Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 10:24 PM JST

PDB ID	:	7X2A
EMDB ID	:	EMD-32963
Title	:	MERS-CoV spike complex with S41 neutralizing antibody Fab Class1 (1u2d RBD with 1Fab)
Authors	:	Zeng, J.W.; Zhang, S.Y.; Zhou, H.X.; Wang, X.W.
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:

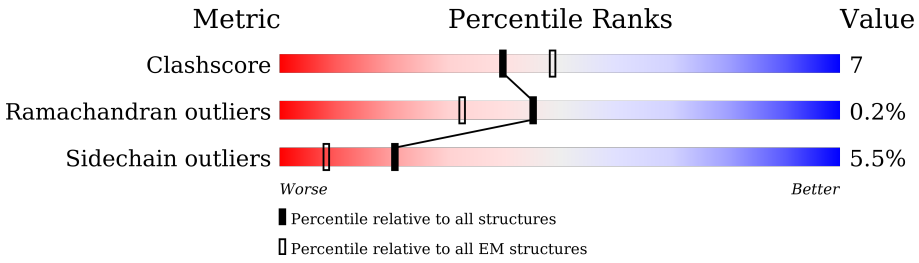
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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	1347	7% 69% 16% 14%
1	B	1347	59% 10% 30%
1	C	1347	6% 57% 13% 30%
2	H	221	25% 71% 26%
3	K	212	35% 69% 28%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26800 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 MERS-CoV Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1159	Total	C	N	O	S	0	0
			8940	5687	1472	1732	49		
1	B	947	Total	C	N	O	S	0	0
			7313	4648	1216	1411	38		
1	C	947	Total	C	N	O	S	0	0
			7313	4648	1216	1411	38		

There are 177 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1060	PRO	VAL	engineered mutation	UNP K0BRG7
A	1061	PRO	LEU	engineered mutation	UNP K0BRG7
A	1291	SER	-	expression tag	UNP K0BRG7
A	1292	ARG	-	expression tag	UNP K0BRG7
A	1293	GLU	-	expression tag	UNP K0BRG7
A	1294	ASN	-	expression tag	UNP K0BRG7
A	1295	LEU	-	expression tag	UNP K0BRG7
A	1296	TYR	-	expression tag	UNP K0BRG7
A	1297	PHE	-	expression tag	UNP K0BRG7
A	1298	GLN	-	expression tag	UNP K0BRG7
A	1299	GLY	-	expression tag	UNP K0BRG7
A	1300	GLY	-	expression tag	UNP K0BRG7
A	1301	GLY	-	expression tag	UNP K0BRG7
A	1302	SER	-	expression tag	UNP K0BRG7
A	1303	ALA	-	expression tag	UNP K0BRG7
A	1304	GLY	-	expression tag	UNP K0BRG7
A	1305	SER	-	expression tag	UNP K0BRG7
A	1306	GLY	-	expression tag	UNP K0BRG7
A	1307	TYR	-	expression tag	UNP K0BRG7
A	1308	ILE	-	expression tag	UNP K0BRG7
A	1309	PRO	-	expression tag	UNP K0BRG7
A	1310	GLU	-	expression tag	UNP K0BRG7
A	1311	ALA	-	expression tag	UNP K0BRG7
A	1312	PRO	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1313	ARG	-	expression tag	UNP K0BRG7
A	1314	ASP	-	expression tag	UNP K0BRG7
A	1315	GLY	-	expression tag	UNP K0BRG7
A	1316	GLN	-	expression tag	UNP K0BRG7
A	1317	ALA	-	expression tag	UNP K0BRG7
A	1318	TYR	-	expression tag	UNP K0BRG7
A	1319	VAL	-	expression tag	UNP K0BRG7
A	1320	ARG	-	expression tag	UNP K0BRG7
A	1321	LYS	-	expression tag	UNP K0BRG7
A	1322	ASP	-	expression tag	UNP K0BRG7
A	1323	GLY	-	expression tag	UNP K0BRG7
A	1324	GLU	-	expression tag	UNP K0BRG7
A	1325	TRP	-	expression tag	UNP K0BRG7
A	1326	VAL	-	expression tag	UNP K0BRG7
A	1327	LEU	-	expression tag	UNP K0BRG7
A	1328	LEU	-	expression tag	UNP K0BRG7
A	1329	SER	-	expression tag	UNP K0BRG7
A	1330	THR	-	expression tag	UNP K0BRG7
A	1331	PHE	-	expression tag	UNP K0BRG7
A	1332	LEU	-	expression tag	UNP K0BRG7
A	1333	GLY	-	expression tag	UNP K0BRG7
A	1334	HIS	-	expression tag	UNP K0BRG7
A	1335	HIS	-	expression tag	UNP K0BRG7
A	1336	HIS	-	expression tag	UNP K0BRG7
A	1337	HIS	-	expression tag	UNP K0BRG7
A	1338	HIS	-	expression tag	UNP K0BRG7
A	1339	HIS	-	expression tag	UNP K0BRG7
A	1340	TRP	-	expression tag	UNP K0BRG7
A	1341	SER	-	expression tag	UNP K0BRG7
A	1342	HIS	-	expression tag	UNP K0BRG7
A	1343	PRO	-	expression tag	UNP K0BRG7
A	1344	GLN	-	expression tag	UNP K0BRG7
A	1345	PHE	-	expression tag	UNP K0BRG7
A	1346	GLU	-	expression tag	UNP K0BRG7
A	1347	LYS	-	expression tag	UNP K0BRG7
B	1060	PRO	VAL	engineered mutation	UNP K0BRG7
B	1061	PRO	LEU	engineered mutation	UNP K0BRG7
B	1291	SER	-	expression tag	UNP K0BRG7
B	1292	ARG	-	expression tag	UNP K0BRG7
B	1293	GLU	-	expression tag	UNP K0BRG7
B	1294	ASN	-	expression tag	UNP K0BRG7
B	1295	LEU	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1296	TYR	-	expression tag	UNP K0BRG7
B	1297	PHE	-	expression tag	UNP K0BRG7
B	1298	GLN	-	expression tag	UNP K0BRG7
B	1299	GLY	-	expression tag	UNP K0BRG7
B	1300	GLY	-	expression tag	UNP K0BRG7
B	1301	GLY	-	expression tag	UNP K0BRG7
B	1302	SER	-	expression tag	UNP K0BRG7
B	1303	ALA	-	expression tag	UNP K0BRG7
B	1304	GLY	-	expression tag	UNP K0BRG7
B	1305	SER	-	expression tag	UNP K0BRG7
B	1306	GLY	-	expression tag	UNP K0BRG7
B	1307	TYR	-	expression tag	UNP K0BRG7
B	1308	ILE	-	expression tag	UNP K0BRG7
B	1309	PRO	-	expression tag	UNP K0BRG7
B	1310	GLU	-	expression tag	UNP K0BRG7
B	1311	ALA	-	expression tag	UNP K0BRG7
B	1312	PRO	-	expression tag	UNP K0BRG7
B	1313	ARG	-	expression tag	UNP K0BRG7
B	1314	ASP	-	expression tag	UNP K0BRG7
B	1315	GLY	-	expression tag	UNP K0BRG7
B	1316	GLN	-	expression tag	UNP K0BRG7
B	1317	ALA	-	expression tag	UNP K0BRG7
B	1318	TYR	-	expression tag	UNP K0BRG7
B	1319	VAL	-	expression tag	UNP K0BRG7
B	1320	ARG	-	expression tag	UNP K0BRG7
B	1321	LYS	-	expression tag	UNP K0BRG7
B	1322	ASP	-	expression tag	UNP K0BRG7
B	1323	GLY	-	expression tag	UNP K0BRG7
B	1324	GLU	-	expression tag	UNP K0BRG7
B	1325	TRP	-	expression tag	UNP K0BRG7
B	1326	VAL	-	expression tag	UNP K0BRG7
B	1327	LEU	-	expression tag	UNP K0BRG7
B	1328	LEU	-	expression tag	UNP K0BRG7
B	1329	SER	-	expression tag	UNP K0BRG7
B	1330	THR	-	expression tag	UNP K0BRG7
B	1331	PHE	-	expression tag	UNP K0BRG7
B	1332	LEU	-	expression tag	UNP K0BRG7
B	1333	GLY	-	expression tag	UNP K0BRG7
B	1334	HIS	-	expression tag	UNP K0BRG7
B	1335	HIS	-	expression tag	UNP K0BRG7
B	1336	HIS	-	expression tag	UNP K0BRG7
B	1337	HIS	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1338	HIS	-	expression tag	UNP K0BRG7
B	1339	HIS	-	expression tag	UNP K0BRG7
B	1340	TRP	-	expression tag	UNP K0BRG7
B	1341	SER	-	expression tag	UNP K0BRG7
B	1342	HIS	-	expression tag	UNP K0BRG7
B	1343	PRO	-	expression tag	UNP K0BRG7
B	1344	GLN	-	expression tag	UNP K0BRG7
B	1345	PHE	-	expression tag	UNP K0BRG7
B	1346	GLU	-	expression tag	UNP K0BRG7
B	1347	LYS	-	expression tag	UNP K0BRG7
C	1060	PRO	VAL	engineered mutation	UNP K0BRG7
C	1061	PRO	LEU	engineered mutation	UNP K0BRG7
C	1291	SER	-	expression tag	UNP K0BRG7
C	1292	ARG	-	expression tag	UNP K0BRG7
C	1293	GLU	-	expression tag	UNP K0BRG7
C	1294	ASN	-	expression tag	UNP K0BRG7
C	1295	LEU	-	expression tag	UNP K0BRG7
C	1296	TYR	-	expression tag	UNP K0BRG7
C	1297	PHE	-	expression tag	UNP K0BRG7
C	1298	GLN	-	expression tag	UNP K0BRG7
C	1299	GLY	-	expression tag	UNP K0BRG7
C	1300	GLY	-	expression tag	UNP K0BRG7
C	1301	GLY	-	expression tag	UNP K0BRG7
C	1302	SER	-	expression tag	UNP K0BRG7
C	1303	ALA	-	expression tag	UNP K0BRG7
C	1304	GLY	-	expression tag	UNP K0BRG7
C	1305	SER	-	expression tag	UNP K0BRG7
C	1306	GLY	-	expression tag	UNP K0BRG7
C	1307	TYR	-	expression tag	UNP K0BRG7
C	1308	ILE	-	expression tag	UNP K0BRG7
C	1309	PRO	-	expression tag	UNP K0BRG7
C	1310	GLU	-	expression tag	UNP K0BRG7
C	1311	ALA	-	expression tag	UNP K0BRG7
C	1312	PRO	-	expression tag	UNP K0BRG7
C	1313	ARG	-	expression tag	UNP K0BRG7
C	1314	ASP	-	expression tag	UNP K0BRG7
C	1315	GLY	-	expression tag	UNP K0BRG7
C	1316	GLN	-	expression tag	UNP K0BRG7
C	1317	ALA	-	expression tag	UNP K0BRG7
C	1318	TYR	-	expression tag	UNP K0BRG7
C	1319	VAL	-	expression tag	UNP K0BRG7
C	1320	ARG	-	expression tag	UNP K0BRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1321	LYS	-	expression tag	UNP K0BRG7
C	1322	ASP	-	expression tag	UNP K0BRG7
C	1323	GLY	-	expression tag	UNP K0BRG7
C	1324	GLU	-	expression tag	UNP K0BRG7
C	1325	TRP	-	expression tag	UNP K0BRG7
C	1326	VAL	-	expression tag	UNP K0BRG7
C	1327	LEU	-	expression tag	UNP K0BRG7
C	1328	LEU	-	expression tag	UNP K0BRG7
C	1329	SER	-	expression tag	UNP K0BRG7
C	1330	THR	-	expression tag	UNP K0BRG7
C	1331	PHE	-	expression tag	UNP K0BRG7
C	1332	LEU	-	expression tag	UNP K0BRG7
C	1333	GLY	-	expression tag	UNP K0BRG7
C	1334	HIS	-	expression tag	UNP K0BRG7
C	1335	HIS	-	expression tag	UNP K0BRG7
C	1336	HIS	-	expression tag	UNP K0BRG7
C	1337	HIS	-	expression tag	UNP K0BRG7
C	1338	HIS	-	expression tag	UNP K0BRG7
C	1339	HIS	-	expression tag	UNP K0BRG7
C	1340	TRP	-	expression tag	UNP K0BRG7
C	1341	SER	-	expression tag	UNP K0BRG7
C	1342	HIS	-	expression tag	UNP K0BRG7
C	1343	PRO	-	expression tag	UNP K0BRG7
C	1344	GLN	-	expression tag	UNP K0BRG7
C	1345	PHE	-	expression tag	UNP K0BRG7
C	1346	GLU	-	expression tag	UNP K0BRG7
C	1347	LYS	-	expression tag	UNP K0BRG7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	221	Total	C	N	O	S	2	0
			1633	1028	274	325	6		

- Molecule 3 is a protein called antibody S41 light chain.

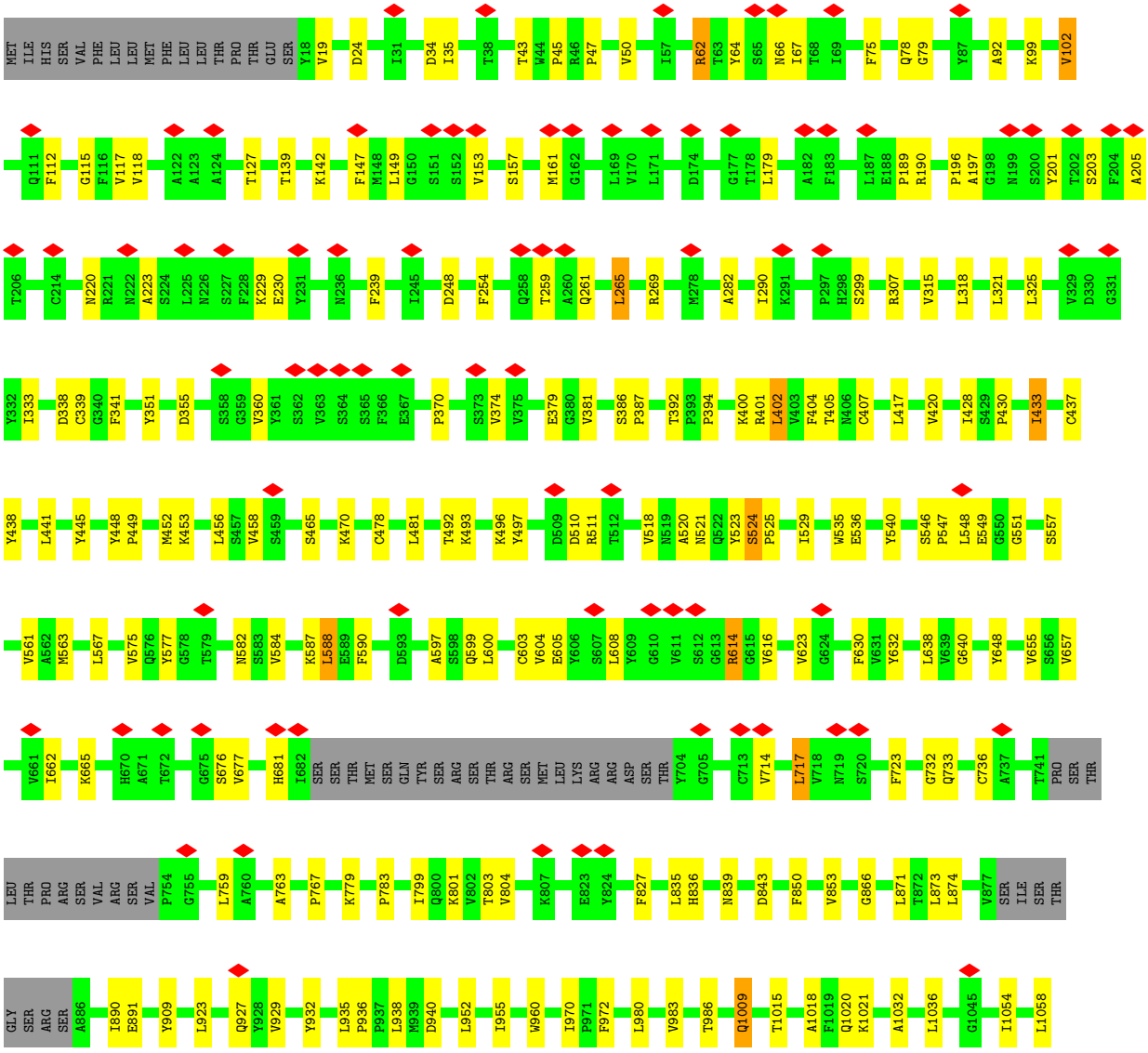
Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	212	Total	C	N	O	S	0	0
			1601	997	277	323	4		

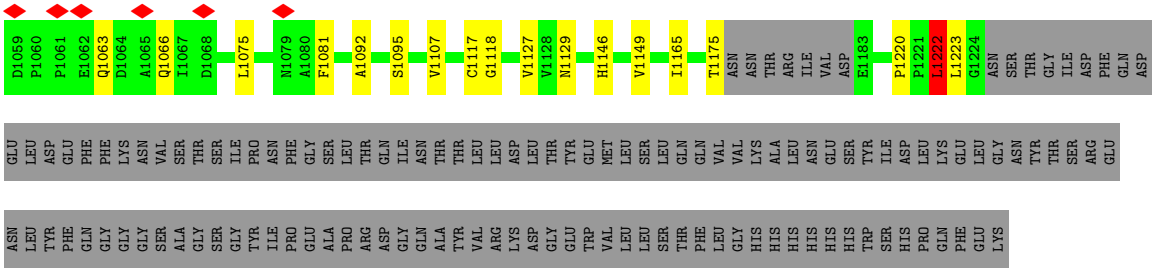
3 Residue-property plots (i)

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: MERS-CoV Spike glycoprotein

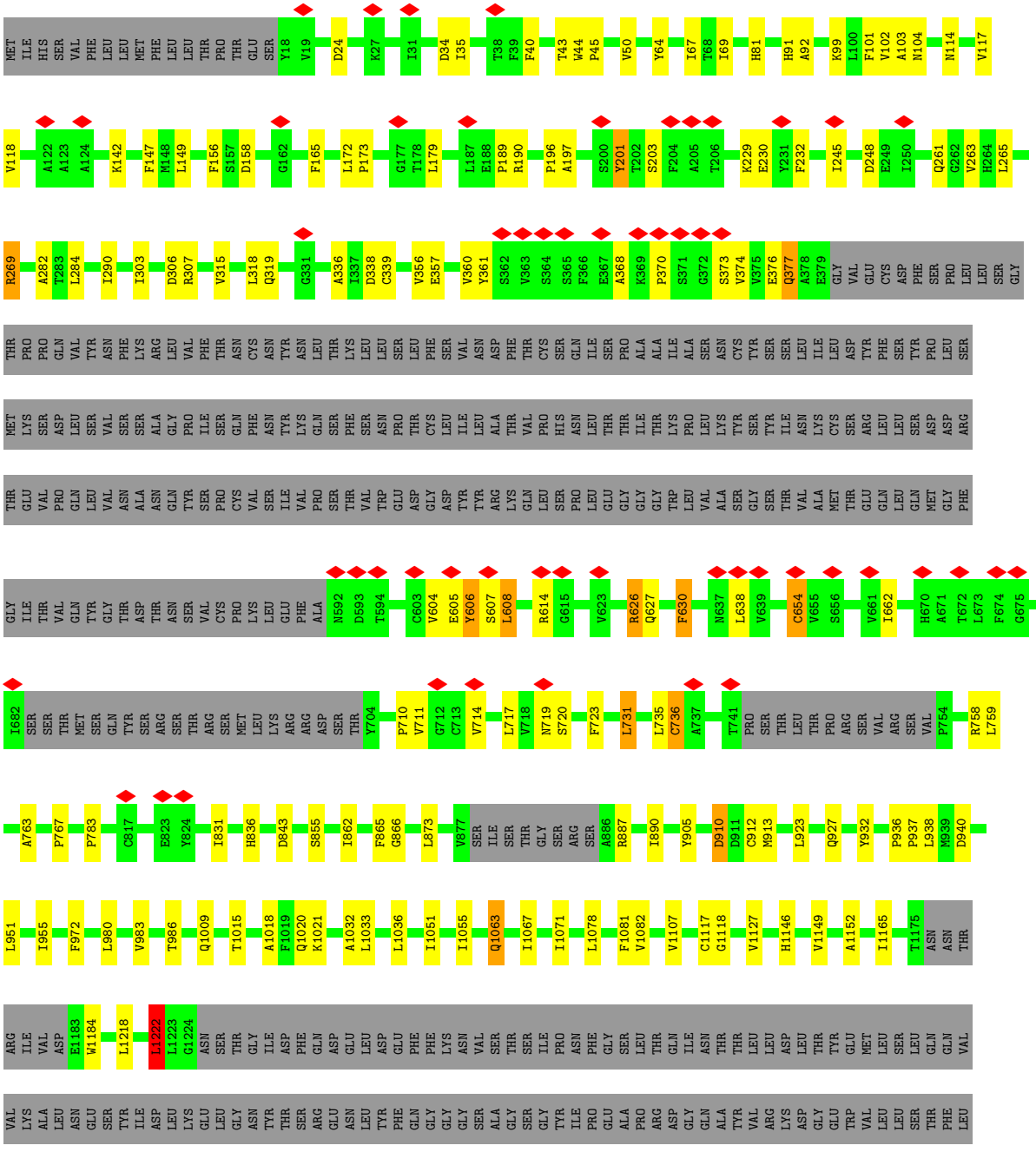
Chain A:





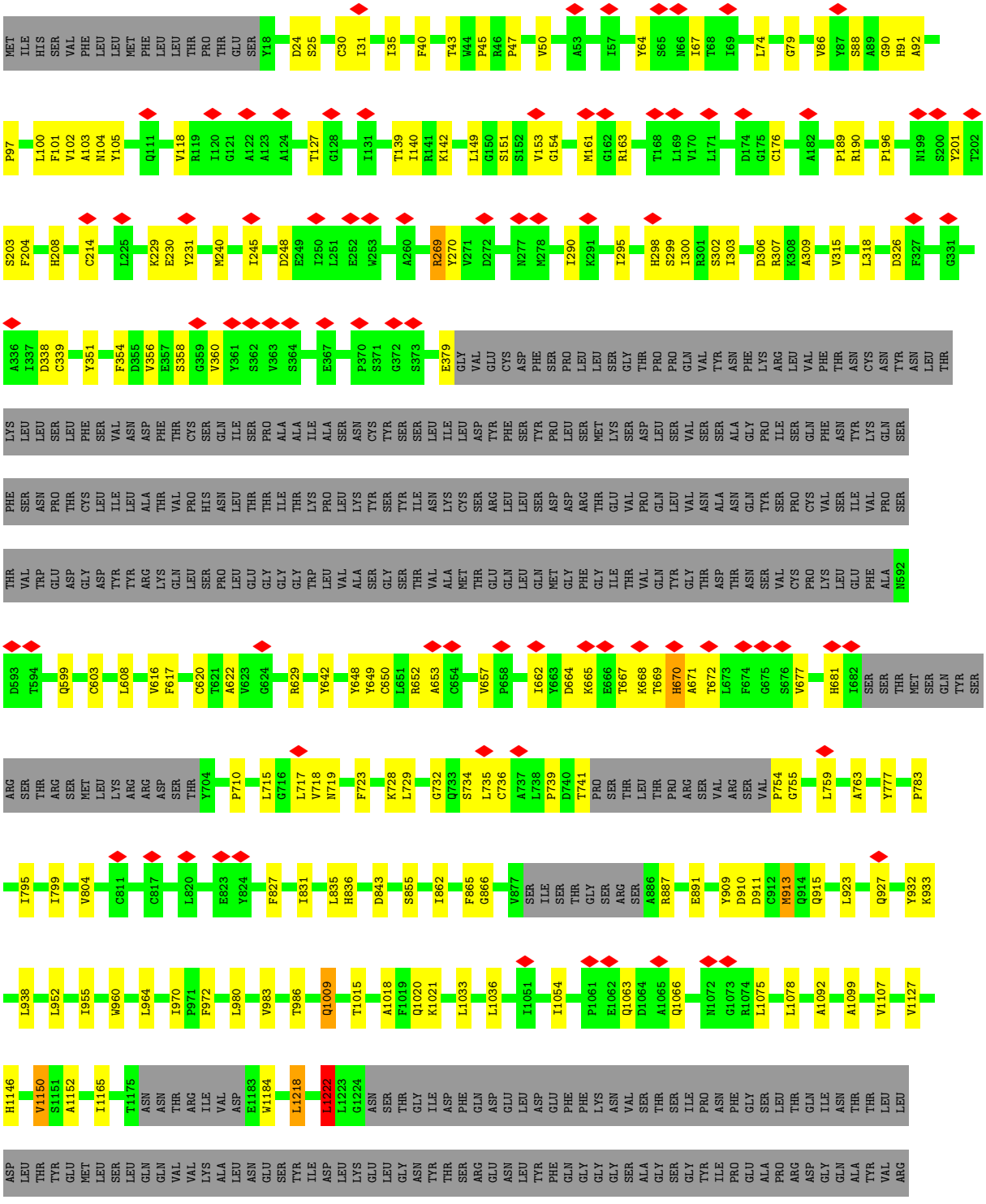
• Molecule 1: MERS-CoV Spike glycoprotein

Chain B:

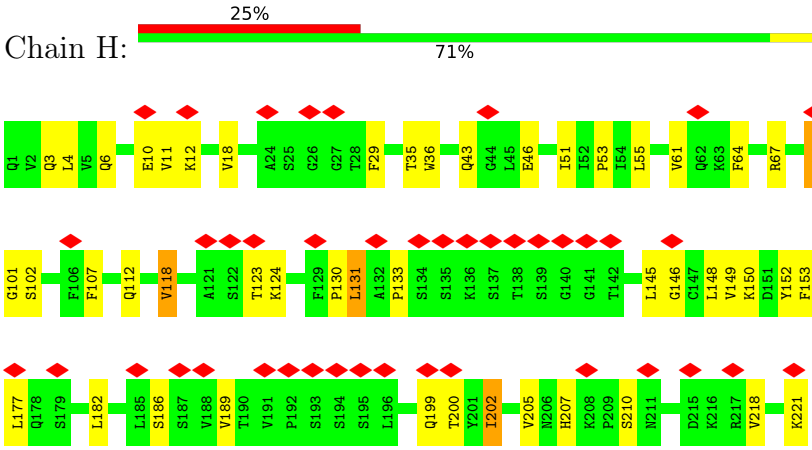


- Molecule 1: MERS-CoV Spike glycoprotein

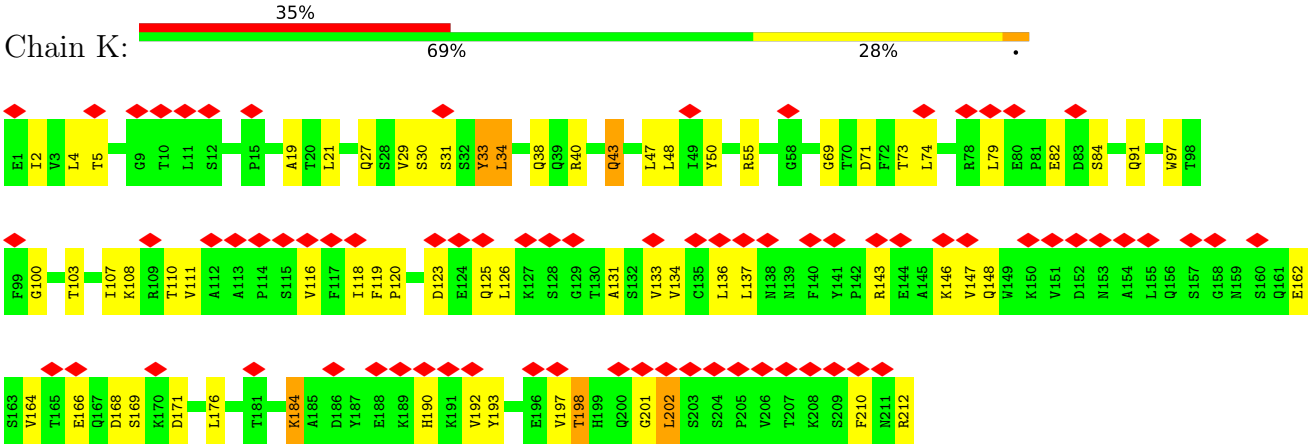
Chain C:



• Molecule 2: antibody S41 heavy chain



• Molecule 3: antibody S41 light chain



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	-0.002	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	0.66	2/9151 (0.0%)	0.63	1/12457 (0.0%)
1	B	0.65	1/7482 (0.0%)	0.63	2/10173 (0.0%)
1	C	0.67	3/7482 (0.0%)	0.65	2/10173 (0.0%)
2	H	0.75	4/1675 (0.2%)	0.74	8/2278 (0.4%)
3	K	0.66	0/1635	0.63	0/2223
All	All	0.67	10/27425 (0.0%)	0.64	13/37304 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	160[A]	SER	C-O	7.07	1.36	1.23
2	H	160[B]	SER	C-O	7.07	1.36	1.23
2	H	186[A]	SER	C-O	6.92	1.36	1.23
2	H	186[B]	SER	C-O	6.92	1.36	1.23
1	A	681	HIS	CB-CG	-6.74	1.38	1.50
1	C	681	HIS	CB-CG	-6.69	1.38	1.50
1	B	681	HIS	CB-CG	-6.68	1.38	1.50
1	C	736	CYS	CB-SG	-5.37	1.73	1.81
1	A	736	CYS	CB-SG	-5.33	1.73	1.81
1	C	891	GLU	CB-CG	-5.11	1.42	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1222	LEU	CD1-CG-CD2	7.38	132.64	110.50
1	A	1222	LEU	CD1-CG-CD2	7.38	132.62	110.50
1	B	1222	LEU	CD1-CG-CD2	7.38	132.62	110.50
1	C	887	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	887	ARG	NE-CZ-NH2	-6.19	117.20	120.30
2	H	186[A]	SER	CA-C-O	5.76	132.19	120.10
2	H	186[B]	SER	CA-C-O	5.76	132.19	120.10
2	H	160[A]	SER	CA-C-O	5.75	132.17	120.10
2	H	160[B]	SER	CA-C-O	5.75	132.17	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	186[A]	SER	O-C-N	-5.12	114.51	122.70
2	H	186[B]	SER	O-C-N	-5.12	114.51	122.70
2	H	160[A]	SER	O-C-N	-5.04	114.64	122.70
2	H	160[B]	SER	O-C-N	-5.04	114.64	122.70

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	8940	0	8622	114	0
1	B	7313	0	7045	91	0
1	C	7313	0	7045	107	0
2	H	1633	0	1621	36	0
3	K	1601	0	1551	32	0
All	All	26800	0	25884	363	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 7.

All (363) 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:B:376:GLU:OE1	1:B:377:GLN:NE2	1.68	1.26
1:B:627:GLN:OE1	1:B:627:GLN:N	1.86	1.09
1:B:376:GLU:CD	1:B:377:GLN:HE21	1.61	1.04
1:B:376:GLU:HG3	1:B:377:GLN:H	1.18	1.04
1:C:92:ALA:HB3	1:C:307:ARG:HH21	1.35	0.91
1:B:376:GLU:CG	1:B:377:GLN:H	1.88	0.86
1:B:376:GLU:HG3	1:B:377:GLN:N	1.90	0.85
1:A:392:THR:HB	1:A:492:THR:HB	1.61	0.82
1:A:804:VAL:H	1:A:835:LEU:HD13	1.46	0.80
1:C:189:PRO:HB3	1:C:196:PRO:HB2	1.65	0.79
1:A:548:LEU:N	1:A:548:LEU:HD22	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:GLU:O	1:B:361:TYR:OH	2.02	0.76
1:C:358:SER:HB3	1:C:664:ASP:HA	1.67	0.75
1:C:92:ALA:HA	1:C:97:PRO:HB3	1.70	0.74
1:C:710:PRO:HD2	1:C:735:LEU:HD11	1.69	0.73
1:C:50:VAL:HG21	1:C:338:ASP:HB2	1.71	0.72
1:C:302:SER:HB3	1:C:306:ASP:HB3	1.72	0.72
1:A:657:VAL:HG13	1:A:677:VAL:HG21	1.72	0.71
1:C:670:HIS:N	1:C:754:PRO:HB2	2.06	0.71
1:C:92:ALA:CB	1:C:307:ARG:HH21	2.04	0.70
1:C:669:THR:HA	1:C:754:PRO:HB2	1.73	0.70
1:B:866:GLY:HA2	1:B:972:PHE:HB3	1.72	0.70
1:C:149:LEU:HB3	1:C:290:ILE:HG21	1.74	0.69
1:C:657:VAL:HG13	1:C:677:VAL:HG21	1.74	0.69
1:B:201:TYR:CG	1:B:201:TYR:O	2.45	0.69
1:B:723:PHE:HB3	1:B:763:ALA:HB2	1.73	0.69
1:C:300:ILE:N	1:C:300:ILE:HD12	2.09	0.68
1:C:866:GLY:HA2	1:C:972:PHE:HB3	1.76	0.68
3:K:84:SER:HB3	3:K:107:ILE:HG12	1.76	0.68
1:B:189:PRO:HB2	1:B:197:ALA:HB2	1.75	0.67
1:C:31:ILE:HB	1:C:100:LEU:CD1	2.24	0.67
1:B:245:ILE:HG23	1:B:269:ARG:HD2	1.77	0.67
1:C:90:GLY:N	1:C:300:ILE:O	2.24	0.67
1:C:358:SER:CB	1:C:664:ASP:HA	2.25	0.67
1:C:664:ASP:HB3	1:C:669:THR:OG1	1.96	0.66
1:B:35:ILE:HD13	1:B:104:ASN:HB3	1.78	0.66
1:C:303:ILE:HG12	1:C:306:ASP:HB2	1.78	0.65
1:C:127:THR:HA	1:C:139:THR:HA	1.78	0.65
3:K:125:GLN:HG3	3:K:131:ALA:HA	1.80	0.64
1:A:548:LEU:HA	1:A:549:GLU:CD	2.18	0.64
1:A:866:GLY:HA2	1:A:972:PHE:HB3	1.80	0.64
1:A:92:ALA:H	1:A:307:ARG:HH21	1.45	0.63
1:A:127:THR:HA	1:A:139:THR:HA	1.80	0.63
1:B:373:SER:HB2	1:B:607:SER:HB2	1.79	0.63
3:K:30:SER:HB3	3:K:33:TYR:HB2	1.78	0.63
1:C:35:ILE:HD13	1:C:104:ASN:HB3	1.81	0.63
1:B:149:LEU:HB3	1:B:290:ILE:HG21	1.80	0.62
1:A:50:VAL:HG21	1:A:338:ASP:HB2	1.81	0.62
1:C:92:ALA:HB3	1:C:307:ARG:NH2	2.10	0.62
1:C:91:HIS:CD2	1:C:101:PHE:HB2	2.34	0.62
1:C:90:GLY:HA2	1:C:101:PHE:H	1.64	0.62
1:B:201:TYR:O	1:B:201:TYR:CD1	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:4:LEU:HD11	3:K:100:GLY:HA2	1.82	0.62
1:A:548:LEU:N	1:A:549:GLU:HA	2.15	0.61
1:C:360:VAL:HG22	1:C:662:ILE:HG23	1.81	0.61
2:H:202:ILE:HG13	2:H:218:VAL:HB	1.81	0.61
1:A:149:LEU:HB3	1:A:290:ILE:HG21	1.83	0.61
1:A:540:TYR:H	2:H:102:SER:HB3	1.65	0.61
1:B:34:ASP:HB2	1:B:99:LYS:HD2	1.81	0.61
1:A:557:SER:HB2	2:H:55:LEU:HD11	1.82	0.61
1:B:92:ALA:H	1:B:307:ARG:HH21	1.46	0.61
1:A:220:ASN:HB3	1:A:223:ALA:HB2	1.82	0.60
1:C:668:LYS:O	1:C:754:PRO:HB3	2.02	0.60
1:B:626:ARG:NH1	1:B:626:ARG:HB2	2.16	0.60
3:K:38:GLN:HB2	3:K:48:LEU:HD11	1.83	0.60
1:A:401:ARG:HH22	1:A:521:ASN:HB3	1.66	0.60
1:B:714:VAL:HG11	1:B:717:LEU:HD12	1.83	0.60
1:A:511:ARG:C	2:H:74:LYS:HE3	2.22	0.60
1:A:873:LEU:HG	1:A:890:ILE:HB	1.84	0.59
1:B:1032:ALA:HB1	1:B:1081:PHE:HE1	1.67	0.59
2:H:130:PRO:HD3	3:K:125:GLN:HE21	1.66	0.59
1:A:546:SER:O	1:A:549:GLU:C	2.41	0.59
2:H:51:ILE:HD12	2:H:72:ALA:HB2	1.85	0.59
1:C:723:PHE:HB3	1:C:763:ALA:HB2	1.84	0.58
1:B:1051:ILE:HG23	1:B:1067:ILE:HG12	1.85	0.58
1:A:394:PRO:HG3	1:A:400:LYS:HG3	1.86	0.58
1:A:510:ASP:O	2:H:74:LYS:NZ	2.32	0.58
3:K:168:ASP:HB3	3:K:171:ASP:HB2	1.85	0.58
1:C:669:THR:HA	1:C:754:PRO:CB	2.34	0.58
2:H:124:LYS:HG2	2:H:182:LEU:HD21	1.85	0.58
2:H:133:PRO:HG2	2:H:221:LYS:H	1.67	0.58
1:A:723:PHE:HB3	1:A:763:ALA:HB2	1.85	0.57
1:A:19:VAL:HG21	1:A:239:PHE:HA	1.87	0.57
1:A:34:ASP:HB2	1:A:99:LYS:HD2	1.86	0.57
1:C:31:ILE:HB	1:C:100:LEU:HD12	1.86	0.57
1:B:711:VAL:HG13	1:B:735:LEU:HD12	1.87	0.57
1:B:630:PHE:HB2	1:B:638:LEU:HD11	1.85	0.57
1:A:35:ILE:HD11	1:A:203:SER:HB2	1.87	0.56
1:C:719:ASN:HA	1:C:759:LEU:HB3	1.86	0.56
1:A:548:LEU:N	1:A:548:LEU:CD2	2.67	0.56
1:A:599:GLN:HB3	1:A:604:VAL:HG11	1.87	0.56
1:B:24:ASP:HA	1:B:229:LYS:HD3	1.88	0.56
1:C:31:ILE:HG21	1:C:100:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:HIS:HB3	2:H:210:SER:HB3	1.87	0.56
1:B:43:THR:HG22	1:B:45:PRO:HD3	1.86	0.56
1:B:710:PRO:HD2	1:B:735:LEU:HD11	1.88	0.56
1:C:31:ILE:CG2	1:C:100:LEU:HD11	2.35	0.56
1:C:64:TYR:HB3	1:C:67:ILE:HD11	1.87	0.56
1:A:437:CYS:HB3	1:A:582:ASN:HB3	1.88	0.56
1:A:497:TYR:HB2	1:A:561:VAL:HG12	1.87	0.56
1:B:843:ASP:HB3	1:B:938:LEU:HD13	1.85	0.56
1:A:24:ASP:HA	1:A:229:LYS:HD3	1.88	0.56
2:H:157:VAL:HB	2:H:207:HIS:HD2	1.71	0.56
3:K:193:TYR:H	3:K:210:PHE:HB3	1.71	0.56
1:C:1054:ILE:HG21	1:C:1066:GLN:HB2	1.88	0.55
1:A:1018:ALA:HA	1:A:1021:LYS:HE2	1.89	0.55
1:C:118:VAL:HG22	1:C:315:VAL:HG22	1.89	0.55
1:B:118:VAL:HG22	1:B:315:VAL:HG22	1.88	0.55
1:C:667:THR:HB	1:C:669:THR:HG23	1.88	0.54
2:H:97:ALA:HB1	2:H:107:PHE:HB3	1.89	0.54
1:A:189:PRO:HB2	1:A:197:ALA:HB2	1.90	0.54
1:A:546:SER:O	1:A:549:GLU:O	2.25	0.54
1:B:1018:ALA:HA	1:B:1021:LYS:HE2	1.90	0.54
1:C:31:ILE:HB	1:C:100:LEU:HD11	1.88	0.54
1:B:158:ASP:OD2	1:B:201:TYR:CE1	2.60	0.53
1:A:843:ASP:HB3	1:A:938:LEU:HD13	1.90	0.53
1:B:156:PHE:CE1	1:B:196:PRO:HB2	2.43	0.53
1:B:263:VAL:HB	1:B:284:LEU:HB2	1.91	0.53
1:B:189:PRO:HB3	1:B:196:PRO:HG2	1.90	0.53
1:C:783:PRO:HA	1:C:1146:HIS:HA	1.90	0.53
1:A:64:TYR:HB3	1:A:67:ILE:HD11	1.91	0.53
1:A:449:PRO:HG2	1:A:452:MET:HG2	1.91	0.53
1:C:664:ASP:HB2	1:C:729:LEU:HD11	1.91	0.53
1:C:1018:ALA:HA	1:C:1021:LYS:HE2	1.90	0.53
1:A:603:CYS:HA	1:A:616:VAL:HG22	1.90	0.52
1:A:402:LEU:HD13	1:A:445:TYR:HE1	1.75	0.52
1:C:298:HIS:HD2	1:C:300:ILE:HD11	1.74	0.52
1:C:1107:VAL:HG21	1:C:1127:VAL:HG23	1.92	0.52
1:C:358:SER:OG	1:C:665:LYS:N	2.43	0.52
1:B:783:PRO:HA	1:B:1146:HIS:HA	1.91	0.52
1:B:720:SER:HB3	1:B:758:ARG:HB3	1.92	0.52
1:C:629:ARG:HA	1:C:642:TYR:HB2	1.92	0.52
1:B:50:VAL:HG21	1:B:338:ASP:HB2	1.91	0.51
2:H:130:PRO:HG2	3:K:125:GLN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:119:PHE:HB2	3:K:134:VAL:HB	1.92	0.51
1:A:355:ASP:HB3	1:A:665:LYS:HE3	1.91	0.51
1:C:31:ILE:CB	1:C:100:LEU:HD11	2.40	0.51
1:C:299:SER:C	1:C:300:ILE:HD12	2.31	0.51
1:B:64:TYR:HB3	1:B:67:ILE:HD11	1.92	0.51
1:A:493:LYS:HG2	1:A:567:LEU:HB2	1.93	0.51
1:B:1107:VAL:HG21	1:B:1127:VAL:HG23	1.92	0.51
1:A:717:LEU:HD12	1:A:759:LEU:HB2	1.93	0.51
1:B:265:LEU:HB2	1:B:282:ALA:HB3	1.91	0.51
1:A:102:VAL:HG21	1:A:205:ALA:HB2	1.92	0.51
1:A:404:PHE:HB3	1:A:407:CYS:SG	2.51	0.51
1:A:783:PRO:HA	1:A:1146:HIS:HA	1.93	0.51
1:B:719:ASN:HA	1:B:759:LEU:HB3	1.93	0.50
2:H:51:ILE:HG21	2:H:70:ILE:HB	1.94	0.50
1:C:245:ILE:HG23	1:C:269:ARG:HD2	1.92	0.50
1:C:24:ASP:HA	1:C:229:LYS:HD3	1.94	0.50
1:A:540:TYR:HD2	2:H:101:GLY:HA2	1.77	0.50
1:A:1165:ILE:HG12	1:A:1222:LEU:HD11	1.94	0.50
1:B:374:VAL:HG22	1:B:606:TYR:HA	1.94	0.50
1:A:803:THR:HG23	1:A:839:ASN:ND2	2.27	0.49
1:C:665:LYS:HA	1:C:668:LYS:HA	1.94	0.49
1:A:676:SER:HA	1:B:905:TYR:O	2.12	0.49
1:C:35:ILE:HD11	1:C:203:SER:HB2	1.93	0.49
1:C:843:ASP:HB3	1:C:938:LEU:HD13	1.95	0.49
2:H:12:LYS:O	2:H:118:VAL:HA	2.12	0.49
1:A:157:SER:HB3	1:A:197:ALA:HA	1.94	0.49
1:C:669:THR:HB	1:C:755:GLY:O	2.12	0.49
2:H:162:ASN:H	2:H:202:ILE:HA	1.78	0.49
1:A:47:PRO:HB2	1:A:79:GLY:HA2	1.95	0.49
1:C:795:ILE:HG21	1:C:1099:ALA:HB2	1.94	0.49
1:B:376:GLU:CG	1:B:377:GLN:N	2.56	0.49
1:C:669:THR:C	1:C:754:PRO:HB2	2.32	0.48
3:K:34:LEU:HD12	3:K:91:GLN:HG2	1.95	0.48
1:C:31:ILE:CG2	1:C:100:LEU:CD1	2.90	0.48
1:C:43:THR:HG22	1:C:45:PRO:HD3	1.96	0.48
1:C:827:PHE:CD1	1:C:1075:LEU:HD22	2.48	0.48
1:A:929:VAL:HG13	1:C:653:ALA:HB3	1.96	0.48
1:A:433:ILE:HD11	1:A:575:VAL:HG21	1.94	0.48
1:A:470:LYS:HB3	1:A:520:ALA:HA	1.95	0.48
1:A:518:VAL:HG23	1:A:525:PRO:HD3	1.93	0.48
1:A:540:TYR:HD1	2:H:55:LEU:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PHE:CE1	1:A:115:GLY:HA2	2.49	0.48
1:A:605:GLU:HG2	1:A:614:ARG:HG3	1.94	0.48
3:K:123:ASP:HA	3:K:126:LEU:HD12	1.96	0.48
1:A:980:LEU:O	1:A:983:VAL:HG22	2.14	0.48
3:K:162:GLU:HB2	3:K:176:LEU:HD21	1.94	0.48
1:A:827:PHE:CD2	1:A:1075:LEU:HD22	2.49	0.47
1:B:1067:ILE:O	1:B:1071:ILE:HG13	2.14	0.47
1:A:43:THR:HG22	1:A:45:PRO:HD3	1.96	0.47
1:A:1054:ILE:HG21	1:A:1066:GLN:HB2	1.95	0.47
1:C:980:LEU:O	1:C:983:VAL:HG22	2.14	0.47
1:B:374:VAL:HG22	1:B:605:GLU:O	2.15	0.47
1:B:1152:ALA:HB2	1:B:1184:TRP:CH2	2.50	0.47
2:H:61:VAL:HG13	2:H:64:PHE:H	1.79	0.47
2:H:149:VAL:HG11	2:H:157:VAL:HG11	1.96	0.47
1:B:873:LEU:HD21	1:B:890:ILE:HD13	1.97	0.47
1:B:980:LEU:O	1:B:983:VAL:HG22	2.14	0.47
1:A:511:ARG:O	2:H:74:LYS:HE3	2.14	0.47
1:C:923:LEU:O	1:C:927:GLN:HG3	2.15	0.47
3:K:2:ILE:HG23	3:K:27:GLN:HB3	1.96	0.47
1:C:105:TYR:HB3	1:C:295:ILE:HB	1.97	0.47
3:K:21:LEU:HD12	3:K:74:LEU:HD23	1.97	0.47
1:A:75:PHE:HB2	1:A:321:LEU:HB2	1.97	0.47
1:A:428:ILE:HD13	1:A:433:ILE:HD13	1.97	0.47
1:C:35:ILE:HG23	1:C:103:ALA:HA	1.97	0.47
1:C:74:LEU:HB3	1:C:318:LEU:HB3	1.97	0.47
1:A:117:VAL:HG13	1:A:318:LEU:HD11	1.97	0.47
1:A:547:PRO:HA	1:A:551:GLY:N	2.30	0.47
1:B:360:VAL:HG22	1:B:662:ILE:HG23	1.97	0.47
1:A:189:PRO:HB3	1:A:196:PRO:HG2	1.97	0.46
1:C:913:MET:HB2	1:C:913:MET:HE2	1.56	0.46
1:C:142:LYS:HD3	1:C:248:ASP:O	2.16	0.46
3:K:146:LYS:HB2	3:K:198:THR:HG23	1.96	0.46
1:A:190:ARG:HD3	1:A:230:GLU:O	2.16	0.46
1:C:151:SER:HA	1:C:290:ILE:HA	1.97	0.46
2:H:88:SER:O	2:H:91:THR:HG22	2.15	0.46
2:H:124:LYS:H	2:H:153:PHE:HB3	1.81	0.46
1:C:300:ILE:N	1:C:300:ILE:CD1	2.78	0.46
1:A:535:TRP:CD1	1:A:536:GLU:HG2	2.51	0.46
1:C:622:ALA:HA	1:C:648:TYR:CD2	2.50	0.46
1:B:1063:GLN:O	1:B:1067:ILE:HG13	2.16	0.46
1:B:50:VAL:HG12	1:B:336:ALA:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:201:GLY:O	3:K:202:LEU:HB2	2.15	0.45
1:B:1165:ILE:HG12	1:B:1222:LEU:HD11	1.98	0.45
1:B:158:ASP:OD2	1:B:201:TYR:CD1	2.69	0.45
1:B:731:LEU:H	1:B:736:CYS:HA	1.81	0.45
1:C:667:THR:HG21	1:C:741:THR:HB	1.98	0.45
1:A:630:PHE:HB3	1:A:632:TYR:CE1	2.52	0.45
1:B:1078:LEU:HD23	1:B:1078:LEU:HA	1.79	0.45
1:A:386:SER:N	1:A:387:PRO:HD2	2.31	0.45
1:A:630:PHE:HB3	1:A:632:TYR:HE1	1.82	0.45
1:C:603:CYS:HA	1:C:616:VAL:HG22	1.98	0.45
2:H:150:LYS:HE3	2:H:150:LYS:HB2	1.83	0.45
1:A:732:GLY:HA3	1:B:936:PRO:HG2	1.98	0.45
1:C:40:PHE:CZ	1:C:88:SER:HB3	2.51	0.45
1:C:669:THR:HG22	1:C:755:GLY:H	1.82	0.45
1:C:1165:ILE:HG12	1:C:1222:LEU:HD11	1.99	0.45
2:H:12:LYS:HG3	2:H:18:VAL:HB	1.97	0.45
1:A:456:LEU:HA	1:A:465:SER:HB3	1.98	0.45
2:H:6:GLN:H	2:H:112:GLN:HE21	1.65	0.45
3:K:120:PRO:HB2	3:K:212:ARG:NH1	2.32	0.45
1:B:368:ALA:HB3	1:B:654:CYS:HB3	2.00	0.45
1:B:927:GLN:HG2	1:B:932:TYR:CE2	2.52	0.45
1:A:360:VAL:HG22	1:A:662:ILE:HG23	1.98	0.44
1:B:608:LEU:H	1:B:608:LEU:HG	1.61	0.44
1:A:370:PRO:HA	1:A:603:CYS:O	2.16	0.44
1:A:265:LEU:HB2	1:A:282:ALA:HB3	1.99	0.44
1:B:117:VAL:HG13	1:B:318:LEU:HD11	1.99	0.44
1:B:261:GLN:H	1:B:261:GLN:HG3	1.56	0.44
1:B:923:LEU:O	1:B:927:GLN:HG3	2.17	0.44
3:K:40:ARG:HH12	3:K:169:SER:HA	1.81	0.44
3:K:119:PHE:HE1	3:K:136:LEU:HB2	1.83	0.44
1:A:927:GLN:HG2	1:A:932:TYR:CE1	2.53	0.44
1:A:142:LYS:HD3	1:A:248:ASP:O	2.16	0.44
1:A:441:LEU:HG	1:A:575:VAL:HG12	1.99	0.44
1:C:25:SER:H	1:C:229:LYS:HB3	1.82	0.44
3:K:47:LEU:HD21	3:K:50:TYR:HB3	1.99	0.44
1:C:140:ILE:HG12	1:C:309:ALA:HB3	2.00	0.44
1:B:370:PRO:HB3	1:B:604:VAL:C	2.38	0.44
1:B:374:VAL:CG2	1:B:606:TYR:HA	2.48	0.44
1:C:40:PHE:HE1	1:C:86:VAL:O	2.00	0.44
1:A:511:ARG:HA	2:H:74:LYS:HE3	1.99	0.44
1:A:588:LEU:HD22	1:A:588:LEU:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:LYS:HD3	1:A:779:LYS:HA	1.90	0.44
1:A:433:ILE:HD12	1:A:433:ILE:HA	1.73	0.43
2:H:53:PRO:HG3	2:H:72:ALA:HB1	2.00	0.43
1:C:326:ASP:HB2	1:C:354:PHE:CE1	2.53	0.43
1:C:672:THR:HB	1:C:715:LEU:HB3	2.00	0.43
1:A:118:VAL:HG21	1:A:147:PHE:CZ	2.52	0.43
1:A:960:TRP:HD1	1:A:970:ILE:HD13	1.81	0.43
1:C:269:ARG:HG3	1:C:270:TYR:N	2.32	0.43
1:B:862:ILE:HG12	1:B:865:PHE:HD1	1.84	0.43
1:B:910:ASP:HA	1:B:913:MET:HE2	1.99	0.43
2:H:152:TYR:HE2	2:H:155:GLU:HA	1.83	0.43
1:A:547:PRO:HA	1:A:551:GLY:CA	2.49	0.43
1:C:831:ILE:HG21	1:C:1078:LEU:HD13	2.00	0.43
1:A:632:TYR:CZ	1:A:638:LEU:HD13	2.53	0.43
1:B:831:ILE:HD12	1:B:1082:VAL:HG21	2.01	0.43
1:A:938:LEU:O	1:A:938:LEU:HG	2.19	0.43
1:A:118:VAL:HG22	1:A:315:VAL:HG22	2.00	0.43
1:A:936:PRO:HG2	1:C:732:GLY:HA3	2.00	0.43
1:A:1117:CYS:HB2	1:A:1118:GLY:H	1.62	0.43
1:C:777:TYR:HB3	1:C:1150:VAL:HG12	2.01	0.43
2:H:64:PHE:HA	2:H:67:ARG:HH11	1.84	0.43
1:A:254:PHE:CZ	1:A:265:LEU:HG	2.54	0.43
1:A:767:PRO:HB3	1:B:855:SER:O	2.19	0.43
1:B:142:LYS:HD3	1:B:248:ASP:O	2.19	0.43
3:K:43:GLN:HE21	3:K:43:GLN:HB3	1.49	0.42
1:A:733:GLN:NE2	1:B:937:PRO:HD2	2.33	0.42
1:A:1107:VAL:HG21	1:A:1127:VAL:HG23	2.01	0.42
1:C:927:GLN:HG2	1:C:932:TYR:CE2	2.55	0.42
2:H:4:LEU:HA	2:H:4:LEU:HD12	1.77	0.42
1:A:799:ILE:HG23	1:A:1092:ALA:HB2	2.00	0.42
1:A:801:LYS:HB2	1:A:935:LEU:HB2	2.01	0.42
1:B:45:PRO:HB2	1:B:81:HIS:HB3	2.01	0.42
1:B:172:LEU:HD12	1:B:173:PRO:HD2	2.01	0.42
3:K:40:ARG:H	3:K:43:GLN:HE21	1.67	0.42
1:A:1220:PRO:HA	1:A:1223:LEU:HD12	2.00	0.42
1:B:951:LEU:O	1:B:955:ILE:HG13	2.20	0.42
1:B:1117:CYS:HB2	1:B:1118:GLY:H	1.64	0.42
1:C:1152:ALA:HB2	1:C:1184:TRP:CH2	2.54	0.42
1:C:1218:LEU:HD13	1:C:1218:LEU:HA	1.92	0.42
3:K:31:SER:HA	3:K:69:GLY:H	1.84	0.42
1:B:35:ILE:HG23	1:B:103:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ASP:OD2	1:B:201:TYR:HE1	2.02	0.42
1:C:154:GLY:O	1:C:163:ARG:HB3	2.19	0.42
1:C:662:ILE:HD12	1:C:671:ALA:HB3	2.01	0.42
1:C:665:LYS:C	1:C:668:LYS:H	2.23	0.42
1:C:804:VAL:H	1:C:835:LEU:HD13	1.85	0.42
1:C:799:ILE:HG23	1:C:1092:ALA:HB2	2.02	0.42
2:H:161:TRP:CE2	2:H:189:VAL:HB	2.55	0.42
1:A:587:LYS:HA	1:A:588:LEU:HA	1.63	0.42
1:C:190:ARG:HD3	1:C:230:GLU:O	2.19	0.42
3:K:184:LYS:HB3	3:K:184:LYS:HE3	1.82	0.42
1:A:78:GLN:HB3	1:A:341:PHE:HB2	2.02	0.42
1:C:862:ILE:HG12	1:C:865:PHE:HD1	1.85	0.42
1:A:597:ALA:HA	1:A:600:LEU:HG	2.02	0.42
1:B:114:ASN:HD22	1:B:319:GLN:HA	1.84	0.42
1:A:430:PRO:O	1:A:433:ILE:HG22	2.20	0.41
1:B:370:PRO:HB3	1:B:604:VAL:CA	2.50	0.41
1:C:204:PHE:HB2	1:C:231:TYR:CD1	2.55	0.41
1:A:891:GLU:OE2	1:A:1129:ASN:HB2	2.20	0.41
1:B:91:HIS:CD2	1:B:101:PHE:HB2	2.55	0.41
2:H:161:TRP:HE3	2:H:202:ILE:HB	1.85	0.41
1:B:303:ILE:HG12	1:B:306:ASP:HB2	2.02	0.41
1:B:376:GLU:OE2	1:B:376:GLU:HA	2.20	0.41
1:C:30:CYS:HB3	1:C:231:TYR:CE1	2.55	0.41
1:C:608:LEU:HD11	1:C:617:PHE:HZ	1.85	0.41
1:A:325:LEU:HD22	1:A:333:ILE:HD13	2.03	0.41
1:A:640:GLY:HA3	1:A:648:TYR:OH	2.20	0.41
1:C:47:PRO:HB2	1:C:79:GLY:HA2	2.01	0.41
1:C:952:LEU:HA	1:C:955:ILE:HD12	2.01	0.41
1:C:960:TRP:HD1	1:C:970:ILE:HD13	1.86	0.41
1:A:102:VAL:HG13	1:A:299:SER:HB2	2.01	0.41
2:H:131:LEU:HA	2:H:146:GLY:O	2.21	0.41
1:A:850:PHE:HA	1:A:853:VAL:HG22	2.02	0.41
1:A:1032:ALA:HB1	1:A:1081:PHE:HE1	1.86	0.41
3:K:79:LEU:HD23	3:K:79:LEU:HA	1.83	0.41
1:A:923:LEU:HD23	1:A:923:LEU:HA	1.96	0.41
1:B:35:ILE:HD11	1:B:203:SER:HB2	2.03	0.41
1:B:614:ARG:HB3	1:B:654:CYS:SG	2.61	0.41
1:C:664:ASP:O	1:C:669:THR:N	2.54	0.41
1:B:118:VAL:HG21	1:B:147:PHE:CZ	2.55	0.41
1:B:190:ARG:HD3	1:B:230:GLU:O	2.20	0.41
1:B:767:PRO:HB3	1:C:855:SER:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:123:THR:HA	2:H:153:PHE:CD2	2.56	0.41
3:K:137:LEU:HD12	3:K:137:LEU:HA	1.87	0.41
1:A:871:LEU:HD22	1:A:874:LEU:HD12	2.02	0.41
1:B:626:ARG:HB2	1:B:626:ARG:HH11	1.82	0.41
2:H:36:TRP:HE1	2:H:51:ILE:HD11	1.85	0.41
3:K:108:LYS:HE2	3:K:111:VAL:HA	2.03	0.41
1:A:952:LEU:HA	1:A:955:ILE:HD12	2.03	0.40
1:C:728:LYS:HD2	1:C:739:PRO:HD2	2.04	0.40
3:K:21:LEU:O	3:K:73:THR:HA	2.21	0.40
1:B:1055:ILE:HA	1:B:1063:GLN:NE2	2.36	0.40
1:C:31:ILE:CB	1:C:100:LEU:CD1	2.95	0.40
1:C:662:ILE:HB	1:C:671:ALA:HB3	2.03	0.40
1:C:670:HIS:HB3	1:C:754:PRO:HG3	2.02	0.40
1:B:370:PRO:HB3	1:B:604:VAL:HA	2.03	0.40
1:B:932:TYR:HE2	1:B:1033:LEU:HD22	1.85	0.40
1:C:927:GLN:HE21	1:C:1033:LEU:HD13	1.86	0.40
1:A:1009:GLN:HE21	1:A:1009:GLN:HB3	1.64	0.40
3:K:19:ALA:HB2	3:K:79:LEU:HD11	2.04	0.40
3:K:29:VAL:HG21	3:K:91:GLN:HB3	2.03	0.40
1:A:448:TYR:HE2	1:A:453:LYS:HA	1.86	0.40
1:A:523:TYR:O	1:A:524:SER:HB3	2.22	0.40
1:C:911:ASP:O	1:C:915:GLN:HB2	2.22	0.40
1:C:1009:GLN:HE21	1:C:1009:GLN:HB3	1.67	0.40
3:K:143:ARG:HH12	3:K:166:GLU:HA	1.85	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	1149/1347 (85%)	1118 (97%)	28 (2%)	3 (0%)	37 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	935/1347 (69%)	924 (99%)	10 (1%)	1 (0%)	48 69
1	C	935/1347 (69%)	917 (98%)	17 (2%)	1 (0%)	48 69
2	H	221/221 (100%)	215 (97%)	5 (2%)	1 (0%)	25 44
3	K	210/212 (99%)	193 (92%)	16 (8%)	1 (0%)	25 44
All	All	3450/4474 (77%)	3367 (98%)	76 (2%)	7 (0%)	45 64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	VAL
1	C	913	MET
1	A	524	SER
1	B	654	CYS
1	A	62	ARG
3	K	202	LEU
2	H	154	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	989/1164 (85%)	938 (95%)	51 (5%)	19 39
1	B	799/1164 (69%)	768 (96%)	31 (4%)	27 52
1	C	799/1164 (69%)	763 (96%)	36 (4%)	23 46
2	H	185/184 (100%)	161 (87%)	24 (13%)	3 6
3	K	178/183 (97%)	157 (88%)	21 (12%)	4 9
All	All	2950/3859 (76%)	2787 (94%)	163 (6%)	20 37

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG

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Mol	Chain	Res	Type
1	A	66	ASN
1	A	102	VAL
1	A	153	VAL
1	A	161	MET
1	A	179	LEU
1	A	201	TYR
1	A	259	THR
1	A	261	GLN
1	A	265	LEU
1	A	269	ARG
1	A	339	CYS
1	A	351	TYR
1	A	374	VAL
1	A	379	GLU
1	A	402	LEU
1	A	405	THR
1	A	417	LEU
1	A	420	VAL
1	A	433	ILE
1	A	438	TYR
1	A	458	VAL
1	A	478	CYS
1	A	481	LEU
1	A	496	LYS
1	A	529	ILE
1	A	563	MET
1	A	577	TYR
1	A	584	VAL
1	A	588	LEU
1	A	590	PHE
1	A	608	LEU
1	A	614	ARG
1	A	623	VAL
1	A	655	VAL
1	A	714	VAL
1	A	717	LEU
1	A	836	HIS
1	A	909	TYR
1	A	940	ASP
1	A	986	THR
1	A	1009	GLN
1	A	1015	THR

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Mol	Chain	Res	Type
1	A	1020	GLN
1	A	1036	LEU
1	A	1058	LEU
1	A	1063	GLN
1	A	1095	SER
1	A	1149	VAL
1	A	1175	THR
1	A	1222	LEU
1	B	40	PHE
1	B	44	TRP
1	B	69	ILE
1	B	102	VAL
1	B	165	PHE
1	B	179	LEU
1	B	201	TYR
1	B	232	PHE
1	B	269	ARG
1	B	339	CYS
1	B	356	VAL
1	B	377	GLN
1	B	606	TYR
1	B	608	LEU
1	B	626	ARG
1	B	630	PHE
1	B	731	LEU
1	B	736	CYS
1	B	836	HIS
1	B	910	ASP
1	B	912	CYS
1	B	940	ASP
1	B	986	THR
1	B	1009	GLN
1	B	1015	THR
1	B	1020	GLN
1	B	1036	LEU
1	B	1063	GLN
1	B	1149	VAL
1	B	1218	LEU
1	B	1222	LEU
1	C	102	VAL
1	C	153	VAL
1	C	161	MET

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Mol	Chain	Res	Type
1	C	176	CYS
1	C	201	TYR
1	C	208	HIS
1	C	214	CYS
1	C	240	MET
1	C	269	ARG
1	C	339	CYS
1	C	351	TYR
1	C	356	VAL
1	C	379	GLU
1	C	599	GLN
1	C	620	CYS
1	C	649	TYR
1	C	650	CYS
1	C	652	ARG
1	C	670	HIS
1	C	717	LEU
1	C	718	VAL
1	C	734	SER
1	C	836	HIS
1	C	909	TYR
1	C	910	ASP
1	C	933	LYS
1	C	964	LEU
1	C	986	THR
1	C	1009	GLN
1	C	1015	THR
1	C	1020	GLN
1	C	1036	LEU
1	C	1063	GLN
1	C	1150	VAL
1	C	1218	LEU
1	C	1222	LEU
2	H	3	GLN
2	H	10	GLU
2	H	11	VAL
2	H	29	PHE
2	H	35	THR
2	H	43	GLN
2	H	46	GLU
2	H	70	ILE
2	H	80	TYR

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Mol	Chain	Res	Type
2	H	81	MET
2	H	91	THR
2	H	118	VAL
2	H	131	LEU
2	H	145	LEU
2	H	148	LEU
2	H	158	THR
2	H	159	VAL
2	H	162	ASN
2	H	170	VAL
2	H	177	LEU
2	H	199	GLN
2	H	200	THR
2	H	202	ILE
2	H	205	VAL
3	K	5	THR
3	K	33	TYR
3	K	34	LEU
3	K	43	GLN
3	K	55	ARG
3	K	71	ASP
3	K	82	GLU
3	K	97	TRP
3	K	103	THR
3	K	110	THR
3	K	116	VAL
3	K	118	ILE
3	K	133	VAL
3	K	147	VAL
3	K	148	GLN
3	K	164	VAL
3	K	184	LYS
3	K	190	HIS
3	K	192	VAL
3	K	197	VAL
3	K	198	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	166	ASN

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Mol	Chain	Res	Type
1	A	236	ASN
1	A	261	GLN
1	A	521	ASN
1	A	576	GLN
1	A	582	ASN
1	A	628	GLN
1	A	733	GLN
1	A	839	ASN
1	A	981	ASN
1	A	1009	GLN
1	A	1056	GLN
1	A	1063	GLN
1	A	1072	ASN
1	A	1213	ASN
1	B	114	ASN
1	B	166	ASN
1	B	236	ASN
1	B	377	GLN
1	B	599	GLN
1	B	628	GLN
1	B	1009	GLN
1	B	1063	GLN
1	B	1072	ASN
1	B	1213	ASN
1	C	36	GLN
1	C	91	HIS
1	C	114	ASN
1	C	166	ASN
1	C	236	ASN
1	C	298	HIS
1	C	592	ASN
1	C	599	GLN
1	C	636	GLN
1	C	981	ASN
1	C	1009	GLN
1	C	1056	GLN
1	C	1063	GLN
1	C	1072	ASN
1	C	1213	ASN
2	H	6	GLN
2	H	162	ASN
2	H	178	GLN

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Mol	Chain	Res	Type
2	H	199	GLN
2	H	207	HIS
3	K	39	GLN
3	K	43	GLN
3	K	125	GLN
3	K	148	GLN
3	K	161	GLN
3	K	199	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

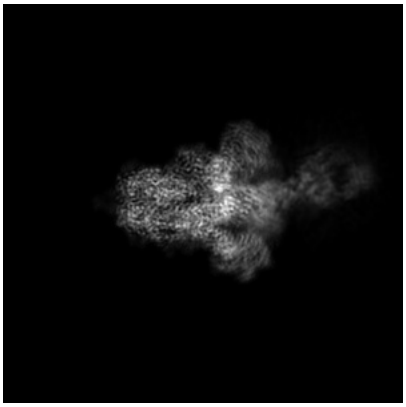
This section contains visualisations of the EMDB entry EMD-32963. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

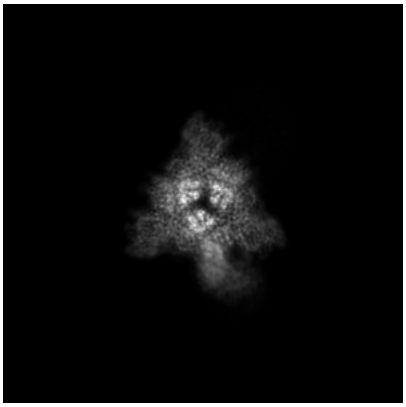
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



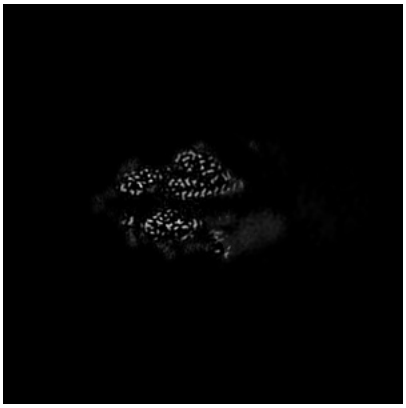
Z

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

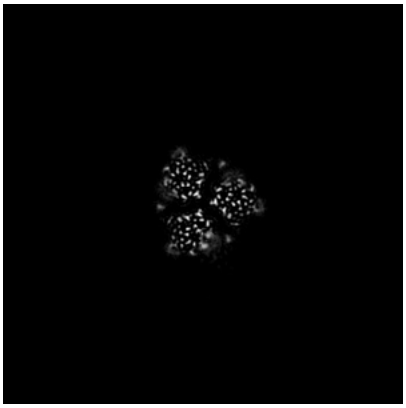
6.2 Central slices

6.2.1 Primary map

X Index: 160



Y Index: 160



Z Index: 160

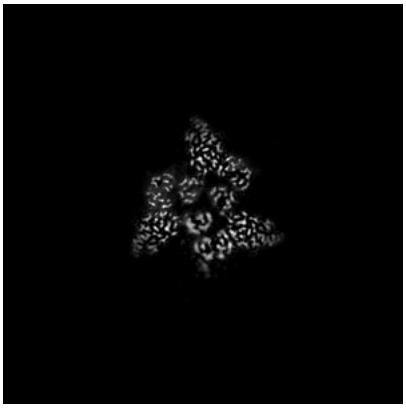
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 154

Y Index: 147



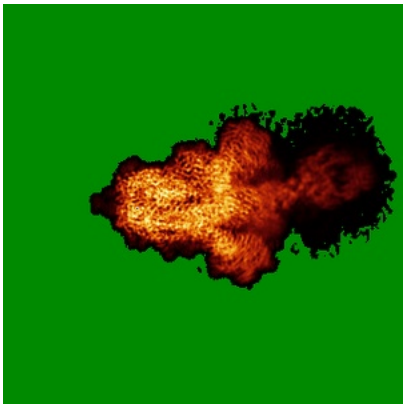
Z Index: 178

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

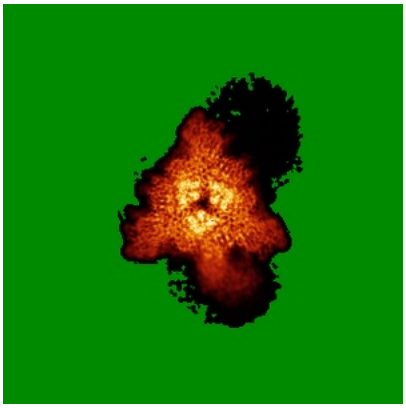
6.4 Orthogonal standard-deviation projections (False-color) (i)

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.

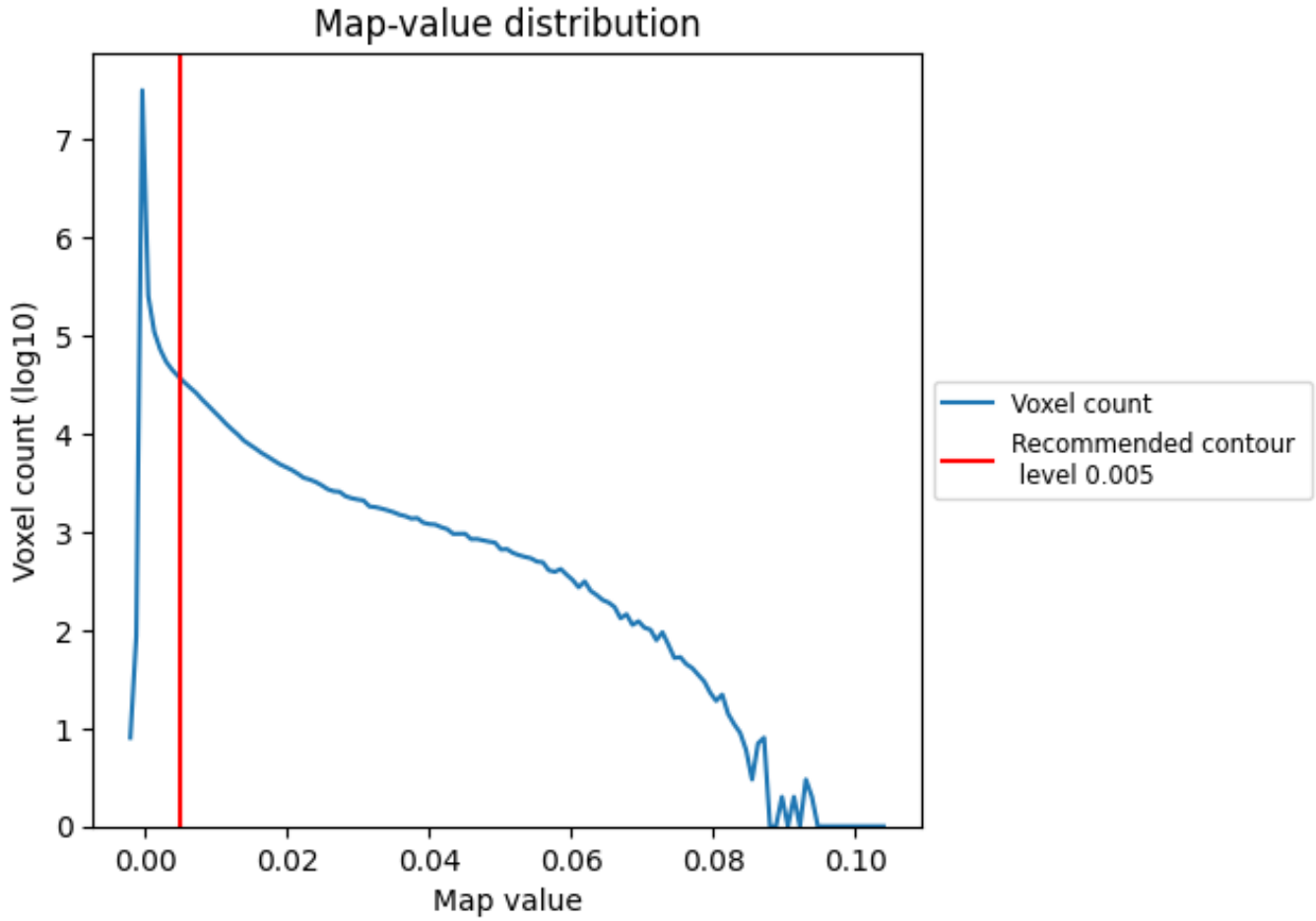
6.6 Mask visualisation (i)

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

7 Map analysis

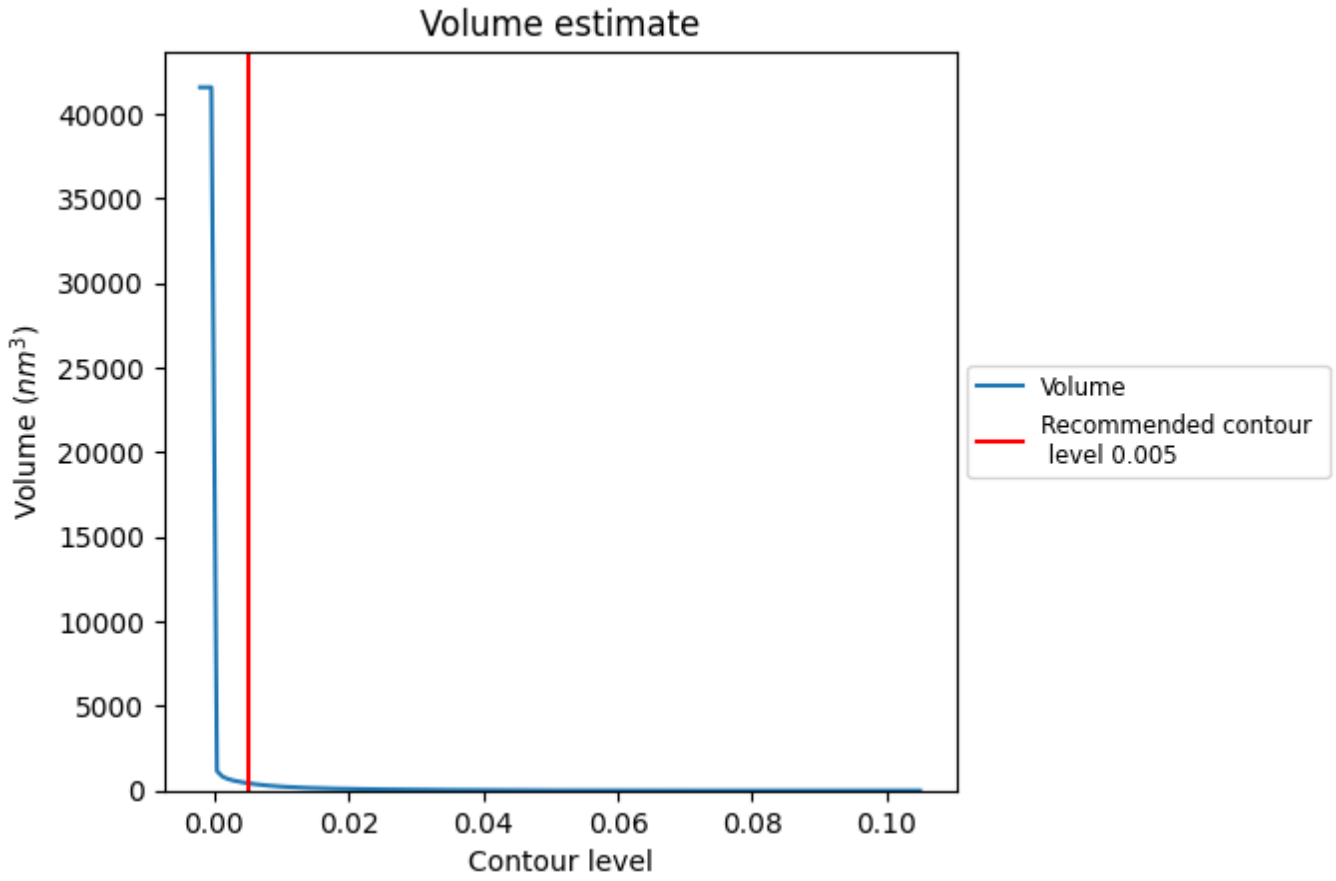
This section contains the results of statistical analysis of the map.

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.

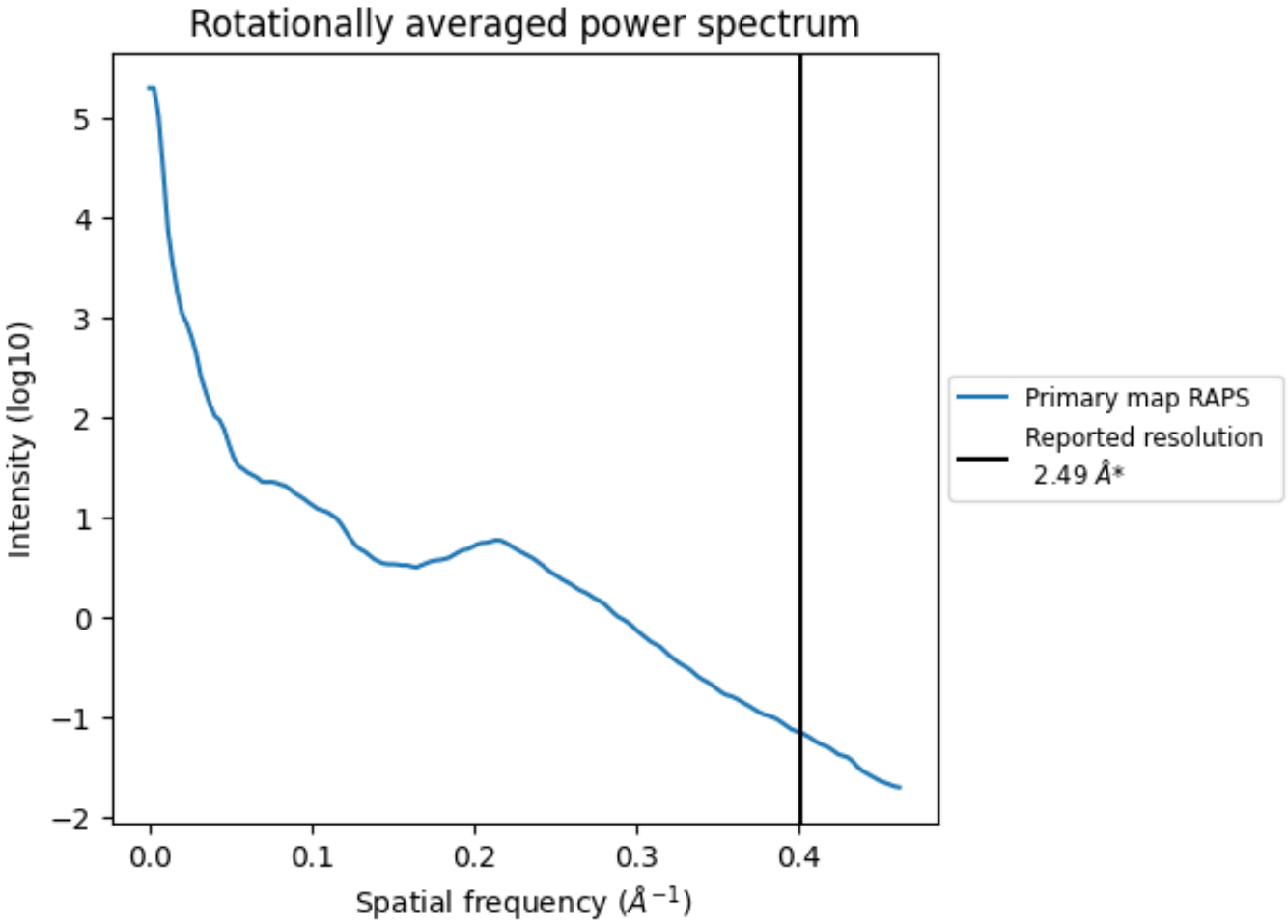
7.2 Volume estimate



The volume at the recommended contour level is 436 nm^3; this corresponds to an approximate mass of 394 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}

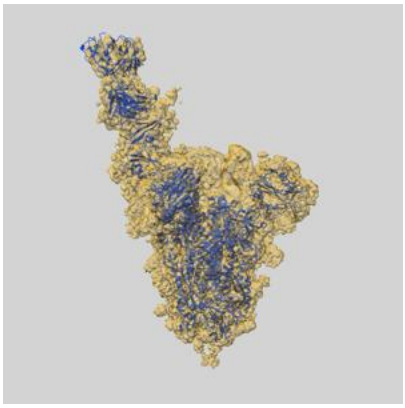
8 Fourier-Shell correlation (i)

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

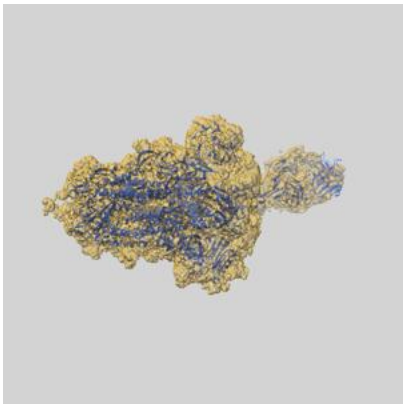
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32963 and PDB model 7X2A. Per-residue inclusion information can be found in section 3 on page 8.

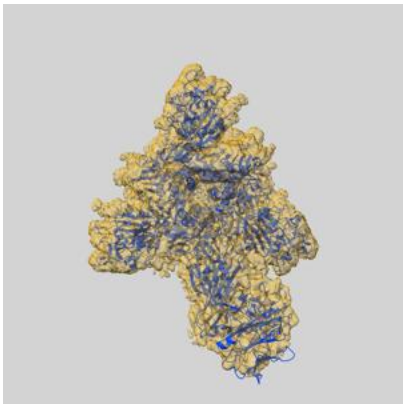
9.1 Map-model overlay



X



Y



Z

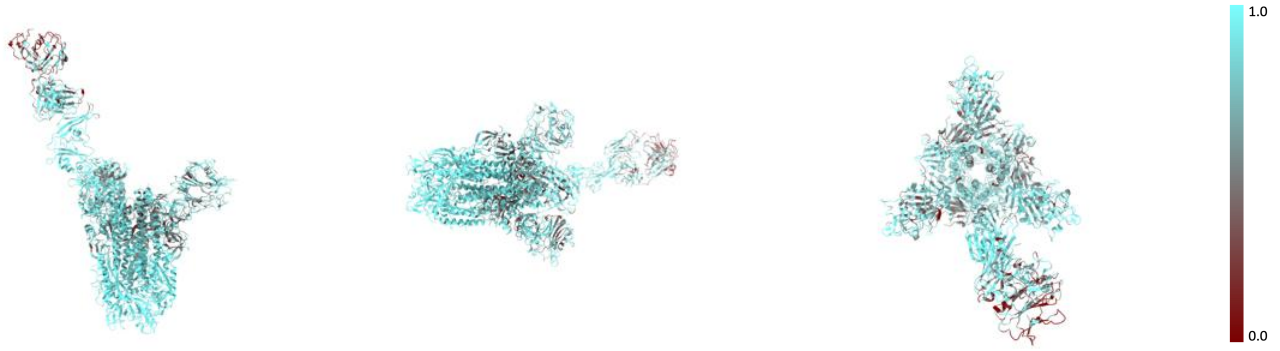
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

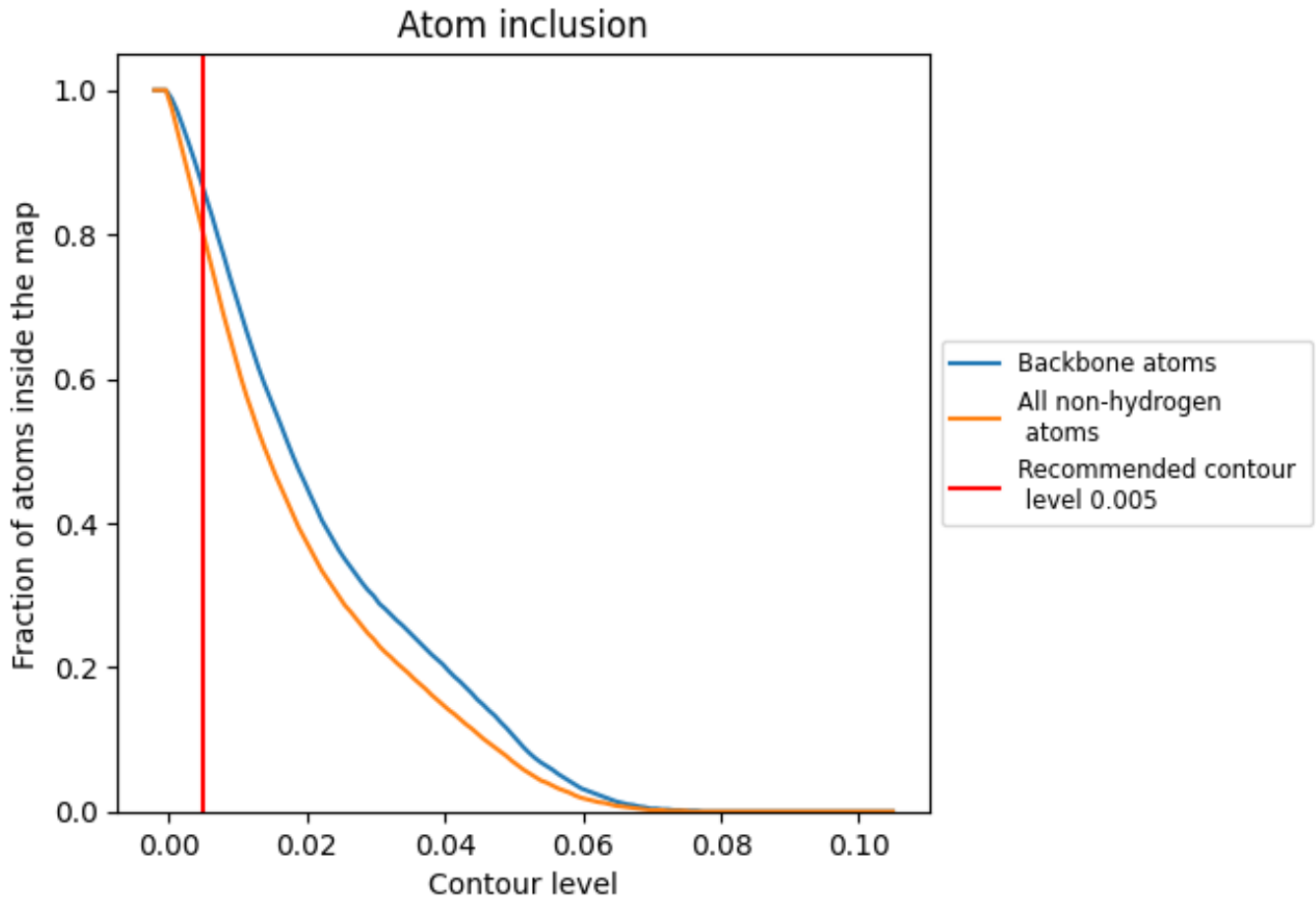
9.3 Atom inclusion mapped to coordinate model (i)



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, 86% of all backbone atoms, 80% 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	0.7980	0.2090
A	0.8290	0.2070
B	0.8450	0.2660
C	0.8040	0.2190
H	0.6330	0.0620
K	0.5440	0.0650