D:882:ILE:HA	1:D:898:PHE:CE1	2.47	0.49
1:A:65:PHE:CE2	1:A:82:PRO:HG3	2.47	0.49
1:A:190:ARG:NH1	1:A:207:HIS:HB2	2.19	0.49
1:D:289:VAL:HG12	1:D:290:ASP:O	2.12	0.49
1:D:874:THR:O	1:D:878:LEU:HD13	2.13	0.49
1:C:190:ARG:HG2	1:C:207:HIS:ND1	2.28	0.49
1:C:278:LYS:HB2	1:C:306:PHE:HE2	1.75	0.49
1:C:739:THR:HG22	1:C:740:MET:HE2	1.95	0.49
1:C:1091:ARG:NH1	1:C:1092:GLU:HB2	2.26	0.49
1:A:140:PHE:HB2	1:A:244:LEU:HD13	1.93	0.49
1:A:438:SER:OG	1:A:442:ASP:OD2	2.30	0.49
1:D:948:LEU:O	1:D:952:VAL:HG23	2.13	0.49
3:K:38:GLN:HA	3:K:44:PRO:HA	1.95	0.49
2:I:59:TYR:CE2	2:I:67:PHE:HB2	2.47	0.49
2:I:83:ARG:HD3	2:I:85:GLU:OE2	2.13	0.49
3:J:14:SER:OG	3:J:17:ASP:OD2	2.26	0.49
1:C:90:VAL:HG21	1:C:238:PHE:CZ	2.47	0.49
1:A:355:ARG:HD3	1:A:396:TYR:HD2	1.77	0.49
1:A:1024:LEU:O	1:A:1028:LYS:HG3	2.12	0.49
1:C:725:GLU:OE1	1:C:1028:LYS:NZ	2.33	0.49
1:D:178:ASP:OD1	1:D:178:ASP:N	2.46	0.49
1:D:329:PHE:HB3	1:D:331:ASN:ND2	2.28	0.49
1:D:898:PHE:O	1:D:901:GLN:HB2	2.13	0.49
2:I:69:ILE:HG13	2:I:78:LEU:HD11	1.95	0.49
1:C:178:ASP:OD1	1:C:207:HIS:NE2	2.45	0.49
1:D:778:THR:HG22	1:D:782:PHE:CD2	2.48	0.49
1:D:880:GLY:HA2	1:D:884:SER:HB2	1.95	0.49
1:C:439:ASN:OD1	1:C:440:ASN:N	2.46	0.48
1:A:662:CYS:SG	1:A:697:MET:HG3	2.53	0.48
1:D:336:CYS:HA	1:D:361:CYS:CB	2.43	0.48
1:D:455:LEU:HA	2:G:97:ARG:HE	1.76	0.48
1:A:245:HIS:O	1:A:259:THR:OG1	2.31	0.48
1:A:821:LEU:O	1:A:825:LYS:HG2	2.13	0.48
1:D:189:LEU:HB2	1:D:210:ILE:HG12	1.95	0.48
1:D:961:THR:O	1:D:965:GLN:N	2.31	0.48
1:D:1076:THR:HB	1:D:1097:SER:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:886:TRP:HB2	1:C:1034:LEU:O	2.13	0.48
1:A:36:VAL:HG11	1:A:220:PHE:CE1	2.48	0.48
1:D:902:MET:HE1	1:D:1049:LEU:HD13	1.94	0.48
2:I:52:TYR:HE1	2:I:58:TYR:HD2	1.62	0.48
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.46	0.48
1:A:246:ARG:HG2	1:A:258:TRP:CE3	2.49	0.48
1:A:318:PHE:CE2	1:A:615:VAL:HG11	2.49	0.48
1:A:1101:HIS:HB2	1:A:1103:PHE:CZ	2.48	0.48
1:D:353:TRP:H	1:D:353:TRP:CD1	2.31	0.48
1:D:674:TYR:HD1	1:D:692:ILE:HG12	1.79	0.48
1:C:377:PHE:CD1	1:C:434:ILE:HG12	2.49	0.48
1:C:890:ALA:HB1	1:A:1046:GLY:HA2	1.96	0.48
1:C:1040:VAL:O	1:D:1030:SER:OG	2.24	0.48
1:D:303:LEU:HD12	1:D:308:VAL:HG13	1.96	0.48
1:D:664:ILE:O	1:D:671:CYS:HB2	2.13	0.48
1:D:1024:LEU:O	1:D:1028:LYS:HG3	2.13	0.48
3:K:21:ILE:HB	3:K:71:PHE:HB3	1.96	0.48
1:D:773:GLU:HA	1:D:776:LYS:NZ	2.28	0.48
1:C:1030:SER:OG	1:A:1041:ASP:HB2	2.14	0.48
1:D:405:ASP:OD1	1:D:405:ASP:N	2.47	0.48
1:D:818:ILE:O	1:D:822:LEU:HG	2.14	0.48
1:C:800:PHE:HZ	1:C:920:GLN:HB3	1.79	0.48
1:C:957:GLN:O	1:C:961:THR:HG23	2.13	0.48
1:A:128:ILE:O	1:A:169:GLU:HA	2.13	0.48
1:A:1033:VAL:HG22	1:A:1051:SER:HB3	1.95	0.48
1:D:448:ASN:OD1	1:D:450:ASN:ND2	2.43	0.48
2:G:68:THR:O	2:G:80:LEU:HA	2.13	0.48
2:I:33:TYR:CE1	2:I:52:TYR:HD2	2.31	0.48
1:A:800:PHE:HB3	1:A:802:PHE:CE1	2.49	0.47
1:A:822:LEU:HD22	1:A:945:LEU:HD11	1.96	0.47
2:G:71:ARG:HB3	2:G:78:LEU:HD13	1.96	0.47
1:A:578:ASP:HB3	1:A:581:THR:O	2.13	0.47
1:A:790:LYS:HA	1:A:790:LYS:HD3	1.69	0.47
1:D:299:THR:HG23	1:D:313:TYR:CD2	2.48	0.47
1:C:386:LYS:HE2	1:C:390:LEU:HD22	1.96	0.47
1:D:273:ARG:CZ	1:D:274:THR:H	2.27	0.47
1:D:1135:ASN:OD1	1:D:1136:THR:N	2.47	0.47
1:C:802:PHE:HA	1:C:804:GLN:HE22	1.79	0.47
1:A:873:TYR:CZ	1:D:699:LEU:HD22	2.49	0.47
1:D:56:LEU:HB2	1:D:91:TYR:CZ	2.49	0.47
1:D:89:GLY:C	1:D:270:LEU:HD13	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:756:TYR:OH	1:D:998:THR:OG1	2.21	0.47
1:C:1078:ALA:HB3	1:C:1095:PHE:HB2	1.96	0.47
1:D:868:GLU:O	1:D:872:GLN:HG3	2.14	0.47
1:A:40:ASP:C	1:A:42:VAL:H	2.23	0.47
1:C:142:ASP:OD1	1:C:142:ASP:O	2.32	0.47
1:A:299:THR:HG22	1:A:308:VAL:HG11	1.97	0.47
1:A:300:LYS:NZ	1:A:602:THR:HG21	2.30	0.47
1:A:864:LEU:HD22	1:D:665:PRO:HB3	1.97	0.47
1:A:928:ASN:HA	1:A:931:ILE:HG12	1.95	0.47
1:A:1014:ARG:O	1:A:1017:GLU:HB2	2.14	0.47
1:D:42:VAL:HB	1:D:44:ARG:HH21	1.80	0.47
1:D:778:THR:HA	1:D:782:PHE:HD2	1.80	0.47
2:G:36:TRP:O	2:G:48:VAL:HB	2.15	0.47
2:G:37:VAL:HG22	2:G:47:TRP:HA	1.96	0.47
1:C:366:SER:OG	1:C:530:SER:N	2.48	0.47
1:C:962:LEU:HD21	1:C:1007:TYR:CG	2.50	0.47
1:A:738:CYS:HB2	1:A:753:LEU:HD21	1.96	0.47
1:D:386:LYS:O	1:D:386:LYS:HG2	2.14	0.47
1:D:930:ALA:O	1:D:934:ILE:HG12	2.13	0.47
1:D:898:PHE:HZ	1:D:1052:PHE:HZ	1.62	0.47
3:J:35:TRP:HB2	3:J:48:ILE:HB	1.95	0.47
1:C:118:LEU:O	1:C:128:ILE:HA	2.15	0.47
1:C:216:LEU:HG	1:C:218:GLN:OE1	2.15	0.47
1:A:382:VAL:HG21	1:A:515:PHE:HZ	1.79	0.47
1:A:905:ARG:O	1:A:906:PHE:HD1	1.97	0.47
1:D:129:LYS:HG2	1:D:169:GLU:HA	1.96	0.47
2:I:18:LEU:HD12	2:I:82(C):LEU:HD22	1.96	0.47
1:C:502:GLY:O	1:C:506:GLN:HG2	2.15	0.46
1:C:953:ASN:HA	1:C:956:ALA:HB3	1.97	0.46
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.97	0.46
1:D:954:GLN:O	1:D:958:ALA:HB2	2.15	0.46
1:C:759:PHE:HA	1:C:762:GLN:OE1	2.16	0.46
1:A:97:LYS:HG2	1:A:186:PHE:CD1	2.50	0.46
1:D:655:HIS:HA	1:D:694:ALA:O	2.15	0.46
1:D:885:GLY:HA2	1:D:901:GLN:NE2	2.31	0.46
1:D:959:LEU:O	1:D:962:LEU:HB3	2.15	0.46
2:I:67:PHE:CG	2:I:80:LEU:HD21	2.51	0.46
1:C:403:ARG:HD3	1:C:505:TYR:CD2	2.51	0.46
1:A:958:ALA:O	1:A:962:LEU:N	2.34	0.46
1:D:106:PHE:HB2	1:D:117:LEU:HB3	1.97	0.46
1:C:951:VAL:HA	1:C:954:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASP:CB	1:A:258:TRP:CZ3	2.79	0.46
1:A:611:LEU:HD22	1:A:666:ILE:CG2	2.45	0.46
1:A:993:ILE:HA	1:A:996:LEU:HD12	1.97	0.46
1:A:1001:LEU:O	1:A:1005:GLN:HG2	2.16	0.46
1:A:1091:ARG:HG3	1:A:1092:GLU:N	2.30	0.46
1:D:802:PHE:HB3	1:D:806:LEU:HD13	1.96	0.46
1:C:403:ARG:HD3	1:C:505:TYR:HD2	1.80	0.46
1:C:819:GLU:HA	1:C:822:LEU:HD12	1.97	0.46
1:C:985:ASP:HB3	1:C:987:PRO:HD2	1.98	0.46
1:A:866:THR:O	1:A:870:ILE:HG13	2.16	0.46
1:D:657:ASN:OD1	1:D:658:ASN:N	2.49	0.46
1:C:1036:GLN:NE2	1:C:1048:HIS:O	2.31	0.46
1:A:42:VAL:HG13	1:A:44:ARG:NH1	2.30	0.46
1:A:111:ASP:OD1	1:A:112:SER:N	2.44	0.46
1:A:913:GLN:O	1:A:916:LEU:HB3	2.15	0.46
1:D:1030:SER:O	1:D:1034:LEU:HB2	2.16	0.46
3:K:61:ARG:HD2	3:K:75:SER:HB3	1.98	0.46
1:C:1089:PHE:HE2	1:C:1124:GLY:HA3	1.81	0.46
1:A:931:ILE:HA	1:A:934:ILE:HD12	1.97	0.46
2:G:40:ALA:HB3	2:G:43:LYS:HB3	1.97	0.46
1:C:453:TYR:CE1	2:I:98:GLU:HG3	2.50	0.46
1:C:866:THR:HG22	1:C:868:GLU:H	1.81	0.46
1:D:902:MET:HG3	1:D:906:PHE:CE2	2.51	0.46
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.97	0.46
1:A:99:ASN:HB3	1:A:102:ARG:NH2	2.31	0.46
1:A:394:ASN:HB3	1:A:396:TYR:HE1	1.80	0.46
1:A:915:VAL:HA	1:A:919:ASN:HB2	1.97	0.46
1:C:726:ILE:HG21	1:C:948:LEU:HG	1.97	0.46
1:A:299:THR:HG21	1:A:599:THR:HG21	1.98	0.46
1:A:451:TYR:HB2	1:A:495:TYR:HB2	1.98	0.46
1:A:969:ASN:HB3	1:A:972:ALA:N	2.30	0.46
1:D:367:VAL:O	1:D:371:SER:HB2	2.16	0.46
1:C:454:ARG:HG3	1:C:491:PRO:HB2	1.97	0.45
1:A:287:ASP:OD1	1:A:288:ALA:N	2.49	0.45
1:D:945:LEU:O	1:D:949:GLN:HG2	2.17	0.45
2:I:9:GLY:HA3	2:I:109:VAL:HG22	1.97	0.45
2:I:59:TYR:HE2	2:I:67:PHE:HB2	1.81	0.45
1:C:47:VAL:H	1:C:279:TYR:HB2	1.81	0.45
1:C:210:ILE:HG22	1:C:211:ASN:N	2.31	0.45
1:C:353:TRP:CZ3	1:C:355:ARG:HB2	2.52	0.45
1:A:281:GLU:H	1:A:281:GLU:CD	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ASN:OD1	1:A:659:SER:N	2.50	0.45
1:D:66:HIS:NE2	1:D:68:ILE:HB	2.31	0.45
2:G:20:LEU:HD13	2:G:36:TRP:CZ2	2.51	0.45
1:C:34:ARG:HH21	1:C:219:GLY:HA3	1.81	0.45
1:C:418:ILE:HG23	1:C:422:ASN:HB2	1.98	0.45
1:C:757:GLY:HA2	1:A:968:SER:HB3	1.97	0.45
1:C:715:PRO:HD3	1:D:894:LEU:HD13	1.98	0.45
1:A:177:MET:SD	1:A:177:MET:N	2.90	0.45
1:A:230:PRO:HB2	1:D:521:PRO:HB3	1.99	0.45
1:D:55:PHE:HB3	1:D:275:PHE:CE2	2.50	0.45
1:D:945:LEU:HB3	1:D:949:GLN:HE21	1.82	0.45
2:I:43:LYS:HG2	2:I:44:GLY:H	1.81	0.45
1:C:206:LYS:HE2	1:C:221:SER:HB3	1.98	0.45
1:C:310:LYS:HD2	1:C:663:ASP:OD2	2.16	0.45
1:C:400:PHE:HE2	1:C:402:ILE:HD13	1.81	0.45
1:C:897:PRO:HB2	1:C:900:MET:HE2	1.97	0.45
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.50	0.45
1:D:977:LEU:HD23	1:D:1000:ARG:HH22	1.80	0.45
1:C:732:THR:HG22	1:C:1058:HIS:CD2	2.51	0.45
1:A:36:VAL:HG11	1:A:220:PHE:CZ	2.51	0.45
1:A:725:GLU:OE2	1:A:1028:LYS:HE2	2.17	0.45
1:A:877:LEU:HD23	1:A:888:PHE:HE2	1.81	0.45
1:D:770:ILE:O	1:D:773:GLU:HB2	2.17	0.45
2:I:39:GLN:NE2	3:J:38:GLN:OE1	2.40	0.45
1:A:311:GLY:HA2	1:A:664:ILE:HG12	1.99	0.45
1:A:755:GLN:O	1:D:970:PHE:N	2.48	0.45
2:I:5:LEU:HG	2:I:23:ALA:HB3	1.99	0.45
2:I:47:TRP:CZ2	2:I:50:VAL:HG13	2.52	0.45
1:C:289:VAL:HG11	1:C:300:LYS:HE2	1.98	0.45
1:C:906:PHE:HB3	1:C:911:VAL:HB	1.98	0.45
1:D:979:ASP:OD1	1:D:980:ILE:HG13	2.17	0.45
1:A:384:PRO:HG2	1:A:385:THR:HG23	1.99	0.45
1:A:295:PRO:HB2	1:A:608:VAL:CG1	2.47	0.44
1:D:789:TYR:HB2	1:D:876:ALA:HB1	1.98	0.44
1:A:354:ASN:OD1	1:A:399:SER:OG	2.36	0.44
1:A:731:MET:HA	1:A:1058:HIS:HB3	1.98	0.44
1:A:738:CYS:SG	1:A:753:LEU:HD21	2.57	0.44
1:A:756:TYR:HA	1:D:970:PHE:HA	1.99	0.44
2:G:82:MET:HG3	2:G:82(C):LEU:HD11	2.00	0.44
3:J:61:ARG:HD2	3:J:75:SER:HB3	1.99	0.44
1:C:957:GLN:O	1:C:961:THR:N	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:HIS:HE2	1:D:68:ILE:HB	1.82	0.44
1:D:643:PHE:HE2	1:D:655:HIS:H	1.66	0.44
1:D:732:THR:HA	1:D:1058:HIS:CE1	2.53	0.44
1:D:979:ASP:OD1	1:D:980:ILE:N	2.51	0.44
1:A:617:CYS:HB2	1:A:649:CYS:HB2	1.81	0.44
1:A:934:ILE:HD13	1:A:1063:LEU:HD22	2.00	0.44
1:D:273:ARG:HH22	1:D:291:CYS:HB2	1.83	0.44
2:G:48:VAL:HG13	2:G:63:VAL:HG21	2.00	0.44
1:C:1014:ARG:O	1:C:1018:ILE:HG12	2.18	0.44
1:A:142:ASP:OD2	1:A:258:TRP:CH2	2.66	0.44
1:D:431:GLY:HA2	1:D:515:PHE:CD1	2.52	0.44
2:G:2:VAL:HG21	2:G:94:ARG:HH12	1.83	0.44
2:G:24:ALA:O	2:G:76:ASN:HB3	2.17	0.44
1:C:761:THR:O	1:C:765:ARG:HD3	2.17	0.44
1:D:611:LEU:HD22	1:D:666:ILE:HG22	2.00	0.44
1:C:31:SER:O	1:C:59:PHE:CA	2.66	0.44
1:C:782:PHE:HA	1:C:877:LEU:HD11	1.99	0.44
1:A:418:ILE:HG23	1:A:422:ASN:HB2	1.98	0.44
1:A:738:CYS:HB2	1:A:742:ILE:HD12	2.00	0.44
1:D:415:THR:HG22	2:G:58:TYR:CD1	2.53	0.44
1:D:718:PHE:CG	1:D:1067:TYR:HE1	2.36	0.44
1:A:874:THR:O	1:A:878:LEU:HG	2.17	0.44
1:D:962:LEU:O	1:D:966:LEU:HG	2.18	0.44
1:C:759:PHE:O	1:C:763:LEU:HD23	2.18	0.44
1:D:403:ARG:HG2	1:D:497:PHE:CE1	2.52	0.44
1:C:117:LEU:HA	1:C:130:VAL:HG22	1.99	0.43
1:C:365:TYR:HB3	1:C:369:TYR:CZ	2.53	0.43
1:C:741:TYR:HA	1:C:857:GLY:HA3	2.00	0.43
1:C:906:PHE:CG	1:C:911:VAL:HB	2.53	0.43
1:A:48:LEU:HD23	1:A:278:LYS:HA	2.00	0.43
1:A:1030:SER:HG	1:D:1040:VAL:C	2.22	0.43
1:C:355:ARG:NH2	1:C:396:TYR:HB3	2.33	0.43
1:C:356:LYS:HG3	1:C:397:ALA:HB3	2.01	0.43
1:A:64:TRP:HD1	1:A:65:PHE:N	2.16	0.43
1:D:205:SER:OG	1:D:226:LEU:HD13	2.17	0.43
1:D:884:SER:HB3	1:D:893:ALA:HB1	2.00	0.43
1:C:807:PRO:HA	1:C:816:SER:HA	2.00	0.43
1:A:903:ALA:HA	1:A:916:LEU:HD21	2.00	0.43
1:D:56:LEU:HD12	1:D:57:PRO:HD2	2.00	0.43
1:D:532:ASN:OD1	1:D:533:LEU:N	2.50	0.43
1:D:995:ARG:HG3	1:D:995:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:100:GLY:HA2	3:K:34:ASN:ND2	2.32	0.43
3:K:29:ILE:HB	3:K:69:PHE:HE2	1.84	0.43
1:C:732:THR:HG22	1:C:1058:HIS:HD2	1.82	0.43
1:D:738:CYS:HB3	1:D:760:CYS:HB2	1.69	0.43
1:D:885:GLY:HA3	1:D:896:ILE:HD12	1.99	0.43
1:C:405:ASP:OD1	1:C:405:ASP:N	2.49	0.43
1:C:865:LEU:HD22	1:C:873:TYR:HE2	1.82	0.43
1:A:30:ASN:OD1	1:A:31:SER:N	2.51	0.43
1:A:96:GLU:O	1:A:188:ASN:HB2	2.19	0.43
1:A:193:VAL:HG12	1:A:195:LYS:HG2	2.00	0.43
1:D:303:LEU:HD11	1:D:313:TYR:CE2	2.54	0.43
1:D:825:LYS:NZ	1:D:938:LEU:O	2.49	0.43
1:D:986:PRO:N	1:D:987:PRO:HD2	2.33	0.43
1:C:797:PHE:CD2	1:C:802:PHE:HB2	2.53	0.43
1:A:334:ASN:OD1	1:A:335:LEU:N	2.52	0.43
1:A:1081:ILE:HD12	1:A:1135:ASN:HB3	1.99	0.43
1:D:182:LYS:NZ	1:D:188:ASN:OD1	2.33	0.43
1:D:329:PHE:CZ	1:D:525:CYS:HB2	2.54	0.43
1:D:712:ILE:HG13	1:D:713:ALA:N	2.34	0.43
1:D:732:THR:O	1:D:734:THR:HG23	2.19	0.43
2:G:89:VAL:HA	2:G:108:THR:HA	2.01	0.43
2:I:34:MET:CE	2:I:78:LEU:HD22	2.47	0.43
1:C:178:ASP:OD1	1:C:178:ASP:N	2.51	0.43
1:C:742:ILE:CG2	1:C:997:ILE:HG23	2.49	0.43
1:C:815:ARG:HB3	1:C:819:GLU:HB3	2.01	0.43
1:C:865:LEU:HA	1:C:869:MET:HE3	2.00	0.43
1:A:318:PHE:O	1:A:319:ARG:NE	2.52	0.43
1:A:720:ILE:HD12	1:A:1049:LEU:HD11	1.99	0.43
1:C:568:ASP:OD1	1:C:570:ALA:N	2.52	0.43
1:C:669:GLY:N	1:D:864:LEU:O	2.48	0.43
1:C:777:ASN:O	1:C:781:VAL:HB	2.19	0.43
1:A:175:PHE:HB3	1:A:177:MET:SD	2.59	0.43
1:A:189:LEU:HD13	1:A:210:ILE:HG21	2.01	0.43
1:A:202:LYS:NZ	1:A:228:ASP:OD2	2.52	0.43
1:A:730:SER:HA	1:A:774:GLN:HG3	2.00	0.43
1:A:1052:PHE:HB2	1:A:1063:LEU:HB2	2.01	0.43
1:D:51:THR:O	1:D:274:THR:HA	2.18	0.43
1:D:176:LEU:O	1:D:177:MET:HE2	2.18	0.43
1:C:123:ALA:HB1	1:C:179:LEU:HD21	2.01	0.43
1:C:421:TYR:HE2	2:I:33:TYR:CE2	2.36	0.43
1:C:733:LYS:NZ	1:C:775:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:773:GLU:HA	1:D:776:LYS:HZ3	1.83	0.43
1:D:912:THR:OG1	1:D:913:GLN:N	2.52	0.43
3:J:78:PRO:HA	3:J:104:ILE:HD13	2.01	0.43
1:C:366:SER:HG	1:C:530:SER:N	2.17	0.43
1:C:425:LEU:HD21	1:C:512:VAL:HG11	2.01	0.43
1:A:34:ARG:HH21	1:A:217:PRO:HG2	1.84	0.43
1:A:81:ASN:ND2	1:A:240:THR:O	2.52	0.43
1:A:756:TYR:HE2	1:A:997:ILE:HG22	1.84	0.43
1:A:1031:GLU:OE2	1:D:1039:ARG:HG3	2.19	0.43
1:A:1083:HIS:HB3	1:A:1088:HIS:NE2	2.33	0.43
1:D:1029:MET:O	1:D:1033:VAL:HB	2.19	0.43
2:G:47:TRP:HE1	2:G:50:VAL:HG13	1.83	0.43
2:I:47:TRP:HZ2	2:I:50:VAL:HG13	1.84	0.43
1:C:356:LYS:CG	1:C:397:ALA:HB3	2.49	0.42
1:A:142:ASP:CB	1:A:258:TRP:CH2	3.02	0.42
1:A:617:CYS:H	1:A:644:GLN:HE22	1.65	0.42
1:D:193:VAL:HG13	1:D:270:LEU:HD11	2.01	0.42
1:D:666:ILE:HD11	1:D:672:ALA:HB2	2.01	0.42
1:D:968:SER:HB2	1:D:970:PHE:CE2	2.54	0.42
3:K:21:ILE:HD12	3:K:71:PHE:HD2	1.84	0.42
1:C:110:LEU:HA	1:C:116:SER:OG	2.19	0.42
1:C:645:THR:OG1	1:C:648:GLY:O	2.26	0.42
1:C:877:LEU:HD23	1:C:888:PHE:HE2	1.85	0.42
1:A:294:ASP:OD1	1:A:294:ASP:N	2.52	0.42
1:A:538:CYS:HB2	1:A:590:CYS:HB2	1.72	0.42
1:A:616:ASN:HA	1:A:644:GLN:OE1	2.19	0.42
1:D:117:LEU:HB2	1:D:130:VAL:HG22	2.00	0.42
1:D:323:THR:N	1:D:538:CYS:O	2.52	0.42
1:D:972:ALA:HB1	1:D:995:ARG:HH12	1.83	0.42
1:C:570:ALA:HB1	1:D:963:VAL:HG21	2.02	0.42
1:C:909:ILE:HG12	1:C:1036:GLN:HE22	1.84	0.42
1:A:37:TYR:HB3	1:A:223:LEU:HB2	2.02	0.42
1:A:353:TRP:HB3	1:A:400:PHE:HB3	2.02	0.42
1:A:355:ARG:HD3	1:A:396:TYR:CD2	2.54	0.42
1:D:393:THR:HA	1:D:522:ALA:HA	2.00	0.42
1:D:671:CYS:O	1:D:694:ALA:HA	2.19	0.42
1:D:866:THR:O	1:D:870:ILE:HG13	2.20	0.42
2:I:96:LEU:HB2	2:I:100:GLY:O	2.19	0.42
3:J:4:MET:HG3	3:J:25:ALA:HA	2.00	0.42
1:C:452:ARG:HG2	1:C:494:SER:HA	2.02	0.42
1:C:906:PHE:CB	1:C:911:VAL:HB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:972:ALA:HB2	1:C:996:LEU:HD21	2.01	0.42
1:A:655:HIS:HA	1:A:694:ALA:O	2.20	0.42
1:A:740:MET:HA	1:A:743:CYS:O	2.19	0.42
1:A:986:PRO:N	1:A:987:PRO:HD2	2.35	0.42
1:D:195:LYS:HE2	1:D:197:ILE:HG22	2.02	0.42
1:D:759:PHE:HA	1:D:762:GLN:HG2	2.02	0.42
1:D:1029:MET:O	1:D:1034:LEU:HG	2.19	0.42
1:D:1077:THR:HA	1:D:1096:VAL:HG12	2.01	0.42
1:C:672:ALA:HA	1:C:693:ILE:O	2.20	0.42
1:A:347:PHE:CD2	1:A:509:ARG:HB3	2.55	0.42
1:A:728:PRO:HG2	1:A:951:VAL:HG21	2.02	0.42
1:D:97:LYS:HE3	1:D:188:ASN:H	1.84	0.42
1:D:190:ARG:HB3	1:D:192:PHE:CE2	2.54	0.42
1:D:957:GLN:HA	1:D:960:ASN:CB	2.43	0.42
2:I:33:TYR:HE1	2:I:52:TYR:HD2	1.67	0.42
1:C:436:TRP:CZ2	1:C:509:ARG:HD2	2.55	0.42
1:C:970:PHE:CE1	1:D:759:PHE:HE2	2.37	0.42
1:D:804:GLN:HB3	1:D:818:ILE:HG13	2.02	0.42
1:D:905:ARG:O	1:D:909:ILE:HG12	2.19	0.42
1:D:1049:LEU:HB2	1:D:1065:VAL:O	2.19	0.42
2:I:87:THR:HG23	2:I:110:THR:HA	2.02	0.42
3:J:2:ILE:HG23	3:J:26:SER:HB2	2.02	0.42
1:C:317:ASN:C	1:C:317:ASN:ND2	2.78	0.42
1:C:405:ASP:N	1:C:504:GLY:O	2.53	0.42
1:A:320:VAL:N	1:A:591:SER:OG	2.36	0.42
1:A:394:ASN:HB3	1:A:396:TYR:CE1	2.55	0.42
1:A:740:MET:HB2	1:D:319:ARG:NH2	2.35	0.42
1:D:97:LYS:HE3	1:D:188:ASN:N	2.35	0.42
1:D:386:LYS:HD3	1:D:390:LEU:HD13	2.01	0.42
1:D:772:VAL:O	1:D:776:LYS:HG2	2.19	0.42
1:D:781:VAL:O	1:D:1029:MET:HG3	2.20	0.42
1:D:992:GLN:HA	1:D:995:ARG:HG2	2.02	0.42
2:G:96:LEU:HD23	2:G:96:LEU:HA	1.90	0.42
1:C:393:THR:HG21	1:D:200:TYR:CD2	2.54	0.42
1:C:873:TYR:CE2	1:A:699:LEU:HD22	2.55	0.42
1:A:296:LEU:HD21	1:A:602:THR:HG22	2.01	0.42
1:A:726:ILE:O	1:A:947:LYS:HB2	2.19	0.42
1:A:915:VAL:HG13	1:A:919:ASN:O	2.19	0.42
1:A:1103:PHE:CG	1:A:1112:PRO:HB3	2.54	0.42
1:D:454:ARG:HH22	1:D:471:GLU:N	2.17	0.42
2:G:38:ARG:NH2	2:G:86:ASP:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:PHE:CD1	1:C:364:ASP:HB2	2.55	0.42
1:C:826:VAL:HB	1:C:1057:PRO:HG2	2.02	0.42
1:A:777:ASN:HA	1:A:780:GLU:HG2	2.02	0.42
1:A:795:LYS:NZ	1:A:807:PRO:O	2.52	0.42
1:A:854:LYS:HA	1:A:858:LEU:O	2.20	0.42
1:D:326:ILE:HD11	1:D:534:VAL:H	1.84	0.42
1:D:433:VAL:HG22	1:D:512:VAL:HG22	2.02	0.42
1:D:440:ASN:OD1	1:D:440:ASN:N	2.53	0.42
1:D:762:GLN:HA	1:D:765:ARG:HG2	2.01	0.42
1:D:804:GLN:O	1:D:818:ILE:HG13	2.20	0.42
1:C:106:PHE:HB3	1:C:235:ILE:HD13	2.02	0.42
1:C:726:ILE:HD12	1:C:1061:VAL:HG22	2.01	0.42
1:A:45:SER:O	1:A:47:VAL:HG13	2.20	0.42
1:A:310:LYS:HD2	1:A:600:PRO:HA	2.02	0.42
1:A:718:PHE:HE1	1:A:720:ILE:HG12	1.85	0.42
1:A:804:GLN:OE1	1:A:817:PHE:HB3	2.20	0.42
1:D:91:TYR:CD1	1:D:193:VAL:HG22	2.55	0.42
1:D:536:ASN:HA	1:D:551:VAL:HG13	2.02	0.42
1:D:808:ASP:HB2	1:D:811:LYS:HZ2	1.84	0.42
1:D:866:THR:HG22	1:D:868:GLU:N	2.33	0.42
1:D:945:LEU:CB	1:D:949:GLN:HE21	2.33	0.42
1:C:804:GLN:CD	1:C:804:GLN:H	2.28	0.41
1:A:1029:MET:HA	1:A:1033:VAL:CG2	2.50	0.41
1:D:91:TYR:CE2	1:D:270:LEU:HD12	2.55	0.41
1:D:329:PHE:HD2	1:D:331:ASN:OD1	2.03	0.41
1:D:1048:HIS:HD2	1:D:1066:THR:HG22	1.85	0.41
1:C:930:ALA:O	1:C:934:ILE:HG12	2.20	0.41
1:D:565:PHE:HB2	1:D:575:ALA:O	2.20	0.41
2:G:38:ARG:HD2	2:G:48:VAL:HG22	2.02	0.41
1:C:497:PHE:CD1	1:C:507:PRO:HB3	2.56	0.41
1:C:611:LEU:HD22	1:C:666:ILE:HG23	2.01	0.41
1:C:947:LYS:HA	1:C:950:ASN:ND2	2.34	0.41
1:C:953:ASN:O	1:C:957:GLN:N	2.49	0.41
1:A:284:THR:HG22	1:D:560:LEU:HD11	2.01	0.41
1:A:740:MET:SD	1:A:744:GLY:HA2	2.60	0.41
1:A:1088:HIS:HA	1:A:1121:PHE:O	2.19	0.41
1:D:54:LEU:HB2	1:D:270:LEU:HD23	2.01	0.41
1:D:131:CYS:HB2	1:D:133:PHE:CE2	2.55	0.41
1:D:144:TYR:HB2	1:D:246:ARG:HH11	1.85	0.41
1:D:912:THR:HG21	1:D:914:ASN:ND2	2.35	0.41
2:G:98:GLU:HB2	3:K:89:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:103:TRP:NE1	3:J:44:PRO:HB2	2.35	0.41
1:C:206:LYS:HB2	1:C:223:LEU:HG	2.02	0.41
1:C:317:ASN:HA	1:C:594:GLY:HA2	2.03	0.41
1:C:737:ASP:OD1	1:C:737:ASP:N	2.50	0.41
1:C:738:CYS:HB2	1:C:753:LEU:HD21	2.02	0.41
1:C:911:VAL:HG13	1:C:1109:PHE:CE2	2.56	0.41
1:C:913:GLN:HA	1:C:916:LEU:HB3	2.02	0.41
1:C:1089:PHE:HD2	1:C:1123:SER:HB3	1.86	0.41
1:A:461:LEU:HD21	1:A:465:GLU:O	2.20	0.41
1:A:963:VAL:O	1:A:966:LEU:HB2	2.20	0.41
1:A:1008:VAL:O	1:A:1012:LEU:HD23	2.20	0.41
1:D:310:LYS:HG3	1:D:600:PRO:HA	2.01	0.41
1:D:329:PHE:CD2	1:D:527:PRO:HA	2.56	0.41
2:G:83:ARG:NE	2:G:83:ARG:HA	2.35	0.41
1:C:346:ARG:NH2	1:C:450:ASN:HB3	2.35	0.41
1:A:361:CYS:H	1:A:524:VAL:HG22	1.84	0.41
1:A:733:LYS:HE3	1:A:861:LEU:HB2	2.01	0.41
1:D:858:LEU:HD21	1:D:959:LEU:HD22	2.02	0.41
2:I:37:VAL:HG13	2:I:46:GLU:O	2.21	0.41
1:C:40:ASP:OD1	1:C:40:ASP:N	2.51	0.41
1:C:877:LEU:O	1:C:881:THR:HG22	2.19	0.41
1:C:905:ARG:HD3	1:C:1049:LEU:O	2.21	0.41
1:A:178:ASP:OD1	1:A:178:ASP:N	2.50	0.41
1:A:455:LEU:HG	1:A:456:PHE:CD1	2.55	0.41
1:A:1100:THR:OG1	1:A:1101:HIS:N	2.54	0.41
1:D:670:ILE:HA	1:D:695:TYR:O	2.20	0.41
3:J:3:VAL:HA	3:J:95:THR:OG1	2.19	0.41
3:J:62:PHE:CD2	3:J:73:ILE:HG12	2.56	0.41
1:C:299:THR:OG1	1:C:597:VAL:HG21	2.21	0.41
1:C:593:GLY:HA3	1:C:613:GLN:O	2.20	0.41
1:C:669:GLY:HA3	1:D:869:MET:SD	2.60	0.41
1:C:735:SER:HB2	1:C:861:LEU:HD11	2.03	0.41
1:C:958:ALA:O	1:C:962:LEU:HG	2.20	0.41
1:C:959:LEU:HA	1:C:962:LEU:HD12	2.02	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.91	0.41
1:D:237:ARG:C	1:D:237:ARG:HD2	2.46	0.41
1:D:1020:ALA:O	1:D:1024:LEU:HB2	2.21	0.41
1:C:766:ALA:O	1:C:770:ILE:HG13	2.21	0.41
1:A:200:TYR:CE2	1:A:230:PRO:HB3	2.56	0.41
1:A:289:VAL:HG12	1:A:290:ASP:O	2.21	0.41
1:A:317:ASN:C	1:A:595:VAL:HG23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.55	0.41
1:A:930:ALA:O	1:A:934:ILE:HG13	2.20	0.41
1:A:950:ASN:HB2	1:A:954:GLN:HE22	1.85	0.41
1:A:1081:ILE:HG13	1:A:1088:HIS:HB2	2.03	0.41
1:A:1105:THR:OG1	1:A:1111:GLU:N	2.34	0.41
1:D:50:SER:HB3	1:D:276:LEU:HD23	2.01	0.41
1:C:95:THR:HG21	1:C:212:LEU:HD13	2.03	0.41
1:C:177:MET:HE1	1:C:190:ARG:HH11	1.85	0.41
1:C:355:ARG:HD3	1:C:355:ARG:C	2.45	0.41
1:C:501:ASN:HA	3:J:28:ASP:CG	2.45	0.41
1:C:731:MET:HE2	1:C:731:MET:HB3	1.84	0.41
1:C:957:GLN:HA	1:C:960:ASN:HB2	2.02	0.41
1:A:671:CYS:O	1:A:694:ALA:HA	2.20	0.41
1:A:720:ILE:HG13	1:A:923:ILE:HD12	2.02	0.41
1:A:726:ILE:HB	1:A:947:LYS:HG3	2.03	0.41
1:A:1053:PRO:O	1:A:1054:GLN:HG2	2.20	0.41
1:A:1105:THR:HG21	1:A:1110:TYR:CD1	2.56	0.41
1:D:299:THR:HG21	1:D:599:THR:HG21	2.02	0.41
1:D:314:GLN:OE1	1:D:314:GLN:N	2.54	0.41
1:D:364:ASP:O	1:D:368:LEU:HG	2.21	0.41
1:D:739:THR:O	1:D:743:CYS:HB2	2.21	0.41
2:G:70:SER:O	2:G:78:LEU:HD12	2.21	0.41
3:K:49:TYR:HE1	3:K:55:GLU:HB2	1.86	0.41
3:J:39:LYS:HB2	3:J:39:LYS:HE2	1.91	0.41
1:A:727:LEU:HD12	1:A:1062:PHE:CD1	2.56	0.41
1:A:966:LEU:HD13	1:A:1000:ARG:HD3	2.03	0.41
1:D:220:PHE:HZ	1:D:288:ALA:HB3	1.86	0.41
1:D:392:PHE:HB2	1:D:524:VAL:HB	2.03	0.41
1:D:715:PRO:HD2	1:D:1109:PHE:HD1	1.86	0.41
2:G:98:GLU:HB2	3:K:89:PHE:HD2	1.86	0.41
3:K:37:GLN:NE2	3:K:47:LEU:HD21	2.36	0.41
1:A:759:PHE:HE1	1:D:1006:THR:HG21	1.86	0.40
1:D:86:PHE:HE2	1:D:196:ASN:HD22	1.69	0.40
1:D:91:TYR:HD1	1:D:193:VAL:HG22	1.84	0.40
1:D:308:VAL:O	1:D:601:GLY:HA2	2.21	0.40
1:D:695:TYR:CE2	1:D:697:MET:HA	2.56	0.40
1:C:194:PHE:CD2	1:C:203:ILE:HG12	2.56	0.40
1:C:949:GLN:HA	1:C:952:VAL:HG22	2.03	0.40
1:A:1034:LEU:HD12	1:D:1040:VAL:HG11	2.03	0.40
1:A:1087:ALA:HB3	1:A:1123:SER:O	2.21	0.40
1:D:97:LYS:HD3	1:D:97:LYS:HA	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LEU:HB2	1:C:289:VAL:HG22	2.04	0.40
1:C:776:LYS:O	1:C:780:GLU:HG2	2.20	0.40
1:A:323:THR:H	1:A:539:VAL:HG12	1.85	0.40
1:A:430:THR:HB	1:A:515:PHE:CE1	2.57	0.40
1:A:957:GLN:O	1:A:961:THR:OG1	2.27	0.40
1:A:1105:THR:HG21	1:A:1110:TYR:CE1	2.55	0.40
1:D:329:PHE:CE1	1:D:525:CYS:HB2	2.56	0.40
1:C:43:PHE:O	1:A:566:GLY:HA2	2.21	0.40
1:C:1091:ARG:NH2	1:C:1118:ASP:O	2.54	0.40
1:A:897:PRO:HG2	1:D:1077:THR:HG21	2.02	0.40
1:D:278:LYS:HE2	1:D:306:PHE:CD1	2.57	0.40
1:D:1101:HIS:CD2	1:D:1102:TRP:N	2.90	0.40
1:C:1027:THR:O	1:C:1031:GLU:CB	2.67	0.40
1:A:756:TYR:CE2	1:A:997:ILE:HG22	2.56	0.40
1:A:959:LEU:O	1:A:963:VAL:N	2.44	0.40
1:D:36:VAL:HG21	1:D:220:PHE:CZ	2.57	0.40
1:D:278:LYS:HE2	1:D:306:PHE:CG	2.55	0.40
1:D:715:PRO:HD2	1:D:1109:PHE:CD1	2.56	0.40
1:D:733:LYS:HB2	1:D:733:LYS:HE3	1.72	0.40
3:J:6:GLN:HG3	3:J:99:GLY:H	1.87	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	1028/1259 (82%)	964 (94%)	64 (6%)	0	100	100
1	C	1009/1259 (80%)	950 (94%)	59 (6%)	0	100	100
1	D	1019/1259 (81%)	962 (94%)	54 (5%)	3 (0%)	36	70
2	G	117/119 (98%)	111 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	116/119 (98%)	105 (90%)	11 (10%)	0	100	100
3	J	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
3	K	104/107 (97%)	94 (90%)	10 (10%)	0	100	100
All	All	3498/4229 (83%)	3287 (94%)	208 (6%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	332	ILE
1	D	337	PRO
1	D	330	PRO

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	908/1091 (83%)	907 (100%)	1 (0%)	88	90
1	C	892/1091 (82%)	891 (100%)	1 (0%)	88	90
1	D	902/1091 (83%)	902 (100%)	0	100	100
2	G	94/95 (99%)	94 (100%)	0	100	100
2	I	94/95 (99%)	94 (100%)	0	100	100
3	J	93/94 (99%)	93 (100%)	0	100	100
3	K	92/94 (98%)	92 (100%)	0	100	100
All	All	3075/3651 (84%)	3073 (100%)	2 (0%)	87	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	317	ASN
1	A	52	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33)

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	317	ASN
1	C	542	ASN
1	C	644	GLN
1	C	774	GLN
1	C	804	GLN
1	C	901	GLN
1	C	913	GLN
1	C	949	GLN
1	A	321	GLN
1	A	440	ASN
1	A	448	ASN
1	A	501	ASN
1	A	544	ASN
1	A	644	GLN
1	A	777	ASN
1	A	784	GLN
1	A	913	GLN
1	A	919	ASN
1	A	949	GLN
1	A	955	ASN
1	A	1074	ASN
1	A	1134	ASN
1	D	239	GLN
1	D	498	GLN
1	D	774	GLN
1	D	824	ASN
1	D	856	ASN
1	D	978	ASN
1	D	1054	GLN
3	K	34	ASN
3	K	37	GLN
3	K	77	GLN
3	J	27	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

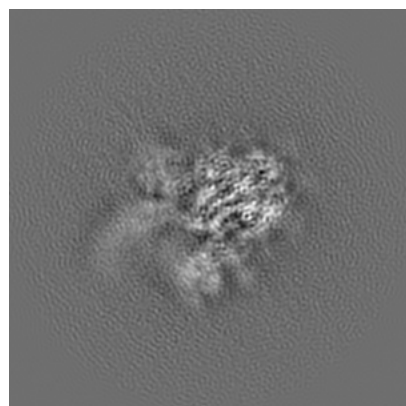
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39685. These allow visual inspection of the internal detail of the map and identification of artifacts.

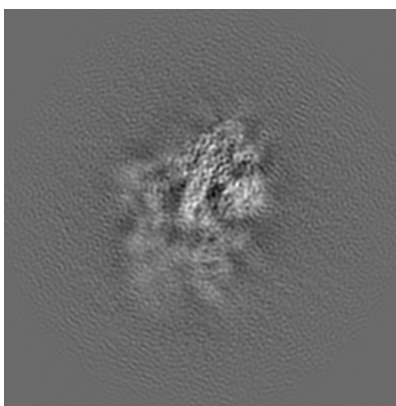
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

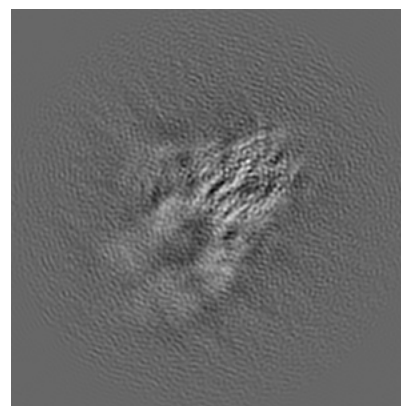
6.1.1 Primary map



X

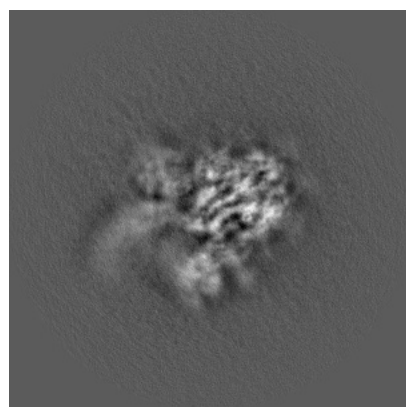


Y

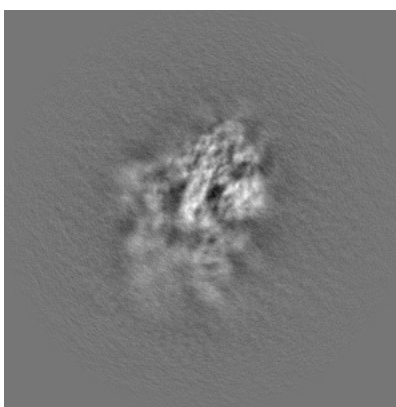


Z

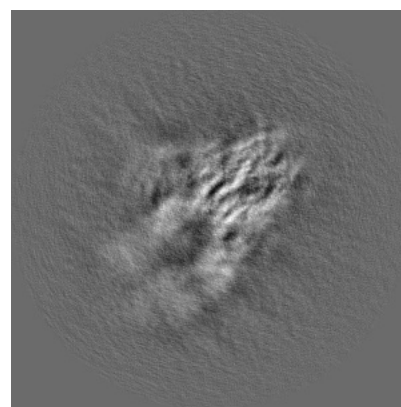
6.1.2 Raw map



X



Y

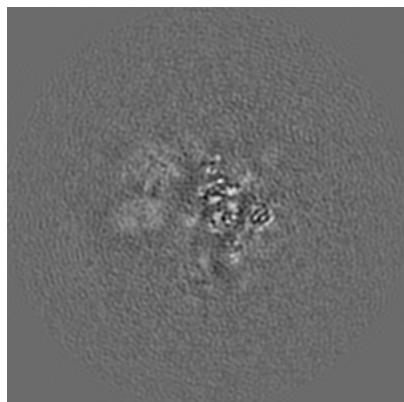


Z

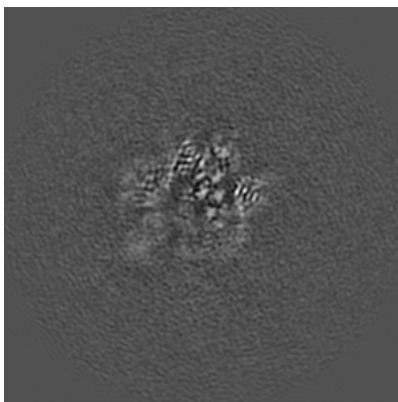
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

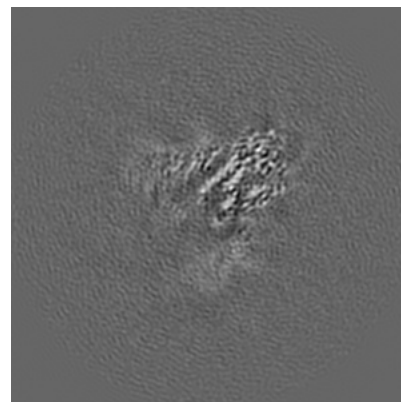
6.2.1 Primary map



X Index: 192

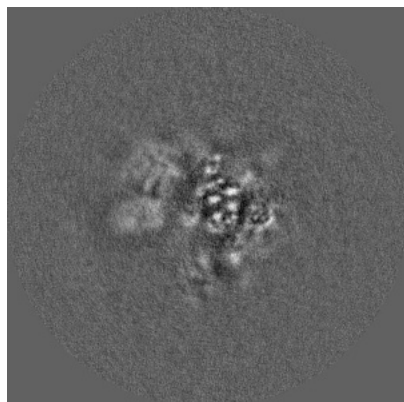


Y Index: 192

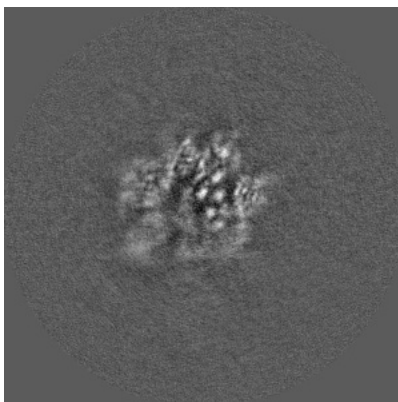


Z Index: 192

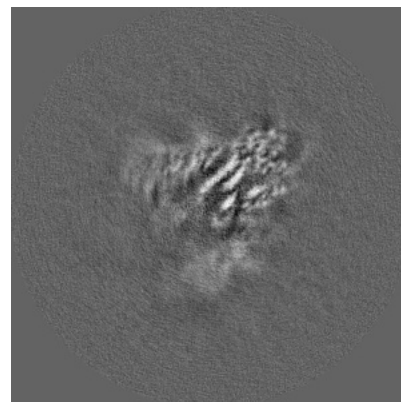
6.2.2 Raw map



X Index: 192



Y Index: 192

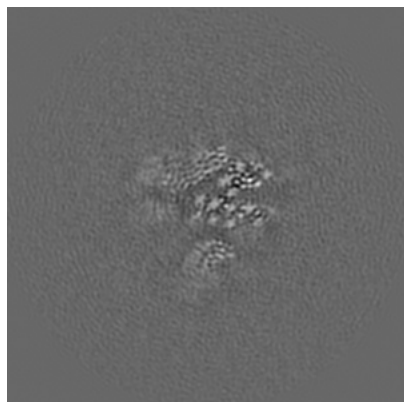


Z Index: 192

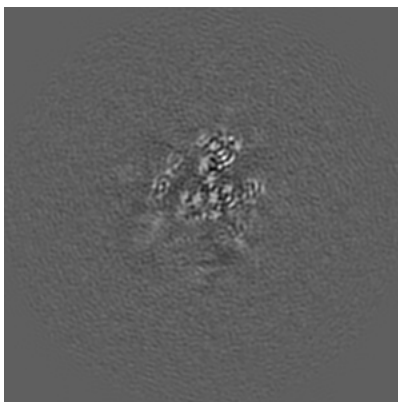
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

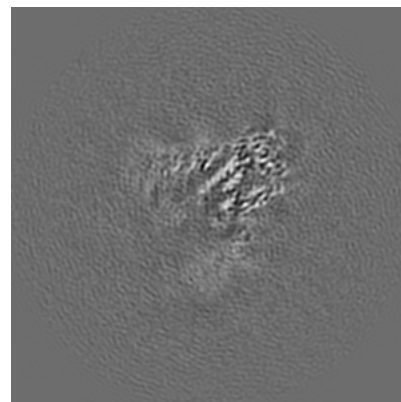
6.3.1 Primary map



X Index: 211

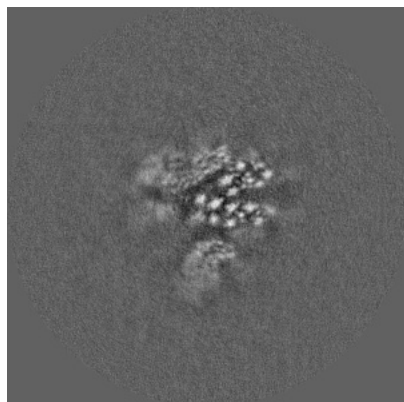


Y Index: 206

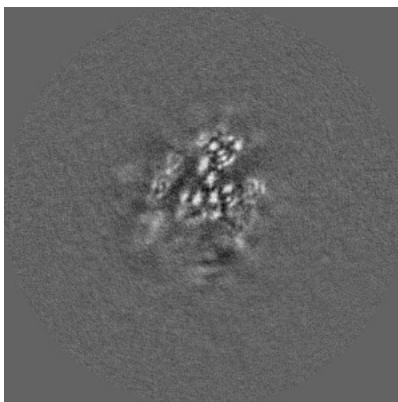


Z Index: 191

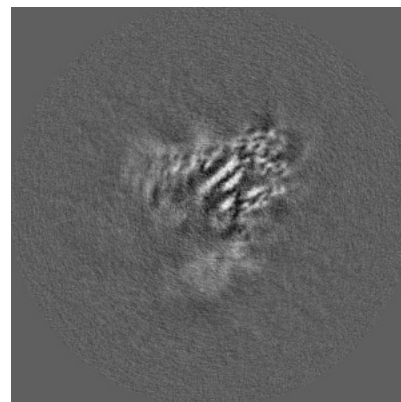
6.3.2 Raw map



X Index: 212



Y Index: 206

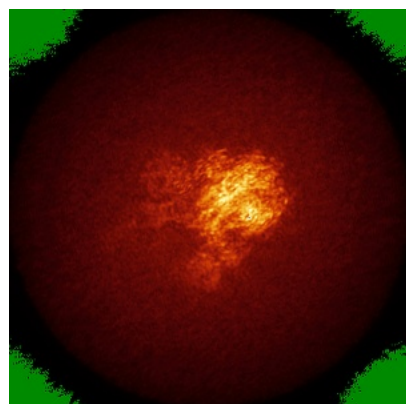


Z Index: 191

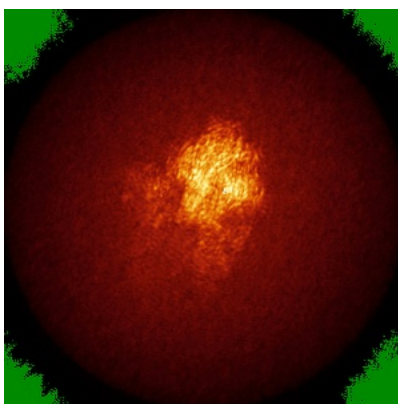
The images above show the largest variance slices of the map in three orthogonal directions.

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

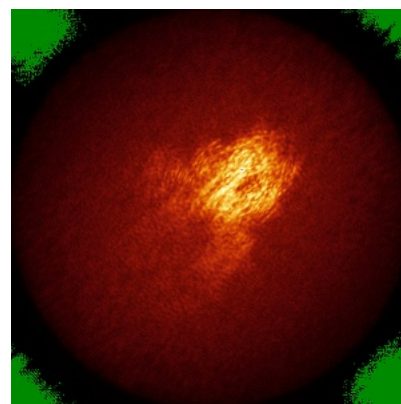
6.4.1 Primary map



X

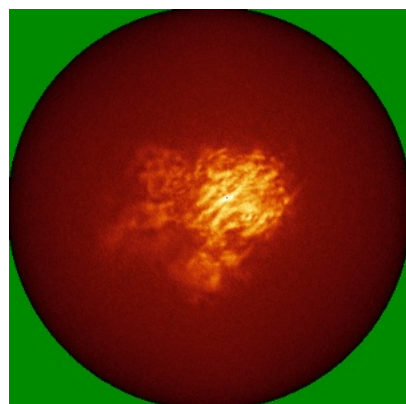


Y

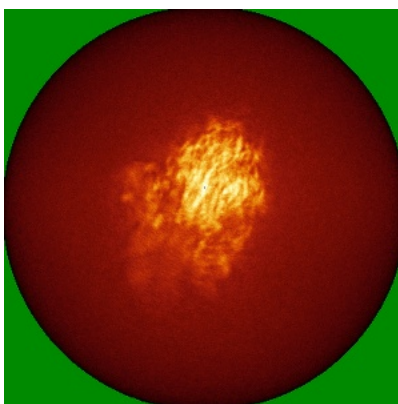


Z

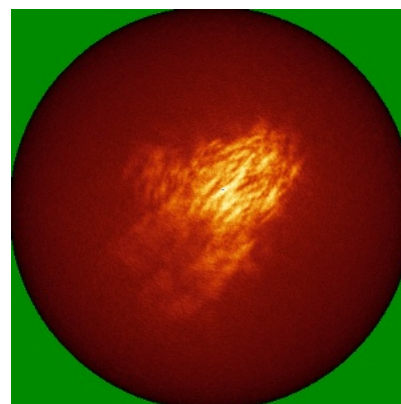
6.4.2 Raw map



X



Y

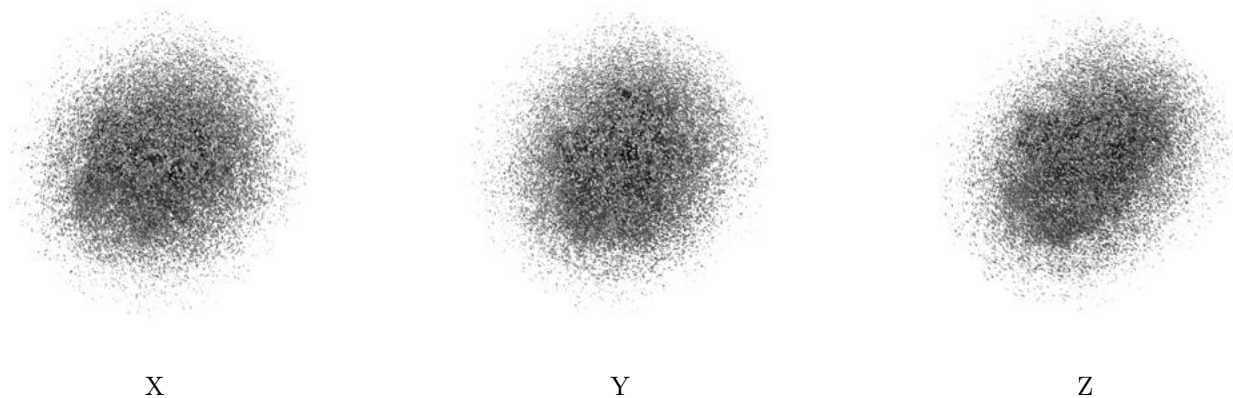


Z

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

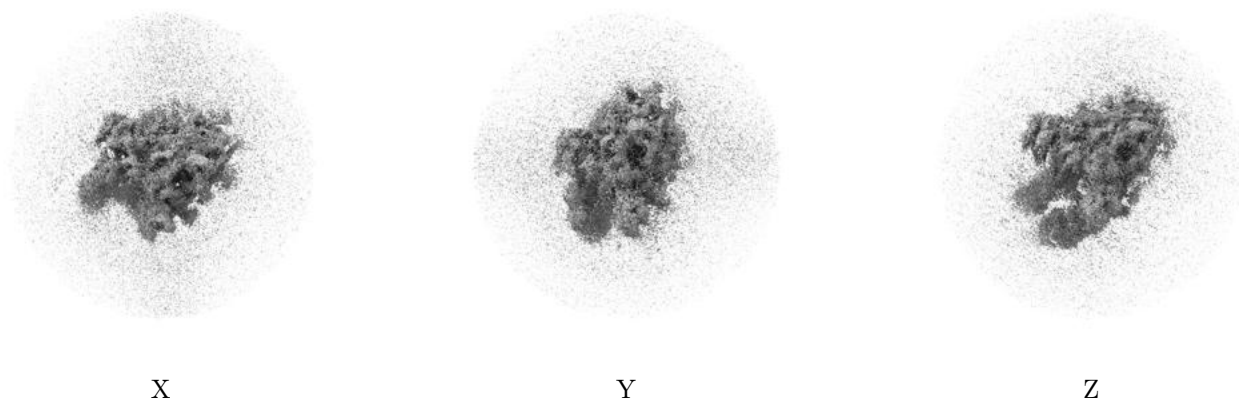
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

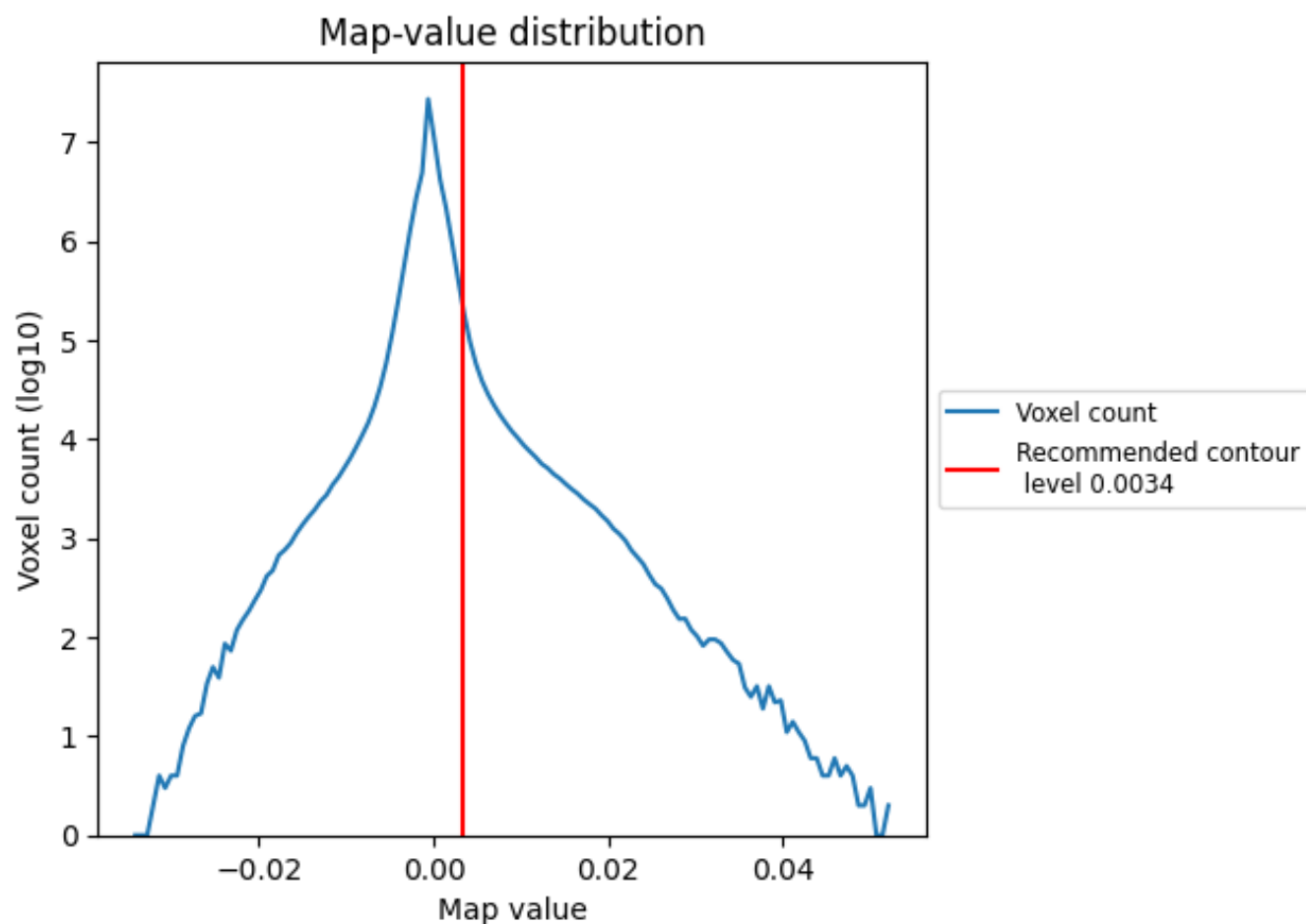
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

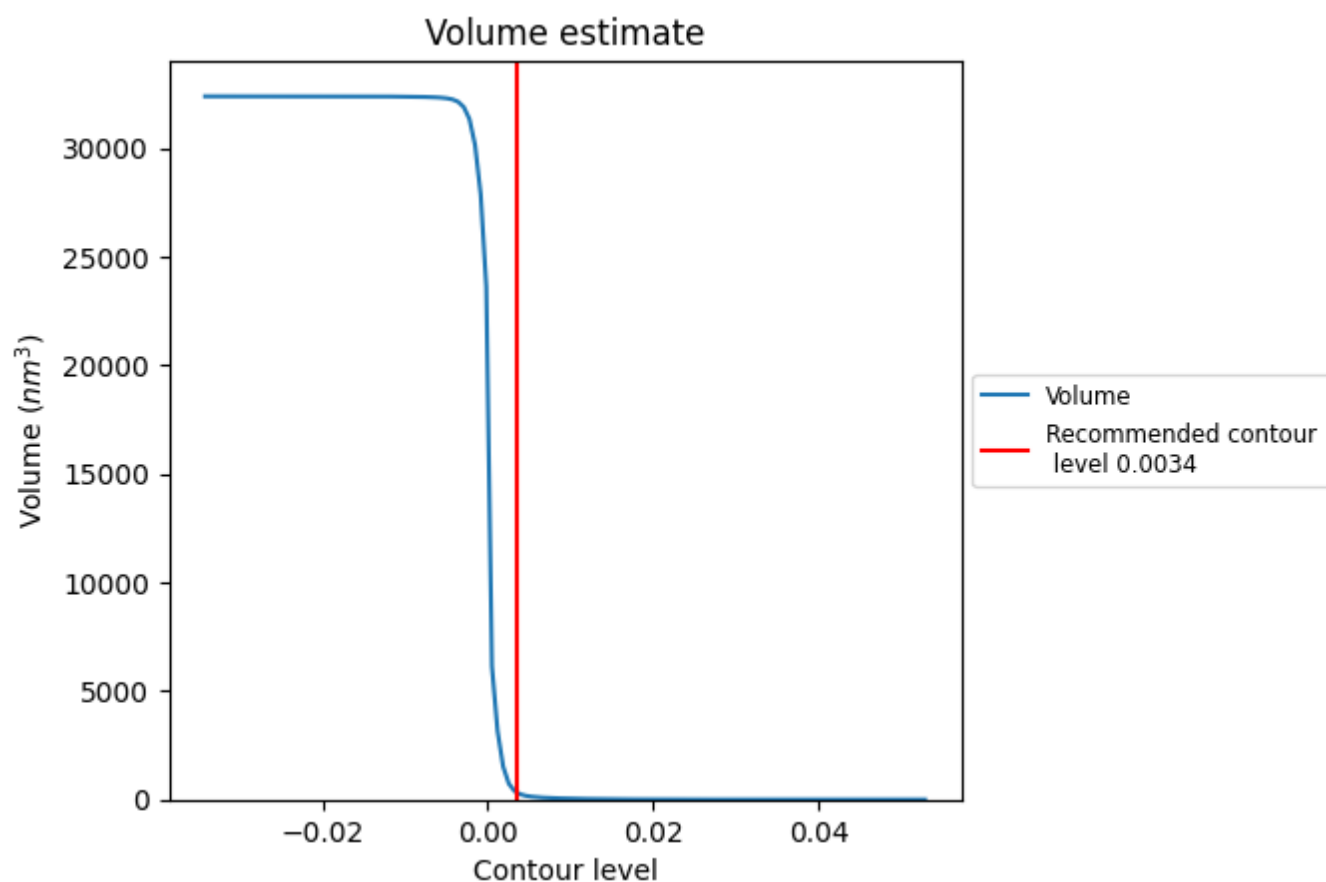
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

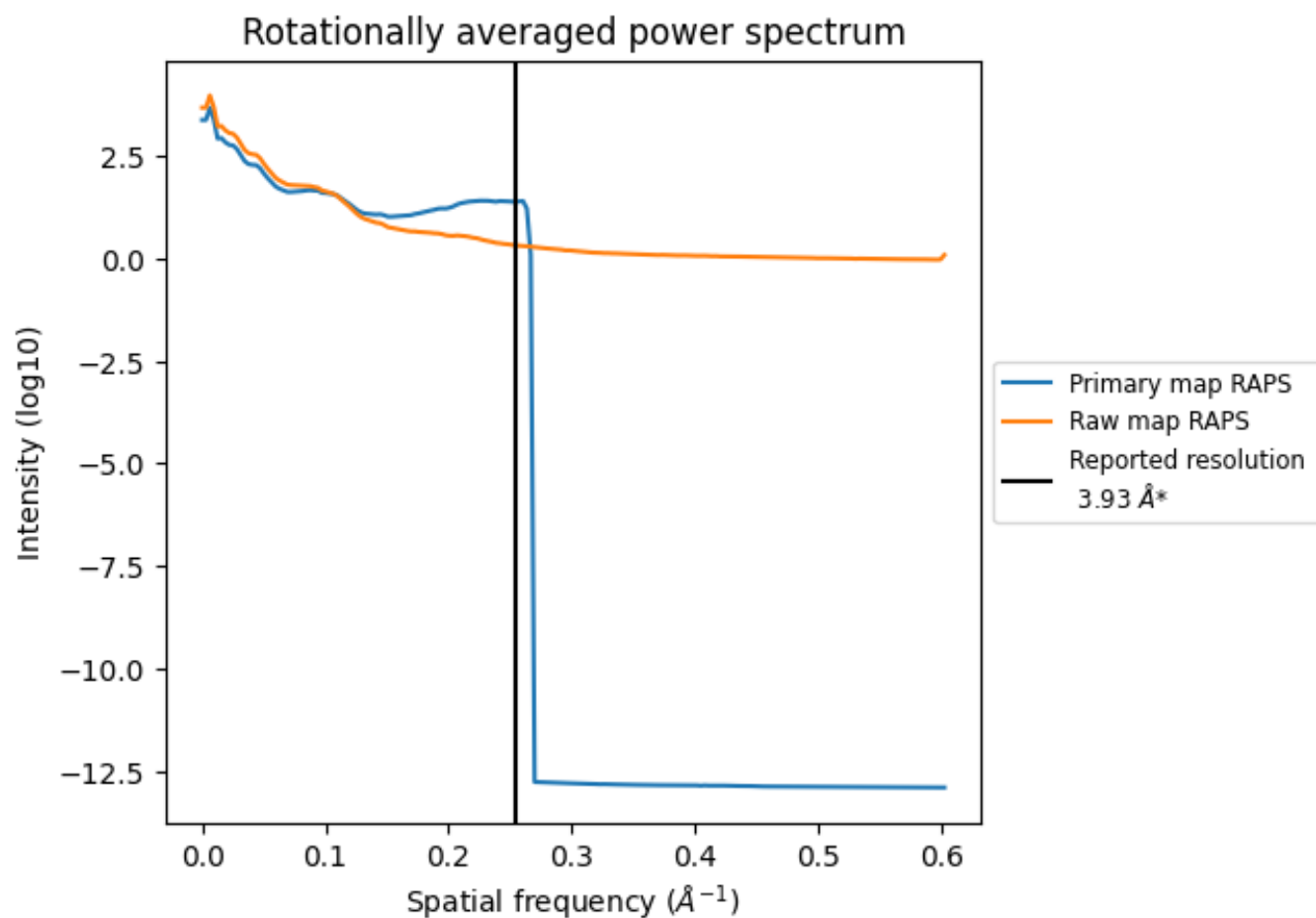
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; this corresponds to an approximate mass of 321 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 ⓘ

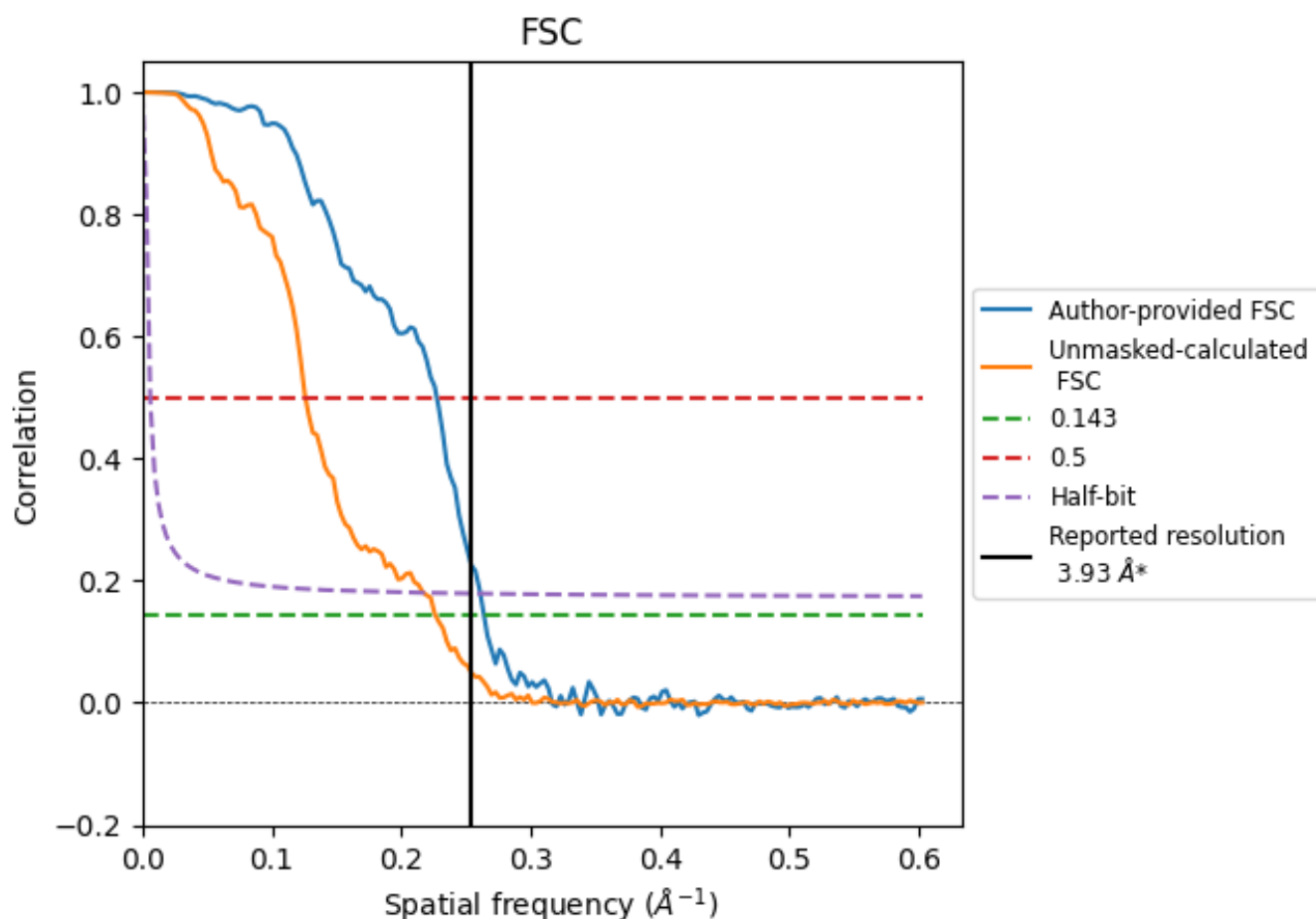


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.254 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

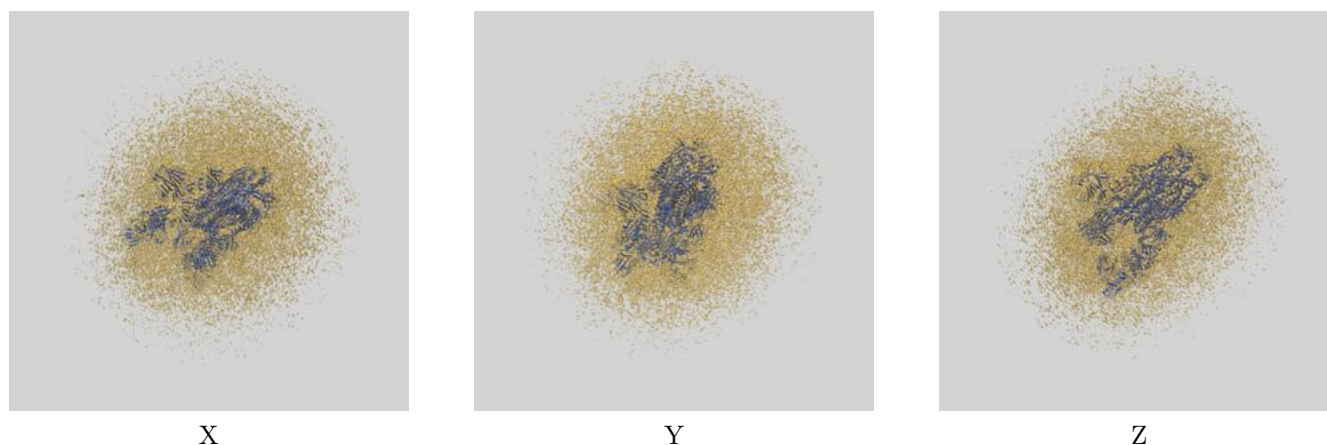
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	3.79	4.40	3.83
Unmasked-calculated*	4.41	7.93	4.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.41 differs from the reported value 3.93 by more than 10 %

9 Map-model fit [i](#)

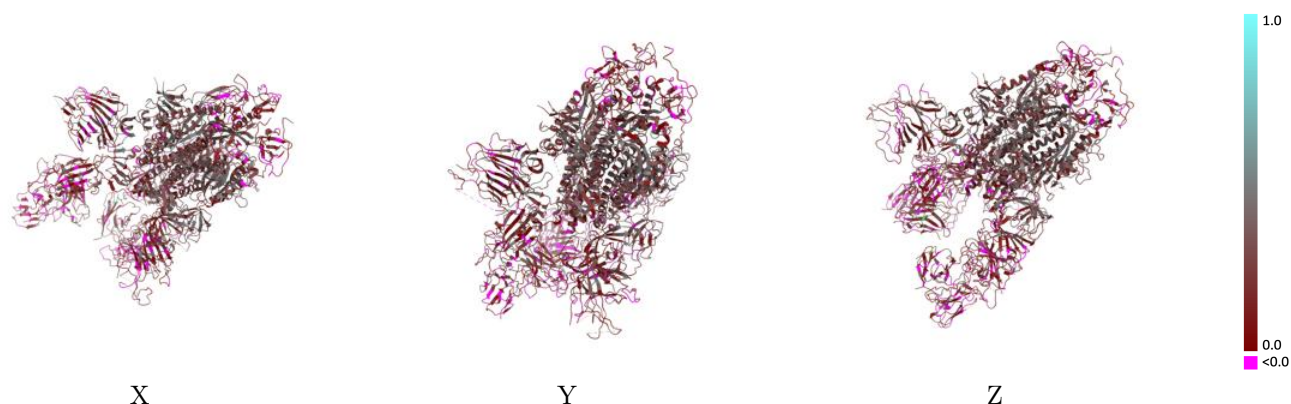
This section contains information regarding the fit between EMDB map EMD-39685 and PDB model 8YZ5. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



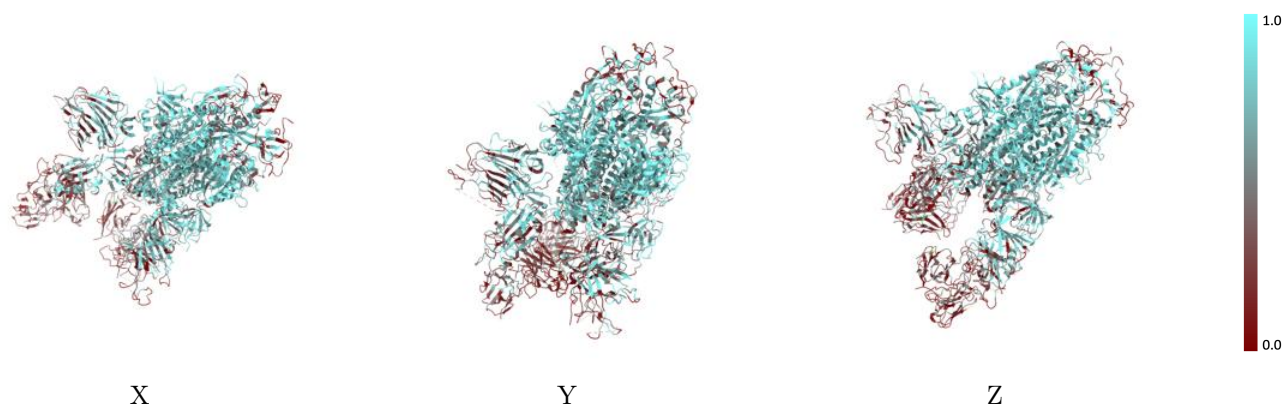
The images above show the 3D surface view of the map at the recommended contour level 0.0034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



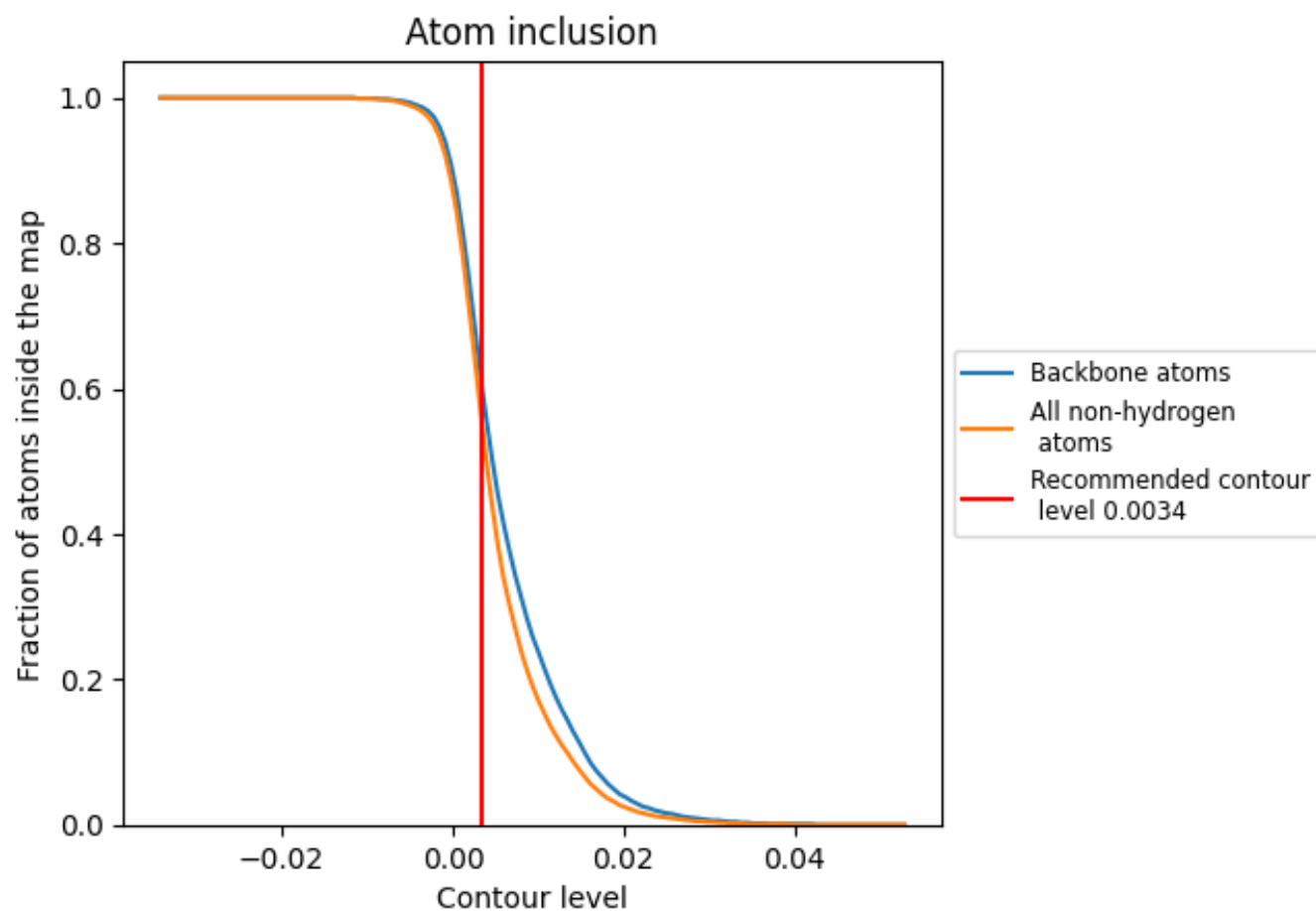
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0034).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 55% 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 (0.0034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5510	0.2340
A	0.5840	0.2450
C	0.6070	0.2490
D	0.5930	0.2450
G	0.2270	0.1510
I	0.1650	0.1590
J	0.3140	0.1480
K	0.2490	0.1370

1.0

0.0

<0.0