Full wwPDB EM Validation Report

Nov 4, 2024 – 08:41 AM JST

PDB ID	:	7X25
EMDB ID	:	EMD-32958
Title	:	MERS-CoV spike complex with S41 neutralizing antibody Fab Class4 (2u1d RBD with 3Fab)
Authors	:	Zeng, J.; Zhang, S.; Zhou, H.; Wang, X.
Deposited on	:	2022-02-25
Resolution	:	2.49 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

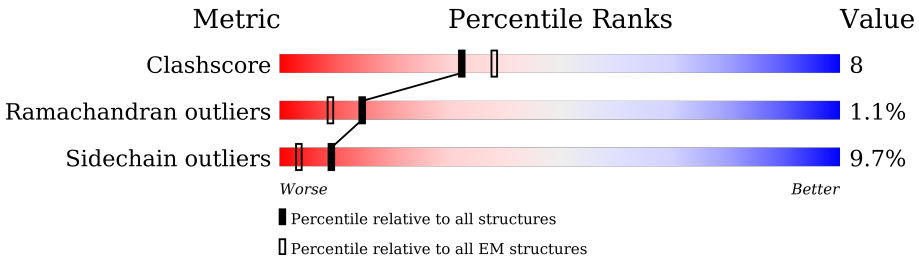
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.49 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	221	33% 69% 27% 5%
1	E	221	24% 66% 26% 5%
1	H	221	66% 26% 6%
2	C	212	38% 68% 28%
2	F	212	34% 69% 28%
2	K	212	5% 69% 27%
3	G	1347	13% 68% 18% 12%
3	I	1347	8% 69% 17% 12%

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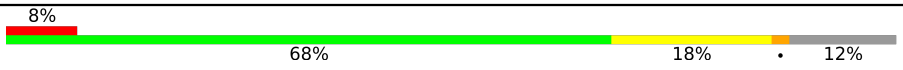
Mol	Chain	Length	Quality of chain
3	J	1347	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 37110 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 antibody S41 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	221	Total	C	N	O	S	2	0
			1633	1028	274	325	6		
1	E	213	Total	C	N	O	S	2	0
			1579	995	265	313	6		
1	H	215	Total	C	N	O	S	1	0
			1585	997	266	316	6		

- Molecule 2 is a protein called antibody S41 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	212	Total	C	N	O	S	0	0
			1601	997	277	323	4		
2	F	212	Total	C	N	O	S	0	0
			1601	997	277	323	4		
2	K	212	Total	C	N	O	S	0	0
			1601	997	277	323	4		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	1189	Total	C	N	O	S	0	0
			9189	5834	1521	1783	51		
3	I	1189	Total	C	N	O	S	0	0
			9189	5834	1521	1783	51		
3	J	1181	Total	C	N	O	S	0	0
			9132	5801	1513	1767	51		

There are 177 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1060	PRO	VAL	engineered mutation	UNP K0BRG7
G	1061	PRO	LEU	engineered mutation	UNP K0BRG7
G	1291	SER	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1292	ARG	-	expression tag	UNP K0BRG7
G	1293	GLU	-	expression tag	UNP K0BRG7
G	1294	ASN	-	expression tag	UNP K0BRG7
G	1295	LEU	-	expression tag	UNP K0BRG7
G	1296	TYR	-	expression tag	UNP K0BRG7
G	1297	PHE	-	expression tag	UNP K0BRG7
G	1298	GLN	-	expression tag	UNP K0BRG7
G	1299	GLY	-	expression tag	UNP K0BRG7
G	1300	GLY	-	expression tag	UNP K0BRG7
G	1301	GLY	-	expression tag	UNP K0BRG7
G	1302	SER	-	expression tag	UNP K0BRG7
G	1303	ALA	-	expression tag	UNP K0BRG7
G	1304	GLY	-	expression tag	UNP K0BRG7
G	1305	SER	-	expression tag	UNP K0BRG7
G	1306	GLY	-	expression tag	UNP K0BRG7
G	1307	TYR	-	expression tag	UNP K0BRG7
G	1308	ILE	-	expression tag	UNP K0BRG7
G	1309	PRO	-	expression tag	UNP K0BRG7
G	1310	GLU	-	expression tag	UNP K0BRG7
G	1311	ALA	-	expression tag	UNP K0BRG7
G	1312	PRO	-	expression tag	UNP K0BRG7
G	1313	ARG	-	expression tag	UNP K0BRG7
G	1314	ASP	-	expression tag	UNP K0BRG7
G	1315	GLY	-	expression tag	UNP K0BRG7
G	1316	GLN	-	expression tag	UNP K0BRG7
G	1317	ALA	-	expression tag	UNP K0BRG7
G	1318	TYR	-	expression tag	UNP K0BRG7
G	1319	VAL	-	expression tag	UNP K0BRG7
G	1320	ARG	-	expression tag	UNP K0BRG7
G	1321	LYS	-	expression tag	UNP K0BRG7
G	1322	ASP	-	expression tag	UNP K0BRG7
G	1323	GLY	-	expression tag	UNP K0BRG7
G	1324	GLU	-	expression tag	UNP K0BRG7
G	1325	TRP	-	expression tag	UNP K0BRG7
G	1326	VAL	-	expression tag	UNP K0BRG7
G	1327	LEU	-	expression tag	UNP K0BRG7
G	1328	LEU	-	expression tag	UNP K0BRG7
G	1329	SER	-	expression tag	UNP K0BRG7
G	1330	THR	-	expression tag	UNP K0BRG7
G	1331	PHE	-	expression tag	UNP K0BRG7
G	1332	LEU	-	expression tag	UNP K0BRG7
G	1333	GLY	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1334	HIS	-	expression tag	UNP K0BRG7
G	1335	HIS	-	expression tag	UNP K0BRG7
G	1336	HIS	-	expression tag	UNP K0BRG7
G	1337	HIS	-	expression tag	UNP K0BRG7
G	1338	HIS	-	expression tag	UNP K0BRG7
G	1339	HIS	-	expression tag	UNP K0BRG7
G	1340	TRP	-	expression tag	UNP K0BRG7
G	1341	SER	-	expression tag	UNP K0BRG7
G	1342	HIS	-	expression tag	UNP K0BRG7
G	1343	PRO	-	expression tag	UNP K0BRG7
G	1344	GLN	-	expression tag	UNP K0BRG7
G	1345	PHE	-	expression tag	UNP K0BRG7
G	1346	GLU	-	expression tag	UNP K0BRG7
G	1347	LYS	-	expression tag	UNP K0BRG7
I	1060	PRO	VAL	engineered mutation	UNP K0BRG7
I	1061	PRO	LEU	engineered mutation	UNP K0BRG7
I	1291	SER	-	expression tag	UNP K0BRG7
I	1292	ARG	-	expression tag	UNP K0BRG7
I	1293	GLU	-	expression tag	UNP K0BRG7
I	1294	ASN	-	expression tag	UNP K0BRG7
I	1295	LEU	-	expression tag	UNP K0BRG7
I	1296	TYR	-	expression tag	UNP K0BRG7
I	1297	PHE	-	expression tag	UNP K0BRG7
I	1298	GLN	-	expression tag	UNP K0BRG7
I	1299	GLY	-	expression tag	UNP K0BRG7
I	1300	GLY	-	expression tag	UNP K0BRG7
I	1301	GLY	-	expression tag	UNP K0BRG7
I	1302	SER	-	expression tag	UNP K0BRG7
I	1303	ALA	-	expression tag	UNP K0BRG7
I	1304	GLY	-	expression tag	UNP K0BRG7
I	1305	SER	-	expression tag	UNP K0BRG7
I	1306	GLY	-	expression tag	UNP K0BRG7
I	1307	TYR	-	expression tag	UNP K0BRG7
I	1308	ILE	-	expression tag	UNP K0BRG7
I	1309	PRO	-	expression tag	UNP K0BRG7
I	1310	GLU	-	expression tag	UNP K0BRG7
I	1311	ALA	-	expression tag	UNP K0BRG7
I	1312	PRO	-	expression tag	UNP K0BRG7
I	1313	ARG	-	expression tag	UNP K0BRG7
I	1314	ASP	-	expression tag	UNP K0BRG7
I	1315	GLY	-	expression tag	UNP K0BRG7
I	1316	GLN	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1317	ALA	-	expression tag	UNP K0BRG7
I	1318	TYR	-	expression tag	UNP K0BRG7
I	1319	VAL	-	expression tag	UNP K0BRG7
I	1320	ARG	-	expression tag	UNP K0BRG7
I	1321	LYS	-	expression tag	UNP K0BRG7
I	1322	ASP	-	expression tag	UNP K0BRG7
I	1323	GLY	-	expression tag	UNP K0BRG7
I	1324	GLU	-	expression tag	UNP K0BRG7
I	1325	TRP	-	expression tag	UNP K0BRG7
I	1326	VAL	-	expression tag	UNP K0BRG7
I	1327	LEU	-	expression tag	UNP K0BRG7
I	1328	LEU	-	expression tag	UNP K0BRG7
I	1329	SER	-	expression tag	UNP K0BRG7
I	1330	THR	-	expression tag	UNP K0BRG7
I	1331	PHE	-	expression tag	UNP K0BRG7
I	1332	LEU	-	expression tag	UNP K0BRG7
I	1333	GLY	-	expression tag	UNP K0BRG7
I	1334	HIS	-	expression tag	UNP K0BRG7
I	1335	HIS	-	expression tag	UNP K0BRG7
I	1336	HIS	-	expression tag	UNP K0BRG7
I	1337	HIS	-	expression tag	UNP K0BRG7
I	1338	HIS	-	expression tag	UNP K0BRG7
I	1339	HIS	-	expression tag	UNP K0BRG7
I	1340	TRP	-	expression tag	UNP K0BRG7
I	1341	SER	-	expression tag	UNP K0BRG7
I	1342	HIS	-	expression tag	UNP K0BRG7
I	1343	PRO	-	expression tag	UNP K0BRG7
I	1344	GLN	-	expression tag	UNP K0BRG7
I	1345	PHE	-	expression tag	UNP K0BRG7
I	1346	GLU	-	expression tag	UNP K0BRG7
I	1347	LYS	-	expression tag	UNP K0BRG7
J	1060	PRO	VAL	engineered mutation	UNP K0BRG7
J	1061	PRO	LEU	engineered mutation	UNP K0BRG7
J	1291	SER	-	expression tag	UNP K0BRG7
J	1292	ARG	-	expression tag	UNP K0BRG7
J	1293	GLU	-	expression tag	UNP K0BRG7
J	1294	ASN	-	expression tag	UNP K0BRG7
J	1295	LEU	-	expression tag	UNP K0BRG7
J	1296	TYR	-	expression tag	UNP K0BRG7
J	1297	PHE	-	expression tag	UNP K0BRG7
J	1298	GLN	-	expression tag	UNP K0BRG7
J	1299	GLY	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1300	GLY	-	expression tag	UNP K0BRG7
J	1301	GLY	-	expression tag	UNP K0BRG7
J	1302	SER	-	expression tag	UNP K0BRG7
J	1303	ALA	-	expression tag	UNP K0BRG7
J	1304	GLY	-	expression tag	UNP K0BRG7
J	1305	SER	-	expression tag	UNP K0BRG7
J	1306	GLY	-	expression tag	UNP K0BRG7
J	1307	TYR	-	expression tag	UNP K0BRG7
J	1308	ILE	-	expression tag	UNP K0BRG7
J	1309	PRO	-	expression tag	UNP K0BRG7
J	1310	GLU	-	expression tag	UNP K0BRG7
J	1311	ALA	-	expression tag	UNP K0BRG7
J	1312	PRO	-	expression tag	UNP K0BRG7
J	1313	ARG	-	expression tag	UNP K0BRG7
J	1314	ASP	-	expression tag	UNP K0BRG7
J	1315	GLY	-	expression tag	UNP K0BRG7
J	1316	GLN	-	expression tag	UNP K0BRG7
J	1317	ALA	-	expression tag	UNP K0BRG7
J	1318	TYR	-	expression tag	UNP K0BRG7
J	1319	VAL	-	expression tag	UNP K0BRG7
J	1320	ARG	-	expression tag	UNP K0BRG7
J	1321	LYS	-	expression tag	UNP K0BRG7
J	1322	ASP	-	expression tag	UNP K0BRG7
J	1323	GLY	-	expression tag	UNP K0BRG7
J	1324	GLU	-	expression tag	UNP K0BRG7
J	1325	TRP	-	expression tag	UNP K0BRG7
J	1326	VAL	-	expression tag	UNP K0BRG7
J	1327	LEU	-	expression tag	UNP K0BRG7
J	1328	LEU	-	expression tag	UNP K0BRG7
J	1329	SER	-	expression tag	UNP K0BRG7
J	1330	THR	-	expression tag	UNP K0BRG7
J	1331	PHE	-	expression tag	UNP K0BRG7
J	1332	LEU	-	expression tag	UNP K0BRG7
J	1333	GLY	-	expression tag	UNP K0BRG7
J	1334	HIS	-	expression tag	UNP K0BRG7
J	1335	HIS	-	expression tag	UNP K0BRG7
J	1336	HIS	-	expression tag	UNP K0BRG7
J	1337	HIS	-	expression tag	UNP K0BRG7
J	1338	HIS	-	expression tag	UNP K0BRG7
J	1339	HIS	-	expression tag	UNP K0BRG7
J	1340	TRP	-	expression tag	UNP K0BRG7
J	1341	SER	-	expression tag	UNP K0BRG7

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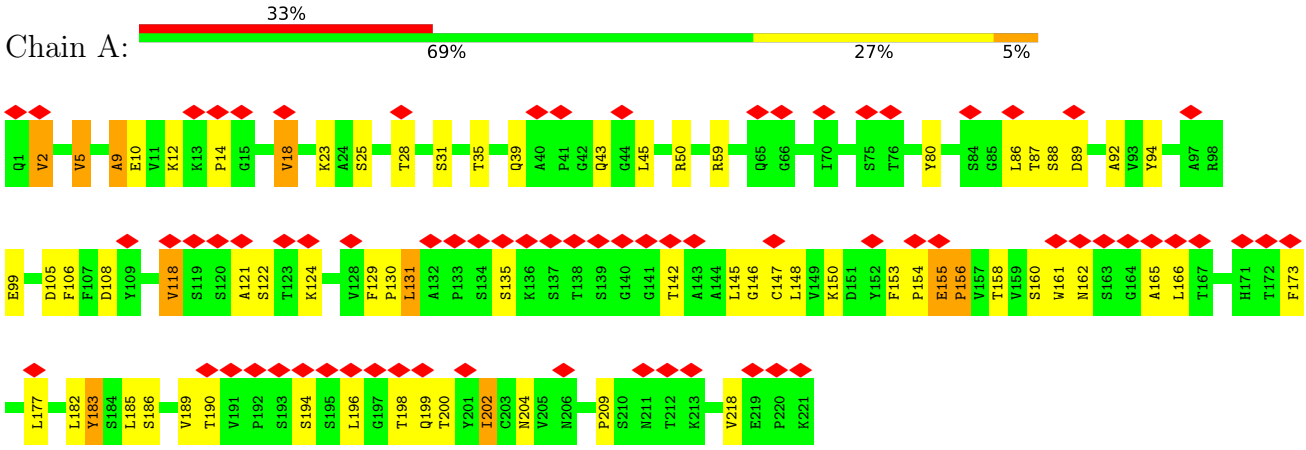
Chain	Residue	Modelled	Actual	Comment	Reference
J	1342	HIS	-	expression tag	UNP K0BRG7
J	1343	PRO	-	expression tag	UNP K0BRG7
J	1344	GLN	-	expression tag	UNP K0BRG7
J	1345	PHE	-	expression tag	UNP K0BRG7
J	1346	GLU	-	expression tag	UNP K0BRG7
J	1347	LYS	-	expression tag	UNP K0BRG7

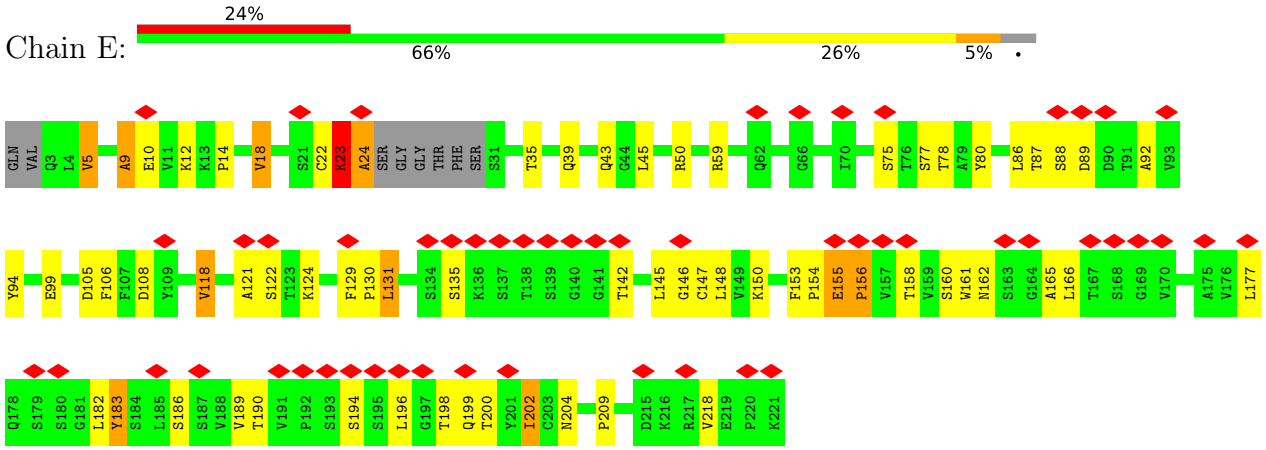
3 Residue-property plots (i)

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

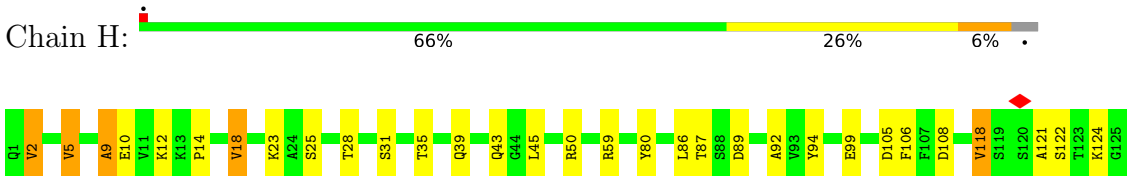
• Molecule 1: antibody S41 heavy chain

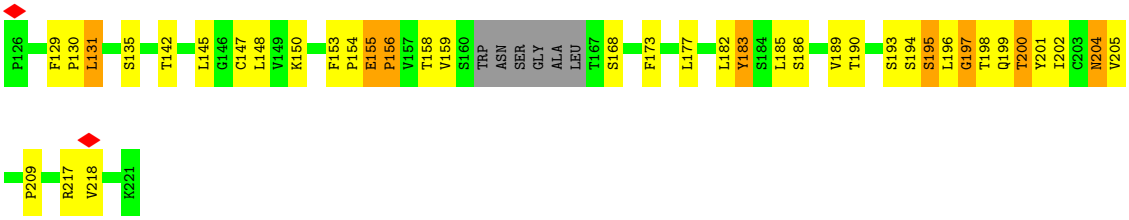


• Molecule 1: antibody S41 heavy chain

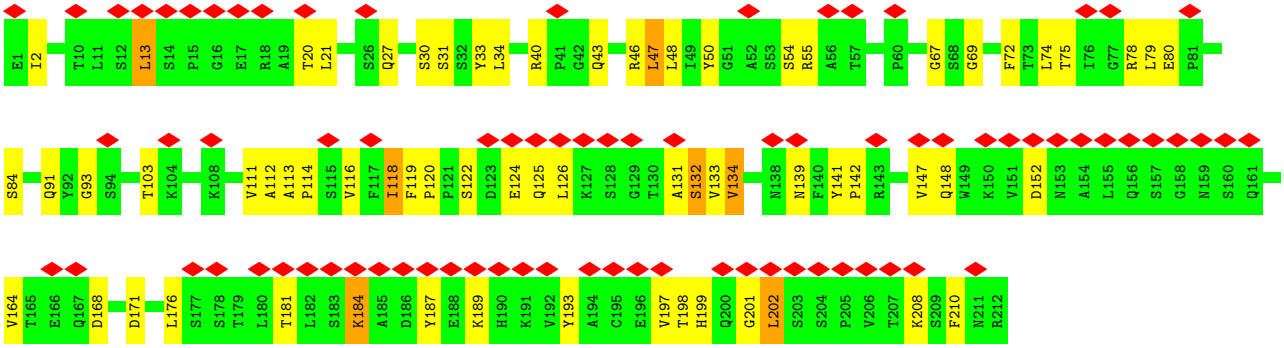


• Molecule 1: antibody S41 heavy chain

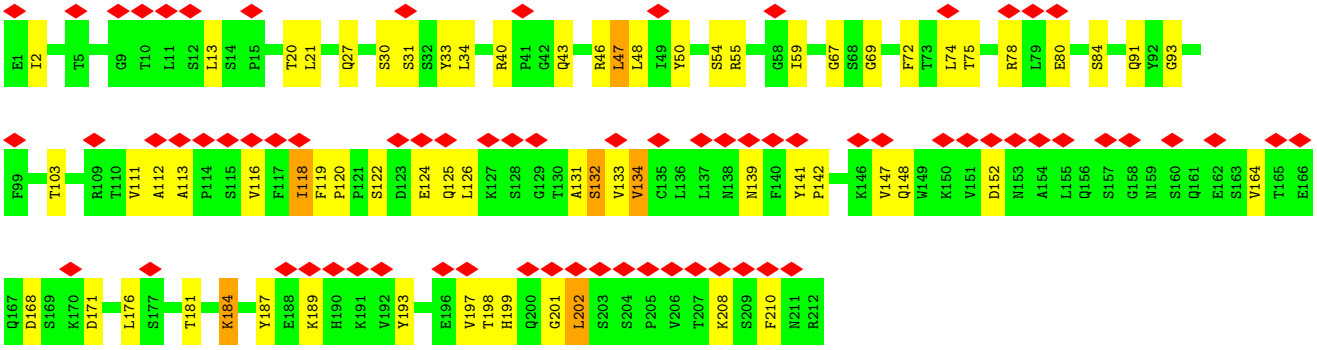




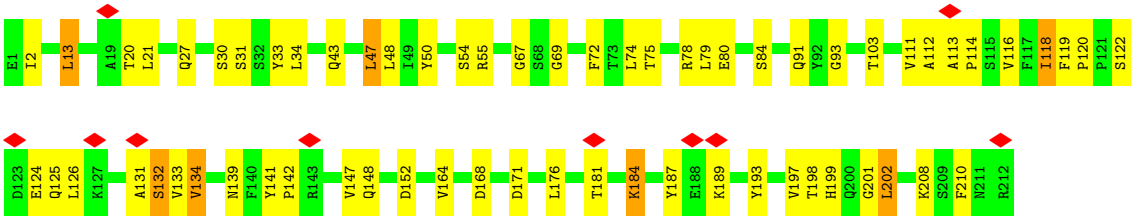
• Molecule 2: antibody S41 light chain



• Molecule 2: antibody S41 light chain



• Molecule 2: antibody S41 light chain

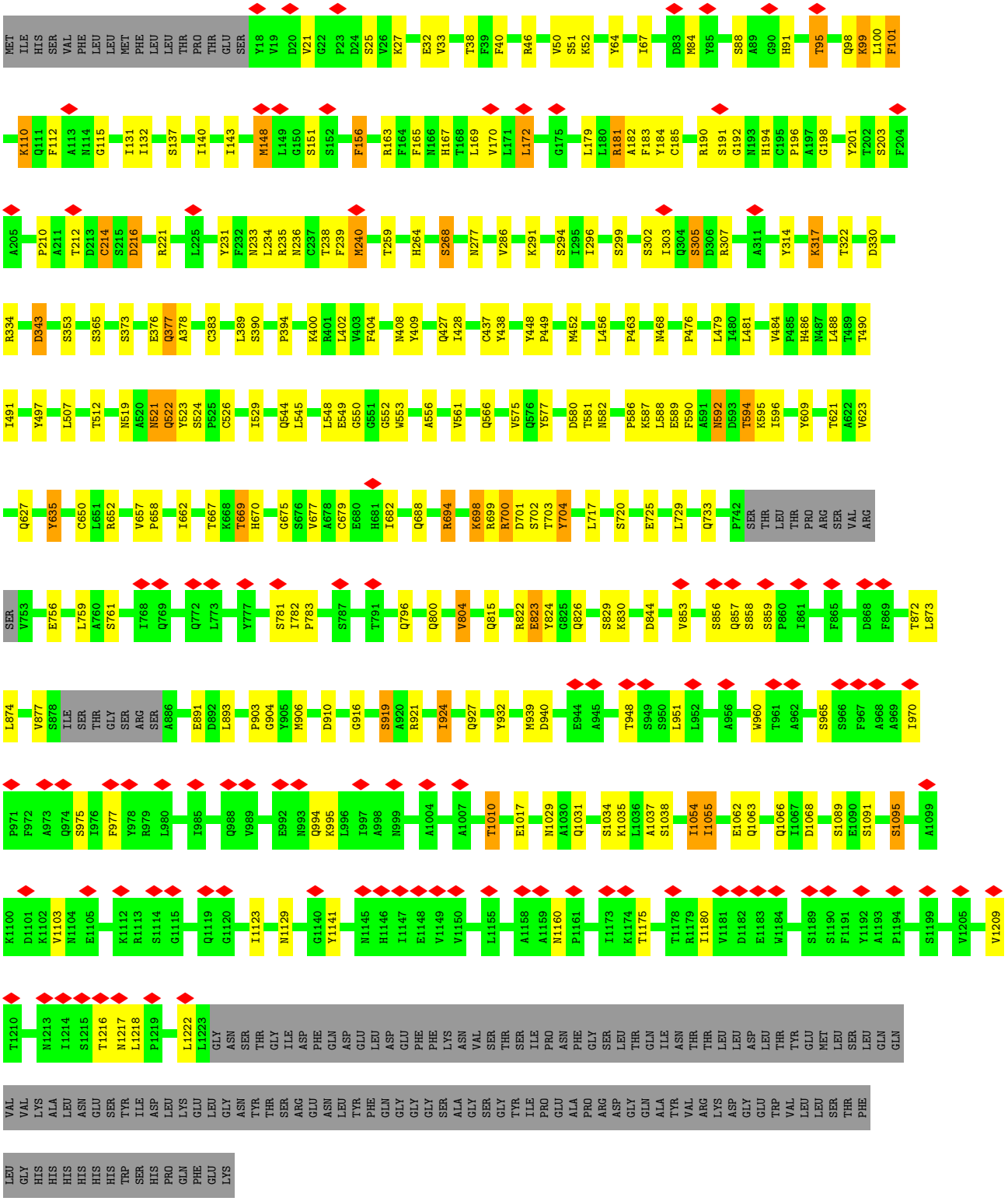


• Molecule 3: Spike glycoprotein

Chain G:

• Molecule 3: Spike glycoprotein

Chain I:



• Molecule 3: Spike glycoprotein

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	424969	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	346.4, 346.4, 346.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.68	4/1675 (0.2%)	0.75	6/2278 (0.3%)
1	E	0.68	4/1619 (0.2%)	0.77	7/2201 (0.3%)
1	H	0.64	2/1621 (0.1%)	0.73	2/2202 (0.1%)
2	C	0.65	0/1635	0.66	0/2223
2	F	0.65	0/1635	0.66	0/2223
2	K	0.65	0/1635	0.66	0/2223
3	G	0.31	0/9405	0.49	0/12803
3	I	0.31	0/9405	0.49	1/12803 (0.0%)
3	J	0.31	0/9346	0.49	0/12719
All	All	0.43	10/37976 (0.0%)	0.55	16/51675 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	H	0	1
3	G	0	4
3	I	0	3
3	J	0	3
All	All	0	13

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	186[A]	SER	C-O	7.05	1.36	1.23
1	E	186[B]	SER	C-O	7.05	1.36	1.23
1	A	186[A]	SER	C-O	7.04	1.36	1.23
1	A	186[B]	SER	C-O	7.04	1.36	1.23
1	H	186[A]	SER	C-O	7.00	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	186[B]	SER	C-O	7.00	1.36	1.23
1	E	160[A]	SER	C-O	6.82	1.36	1.23
1	E	160[B]	SER	C-O	6.82	1.36	1.23
1	A	160[A]	SER	C-O	6.79	1.36	1.23
1	A	160[B]	SER	C-O	6.79	1.36	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	24	ALA	N-CA-C	-6.43	93.65	111.00
1	A	160[A]	SER	CA-C-O	6.29	133.31	120.10
1	A	160[B]	SER	CA-C-O	6.29	133.31	120.10
1	E	160[A]	SER	CA-C-O	6.29	133.31	120.10
1	E	160[B]	SER	CA-C-O	6.29	133.31	120.10
1	A	160[A]	SER	CA-C-N	-5.85	104.33	117.20
1	A	160[B]	SER	CA-C-N	-5.85	104.33	117.20
1	E	160[A]	SER	CA-C-N	-5.83	104.37	117.20
1	E	160[B]	SER	CA-C-N	-5.83	104.37	117.20
1	A	186[A]	SER	CA-C-O	5.77	132.23	120.10
1	A	186[B]	SER	CA-C-O	5.77	132.23	120.10
1	H	186[A]	SER	CA-C-O	5.77	132.21	120.10
1	H	186[B]	SER	CA-C-O	5.77	132.21	120.10
1	E	186[A]	SER	CA-C-O	5.75	132.18	120.10
1	E	186[B]	SER	CA-C-O	5.75	132.18	120.10
3	I	650	CYS	CA-CB-SG	5.69	124.24	114.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	GLU	Peptide
1	E	155	GLU	Peptide
3	G	1217	ASN	Peptide
3	G	165	PHE	Peptide
3	G	380	GLY	Peptide
3	G	521	ASN	Peptide
1	H	155	GLU	Peptide
3	I	1217	ASN	Peptide
3	I	165	PHE	Peptide
3	I	521	ASN	Peptide
3	J	1217	ASN	Peptide
3	J	165	PHE	Peptide

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Mol	Chain	Res	Type	Group
3	J	521	ASN	Peptide

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	1633	0	1621	37	0
1	E	1579	0	1568	47	0
1	H	1585	0	1575	48	0
2	C	1601	0	1551	31	0
2	F	1601	0	1551	29	0
2	K	1601	0	1551	29	0
3	G	9189	0	8877	145	0
3	I	9189	0	8875	145	0
3	J	9132	0	8832	139	0
All	All	37110	0	36001	605	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 8.

All (605) 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)
3:I:580:ASP:OD2	3:J:62:ARG:NH2	1.59	1.34
3:I:377:GLN:HG2	3:I:408:ASN:ND2	1.64	1.10
1:E:75:SER:O	1:H:168:SER:OG	1.66	1.09
1:E:75:SER:O	1:H:168:SER:CB	2.04	1.04
3:I:580:ASP:OD2	3:J:62:ARG:CZ	2.05	1.03
3:I:580:ASP:CG	3:J:62:ARG:NH2	2.14	1.00
3:I:377:GLN:HG2	3:I:408:ASN:HD22	1.22	0.97
3:I:377:GLN:CG	3:I:408:ASN:ND2	2.31	0.93
3:J:181:ARG:HH11	3:J:240:MET:HE1	1.43	0.84
3:G:185:CYS:HB3	3:G:234:LEU:HD12	1.59	0.83
3:J:1125:SER:HG	3:J:1138:HIS:HD1	1.25	0.81
3:I:658:PRO:HG2	3:I:675:GLY:HA3	1.63	0.80
3:J:185:CYS:HB3	3:J:234:LEU:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:658:PRO:HG2	3:G:675:GLY:HA3	1.66	0.78
3:J:658:PRO:HG2	3:J:675:GLY:HA3	1.66	0.78
1:A:162:ASN:HB3	1:A:165:ALA:HB3	1.66	0.78
3:J:181:ARG:NH2	3:J:221:ARG:O	2.16	0.78
1:E:162:ASN:HB3	1:E:165:ALA:HB3	1.66	0.77
3:I:216:ASP:OD1	3:I:216:ASP:N	2.18	0.77
3:J:216:ASP:OD1	3:J:216:ASP:N	2.17	0.77
2:C:34:LEU:HD12	2:C:91:GLN:HG2	1.67	0.77
2:F:34:LEU:HD12	2:F:91:GLN:HG2	1.67	0.77
2:K:34:LEU:HD12	2:K:91:GLN:HG2	1.66	0.76
3:I:394:PRO:HG3	3:I:400:LYS:HG3	1.67	0.76
3:I:521:ASN:O	3:I:523:TYR:N	2.19	0.75
3:J:698:LYS:HA	3:J:698:LYS:HE2	1.68	0.75
3:G:394:PRO:HG3	3:G:400:LYS:HG3	1.67	0.75
3:J:521:ASN:O	3:J:523:TYR:N	2.19	0.75
3:J:394:PRO:HG3	3:J:400:LYS:HG3	1.67	0.74
3:G:698:LYS:HE2	3:G:698:LYS:HA	1.68	0.73
3:G:521:ASN:O	3:G:523:TYR:N	2.19	0.72
1:H:198:THR:HG22	1:H:217:ARG:HH11	1.55	0.72
3:G:667:THR:HG1	3:G:669:THR:HG1	1.28	0.72
3:I:698:LYS:HE2	3:I:698:LYS:HA	1.70	0.71
3:G:343:ASP:OD1	3:G:343:ASP:N	2.22	0.70
3:G:830:LYS:HE3	3:G:830:LYS:HA	1.73	0.70
2:K:132:SER:HA	2:K:181:THR:HA	1.75	0.69
3:J:910:ASP:HA	3:J:913:MET:HG3	1.73	0.69
1:H:198:THR:HG22	1:H:217:ARG:NH1	2.08	0.68
3:J:343:ASP:OD1	3:J:343:ASP:N	2.23	0.68
1:H:87:THR:HG23	1:H:89:ASP:H	1.58	0.68
3:J:37:GLN:NE2	3:J:104:ASN:OD1	2.26	0.68
3:J:169:LEU:HD22	3:J:286:VAL:HG21	1.75	0.68
2:F:132:SER:HA	2:F:181:THR:HA	1.75	0.68
1:H:50:ARG:HH11	1:H:59:ARG:HE	1.43	0.67
1:A:87:THR:HG23	1:A:89:ASP:H	1.58	0.67
1:E:86:LEU:HD11	1:E:118:VAL:HG11	1.76	0.67
3:G:826:GLN:OE1	3:G:826:GLN:N	2.22	0.67
1:H:86:LEU:HD11	1:H:118:VAL:HG11	1.76	0.67
3:I:463:PRO:O	3:I:468:ASN:ND2	2.27	0.67
1:A:50:ARG:HH11	1:A:59:ARG:HE	1.43	0.67
1:E:87:THR:HG23	1:E:89:ASP:H	1.59	0.67
2:C:132:SER:HA	2:C:181:THR:HA	1.75	0.67
3:I:343:ASP:OD1	3:I:343:ASP:N	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:377:GLN:HE22	3:I:588:LEU:H	1.43	0.66
2:C:118:ILE:HD11	2:C:208:LYS:HB3	1.78	0.66
3:G:216:ASP:OD1	3:G:216:ASP:N	2.17	0.66
2:F:118:ILE:HD11	2:F:208:LYS:HB3	1.78	0.66
1:A:86:LEU:HD11	1:A:118:VAL:HG11	1.76	0.66
3:I:580:ASP:CG	3:J:62:ARG:HH21	1.98	0.66
1:A:124:LYS:HG2	1:A:182:LEU:HD21	1.78	0.65
1:E:124:LYS:HG2	1:E:182:LEU:HD21	1.78	0.65
3:G:463:PRO:O	3:G:468:ASN:ND2	2.27	0.65
3:I:156:PHE:CD1	3:I:163:ARG:HB2	2.32	0.65
3:I:702:SER:HB2	3:I:704:TYR:CZ	2.32	0.65
3:J:657:VAL:HG13	3:J:677:VAL:HG21	1.79	0.65
3:I:428:ILE:HG13	3:J:1057:ARG:O	1.96	0.65
1:E:50:ARG:HH11	1:E:59:ARG:HE	1.43	0.64
2:C:193:TYR:H	2:C:210:PHE:HB3	1.63	0.64
1:H:124:LYS:HG2	1:H:182:LEU:HD21	1.78	0.64
3:J:463:PRO:O	3:J:468:ASN:ND2	2.27	0.64
2:K:118:ILE:HD11	2:K:208:LYS:HB3	1.78	0.64
2:F:193:TYR:H	2:F:210:PHE:HB3	1.63	0.64
1:A:131:LEU:HD22	1:A:218:VAL:HG22	1.80	0.64
1:E:50:ARG:NH1	1:E:59:ARG:HE	1.96	0.64
2:K:193:TYR:H	2:K:210:PHE:HB3	1.63	0.64
3:J:702:SER:HB2	3:J:704:TYR:CZ	2.33	0.64
1:H:50:ARG:NH1	1:H:59:ARG:HE	1.96	0.64
1:H:131:LEU:HD22	1:H:218:VAL:HG22	1.80	0.63
3:G:1155:LEU:HD22	3:G:1214:ILE:HD11	1.79	0.63
3:J:1155:LEU:HD22	3:J:1214:ILE:HD11	1.79	0.63
1:A:50:ARG:NH1	1:A:59:ARG:HE	1.96	0.62
1:E:22:CYS:O	1:E:24:ALA:N	2.32	0.62
2:F:168:ASP:HB3	2:F:171:ASP:HB2	1.81	0.62
1:H:130:PRO:HG3	2:K:124:GLU:HB3	1.82	0.62
1:E:131:LEU:HD22	1:E:218:VAL:HG22	1.80	0.62
3:J:156:PHE:CD1	3:J:163:ARG:HB2	2.34	0.62
3:G:156:PHE:CD1	3:G:163:ARG:HB2	2.34	0.62
1:E:130:PRO:HG3	2:F:124:GLU:HB3	1.82	0.61
3:G:181:ARG:HG3	3:G:183:PHE:HE2	1.65	0.61
3:G:702:SER:HB2	3:G:704:TYR:CZ	2.36	0.61
3:I:169:LEU:HD22	3:I:286:VAL:HG21	1.80	0.61
3:G:190:ARG:NH1	3:G:233:ASN:OD1	2.33	0.61
3:G:389:LEU:HA	3:G:491:ILE:HD11	1.82	0.61
2:C:168:ASP:HB3	2:C:171:ASP:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:168:ASP:HB3	2:K:171:ASP:HB2	1.81	0.61
1:E:23:LYS:HA	1:E:78:THR:HG23	1.82	0.60
3:J:190:ARG:NH1	3:J:233:ASN:OD1	2.33	0.60
3:I:389:LEU:HA	3:I:491:ILE:HD11	1.82	0.60
3:I:100:LEU:HD22	3:I:299:SER:HB3	1.83	0.60
3:I:635:TYR:CZ	3:J:921:ARG:HD2	2.37	0.60
1:A:130:PRO:HG3	2:C:124:GLU:HB3	1.82	0.60
3:I:101:PHE:CD2	3:I:132:ILE:HG22	2.36	0.60
3:I:183:PHE:HD1	3:I:185:CYS:HB2	1.65	0.60
3:J:389:LEU:HA	3:J:491:ILE:HD11	1.82	0.60
3:I:181:ARG:NH1	3:I:221:ARG:O	2.27	0.60
3:I:210:PRO:HA	3:I:214:CYS:HB2	1.84	0.59
3:J:261:GLN:N	3:J:261:GLN:OE1	2.35	0.59
3:I:190:ARG:NH1	3:I:233:ASN:OD1	2.35	0.59
3:I:259:THR:OG1	3:I:264:HIS:NE2	2.24	0.59
3:I:581:THR:HG22	3:J:61:GLY:HA3	1.84	0.59
3:I:91:HIS:O	3:I:98:GLN:N	2.32	0.59
3:G:132:ILE:HD11	3:G:307:ARG:CZ	2.32	0.59
3:J:1054:ILE:HD13	3:J:1066:GLN:HB2	1.85	0.59
3:G:456:LEU:HG	3:G:479:LEU:HD21	1.85	0.58
3:J:1055:ILE:O	3:J:1063:GLN:NE2	2.36	0.58
3:I:132:ILE:HD11	3:I:307:ARG:CZ	2.33	0.58
3:I:456:LEU:HG	3:I:479:LEU:HD21	1.85	0.58
2:F:119:PHE:HB2	2:F:134:VAL:HG23	1.85	0.58
3:G:181:ARG:HE	3:G:240:MET:HE1	1.67	0.58
1:E:22:CYS:C	1:E:24:ALA:H	2.07	0.58
2:K:119:PHE:HB2	2:K:134:VAL:HG23	1.85	0.58
2:F:31:SER:HA	2:F:69:GLY:H	1.69	0.58
3:G:101:PHE:CD2	3:G:132:ILE:HG22	2.39	0.58
2:F:131:ALA:HB3	2:F:187:TYR:OH	2.04	0.57
2:K:131:ALA:HB3	2:K:187:TYR:OH	2.04	0.57
2:C:119:PHE:HB2	2:C:134:VAL:HG23	1.85	0.57
3:J:804:VAL:HA	3:J:932:TYR:HA	1.86	0.57
2:C:199:HIS:CD2	2:C:201:GLY:H	2.22	0.57
3:G:91:HIS:O	3:G:98:GLN:N	2.33	0.57
3:J:33:VAL:HG12	3:J:100:LEU:HD12	1.87	0.57
2:K:199:HIS:CD2	2:K:201:GLY:H	2.22	0.57
2:C:131:ALA:HB3	2:C:187:TYR:OH	2.04	0.57
2:C:31:SER:HA	2:C:69:GLY:H	1.69	0.57
3:I:33:VAL:HG12	3:I:100:LEU:HD12	1.87	0.57
3:I:484:VAL:HG23	3:I:488:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:456:LEU:HG	3:J:479:LEU:HD21	1.85	0.56
3:G:118:VAL:HG22	3:G:315:VAL:HG22	1.87	0.56
3:G:733:GLN:O	3:I:940:ASP:N	2.39	0.56
3:I:377:GLN:HG3	3:I:408:ASN:ND2	2.19	0.56
3:J:246:THR:O	3:J:269:ARG:NH2	2.38	0.56
2:F:199:HIS:CD2	2:F:201:GLY:H	2.22	0.56
2:K:31:SER:HA	2:K:69:GLY:H	1.69	0.56
3:G:804:VAL:HA	3:G:932:TYR:HA	1.88	0.56
3:J:84:MET:HG3	3:J:314:TYR:CE2	2.41	0.56
3:G:100:LEU:HD22	3:G:299:SER:HB3	1.86	0.56
3:J:259:THR:OG1	3:J:264:HIS:NE2	2.24	0.56
3:J:484:VAL:HG23	3:J:488:LEU:HD23	1.87	0.56
3:I:826:GLN:OE1	3:I:826:GLN:N	2.26	0.56
1:A:10:GLU:HG3	1:A:18:VAL:HG23	1.88	0.56
3:G:725:GLU:OE1	3:G:725:GLU:N	2.24	0.56
3:I:181:ARG:HH21	3:I:240:MET:HE1	1.70	0.56
3:G:484:VAL:HG23	3:G:488:LEU:HD23	1.87	0.56
3:I:1055:ILE:O	3:I:1063:GLN:NE2	2.39	0.56
3:I:652:ARG:HE	3:J:915:GLN:HB3	1.71	0.56
3:I:657:VAL:HG13	3:I:677:VAL:HG11	1.87	0.56
3:G:303:ILE:HG22	3:G:305:SER:H	1.71	0.55
3:G:824:TYR:OH	3:G:1068:ASP:OD1	2.22	0.55
3:J:183:PHE:HD1	3:J:185:CYS:HB2	1.71	0.55
3:J:303:ILE:HG22	3:J:305:SER:H	1.71	0.55
1:A:162:ASN:HD21	1:A:199:GLN:HB3	1.72	0.55
3:J:853:VAL:HG13	3:J:951:LEU:HD22	1.88	0.55
3:I:303:ILE:HG22	3:I:305:SER:H	1.71	0.55
3:I:185:CYS:HB3	3:I:234:LEU:HD12	1.90	0.54
1:A:5:VAL:HG23	1:A:23:LYS:HB3	1.90	0.54
1:E:10:GLU:HG3	1:E:18:VAL:HG23	1.88	0.54
3:G:259:THR:OG1	3:G:264:HIS:NE2	2.24	0.54
1:H:10:GLU:HG3	1:H:18:VAL:HG23	1.88	0.54
3:J:796:GLN:O	3:J:1095:SER:HB3	2.06	0.54
3:I:322:THR:OG1	3:J:822:ARG:NH1	2.41	0.54
2:F:120:PRO:HA	2:F:133:VAL:HG13	1.90	0.54
3:G:657:VAL:HG13	3:G:677:VAL:HG11	1.89	0.54
1:H:202:ILE:HG22	1:H:204:ASN:HB3	1.89	0.54
3:G:101:PHE:HD2	3:G:132:ILE:HG22	1.73	0.54
1:H:201:TYR:HA	1:H:217:ARG:HA	1.89	0.54
3:I:804:VAL:HA	3:I:932:TYR:HA	1.90	0.54
3:G:1055:ILE:O	3:G:1063:GLN:NE2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:120:PRO:HA	2:K:133:VAL:HG13	1.90	0.53
3:J:960:TRP:CZ2	3:J:970:ILE:HD13	2.44	0.53
1:E:162:ASN:HD21	1:E:199:GLN:HB3	1.72	0.53
3:I:238:THR:HG22	3:I:239:PHE:H	1.74	0.53
3:I:594:THR:O	3:I:594:THR:OG1	2.16	0.53
3:G:686:MET:HE3	3:G:689:TYR:CD2	2.43	0.53
1:H:121:ALA:O	1:H:122:SER:OG	2.26	0.53
3:J:91:HIS:O	3:J:98:GLN:N	2.34	0.53
3:G:248:ASP:OD1	3:G:269:ARG:NH2	2.40	0.53
3:G:709:THR:OG1	3:G:712:GLY:O	2.18	0.53
3:G:449:PRO:HG3	3:G:561:VAL:HG11	1.90	0.53
3:G:238:THR:HG22	3:G:239:PHE:H	1.73	0.53
1:H:5:VAL:HG23	1:H:23:LYS:HB3	1.90	0.53
3:J:268:SER:O	3:J:268:SER:OG	2.27	0.52
3:I:592:ASN:O	3:I:592:ASN:ND2	2.41	0.52
3:I:824:TYR:OH	3:I:1068:ASP:OD1	2.27	0.52
3:I:919:SER:O	3:I:919:SER:OG	2.28	0.52
1:E:130:PRO:HB3	2:F:122:SER:HB3	1.92	0.52
3:J:449:PRO:HG3	3:J:561:VAL:HG11	1.91	0.52
2:C:120:PRO:HA	2:C:133:VAL:HG13	1.90	0.52
1:H:106:PHE:HB2	2:K:47:LEU:HD11	1.92	0.52
3:G:84:MET:HG3	3:G:314:TYR:CE2	2.45	0.52
3:J:238:THR:HG22	3:J:239:PHE:H	1.75	0.52
3:J:117:VAL:HG12	3:J:278:MET:HE1	1.91	0.52
2:K:91:GLN:C	2:K:93:GLY:H	2.13	0.52
3:I:733:GLN:O	3:J:940:ASP:N	2.43	0.52
1:A:130:PRO:HB3	2:C:122:SER:HB3	1.92	0.51
1:E:22:CYS:C	1:E:24:ALA:N	2.64	0.51
3:G:183:PHE:HD1	3:G:185:CYS:HB2	1.74	0.51
3:I:449:PRO:HG3	3:I:561:VAL:HG11	1.91	0.51
3:G:519:ASN:HB2	3:G:522:GLN:CD	2.31	0.51
3:J:826:GLN:OE1	3:J:826:GLN:N	2.37	0.51
3:G:1054:ILE:HD13	3:G:1066:GLN:HB2	1.93	0.51
2:C:21:LEU:HD12	2:C:74:LEU:HD23	1.93	0.51
2:F:21:LEU:HD12	2:F:74:LEU:HD23	1.93	0.51
1:H:130:PRO:HB3	2:K:122:SER:HB3	1.92	0.51
3:J:215:SER:OG	3:J:218:ASN:O	2.28	0.51
1:E:162:ASN:HB2	1:E:166:LEU:H	1.76	0.51
3:G:427:GLN:HB2	3:G:476:PRO:HA	1.93	0.51
3:G:796:GLN:O	3:G:1095:SER:HB3	2.11	0.51
3:G:921:ARG:NH2	3:G:1037:ALA:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:939:MET:HG2	3:G:943:MET:HG2	1.91	0.51
3:I:667:THR:OG1	3:I:669:THR:OG1	2.25	0.51
1:A:155:GLU:HG2	1:A:156:PRO:HA	1.93	0.51
3:G:91:HIS:HB2	3:G:99:LYS:HG3	1.93	0.51
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.93	0.51
3:I:796:GLN:O	3:I:1095:SER:HB3	2.11	0.51
3:I:1054:ILE:HD13	3:I:1066:GLN:HB2	1.93	0.51
3:J:169:LEU:HD12	3:J:170:VAL:N	2.26	0.51
1:H:9:ALA:CB	1:H:156:PRO:HD3	2.41	0.51
3:I:652:ARG:HG3	3:I:652:ARG:HH11	1.76	0.51
3:J:235:ARG:HG2	3:J:235:ARG:HH11	1.75	0.51
1:A:162:ASN:HB2	1:A:166:LEU:H	1.76	0.51
3:G:919:SER:O	3:G:919:SER:OG	2.28	0.51
3:J:519:ASN:HB2	3:J:522:GLN:CD	2.31	0.51
2:F:91:GLN:C	2:F:93:GLY:H	2.13	0.51
3:G:181:ARG:NH1	3:G:221:ARG:O	2.26	0.51
3:G:822:ARG:HH12	3:J:72:GLN:HG2	1.76	0.51
1:H:155:GLU:HG2	1:H:156:PRO:HA	1.93	0.51
1:A:106:PHE:HB2	2:C:47:LEU:HD11	1.92	0.50
1:E:155:GLU:HG2	1:E:156:PRO:HA	1.93	0.50
3:G:235:ARG:HG2	3:G:235:ARG:HH11	1.76	0.50
3:G:665:LYS:O	3:G:668:LYS:HD3	2.11	0.50
2:K:21:LEU:HD12	2:K:74:LEU:HD23	1.93	0.50
1:A:9:ALA:CB	1:A:156:PRO:HD3	2.41	0.50
1:E:75:SER:O	1:H:168:SER:HB2	2.05	0.50
1:E:106:PHE:HB2	2:F:47:LEU:HD11	1.92	0.50
3:I:1010:THR:O	3:I:1010:THR:OG1	2.29	0.50
3:J:132:ILE:HD11	3:J:307:ARG:CZ	2.42	0.50
3:J:427:GLN:HB2	3:J:476:PRO:HA	1.93	0.50
3:J:728:LYS:HA	3:J:728:LYS:HE2	1.93	0.50
2:C:91:GLN:C	2:C:93:GLY:H	2.13	0.50
3:G:1010:THR:O	3:G:1010:THR:OG1	2.28	0.50
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.93	0.50
1:E:39:GLN:HB2	1:E:45:LEU:HD23	1.93	0.50
3:I:268:SER:O	3:I:268:SER:OG	2.21	0.50
3:J:1035:LYS:HB2	3:J:1035:LYS:NZ	2.27	0.50
1:E:9:ALA:CB	1:E:156:PRO:HD3	2.41	0.50
3:G:486:HIS:CE1	3:G:566:GLN:HE21	2.30	0.50
3:G:1062:GLU:OE2	3:G:1062:GLU:N	2.42	0.50
3:I:402:LEU:HB3	3:I:404:PHE:CE1	2.47	0.50
3:J:701:ASP:O	3:J:703:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:486:HIS:CE1	3:J:566:GLN:HE21	2.30	0.50
3:J:1060:PRO:HA	3:J:1063:GLN:HB2	1.93	0.50
3:I:519:ASN:HB2	3:I:522:GLN:CD	2.31	0.50
3:I:717:LEU:HD13	3:I:759:LEU:HB2	1.93	0.49
3:I:91:HIS:HB2	3:I:99:LYS:HG3	1.93	0.49
3:I:437:CYS:O	3:I:582:ASN:ND2	2.45	0.49
3:J:402:LEU:HB3	3:J:404:PHE:CE1	2.47	0.49
3:G:437:CYS:O	3:G:582:ASN:ND2	2.45	0.49
1:H:198:THR:CG2	1:H:217:ARG:NH1	2.74	0.49
1:E:121:ALA:O	1:E:122:SER:OG	2.26	0.49
3:I:88:SER:HB2	3:I:131:ILE:HB	1.94	0.49
3:I:95:THR:HA	3:I:303:ILE:HD12	1.95	0.49
3:I:486:HIS:CE1	3:I:566:GLN:HE21	2.30	0.49
3:G:824:TYR:OH	3:G:1072:ASN:ND2	2.45	0.49
3:G:916:GLY:O	3:J:652:ARG:NH1	2.39	0.49
3:I:151:SER:O	3:I:291:LYS:NZ	2.45	0.49
3:I:427:GLN:HB2	3:I:476:PRO:HA	1.93	0.49
3:I:702:SER:OG	3:I:756:GLU:OE2	2.27	0.49
3:J:824:TYR:OH	3:J:1072:ASN:ND2	2.46	0.49
1:A:121:ALA:O	1:A:122:SER:OG	2.26	0.49
3:I:46:ARG:HG3	3:I:314:TYR:CZ	2.47	0.49
1:A:92:ALA:HB3	1:A:94:TYR:HE1	1.78	0.49
3:G:402:LEU:HB3	3:G:404:PHE:CE1	2.47	0.49
3:I:383:CYS:SG	3:I:409:TYR:HB3	2.53	0.49
3:I:524:SER:O	3:I:526:CYS:N	2.46	0.49
3:J:88:SER:HB2	3:J:131:ILE:HB	1.95	0.49
1:A:9:ALA:HB3	1:A:156:PRO:HD3	1.95	0.49
1:E:92:ALA:HB3	1:E:94:TYR:HE1	1.78	0.49
1:E:155:GLU:HB2	1:E:183:TYR:CE1	2.48	0.49
3:G:259:THR:HG1	3:G:264:HIS:HE2	1.56	0.49
3:G:524:SER:O	3:G:526:CYS:N	2.46	0.49
3:I:40:PHE:HE1	3:I:88:SER:HB3	1.77	0.49
1:H:92:ALA:HB3	1:H:94:TYR:HE1	1.78	0.48
3:I:112:PHE:CZ	3:I:115:GLY:HA2	2.48	0.48
3:G:40:PHE:HE1	3:G:88:SER:HB3	1.77	0.48
3:G:1125:SER:OG	3:G:1138:HIS:ND1	2.40	0.48
3:J:620:CYS:SG	3:J:650:CYS:N	2.86	0.48
2:K:126:LEU:HD23	2:K:131:ALA:HB2	1.95	0.48
1:A:155:GLU:HB2	1:A:183:TYR:CE1	2.48	0.48
3:J:800:GLN:HB2	3:J:1029:ASN:ND2	2.28	0.48
3:G:800:GLN:HB2	3:G:1029:ASN:ND2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:170:VAL:O	3:I:182:ALA:HA	2.14	0.48
3:I:377:GLN:C	3:I:609:TYR:CZ	2.87	0.48
3:J:91:HIS:HB2	3:J:99:LYS:HG3	1.96	0.48
3:J:101:PHE:CD2	3:J:132:ILE:HG22	2.49	0.48
3:J:1010:THR:O	3:J:1010:THR:OG1	2.27	0.48
3:G:268:SER:O	3:G:268:SER:OG	2.28	0.48
3:G:277:ASN:N	3:G:277:ASN:HD22	2.11	0.48
1:H:2:VAL:HG23	1:H:25:SER:O	2.14	0.48
3:J:919:SER:O	3:J:919:SER:OG	2.27	0.48
3:I:652:ARG:NH2	3:J:914:GLN:O	2.47	0.48
1:A:131:LEU:HD23	1:A:147:CYS:HB3	1.96	0.48
1:E:9:ALA:HB3	1:E:156:PRO:HD3	1.95	0.48
2:F:126:LEU:HD23	2:F:131:ALA:HB2	1.95	0.48
1:H:131:LEU:HD23	1:H:147:CYS:HB3	1.96	0.48
1:H:155:GLU:HB2	1:H:183:TYR:CE1	2.48	0.48
3:I:169:LEU:HD12	3:I:170:VAL:N	2.29	0.48
3:I:580:ASP:OD1	3:J:62:ARG:NH2	2.44	0.48
1:E:131:LEU:HD23	1:E:147:CYS:HB3	1.96	0.47
1:H:9:ALA:HB3	1:H:156:PRO:HD3	1.95	0.47
3:I:378:ALA:HB2	3:I:609:TYR:HE2	1.79	0.47
3:J:374:VAL:HG11	3:J:596:ILE:HG12	1.96	0.47
3:I:577:TYR:CZ	3:J:1057:ARG:NE	2.83	0.47
3:J:594:THR:O	3:J:594:THR:OG1	2.31	0.47
1:A:2:VAL:HG23	1:A:25:SER:O	2.14	0.47
3:J:112:PHE:CZ	3:J:115:GLY:HA2	2.49	0.47
3:G:262:GLY:HA2	3:G:286:VAL:O	2.15	0.47
1:H:12:LYS:HB2	1:H:118:VAL:HG12	1.97	0.47
3:I:181:ARG:HG3	3:I:183:PHE:HE2	1.79	0.47
3:J:720:SER:HB3	3:J:758:ARG:HB3	1.96	0.47
3:G:526:CYS:SG	3:G:556:ALA:HB2	2.54	0.47
3:I:662:ILE:O	3:I:670:HIS:HA	2.14	0.47
1:A:129:PHE:CZ	2:C:125:GLN:HG2	2.50	0.47
1:A:129:PHE:CE2	2:C:125:GLN:HG2	2.50	0.47
1:E:50:ARG:HH11	1:E:59:ARG:NE	2.11	0.47
3:G:88:SER:HB2	3:G:131:ILE:HB	1.96	0.47
1:H:129:PHE:CE2	2:K:125:GLN:HG2	2.50	0.47
3:I:526:CYS:SG	3:I:556:ALA:HB2	2.54	0.47
3:I:652:ARG:NH2	3:J:916:GLY:O	2.48	0.47
1:E:148:LEU:HD21	1:E:150:LYS:HE3	1.97	0.47
3:G:212:THR:O	3:G:215:SER:OG	2.31	0.47
1:E:12:LYS:HB2	1:E:118:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:PHE:CE2	2:F:125:GLN:HG2	2.50	0.47
3:I:652:ARG:HG3	3:I:652:ARG:NH1	2.30	0.47
3:J:40:PHE:HE1	3:J:88:SER:HB3	1.78	0.47
1:A:129:PHE:CE1	1:A:150:LYS:HB3	2.50	0.47
2:C:126:LEU:HD23	2:C:131:ALA:HB2	1.95	0.47
1:E:129:PHE:CZ	2:F:125:GLN:HG2	2.50	0.47
3:G:169:LEU:HD12	3:G:170:VAL:N	2.30	0.47
3:I:782:ILE:HG13	3:I:783:PRO:HD2	1.95	0.47
3:G:701:ASP:O	3:G:703:THR:HG22	2.15	0.46
3:G:826:GLN:O	3:G:830:LYS:HG2	2.14	0.46
3:G:907:GLN:HB3	3:J:678:ALA:HB2	1.96	0.46
1:H:129:PHE:CE1	1:H:150:LYS:HB3	2.50	0.46
3:J:95:THR:HA	3:J:303:ILE:HD12	1.97	0.46
1:E:75:SER:C	1:H:168:SER:OG	2.47	0.46
1:E:129:PHE:CE1	1:E:150:LYS:HB3	2.50	0.46
3:G:549:GLU:HA	3:G:550:GLY:HA2	1.64	0.46
3:G:587:LYS:HB2	3:G:587:LYS:HE3	1.36	0.46
1:H:148:LEU:HD21	1:H:150:LYS:HE3	1.97	0.46
3:G:168:THR:O	3:G:168:THR:OG1	2.32	0.46
3:G:192:GLY:O	3:G:198:GLY:HA3	2.16	0.46
3:J:709:THR:OG1	3:J:712:GLY:O	2.19	0.46
1:A:12:LYS:HB2	1:A:118:VAL:HG12	1.97	0.46
3:I:172:LEU:O	3:I:181:ARG:HG2	2.16	0.46
3:J:662:ILE:O	3:J:670:HIS:HA	2.16	0.46
3:G:102:VAL:HB	3:G:297:PRO:HB3	1.97	0.46
3:I:277:ASN:HD22	3:I:277:ASN:H	1.63	0.46
3:J:291:LYS:HB2	3:J:292:TYR:CE1	2.51	0.46
2:F:47:LEU:HD21	2:F:50:TYR:HB3	1.98	0.46
3:J:192:GLY:O	3:J:198:GLY:HA3	2.16	0.46
3:J:824:TYR:OH	3:J:1068:ASP:OD1	2.27	0.46
1:A:129:PHE:CZ	1:A:150:LYS:HB3	2.51	0.46
3:G:112:PHE:CZ	3:G:115:GLY:HA2	2.50	0.46
3:I:234:LEU:H	3:I:234:LEU:HD22	1.81	0.46
3:I:507:LEU:HD12	3:I:512:THR:HB	1.98	0.46
2:C:78:ARG:HH11	2:C:80:GLU:HG3	1.81	0.46
3:G:620:CYS:SG	3:G:650:CYS:N	2.88	0.46
1:H:129:PHE:CZ	2:K:125:GLN:HG2	2.50	0.46
3:J:376:GLU:HB2	3:J:608:LEU:HD23	1.98	0.46
1:H:129:PHE:CZ	1:H:150:LYS:HB3	2.51	0.46
3:I:701:ASP:O	3:I:703:THR:HG22	2.15	0.46
3:G:156:PHE:HD2	3:G:201:TYR:CE2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:807:LYS:NZ	3:J:692:SER:OG	2.48	0.45
3:I:101:PHE:HD2	3:I:132:ILE:HG22	1.79	0.45
3:I:1062:GLU:OE2	3:I:1062:GLU:N	2.47	0.45
3:J:69:ILE:HD11	3:J:327:PHE:HE1	1.81	0.45
3:J:192:GLY:H	3:J:198:GLY:HA3	1.81	0.45
3:J:939:MET:HE3	3:J:944:GLU:HG3	1.97	0.45
1:H:50:ARG:HH11	1:H:59:ARG:NE	2.11	0.45
3:I:183:PHE:CD1	3:I:185:CYS:HB2	2.50	0.45
3:J:891:GLU:OE1	3:J:1129:ASN:HB2	2.16	0.45
2:K:78:ARG:HH11	2:K:80:GLU:HG3	1.81	0.45
3:I:156:PHE:HD2	3:I:201:TYR:CE2	2.34	0.45
3:J:156:PHE:HD2	3:J:201:TYR:CE2	2.35	0.45
2:K:47:LEU:HD21	2:K:50:TYR:HB3	1.98	0.45
3:G:383:CYS:SG	3:G:409:TYR:HB3	2.56	0.45
3:I:32:GLU:HB2	3:I:194:HIS:CD2	2.52	0.45
3:I:577:TYR:CE2	3:J:1057:ARG:NH2	2.84	0.45
3:I:800:GLN:HB2	3:I:1029:ASN:ND2	2.31	0.45
3:J:110:LYS:HE2	3:J:110:LYS:HB3	1.56	0.45
2:K:48:LEU:HD23	2:K:48:LEU:HA	1.82	0.45
1:E:129:PHE:CZ	1:E:150:LYS:HB3	2.51	0.45
3:I:192:GLY:O	3:I:198:GLY:HA3	2.15	0.45
1:A:148:LEU:HD21	1:A:150:LYS:HE3	1.97	0.45
2:C:47:LEU:HD21	2:C:50:TYR:HB3	1.98	0.45
3:I:438:TYR:CD2	3:I:575:VAL:HB	2.52	0.45
3:I:853:VAL:HG13	3:I:951:LEU:HD22	1.99	0.45
3:I:904:GLY:C	3:I:906:MET:H	2.20	0.45
3:J:184:TYR:OH	3:J:286:VAL:HG13	2.17	0.45
3:J:1180:ILE:H	3:J:1180:ILE:HG12	1.41	0.45
3:G:300:ILE:HD13	3:G:310:TRP:NE1	2.31	0.45
3:G:334:ARG:HD3	3:G:334:ARG:HA	1.64	0.45
3:G:438:TYR:CD2	3:G:575:VAL:HB	2.52	0.45
3:G:507:LEU:HD12	3:G:512:THR:HB	1.98	0.45
3:I:110:LYS:HB3	3:I:110:LYS:HE2	1.59	0.45
3:I:549:GLU:HA	3:I:550:GLY:HA2	1.64	0.45
3:I:903:PRO:HA	3:I:924:ILE:HG13	1.99	0.45
3:G:904:GLY:C	3:G:906:MET:H	2.21	0.45
3:G:1123:ILE:HD11	3:G:1141:TYR:HB2	1.98	0.45
3:I:891:GLU:OE1	3:I:1129:ASN:HB2	2.17	0.45
3:J:438:TYR:CD2	3:J:575:VAL:HB	2.52	0.45
3:G:822:ARG:NH1	3:J:72:GLN:HG2	2.33	0.44
3:I:977:PHE:CZ	3:I:994:GLN:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:VAL:HG23	1:E:23:LYS:HB2	1.98	0.44
2:F:78:ARG:HH11	2:F:80:GLU:HG3	1.81	0.44
3:G:1180:ILE:H	3:G:1180:ILE:HG12	1.41	0.44
3:I:64:TYR:HB3	3:I:67:ILE:HD11	1.98	0.44
3:J:40:PHE:CE1	3:J:131:ILE:HG21	2.53	0.44
3:J:155:ASN:HB3	3:J:159:GLY:HA2	1.99	0.44
3:I:627:GLN:OE1	3:I:627:GLN:N	2.46	0.44
3:J:300:ILE:HG22	3:J:302:SER:HB3	2.00	0.44
1:A:146:GLY:HA2	1:A:161:TRP:CH2	2.53	0.44
2:C:67:GLY:HA3	2:C:72:PHE:HA	2.00	0.44
1:H:202:ILE:CG2	1:H:204:ASN:HB3	2.47	0.44
3:I:481:LEU:HD12	3:I:481:LEU:HA	1.84	0.44
2:C:184:LYS:HE3	2:C:184:LYS:HB3	1.77	0.44
3:G:155:ASN:HB3	3:G:159:GLY:HA2	1.99	0.44
3:G:169:LEU:HD22	3:G:286:VAL:HG21	1.99	0.44
3:G:184:TYR:OH	3:G:286:VAL:HG13	2.18	0.44
3:J:448:TYR:OH	3:J:452:MET:HG3	2.18	0.44
2:F:67:GLY:HA3	2:F:72:PHE:HA	2.00	0.44
3:I:27:LYS:HE2	3:I:27:LYS:HB2	1.70	0.44
3:J:526:CYS:SG	3:J:556:ALA:HB2	2.58	0.44
3:G:36:GLN:HG3	3:G:101:PHE:HE1	1.82	0.43
3:G:344:LEU:HD23	3:G:344:LEU:HA	1.82	0.43
3:I:544:GLN:HB2	3:I:553:TRP:CZ3	2.53	0.43
1:E:146:GLY:HA2	1:E:161:TRP:CH2	2.53	0.43
2:F:184:LYS:HB3	2:F:184:LYS:HE3	1.77	0.43
3:G:145:PRO:HB3	3:G:313:PHE:CE2	2.53	0.43
3:G:330:ASP:OD1	3:G:330:ASP:N	2.51	0.43
1:H:202:ILE:HG22	1:H:204:ASN:H	1.83	0.43
3:I:702:SER:OG	3:I:703:THR:N	2.51	0.43
3:J:524:SER:O	3:J:526:CYS:N	2.50	0.43
1:A:50:ARG:HH11	1:A:59:ARG:NE	2.11	0.43
2:F:2:ILE:HG12	2:F:27:GLN:HB3	2.00	0.43
3:G:448:TYR:OH	3:G:452:MET:HG3	2.18	0.43
3:G:903:PRO:HA	3:G:924:ILE:HG13	2.00	0.43
3:J:544:GLN:HB2	3:J:553:TRP:CZ3	2.53	0.43
2:K:67:GLY:HA3	2:K:72:PHE:HA	2.00	0.43
3:G:702:SER:OG	3:G:703:THR:N	2.51	0.43
3:J:1223:LEU:HD23	3:J:1223:LEU:HA	1.87	0.43
3:G:291:LYS:HB2	3:G:292:TYR:CD1	2.54	0.43
3:J:170:VAL:O	3:J:182:ALA:HA	2.17	0.43
3:J:782:ILE:HG13	3:J:783:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:148:MET:HB2	3:I:296:ILE:HD11	2.00	0.43
3:I:330:ASP:N	3:I:330:ASP:OD1	2.50	0.43
3:I:377:GLN:O	3:I:609:TYR:OH	2.31	0.43
3:I:548:LEU:HA	3:I:549:GLU:HA	1.71	0.43
3:I:927:GLN:HB2	3:I:932:TYR:O	2.19	0.43
3:J:548:LEU:HA	3:J:549:GLU:HA	1.71	0.43
3:J:903:PRO:HA	3:J:924:ILE:HG13	1.99	0.43
3:J:1218:LEU:HD23	3:J:1218:LEU:HA	1.71	0.43
3:G:544:GLN:HB2	3:G:553:TRP:CZ3	2.53	0.43
3:I:924:ILE:O	3:I:927:GLN:HG2	2.19	0.43
3:I:1035:LYS:HE3	3:I:1035:LYS:HB2	1.83	0.43
3:J:702:SER:OG	3:J:703:THR:N	2.52	0.43
2:C:2:ILE:HG12	2:C:27:GLN:HB3	2.00	0.43
2:C:30:SER:HB3	2:C:33:TYR:HB2	2.01	0.43
3:G:758:ARG:HG3	3:G:758:ARG:HH11	1.84	0.43
3:I:235:ARG:HH11	3:I:235:ARG:HG2	1.83	0.43
2:K:30:SER:HB3	2:K:33:TYR:HB2	2.01	0.43
2:F:112:ALA:HB3	2:F:141:TYR:N	2.34	0.43
3:G:102:VAL:HG23	3:G:103:ALA:O	2.19	0.43
3:J:686:MET:HE3	3:J:686:MET:HB3	1.75	0.43
2:C:112:ALA:HB3	2:C:141:TYR:N	2.34	0.42
2:C:113:ALA:HA	2:C:114:PRO:HD3	1.87	0.42
3:G:548:LEU:HA	3:G:549:GLU:HA	1.71	0.42
3:I:1123:ILE:HD11	3:I:1141:TYR:HB2	2.01	0.42
3:G:347:LEU:HD23	3:G:347:LEU:HA	1.91	0.42
3:I:317:LYS:HA	3:I:317:LYS:HD2	1.77	0.42
3:I:592:ASN:ND2	3:I:592:ASN:C	2.73	0.42
2:K:113:ALA:HA	2:K:114:PRO:HD3	1.87	0.42
3:G:95:THR:HA	3:G:303:ILE:HD12	2.01	0.42
3:G:720:SER:HB3	3:G:758:ARG:HB3	2.01	0.42
3:I:448:TYR:OH	3:I:452:MET:HG3	2.18	0.42
2:C:113:ALA:HA	2:C:201:GLY:HA3	2.01	0.42
1:H:159:VAL:HG23	1:H:205:VAL:HG12	2.01	0.42
3:I:960:TRP:CZ2	3:I:970:ILE:HD13	2.54	0.42
3:J:167:HIS:HB3	3:J:184:TYR:CE1	2.54	0.42
2:K:184:LYS:HB3	2:K:184:LYS:HE3	1.77	0.42
2:F:30:SER:HB3	2:F:33:TYR:HB2	2.01	0.42
3:G:587:LYS:H	3:G:587:LYS:HG3	1.58	0.42
3:G:662:ILE:O	3:G:670:HIS:HA	2.18	0.42
3:G:782:ILE:HG13	3:G:783:PRO:HD2	2.02	0.42
3:J:100:LEU:HD22	3:J:299:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:ILE:HG12	2:K:27:GLN:HB3	2.00	0.42
2:K:112:ALA:HB3	2:K:141:TYR:N	2.34	0.42
1:A:50:ARG:HD3	1:A:99:GLU:OE2	2.20	0.42
3:I:40:PHE:CE1	3:I:131:ILE:HG21	2.54	0.42
2:C:13:LEU:HD13	2:C:79:LEU:HD13	2.02	0.42
3:G:156:PHE:HD1	3:G:156:PHE:HA	1.74	0.42
3:G:181:ARG:HH21	3:G:240:MET:HE1	1.84	0.42
3:G:638:LEU:HD23	3:G:651:LEU:HD23	2.02	0.42
3:G:891:GLU:OE1	3:G:1129:ASN:HB2	2.19	0.42
3:I:545:LEU:HD23	3:I:552:GLY:O	2.20	0.42
1:E:153:PHE:HB3	1:E:154:PRO:HD3	2.02	0.42
2:F:48:LEU:HD23	2:F:48:LEU:HA	1.82	0.42
2:F:59:ILE:HD13	2:F:59:ILE:HA	1.90	0.42
3:G:172:LEU:O	3:G:181:ARG:HG2	2.20	0.42
3:J:285:PRO:O	3:J:287:TYR:HD1	2.03	0.42
1:E:87:THR:OG1	1:E:88:SER:N	2.52	0.42
3:G:110:LYS:HB3	3:G:110:LYS:HE2	1.59	0.42
3:G:979:ARG:HD3	3:G:1123:ILE:O	2.20	0.42
3:I:921:ARG:NH2	3:I:1037:ALA:O	2.53	0.42
3:J:595:LYS:HE2	3:J:595:LYS:HB2	1.92	0.42
2:K:13:LEU:HD13	2:K:79:LEU:HD13	2.02	0.42
3:G:156:PHE:CE1	3:G:163:ARG:HB2	2.54	0.41
3:G:170:VAL:O	3:G:182:ALA:HA	2.20	0.41
3:G:545:LEU:HD23	3:G:552:GLY:O	2.20	0.41
1:H:145:LEU:HD13	1:H:218:VAL:HG11	2.02	0.41
1:H:196:LEU:O	1:H:197:GLY:C	2.58	0.41
3:J:823:GLU:H	3:J:823:GLU:HG3	1.68	0.41
1:A:145:LEU:HD13	1:A:218:VAL:HG11	2.02	0.41
1:E:75:SER:C	1:H:168:SER:HG	2.11	0.41
3:G:768:ILE:HB	3:I:857:GLN:HG2	2.02	0.41
3:I:184:TYR:OH	3:I:286:VAL:HG13	2.20	0.41
3:I:700:ARG:H	3:I:700:ARG:HD2	1.85	0.41
3:G:178:THR:HG22	3:G:247:GLU:OE1	2.21	0.41
3:J:481:LEU:HD12	3:J:481:LEU:HA	1.84	0.41
3:J:545:LEU:HD23	3:J:552:GLY:O	2.20	0.41
3:G:300:ILE:HG22	3:G:302:SER:HB3	2.02	0.41
3:G:449:PRO:HD3	3:G:497:TYR:CG	2.55	0.41
3:G:1040:LEU:HD23	3:G:1040:LEU:HA	1.88	0.41
3:J:262:GLY:HA2	3:J:286:VAL:O	2.19	0.41
2:K:113:ALA:HA	2:K:201:GLY:HA3	2.01	0.41
1:E:50:ARG:HD3	1:E:99:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:SER:O	1:H:168:SER:HB3	2.11	0.41
3:G:622:ALA:HA	3:G:648:TYR:CD2	2.55	0.41
1:H:50:ARG:HD3	1:H:99:GLU:OE2	2.20	0.41
3:I:196:PRO:HD3	3:I:231:TYR:HD2	1.85	0.41
3:I:694:ARG:HG2	3:I:694:ARG:HH11	1.86	0.41
3:J:702:SER:OG	3:J:756:GLU:OE2	2.37	0.41
3:J:904:GLY:C	3:J:906:MET:H	2.24	0.41
1:H:153:PHE:HB3	1:H:154:PRO:HD3	2.02	0.41
2:F:113:ALA:HA	2:F:201:GLY:HA3	2.01	0.41
3:G:738:LEU:HD23	3:G:738:LEU:HA	1.91	0.41
3:I:853:VAL:HG22	3:I:1103:VAL:HG11	2.03	0.41
1:H:177:LEU:HA	1:H:183:TYR:HB3	2.02	0.41
3:I:409:TYR:O	3:I:586:PRO:HA	2.21	0.41
3:J:145:PRO:HB3	3:J:313:PHE:CE2	2.56	0.41
1:A:87:THR:OG1	1:A:88:SER:N	2.53	0.41
1:A:153:PHE:HB3	1:A:154:PRO:HD3	2.02	0.41
2:C:48:LEU:HD23	2:C:48:LEU:HA	1.82	0.41
1:E:177:LEU:HA	1:E:183:TYR:HB3	2.02	0.41
3:G:322:THR:OG1	3:I:822:ARG:NH1	2.50	0.41
3:G:652:ARG:NH1	3:I:916:GLY:O	2.49	0.41
3:G:702:SER:OG	3:G:756:GLU:OE2	2.33	0.41
3:G:815:GLN:O	3:G:815:GLN:NE2	2.54	0.41
3:G:893:LEU:HD23	3:G:897:LYS:HG3	2.03	0.41
1:H:173:PHE:O	1:H:185:LEU:HB2	2.21	0.41
3:I:449:PRO:HD3	3:I:497:TYR:CG	2.55	0.41
3:I:595:LYS:HD2	3:I:595:LYS:HA	1.91	0.41
3:I:823:GLU:H	3:I:823:GLU:HG3	1.70	0.41
3:J:449:PRO:HD3	3:J:497:TYR:CG	2.55	0.41
3:J:667:THR:OG1	3:J:669:THR:OG1	2.25	0.41
3:J:178:THR:HG22	3:J:247:GLU:OE2	2.21	0.41
1:A:177:LEU:HA	1:A:183:TYR:HB3	2.03	0.40
1:E:77:SER:O	1:E:77:SER:OG	2.38	0.40
3:G:40:PHE:CE1	3:G:131:ILE:HG21	2.56	0.40
3:I:84:MET:HG3	3:I:314:TYR:CE2	2.56	0.40
3:J:365:SER:HA	3:J:659:VAL:HG23	2.03	0.40
1:A:173:PHE:O	1:A:185:LEU:HB2	2.21	0.40
1:E:145:LEU:HD13	1:E:218:VAL:HG11	2.02	0.40
3:G:93:THR:HG23	3:G:98:GLN:HG2	2.02	0.40
3:G:694:ARG:HG2	3:G:694:ARG:HH11	1.86	0.40
3:G:794:TYR:CD1	3:G:1022:VAL:HG22	2.56	0.40
1:H:195:SER:C	1:H:197:GLY:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:40:ARG:HD3	2:F:46:ARG:HH21	1.86	0.40
3:G:32:GLU:HB2	3:G:194:HIS:CD2	2.55	0.40
3:G:415:LEU:HD23	3:G:415:LEU:HA	1.87	0.40
3:J:93:THR:HG23	3:J:98:GLN:HG2	2.03	0.40
3:J:109:VAL:HG21	3:J:153:VAL:HG11	2.02	0.40
2:C:40:ARG:HD3	2:C:46:ARG:HH21	1.86	0.40
2:C:208:LYS:HA	2:C:208:LYS:HD3	1.93	0.40
3:G:167:HIS:HB3	3:G:184:TYR:CE1	2.57	0.40
3:G:466:GLN:O	3:G:518:VAL:HG12	2.22	0.40
3:I:365:SER:HB3	3:I:658:PRO:HA	2.03	0.40
3:I:390:SER:HA	3:I:490:THR:O	2.22	0.40
3:J:77:TYR:HE1	3:J:321:LEU:HD21	1.85	0.40
3:J:87:TYR:OH	3:J:296:ILE:O	2.28	0.40
3:J:142:LYS:NZ	3:J:144:TYR:OH	2.38	0.40
3:J:638:LEU:HD23	3:J:651:LEU:HD23	2.03	0.40
1:E:155:GLU:CG	1:E:156:PRO:HA	2.52	0.40
3:G:390:SER:HA	3:G:490:THR:O	2.22	0.40
3:J:419:SER:OG	3:J:483:THR:HB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	221/221 (100%)	173 (78%)	37 (17%)	11 (5%)	1 2
1	E	211/221 (96%)	166 (79%)	34 (16%)	11 (5%)	1 2
1	H	212/221 (96%)	165 (78%)	37 (18%)	10 (5%)	2 2
2	C	210/212 (99%)	168 (80%)	37 (18%)	5 (2%)	5 8
2	F	210/212 (99%)	168 (80%)	37 (18%)	5 (2%)	5 8
2	K	210/212 (99%)	168 (80%)	37 (18%)	5 (2%)	5 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	G	1183/1347 (88%)	1087 (92%)	94 (8%)	2 (0%)	44 64
3	I	1183/1347 (88%)	1086 (92%)	96 (8%)	1 (0%)	48 69
3	J	1173/1347 (87%)	1083 (92%)	88 (8%)	2 (0%)	44 64
All	All	4813/5340 (90%)	4264 (89%)	497 (10%)	52 (1%)	15 23

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	THR
1	E	198	THR
3	G	381	VAL
3	G	522	GLN
3	I	522	GLN
3	J	522	GLN
1	A	108	ASP
1	A	196	LEU
1	E	23	LYS
1	E	108	ASP
1	E	196	LEU
1	H	108	ASP
1	H	197	GLY
1	H	199	GLN
1	A	9	ALA
1	A	135	SER
2	C	139	ASN
1	E	9	ALA
1	E	135	SER
2	F	139	ASN
1	H	9	ALA
1	H	135	SER
2	K	139	ASN
1	A	194	SER
2	C	84	SER
2	C	142	PRO
1	E	194	SER
2	F	84	SER
2	F	142	PRO
1	H	200	THR
3	J	380	GLY
2	K	84	SER
2	K	142	PRO

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Mol	Chain	Res	Type
1	A	31	SER
2	C	132	SER
2	C	202	LEU
2	F	132	SER
2	F	202	LEU
1	H	31	SER
2	K	132	SER
2	K	202	LEU
1	A	156	PRO
1	A	209	PRO
1	E	156	PRO
1	E	209	PRO
1	H	156	PRO
1	H	209	PRO
1	A	14	PRO
1	A	202	ILE
1	E	14	PRO
1	E	202	ILE
1	H	14	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	185/184 (100%)	167 (90%)	18 (10%)	6 14
1	E	179/184 (97%)	162 (90%)	17 (10%)	7 14
1	H	180/184 (98%)	160 (89%)	20 (11%)	5 10
2	C	178/183 (97%)	156 (88%)	22 (12%)	4 7
2	F	178/183 (97%)	156 (88%)	22 (12%)	4 7
2	K	178/183 (97%)	156 (88%)	22 (12%)	4 7
3	G	1021/1164 (88%)	927 (91%)	94 (9%)	7 15
3	I	1021/1164 (88%)	921 (90%)	100 (10%)	6 13
3	J	1014/1164 (87%)	930 (92%)	84 (8%)	9 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4134/4593 (90%)	3735 (90%)	399 (10%)	9 14

All (399) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	5	VAL
1	A	18	VAL
1	A	28	THR
1	A	35	THR
1	A	43	GLN
1	A	80	TYR
1	A	105	ASP
1	A	118	VAL
1	A	131	LEU
1	A	142	THR
1	A	158	THR
1	A	183	TYR
1	A	189	VAL
1	A	190	THR
1	A	200	THR
1	A	202	ILE
1	A	204	ASN
2	C	13	LEU
2	C	20	THR
2	C	43	GLN
2	C	47	LEU
2	C	54	SER
2	C	55	ARG
2	C	75	THR
2	C	103	THR
2	C	111	VAL
2	C	116	VAL
2	C	118	ILE
2	C	134	VAL
2	C	147	VAL
2	C	148	GLN
2	C	152	ASP
2	C	164	VAL
2	C	176	LEU
2	C	184	LYS
2	C	189	LYS

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Mol	Chain	Res	Type
2	C	197	VAL
2	C	198	THR
2	C	202	LEU
1	E	5	VAL
1	E	18	VAL
1	E	23	LYS
1	E	35	THR
1	E	43	GLN
1	E	80	TYR
1	E	105	ASP
1	E	118	VAL
1	E	131	LEU
1	E	142	THR
1	E	158	THR
1	E	183	TYR
1	E	189	VAL
1	E	190	THR
1	E	200	THR
1	E	202	ILE
1	E	204	ASN
2	F	13	LEU
2	F	20	THR
2	F	43	GLN
2	F	47	LEU
2	F	54	SER
2	F	55	ARG
2	F	75	THR
2	F	103	THR
2	F	111	VAL
2	F	116	VAL
2	F	118	ILE
2	F	134	VAL
2	F	147	VAL
2	F	148	GLN
2	F	152	ASP
2	F	164	VAL
2	F	176	LEU
2	F	184	LYS
2	F	189	LYS
2	F	197	VAL
2	F	198	THR
2	F	202	LEU

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Mol	Chain	Res	Type
3	G	25	SER
3	G	38	THR
3	G	48	ILE
3	G	50	VAL
3	G	52	LYS
3	G	95	THR
3	G	101	PHE
3	G	110	LYS
3	G	131	ILE
3	G	137	SER
3	G	140	ILE
3	G	143	ILE
3	G	156	PHE
3	G	167	HIS
3	G	168	THR
3	G	172	LEU
3	G	179	LEU
3	G	203	SER
3	G	216	ASP
3	G	235	ARG
3	G	236	ASN
3	G	240	MET
3	G	246	THR
3	G	277	ASN
3	G	294	SER
3	G	302	SER
3	G	305	SER
3	G	343	ASP
3	G	353	SER
3	G	364	SER
3	G	373	SER
3	G	376	GLU
3	G	377	GLN
3	G	384	ASP
3	G	529	ILE
3	G	587	LYS
3	G	590	PHE
3	G	592	ASN
3	G	593	ASP
3	G	594	THR
3	G	595	LYS
3	G	620	CYS

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Mol	Chain	Res	Type
3	G	621	THR
3	G	628	GLN
3	G	629	ARG
3	G	669	THR
3	G	677	VAL
3	G	679	CYS
3	G	694	ARG
3	G	698	LYS
3	G	699	ARG
3	G	700	ARG
3	G	704	TYR
3	G	720	SER
3	G	721	SER
3	G	729	LEU
3	G	740	ASP
3	G	761	SER
3	G	781	SER
3	G	802	VAL
3	G	804	VAL
3	G	807	LYS
3	G	815	GLN
3	G	823	GLU
3	G	829	SER
3	G	856	SER
3	G	858	SER
3	G	859	SER
3	G	871	LEU
3	G	872	THR
3	G	873	LEU
3	G	874	LEU
3	G	877	VAL
3	G	919	SER
3	G	924	ILE
3	G	960	TRP
3	G	985	ILE
3	G	995	LYS
3	G	1010	THR
3	G	1017	GLU
3	G	1031	GLN
3	G	1034	SER
3	G	1038	SER
3	G	1054	ILE

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Mol	Chain	Res	Type
3	G	1055	ILE
3	G	1089	SER
3	G	1095	SER
3	G	1111	SER
3	G	1175	THR
3	G	1180	ILE
3	G	1203	LYS
3	G	1209	VAL
3	G	1216	THR
3	G	1218	LEU
1	H	2	VAL
1	H	5	VAL
1	H	18	VAL
1	H	28	THR
1	H	35	THR
1	H	43	GLN
1	H	80	TYR
1	H	105	ASP
1	H	118	VAL
1	H	131	LEU
1	H	142	THR
1	H	158	THR
1	H	183	TYR
1	H	189	VAL
1	H	190	THR
1	H	193	SER
1	H	194	SER
1	H	195	SER
1	H	200	THR
1	H	204	ASN
3	I	21	VAL
3	I	25	SER
3	I	38	THR
3	I	50	VAL
3	I	51	SER
3	I	52	LYS
3	I	95	THR
3	I	99	LYS
3	I	101	PHE
3	I	110	LYS
3	I	137	SER
3	I	140	ILE

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Mol	Chain	Res	Type
3	I	143	ILE
3	I	148	MET
3	I	156	PHE
3	I	167	HIS
3	I	172	LEU
3	I	179	LEU
3	I	181	ARG
3	I	191	SER
3	I	203	SER
3	I	212	THR
3	I	214	CYS
3	I	216	ASP
3	I	236	ASN
3	I	240	MET
3	I	268	SER
3	I	294	SER
3	I	302	SER
3	I	305	SER
3	I	317	LYS
3	I	334	ARG
3	I	343	ASP
3	I	353	SER
3	I	373	SER
3	I	376	GLU
3	I	377	GLN
3	I	529	ILE
3	I	587	LYS
3	I	589	GLU
3	I	590	PHE
3	I	592	ASN
3	I	594	THR
3	I	596	ILE
3	I	621	THR
3	I	623	VAL
3	I	635	TYR
3	I	669	THR
3	I	679	CYS
3	I	682	ILE
3	I	688	GLN
3	I	694	ARG
3	I	698	LYS
3	I	699	ARG

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Mol	Chain	Res	Type
3	I	700	ARG
3	I	704	TYR
3	I	720	SER
3	I	725	GLU
3	I	729	LEU
3	I	761	SER
3	I	781	SER
3	I	804	VAL
3	I	815	GLN
3	I	823	GLU
3	I	829	SER
3	I	830	LYS
3	I	844	ASP
3	I	856	SER
3	I	858	SER
3	I	859	SER
3	I	872	THR
3	I	873	LEU
3	I	874	LEU
3	I	877	VAL
3	I	893	LEU
3	I	910	ASP
3	I	919	SER
3	I	924	ILE
3	I	939	MET
3	I	948	THR
3	I	965	SER
3	I	975	SER
3	I	995	LYS
3	I	1010	THR
3	I	1017	GLU
3	I	1031	GLN
3	I	1034	SER
3	I	1038	SER
3	I	1054	ILE
3	I	1055	ILE
3	I	1089	SER
3	I	1091	SER
3	I	1095	SER
3	I	1160	ASN
3	I	1175	THR
3	I	1180	ILE

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Mol	Chain	Res	Type
3	I	1209	VAL
3	I	1216	THR
3	I	1218	LEU
3	I	1222	LEU
3	J	25	SER
3	J	38	THR
3	J	50	VAL
3	J	52	LYS
3	J	95	THR
3	J	110	LYS
3	J	137	SER
3	J	143	ILE
3	J	153	VAL
3	J	156	PHE
3	J	167	HIS
3	J	184	TYR
3	J	191	SER
3	J	203	SER
3	J	212	THR
3	J	216	ASP
3	J	240	MET
3	J	257	THR
3	J	294	SER
3	J	302	SER
3	J	305	SER
3	J	334	ARG
3	J	343	ASP
3	J	353	SER
3	J	373	SER
3	J	376	GLU
3	J	379	GLU
3	J	528	SER
3	J	529	ILE
3	J	583	SER
3	J	584	VAL
3	J	588	LEU
3	J	620	CYS
3	J	621	THR
3	J	623	VAL
3	J	628	GLN
3	J	629	ARG
3	J	635	TYR

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Mol	Chain	Res	Type
3	J	669	THR
3	J	679	CYS
3	J	694	ARG
3	J	699	ARG
3	J	700	ARG
3	J	704	TYR
3	J	720	SER
3	J	721	SER
3	J	725	GLU
3	J	729	LEU
3	J	740	ASP
3	J	804	VAL
3	J	815	GLN
3	J	823	GLU
3	J	829	SER
3	J	856	SER
3	J	858	SER
3	J	859	SER
3	J	871	LEU
3	J	872	THR
3	J	873	LEU
3	J	874	LEU
3	J	877	VAL
3	J	907	GLN
3	J	910	ASP
3	J	924	ILE
3	J	948	THR
3	J	995	LYS
3	J	1010	THR
3	J	1031	GLN
3	J	1034	SER
3	J	1038	SER
3	J	1050	SER
3	J	1054	ILE
3	J	1055	ILE
3	J	1089	SER
3	J	1091	SER
3	J	1095	SER
3	J	1111	SER
3	J	1131	PRO
3	J	1160	ASN
3	J	1175	THR

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Mol	Chain	Res	Type
3	J	1180	ILE
3	J	1185	SER
3	J	1209	VAL
3	J	1216	THR
2	K	13	LEU
2	K	20	THR
2	K	43	GLN
2	K	47	LEU
2	K	54	SER
2	K	55	ARG
2	K	75	THR
2	K	103	THR
2	K	111	VAL
2	K	116	VAL
2	K	118	ILE
2	K	134	VAL
2	K	147	VAL
2	K	148	GLN
2	K	152	ASP
2	K	164	VAL
2	K	176	LEU
2	K	184	LYS
2	K	189	LYS
2	K	197	VAL
2	K	198	THR
2	K	202	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	178	GLN
1	A	199	GLN
2	C	43	GLN
2	C	91	GLN
2	C	148	GLN
2	C	199	HIS
1	E	162	ASN
1	E	178	GLN
1	E	199	GLN
2	F	43	GLN
2	F	91	GLN

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Mol	Chain	Res	Type
2	F	148	GLN
2	F	199	HIS
3	G	486	HIS
3	G	566	GLN
3	G	819	GLN
1	H	178	GLN
3	I	377	GLN
3	I	408	ASN
3	I	486	HIS
3	I	566	GLN
3	I	592	ASN
3	J	486	HIS
3	J	566	GLN
2	K	43	GLN
2	K	91	GLN
2	K	148	GLN
2	K	199	HIS

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

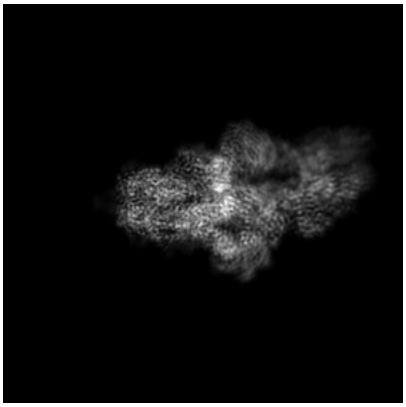
This section contains visualisations of the EMDB entry EMD-32958. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

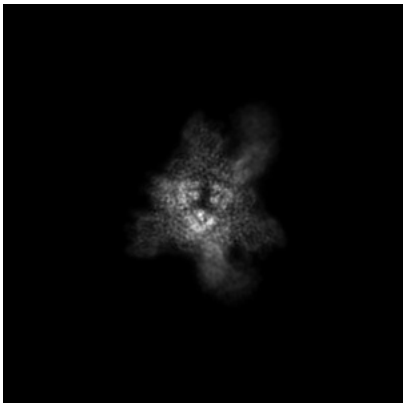
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



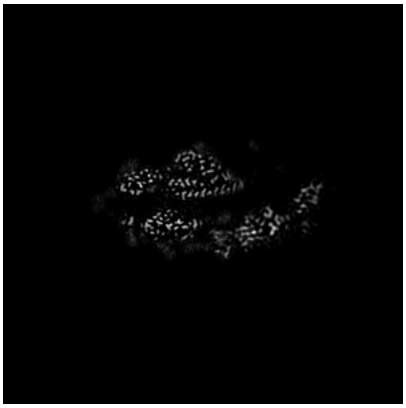
Z

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

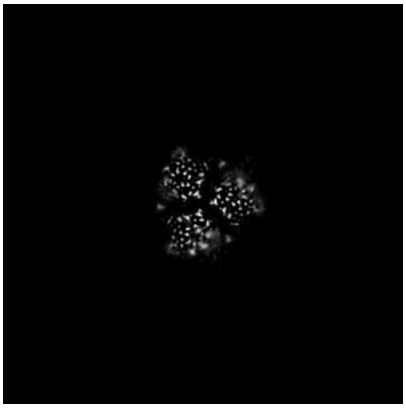
6.2 Central slices

6.2.1 Primary map

X Index: 160



Y Index: 160



Z Index: 160

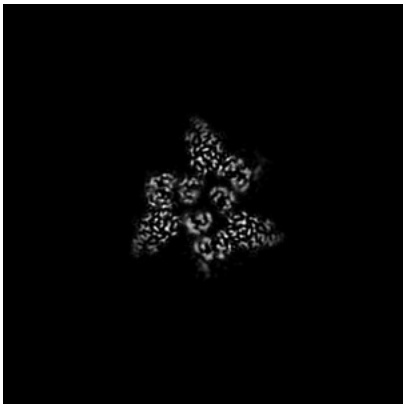
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 154

Y Index: 147

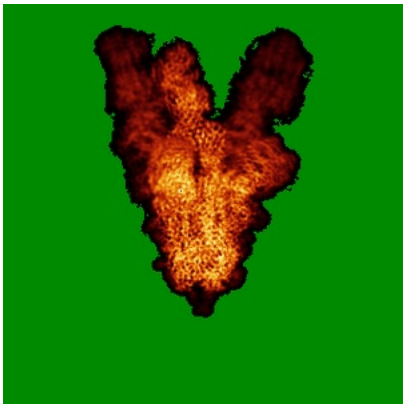


Z Index: 178

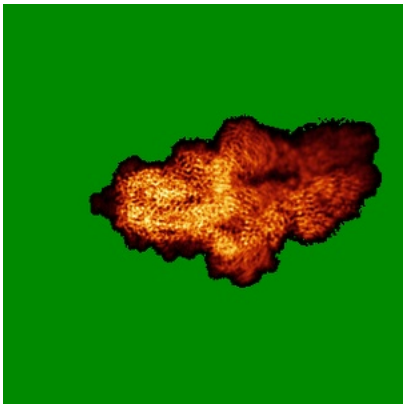
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

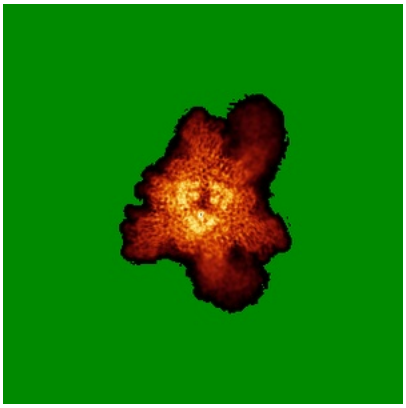
6.4.1 Primary map



X



Y

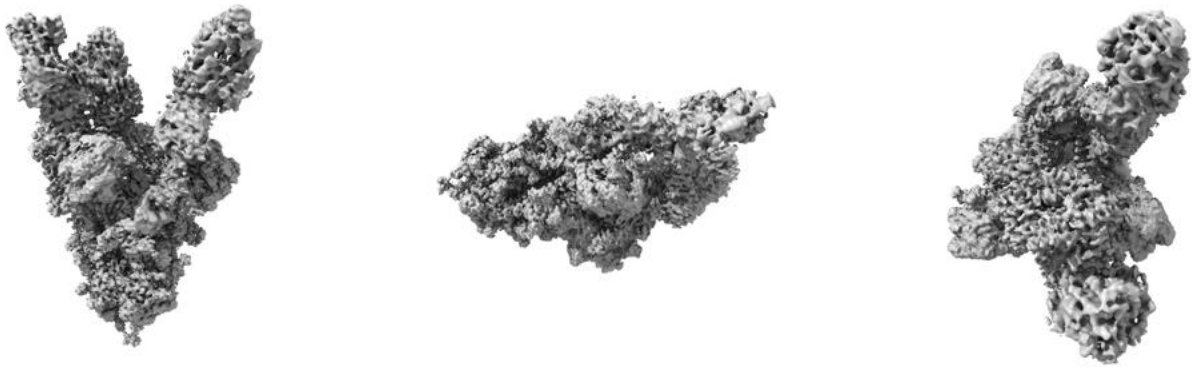


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

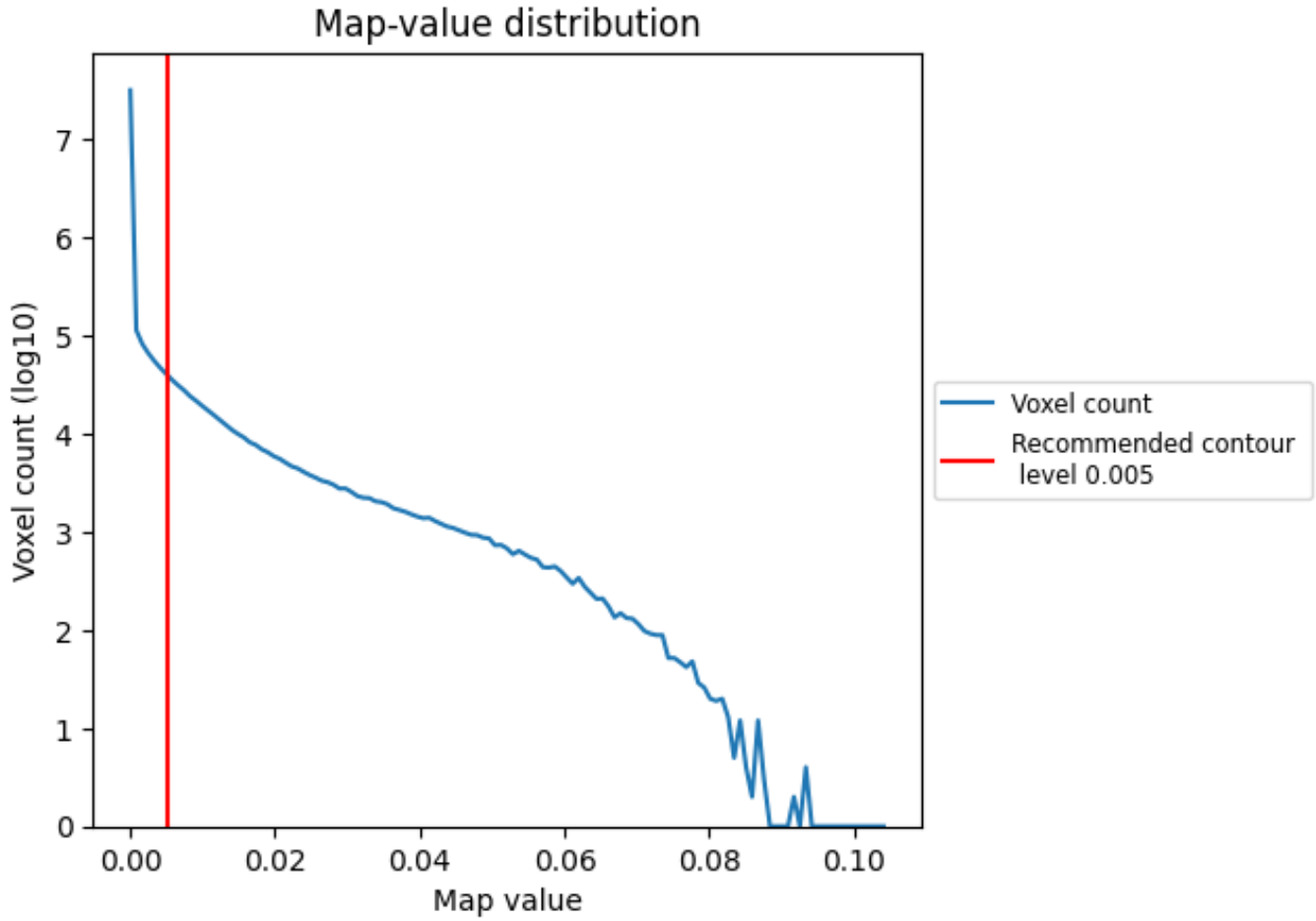
6.6 Mask visualisation (i)

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

7 Map analysis

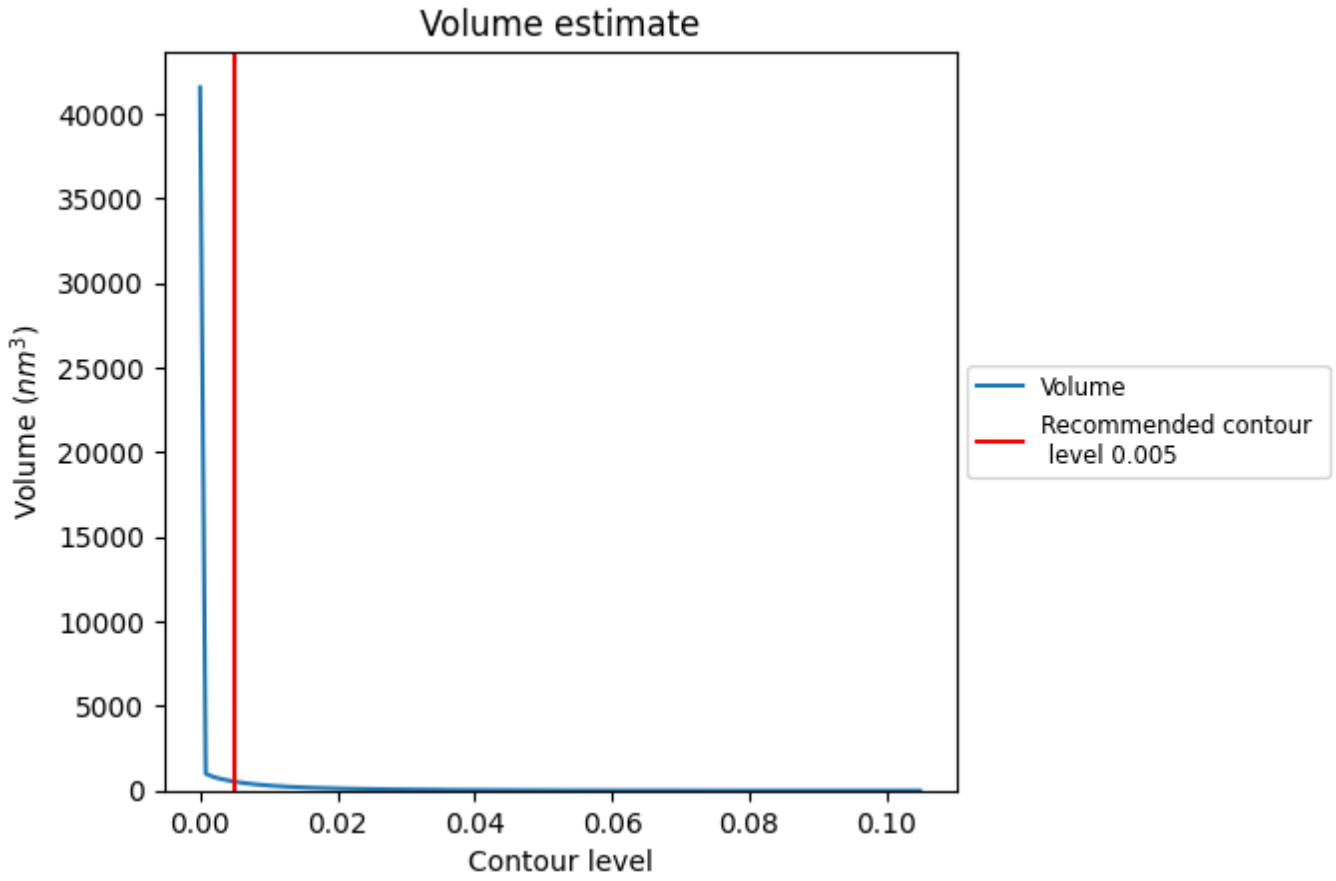
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

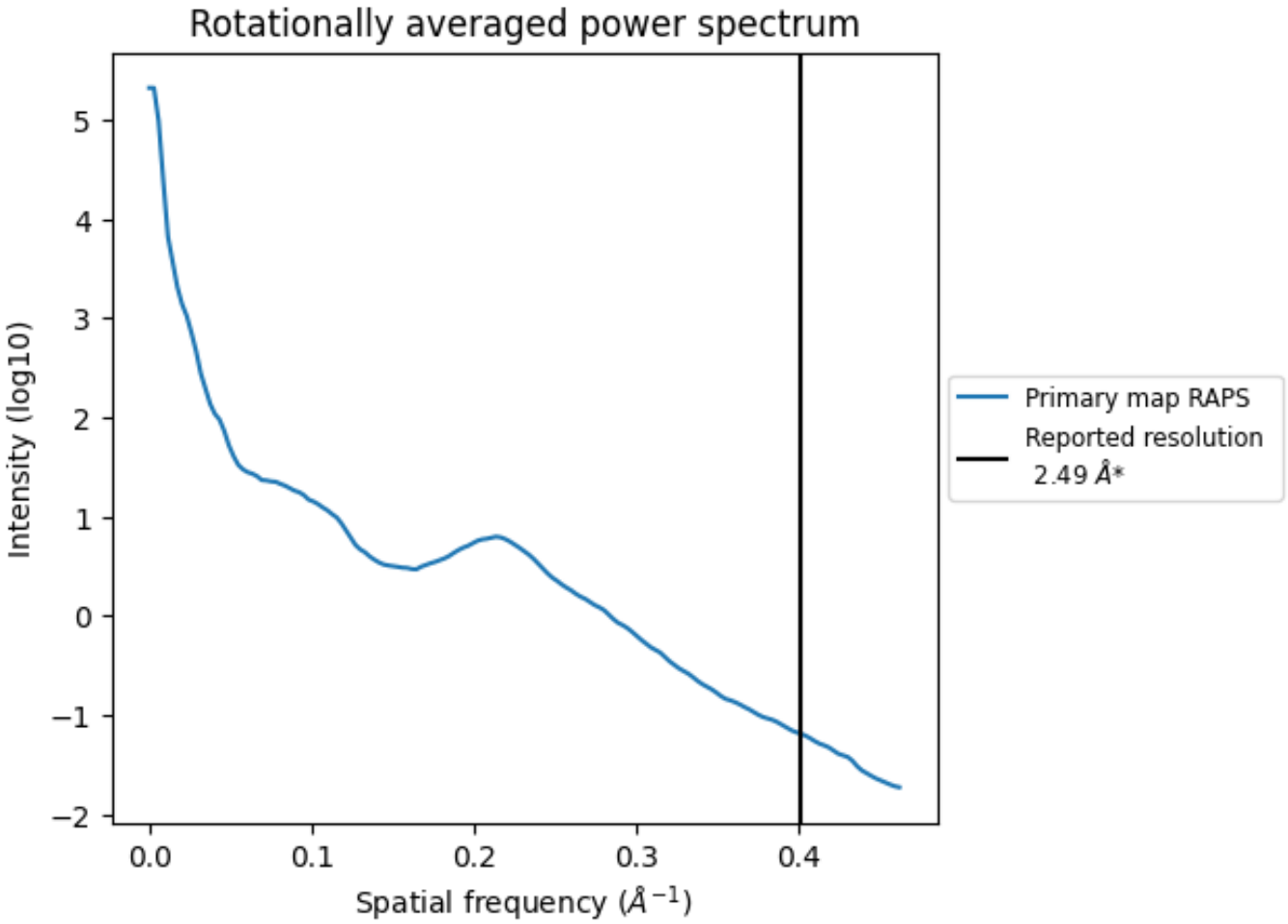
7.2 Volume estimate



The volume at the recommended contour level is 529 nm^3; this corresponds to an approximate mass of 478 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.402 $Å^{-1}$

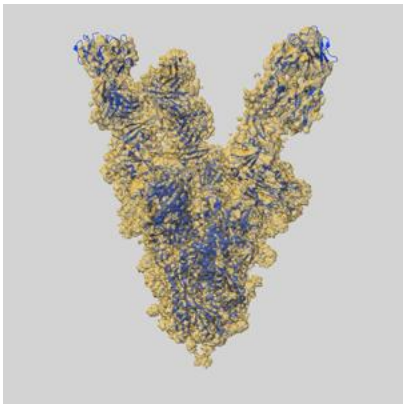
8 Fourier-Shell correlation

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

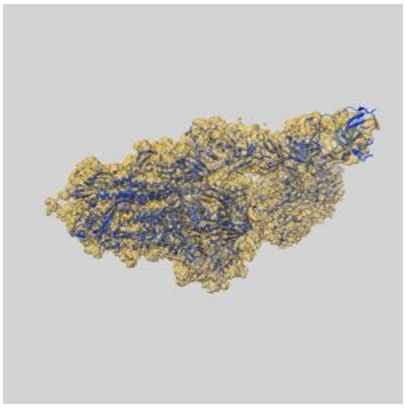
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32958 and PDB model 7X25. Per-residue inclusion information can be found in section 3 on page 10.

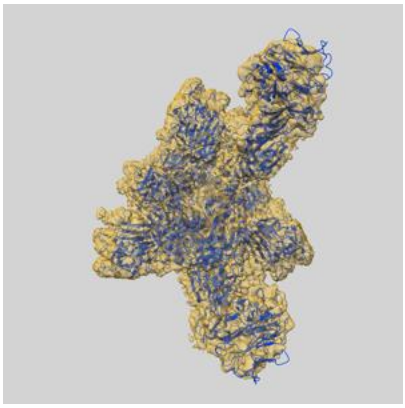
9.1 Map-model overlay



X



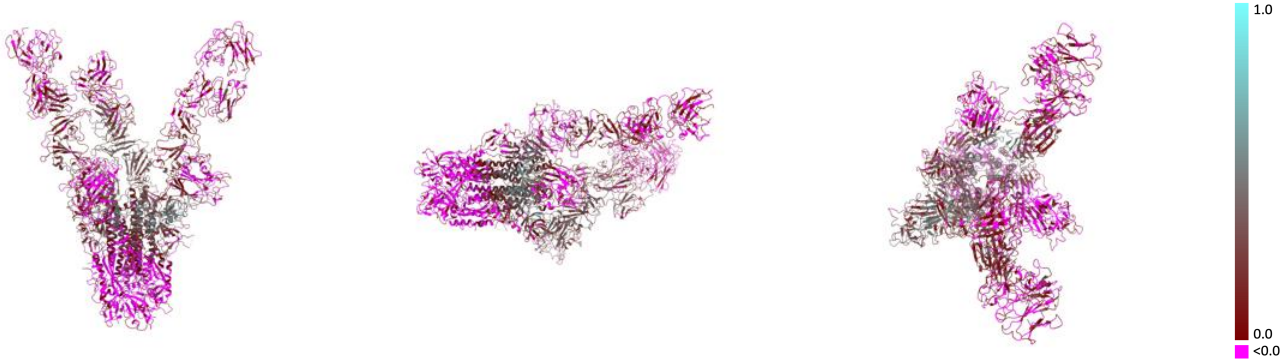
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

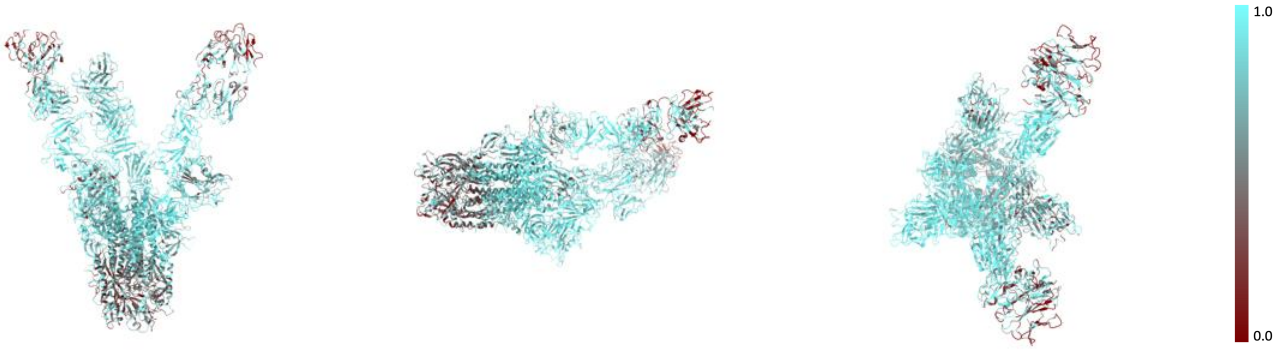
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

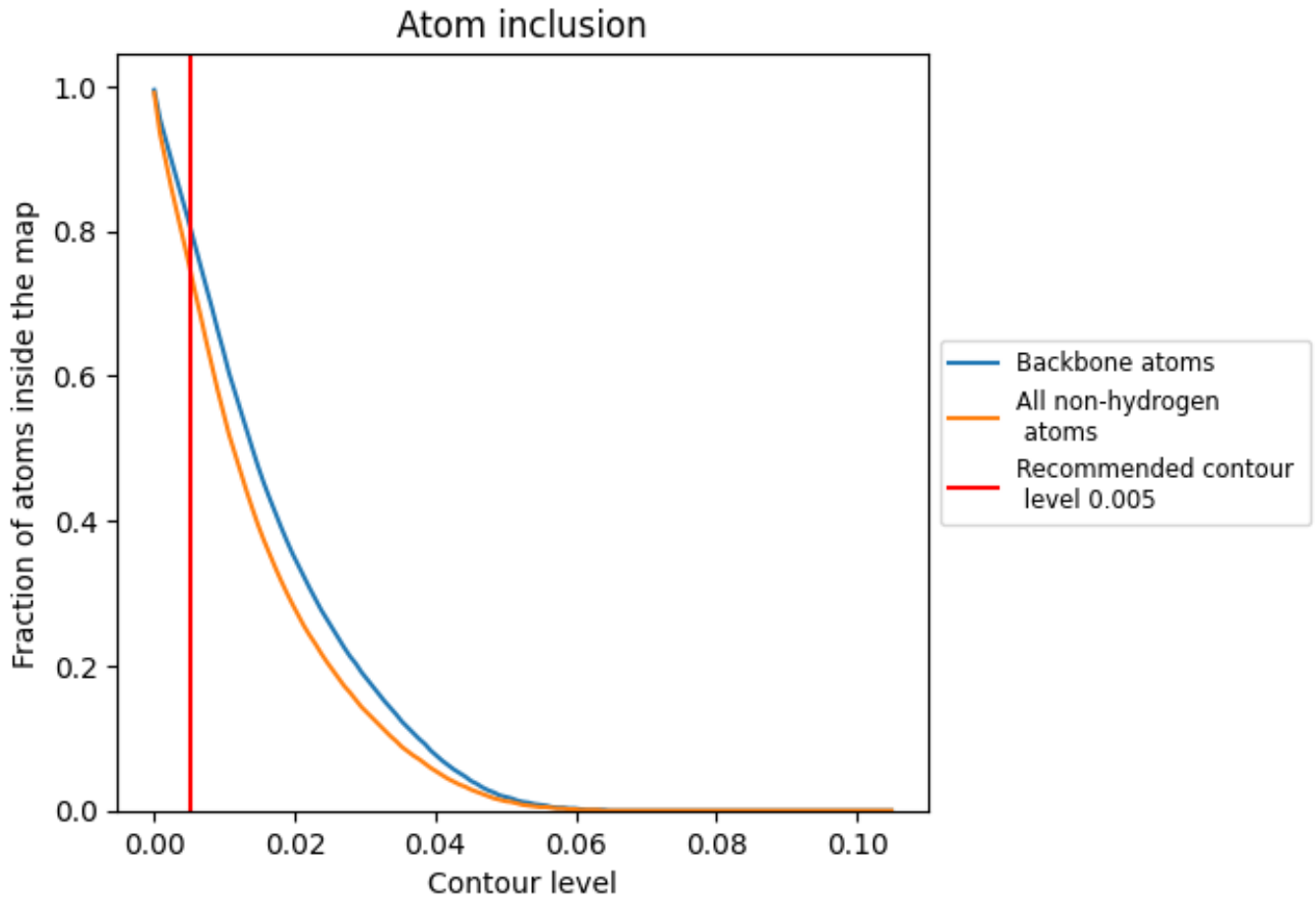
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 75% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.1290
A	0.5980	0.0420
C	0.5510	0.0670
E	0.6430	0.0650
F	0.5380	0.0580
G	0.7330	0.0690
H	0.8340	0.1730
I	0.7930	0.1510
J	0.8260	0.2050
K	0.8000	0.1480