



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 07:02 PM UTC

PDB ID : 7X29 / pdb_00007x29
EMDB ID : EMD-32962
Title : MERS-CoV spike complex with S41 neutralizing antibody Fab Class2 (1u2d RBD with 2Fab)
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:

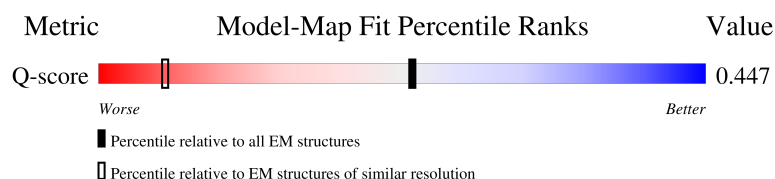
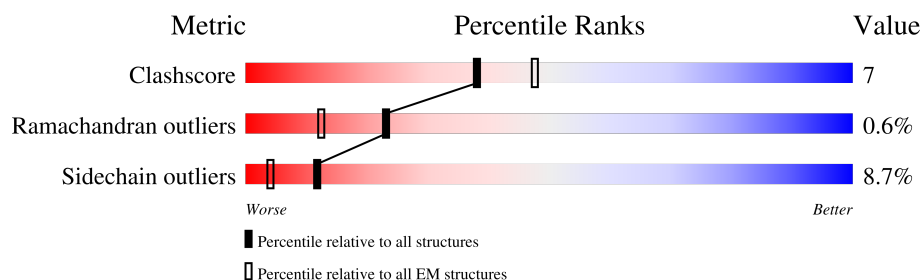
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6237 (2.00 - 2.99)

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

Mol	Chain	Length	Quality of chain
1	A	1347	
1	B	1347	
1	C	1347	
2	F	221	

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Mol	Chain	Length	Quality of chain
2	H	221	
3	G	212	
3	K	212	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32453 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	991	Total	C	N	O	S	0	0
			7657	4852	1281	1483	41		
1	B	1190	Total	C	N	O	S	0	0
			9186	5830	1522	1783	51		
1	C	1190	Total	C	N	O	S	0	0
			9186	5830	1522	1783	51		

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	F	214	Total	C	N	O	S	2	0
			1589	1002	267	314	6		
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	G	212	Total	C	N	O	S	0	0
			1601	997	277	323	4		

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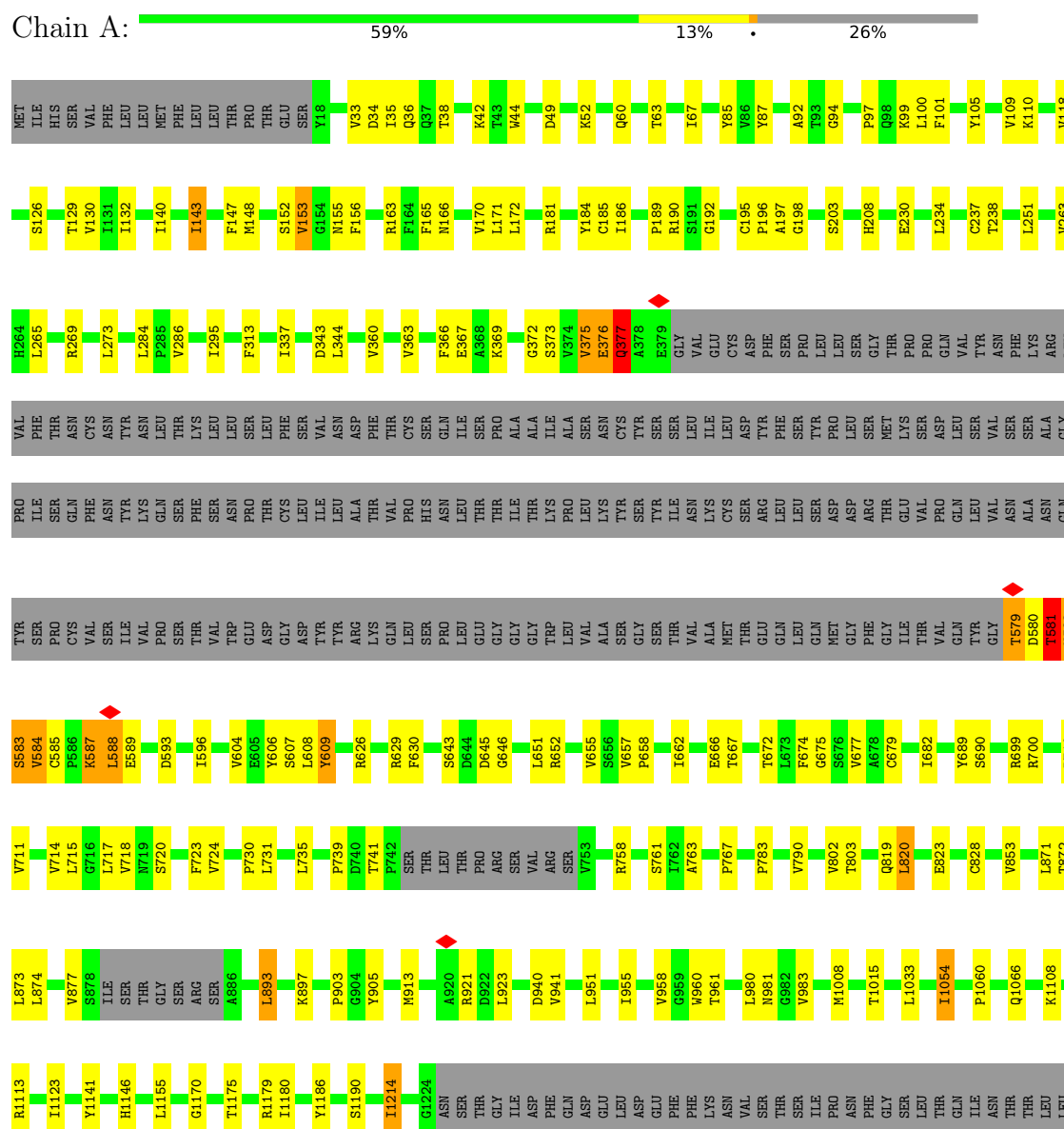
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	212	Total	C	N	O	S	0	0
			1601	997	277	323	4		

3 Residue-property plots

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

• Molecule 1: Spike glycoprotein



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

• Molecule 1: Spike glycoprotein

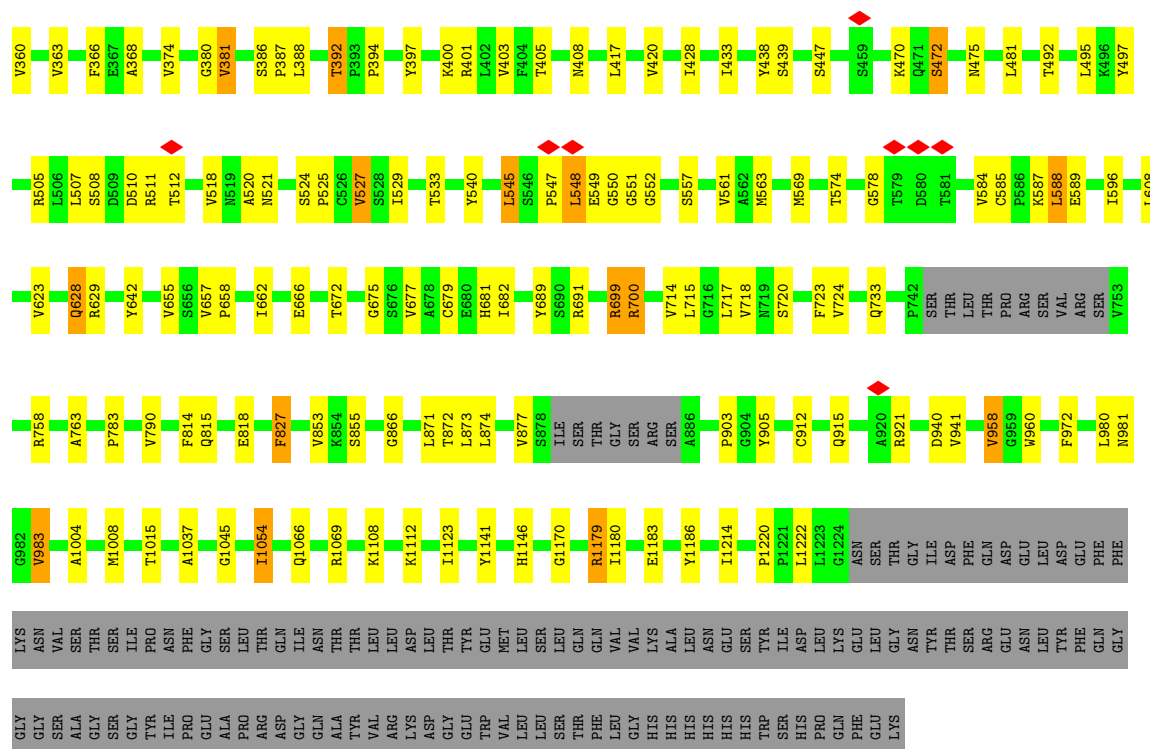
Chain B:  71% 16% 12%

VAL	MET	LEU	LEU	LEU	SER	LEU	GLN	THR	PHE	LEU	GLY	HIS	HIS	HIS	ALA	LYS	VAL	ASP	LEU	LEU	GLY	ASN	THR	THR	ASP	THR	SER	ARG	GLN	ASP	GLU	ASN	LEU	LEU	TYR	PHE	GLN	GLY	GLY	LYS	GLY	ASN	SER	VAL	ALA	SER	GLY	THR	SER	GLY	ILE	PRO	TYR	ILE	ASN	GLY	PRO	GLU	GLY	ALA	PRO	GLU	GLU	ARG	ASP	GLN	GLY	ILE	ASN	GLN	ALA	THR	THR	THR	VAL	VAL	LYS	ASP	LEU	GLY	THR	GLU	TRP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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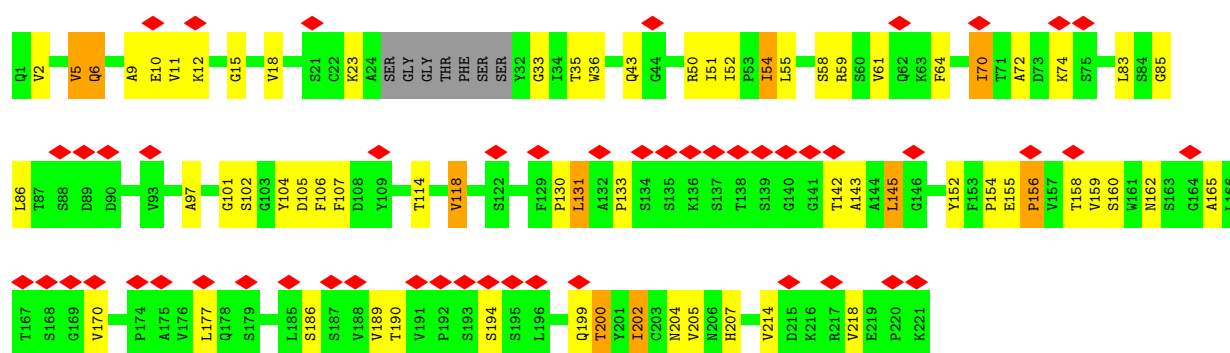
• Molecule 1: Spike glycoprotein

Chain C:  73% 14% 12%

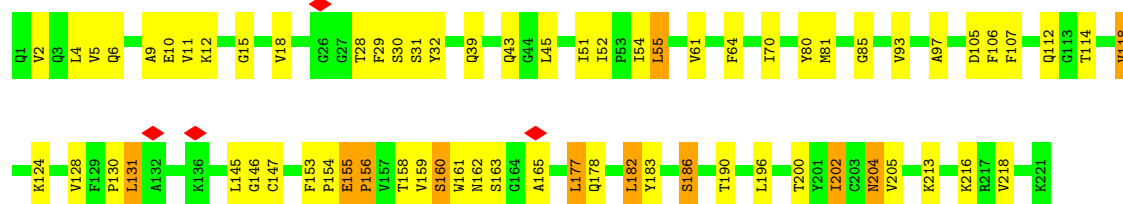
MET	ILE	HIS	SER	VAL	PHE	LEU	LEU	MET	PHE	LEU	LEU	GLU	SER	Y18	K27	S28	V33	V50	Q60	T63	I67	Y87	A92	P97	V109	K110	G115	F116	V117	T129	I132	I143	G150	V153	G154	M155	F156	R163	F164
L171	L179	L180	R181	A182	F183	Y184	C185	P189	R190	S191	G192	C195	P196	A197	G198	S203	H208	R221	E230	L234	C237	T238	F239	M240	Y243	T246	L251	L256	T257	Q258	V263	M278	L284	P285	T289	A336	I337	D343	



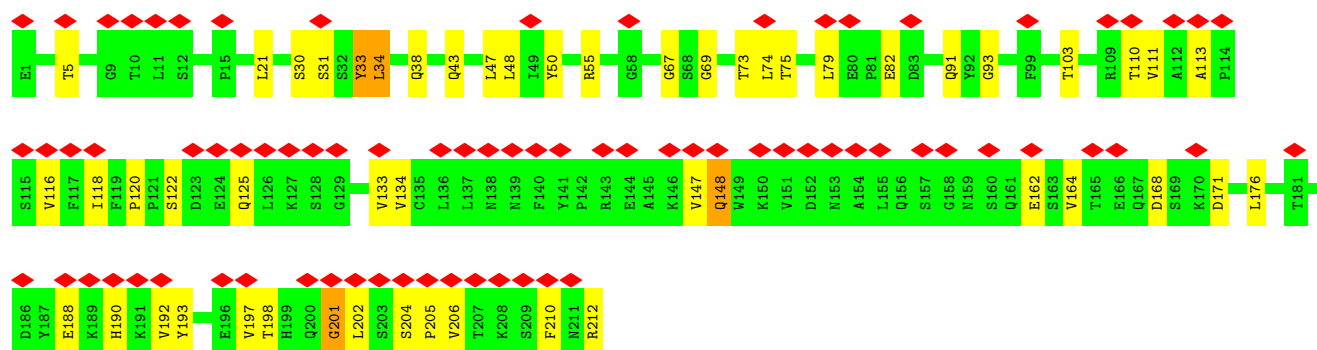
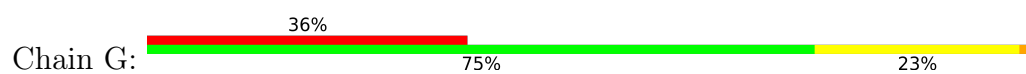
• Molecule 2: antibody S41 heavy chain



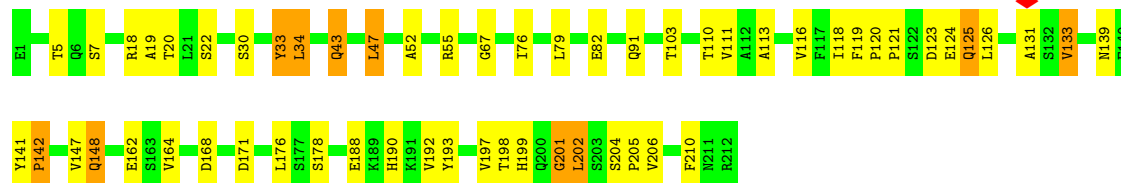
• Molecule 2: antibody S41 heavy chain



• Molecule 3: antibody S41 light chain



- Molecule 3: antibody S41 light chain



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	1.12	3/7832 (0.0%)	1.79	10/10650 (0.1%)
1	B	1.00	0/9401	1.16	2/12797 (0.0%)
1	C	1.00	0/9401	1.15	2/12797 (0.0%)
2	F	1.18	4/1629 (0.2%)	1.36	12/2215 (0.5%)
2	H	1.18	4/1675 (0.2%)	1.36	12/2278 (0.5%)
3	G	1.02	0/1635	1.16	2/2223 (0.1%)
3	K	1.01	0/1635	1.17	2/2223 (0.1%)
All	All	1.05	11/33208 (0.0%)	1.35	42/45183 (0.1%)

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	B	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	GLN	CD-OE1	34.88	1.89	1.23
1	A	377	GLN	CG-CD	28.48	2.23	1.52
1	A	377	GLN	CD-NE2	19.01	1.73	1.33
2	F	160[A]	SER	C-O	11.54	1.37	1.24
2	F	160[B]	SER	C-O	11.54	1.37	1.24
2	H	160[A]	SER	C-O	11.09	1.37	1.24
2	H	160[B]	SER	C-O	11.09	1.37	1.24
2	F	186[A]	SER	C-O	10.49	1.36	1.24
2	F	186[B]	SER	C-O	10.49	1.36	1.24
2	H	186[A]	SER	C-O	10.40	1.36	1.24
2	H	186[B]	SER	C-O	10.40	1.36	1.24

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	GLN	OE1-CD-NE2	-111.64	10.96	122.60
1	A	377	GLN	CG-CD-NE2	-70.90	10.05	116.40
1	A	377	GLN	CG-CD-OE1	-50.06	20.68	120.80
2	F	186[A]	SER	CA-C-O	11.03	132.27	120.36
2	F	186[B]	SER	CA-C-O	11.03	132.27	120.36
2	H	186[A]	SER	CA-C-O	10.99	132.35	120.38
2	H	186[B]	SER	CA-C-O	10.99	132.35	120.38
2	F	160[A]	SER	CA-C-O	10.46	131.93	120.32
2	F	160[B]	SER	CA-C-O	10.46	131.93	120.32
2	H	160[A]	SER	CA-C-O	10.33	131.68	120.32
2	H	160[B]	SER	CA-C-O	10.33	131.68	120.32
1	A	377	GLN	CB-CG-CD	9.97	129.55	112.60
2	H	186[A]	SER	N-CA-C	8.83	123.28	109.07
2	H	186[B]	SER	N-CA-C	8.83	123.28	109.07
2	F	186[A]	SER	N-CA-C	8.77	123.19	108.90
2	F	186[B]	SER	N-CA-C	8.77	123.19	108.90
1	A	377	GLN	CB-CA-C	8.69	127.71	110.42
1	A	377	GLN	N-CA-CB	8.17	124.30	110.49
2	F	160[A]	SER	N-CA-C	7.89	122.09	108.76
2	F	160[B]	SER	N-CA-C	7.89	122.09	108.76
2	H	160[A]	SER	N-CA-C	7.50	120.74	108.52
2	H	160[B]	SER	N-CA-C	7.50	120.74	108.52
2	H	186[A]	SER	O-C-N	-7.43	114.53	123.29
2	H	186[B]	SER	O-C-N	-7.43	114.53	123.29
2	F	186[A]	SER	O-C-N	-7.30	114.61	123.30
2	F	186[B]	SER	O-C-N	-7.30	114.61	123.30
2	F	160[A]	SER	O-C-N	-7.17	114.92	123.31
2	F	160[B]	SER	O-C-N	-7.17	114.92	123.31
2	H	160[A]	SER	O-C-N	-6.86	115.18	123.27
2	H	160[B]	SER	O-C-N	-6.86	115.18	123.27
1	A	582	ASN	N-CA-CB	6.45	121.46	110.50
1	A	580	ASP	N-CA-C	6.39	119.56	108.76
1	A	377	GLN	CA-CB-CG	6.30	126.70	114.10
1	B	115	GLY	CA-C-O	-6.21	117.84	122.37
1	C	115	GLY	CA-C-O	-6.12	117.90	122.37
1	A	1060	PRO	N-CA-C	5.86	117.85	110.70
3	K	201	GLY	CA-C-O	-5.69	116.46	121.58
1	B	1060	PRO	N-CA-C	5.69	117.64	110.70
3	G	201	GLY	CA-C-O	-5.68	116.46	121.58
1	C	1220	PRO	N-CA-C	5.33	117.20	110.70
3	G	67	GLY	CA-C-O	-5.32	117.98	122.29
3	K	67	GLY	CA-C-O	-5.20	118.08	122.29

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	588	LEU	Peptide
1	B	548	LEU	Peptide

5.2 Too-close contacts

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	7657	0	7387	162	0
1	B	9186	0	8873	102	0
1	C	9186	0	8873	103	0
2	F	1589	0	1583	39	0
2	H	1633	0	1621	53	0
3	G	1601	0	1551	21	0
3	K	1601	0	1551	25	0
All	All	32453	0	31439	475	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 (475) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLN:NE2	1:A:377:GLN:CD	1.73	1.47
1:A:377:GLN:CG	1:A:585:CYS:H	1.46	1.29
2:H:178:GLN:HG2	2:H:182:LEU:O	1.29	1.27
1:A:377:GLN:HE21	1:A:377:GLN:CB	1.49	1.25
2:H:178:GLN:CG	2:H:182:LEU:O	1.86	1.21
1:A:377:GLN:OE1	1:A:377:GLN:HG2	1.38	1.17
1:A:152:SER:C	1:A:165:PHE:HD2	1.50	1.17
1:A:153:VAL:C	1:A:165:PHE:CE2	2.23	1.17
1:A:377:GLN:CD	1:A:585:CYS:N	2.04	1.16
1:A:377:GLN:CD	1:A:377:GLN:OE1	1.89	1.14
1:A:377:GLN:CD	1:A:377:GLN:CG	2.23	1.10
1:A:377:GLN:CG	1:A:377:GLN:OE1	0.81	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLN:CD	1:A:585:CYS:O	1.94	1.10
1:A:377:GLN:NE2	1:A:585:CYS:H	1.50	1.10
1:A:152:SER:C	1:A:165:PHE:CD2	2.31	1.09
1:A:49:ASP:HB3	1:A:52:LYS:HG2	1.32	1.08
1:A:153:VAL:O	1:A:165:PHE:CE2	2.11	1.04
1:A:49:ASP:HB3	1:A:52:LYS:CG	1.61	1.02
1:A:377:GLN:NE2	1:A:377:GLN:CB	2.14	1.02
2:H:196:LEU:HD12	2:H:200:THR:HG22	1.43	1.00
1:A:153:VAL:N	1:A:165:PHE:CE2	2.30	1.00
1:A:377:GLN:CG	1:A:585:CYS:N	2.25	0.99
1:C:548:LEU:HA	1:C:549:GLU:CD	1.87	0.99
1:A:583:SER:O	1:A:584:VAL:HG23	1.60	0.98
1:A:377:GLN:NE2	1:A:585:CYS:O	1.97	0.97
1:A:583:SER:O	1:A:584:VAL:CG2	2.14	0.96
2:H:178:GLN:CD	2:H:182:LEU:O	2.09	0.94
1:A:710:PRO:HD2	1:A:735:LEU:HD11	1.53	0.90
1:A:377:GLN:NE2	1:A:585:CYS:N	2.20	0.89
1:B:306:ASP:OD1	1:B:308:LYS:NZ	2.05	0.89
1:C:511:ARG:C	2:F:74:LYS:HE3	1.98	0.89
1:A:153:VAL:N	1:A:165:PHE:HE2	1.70	0.89
1:A:377:GLN:NE2	1:A:377:GLN:HG2	1.22	0.89
1:A:581:THR:CG2	1:A:582:ASN:HA	2.05	0.87
1:A:153:VAL:O	1:A:165:PHE:CZ	2.28	0.85
2:H:177:LEU:HD13	2:H:183:TYR:CD2	2.12	0.85
1:A:377:GLN:OE1	1:A:585:CYS:O	1.95	0.84
1:A:49:ASP:CB	1:A:52:LYS:HG2	2.08	0.83
1:A:377:GLN:CD	1:A:585:CYS:H	1.83	0.83
1:A:42:LYS:HD3	1:A:44:TRP:CH2	2.14	0.83
1:A:377:GLN:HE21	1:A:377:GLN:HG2	0.83	0.83
1:A:711:VAL:HG22	1:A:735:LEU:HD12	1.62	0.81
2:H:196:LEU:CD1	2:H:200:THR:HG22	2.10	0.81
1:C:392:THR:HB	1:C:492:THR:HB	1.62	0.80
1:A:152:SER:O	1:A:165:PHE:HD2	1.65	0.79
1:A:153:VAL:N	1:A:165:PHE:CD2	2.47	0.79
2:H:124:LYS:HG2	2:H:182:LEU:HD23	1.66	0.78
1:C:699:ARG:HD2	1:C:715:LEU:HG	1.66	0.78
1:A:377:GLN:HG2	1:A:585:CYS:HB2	1.62	0.78
2:H:97:ALA:HB1	2:H:107:PHE:HB3	1.64	0.78
1:A:583:SER:C	1:A:584:VAL:HG23	2.09	0.77
2:H:177:LEU:CD1	2:H:183:TYR:CD2	2.68	0.77
2:H:124:LYS:HG2	2:H:182:LEU:CD2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:177:LEU:HA	2:H:183:TYR:HB3	1.67	0.77
1:B:300:ILE:HD12	1:B:300:ILE:N	1.99	0.76
1:B:107:GLN:HE22	1:B:160:LYS:HB3	1.51	0.76
1:A:49:ASP:O	1:A:52:LYS:HG2	1.86	0.76
1:A:714:VAL:HG21	1:A:717:LEU:HD12	1.67	0.75
1:C:548:LEU:N	1:C:548:LEU:HD22	2.02	0.74
1:A:42:LYS:HE3	1:A:44:TRP:CZ2	2.23	0.74
1:A:582:ASN:O	1:A:583:SER:HB3	1.86	0.74
1:A:153:VAL:CA	1:A:165:PHE:CE2	2.72	0.72
1:A:377:GLN:NE2	1:A:377:GLN:CG	0.61	0.72
2:H:182:LEU:HD12	2:H:182:LEU:N	2.04	0.72
1:A:723:PHE:HB3	1:A:763:ALA:HB2	1.71	0.72
1:A:581:THR:CG2	1:A:582:ASN:ND2	2.53	0.71
1:A:49:ASP:O	1:A:52:LYS:CG	2.39	0.71
2:H:177:LEU:N	2:H:177:LEU:HD22	2.06	0.71
1:A:377:GLN:HG2	1:A:585:CYS:CB	2.21	0.70
1:A:377:GLN:CD	1:A:584:VAL:C	2.58	0.70
1:A:582:ASN:O	1:A:583:SER:CB	2.39	0.70
1:A:581:THR:HG23	1:A:582:ASN:ND2	2.06	0.70
1:C:657:VAL:HG13	1:C:677:VAL:HG21	1.74	0.69
1:A:377:GLN:HG2	1:A:585:CYS:CA	2.23	0.69
1:A:581:THR:HG22	1:A:582:ASN:HA	1.73	0.69
1:B:1054:ILE:HD13	1:B:1066:GLN:HB2	1.75	0.69
1:C:723:PHE:HB3	1:C:763:ALA:HB2	1.74	0.68
1:C:92:ALA:HA	1:C:97:PRO:HA	1.74	0.68
1:B:94:GLY:N	1:B:304:GLN:OE1	2.19	0.68
1:A:581:THR:CG2	1:A:582:ASN:HD22	2.06	0.67
2:H:106:PHE:HB2	3:K:47:LEU:HD11	1.75	0.67
1:B:658:PRO:HG2	1:B:675:GLY:HA3	1.77	0.67
1:A:42:LYS:CE	1:A:44:TRP:CZ2	2.77	0.67
1:A:377:GLN:HE22	1:A:377:GLN:HG3	0.57	0.66
2:H:196:LEU:CD1	2:H:200:THR:CG2	2.72	0.66
1:A:377:GLN:CD	1:A:585:CYS:C	2.63	0.66
1:A:643:SER:HB2	1:A:645:ASP:OD1	1.95	0.65
3:G:193:TYR:H	3:G:210:PHE:HB3	1.62	0.65
1:A:377:GLN:CG	1:A:377:GLN:HE21	0.40	0.64
2:H:178:GLN:OE1	2:H:182:LEU:HB2	1.98	0.64
2:H:177:LEU:HD22	2:H:177:LEU:H	1.60	0.64
1:A:377:GLN:CG	1:A:585:CYS:O	2.44	0.64
3:G:168:ASP:HB3	3:G:171:ASP:HB2	1.79	0.64
3:K:193:TYR:H	3:K:210:PHE:HB3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLN:NE2	1:A:377:GLN:HG3	1.04	0.63
1:C:401:ARG:HH22	1:C:521:ASN:HB3	1.62	0.63
2:H:15:GLY:HA2	2:H:85:GLY:HA2	1.79	0.63
1:C:394:PRO:HG3	1:C:400:LYS:HG3	1.80	0.63
1:A:269:ARG:HG2	1:A:273:LEU:HD13	1.80	0.63
1:B:720:SER:HB3	1:B:758:ARG:HB3	1.80	0.63
1:C:507:LEU:HD13	1:C:507:LEU:O	1.98	0.63
3:G:30:SER:HB3	3:G:33:TYR:HB2	1.78	0.63
2:H:177:LEU:H	2:H:177:LEU:CD2	2.12	0.62
1:B:394:PRO:HG3	1:B:400:LYS:HG3	1.79	0.62
2:H:130:PRO:HD3	3:K:125:GLN:HE21	1.62	0.62
1:B:366:PHE:HB3	1:B:689:TYR:HB3	1.82	0.62
1:C:548:LEU:N	1:C:549:GLU:HA	2.12	0.62
1:A:33:VAL:HG12	1:A:100:LEU:HB2	1.82	0.62
1:A:152:SER:CB	1:A:165:PHE:CD2	2.83	0.62
1:C:658:PRO:HG2	1:C:675:GLY:HA3	1.82	0.62
1:A:153:VAL:O	1:A:165:PHE:HE2	1.77	0.61
3:K:168:ASP:HB3	3:K:171:ASP:HB2	1.81	0.61
1:A:92:ALA:HA	1:A:97:PRO:HA	1.80	0.61
1:A:153:VAL:C	1:A:165:PHE:CZ	2.75	0.61
1:A:49:ASP:CB	1:A:52:LYS:CG	2.55	0.61
1:A:377:GLN:OE1	1:A:377:GLN:HG3	0.80	0.61
1:C:549:GLU:HB3	1:C:550:GLY:HA2	1.80	0.61
2:F:97:ALA:HB1	2:F:107:PHE:HB3	1.82	0.60
1:B:100:LEU:HD22	1:B:299:SER:HB3	1.82	0.60
1:C:366:PHE:HA	1:C:691:ARG:HB3	1.84	0.60
1:C:1054:ILE:HD13	1:C:1066:GLN:HB2	1.84	0.60
2:H:182:LEU:H	2:H:182:LEU:CD1	2.14	0.60
1:B:343:ASP:HB3	1:B:363:VAL:HG11	1.84	0.60
1:A:581:THR:HG22	1:A:582:ASN:CA	2.31	0.60
2:H:153:PHE:HA	2:H:182:LEU:HA	1.82	0.60
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.84	0.60
1:C:507:LEU:HD13	1:C:507:LEU:C	2.27	0.60
1:C:700:ARG:HD3	1:C:700:ARG:H	1.66	0.59
2:H:130:PRO:HG3	3:K:124:GLU:HB3	1.83	0.59
1:B:401:ARG:HH22	1:B:521:ASN:HB3	1.67	0.59
2:F:15:GLY:HA2	2:F:85:GLY:HA2	1.83	0.59
3:G:38:GLN:HB2	3:G:48:LEU:HD11	1.84	0.59
1:B:298:HIS:HD2	1:B:300:ILE:HD11	1.67	0.59
2:F:131:LEU:HD22	2:F:218:VAL:HG22	1.84	0.59
1:A:377:GLN:CB	1:A:585:CYS:H	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:PRO:HG2	1:A:675:GLY:HA3	1.84	0.58
1:A:581:THR:HG23	1:A:582:ASN:HA	1.85	0.58
2:H:182:LEU:N	2:H:182:LEU:CD1	2.66	0.58
2:H:178:GLN:OE1	2:H:182:LEU:O	2.21	0.58
2:H:196:LEU:HD11	2:H:200:THR:CG2	2.33	0.58
1:B:557:SER:HB2	2:H:55:LEU:HD23	1.84	0.58
1:A:377:GLN:HG2	1:A:585:CYS:N	2.17	0.57
2:H:182:LEU:HD12	2:H:182:LEU:H	1.69	0.57
1:B:392:THR:HB	1:B:492:THR:HB	1.86	0.57
3:K:125:GLN:HB3	3:K:131:ALA:HA	1.86	0.57
1:A:606:TYR:CD1	1:A:608:LEU:HB2	2.39	0.57
1:A:652:ARG:HD3	1:B:915:GLN:HB3	1.86	0.57
1:A:657:VAL:HG13	1:A:677:VAL:HG11	1.87	0.57
1:A:377:GLN:HE21	1:A:585:CYS:H	1.17	0.57
1:A:583:SER:C	1:A:584:VAL:CG2	2.74	0.57
1:C:366:PHE:HB3	1:C:689:TYR:HB3	1.86	0.57
3:G:162:GLU:HB2	3:G:176:LEU:HD21	1.87	0.57
1:C:258:GLN:HE22	1:C:289:THR:HA	1.69	0.57
3:K:34:LEU:HD12	3:K:91:GLN:HG2	1.87	0.57
1:A:377:GLN:CG	1:A:585:CYS:CA	2.82	0.56
1:B:97:PRO:HB2	1:B:301:ARG:HE	1.70	0.56
1:B:628:GLN:HB2	1:C:63:THR:HB	1.87	0.56
2:H:153:PHE:O	2:H:183:TYR:CZ	2.58	0.56
1:C:714:VAL:HG21	1:C:717:LEU:HD12	1.87	0.56
1:A:583:SER:HB2	1:A:609:TYR:CA	2.35	0.56
1:B:366:PHE:HA	1:B:691:ARG:HB3	1.88	0.56
1:C:510:ASP:OD2	2:H:162:ASN:HB3	2.05	0.56
1:A:343:ASP:HB3	1:A:363:VAL:HG11	1.86	0.56
1:B:102:VAL:HB	1:B:297:PRO:HB3	1.88	0.56
3:G:34:LEU:HD12	3:G:91:GLN:HG2	1.87	0.56
2:F:51:ILE:HD12	2:F:72:ALA:HB2	1.87	0.56
1:A:375:VAL:HG23	1:A:607:SER:HB3	1.89	0.55
2:F:50:ARG:HH11	2:F:59:ARG:HB2	1.70	0.55
1:C:511:ARG:O	2:F:74:LYS:HE3	2.07	0.55
1:C:548:LEU:N	1:C:548:LEU:CD2	2.69	0.55
1:A:606:TYR:HD1	1:A:608:LEU:HB2	1.72	0.55
3:K:113:ALA:HB1	3:K:202:LEU:HD23	1.89	0.55
3:K:121:PRO:HD3	3:K:133:VAL:HG13	1.89	0.55
1:B:714:VAL:HG21	1:B:717:LEU:HD12	1.88	0.55
1:C:508:SER:HB2	1:C:512:THR:HB	1.88	0.55
1:A:263:VAL:HB	1:A:284:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:PHE:HB3	1:A:689:TYR:HB3	1.89	0.54
1:A:377:GLN:NE2	1:A:585:CYS:C	2.63	0.54
1:A:153:VAL:H	1:A:165:PHE:HE2	1.52	0.54
1:B:464:ILE:HA	1:B:468:ASN:HD22	1.73	0.54
1:C:343:ASP:HB3	1:C:363:VAL:HG11	1.89	0.54
1:C:189:PRO:HB2	1:C:197:ALA:HB2	1.90	0.54
1:C:511:ARG:C	2:F:74:LYS:CE	2.76	0.54
1:C:720:SER:HB3	1:C:758:ARG:HB3	1.89	0.54
2:H:153:PHE:HB2	2:H:182:LEU:HG	1.90	0.54
2:F:130:PRO:HD3	3:G:125:GLN:NE2	2.22	0.54
1:A:49:ASP:C	1:A:52:LYS:HG2	2.33	0.54
1:A:1155:LEU:HB3	1:A:1214:ILE:HD11	1.90	0.54
2:H:146:GLY:HA2	2:H:161:TRP:HZ2	1.72	0.54
1:A:820:LEU:O	1:A:823:GLU:HG3	2.07	0.53
1:A:583:SER:O	1:A:584:VAL:HG22	2.03	0.53
3:K:162:GLU:HB2	3:K:176:LEU:HD21	1.88	0.53
1:A:643:SER:CB	1:A:645:ASP:OD1	2.56	0.53
1:C:548:LEU:HA	1:C:549:GLU:CG	2.37	0.53
1:A:49:ASP:O	1:A:52:LYS:HG3	2.09	0.53
1:C:397:TYR:HD1	1:C:527:VAL:HG23	1.74	0.53
3:K:34:LEU:HB3	3:K:52:ALA:HB2	1.91	0.53
1:B:958:VAL:HG11	1:B:1108:LYS:O	2.09	0.53
1:C:28:SER:HA	1:C:190:ARG:HH21	1.74	0.53
1:B:36:GLN:HB2	1:B:101:PHE:CZ	2.44	0.52
1:A:958:VAL:HG11	1:A:1108:LYS:O	2.10	0.52
1:B:1179:ARG:HG2	1:B:1183:GLU:HG2	1.91	0.52
3:G:47:LEU:HD21	3:G:50:TYR:HB3	1.92	0.52
1:B:476:PRO:HG2	1:B:577:TYR:HE2	1.75	0.52
2:F:104:TYR:HB3	2:F:106:PHE:CE2	2.44	0.52
1:A:720:SER:HB3	1:A:758:ARG:HB3	1.92	0.52
1:B:1123:ILE:HD11	1:B:1141:TYR:HB2	1.91	0.52
2:H:177:LEU:CD1	2:H:183:TYR:HD2	2.20	0.52
3:G:21:LEU:HD12	3:G:74:LEU:HD23	1.91	0.52
1:A:377:GLN:NE2	1:A:377:GLN:OE1	0.38	0.52
1:A:36:GLN:HB2	1:A:101:PHE:CZ	2.44	0.51
1:A:152:SER:O	1:A:165:PHE:CD2	2.55	0.51
3:G:120:PRO:HB2	3:G:212:ARG:NH1	2.25	0.51
2:H:177:LEU:N	2:H:177:LEU:CD2	2.70	0.51
1:A:189:PRO:HB2	1:A:197:ALA:HB2	1.92	0.51
2:H:131:LEU:HD22	2:H:218:VAL:HG22	1.93	0.51
1:B:300:ILE:N	1:B:300:ILE:CD1	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:VAL:HG13	1:B:677:VAL:HG11	1.93	0.51
1:C:540:TYR:CD2	2:F:101:GLY:HA2	2.46	0.51
1:C:958:VAL:HG11	1:C:1108:LYS:O	2.11	0.51
1:C:263:VAL:HB	1:C:284:LEU:HB2	1.93	0.51
1:A:581:THR:HG22	1:A:582:ASN:CB	2.41	0.50
1:B:723:PHE:HB3	1:B:763:ALA:HB2	1.94	0.50
1:C:548:LEU:HD13	1:C:549:GLU:OE2	2.12	0.50
1:A:376:GLU:O	1:A:609:TYR:HD2	1.95	0.50
2:H:31:SER:HA	2:H:54:ILE:HG13	1.92	0.50
1:C:33:VAL:HG21	1:C:203:SER:HB3	1.92	0.50
2:F:61:VAL:HG13	2:F:64:PHE:H	1.76	0.50
3:K:123:ASP:HA	3:K:126:LEU:HB2	1.93	0.50
1:C:190:ARG:HD3	1:C:230:GLU:O	2.12	0.50
1:B:518:VAL:HG23	1:B:525:PRO:HD3	1.94	0.50
2:H:124:LYS:HG2	2:H:182:LEU:HD21	1.90	0.50
1:A:42:LYS:CD	1:A:44:TRP:CH2	2.93	0.49
2:H:6:GLN:H	2:H:112:GLN:HE21	1.59	0.49
1:A:593:ASP:OD1	1:A:593:ASP:N	2.39	0.49
1:C:866:GLY:HA2	1:C:972:PHE:HB3	1.94	0.49
2:F:12:LYS:O	2:F:118:VAL:HA	2.13	0.49
1:A:377:GLN:HG2	1:A:585:CYS:C	2.36	0.49
2:F:130:PRO:HD3	3:G:125:GLN:HE21	1.77	0.49
2:F:133:PRO:HB3	2:F:145:LEU:HB3	1.93	0.49
2:H:130:PRO:HD3	3:K:125:GLN:HB2	1.95	0.49
1:A:377:GLN:HE21	1:A:585:CYS:N	1.95	0.49
1:B:207:TYR:HA	1:B:299:SER:O	2.13	0.49
2:H:131:LEU:HD23	2:H:147:CYS:HB3	1.94	0.49
2:F:5:VAL:HG23	2:F:23:LYS:HB3	1.94	0.49
2:F:52:ILE:HG22	2:F:55:LEU:H	1.77	0.49
1:B:526:CYS:HB3	1:B:556:ALA:HB2	1.95	0.49
1:B:263:VAL:HB	1:B:284:LEU:HB2	1.94	0.49
1:C:549:GLU:CB	1:C:550:GLY:HA2	2.41	0.49
1:A:109:VAL:HG11	1:A:153:VAL:HG21	1.94	0.48
1:B:100:LEU:HD22	1:B:299:SER:CB	2.43	0.48
1:B:404:PHE:HB3	1:B:407:CYS:SG	2.53	0.48
1:A:377:GLN:NE2	1:A:585:CYS:CA	2.76	0.48
1:A:1123:ILE:HD11	1:A:1141:TYR:HB2	1.94	0.48
3:G:204:SER:HB3	3:G:205:PRO:HD2	1.93	0.48
1:B:1219:PRO:HG2	1:B:1222:LEU:HB2	1.96	0.48
1:B:387:PRO:HG2	1:B:402:LEU:HD21	1.95	0.48
1:C:183:PHE:CD1	1:C:185:CYS:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:LYS:HB3	1:C:520:ALA:HA	1.96	0.48
1:C:1123:ILE:HD11	1:C:1141:TYR:HB2	1.94	0.48
1:C:109:VAL:HG11	1:C:153:VAL:HG21	1.96	0.48
3:G:33:TYR:HD2	3:G:93:GLY:HA2	1.78	0.48
1:B:700:ARG:H	1:B:700:ARG:HD3	1.78	0.48
2:H:52:ILE:HG22	2:H:55:LEU:H	1.79	0.48
1:B:862:ILE:HG12	1:B:865:PHE:HD1	1.79	0.48
1:A:583:SER:HB2	1:A:609:TYR:HA	1.96	0.48
2:F:162:ASN:HB3	2:F:165:ALA:HB3	1.96	0.48
1:B:430:PRO:O	1:B:433:ILE:HG22	2.14	0.47
1:C:360:VAL:HG22	1:C:662:ILE:HG23	1.96	0.47
1:A:667:THR:HG21	1:A:739:PRO:HB2	1.96	0.47
1:B:629:ARG:HA	1:B:642:TYR:HB2	1.96	0.47
1:A:731:LEU:HB2	1:A:735:LEU:HB2	1.95	0.47
1:B:783:PRO:HA	1:B:1146:HIS:HA	1.96	0.47
2:F:143:ALA:HB2	2:F:194:SER:HA	1.96	0.47
3:K:162:GLU:HA	3:K:178:SER:HA	1.97	0.47
1:B:866:GLY:HA2	1:B:972:PHE:HB3	1.97	0.47
1:B:360:VAL:HG22	1:B:662:ILE:HG23	1.97	0.47
2:F:51:ILE:HG21	2:F:70:ILE:HB	1.97	0.47
1:B:298:HIS:CD2	1:B:300:ILE:HD11	2.49	0.47
3:K:43:GLN:HE21	3:K:43:GLN:HB3	1.49	0.47
1:A:923:LEU:HD13	1:A:1033:LEU:HB2	1.96	0.47
1:B:156:PHE:CE1	1:B:196:PRO:HB3	2.49	0.47
1:A:377:GLN:CD	1:A:585:CYS:CA	2.83	0.47
1:B:1053:ASP:HA	1:B:1056:GLN:HE21	1.79	0.47
3:K:19:ALA:HB2	3:K:79:LEU:HD11	1.95	0.47
3:K:204:SER:HB3	3:K:205:PRO:HD2	1.98	0.47
1:A:609:TYR:HE1	1:A:629:ARG:HE	1.61	0.46
1:B:448:TYR:HE1	1:B:464:ILE:HG21	1.79	0.46
1:B:767:PRO:HB3	1:C:855:SER:O	2.15	0.46
1:B:417:LEU:HD12	1:B:488:LEU:HD13	1.97	0.46
1:C:368:ALA:HA	1:C:689:TYR:HD1	1.79	0.46
2:H:61:VAL:HG13	2:H:64:PHE:H	1.80	0.46
1:C:783:PRO:HA	1:C:1146:HIS:HA	1.98	0.46
3:K:199:HIS:CD2	3:K:201:GLY:H	2.33	0.46
1:A:63:THR:HB	1:C:628:GLN:HB2	1.98	0.46
1:A:152:SER:HB2	1:A:165:PHE:CD2	2.49	0.46
2:F:205:VAL:HG22	2:F:214:VAL:H	1.81	0.46
1:C:557:SER:HB2	2:F:55:LEU:HD21	1.97	0.46
1:A:35:ILE:HD11	1:A:203:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:LYS:O	2:H:118:VAL:HA	2.16	0.46
1:B:258:GLN:HE22	1:B:289:THR:HA	1.81	0.46
1:B:118:VAL:HG21	1:B:147:PHE:CZ	2.50	0.46
1:C:814:PHE:O	1:C:818:GLU:HG2	2.15	0.46
1:A:1170:GLY:HA3	1:A:1186:TYR:CE2	2.51	0.46
1:B:1179:ARG:HH22	1:B:1194:PRO:HB2	1.80	0.46
2:H:9:ALA:HA	2:H:114:THR:HG23	1.98	0.46
1:C:540:TYR:H	2:F:102:SER:HB3	1.80	0.45
2:F:152:TYR:HD2	2:F:207:HIS:HE2	1.65	0.45
1:C:386:SER:N	1:C:387:PRO:HD2	2.30	0.45
2:H:130:PRO:CD	3:K:125:GLN:HB2	2.46	0.45
1:C:507:LEU:C	1:C:507:LEU:CD1	2.90	0.45
1:A:360:VAL:HG22	1:A:662:ILE:HG23	1.99	0.45
1:C:183:PHE:HD1	1:C:185:CYS:HB2	1.80	0.45
1:C:439:SER:HB2	1:C:578:GLY:H	1.82	0.45
2:F:9:ALA:HA	2:F:114:THR:HG23	1.97	0.45
2:F:54:ILE:HG23	2:F:74:LYS:HD2	1.98	0.45
1:B:1222:LEU:HD12	1:B:1222:LEU:HA	1.77	0.45
1:A:87:TYR:HD2	1:A:143:ILE:HD12	1.82	0.45
1:B:299:SER:C	1:B:300:ILE:HD12	2.40	0.45
1:C:179:LEU:HD11	1:C:181:ARG:HH22	1.82	0.45
1:C:185:CYS:HA	1:C:237:CYS:HA	1.99	0.45
1:C:545:LEU:HD13	1:C:545:LEU:HA	1.88	0.45
2:F:200:THR:HG22	2:F:218:VAL:HB	1.99	0.45
3:K:30:SER:HB3	3:K:33:TYR:HB2	1.98	0.45
1:A:34:ASP:HB2	1:A:99:LYS:HD3	1.99	0.45
1:B:183:PHE:HB3	1:B:240:MET:HG2	1.99	0.45
1:C:408:ASN:HA	1:C:585:CYS:O	2.17	0.45
1:C:540:TYR:HD2	2:F:101:GLY:HA2	1.80	0.45
1:A:153:VAL:CA	1:A:165:PHE:CD2	2.99	0.44
1:A:767:PRO:HB3	1:B:855:SER:O	2.16	0.44
1:C:87:TYR:HD2	1:C:143:ILE:HD12	1.82	0.44
1:C:587:LYS:HA	1:C:588:LEU:HA	1.75	0.44
1:C:903:PRO:HG2	1:C:905:TYR:CZ	2.52	0.44
1:C:790:VAL:HG11	1:C:1008:MET:SD	2.58	0.44
1:B:506:LEU:HD22	2:H:31:SER:HB3	1.98	0.44
1:A:166:ASN:HA	1:A:186:ILE:HG23	1.98	0.44
3:G:204:SER:HB3	3:G:205:PRO:CD	2.48	0.44
1:A:369:LYS:HE2	1:A:690:SER:HB3	1.99	0.44
2:F:55:LEU:HD12	2:F:55:LEU:HA	1.82	0.44
1:A:192:GLY:O	1:A:198:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PRO:HD3	1:B:333:ILE:HD11	1.98	0.44
1:B:386:SER:N	1:B:387:PRO:HD2	2.32	0.44
1:C:185:CYS:HB3	1:C:234:LEU:HD12	1.99	0.44
2:F:36:TRP:HE1	2:F:51:ILE:HD11	1.82	0.44
3:K:148:GLN:HE21	3:K:148:GLN:HB2	1.57	0.44
1:B:126:SER:O	1:B:140:ILE:HG13	2.18	0.44
1:B:374:VAL:HG11	1:B:596:ILE:HG12	1.99	0.44
1:C:374:VAL:HG11	1:C:596:ILE:HG12	2.00	0.44
1:C:505:ARG:NH1	1:C:552:GLY:HA3	2.33	0.44
1:A:626:ARG:HH12	1:A:646:GLY:HA2	1.82	0.43
1:C:629:ARG:HA	1:C:642:TYR:HB2	2.00	0.43
1:A:126:SER:O	1:A:140:ILE:HG13	2.18	0.43
1:A:155:ASN:O	1:A:163:ARG:HG2	2.18	0.43
1:A:913:MET:HE2	1:C:681:HIS:CE1	2.53	0.43
1:B:92:ALA:HA	1:B:97:PRO:HA	2.00	0.43
1:B:452:MET:HE2	1:B:452:MET:HB3	1.88	0.43
1:C:447:SER:HA	1:C:569:MET:HA	2.00	0.43
1:C:547:PRO:HA	1:C:551:GLY:CA	2.48	0.43
2:F:54:ILE:H	2:F:54:ILE:HG12	1.49	0.43
1:A:1054:ILE:HD13	1:A:1066:GLN:HB2	2.00	0.43
2:H:30:SER:HB3	2:H:32:TYR:HD2	1.82	0.43
1:B:981:ASN:HD22	1:B:981:ASN:HA	1.61	0.43
3:G:31:SER:HA	3:G:69:GLY:H	1.83	0.43
1:B:667:THR:HG22	1:B:742:PRO:HD3	2.00	0.43
1:C:401:ARG:NH2	1:C:521:ASN:HB3	2.31	0.43
3:G:113:ALA:HA	3:G:201:GLY:HA3	2.00	0.43
1:C:912:CYS:O	1:C:915:GLN:HB2	2.19	0.43
2:F:51:ILE:HG22	2:F:58:SER:HA	2.00	0.43
1:B:105:TYR:HB3	1:B:295:ILE:HB	2.01	0.43
1:C:380:GLY:O	1:C:381:VAL:HB	2.18	0.43
2:F:130:PRO:HB3	3:G:122:SER:HB3	2.00	0.43
1:A:190:ARG:HD3	1:A:230:GLU:O	2.19	0.43
1:C:181:ARG:NH2	1:C:221:ARG:O	2.52	0.43
1:C:497:TYR:HB2	1:C:561:VAL:HG12	2.01	0.43
2:H:146:GLY:HA2	2:H:161:TRP:CZ2	2.52	0.43
1:B:799:ILE:HG23	1:B:1092:ALA:HB2	2.01	0.42
3:K:7:SER:HB3	3:K:22:SER:H	1.84	0.42
1:A:790:VAL:HG11	1:A:1008:MET:SD	2.60	0.42
1:B:34:ASP:HB2	1:B:99:LYS:HD3	2.00	0.42
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.84	0.42
1:B:470:LYS:HB3	1:B:520:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ASN:HB2	1:B:318:LEU:O	2.19	0.42
1:C:397:TYR:CD1	1:C:527:VAL:HG23	2.55	0.42
2:F:83:LEU:HG	2:F:86:LEU:HB3	2.01	0.42
1:A:372:GLY:H	1:A:604:VAL:HG12	1.84	0.42
1:A:758:ARG:HG3	1:A:758:ARG:HH11	1.84	0.42
1:A:105:TYR:HB3	1:A:295:ILE:HB	2.01	0.42
1:B:740:ASP:HB3	1:B:755:GLY:H	1.84	0.42
1:B:1170:GLY:HA3	1:B:1186:TYR:CE2	2.54	0.42
1:C:192:GLY:O	1:C:198:GLY:HA3	2.19	0.42
1:C:518:VAL:HG23	1:C:525:PRO:HD3	2.01	0.42
3:K:18:ARG:HA	3:K:76:ILE:O	2.19	0.42
2:F:33:GLY:HA3	2:F:52:ILE:HG13	2.01	0.42
2:H:163:SER:HA	2:H:204:ASN:HB3	2.02	0.42
1:A:85:TYR:HB2	1:A:313:PHE:CZ	2.55	0.42
1:A:118:VAL:HG21	1:A:147:PHE:CZ	2.54	0.42
1:B:719:ASN:HA	1:B:759:LEU:HB3	2.01	0.42
1:C:1222:LEU:HD23	1:C:1222:LEU:HA	1.90	0.42
1:A:587:LYS:HE3	1:A:587:LYS:HB2	1.53	0.42
1:C:1170:GLY:HA3	1:C:1186:TYR:CE2	2.55	0.42
1:A:263:VAL:HG23	1:A:286:VAL:HB	2.02	0.42
1:B:25:SER:HB3	1:B:190:ARG:HH12	1.85	0.42
1:B:190:ARG:HD3	1:B:230:GLU:O	2.20	0.42
1:A:33:VAL:HG12	1:A:100:LEU:HD12	2.02	0.42
1:A:185:CYS:HA	1:A:237:CYS:HA	2.00	0.42
1:A:377:GLN:CG	1:A:585:CYS:C	2.92	0.42
1:A:674:PHE:HE2	1:A:715:LEU:HD12	1.85	0.42
1:A:951:LEU:O	1:A:955:ILE:HG13	2.20	0.42
1:B:154:GLY:O	1:B:163:ARG:HB3	2.19	0.42
1:B:549:GLU:HA	1:B:550:GLY:HA2	1.78	0.42
1:C:549:GLU:HA	1:C:549:GLU:OE1	2.20	0.42
1:B:951:LEU:O	1:B:955:ILE:HG13	2.20	0.41
1:C:117:VAL:HG12	1:C:278:MET:HE1	2.01	0.41
1:C:1045:GLY:HA3	1:C:1069:ARG:HH21	1.85	0.41
1:A:783:PRO:HA	1:A:1146:HIS:HA	2.00	0.41
1:B:449:PRO:HG3	1:B:561:VAL:HG11	2.02	0.41
1:C:439:SER:HB2	1:C:578:GLY:N	2.35	0.41
1:B:497:TYR:HB2	1:B:561:VAL:HG12	2.02	0.41
1:B:606:TYR:CZ	1:B:651:LEU:HD21	2.55	0.41
1:B:652:ARG:HD3	1:C:915:GLN:HB3	2.01	0.41
1:C:150:GLY:HA3	1:C:164:PHE:CD1	2.56	0.41
1:C:428:ILE:HG21	1:C:433:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LYS:HD3	1:A:44:TRP:HH2	1.77	0.41
1:A:913:MET:HE2	1:C:681:HIS:HE1	1.85	0.41
1:A:1113:ARG:H	1:A:1113:ARG:HG2	1.73	0.41
1:B:87:TYR:HD2	1:B:143:ILE:HD12	1.85	0.41
1:B:493:LYS:HG2	1:B:567:LEU:HB2	2.01	0.41
1:C:921:ARG:HE	1:C:1037:ALA:HB1	1.85	0.41
2:F:131:LEU:HD13	2:F:218:VAL:HA	2.02	0.41
1:B:185:CYS:HA	1:B:237:CYS:HA	2.01	0.41
1:C:587:LYS:HG3	1:C:588:LEU:HG	2.01	0.41
3:G:79:LEU:HD23	3:G:79:LEU:HA	1.88	0.41
3:G:148:GLN:HE21	3:G:148:GLN:HB2	1.55	0.41
2:H:205:VAL:O	2:H:213:LYS:HA	2.20	0.41
3:K:141:TYR:HA	3:K:142:PRO:HA	1.86	0.41
1:A:893:LEU:HD23	1:A:897:LYS:HG3	2.02	0.41
1:B:143:ILE:HD13	1:B:144:TYR:H	1.86	0.41
2:F:130:PRO:CG	3:G:125:GLN:HB2	2.49	0.41
1:A:903:PRO:HG2	1:A:905:TYR:CZ	2.55	0.41
1:B:166:ASN:HA	1:B:186:ILE:HG23	2.02	0.41
1:C:156:PHE:CE1	1:C:196:PRO:HB3	2.55	0.41
1:A:344:LEU:HA	1:A:344:LEU:HD23	1.83	0.41
1:A:579:THR:HG22	1:B:62:ARG:CZ	2.51	0.41
1:A:156:PHE:CE1	1:A:196:PRO:HB3	2.55	0.41
1:B:87:TYR:CG	1:B:298:HIS:HB3	2.56	0.41
1:C:1179:ARG:HG2	1:C:1183:GLU:HG2	2.02	0.41
3:G:21:LEU:O	3:G:73:THR:HA	2.20	0.41
1:A:609:TYR:HB3	1:A:630:PHE:CE2	2.55	0.41
1:B:306:ASP:CG	1:B:308:LYS:NZ	2.78	0.41
2:F:6:GLN:HE21	2:F:6:GLN:HB2	1.64	0.41
2:H:128:VAL:HG11	2:H:216:LYS:HD2	2.03	0.41
1:A:148:MET:HG3	1:A:170:VAL:HG22	2.03	0.40
1:A:819:GLN:HE21	1:A:819:GLN:HB2	1.59	0.40
1:A:853:VAL:HG13	1:A:951:LEU:HD22	2.03	0.40
1:A:980:LEU:O	1:A:983:VAL:HG22	2.21	0.40
1:B:985:ILE:HD11	1:B:1141:TYR:CE2	2.56	0.40
1:C:790:VAL:HG23	1:C:1004:ALA:HB1	2.03	0.40
1:B:733:GLN:O	1:C:940:ASP:HB2	2.21	0.40
1:B:980:LEU:O	1:B:983:VAL:HG22	2.22	0.40
1:C:50:VAL:HG13	1:C:336:ALA:O	2.21	0.40
2:F:155:GLU:HA	2:F:156:PRO:HA	1.87	0.40
3:K:119:PHE:HA	3:K:120:PRO:HD3	1.88	0.40
1:B:470:LYS:HE3	1:B:470:LYS:HB2	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:740:ASP:HB2	1:B:758:ARG:HH12	1.87	0.40
1:C:472:SER:HB2	1:C:475:ASN:OD1	2.22	0.40
1:A:583:SER:CB	1:A:609:TYR:CG	3.05	0.40
1:B:472:SER:HB2	1:B:475:ASN:OD1	2.21	0.40
1:C:284:LEU:HA	1:C:285:PRO:HD3	1.93	0.40
1:A:940:ASP:HB2	1:C:733:GLN:O	2.21	0.40
1:B:19:VAL:O	1:B:237:CYS:HB3	2.22	0.40
1:B:482:ALA:HB3	1:B:571:PHE:HE2	1.86	0.40
1:B:1054:ILE:HG13	1:B:1055:ILE:N	2.37	0.40
1:C:154:GLY:O	1:C:163:ARG:HB3	2.22	0.40
1:C:980:LEU:O	1:C:983:VAL:HG22	2.22	0.40
2:H:155:GLU:HA	2:H:156:PRO:HA	1.86	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	983/1347 (73%)	954 (97%)	20 (2%)	9 (1%)	14	27
1	B	1184/1347 (88%)	1157 (98%)	23 (2%)	4 (0%)	36	55
1	C	1184/1347 (88%)	1155 (98%)	26 (2%)	3 (0%)	36	55
2	F	212/221 (96%)	204 (96%)	5 (2%)	3 (1%)	9	17
2	H	221/221 (100%)	213 (96%)	4 (2%)	4 (2%)	6	12
3	G	210/212 (99%)	192 (91%)	18 (9%)	0	100	100
3	K	210/212 (99%)	192 (91%)	16 (8%)	2 (1%)	12	24
All	All	4204/4907 (86%)	4067 (97%)	112 (3%)	25 (1%)	23	38

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	583	SER
1	A	584	VAL
1	A	589	GLU
1	B	592	ASN
1	B	827	PHE
1	C	381	VAL
1	C	827	PHE
2	F	202	ILE
2	H	202	ILE
3	K	139	ASN
1	C	524	SER
2	H	165	ALA
3	K	142	PRO
1	A	581	THR
1	A	376	GLU
1	A	377	GLN
1	A	700	ARG
1	A	730	PRO
1	B	524	SER
1	B	94	GLY
2	F	154	PRO
1	A	94	GLY
2	H	154	PRO
2	F	156	PRO
2	H	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	842/1164 (72%)	780 (93%)	62 (7%)	13	27
1	B	1020/1164 (88%)	943 (92%)	77 (8%)	12	26
1	C	1020/1164 (88%)	948 (93%)	72 (7%)	13	29
2	F	180/184 (98%)	155 (86%)	25 (14%)	3	7
2	H	185/184 (100%)	154 (83%)	31 (17%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	178/183 (97%)	154 (86%)	24 (14%)	4	8
3	K	178/183 (97%)	153 (86%)	25 (14%)	3	7
All	All	3603/4226 (85%)	3287 (91%)	316 (9%)	12	20

All (316) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	60	GLN
1	A	67	ILE
1	A	110	LYS
1	A	129	THR
1	A	130	VAL
1	A	132	ILE
1	A	143	ILE
1	A	153	VAL
1	A	171	LEU
1	A	172	LEU
1	A	181	ARG
1	A	184	TYR
1	A	195	CYS
1	A	208	HIS
1	A	234	LEU
1	A	238	THR
1	A	251	LEU
1	A	265	LEU
1	A	337	ILE
1	A	367	GLU
1	A	373	SER
1	A	375	VAL
1	A	579	THR
1	A	581	THR
1	A	587	LYS
1	A	588	LEU
1	A	596	ILE
1	A	609	TYR
1	A	651	LEU
1	A	655	VAL
1	A	666	GLU
1	A	672	THR
1	A	679	CYS

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Mol	Chain	Res	Type
1	A	682	ILE
1	A	699	ARG
1	A	718	VAL
1	A	724	VAL
1	A	741	THR
1	A	761	SER
1	A	802	VAL
1	A	803	THR
1	A	820	LEU
1	A	828	CYS
1	A	871	LEU
1	A	872	THR
1	A	873	LEU
1	A	874	LEU
1	A	877	VAL
1	A	893	LEU
1	A	921	ARG
1	A	941	VAL
1	A	960	TRP
1	A	961	THR
1	A	981	ASN
1	A	1015	THR
1	A	1054	ILE
1	A	1175	THR
1	A	1179	ARG
1	A	1180	ILE
1	A	1190	SER
1	A	1214	ILE
1	B	33	VAL
1	B	38	THR
1	B	50	VAL
1	B	69	ILE
1	B	86	VAL
1	B	95	THR
1	B	110	LYS
1	B	129	THR
1	B	132	ILE
1	B	143	ILE
1	B	171	LEU
1	B	172	LEU
1	B	181	ARG
1	B	184	TYR

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Mol	Chain	Res	Type
1	B	195	CYS
1	B	208	HIS
1	B	214	CYS
1	B	234	LEU
1	B	238	THR
1	B	240	MET
1	B	251	LEU
1	B	300	ILE
1	B	317	LYS
1	B	337	ILE
1	B	392	THR
1	B	403	VAL
1	B	405	THR
1	B	417	LEU
1	B	420	VAL
1	B	438	TYR
1	B	478	CYS
1	B	481	LEU
1	B	495	LEU
1	B	512	THR
1	B	529	ILE
1	B	545	LEU
1	B	548	LEU
1	B	555	VAL
1	B	563	MET
1	B	574	THR
1	B	584	VAL
1	B	594	THR
1	B	596	ILE
1	B	608	LEU
1	B	623	VAL
1	B	650	CYS
1	B	679	CYS
1	B	682	ILE
1	B	686	MET
1	B	688	GLN
1	B	699	ARG
1	B	711	VAL
1	B	714	VAL
1	B	724	VAL
1	B	741	THR
1	B	823	GLU

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Mol	Chain	Res	Type
1	B	827	PHE
1	B	853	VAL
1	B	872	THR
1	B	874	LEU
1	B	877	VAL
1	B	893	LEU
1	B	921	ARG
1	B	958	VAL
1	B	960	TRP
1	B	981	ASN
1	B	983	VAL
1	B	1015	THR
1	B	1054	ILE
1	B	1100	LYS
1	B	1105	GLU
1	B	1112	LYS
1	B	1179	ARG
1	B	1180	ILE
1	B	1190	SER
1	B	1214	ILE
1	B	1222	LEU
1	C	27	LYS
1	C	33	VAL
1	C	60	GLN
1	C	67	ILE
1	C	110	LYS
1	C	129	THR
1	C	132	ILE
1	C	143	ILE
1	C	171	LEU
1	C	181	ARG
1	C	184	TYR
1	C	195	CYS
1	C	208	HIS
1	C	234	LEU
1	C	238	THR
1	C	240	MET
1	C	243	TYR
1	C	246	THR
1	C	251	LEU
1	C	256	ILE
1	C	337	ILE

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Mol	Chain	Res	Type
1	C	388	LEU
1	C	392	THR
1	C	403	VAL
1	C	405	THR
1	C	417	LEU
1	C	420	VAL
1	C	438	TYR
1	C	472	SER
1	C	481	LEU
1	C	495	LEU
1	C	527	VAL
1	C	529	ILE
1	C	533	THR
1	C	545	LEU
1	C	548	LEU
1	C	563	MET
1	C	574	THR
1	C	584	VAL
1	C	588	LEU
1	C	589	GLU
1	C	608	LEU
1	C	623	VAL
1	C	628	GLN
1	C	655	VAL
1	C	666	GLU
1	C	672	THR
1	C	679	CYS
1	C	682	ILE
1	C	699	ARG
1	C	700	ARG
1	C	718	VAL
1	C	724	VAL
1	C	815	GLN
1	C	827	PHE
1	C	853	VAL
1	C	871	LEU
1	C	872	THR
1	C	873	LEU
1	C	874	LEU
1	C	877	VAL
1	C	941	VAL
1	C	958	VAL

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Mol	Chain	Res	Type
1	C	960	TRP
1	C	981	ASN
1	C	983	VAL
1	C	1015	THR
1	C	1054	ILE
1	C	1112	LYS
1	C	1179	ARG
1	C	1180	ILE
1	C	1214	ILE
2	F	2	VAL
2	F	5	VAL
2	F	6	GLN
2	F	10	GLU
2	F	11	VAL
2	F	18	VAL
2	F	35	THR
2	F	43	GLN
2	F	54	ILE
2	F	70	ILE
2	F	105	ASP
2	F	118	VAL
2	F	131	LEU
2	F	142	THR
2	F	145	LEU
2	F	158	THR
2	F	159	VAL
2	F	170	VAL
2	F	177	LEU
2	F	189	VAL
2	F	190	THR
2	F	199	GLN
2	F	200	THR
2	F	202	ILE
2	F	204	ASN
3	G	5	THR
3	G	33	TYR
3	G	34	LEU
3	G	43	GLN
3	G	55	ARG
3	G	75	THR
3	G	82	GLU
3	G	103	THR

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Mol	Chain	Res	Type
3	G	110	THR
3	G	111	VAL
3	G	116	VAL
3	G	118	ILE
3	G	133	VAL
3	G	134	VAL
3	G	147	VAL
3	G	148	GLN
3	G	164	VAL
3	G	188	GLU
3	G	190	HIS
3	G	192	VAL
3	G	197	VAL
3	G	198	THR
3	G	202	LEU
3	G	206	VAL
2	H	2	VAL
2	H	4	LEU
2	H	5	VAL
2	H	10	GLU
2	H	11	VAL
2	H	18	VAL
2	H	28	THR
2	H	29	PHE
2	H	43	GLN
2	H	51	ILE
2	H	55	LEU
2	H	70	ILE
2	H	80	TYR
2	H	81	MET
2	H	93	VAL
2	H	105	ASP
2	H	118	VAL
2	H	131	LEU
2	H	145	LEU
2	H	155	GLU
2	H	158	THR
2	H	159	VAL
2	H	160[A]	SER
2	H	160[B]	SER
2	H	177	LEU
2	H	182	LEU

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Mol	Chain	Res	Type
2	H	186[A]	SER
2	H	186[B]	SER
2	H	190	THR
2	H	202	ILE
2	H	204	ASN
3	K	5	THR
3	K	20	THR
3	K	33	TYR
3	K	34	LEU
3	K	43	GLN
3	K	47	LEU
3	K	55	ARG
3	K	82	GLU
3	K	103	THR
3	K	110	THR
3	K	111	VAL
3	K	116	VAL
3	K	118	ILE
3	K	125	GLN
3	K	133	VAL
3	K	147	VAL
3	K	148	GLN
3	K	164	VAL
3	K	188	GLU
3	K	190	HIS
3	K	192	VAL
3	K	197	VAL
3	K	198	THR
3	K	202	LEU
3	K	206	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	91	HIS
1	A	98	GLN
1	A	277	ASN
1	A	377	GLN
1	A	582	ASN
1	A	618	GLN
1	A	628	GLN

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Mol	Chain	Res	Type
1	A	647	ASN
1	A	708	GLN
1	A	719	ASN
1	A	808	GLN
1	A	819	GLN
1	A	857	GLN
1	A	981	ASN
1	A	994	GLN
1	A	1056	GLN
1	A	1145	ASN
1	A	1160	ASN
1	A	1177	ASN
1	A	1208	GLN
1	A	1212	GLN
1	B	98	GLN
1	B	244	ASN
1	B	277	ASN
1	B	298	HIS
1	B	319	GLN
1	B	421	ASN
1	B	427	GLN
1	B	516	GLN
1	B	592	ASN
1	B	602	ASN
1	B	636	GLN
1	B	637	ASN
1	B	688	GLN
1	B	848	ASN
1	B	981	ASN
1	B	987	GLN
1	B	994	GLN
1	B	1020	GLN
1	B	1031	GLN
1	B	1056	GLN
1	B	1072	ASN
1	B	1097	GLN
1	B	1145	ASN
1	B	1160	ASN
1	B	1177	ASN
1	B	1212	GLN
1	C	37	GLN
1	C	72	GLN

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Mol	Chain	Res	Type
1	C	277	ASN
1	C	516	GLN
1	C	592	ASN
1	C	618	GLN
1	C	628	GLN
1	C	636	GLN
1	C	681	HIS
1	C	708	GLN
1	C	808	GLN
1	C	812	ASN
1	C	819	GLN
1	C	826	GLN
1	C	848	ASN
1	C	981	ASN
1	C	987	GLN
1	C	994	GLN
1	C	1020	GLN
1	C	1031	GLN
1	C	1085	GLN
1	C	1145	ASN
1	C	1160	ASN
1	C	1177	ASN
1	C	1212	GLN
1	C	1217	ASN
2	F	6	GLN
2	F	178	GLN
2	F	199	GLN
3	G	43	GLN
3	G	125	GLN
3	G	148	GLN
3	G	161	GLN
2	H	1	GLN
2	H	6	GLN
2	H	62	GLN
2	H	112	GLN
2	H	199	GLN
3	K	43	GLN
3	K	125	GLN
3	K	148	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32962. These allow visual inspection of the internal detail of the map and identification of artifacts.

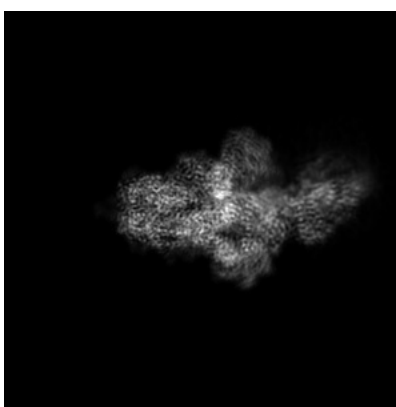
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

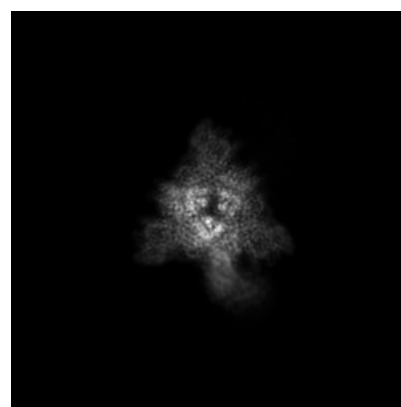
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 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](#)

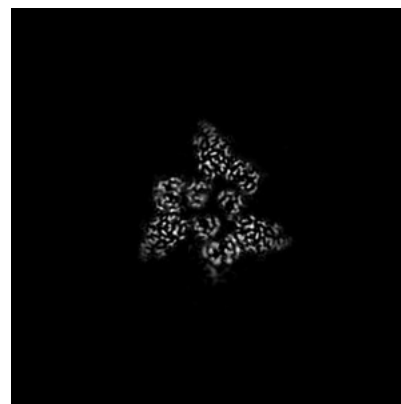
6.3.1 Primary map



X Index: 154



Y Index: 147

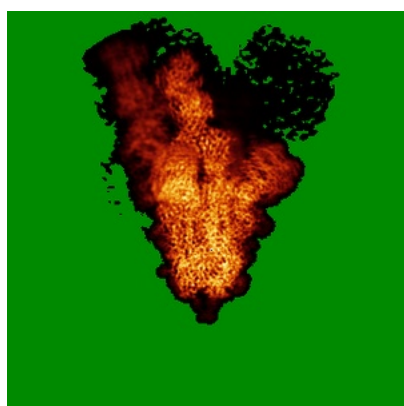


Z Index: 178

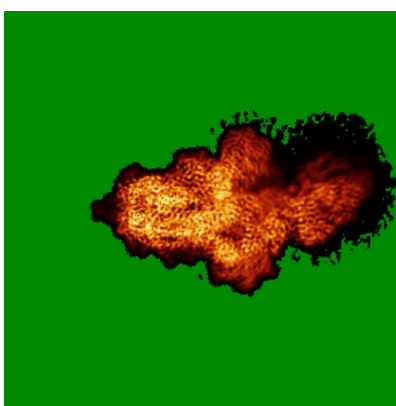
The images above show the largest variance slices of the map in three orthogonal directions.

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

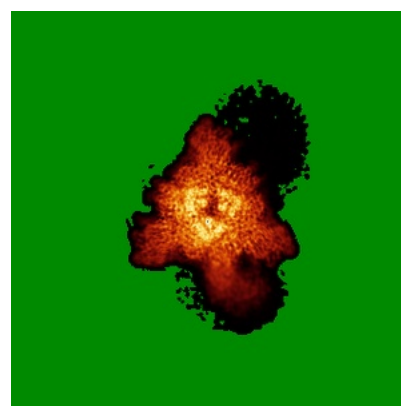
6.4.1 Primary map



X



Y

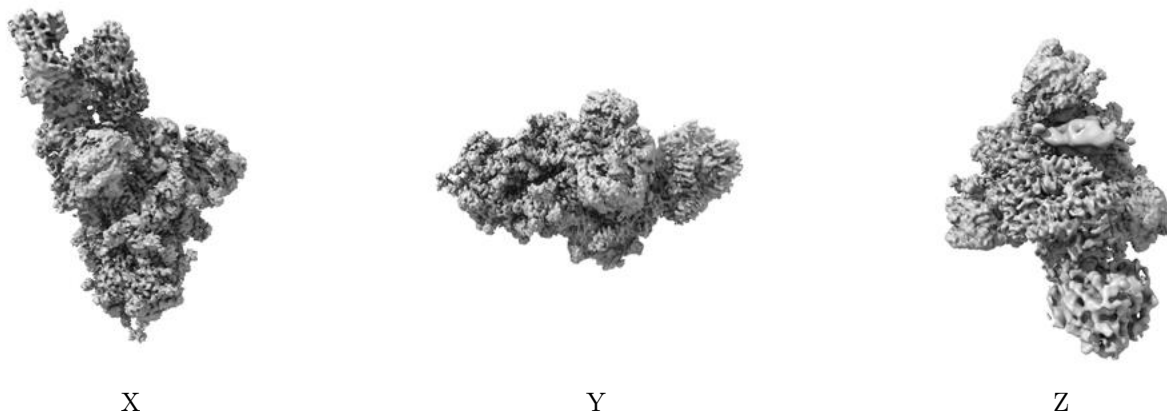


Z

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



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.

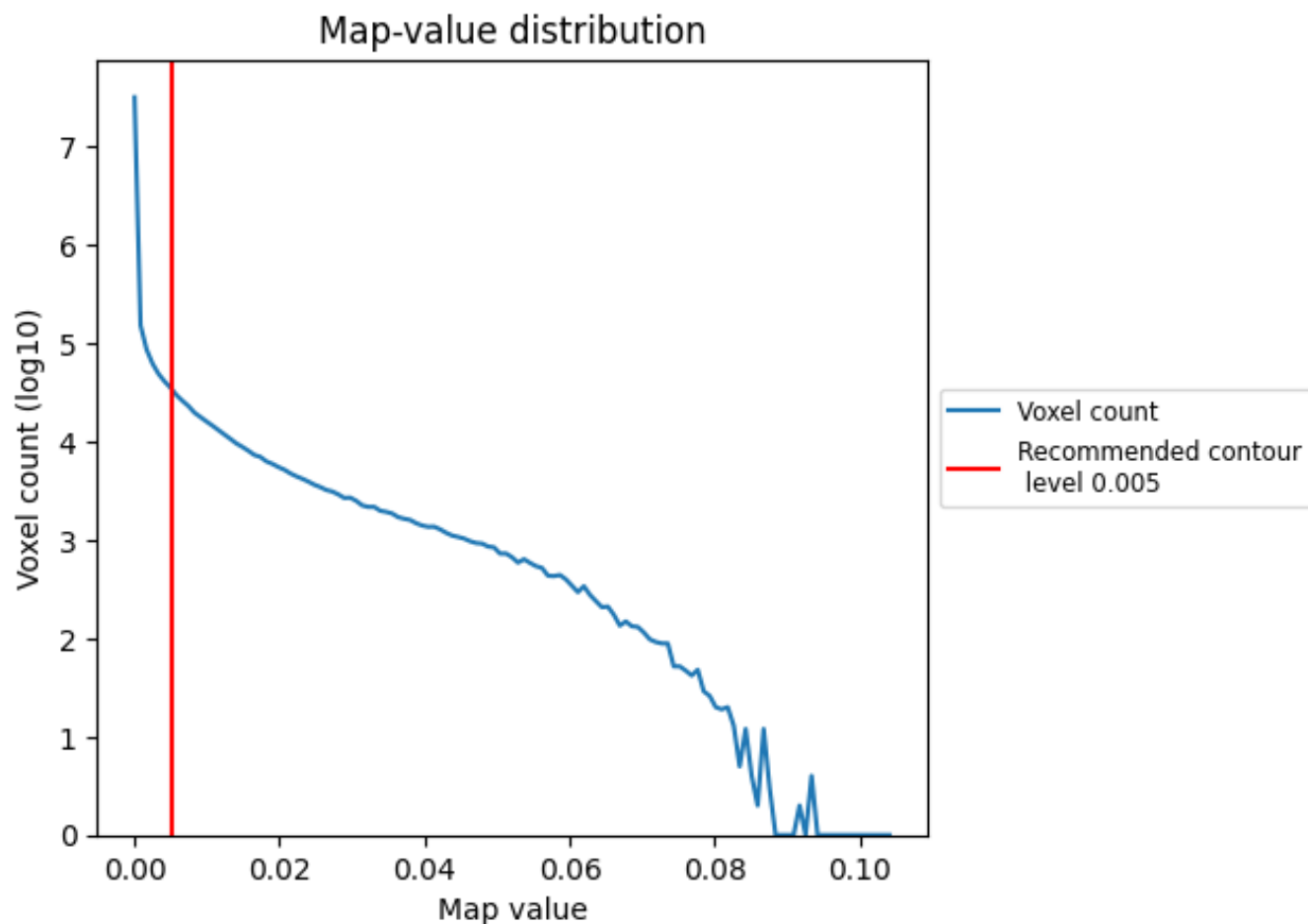
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

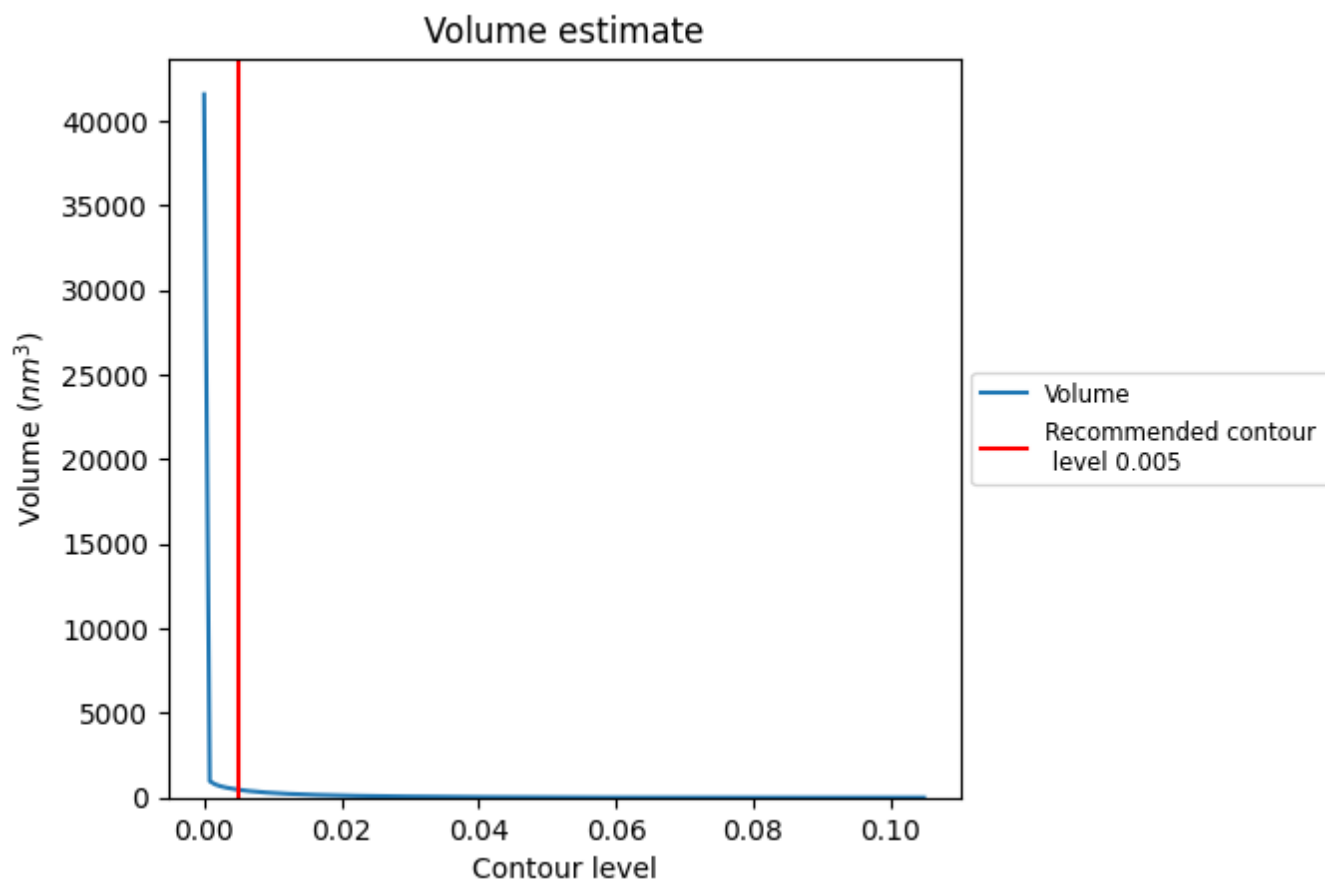
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

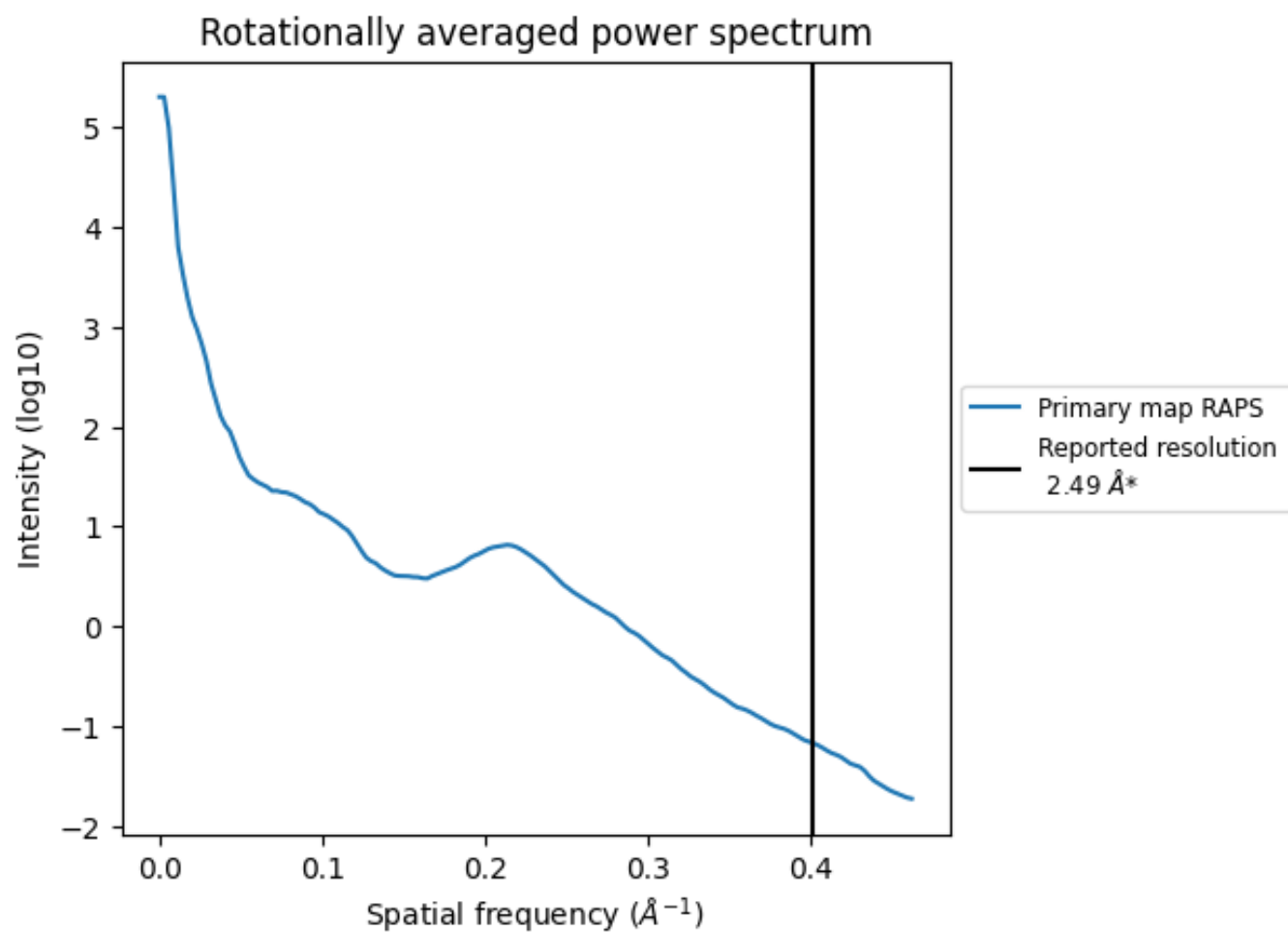
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 465 nm^3 ; this corresponds to an approximate mass of 420 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.402 Å⁻¹

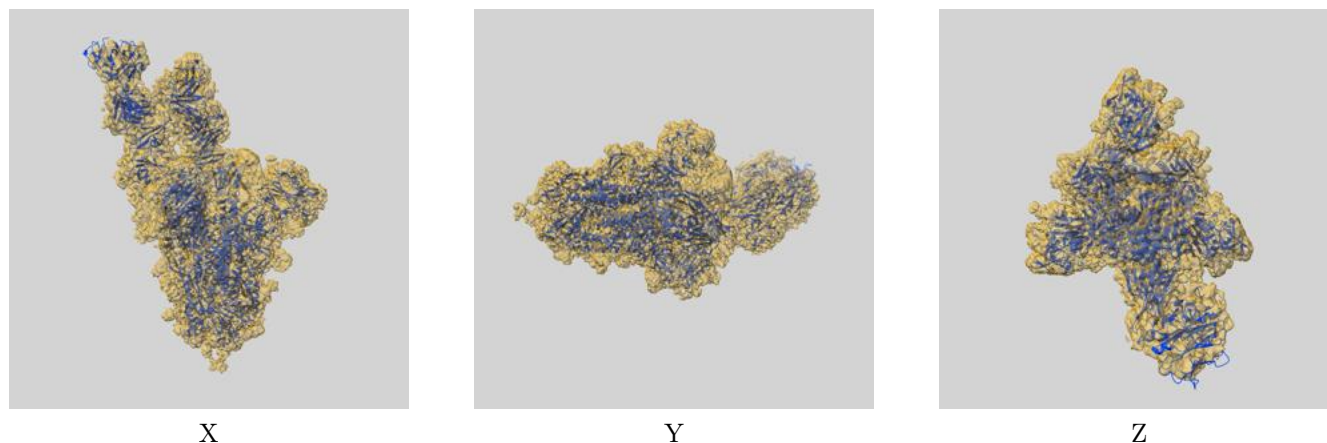
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

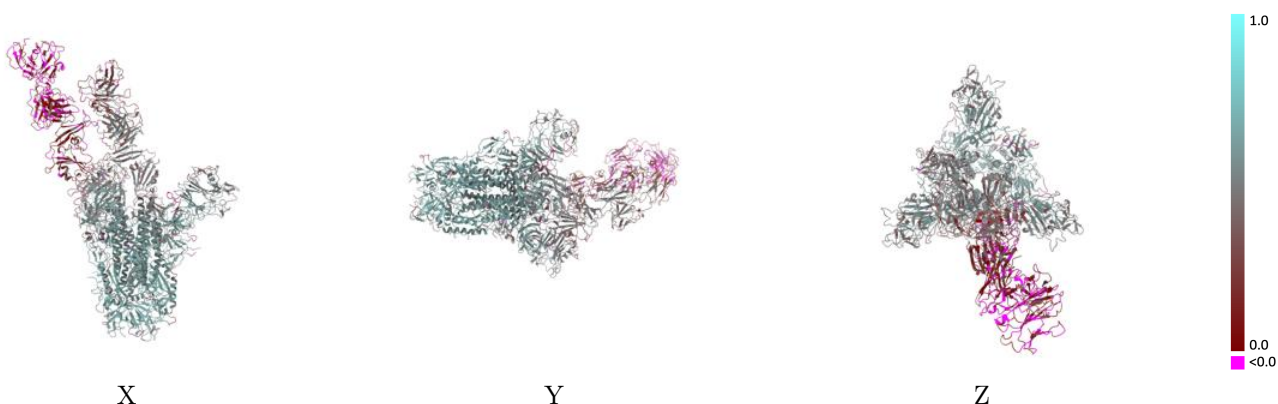
This section contains information regarding the fit between EMDB map EMD-32962 and PDB model 7X29. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



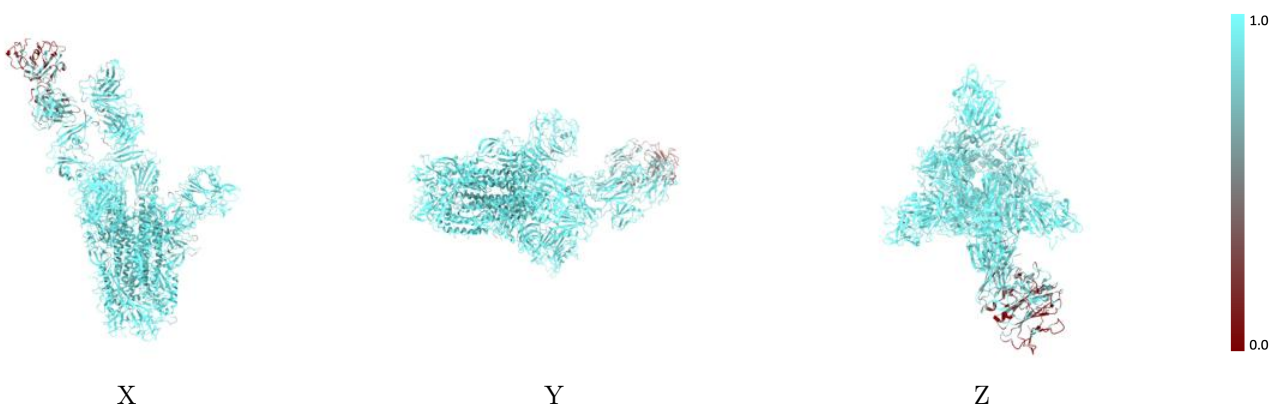
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



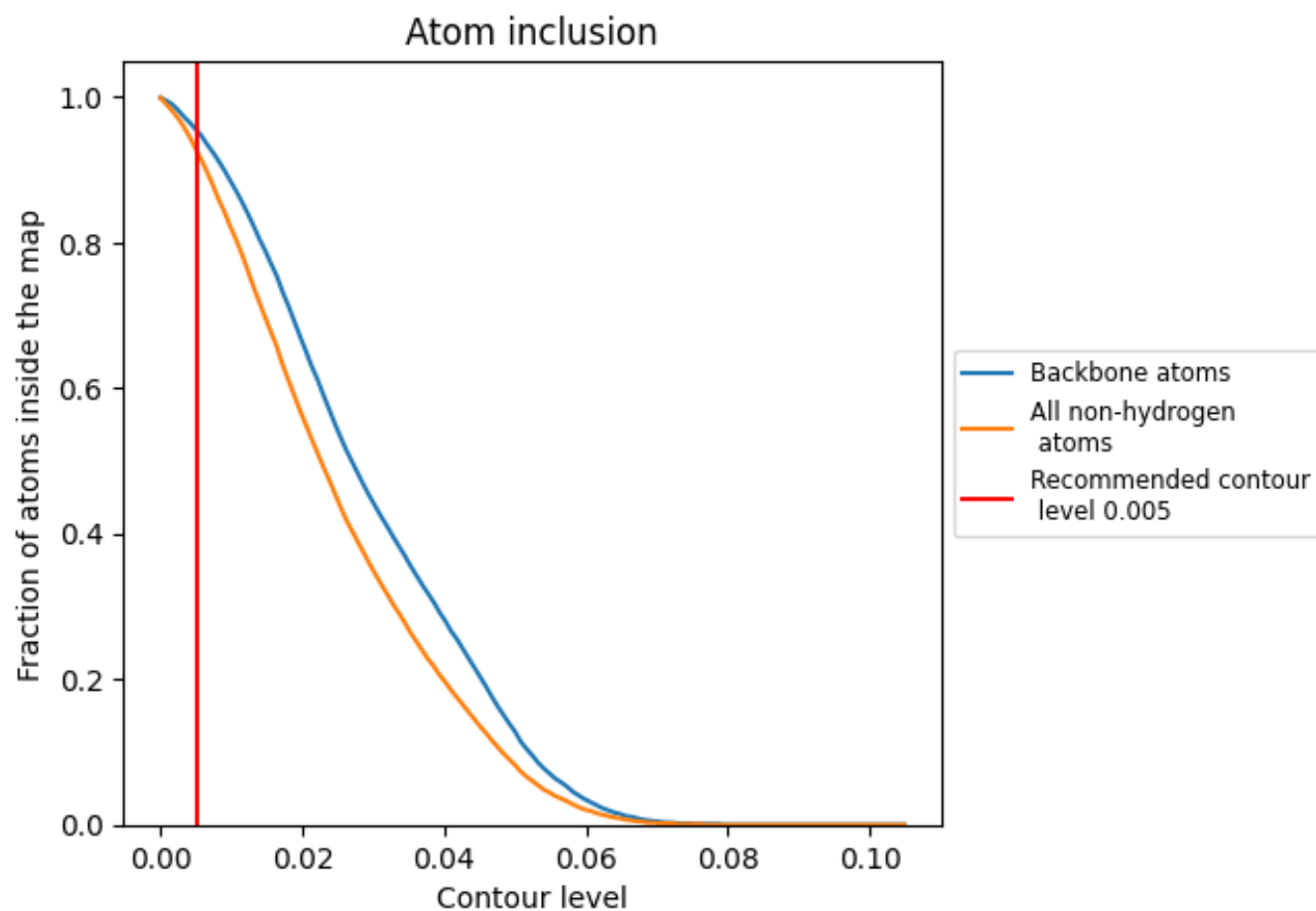
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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	0.9280	0.4470
A	0.9730	0.5290
B	0.9750	0.5170
C	0.9640	0.4700
F	0.6450	0.0750
G	0.5350	0.0680
H	0.9280	0.3630
K	0.9130	0.3460

1.0

0.0

<0.0