



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 04:12 PM UTC

PDB ID : 6ACJ / pdb_00006acj
EMDB ID : EMD-9593
Title : Trypsin-cleaved and low pH-treated SARS-CoV spike glycoprotein and ACE2 complex, ACE2-bound conformation 2
Authors : Gui, M.; Song, W.
Deposited on : 2018-07-26
Resolution : 4.20 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

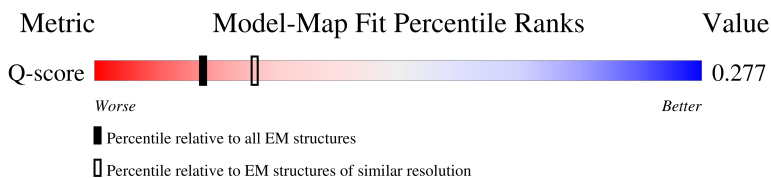
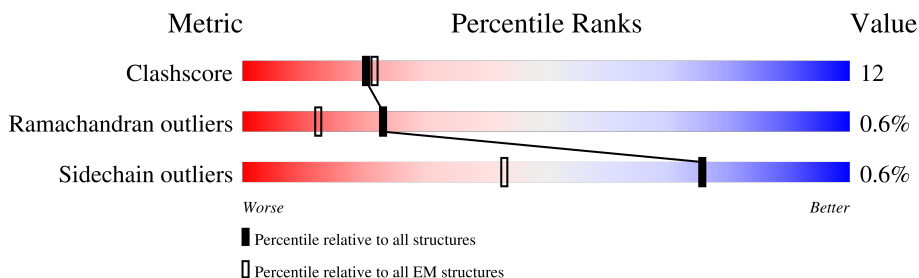
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	5410 (3.70 - 4.70)

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	1203	
1	B	1203	
1	C	1203	
2	D	603	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29715 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	1065	Total	C	N	O	S	0	0
			8302	5304	1374	1579	45		
1	B	1065	Total	C	N	O	S	0	0
			8302	5304	1374	1579	45		
1	C	1057	Total	C	N	O	S	0	0
			8241	5264	1364	1568	45		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1197	SER	-	expression tag	UNP P59594
A	1198	HIS	-	expression tag	UNP P59594
A	1199	PRO	-	expression tag	UNP P59594
A	1200	GLN	-	expression tag	UNP P59594
A	1201	PHE	-	expression tag	UNP P59594
A	1202	GLU	-	expression tag	UNP P59594
A	1203	LYS	-	expression tag	UNP P59594
B	1197	SER	-	expression tag	UNP P59594
B	1198	HIS	-	expression tag	UNP P59594
B	1199	PRO	-	expression tag	UNP P59594
B	1200	GLN	-	expression tag	UNP P59594
B	1201	PHE	-	expression tag	UNP P59594
B	1202	GLU	-	expression tag	UNP P59594
B	1203	LYS	-	expression tag	UNP P59594
C	1197	SER	-	expression tag	UNP P59594
C	1198	HIS	-	expression tag	UNP P59594
C	1199	PRO	-	expression tag	UNP P59594
C	1200	GLN	-	expression tag	UNP P59594
C	1201	PHE	-	expression tag	UNP P59594
C	1202	GLU	-	expression tag	UNP P59594
C	1203	LYS	-	expression tag	UNP P59594

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

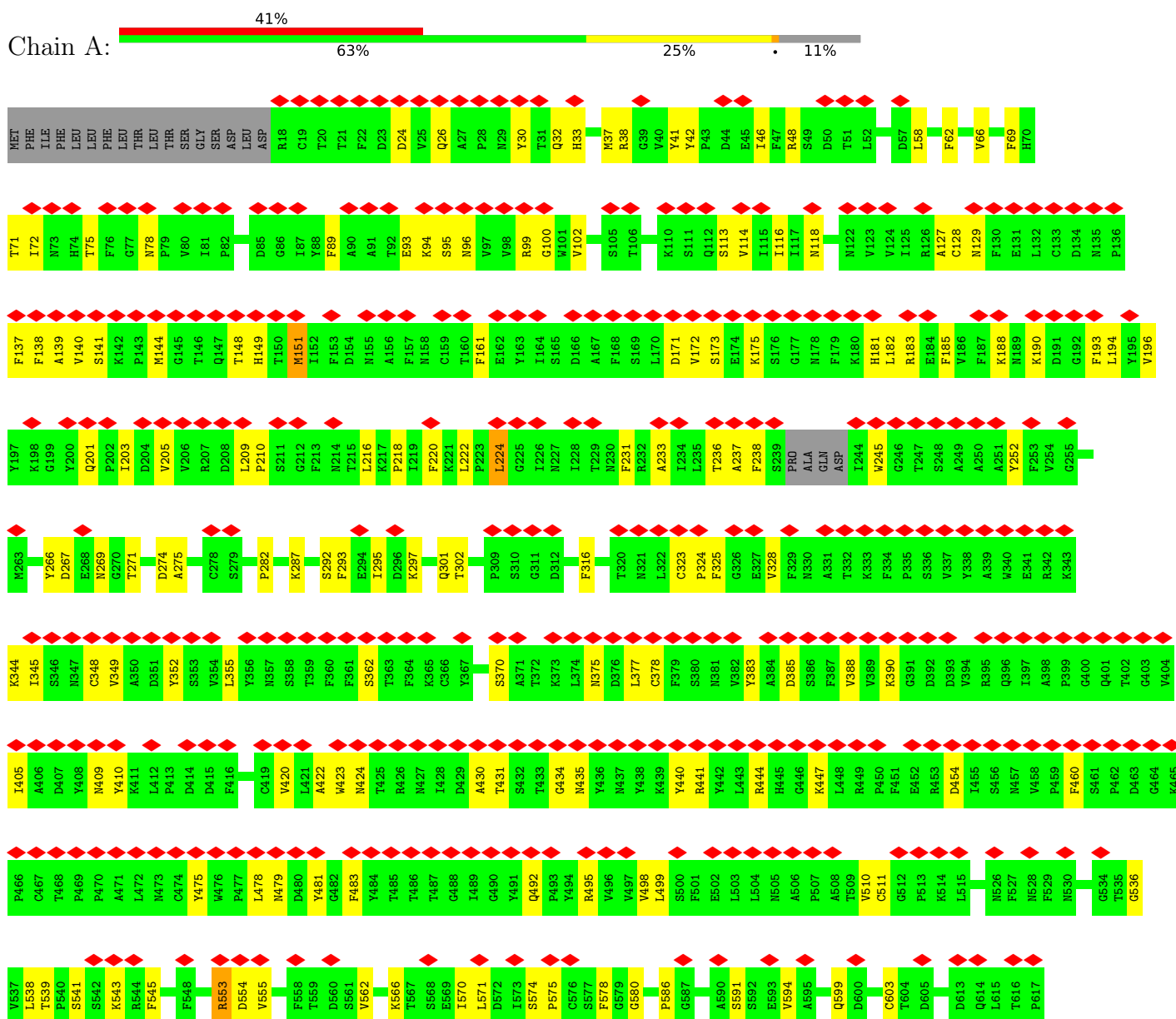
There are 6 discrepancies between the modelled and reference sequences:

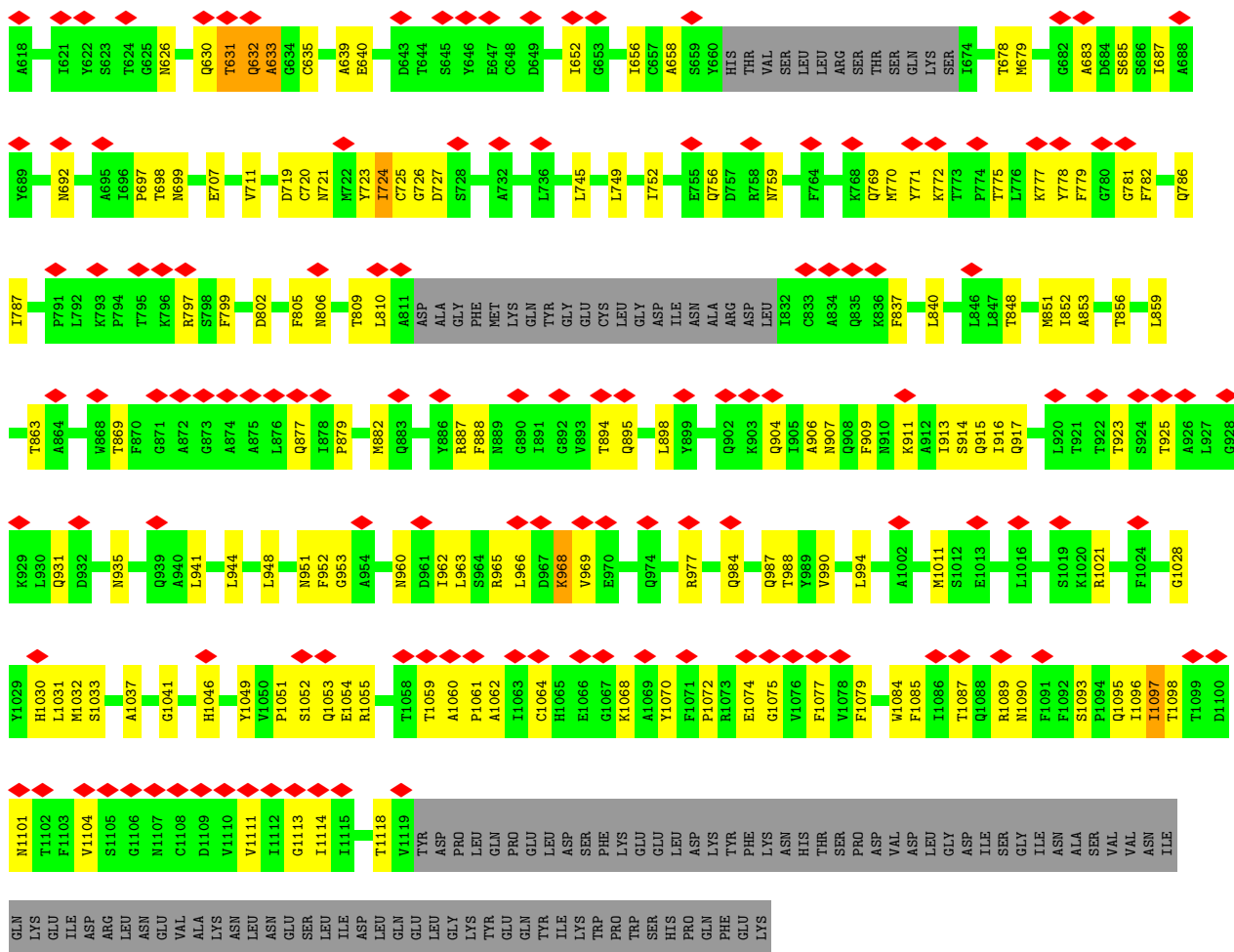
Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1

3 Residue-property plots

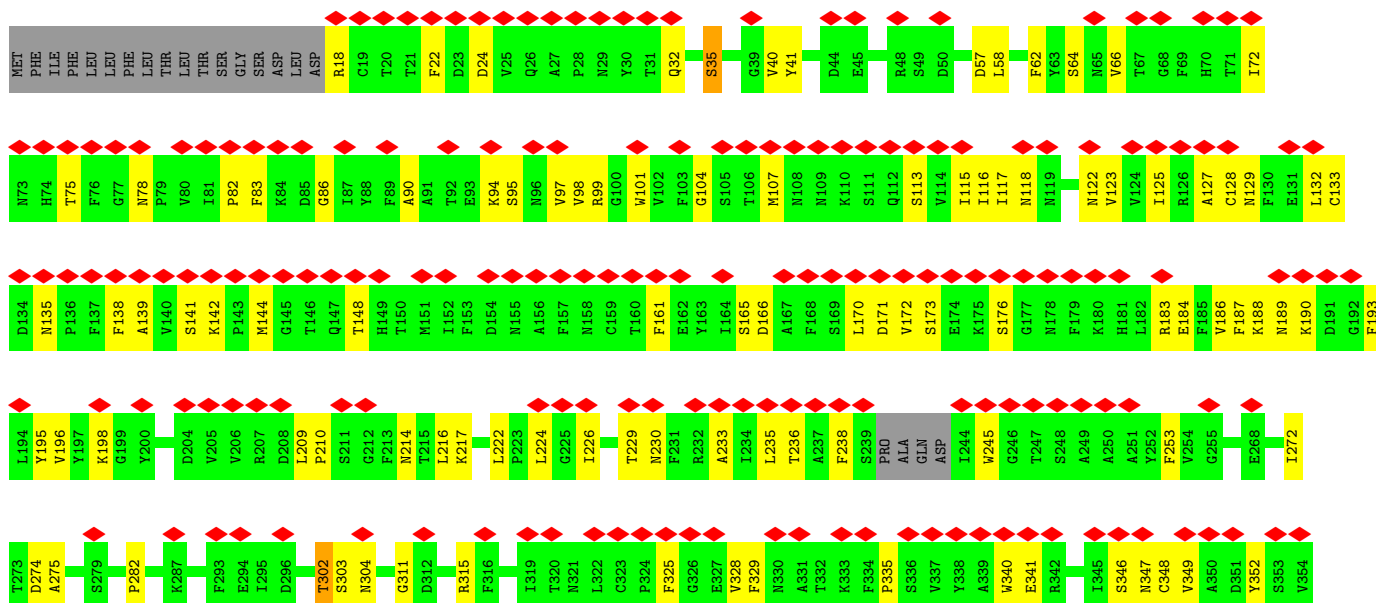
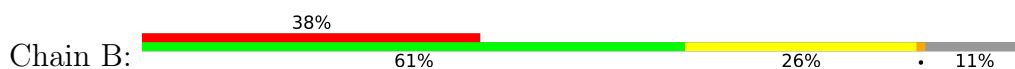
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

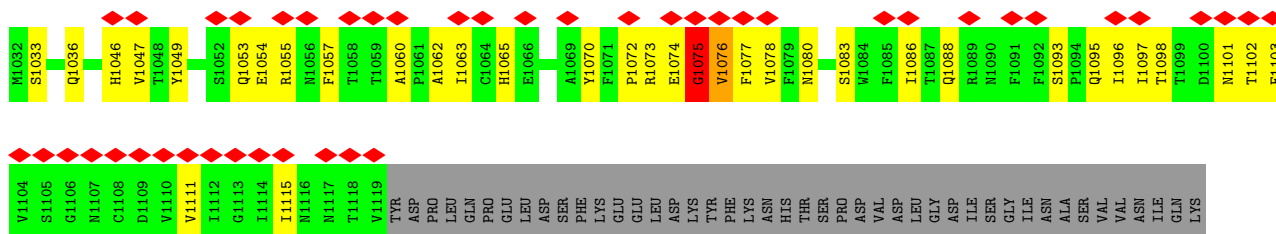




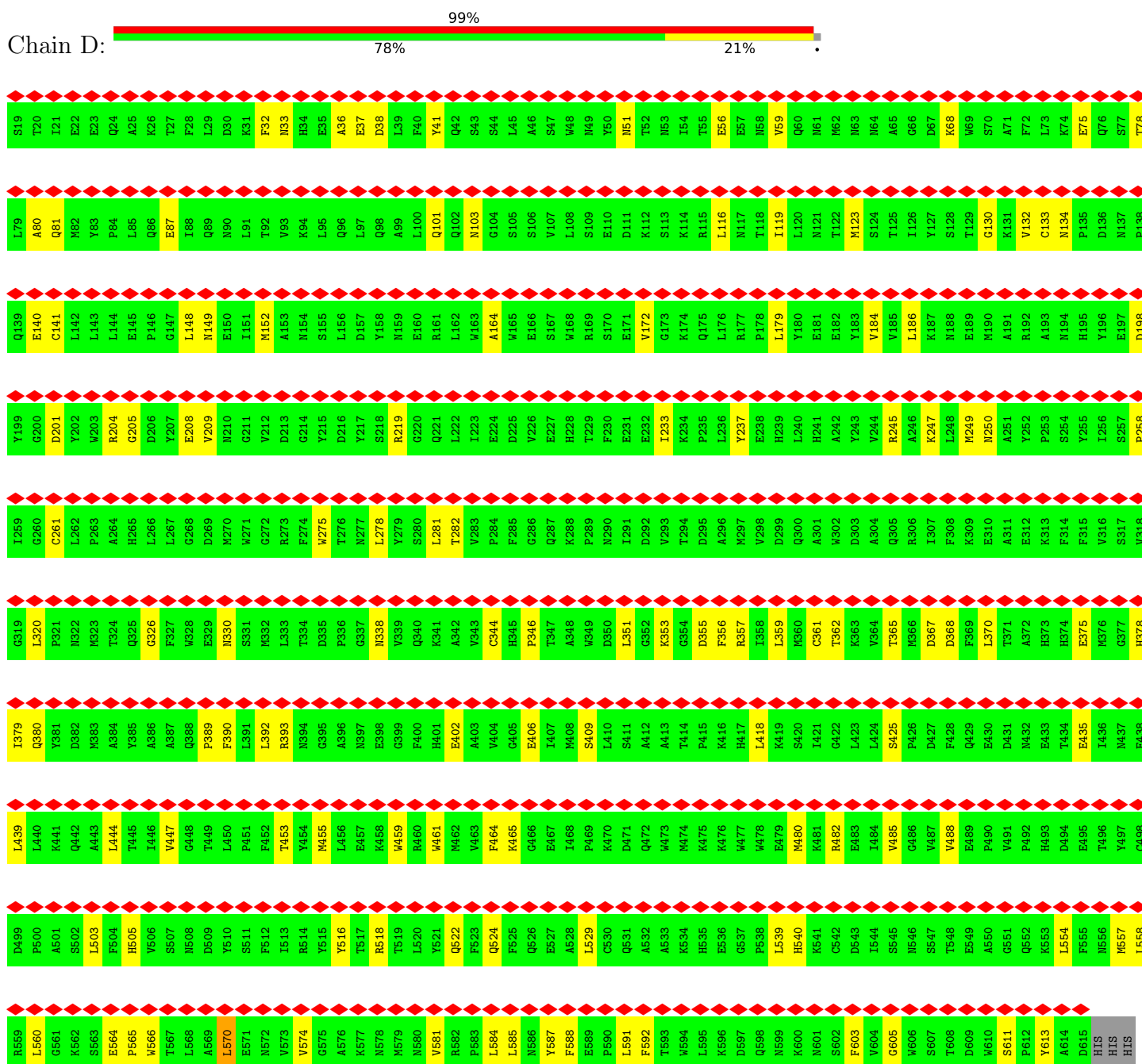
• Molecule 1: Spike glycoprotein



Q939	I852	M770	L519	P459	F399	A339	T261	G192	F130	G68
T943	G862	Y771	D605	F460	G400	V340	Y266	F193	E131	F69
L944	T863	K772	A609	S461	Q401	E341	D267	L194	L132	H70
Q947	T863	T775	D613	P462	T402	R342	E268	Y195	C133	I71
N951	T865	K777	D614	D463	G403	R343	D274	V196	D134	I72
F952	S686	Y778	L615	G464	V404	K344	D274	K198	N135	N73
	S687		T616	K465	T405	I345	D274		P136	H74
S956	G868	G781	P617	P466	A406	S346	D277	Q201	F137	T75
N960	T869	F782	A618	P467	D407	N347	C278	I202	F138	F76
D961	N783	N783	G630	T468	Y408	C348		I203	A139	G77
I962	N691	F784	R620	P469	N409	V349	N281	D204	V140	N78
G872	N692		I621	P470	Y410	A350	P282	V205	S141	F79
G873	T693		G625	A471	K411	D351	L283	V206	K142	V80
G874	I694		V628	L472	L412	Y352	A284	R207	P143	I81
G875	A695		F545	N473	F413	S353	E285	D208	M144	P82
L966	I696		G546	C474	D414	L355	L286	L209	G145	F83
L876	T696		G547	Y475	D415	Y356	K287	P210	T146	K84
L877	F629		F547	Y476	F416	N357	S292	S211	Q147	D85
L878	G630		T631	N477	N417	S358	F293	G212	T148	G86
L879	T632		G549	L478	G418	T359	E294	L216	H149	I87
F880	A633		G550	N479	C419	F360	I295		T150	A90
	E640		F551	D480	V420	F361	D296	K221	M151	A91
Q883	H641		G552	D481	L421	S622		L222	I152	T92
N884	V642		R553	Y481	A422	Y362	Y299	P223	F153	E93
A885	D643		D554	G482	N423	T363	Y300	L224	D154	K94
Y886	T644		V555	F483	Y423	F364	Q302	G225	N155	S95
F888	S645		S556	N424	T425	K365	T301	I226	A156	N96
N889	Y646		D557	T426	R426	C366	N304	N227	F157	V97
G890	E847		F558	T427	N427	Y367	G311	I228	N158	V98
I891	C648		T559	T428	L428	G368	D312	T229	C159	R99
G892	D649		D560	G488	D429	V369	R315	N730	T160	G100
			V562	I489	A430	S370	F316	F231	F161	W101
Q895	L652		R563	G490	A431	A371	P317	R232	E162	V102
L898	G655		D564	Y491	T431	T372	N318	A233	Y163	F103
Y899	T656		T567	Q492	S432	K373	I1E	I234	I164	G104
E900	G657		S568	P493	T433	L374	THR	L235	S165	S105
N901	A658		E569	Y494	G434	N375	ASN	T236	D166	T106
Q902	S659		Y660	R495	N435	D376	LEU	A237	A167	M107
K903	HIS		L571	N496	Y436	L377	C223	F238	F168	M108
Q904	THR		D572	V497	N437	P324	P324	PR0	S169	N109
	D573		I573	V498	Y438	F325	F325	ALA	L170	K110
E1013	VAL		S574	L499	K439	G326	G326	GLN	D171	S111
C1014	SER		P575	S500	Y440	E327	E327	ASP	V172	Q112
	LEU					V328	V328	GLN	S113	Q113
G1017	ARG		F576	F501	R441	N381	N381	I244	V173	V114
S919	SER		D579	E502	Y442	V382	V382	W245	S173	V115
L920	THR		G580	L503	L443	Y383	N330	G246	E174	I115
T921	SER			L504	R444	A384	A331	T247	K175	I116
T922	GLN		S591	N505	H445	D385	T332	S248	S176	I117
T923	LYS		S592	N506	G446	S386	K333	A249	G177	N118
S924	SER		E593	A506	K447	F387	F334	A250	M178	T121
T925	LYS		P507	P507	L448	V388	F335	A251	F179	W122
S926	THR		V675	A508	R449	S387	S336	Y252	K180	W123
A926	SER		V676	T509	P450	V389	V337	F253	H181	V124
	A676		V677	V510	F451	K390	Y338	W254	L182	I125
V934			W602	C511	D452	G391	G255	R183	A127	R126
N937				G512	E452	D392			F187	C128
A938				PRO	R453	D393			K188	N129
				LYS	D454	V394			N189	
				LEU	I455	R395			K190	
				SER	S456	Q396			D191	
				T617	N457	I397				
				D518	V468	A398				



● Molecule 2: Angiotensin-converting enzyme 2



HIS
HIS
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	129462	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	33.479	Depositor
Minimum map value	-16.130	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.871	Depositor
Recommended contour level	8	Depositor
Map size ($\text{\AA}$)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	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	0.46	0/8499	0.81	3/11568 (0.0%)
1	B	0.46	0/8499	0.83	10/11568 (0.1%)
1	C	0.58	11/8435 (0.1%)	0.88	20/11477 (0.2%)
2	D	0.26	0/5007	0.66	5/6803 (0.1%)
All	All	0.47	11/30440 (0.0%)	0.81	38/41416 (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	14
1	B	0	19
1	C	0	21
2	D	0	1
All	All	0	55

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	678	THR	CA-C	-11.37	1.37	1.52
1	C	677	TYR	CA-C	-9.98	1.39	1.52
1	C	676	ALA	C-O	-9.06	1.12	1.24
1	C	642	VAL	N-CA	-8.60	1.35	1.46
1	C	677	TYR	C-O	-7.83	1.14	1.24
1	C	675	VAL	CA-CB	-7.40	1.44	1.54
1	C	642	VAL	CA-CB	-6.78	1.46	1.54
1	C	677	TYR	CA-CB	-6.46	1.42	1.53
1	C	676	ALA	N-CA	5.91	1.53	1.46
1	C	675	VAL	C-O	-5.28	1.17	1.24
1	C	647	GLU	CA-C	-5.15	1.45	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	647	GLU	CA-C-N	-9.37	103.65	121.54
1	C	647	GLU	C-N-CA	-9.37	103.65	121.54
1	C	642	VAL	CB-CA-C	-9.12	97.40	111.26
1	B	891	ILE	N-CA-C	-9.11	104.27	113.47
1	C	641	HIS	O-C-N	8.13	133.67	122.29
1	C	646	TYR	N-CA-C	7.63	127.06	110.80
1	C	675	VAL	CA-C-N	6.86	134.65	121.54
1	C	675	VAL	C-N-CA	6.86	134.65	121.54
1	C	678	THR	CA-C-N	-6.85	108.46	121.54
1	C	678	THR	C-N-CA	-6.85	108.46	121.54
1	C	642	VAL	N-CA-C	-6.76	100.85	109.58
1	B	729	THR	N-CA-C	-6.56	107.14	114.62
2	D	133	CYS	CA-C-N	6.39	129.34	120.65
2	D	133	CYS	C-N-CA	6.39	129.34	120.65
1	C	647	GLU	N-CA-C	-6.13	97.75	110.80
1	C	677	TYR	N-CA-C	6.08	123.74	110.80
1	C	675	VAL	CA-C-O	-5.92	113.38	120.78
1	B	491	TYR	CA-C-N	-5.92	112.53	123.65
1	B	491	TYR	C-N-CA	-5.92	112.53	123.65
1	C	630	GLN	N-CA-C	-5.81	101.81	108.49
1	B	1012	SER	CA-C-N	5.70	128.17	120.65
1	B	1012	SER	C-N-CA	5.70	128.17	120.65
2	D	87	GLU	N-CA-C	-5.62	107.42	114.56
1	A	224	LEU	N-CA-C	5.59	117.24	111.03
1	C	1076	VAL	N-CA-C	5.53	120.85	109.34
1	C	121	THR	N-CA-C	-5.30	107.47	114.31
1	C	1075	GLY	CA-C-N	5.26	131.43	121.97
1	C	1075	GLY	C-N-CA	5.26	131.43	121.97
1	B	553	ARG	N-CA-C	5.22	118.40	111.30
2	D	338	ASN	CA-C-N	5.18	127.28	120.60
2	D	338	ASN	C-N-CA	5.18	127.28	120.60
1	C	646	TYR	CA-C-N	-5.07	111.86	121.54
1	C	646	TYR	C-N-CA	-5.07	111.86	121.54
1	A	787	ILE	CA-C-N	5.05	135.60	120.69
1	A	787	ILE	C-N-CA	5.05	135.60	120.69
1	B	428	ILE	N-CA-C	-5.05	107.88	112.12
1	B	926	ALA	CA-C-N	5.02	129.21	121.53
1	B	926	ALA	C-N-CA	5.02	129.21	121.53

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1052	SER	Peptide
1	A	1074	GLU	Peptide
1	A	1077	PHE	Peptide
1	A	151	MET	Peptide
1	A	553	ARG	Peptide
1	A	62	PHE	Peptide
1	A	631	THR	Peptide
1	A	633	ALA	Peptide
1	A	724	ILE	Peptide
1	A	725	CYS	Peptide
1	A	726	GLY	Peptide
1	A	727	ASP	Peptide
1	A	923	THR	Peptide
1	A	968	LYS	Peptide
1	B	1052	SER	Peptide
1	B	1074	GLU	Peptide
1	B	1075	GLY	Peptide
1	B	35	SER	Peptide
1	B	507	PRO	Peptide
1	B	553	ARG	Peptide
1	B	558	PHE	Peptide
1	B	576	CYS	Peptide
1	B	62	PHE	Peptide
1	B	629	PHE	Peptide
1	B	631	THR	Peptide
1	B	722	MET	Peptide
1	B	724	ILE	Peptide
1	B	726	GLY	Peptide
1	B	727	ASP	Peptide
1	B	776	LEU	Peptide
1	B	781	GLY	Peptide
1	B	837	PHE	Peptide
1	B	968	LYS	Peptide
1	C	1073	ARG	Peptide
1	C	1074	GLU	Peptide
1	C	1075	GLY	Peptide
1	C	1077	PHE	Peptide
1	C	151	MET	Peptide
1	C	206	VAL	Peptide
1	C	292	SER	Peptide
1	C	316	PHE	Peptide
1	C	347	ASN	Peptide
1	C	35	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	465	LYS	Peptide
1	C	511	CYS	Peptide
1	C	527	PHE	Peptide
1	C	54	LEU	Peptide
1	C	548	PHE	Peptide
1	C	567	THR	Peptide
1	C	573	ILE	Peptide
1	C	837	PHE	Peptide
1	C	865	THR	Peptide
1	C	95	SER	Peptide
1	C	97	VAL	Peptide
2	D	425	SER	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	8302	0	8082	205	0
1	B	8302	0	8082	215	0
1	C	8241	0	8011	260	0
2	D	4870	0	4643	78	0
All	All	29715	0	28818	711	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (711) 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:C:646:TYR:HB2	1:C:677:TYR:CE2	1.33	1.59
1:C:646:TYR:CB	1:C:677:TYR:CE2	1.90	1.53
1:C:647:GLU:O	1:C:648:CYS:CB	1.77	1.26
1:C:646:TYR:HB2	1:C:677:TYR:CD2	1.78	1.17
1:C:646:TYR:CA	1:C:677:TYR:CE2	2.28	1.16
1:C:646:TYR:CB	1:C:677:TYR:CZ	2.29	1.15
1:C:646:TYR:CA	1:C:677:TYR:HE2	1.57	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:TYR:HB2	1:C:677:TYR:CZ	1.85	1.12
1:C:678:THR:O	1:C:679:MET:HB2	1.40	1.08
1:C:647:GLU:O	1:C:648:CYS:HB3	1.49	1.07
1:C:647:GLU:OE1	1:C:680:SER:OG	1.73	1.06
1:C:656:ILE:HG12	1:C:677:TYR:O	1.57	1.04
1:C:655:GLY:O	1:C:678:THR:O	1.83	0.97
1:C:646:TYR:N	1:C:677:TYR:CE2	2.34	0.95
1:C:646:TYR:HB3	1:C:677:TYR:CZ	1.98	0.95
1:C:647:GLU:O	1:C:648:CYS:HB2	1.67	0.94
1:C:640:GLU:O	1:C:642:VAL:HG23	1.68	0.92
1:C:678:THR:O	1:C:679:MET:CB	2.16	0.92
1:C:678:THR:OG1	1:C:679:MET:N	2.03	0.87
2:D:346:PRO:HA	2:D:359:LEU:O	1.75	0.87
1:C:93:GLU:O	1:C:181:HIS:HB2	1.77	0.84
1:C:18:ARG:N	1:C:133:CYS:HG	1.77	0.83
1:A:190:LYS:O	1:A:193:PHE:HB2	1.80	0.81
1:C:646:TYR:N	1:C:677:TYR:CD2	2.49	0.81
1:B:113:SER:O	1:B:127:ALA:HA	1.81	0.80
1:C:647:GLU:N	1:C:677:TYR:OH	2.15	0.79
1:B:115:ILE:O	1:B:125:ILE:HA	1.82	0.79
1:B:190:LYS:O	1:B:193:PHE:HB2	1.82	0.79
1:C:418:GLY:HA3	1:C:499:LEU:O	1.84	0.78
1:C:1088:GLN:HE22	1:C:1093:SER:HB2	1.48	0.78
1:C:646:TYR:N	1:C:677:TYR:HE2	1.78	0.77
1:A:913:ILE:O	1:A:916:ILE:HB	1.85	0.77
1:B:909:PHE:O	1:B:912:ALA:HB3	1.85	0.77
2:D:566:TRP:O	2:D:570:LEU:HB2	1.85	0.76
1:C:564:ASP:HB3	1:C:568:SER:H	1.50	0.76
1:B:118:ASN:HB3	1:B:170:LEU:HD21	1.68	0.75
1:C:646:TYR:HB3	1:C:677:TYR:OH	1.87	0.74
1:C:646:TYR:O	1:C:647:GLU:CG	2.36	0.73
1:C:648:CYS:N	1:C:677:TYR:OH	2.22	0.73
1:A:100:GLY:HA2	1:A:116:ILE:O	1.89	0.72
1:C:647:GLU:OE1	1:C:647:GLU:HA	1.90	0.71
1:C:677:TYR:HD1	1:C:677:TYR:H	1.38	0.71
1:C:713:MET:HG2	1:C:756:GLN:HE22	1.55	0.70
1:A:348:CYS:SG	1:A:349:VAL:N	2.64	0.69
1:A:895:GLN:HG3	1:B:1074:GLU:HG2	1.75	0.69
1:A:906:ALA:O	1:A:909:PHE:HB3	1.92	0.69
1:A:94:LYS:HB3	1:A:175:LYS:HB2	1.76	0.68
1:C:422:ALA:HA	1:C:495:ARG:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:835:GLN:NE2	1:C:575:PRO:O	2.26	0.68
1:C:1030:HIS:HE1	1:C:1033:SER:HB2	1.58	0.68
1:A:128:CYS:SG	1:A:129:ASN:N	2.67	0.67
1:C:707:GLU:OE1	1:C:1046:HIS:NE2	2.28	0.67
1:C:299:ILE:HD11	1:C:652:ILE:HG12	1.77	0.67
1:A:837:PHE:HB3	1:B:575:PRO:HD3	1.77	0.66
1:B:99:ARG:HH22	1:B:172:VAL:HA	1.60	0.66
1:A:1064:CYS:HB3	1:A:1114:ILE:HG23	1.77	0.66
1:B:18:ARG:N	1:B:133:CYS:HG	1.93	0.65
1:A:1061:PRO:HD2	1:A:1113:GLY:H	1.61	0.65
1:A:707:GLU:OE1	1:A:1046:HIS:NE2	2.29	0.65
1:A:149:HIS:NE2	1:A:151:MET:SD	2.69	0.65
1:C:1063:ILE:HB	1:C:1070:TYR:HB2	1.79	0.64
1:A:960:ASN:H	1:A:963:LEU:HD13	1.62	0.64
1:C:656:ILE:CG1	1:C:677:TYR:O	2.39	0.64
1:B:340:TRP:O	1:B:453:ARG:NH1	2.31	0.64
1:C:722:MET:HA	1:C:726:GLY:HA2	1.80	0.64
1:A:58:LEU:HB2	1:A:188:LYS:HE3	1.80	0.64
1:A:1096:ILE:O	1:A:1101:ASN:ND2	2.30	0.64
1:C:887:ARG:NH1	1:C:1031:LEU:O	2.29	0.63
2:D:406:GLU:HG3	2:D:518:ARG:HD3	1.80	0.63
1:B:1059:THR:O	1:B:1080:ASN:ND2	2.31	0.63
1:C:347:ASN:H	1:C:509:THR:HB	1.62	0.63
1:C:1062:ALA:HB3	1:C:1111:VAL:HG13	1.81	0.63
1:A:887:ARG:NH1	1:A:1031:LEU:O	2.29	0.63
1:A:325:PHE:HA	1:A:328:VAL:HG12	1.80	0.63
1:A:1097:ILE:HD13	1:A:1118:THR:HA	1.81	0.63
1:B:107:MET:HA	1:B:132:LEU:HD12	1.80	0.62
1:B:348:CYS:SG	1:B:349:VAL:N	2.71	0.62
1:C:385:ASP:O	1:C:497:VAL:HA	1.98	0.62
1:A:869:THR:OG1	1:B:1089:ARG:NH1	2.32	0.62
1:A:632:GLN:NE2	1:C:833:CYS:SG	2.69	0.62
1:A:536:GLY:HA3	1:A:574:SER:HA	1.80	0.62
1:A:786:GLN:HB3	1:A:799:PHE:HB3	1.81	0.62
1:A:41:TYR:OH	1:A:188:LYS:NZ	2.29	0.62
1:C:704:ILE:HG12	1:C:1047:VAL:HG22	1.82	0.62
1:B:707:GLU:OE1	1:B:1046:HIS:NE2	2.33	0.62
1:C:1096:ILE:O	1:C:1101:ASN:ND2	2.27	0.62
1:C:361:PHE:HA	1:C:423:TRP:HB3	1.83	0.61
1:B:127:ALA:HB3	1:B:161:PHE:HB3	1.82	0.61
1:B:652:ILE:HD11	1:B:658:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:TYR:HB3	1:C:677:TYR:CE2	2.12	0.61
1:B:101:TRP:HB2	1:B:116:ILE:HB	1.82	0.61
1:A:96:ASN:OD1	1:A:183:ARG:NH1	2.34	0.60
1:A:779:PHE:HB2	1:A:782:PHE:HB2	1.82	0.60
1:B:541:SER:HA	1:B:571:LEU:HG	1.83	0.60
1:A:139:ALA:HB3	1:A:148:THR:HB	1.83	0.60
1:C:363:THR:HB	1:C:422:ALA:HB3	1.83	0.60
1:B:94:LYS:HD2	1:B:176:SER:HA	1.82	0.60
1:B:484:TYR:HB2	1:B:487:THR:HB	1.83	0.60
1:A:182:LEU:HD23	1:A:201:GLN:HB3	1.82	0.60
1:A:1030:HIS:HE1	1:A:1033:SER:HB2	1.67	0.60
1:A:1097:ILE:HB	1:A:1118:THR:HG23	1.83	0.60
1:B:835:GLN:NE2	1:C:573:ILE:O	2.35	0.60
1:B:302:THR:HG23	1:B:581:VAL:HG23	1.82	0.60
1:C:524:CYS:HA	1:C:536:GLY:O	2.02	0.60
1:C:646:TYR:O	1:C:647:GLU:OE1	2.20	0.60
1:A:756:GLN:HA	1:A:759:ASN:HD22	1.67	0.60
1:C:656:ILE:HG13	1:C:678:THR:HA	1.82	0.60
1:A:378:CYS:HA	1:A:511:CYS:HA	1.83	0.59
1:B:385:ASP:HB2	1:B:498:VAL:HB	1.84	0.59
1:A:575:PRO:HD3	1:C:837:PHE:HB3	1.84	0.59
1:B:745:LEU:HD22	1:B:990:VAL:HG21	1.82	0.59
1:A:553:ARG:HE	1:C:46:ILE:HD13	1.67	0.59
1:A:435:ASN:HB3	1:A:483:PHE:HB2	1.84	0.59
1:B:315:ARG:NH1	1:B:517:THR:O	2.34	0.59
1:B:41:TYR:HB3	1:B:216:LEU:HD12	1.85	0.58
1:A:1054:GLU:O	1:A:1055:ARG:NH1	2.35	0.58
1:A:541:SER:HB3	1:A:543:LYS:HG2	1.84	0.58
1:B:209:LEU:HB2	1:B:253:PHE:HE2	1.69	0.58
1:B:913:ILE:O	1:B:916:ILE:HB	2.03	0.58
1:A:95:SER:HB3	1:A:175:LYS:HE3	1.86	0.58
1:A:138:PHE:HB2	1:A:236:THR:HA	1.85	0.58
1:A:316:PHE:O	1:A:566:LYS:NZ	2.36	0.58
1:A:887:ARG:NH1	1:A:1032:MET:SD	2.77	0.58
1:A:30:TYR:O	1:A:32:GLN:NE2	2.34	0.58
1:B:117:ILE:O	1:B:123:VAL:HA	2.03	0.58
1:A:626:ASN:ND2	1:A:640:GLU:OE2	2.35	0.58
1:C:686:SER:OG	1:C:687:ILE:N	2.31	0.58
1:C:398:ALA:HB3	1:C:401:GLN:HG3	1.85	0.58
1:A:325:PHE:HE1	1:A:345:ILE:HD13	1.67	0.57
1:C:281:ASN:H	1:C:284:ALA:HB3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ASN:H	1:C:509:THR:HG1	1.50	0.57
1:B:1064:CYS:HB3	1:B:1114:ILE:HG23	1.86	0.57
1:B:282:PRO:HB2	1:B:594:VAL:HG21	1.86	0.57
1:B:887:ARG:NH1	1:B:1031:LEU:O	2.36	0.57
1:C:124:VAL:HG22	1:C:164:ILE:HG12	1.85	0.57
1:C:646:TYR:O	1:C:647:GLU:HG2	2.03	0.57
1:C:677:TYR:N	1:C:677:TYR:CD1	2.70	0.57
1:C:25:VAL:HA	1:C:76:PHE:HB3	1.85	0.57
1:A:196:VAL:HB	1:A:220:PHE:HB2	1.87	0.57
1:B:777:LYS:NZ	1:B:789:PRO:O	2.37	0.57
1:A:99:ARG:HD3	1:A:118:ASN:HB2	1.85	0.57
2:D:132:VAL:O	2:D:141:CYS:HA	2.05	0.57
1:C:383:TYR:HB2	1:C:500:SER:HB2	1.86	0.57
1:B:755:GLU:OE1	1:B:1001:ARG:NH2	2.38	0.57
1:B:756:GLN:HA	1:B:759:ASN:HD22	1.69	0.57
1:C:58:LEU:HB2	1:C:188:LYS:HE3	1.86	0.57
1:C:1029:TYR:HB2	1:C:1049:TYR:HB3	1.85	0.57
1:A:711:VAL:HG22	1:A:1041:GLY:HA2	1.87	0.56
1:B:424:ASN:ND2	1:B:492:GLN:OE1	2.38	0.56
1:B:1060:ALA:HB2	1:B:1080:ASN:HD22	1.69	0.56
1:C:390:LYS:HE3	1:C:392:ASP:HB2	1.87	0.56
2:D:237:TYR:OH	2:D:485:VAL:O	2.20	0.56
1:B:128:CYS:SG	1:B:129:ASN:N	2.77	0.56
1:C:644:THR:HG22	1:C:644:THR:O	2.05	0.56
1:C:1054:GLU:O	1:C:1055:ARG:NH1	2.37	0.56
2:D:245:ARG:NH2	2:D:605:GLY:O	2.36	0.56
2:D:278:LEU:O	2:D:282:THR:N	2.38	0.56
2:D:389:PRO:HG2	2:D:392:LEU:HB2	1.88	0.56
1:B:563:ARG:HG3	1:B:569:GLU:HG3	1.86	0.56
1:B:184:GLU:OE1	1:B:214:ASN:ND2	2.34	0.56
1:C:405:ILE:HG23	1:C:409:ASN:HD22	1.70	0.56
1:B:740:SER:OG	1:C:947:GLN:NE2	2.39	0.56
1:B:1030:HIS:CE1	1:B:1033:SER:HB2	2.41	0.56
1:B:1086:ILE:O	1:B:1095:GLN:NE2	2.38	0.56
1:C:642:VAL:HG21	1:C:675:VAL:CB	2.35	0.56
1:B:720:CYS:SG	1:B:721:ASN:N	2.78	0.56
2:D:51:ASN:HB3	2:D:359:LEU:HG	1.87	0.56
1:A:720:CYS:SG	1:A:721:ASN:N	2.79	0.56
1:C:128:CYS:SG	1:C:129:ASN:N	2.79	0.56
1:B:536:GLY:HA3	1:B:574:SER:HA	1.87	0.55
1:B:719:ASP:OD1	1:C:304:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:GLN:NE2	1:B:988:THR:OG1	2.39	0.55
1:B:423:TRP:O	1:B:494:TYR:HA	2.07	0.55
1:A:440:TYR:O	1:A:478:LEU:HA	2.05	0.55
1:C:642:VAL:HG21	1:C:675:VAL:HB	1.87	0.55
1:A:745:LEU:HD22	1:A:990:VAL:HG21	1.87	0.55
1:A:769:GLN:HE21	1:B:685:SER:HB2	1.71	0.55
1:A:1098:THR:OG1	1:A:1101:ASN:ND2	2.40	0.55
1:B:698:THR:OG1	1:B:1053:GLN:OE1	2.23	0.55
2:D:402:GLU:HG3	2:D:518:ARG:HG3	1.88	0.55
1:A:631:THR:O	1:A:633:ALA:N	2.40	0.55
1:A:699:ASN:H	1:A:1053:GLN:HB2	1.72	0.55
1:B:32:GLN:HA	1:B:66:VAL:O	2.07	0.55
1:B:99:ARG:HH12	1:B:172:VAL:HG13	1.71	0.55
1:B:959:LEU:HD23	1:B:962:ILE:HD11	1.89	0.54
1:C:188:LYS:HB3	1:C:195:TYR:HB2	1.88	0.54
1:C:380:SER:HA	1:C:509:THR:H	1.71	0.54
1:B:866:ALA:HB2	1:C:689:TYR:HE1	1.72	0.54
1:A:1062:ALA:HB3	1:A:1111:VAL:HG13	1.89	0.54
1:A:1064:CYS:HB2	1:A:1111:VAL:HG11	1.88	0.54
1:B:186:VAL:O	1:B:196:VAL:HA	2.07	0.54
1:C:394:VAL:HG21	1:C:494:TYR:HD2	1.72	0.54
1:C:648:CYS:H	1:C:677:TYR:HH	1.53	0.54
2:D:524:GLN:HB3	2:D:574:VAL:HG11	1.90	0.54
1:B:879:PRO:HB3	1:C:691:ASN:HA	1.88	0.54
1:C:362:SER:N	1:C:422:ALA:O	2.37	0.54
1:B:1093:SER:O	1:B:1095:GLN:NE2	2.40	0.54
1:A:441:ARG:NH1	1:A:454:ASP:O	2.41	0.54
1:A:953:GLY:O	1:A:977:ARG:NH1	2.39	0.54
1:C:141:SER:HB3	1:C:145:GLY:H	1.72	0.54
1:C:646:TYR:O	1:C:680:SER:OG	2.26	0.54
1:C:698:THR:OG1	1:C:1055:ARG:NH2	2.41	0.54
1:B:99:ARG:NH2	1:B:171:ASP:O	2.41	0.54
1:B:325:PHE:HA	1:B:328:VAL:HG12	1.89	0.54
1:B:378:CYS:HA	1:B:511:CYS:HA	1.90	0.54
1:B:90:ALA:HA	1:B:183:ARG:O	2.08	0.54
1:C:960:ASN:H	1:C:963:LEU:HD13	1.73	0.54
1:B:524:CYS:HA	1:B:536:GLY:O	2.08	0.54
1:A:113:SER:O	1:A:127:ALA:HA	2.08	0.53
1:A:652:ILE:HD11	1:A:658:ALA:HB2	1.89	0.53
1:B:1005:ASN:O	1:B:1009:THR:OG1	2.23	0.53
1:A:888:PHE:HE2	1:A:898:LEU:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ARG:HG3	1:C:477:PRO:HB2	1.91	0.53
2:D:119:ILE:HD12	2:D:179:LEU:HD22	1.88	0.53
1:A:323:CYS:N	1:A:348:CYS:SG	2.82	0.53
1:A:420:VAL:HG22	1:A:498:VAL:HG22	1.90	0.53
2:D:378:HIS:HE1	2:D:402:GLU:HA	1.73	0.53
1:A:749:LEU:HD23	1:A:752:ILE:HD12	1.91	0.53
1:B:905:ILE:O	1:B:909:PHE:N	2.38	0.53
1:C:90:ALA:HB3	1:C:253:PHE:HB2	1.90	0.53
1:C:411:LYS:HB2	1:C:448:LEU:HB2	1.90	0.53
1:C:934:VAL:HA	1:C:937:ASN:HD22	1.74	0.53
1:A:431:THR:OG1	1:A:434:GLY:O	2.26	0.53
1:B:392:ASP:OD1	1:B:395:ARG:NH2	2.41	0.53
1:B:960:ASN:HA	1:B:963:LEU:HB2	1.90	0.53
1:B:1063:ILE:HD11	1:B:1078:VAL:HG11	1.91	0.53
1:B:1097:ILE:HD13	1:B:1118:THR:HA	1.91	0.53
1:C:538:LEU:HD22	1:C:570:ILE:HD12	1.90	0.53
1:C:100:GLY:HA3	1:C:234:ILE:HB	1.89	0.53
1:C:283:LEU:HD22	1:C:592:SER:HB2	1.89	0.53
2:D:75:GLU:O	2:D:78:THR:OG1	2.26	0.53
2:D:119:ILE:HG22	2:D:123:MET:HE2	1.89	0.53
2:D:439:LEU:HB3	2:D:591:LEU:HD22	1.91	0.53
1:A:1079:PHE:HB2	1:A:1087:THR:HG23	1.91	0.53
1:B:78:ASN:ND2	1:B:233:ALA:O	2.36	0.53
1:B:377:LEU:HD22	1:B:531:GLY:HA2	1.89	0.53
1:C:337:VAL:HG22	1:C:389:VAL:HG12	1.91	0.53
1:B:626:ASN:ND2	1:B:639:ALA:O	2.42	0.52
1:C:432:SER:HA	1:C:484:TYR:HB3	1.91	0.52
1:C:646:TYR:O	1:C:647:GLU:CB	2.53	0.52
1:C:646:TYR:O	1:C:647:GLU:CD	2.53	0.52
1:C:1078:VAL:HG22	1:C:1086:ILE:HG12	1.91	0.52
1:A:1051:PRO:HB3	1:A:1090:ASN:HD21	1.74	0.52
1:C:99:ARG:HE	1:C:118:ASN:HD22	1.58	0.52
2:D:233:ILE:HD11	2:D:581:VAL:HG21	1.91	0.52
1:A:543:LYS:HB3	1:A:545:PHE:HB2	1.91	0.52
1:B:444:ARG:NH1	1:B:447:LYS:O	2.42	0.52
2:D:351:LEU:HB2	2:D:355:ASP:O	2.09	0.52
1:A:352:TYR:HD1	1:A:355:LEU:HD12	1.74	0.52
1:B:99:ARG:HE	1:B:118:ASN:HD22	1.58	0.52
2:D:37:GLU:OE1	2:D:393:ARG:NH1	2.43	0.52
1:C:101:TRP:HB2	1:C:116:ILE:HB	1.91	0.52
1:C:486:THR:O	2:D:330:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:ASN:ND2	2:D:140:GLU:OE1	2.43	0.52
1:A:538:LEU:HD22	1:A:570:ILE:HD12	1.91	0.52
1:A:769:GLN:NE2	1:B:683:ALA:O	2.42	0.52
1:C:41:TYR:OH	1:C:188:LYS:NZ	2.43	0.52
1:B:302:THR:OG1	1:B:303:SER:N	2.43	0.52
1:C:473:ASN:ND2	1:C:475:TYR:OH	2.42	0.52
1:C:646:TYR:C	1:C:680:SER:OG	2.53	0.52
1:A:370:SER:OG	1:C:965:ARG:O	2.28	0.52
1:A:430:ALA:HA	1:A:435:ASN:HB2	1.92	0.52
1:B:35:SER:OG	1:B:64:SER:N	2.42	0.52
1:C:99:ARG:HD2	1:C:147:GLN:HE22	1.74	0.52
1:C:193:PHE:HA	1:C:222:LEU:O	2.10	0.52
1:B:397:ILE:HG23	1:B:412:LEU:HD11	1.92	0.51
1:C:292:SER:OG	1:C:293:PHE:N	2.43	0.51
1:A:301:GLN:NE2	1:A:302:THR:O	2.43	0.51
1:A:771:TYR:HD1	1:B:687:ILE:HG12	1.74	0.51
1:B:987:GLN:NE2	1:C:988:THR:OG1	2.42	0.51
1:C:238:PHE:HB2	1:C:246:GLY:H	1.74	0.51
1:C:436:TYR:OH	2:D:38:ASP:OD1	2.25	0.51
1:A:1093:SER:O	1:A:1095:GLN:NE2	2.42	0.51
1:B:439:LYS:HD3	1:B:478:LEU:HB3	1.92	0.51
1:B:539:THR:HG23	1:B:571:LEU:HB2	1.91	0.51
1:C:302:THR:OG1	1:C:303:SER:N	2.42	0.51
1:B:116:ILE:HG13	1:B:125:ILE:HG12	1.92	0.51
1:B:303:SER:OG	1:B:304:ASN:N	2.43	0.51
1:C:646:TYR:H	1:C:677:TYR:HD2	1.51	0.51
2:D:208:GLU:OE2	2:D:219:ARG:NH1	2.44	0.51
1:A:988:THR:OG1	1:C:987:GLN:NE2	2.43	0.51
1:C:645:SER:HB3	1:C:680:SER:N	2.26	0.51
1:C:755:GLU:OE1	1:C:1001:ARG:NH2	2.44	0.51
2:D:148:LEU:HG	2:D:164:ALA:HB1	1.93	0.51
1:B:956:SER:OG	1:B:957:SER:N	2.41	0.51
1:C:440:TYR:O	1:C:478:LEU:HA	2.11	0.51
1:C:1063:ILE:H	1:C:1070:TYR:H	1.59	0.51
1:A:69:PHE:HB2	1:A:252:TYR:O	2.11	0.51
1:B:1063:ILE:HB	1:B:1070:TYR:HB2	1.91	0.51
1:A:26:GLN:HB2	1:A:75:THR:HA	1.93	0.50
1:C:138:PHE:HB2	1:C:236:THR:HG22	1.92	0.50
1:C:419:CYS:HB2	1:C:499:LEU:HD12	1.91	0.50
1:C:1086:ILE:O	1:C:1095:GLN:NE2	2.44	0.50
2:D:554:LEU:O	2:D:558:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:ND2	1:A:233:ALA:O	2.42	0.50
1:A:580:GLY:H	1:A:599:GLN:HB2	1.76	0.50
1:B:562:VAL:HG23	1:B:570:ILE:HG13	1.92	0.50
1:C:777:LYS:NZ	1:C:789:PRO:O	2.44	0.50
1:C:968:LYS:O	1:C:971:ALA:N	2.39	0.50
1:A:267:ASP:OD1	1:A:271:THR:N	2.40	0.50
1:B:1030:HIS:HE1	1:B:1033:SER:HB2	1.76	0.50
2:D:330:ASN:HB3	2:D:357:ARG:HE	1.76	0.50
1:A:1089:ARG:NH1	1:C:869:THR:OG1	2.44	0.50
1:C:174:GLU:HG3	1:C:248:SER:HB3	1.93	0.50
2:D:245:ARG:NH1	2:D:603:PHE:O	2.44	0.50
1:A:33:HIS:HB2	1:A:66:VAL:HB	1.93	0.50
1:C:1031:LEU:N	1:C:1047:VAL:O	2.45	0.50
1:C:1083:SER:HB3	1:C:1115:ILE:HG23	1.94	0.50
2:D:80:ALA:O	2:D:101:GLN:NE2	2.38	0.50
2:D:529:LEU:HD21	2:D:554:LEU:HD22	1.93	0.50
1:B:165:SER:OG	1:B:166:ASP:N	2.45	0.50
1:B:694:ILE:O	1:B:1057:PHE:N	2.39	0.50
1:C:591:SER:OG	1:C:592:SER:N	2.45	0.50
1:A:89:PHE:HB3	1:A:185:PHE:O	2.12	0.50
1:A:99:ARG:NH2	1:A:171:ASP:O	2.44	0.50
1:A:848:THR:O	1:A:852:ILE:N	2.36	0.50
1:C:190:LYS:O	1:C:193:PHE:HB2	2.12	0.50
1:C:380:SER:HB2	1:C:508:ALA:HA	1.94	0.50
1:C:723:TYR:OH	1:C:944:LEU:O	2.29	0.49
1:A:656:ILE:HA	1:A:678:THR:HA	1.94	0.49
1:A:685:SER:HB2	1:C:769:GLN:HE21	1.76	0.49
1:B:612:ALA:O	1:B:614:GLN:NE2	2.41	0.49
1:B:803:LEU:HD13	1:B:921:THR:HG22	1.93	0.49
1:C:646:TYR:C	1:C:677:TYR:HE2	2.17	0.49
1:B:962:ILE:HG13	1:B:963:LEU:HD12	1.94	0.49
1:C:145:GLY:HA3	1:C:173:SER:HB3	1.94	0.49
1:C:887:ARG:NH2	1:C:1017:GLY:O	2.45	0.49
2:D:275:TRP:HB3	2:D:444:LEU:HD12	1.94	0.49
1:C:527:PHE:HE1	1:C:538:LEU:HD11	1.77	0.49
1:A:362:SER:N	1:A:422:ALA:O	2.44	0.49
1:B:125:ILE:HD13	1:B:222:LEU:HD11	1.93	0.49
1:B:529:PHE:HE2	1:B:562:VAL:HG21	1.78	0.49
1:B:1031:LEU:N	1:B:1047:VAL:O	2.46	0.49
1:C:640:GLU:O	1:C:642:VAL:CG2	2.52	0.49
2:D:356:PHE:HB3	2:D:379:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ALA:HB3	1:A:161:PHE:HB3	1.93	0.49
1:B:962:ILE:O	1:B:966:LEU:N	2.46	0.49
1:A:140:VAL:O	1:A:238:PHE:HA	2.13	0.49
1:B:960:ASN:O	1:B:964:SER:N	2.41	0.49
1:C:103:PHE:CD1	1:C:231:PHE:HB2	2.48	0.49
1:C:580:GLY:H	1:C:599:GLN:HB2	1.78	0.49
1:C:775:THR:HA	1:C:777:LYS:HE3	1.94	0.49
2:D:281:LEU:HD12	2:D:282:THR:HG23	1.94	0.49
2:D:435:GLU:OE2	2:D:540:HIS:NE2	2.46	0.49
1:B:609:ALA:HA	1:B:614:GLN:HB2	1.94	0.49
1:C:99:ARG:HE	1:C:118:ASN:HB2	1.77	0.49
1:B:903:LYS:O	1:B:906:ALA:HB3	2.13	0.49
1:C:285:GLU:OE2	1:C:302:THR:OG1	2.31	0.49
1:C:381:ASN:N	1:C:509:THR:HG1	2.11	0.49
1:A:405:ILE:O	1:A:409:ASN:N	2.46	0.48
1:B:859:LEU:O	1:B:863:THR:OG1	2.21	0.48
2:D:588:PHE:O	2:D:592:PHE:N	2.46	0.48
1:A:292:SER:OG	1:A:293:PHE:N	2.45	0.48
1:A:882:MET:HE3	1:B:1076:VAL:HB	1.94	0.48
1:A:960:ASN:HA	1:A:963:LEU:HD22	1.95	0.48
1:A:352:TYR:HD2	1:A:375:ASN:HB3	1.78	0.48
1:A:994:LEU:HG	1:B:995:ILE:HG21	1.95	0.48
1:A:1097:ILE:H	1:A:1097:ILE:HG13	1.45	0.48
2:D:365:THR:HG22	2:D:367:ASP:H	1.78	0.48
1:A:46:ILE:HD13	1:B:553:ARG:HE	1.78	0.48
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.94	0.48
1:A:41:TYR:HB3	1:A:216:LEU:HB2	1.94	0.48
1:A:692:ASN:HA	1:A:1059:THR:HG22	1.95	0.48
1:C:21:THR:HA	1:C:135:ASN:HD22	1.78	0.48
1:C:139:ALA:HB1	1:C:239:SER:HB2	1.95	0.48
2:D:482:ARG:NH2	2:D:613:TYR:OH	2.47	0.48
1:B:82:PRO:HA	1:B:230:ASN:HA	1.95	0.48
1:B:188:LYS:HB3	1:B:195:TYR:HB2	1.94	0.48
1:C:129:ASN:ND2	1:C:157:PHE:O	2.47	0.48
1:C:605:ASP:O	1:C:609:ALA:HB2	2.13	0.48
1:C:968:LYS:HG3	1:C:969:VAL:HG23	1.96	0.48
1:B:894:THR:HG23	1:B:896:ASN:H	1.79	0.48
1:B:912:ALA:O	1:B:916:ILE:N	2.35	0.48
1:B:1064:CYS:HB2	1:B:1111:VAL:HG21	1.95	0.48
1:C:898:LEU:O	1:C:901:ASN:N	2.35	0.48
1:A:222:LEU:HB3	1:A:224:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:LYS:HB2	1:B:686:SER:HA	1.96	0.48
1:A:914:SER:O	1:A:917:GLN:HB2	2.14	0.48
1:A:444:ARG:NH1	1:A:447:LYS:O	2.46	0.48
1:C:115:ILE:O	1:C:125:ILE:HA	2.13	0.48
1:C:127:ALA:HB3	1:C:161:PHE:HB3	1.96	0.48
2:D:503:LEU:HD23	2:D:505:HIS:H	1.79	0.48
1:A:539:THR:HG23	1:A:571:LEU:HB2	1.95	0.48
1:A:887:ARG:HH12	1:A:1032:MET:HA	1.78	0.48
1:C:694:ILE:N	1:C:1057:PHE:O	2.45	0.48
1:A:141:SER:HB3	1:A:144:MET:HB2	1.96	0.47
1:A:203:ILE:HD13	1:A:210:PRO:HG3	1.94	0.47
2:D:247:LYS:HD2	2:D:250:ASN:HD22	1.79	0.47
1:A:203:ILE:HD12	1:A:205:VAL:HG23	1.96	0.47
1:A:859:LEU:O	1:A:863:THR:OG1	2.27	0.47
1:A:879:PRO:HB3	1:B:691:ASN:HA	1.97	0.47
1:A:984:GLN:HE21	1:B:984:GLN:HE22	1.62	0.47
1:B:1062:ALA:HB3	1:B:1111:VAL:HG13	1.95	0.47
2:D:198:ASP:OD1	2:D:201:ASP:N	2.46	0.47
1:B:139:ALA:HB3	1:B:148:THR:HB	1.96	0.47
1:B:188:LYS:HE2	1:B:190:LYS:HB2	1.96	0.47
1:B:652:ILE:HB	1:B:656:ILE:HG22	1.96	0.47
1:C:315:ARG:HH22	1:C:519:LEU:HB3	1.80	0.47
1:C:745:LEU:HD22	1:C:990:VAL:HG21	1.96	0.47
1:C:968:LYS:HG3	1:C:969:VAL:H	1.79	0.47
1:A:697:PRO:HB3	1:A:1053:GLN:H	1.80	0.47
1:A:1060:ALA:HA	1:A:1113:GLY:HA3	1.96	0.47
1:B:86:GLY:CA	1:B:187:PHE:O	2.63	0.47
1:C:1065:HIS:HB3	1:C:1070:TYR:HE2	1.79	0.47
2:D:344:CYS:HB3	2:D:361:CYS:HB2	1.76	0.47
1:A:575:PRO:HG2	1:C:835:GLN:HG2	1.95	0.47
1:B:329:PHE:HZ	1:B:499:LEU:HD11	1.79	0.47
1:B:390:LYS:HE2	1:B:481:TYR:HA	1.95	0.47
1:C:605:ASP:O	1:C:609:ALA:CB	2.63	0.47
1:C:628:VAL:HG13	1:C:641:HIS:CE1	2.49	0.47
1:C:628:VAL:HG13	1:C:641:HIS:NE2	2.30	0.47
1:C:784:PHE:O	1:C:788:LEU:N	2.42	0.47
2:D:184:VAL:HG12	2:D:464:PHE:HE1	1.80	0.47
1:A:698:THR:OG1	1:A:1053:GLN:OE1	2.19	0.47
1:B:24:ASP:O	1:B:245:TRP:NE1	2.40	0.47
1:B:628:VAL:HG22	1:B:641:HIS:CE1	2.49	0.47
1:C:1060:ALA:HB3	1:C:1080:ASN:HD22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LEU:HD11	1:C:964:SER:HB2	1.96	0.47
1:B:22:PHE:H	1:B:135:ASN:HD22	1.61	0.47
1:B:770:MET:N	1:C:683:ALA:O	2.48	0.47
1:C:165:SER:OG	1:C:166:ASP:N	2.46	0.47
1:C:418:GLY:CA	1:C:499:LEU:O	2.60	0.47
1:C:713:MET:SD	1:C:993:GLN:NE2	2.88	0.47
1:C:790:ASP:HB2	1:C:793:LYS:HG2	1.96	0.47
1:A:460:PHE:N	1:A:475:TYR:O	2.48	0.47
1:A:633:ALA:HB2	1:C:844:PRO:HG3	1.97	0.47
1:C:131:GLU:OE1	1:C:155:ASN:ND2	2.48	0.47
1:C:979:ILE:O	1:C:983:LEU:HB2	2.15	0.47
1:A:114:VAL:HG23	1:A:127:ALA:HB2	1.96	0.47
1:A:424:ASN:ND2	1:A:492:GLN:OE1	2.43	0.47
1:A:1079:PHE:HB3	1:A:1085:PHE:C	2.39	0.47
1:B:97:VAL:HG12	1:B:98:VAL:HG13	1.98	0.47
2:D:116:LEU:HD13	2:D:186:LEU:HB2	1.97	0.47
1:B:1013:GLU:OE2	1:C:1021:ARG:NE	2.46	0.46
1:B:769:GLN:HE22	1:C:685:SER:HB3	1.81	0.46
1:B:861:SER:O	1:B:865:THR:OG1	2.32	0.46
1:B:960:ASN:H	1:B:963:LEU:HD13	1.80	0.46
1:C:194:LEU:O	1:C:221:LYS:HA	2.14	0.46
1:C:849:ASP:HA	1:C:852:ILE:HD12	1.96	0.46
1:C:884:MET:HE3	1:C:1031:LEU:HD21	1.97	0.46
1:A:99:ARG:HH12	1:A:172:VAL:HG13	1.81	0.46
1:B:784:PHE:HA	1:B:787:ILE:HD12	1.97	0.46
1:C:24:ASP:OD2	1:C:74:HIS:ND1	2.36	0.46
1:C:645:SER:HB3	1:C:680:SER:CA	2.45	0.46
1:C:787:ILE:HG23	1:C:1036:GLN:HE22	1.81	0.46
1:B:198:LYS:O	1:B:217:LYS:N	2.34	0.46
1:B:911:LYS:O	1:B:915:GLN:N	2.42	0.46
1:C:91:ALA:HB3	1:C:183:ARG:HB2	1.98	0.46
1:A:370:SER:OG	1:C:970:GLU:OE2	2.25	0.46
1:B:603:CYS:HB3	1:B:627:ASN:HD21	1.79	0.46
1:C:95:SER:H	1:C:181:HIS:CD2	2.34	0.46
1:C:646:TYR:N	1:C:677:TYR:HD2	2.07	0.46
1:A:575:PRO:O	1:C:835:GLN:NE2	2.36	0.46
1:C:286:LEU:HD11	1:C:300:TYR:HD2	1.81	0.46
1:C:287:LYS:HA	1:C:295:ILE:HD11	1.98	0.46
1:C:381:ASN:N	1:C:509:THR:OG1	2.43	0.46
1:A:93:GLU:HG3	1:A:183:ARG:HH22	1.81	0.46
1:A:626:ASN:ND2	1:A:639:ALA:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:453:THR:HG21	2:D:516:TYR:HB2	1.98	0.46
1:B:104:GLY:O	1:B:229:THR:N	2.41	0.46
1:B:346:SER:OG	1:B:347:ASN:N	2.48	0.46
1:A:775:THR:HA	1:A:777:LYS:HG3	1.97	0.46
1:C:116:ILE:HA	1:C:125:ILE:HG12	1.98	0.46
1:B:340:TRP:CE2	1:B:453:ARG:HD3	2.51	0.45
1:B:398:ALA:HB3	1:B:401:GLN:HG3	1.98	0.45
1:A:274:ASP:OD1	1:A:275:ALA:N	2.48	0.45
1:C:807:LYS:NZ	1:C:920:LEU:O	2.38	0.45
1:A:809:THR:OG1	1:A:810:LEU:N	2.50	0.45
2:D:539:LEU:HD23	2:D:587:TYR:HB2	1.97	0.45
1:A:324:PRO:O	1:A:328:VAL:N	2.39	0.45
1:A:440:TYR:HB3	1:A:481:TYR:HE1	1.82	0.45
1:B:18:ARG:N	1:B:133:CYS:SG	2.88	0.45
1:B:311:GLY:H	1:B:525:VAL:HG12	1.80	0.45
1:B:631:THR:O	1:B:633:ALA:N	2.40	0.45
1:B:770:MET:HE2	1:B:770:MET:HB3	1.85	0.45
1:C:371:ALA:HA	1:C:374:LEU:HD22	1.98	0.45
1:A:72:ILE:H	1:A:75:THR:HB	1.82	0.45
1:C:698:THR:OG1	1:C:1053:GLN:OE1	2.20	0.45
2:D:32:PHE:O	2:D:36:ALA:CB	2.64	0.45
1:A:802:ASP:O	1:A:806:ASN:ND2	2.49	0.45
1:B:362:SER:N	1:B:422:ALA:O	2.47	0.45
1:B:366:CYS:HB3	1:B:369:VAL:HG23	1.99	0.45
1:B:660:TYR:HB2	1:B:674:ILE:HA	1.98	0.45
1:B:721:ASN:HD22	1:C:304:ASN:HD22	1.65	0.45
2:D:81:GLN:NE2	2:D:103:ASN:OD1	2.49	0.45
1:A:554:ASP:OD1	1:A:555:VAL:N	2.49	0.45
1:B:138:PHE:HB2	1:B:236:THR:HG22	1.98	0.45
1:B:224:LEU:HB3	1:B:226:ILE:HG12	1.98	0.45
1:B:363:THR:HB	1:B:422:ALA:HB3	1.97	0.45
1:C:71:THR:OG1	1:C:75:THR:O	2.28	0.45
1:A:269:ASN:OD1	1:B:544:ARG:NE	2.49	0.45
1:A:344:LYS:HG3	1:A:383:TYR:HE1	1.81	0.45
1:B:435:ASN:HB3	1:B:483:PHE:HB2	1.99	0.45
1:B:563:ARG:NE	1:B:569:GLU:OE2	2.49	0.45
1:C:951:ASN:OD1	1:C:952:PHE:N	2.49	0.45
2:D:518:ARG:O	2:D:522:GLN:HB2	2.16	0.45
1:A:37:MET:HE2	1:A:37:MET:HB3	1.87	0.45
1:A:948:LEU:HD23	1:A:948:LEU:HA	1.75	0.45
1:C:642:VAL:HG21	1:C:675:VAL:CA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:LYS:HA	2:D:250:ASN:HD22	1.81	0.45
2:D:455:MET:HE2	2:D:459:TRP:HB2	1.99	0.45
2:D:370:LEU:HB3	2:D:409:SER:HB2	1.99	0.44
1:A:848:THR:HB	1:A:851:MET:HB2	1.98	0.44
1:B:678:THR:OG1	1:B:679:MET:N	2.34	0.44
1:B:775:THR:HA	1:B:777:LYS:HE3	1.99	0.44
1:C:209:LEU:HD12	1:C:210:PRO:HD2	1.99	0.44
1:C:397:ILE:HA	1:C:412:LEU:HD21	1.98	0.44
1:C:426:ARG:HA	1:C:430:ALA:HB3	1.99	0.44
1:C:674:ILE:HD12	1:C:675:VAL:O	2.17	0.44
1:B:95:SER:OG	1:B:173:SER:O	2.27	0.44
1:B:951:ASN:OD1	1:B:952:PHE:N	2.50	0.44
1:A:24:ASP:HB3	1:A:245:TRP:HE1	1.83	0.44
1:A:352:TYR:HA	1:A:355:LEU:HD12	1.99	0.44
1:A:405:ILE:HG23	1:A:409:ASN:HD22	1.82	0.44
1:B:978:LEU:HD23	1:B:978:LEU:HA	1.85	0.44
1:C:35:SER:HB2	1:C:60:LEU:HD21	1.98	0.44
1:A:951:ASN:OD1	1:A:952:PHE:N	2.48	0.44
1:B:1080:ASN:HA	1:B:1083:SER:HA	2.00	0.44
1:C:187:PHE:HE1	1:C:196:VAL:HG13	1.81	0.44
2:D:38:ASP:OD1	2:D:353:LYS:NZ	2.46	0.44
1:A:282:PRO:HB2	1:A:594:VAL:HG21	2.00	0.44
1:A:385:ASP:OD2	1:A:410:TYR:OH	2.33	0.44
1:A:770:MET:HE2	1:A:770:MET:HB3	1.83	0.44
1:C:19:CYS:HB3	1:C:134:ASP:HB2	1.99	0.44
1:C:441:ARG:HH22	1:C:457:ASN:HA	1.82	0.44
1:C:615:LEU:HB3	1:C:617:PRO:HD2	2.00	0.44
1:A:71:THR:OG1	1:A:75:THR:O	2.30	0.44
1:B:86:GLY:HA3	1:B:187:PHE:O	2.17	0.44
1:B:335:PRO:HG3	1:B:341:GLU:HB2	1.98	0.44
1:C:38:ARG:NH2	1:C:210:PRO:O	2.40	0.44
2:D:237:TYR:HD1	2:D:447:VAL:HG12	1.82	0.44
2:D:566:TRP:O	2:D:570:LEU:CB	2.63	0.44
1:A:209:LEU:HD12	1:A:210:PRO:HD2	2.00	0.44
1:B:352:TYR:HD2	1:B:375:ASN:HB3	1.81	0.44
1:B:1051:PRO:HG3	1:B:1090:ASN:HD21	1.83	0.44
1:C:561:SER:HB3	1:C:571:LEU:HD23	1.99	0.44
1:A:1079:PHE:CE2	1:A:1084:TRP:HB2	2.53	0.44
1:B:78:ASN:HB2	1:B:235:LEU:HD13	1.99	0.44
1:B:1031:LEU:HD12	1:B:1031:LEU:HA	1.85	0.44
1:C:323:CYS:O	1:C:325:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:PHE:N	1:B:475:TYR:O	2.51	0.43
1:C:631:THR:O	1:C:633:ALA:N	2.52	0.43
1:A:96:ASN:HA	1:A:183:ARG:HH12	1.83	0.43
1:A:698:THR:H	1:A:1053:GLN:HB2	1.84	0.43
1:A:778:TYR:CZ	1:A:781:GLY:HA2	2.53	0.43
1:C:1102:THR:OG1	1:C:1103:PHE:N	2.50	0.43
2:D:33:ASN:ND2	2:D:390:PHE:H	2.16	0.43
2:D:482:ARG:NH2	2:D:611:SER:OG	2.51	0.43
1:C:72:ILE:H	1:C:75:THR:HB	1.82	0.43
1:A:370:SER:H	1:C:965:ARG:HB2	1.83	0.43
1:A:968:LYS:HD3	1:A:968:LYS:HA	1.91	0.43
1:B:139:ALA:O	1:B:148:THR:OG1	2.32	0.43
1:C:99:ARG:NE	1:C:118:ASN:HB2	2.33	0.43
1:A:1070:TYR:HE1	1:A:1104:VAL:HA	1.84	0.43
1:B:224:LEU:HD13	1:B:226:ILE:HD11	2.01	0.43
1:A:390:LYS:HG2	1:A:483:PHE:HZ	1.83	0.43
1:B:656:ILE:HG12	1:B:678:THR:HA	2.00	0.43
1:B:915:GLN:O	1:B:918:GLU:HB2	2.17	0.43
1:B:1032:MET:HE3	1:B:1032:MET:HB3	1.81	0.43
1:C:546:GLN:HB2	1:C:549:GLN:OE1	2.19	0.43
1:A:390:LYS:HG2	1:A:483:PHE:CZ	2.53	0.43
1:A:575:PRO:HB3	1:A:578:PHE:HE1	1.84	0.43
1:A:856:THR:HG21	1:A:1037:ALA:HB2	2.00	0.43
1:A:348:CYS:HB3	1:A:510:VAL:HG22	2.01	0.43
1:A:895:GLN:HB2	1:B:1071:PHE:CD2	2.53	0.43
1:A:1021:ARG:H	1:A:1021:ARG:HG2	1.71	0.43
1:B:72:ILE:H	1:B:75:THR:HB	1.84	0.43
2:D:249:MET:HE1	2:D:258:PRO:HG3	2.00	0.43
1:A:287:LYS:HA	1:A:295:ILE:HD11	2.01	0.43
1:A:965:ARG:HB2	1:B:369:VAL:HA	2.01	0.43
1:C:1030:HIS:CE1	1:C:1033:SER:HB2	2.46	0.43
1:A:95:SER:OG	1:A:173:SER:O	2.37	0.43
1:A:1011:MET:HB2	1:A:1011:MET:HE3	1.78	0.43
1:A:1028:GLY:HA3	1:A:1049:TYR:H	1.82	0.43
1:B:274:ASP:OD1	1:B:275:ALA:N	2.51	0.43
1:B:959:LEU:O	1:B:961:ASP:N	2.52	0.43
1:C:99:ARG:HH22	1:C:172:VAL:HG22	1.84	0.43
1:C:261:THR:HB	1:C:278:CYS:HB2	2.01	0.43
1:C:315:ARG:HH12	1:C:519:LEU:HB3	1.83	0.43
1:C:544:ARG:O	1:C:546:GLN:NE2	2.52	0.43
1:C:862:GLY:HA2	1:C:866:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:LEU:HD13	1:A:941:LEU:HD11	2.01	0.42
1:A:1079:PHE:HE2	1:A:1084:TRP:HB2	1.84	0.42
1:C:659:SER:OG	1:C:660:TYR:N	2.52	0.42
1:C:961:ASP:O	1:C:964:SER:OG	2.31	0.42
2:D:375:GLU:HA	2:D:378:HIS:HD2	1.84	0.42
1:A:137:PHE:HB2	1:A:237:ALA:HB2	2.00	0.42
1:A:562:VAL:HG23	1:A:570:ILE:HG13	2.00	0.42
1:C:94:LYS:NZ	1:C:249:ALA:O	2.40	0.42
1:C:197:TYR:HB3	1:C:216:LEU:HB3	2.01	0.42
1:C:640:GLU:O	1:C:642:VAL:N	2.46	0.42
2:D:209:VAL:HG11	2:D:565:PRO:HB3	2.00	0.42
1:B:142:LYS:HB2	1:B:238:PHE:HB3	2.01	0.42
1:B:721:ASN:ND2	1:C:304:ASN:HD22	2.17	0.42
1:B:724:ILE:HG22	1:B:725:CYS:HB2	2.01	0.42
1:B:1072:PRO:HB3	1:B:1078:VAL:HG22	1.99	0.42
2:D:205:GLY:HA2	2:D:208:GLU:HB2	2.00	0.42
1:C:292:SER:OG	1:C:294:GLU:N	2.52	0.42
1:B:209:LEU:HD12	1:B:210:PRO:HD2	2.01	0.42
1:B:853:ALA:O	1:B:856:THR:OG1	2.30	0.42
1:B:1054:GLU:O	1:B:1055:ARG:NH1	2.52	0.42
1:C:756:GLN:HA	1:C:759:ASN:HD22	1.84	0.42
2:D:247:LYS:HB2	2:D:282:THR:HG22	2.00	0.42
2:D:455:MET:HE3	2:D:480:MET:HB2	2.01	0.42
1:A:362:SER:H	1:A:423:TRP:HA	1.84	0.42
1:B:122:ASN:OD1	1:B:123:VAL:N	2.52	0.42
1:B:996:ARG:O	1:B:1000:ILE:HB	2.20	0.42
1:C:382:VAL:H	1:C:510:VAL:HG11	1.84	0.42
1:C:1098:THR:H	1:C:1101:ASN:ND2	2.18	0.42
2:D:362:THR:HG23	2:D:368:ASP:HB3	2.01	0.42
1:B:138:PHE:HB2	1:B:236:THR:HA	2.01	0.42
1:C:78:ASN:HD21	1:C:136:PRO:HG2	1.85	0.42
2:D:461:TRP:O	2:D:465:LYS:CB	2.68	0.42
1:A:603:CYS:N	1:A:635:CYS:SG	2.92	0.42
1:B:40:VAL:HG11	1:B:272:ILE:HG21	2.00	0.42
1:B:751:GLY:O	1:B:755:GLU:HG2	2.20	0.42
1:C:398:ALA:H	1:C:412:LEU:HG	1.84	0.42
1:A:95:SER:H	1:A:181:HIS:CD2	2.37	0.42
1:A:911:LYS:O	1:A:915:GLN:N	2.46	0.42
1:B:749:LEU:HD23	1:B:749:LEU:HA	1.86	0.42
1:B:1097:ILE:H	1:B:1097:ILE:HG13	1.52	0.42
1:C:707:GLU:OE2	1:C:1010:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:960:ASN:HA	1:C:963:LEU:HD22	2.02	0.42
2:D:320:LEU:HD13	2:D:380:GLN:HG2	2.02	0.42
1:B:786:GLN:OE1	1:B:917:GLN:NE2	2.53	0.42
1:C:33:HIS:HD2	1:C:68:GLY:HA3	1.84	0.42
1:C:880:PHE:HA	1:C:883:GLN:HB2	2.02	0.42
2:D:56:GLU:HA	2:D:59:VAL:HG12	2.01	0.42
2:D:557:MET:HA	2:D:560:LEU:HD13	2.02	0.42
1:A:38:ARG:NH2	1:A:210:PRO:O	2.42	0.41
1:A:42:TYR:HB2	1:A:218:PRO:HD3	2.01	0.41
1:A:630:GLN:HG2	1:A:631:THR:H	1.84	0.41
1:B:801:GLU:HA	1:B:804:LEU:HD12	2.01	0.41
1:B:916:ILE:HD13	1:B:916:ILE:HA	1.88	0.41
1:B:1079:PHE:HB3	1:B:1085:PHE:C	2.45	0.41
2:D:581:VAL:HG13	2:D:585:LEU:HD23	2.02	0.41
1:B:83:PHE:HE2	1:B:189:ASN:HB2	1.86	0.41
1:B:968:LYS:HD3	1:B:968:LYS:HA	1.83	0.41
1:A:678:THR:OG1	1:A:679:MET:N	2.38	0.41
1:A:683:ALA:O	1:C:770:MET:N	2.53	0.41
1:A:904:GLN:HA	1:A:907:ASN:HD22	1.85	0.41
1:B:961:ASP:OD1	1:B:965:ARG:NH1	2.38	0.41
1:B:1060:ALA:HB2	1:B:1080:ASN:ND2	2.34	0.41
1:C:78:ASN:ND2	1:C:136:PRO:HG2	2.35	0.41
1:C:645:SER:CB	1:C:680:SER:HB3	2.50	0.41
1:A:1068:LYS:NZ	1:A:1104:VAL:HG13	2.35	0.41
1:C:48:ARG:HB2	1:C:266:TYR:CE2	2.55	0.41
2:D:198:ASP:OD1	2:D:204:ARG:NH2	2.53	0.41
1:A:853:ALA:O	1:A:856:THR:OG1	2.32	0.41
1:A:877:GLN:HE21	1:B:695:ALA:HB3	1.85	0.41
1:B:832:ILE:O	1:C:632:GLN:NE2	2.53	0.41
1:C:432:SER:HB3	1:C:485:THR:HB	2.03	0.41
2:D:326:GLY:O	2:D:330:ASN:HB2	2.20	0.41
1:A:719:ASP:OD1	1:A:721:ASN:N	2.50	0.41
1:B:141:SER:HB3	1:B:144:MET:HB2	2.02	0.41
1:A:102:VAL:O	1:A:231:PHE:HA	2.20	0.41
1:B:1085:PHE:HB3	1:B:1095:GLN:H	1.85	0.41
1:C:131:GLU:HB2	1:C:155:ASN:HD22	1.84	0.41
1:C:915:GLN:O	1:C:919:SER:OG	2.30	0.41
1:A:89:PHE:HD2	1:A:185:PHE:HB2	1.86	0.41
1:A:499:LEU:HA	1:A:499:LEU:HD23	1.90	0.41
1:A:692:ASN:HD22	1:A:1059:THR:HG22	1.85	0.41
1:B:545:PHE:HZ	1:B:550:GLN:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:ILE:O	1:B:804:LEU:HG	2.21	0.41
1:C:136:PRO:HB2	1:C:234:ILE:HG12	2.01	0.41
2:D:581:VAL:HG22	2:D:584:LEU:HB3	2.02	0.41
1:A:48:ARG:HB2	1:A:266:TYR:CD2	2.56	0.41
1:A:440:TYR:OH	1:A:479:ASN:ND2	2.54	0.41
1:A:962:ILE:O	1:A:966:LEU:N	2.54	0.41
1:B:835:GLN:HE21	1:C:575:PRO:HG2	1.85	0.41
1:B:890:GLY:O	1:B:1018:GLN:NE2	2.54	0.41
1:C:44:ASP:OD2	1:C:48:ARG:NH1	2.54	0.41
1:C:695:ALA:HB1	1:C:1055:ARG:H	1.86	0.41
1:C:741:PHE:CD2	1:C:983:LEU:HD21	2.56	0.41
2:D:32:PHE:O	2:D:36:ALA:HB3	2.20	0.41
2:D:41:TYR:CG	2:D:353:LYS:HD2	2.56	0.41
2:D:149:ASN:HA	2:D:152:MET:HB2	2.03	0.41
2:D:406:GLU:HG3	2:D:518:ARG:HH21	1.86	0.41
2:D:418:LEU:HD13	2:D:418:LEU:HA	1.91	0.41
1:A:931:GLN:O	1:A:935:ASN:ND2	2.54	0.41
1:B:315:ARG:HB3	1:B:565:PRO:HD2	2.03	0.41
1:C:389:VAL:HB	1:C:393:ASP:HB2	2.02	0.41
1:C:736:LEU:HD23	1:C:736:LEU:HA	1.85	0.41
1:A:586:PRO:HG2	1:A:591:SER:HB3	2.03	0.40
1:A:723:TYR:CE1	1:A:944:LEU:HG	2.56	0.40
1:A:1068:LYS:HB2	1:A:1068:LYS:HE3	1.87	0.40
1:B:758:ARG:CZ	1:B:1001:ARG:HH12	2.34	0.40
1:B:909:PHE:HZ	1:B:1034:PHE:HE2	1.69	0.40
1:C:94:LYS:HA	1:C:181:HIS:CD2	2.56	0.40
1:C:382:VAL:HG22	1:C:510:VAL:HG11	2.03	0.40
1:C:749:LEU:HD23	1:C:749:LEU:HA	1.90	0.40
1:A:297:LYS:HG3	1:A:586:PRO:HA	2.03	0.40
1:C:747:ARG:O	1:C:750:SER:OG	2.30	0.40
1:C:888:PHE:CZ	1:C:898:LEU:HB2	2.56	0.40
1:A:749:LEU:HD23	1:A:749:LEU:HA	1.77	0.40
1:B:441:ARG:NH2	1:B:443:LEU:O	2.53	0.40
1:B:626:ASN:HD21	1:B:639:ALA:C	2.28	0.40
1:B:847:LEU:HD11	1:B:855:TYR:HE2	1.86	0.40
1:B:1063:ILE:HG21	1:B:1118:THR:HG21	2.03	0.40
1:C:94:LYS:HD2	1:C:179:PHE:HA	2.04	0.40
1:C:939:GLN:O	1:C:943:THR:OG1	2.20	0.40
2:D:560:LEU:HD23	2:D:564:GLU:HB2	2.02	0.40
1:A:194:LEU:HD12	1:A:194:LEU:HA	1.91	0.40
1:A:797:ARG:HD2	1:A:805:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ASP:OD1	1:B:58:LEU:N	2.54	0.40
2:D:130:GLY:HA3	2:D:172:VAL:HG11	2.03	0.40
2:D:261:CYS:HB2	2:D:488:VAL:HG13	2.03	0.40
1:B:749:LEU:HD23	1:B:752:ILE:HD12	2.03	0.40
1:B:901:ASN:O	1:B:904:GLN:HB3	2.22	0.40
1:B:941:LEU:HA	1:B:941:LEU:HD12	1.83	0.40
1:C:95:SER:H	1:C:181:HIS:CG	2.40	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	1057/1203 (88%)	853 (81%)	199 (19%)	5 (0%)	24	62
1	B	1057/1203 (88%)	848 (80%)	204 (19%)	5 (0%)	24	62
1	C	1045/1203 (87%)	840 (80%)	193 (18%)	12 (1%)	11	45
2	D	595/603 (99%)	562 (94%)	33 (6%)	0	100	100
All	All	3754/4212 (89%)	3103 (83%)	629 (17%)	22 (1%)	23	58

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	632	GLN
1	C	648	CYS
1	C	676	ALA
1	A	632	GLN
1	A	1072	PRO
1	B	1072	PRO
1	C	647	GLU
1	C	679	MET

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Mol	Chain	Res	Type
1	C	1072	PRO
1	B	925	THR
1	C	632	GLN
1	C	645	SER
1	C	1076	VAL
1	A	925	THR
1	B	969	VAL
1	C	675	VAL
1	C	692	ASN
1	A	969	VAL
1	C	557	ASP
1	B	1075	GLY
1	C	1075	GLY
1	A	1075	GLY

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	922/1048 (88%)	918 (100%)	4 (0%)	84	82
1	B	922/1048 (88%)	915 (99%)	7 (1%)	73	77
1	C	914/1048 (87%)	907 (99%)	7 (1%)	73	77
2	D	527/533 (99%)	525 (100%)	2 (0%)	84	82
All	All	3285/3677 (89%)	3265 (99%)	20 (1%)	76	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	687	ILE
1	A	724	ILE
1	A	894	THR
1	A	1097	ILE
1	B	302	THR
1	B	674	ILE
1	B	687	ILE

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Mol	Chain	Res	Type
1	B	711	VAL
1	B	865	THR
1	B	1087	THR
1	B	1097	ILE
1	C	318	ASN
1	C	510	VAL
1	C	647	GLU
1	C	656	ILE
1	C	677	TYR
1	C	678	THR
1	C	1097	ILE
2	D	68	LYS
2	D	570	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	129	ASN
1	A	181	HIS
1	A	301	GLN
1	A	304	ASN
1	A	330	ASN
1	A	589	ASN
1	A	632	GLN
1	A	692	ASN
1	A	746	ASN
1	A	759	ASN
1	A	769	GLN
1	A	806	ASN
1	A	907	ASN
1	A	935	ASN
1	A	987	GLN
1	A	1090	ASN
1	A	1101	ASN
1	B	33	HIS
1	B	118	ASN
1	B	611	HIS
1	B	627	ASN
1	B	699	ASN
1	B	746	ASN
1	B	759	ASN

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Mol	Chain	Res	Type
1	B	769	GLN
1	B	806	ASN
1	B	835	GLN
1	B	904	GLN
1	B	917	GLN
1	B	935	ASN
1	B	984	GLN
1	B	987	GLN
1	B	1101	ASN
1	C	112	GLN
1	C	135	ASN
1	C	147	GLN
1	C	155	ASN
1	C	181	HIS
1	C	304	ASN
1	C	318	ASN
1	C	473	ASN
1	C	479	ASN
1	C	632	GLN
1	C	699	ASN
1	C	759	ASN
1	C	769	GLN
1	C	838	ASN
1	C	937	ASN
1	C	947	GLN
1	C	960	ASN
1	C	987	GLN
1	C	1018	GLN
1	C	1030	HIS
1	C	1095	GLN
2	D	53	ASN
2	D	58	ASN
2	D	89	GLN
2	D	96	GLN
2	D	102	GLN
2	D	154	ASN
2	D	210	ASN
2	D	239	HIS
2	D	250	ASN
2	D	322	ASN
2	D	437	ASN
2	D	556	ASN

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Mol	Chain	Res	Type
2	D	586	ASN

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.

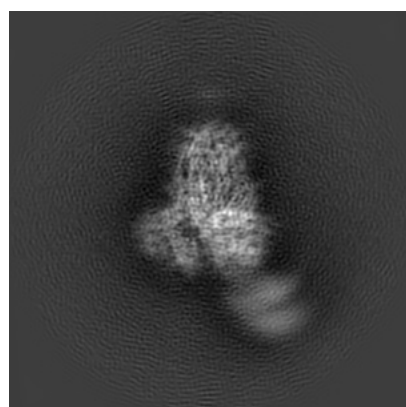
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9593. These allow visual inspection of the internal detail of the map and identification of artifacts.

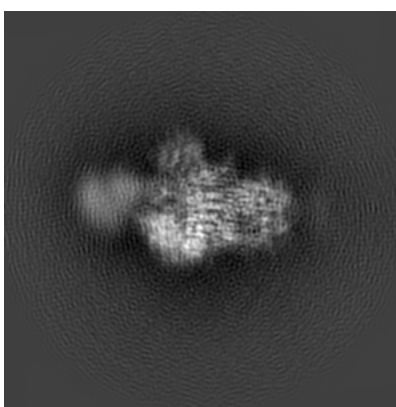
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

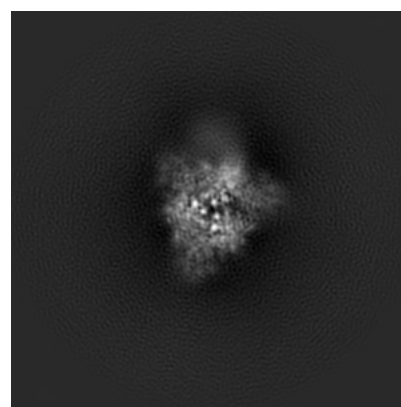
6.1.1 Primary map



X



Y

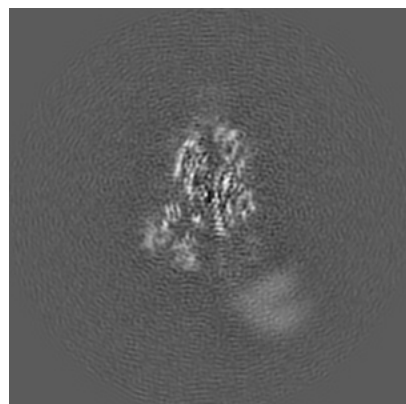


Z

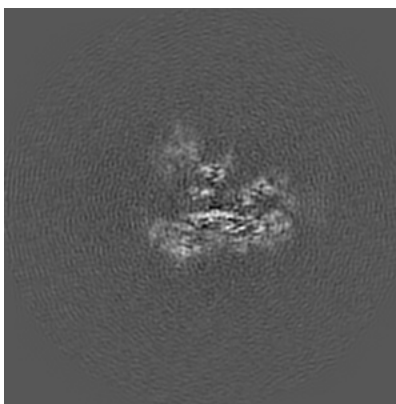
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

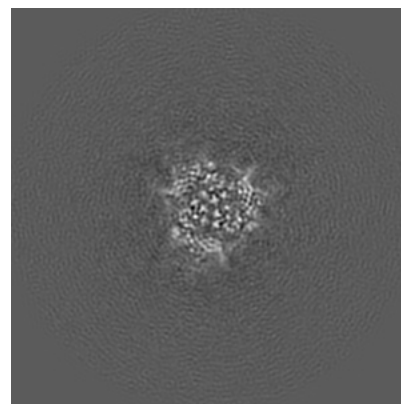
6.2.1 Primary map



X Index: 144



Y Index: 144

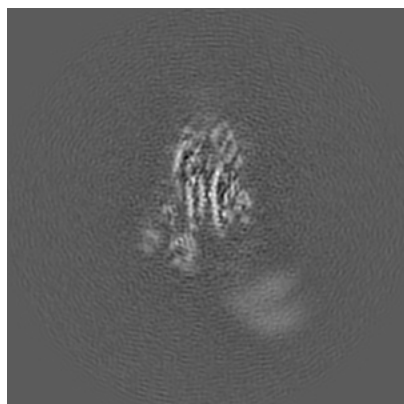


Z Index: 144

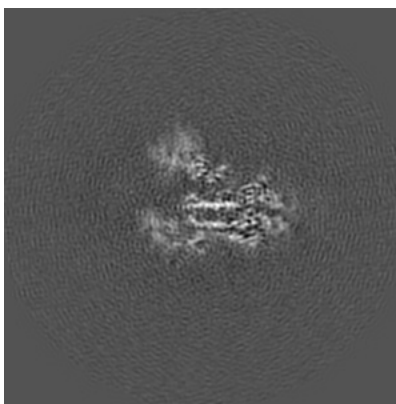
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

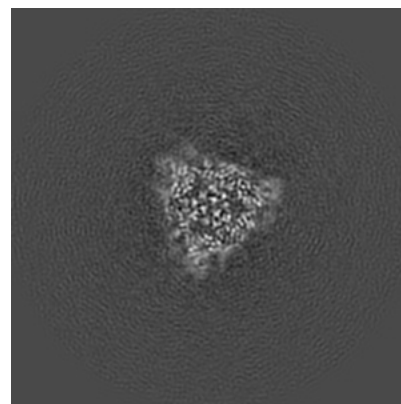
6.3.1 Primary map



X Index: 146



Y Index: 149

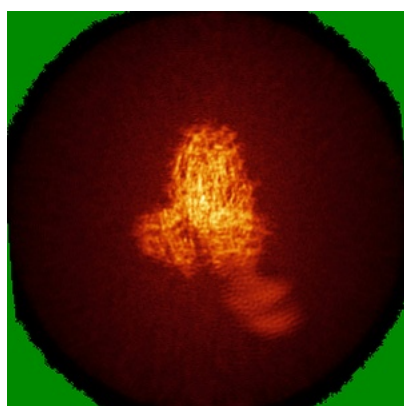


Z Index: 141

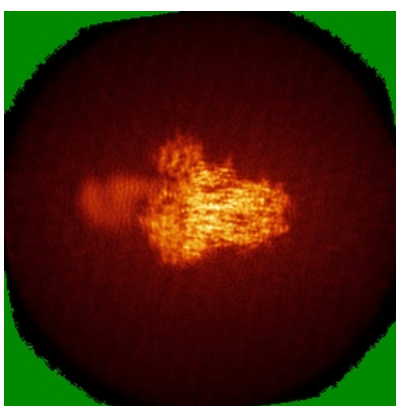
The images above show the largest variance slices of the map in three orthogonal directions.

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

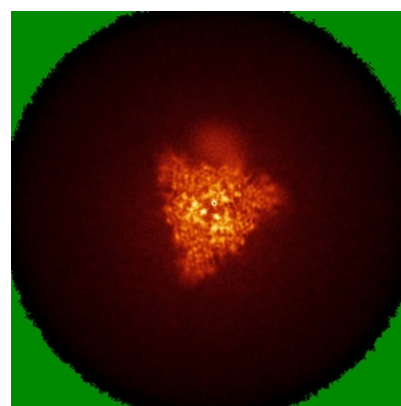
6.4.1 Primary map



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 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

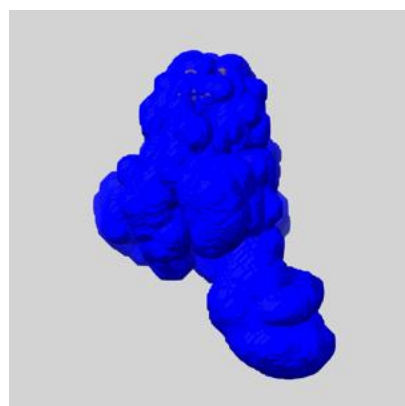
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

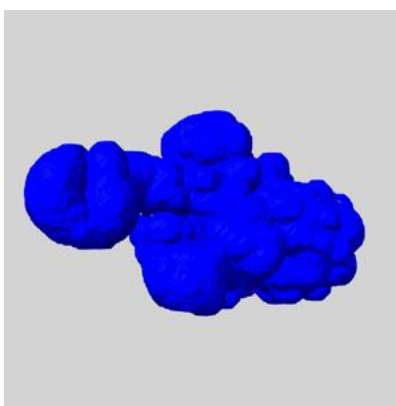
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

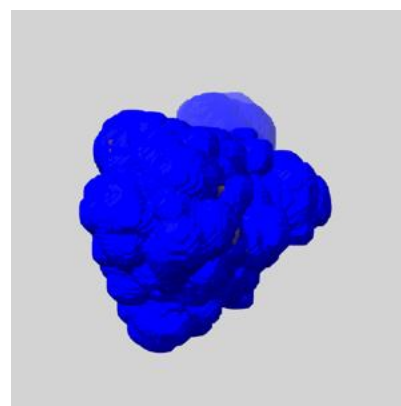
6.6.1 emd_9593_msk_1.map [i](#)



X



Y

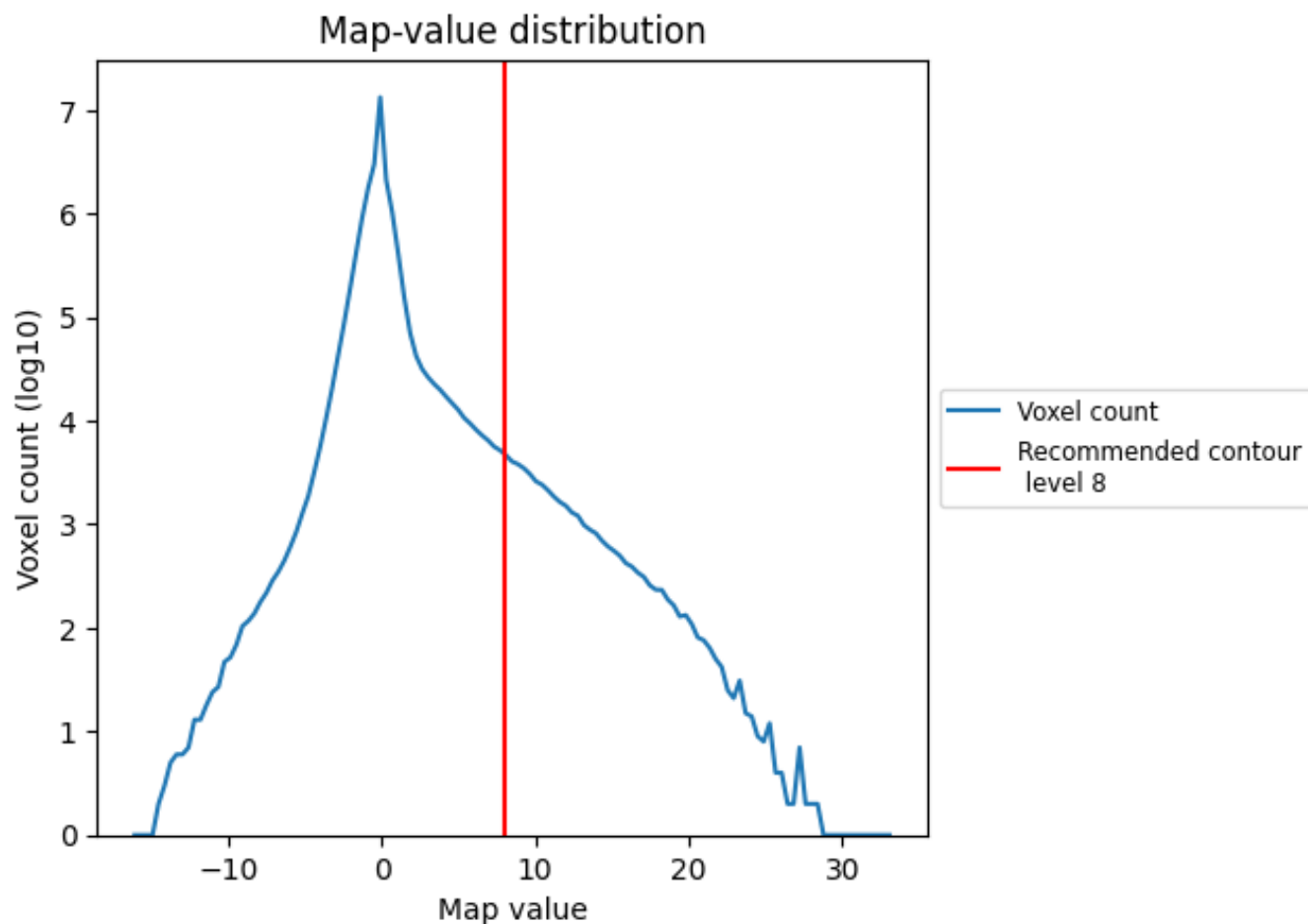


Z

7 Map analysis [i](#)

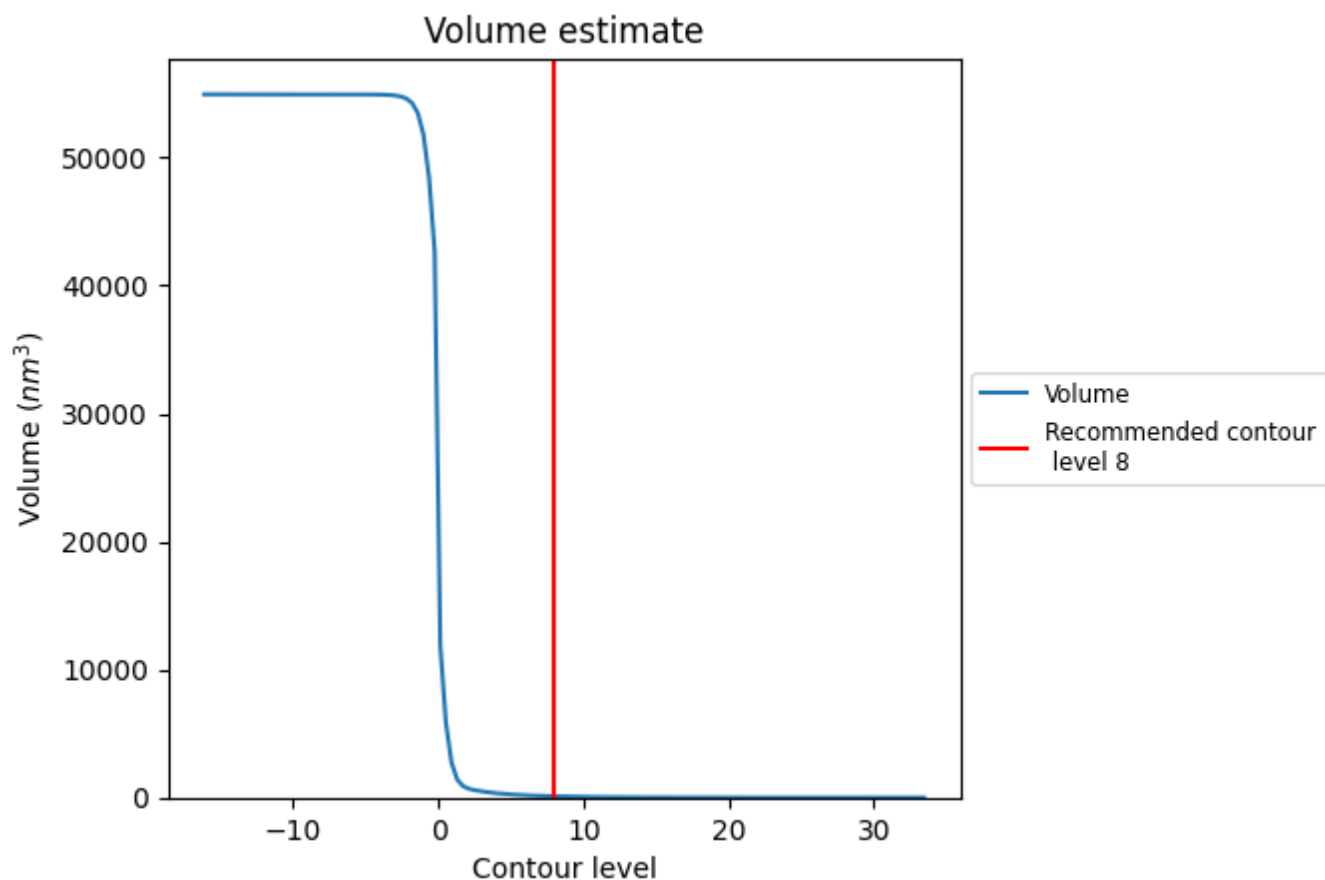
This section contains the results of statistical analysis of the map.

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.

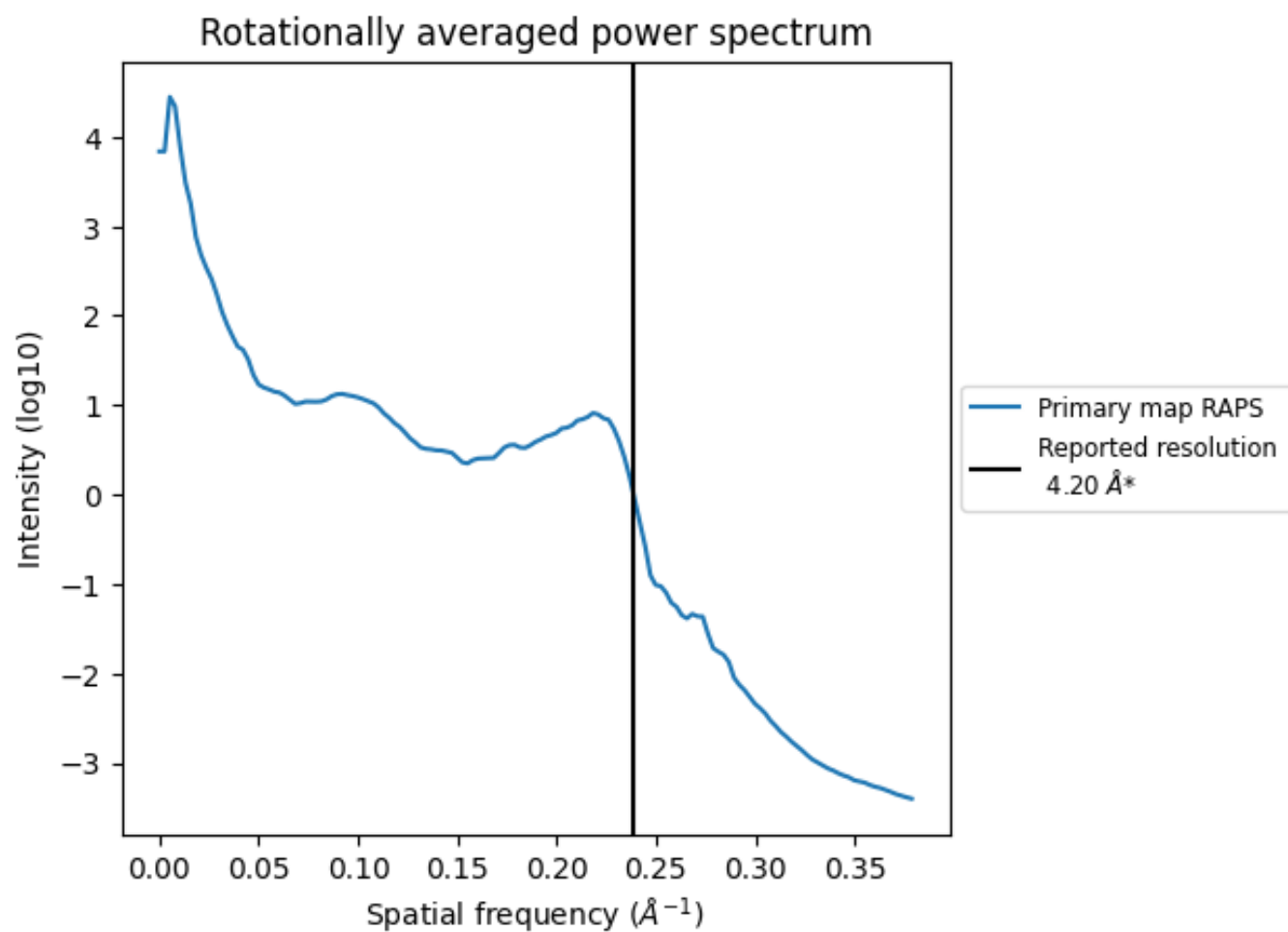
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 90 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 ⓘ

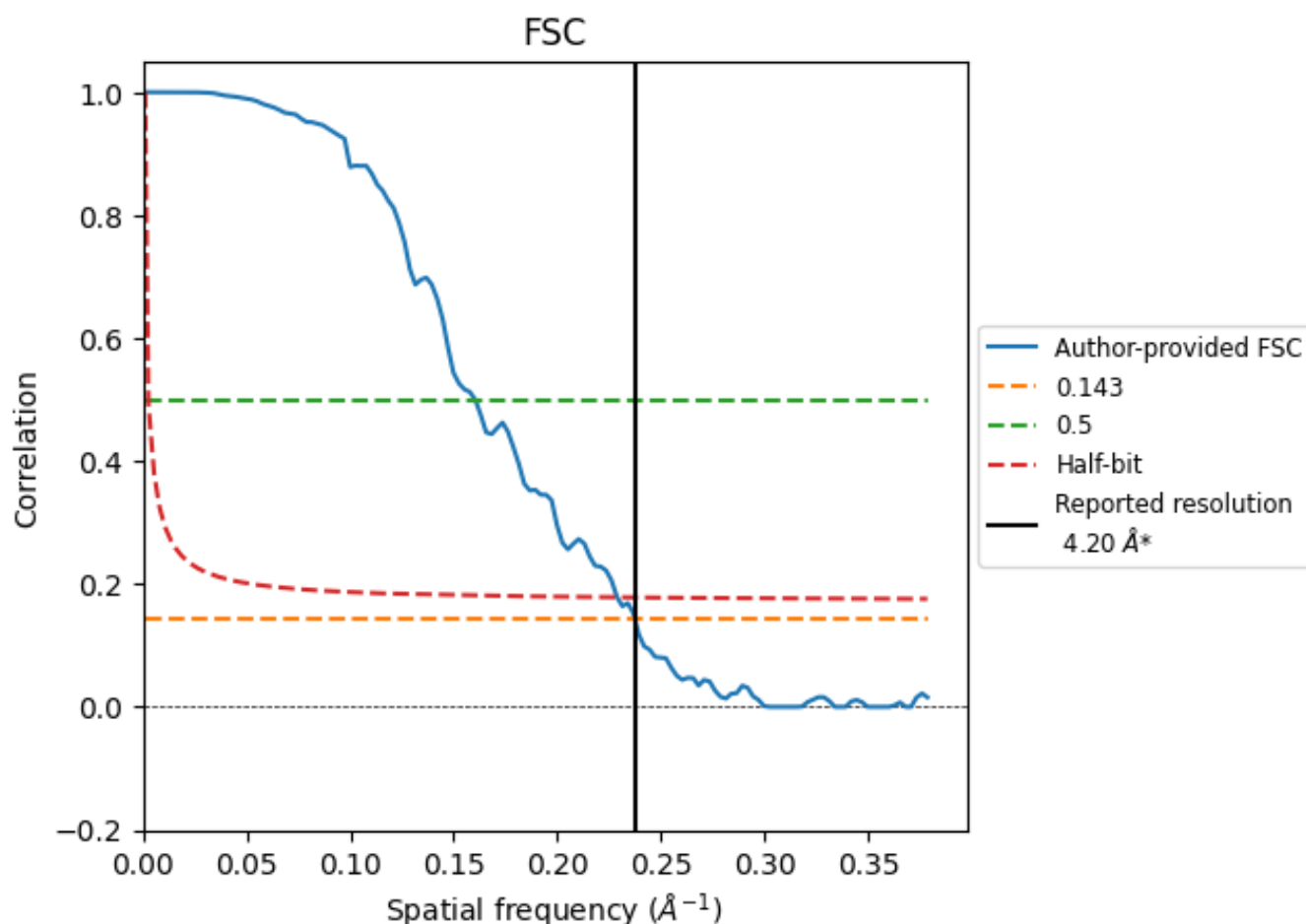


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

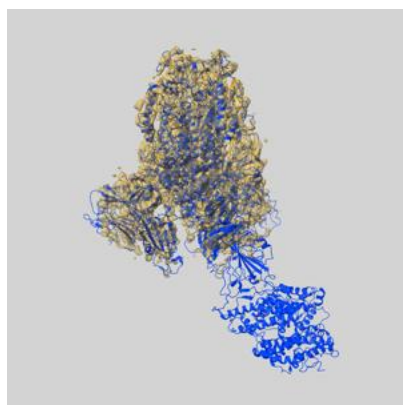
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.21	6.24	4.37
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

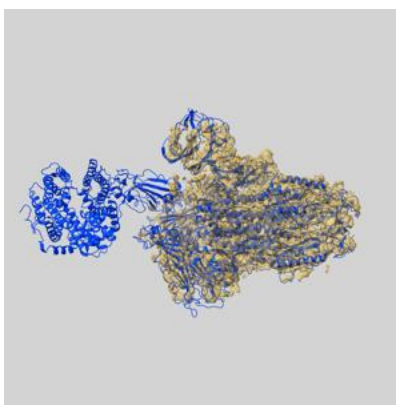
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9593 and PDB model 6ACJ. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

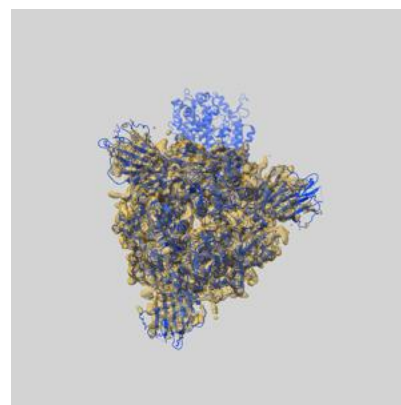
9.1 Map-model overlay [i](#)



X



Y



Z

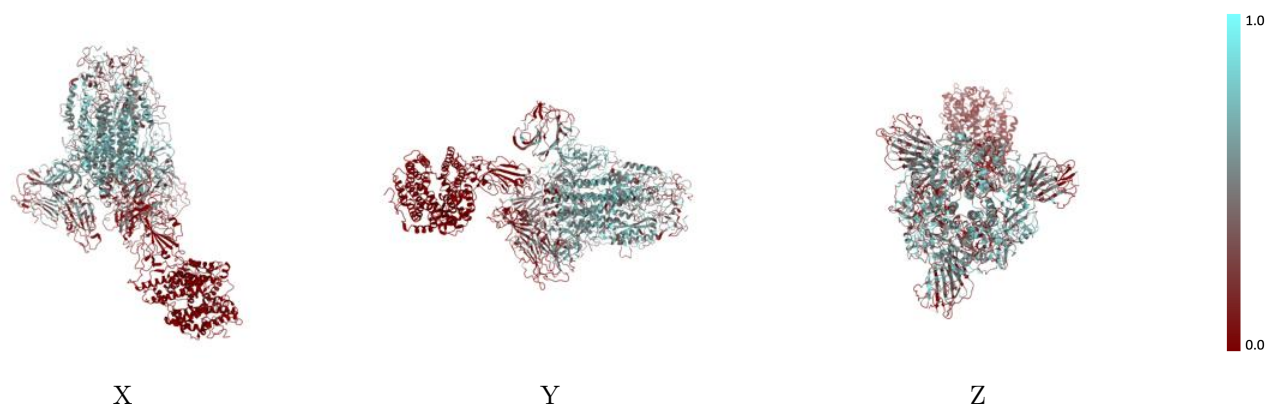
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



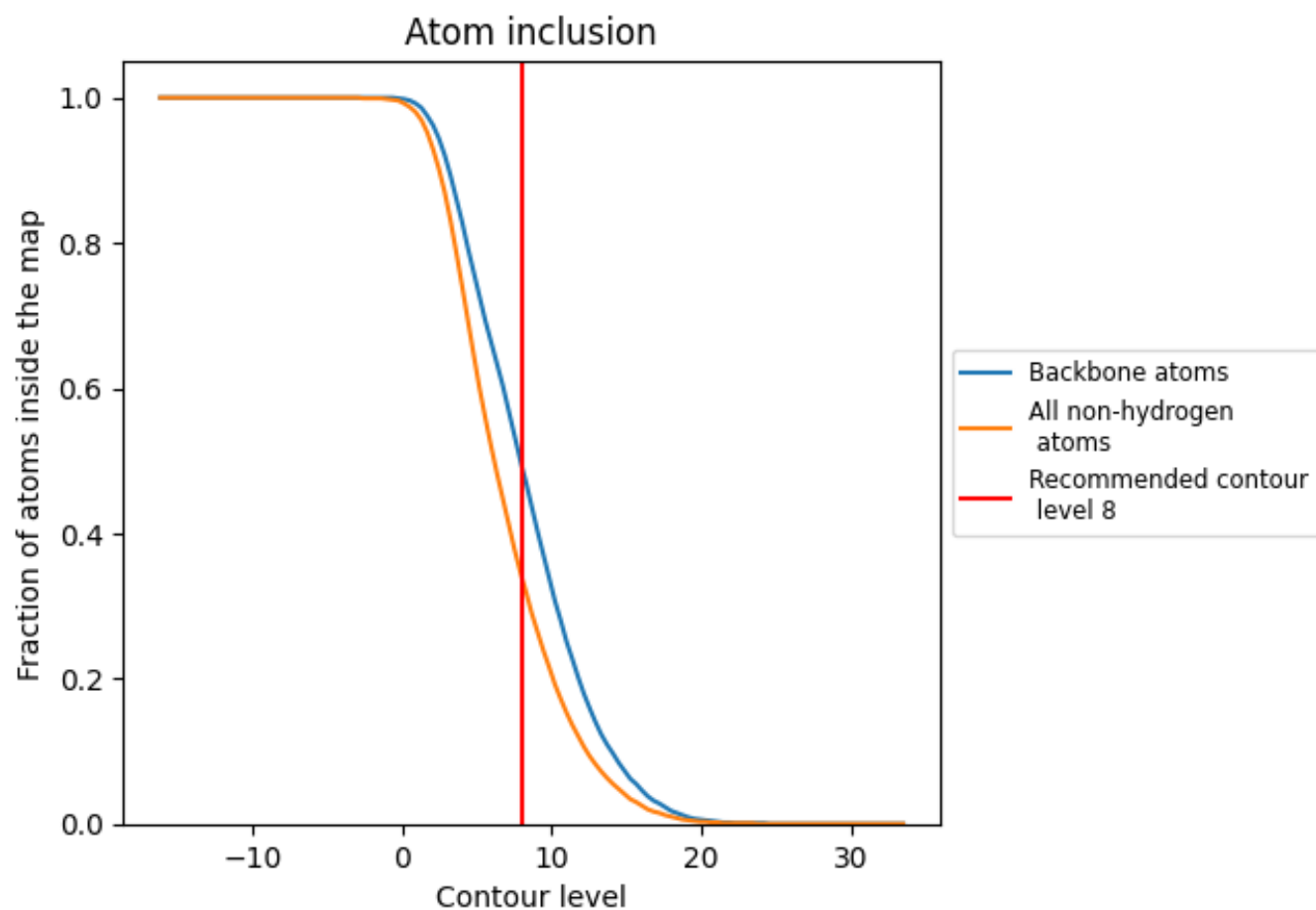
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 34% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3400	0.2770
A	0.4190	0.3200
B	0.4250	0.3080
C	0.3750	0.2960
D	0.0000	0.1150

