



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 12:39 AM JST

PDB ID : 6ACG  
EMDB ID : EMD-9591  
Title : Trypsin-cleaved and low pH-treated SARS-CoV spike glycoprotein and ACE2 complex, ACE2-bound conformation 1  
Authors : Gui, M.; Song, W.  
Deposited on : 2018-07-26  
Resolution : 5.40 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](mailto: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>.

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

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

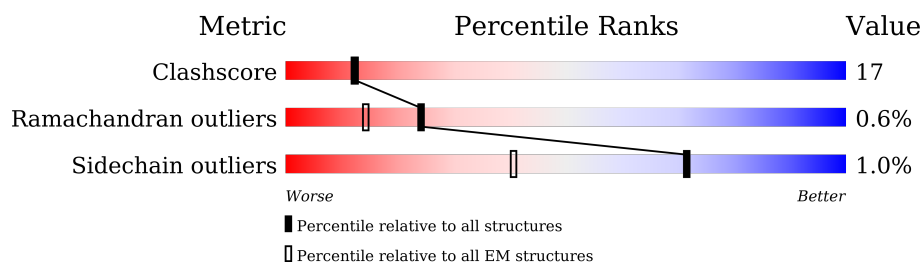
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>43%</div> <div>51%</div> <div>36%</div> <div>•</div> <div>11%</div> </div>
1	B	1203	<div> <div>37%</div> <div>52%</div> <div>35%</div> <div>•</div> <div>11%</div> </div>
1	C	1203	<div> <div>45%</div> <div>53%</div> <div>33%</div> <div>••</div> <div>12%</div> </div>
2	D	603	<div> <div>99%</div> <div>75%</div> <div>24%</div> <div>•</div> </div>

## 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

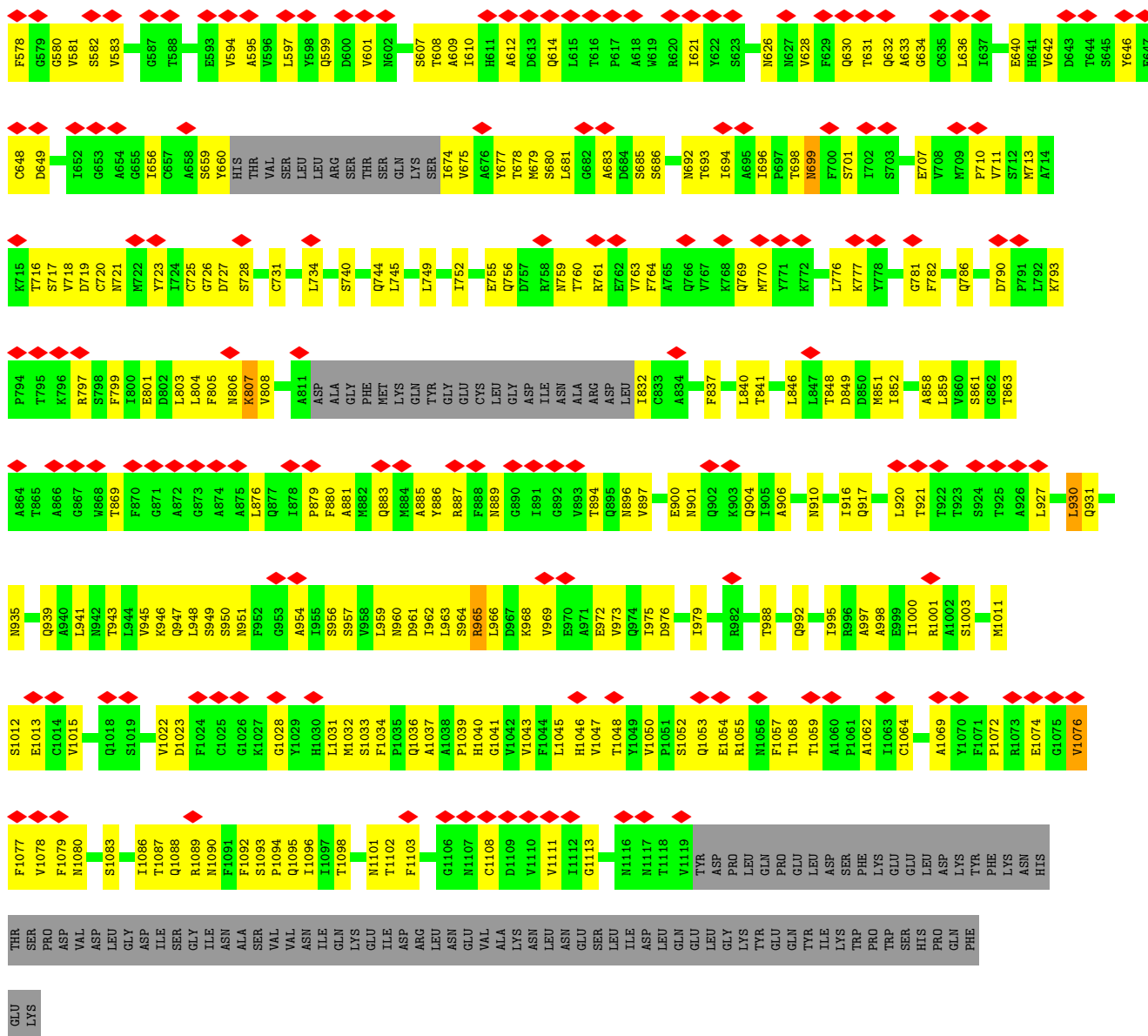
- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

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

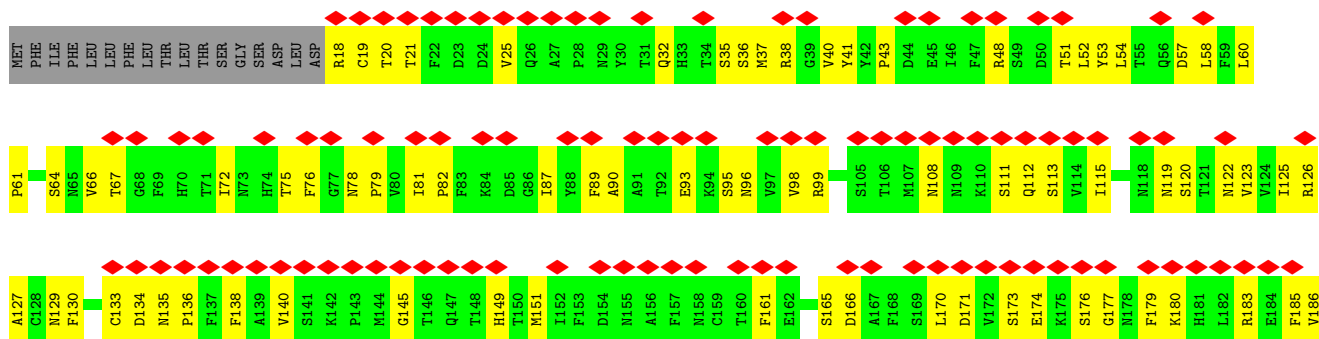
There are 6 discrepancies between the modelled and reference sequences:

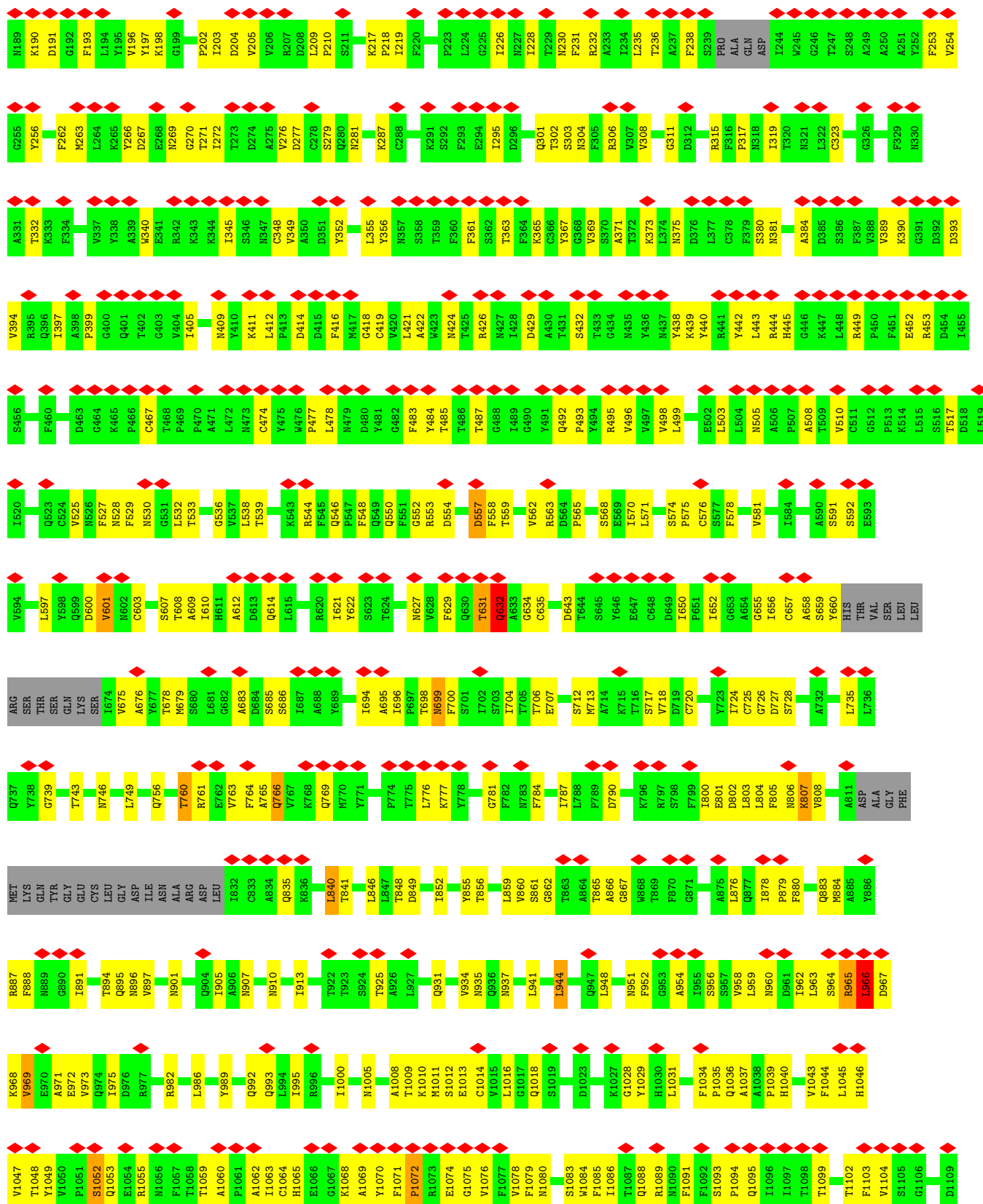
Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1

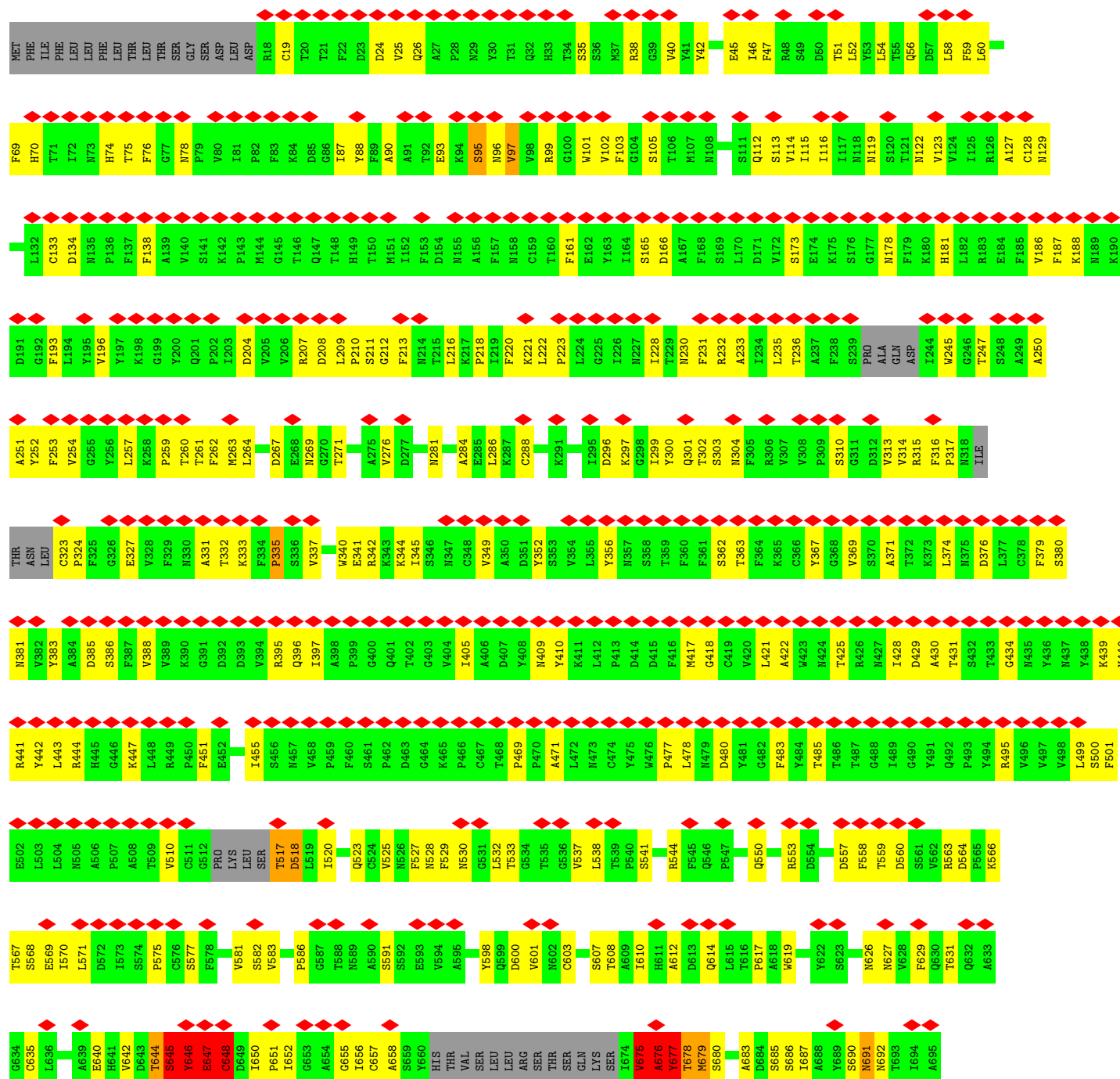




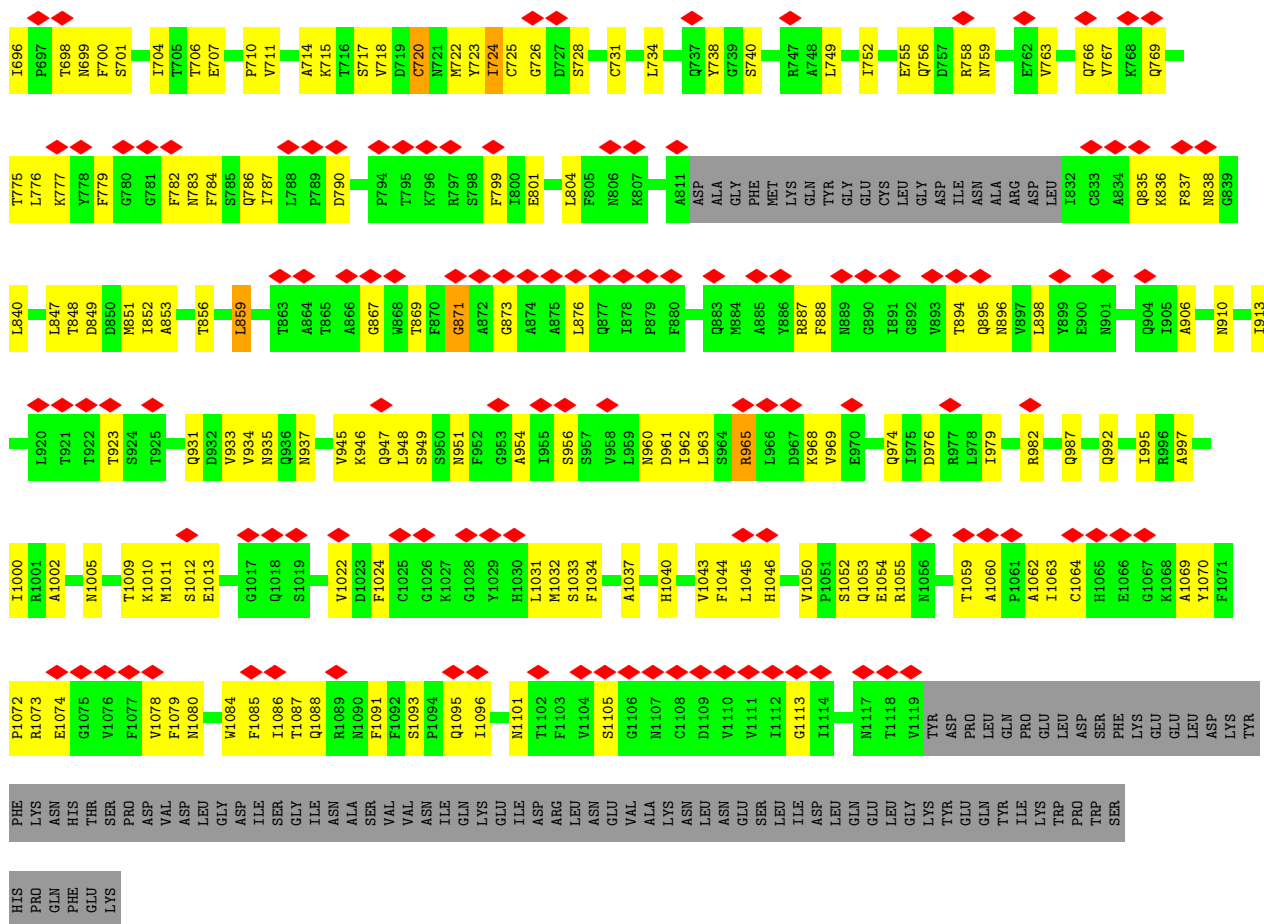
• Molecule 1: Spike glycoprotein



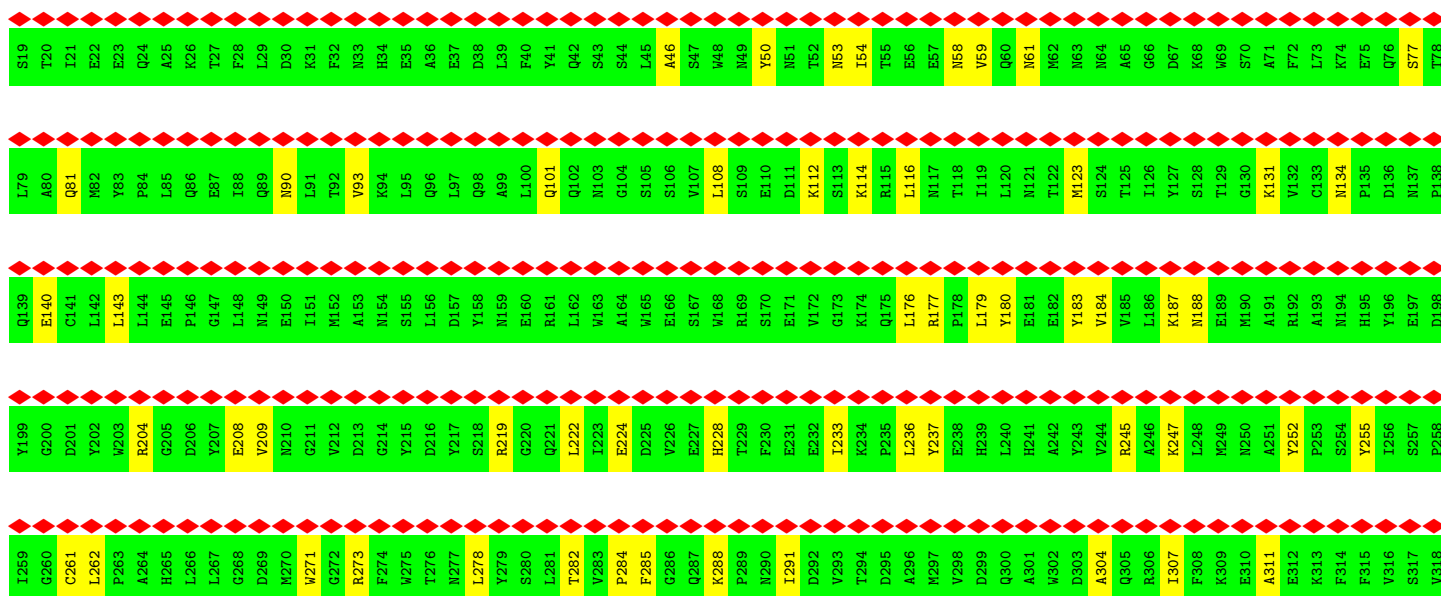
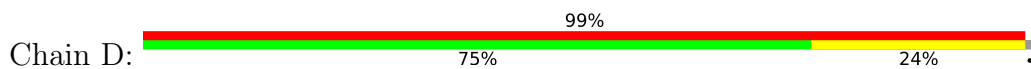








• Molecule 2: Angiotensin-converting enzyme 2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53189	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	28.981	Depositor
Minimum map value	-13.647	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.921	Depositor
Recommended contour level	8	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.55	3/8499 (0.0%)	0.75	6/11568 (0.1%)
1	B	0.55	0/8499	0.76	6/11568 (0.1%)
1	C	0.59	4/8435 (0.0%)	0.80	9/11477 (0.1%)
2	D	0.33	0/5007	0.58	3/6803 (0.0%)
All	All	0.53	7/30440 (0.0%)	0.74	24/41416 (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	17
1	B	0	17
1	C	0	19
2	D	0	2
All	All	0	55

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	677	TYR	CE2-CZ	-8.28	1.27	1.38
1	A	725	CYS	CB-SG	-6.81	1.70	1.82
1	A	731	CYS	CB-SG	-6.41	1.71	1.82
1	C	676	ALA	C-O	-5.93	1.12	1.23
1	A	411	LYS	C-N	-5.48	1.21	1.34
1	C	677	TYR	CD2-CE2	-5.34	1.31	1.39
1	C	677	TYR	CA-CB	-5.11	1.42	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	518	ASP	CB-CG-OD1	9.91	127.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	944	LEU	CA-CB-CG	9.05	136.12	115.30
1	A	557	ASP	CB-CG-OD1	8.32	125.78	118.30
1	A	966	LEU	CA-CB-CG	6.80	130.93	115.30
1	C	644	THR	CA-C-N	-6.62	102.64	117.20
1	C	859	LEU	CA-CB-CG	-6.44	100.49	115.30
1	C	677	TYR	CB-CG-CD2	-6.22	117.27	121.00
2	D	503	LEU	CA-CB-CG	6.22	129.60	115.30
1	A	930	LEU	CB-CG-CD2	-6.10	100.63	111.00
1	C	677	TYR	N-CA-C	5.84	126.76	111.00
1	C	648	CYS	CA-CB-SG	-5.80	103.56	114.00
1	C	675	VAL	C-N-CA	5.75	136.09	121.70
1	C	647	GLU	C-N-CA	-5.59	107.73	121.70
2	D	558	LEU	CB-CG-CD1	-5.56	101.56	111.00
1	A	745	LEU	CA-CB-CG	-5.37	102.94	115.30
1	C	646	TYR	N-CA-CB	-5.37	100.94	110.60
2	D	558	LEU	CA-CB-CG	5.35	127.61	115.30
1	B	840	LEU	CA-CB-CG	-5.27	103.17	115.30
1	B	411	LYS	C-N-CA	5.23	134.78	121.70
1	B	966	LEU	CB-CG-CD1	5.19	119.83	111.00
1	B	557	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	216	LEU	CA-CB-CG	-5.10	103.58	115.30
1	A	504	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	735	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1023	ASP	Peptide
1	A	1052	SER	Peptide
1	A	1074	GLU	Peptide
1	A	172	VAL	Peptide
1	A	206	VAL	Peptide
1	A	415	ASP	Peptide
1	A	416	PHE	Peptide
1	A	558	PHE	Peptide
1	A	621	ILE	Peptide
1	A	632	GLN	Peptide
1	A	726	GLY	Peptide
1	A	727	ASP	Peptide
1	A	728	SER	Peptide
1	A	763	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	776	LEU	Peptide
1	A	781	GLY	Peptide
1	A	968	LYS	Peptide
1	B	1052	SER	Peptide
1	B	1074	GLU	Peptide
1	B	412	LEU	Peptide
1	B	548	PHE	Peptide
1	B	562	VAL	Peptide
1	B	632	GLN	Peptide
1	B	706	THR	Peptide
1	B	726	GLY	Peptide
1	B	727	ASP	Peptide
1	B	728	SER	Peptide
1	B	766	GLN	Peptide
1	B	776	LEU	Peptide
1	B	781	GLY	Peptide
1	B	879	PRO	Peptide
1	B	966	LEU	Peptide
1	B	967	ASP	Peptide
1	B	968	LYS	Peptide
1	C	1074	GLU	Peptide
1	C	221	LYS	Peptide
1	C	327	GLU	Peptide
1	C	335	PRO	Peptide
1	C	380	SER	Peptide
1	C	455	ILE	Peptide
1	C	510	VAL	Peptide
1	C	517	THR	Peptide
1	C	527	PHE	Peptide
1	C	558	PHE	Peptide
1	C	559	THR	Peptide
1	C	629	PHE	Peptide
1	C	644	THR	Mainchain
1	C	724	ILE	Peptide
1	C	776	LEU	Peptide
1	C	871	GLY	Peptide
1	C	923	THR	Peptide
1	C	95	SER	Peptide
1	C	97	VAL	Peptide
2	D	338	ASN	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	299	0
1	B	8302	0	8082	300	0
1	C	8241	0	8011	339	0
2	D	4870	0	4643	87	0
All	All	29715	0	28818	983	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (983) 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:656:ILE:CG1	1:C:677:TYR:O	1.89	1.21
1:C:678:THR:O	1:C:679:MET:HB2	1.43	1.18
1:C:656:ILE:HG12	1:C:677:TYR:O	1.00	1.17
1:C:647:GLU:O	1:C:648:CYS:CB	1.91	1.14
1:C:646:TYR:C	1:C:680:SER:OG	1.94	1.06
1:C:645:SER:HB3	1:C:679:MET:C	1.74	1.05
1:C:645:SER:OG	1:C:677:TYR:HD2	1.39	1.05
1:C:646:TYR:N	1:C:680:SER:H	1.57	1.03
1:C:69:PHE:HB2	1:C:252:TYR:O	1.60	1.01
1:C:645:SER:OG	1:C:677:TYR:CD2	2.11	1.01
1:C:678:THR:O	1:C:679:MET:CB	2.07	0.99
1:C:645:SER:OG	1:C:679:MET:N	1.96	0.98
1:A:194:LEU:O	1:A:221:LYS:HA	1.63	0.98
1:C:193:PHE:HA	1:C:222:LEU:O	1.68	0.94
1:C:647:GLU:O	1:C:648:CYS:HB3	1.68	0.93
2:D:554:LEU:O	2:D:558:LEU:HB2	1.69	0.93
1:C:642:VAL:CG1	1:C:675:VAL:HG12	2.00	0.92
1:C:418:GLY:HA3	1:C:499:LEU:O	1.69	0.91
1:C:103:PHE:HB2	1:C:114:VAL:O	1.70	0.91
1:B:140:VAL:O	1:B:238:PHE:HA	1.70	0.90
1:A:524:CYS:HA	1:A:536:GLY:O	1.73	0.89
1:B:345:ILE:O	1:B:381:ASN:HA	1.74	0.88
1:C:647:GLU:O	1:C:648:CYS:HB2	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLU:O	1:C:181:HIS:HB2	1.74	0.87
1:B:115:ILE:O	1:B:125:ILE:HA	1.76	0.86
1:B:113:SER:O	1:B:127:ALA:HA	1.75	0.85
1:A:386:SER:HA	1:A:496:VAL:O	1.77	0.84
1:B:897:VAL:O	1:B:901:ASN:HB2	1.79	0.83
1:C:196:VAL:O	1:C:220:PHE:HB2	1.78	0.83
1:C:363:THR:O	1:C:421:LEU:HA	1.79	0.82
1:B:760:THR:O	1:B:764:PHE:HB2	1.80	0.82
1:C:646:TYR:C	1:C:680:SER:HG	1.78	0.82
1:C:646:TYR:N	1:C:680:SER:N	2.27	0.82
1:C:706:THR:HA	1:C:1044:PHE:O	1.79	0.81
1:C:645:SER:CB	1:C:679:MET:H	1.93	0.81
1:C:646:TYR:N	1:C:677:TYR:HE2	1.78	0.80
1:C:677:TYR:HD1	1:C:677:TYR:H	1.32	0.78
1:C:646:TYR:HA	1:C:680:SER:OG	1.83	0.77
1:A:423:TRP:O	1:A:494:TYR:HA	1.84	0.77
1:A:1059:THR:HA	1:A:1080:ASN:H	1.48	0.76
1:B:878:ILE:HB	1:B:883:GLN:HE21	1.51	0.76
1:A:363:THR:HB	1:A:422:ALA:O	1.87	0.75
1:C:646:TYR:CA	1:C:680:SER:OG	2.35	0.74
1:A:140:VAL:O	1:A:238:PHE:HA	1.87	0.74
1:B:90:ALA:HA	1:B:183:ARG:O	1.86	0.74
1:A:102:VAL:HA	1:A:114:VAL:O	1.88	0.73
2:D:291:ILE:HG13	2:D:438:PHE:HB2	1.71	0.73
2:D:346:PRO:HA	2:D:359:LEU:O	1.88	0.73
1:B:389:VAL:O	1:B:493:PRO:HA	1.88	0.73
2:D:378:HIS:HE1	2:D:402:GLU:HA	1.53	0.72
1:C:696:ILE:H	1:C:1055:ARG:H	1.37	0.72
1:C:642:VAL:HG11	1:C:675:VAL:HG12	1.69	0.72
1:C:646:TYR:H	1:C:680:SER:H	1.37	0.72
1:B:133:CYS:HB2	1:B:136:PRO:HD3	1.72	0.71
1:A:335:PRO:HG3	1:A:341:GLU:HB2	1.72	0.71
1:C:646:TYR:HA	1:C:680:SER:CB	2.20	0.71
1:C:646:TYR:HB2	1:C:677:TYR:CE2	2.24	0.71
1:A:87:ILE:HD11	1:A:187:PHE:HB2	1.71	0.71
1:C:113:SER:O	1:C:127:ALA:HA	1.90	0.71
1:A:965:ARG:HB2	1:B:369:VAL:HA	1.73	0.70
1:C:101:TRP:HB2	1:C:116:ILE:O	1.90	0.70
1:C:102:VAL:HA	1:C:115:ILE:HG12	1.72	0.70
1:C:101:TRP:O	1:C:115:ILE:HA	1.91	0.70
1:C:405:ILE:HG23	1:C:409:ASN:HD22	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:TYR:CA	1:C:680:SER:H	2.06	0.69
1:A:67:THR:HB	1:A:254:VAL:HB	1.75	0.69
1:B:699:ASN:H	1:B:1053:GLN:HB2	1.57	0.69
1:B:32:GLN:HA	1:B:66:VAL:O	1.93	0.69
1:A:182:LEU:HD23	1:A:201:GLN:HB3	1.73	0.69
1:B:856:THR:HG21	1:B:1037:ALA:HB2	1.75	0.68
1:C:323:CYS:HB2	1:C:349:VAL:H	1.57	0.68
1:A:383:TYR:HB2	1:A:500:SER:HB3	1.75	0.68
1:C:528:ASN:HA	1:C:533:THR:HA	1.75	0.68
1:C:696:ILE:HB	1:C:1055:ARG:HB2	1.75	0.67
1:B:190:LYS:O	1:B:193:PHE:HB2	1.94	0.67
1:C:646:TYR:H	1:C:677:TYR:HE2	1.43	0.67
1:C:383:TYR:HB2	1:C:500:SER:HB2	1.77	0.67
1:A:47:PHE:HB3	1:B:552:GLY:HA2	1.77	0.67
1:A:541:SER:HA	1:A:571:LEU:HG	1.76	0.67
1:C:645:SER:HA	1:C:677:TYR:CD2	2.29	0.67
1:C:646:TYR:O	1:C:680:SER:O	2.13	0.66
1:A:960:ASN:HA	1:A:963:LEU:HB2	1.77	0.66
1:B:127:ALA:HB3	1:B:161:PHE:HB3	1.78	0.65
1:C:779:PHE:H	1:C:782:PHE:H	1.43	0.65
2:D:261:CYS:HB2	2:D:488:VAL:HG13	1.78	0.65
1:C:341:GLU:HB2	1:C:386:SER:HB2	1.79	0.65
1:A:549:GLN:O	1:A:563:ARG:NH1	2.29	0.65
1:B:165:SER:OG	1:B:166:ASP:N	2.28	0.65
1:B:608:THR:O	1:B:612:ALA:N	2.29	0.65
1:C:646:TYR:N	1:C:677:TYR:CE2	2.64	0.65
1:A:311:GLY:H	1:A:525:VAL:HG12	1.60	0.65
1:A:887:ARG:NH1	1:A:1032:MET:SD	2.70	0.65
1:B:603:CYS:N	1:B:635:CYS:SG	2.69	0.65
1:A:583:VAL:HA	1:A:595:ALA:O	1.97	0.65
1:B:311:GLY:H	1:B:525:VAL:HG12	1.60	0.65
1:B:95:SER:HB2	1:B:171:ASP:HB3	1.79	0.64
1:A:1036:GLN:HB2	1:A:1043:VAL:HB	1.78	0.64
1:C:301:GLN:NE2	1:C:302:THR:O	2.29	0.64
1:C:388:VAL:HG22	1:C:495:ARG:HG2	1.79	0.64
2:D:208:GLU:OE1	2:D:219:ARG:NH1	2.30	0.64
1:A:683:ALA:HB3	1:C:769:GLN:HA	1.79	0.64
1:B:784:PHE:HA	1:B:787:ILE:HD12	1.78	0.64
1:A:378:CYS:HA	1:A:511:CYS:HA	1.80	0.64
1:A:1062:ALA:O	1:A:1113:GLY:N	2.30	0.64
1:B:18:ARG:N	1:B:133:CYS:HG	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:CYS:O	1:B:499:LEU:HB2	1.98	0.64
1:C:656:ILE:CD1	1:C:677:TYR:O	2.45	0.64
1:B:700:PHE:HA	1:B:1052:SER:H	1.62	0.64
1:C:992:GLN:HA	1:C:995:ILE:HD12	1.79	0.63
1:B:82:PRO:HA	1:B:230:ASN:HA	1.80	0.63
1:B:89:PHE:HB3	1:B:185:PHE:HB2	1.80	0.63
1:B:340:TRP:O	1:B:453:ARG:NH1	2.30	0.63
1:A:325:PHE:HA	1:A:328:VAL:HG12	1.81	0.63
1:A:581:VAL:HA	1:A:597:LEU:O	1.98	0.62
1:A:441:ARG:NH1	1:A:455:ILE:O	2.33	0.62
1:B:650:ILE:HB	1:B:658:ALA:HB3	1.81	0.62
1:A:786:GLN:OE1	1:A:917:GLN:NE2	2.32	0.62
1:A:102:VAL:HG22	1:A:115:ILE:HA	1.81	0.62
1:A:348:CYS:SG	1:A:349:VAL:N	2.72	0.62
1:B:992:GLN:HA	1:B:995:ILE:HD12	1.80	0.62
1:C:645:SER:CB	1:C:679:MET:N	2.59	0.62
1:B:1010:LYS:O	1:B:1014:CYS:N	2.31	0.62
1:C:749:LEU:HA	1:C:752:ILE:HD12	1.81	0.62
1:A:711:VAL:H	1:A:1041:GLY:HA2	1.65	0.62
1:B:763:VAL:HG22	1:B:1008:ALA:HB2	1.81	0.61
1:C:656:ILE:HG13	1:C:678:THR:HA	1.82	0.61
1:A:41:TYR:OH	1:A:188:LYS:NZ	2.31	0.61
1:A:1033:SER:HA	1:A:1045:LEU:O	2.00	0.61
1:C:1063:ILE:HB	1:C:1070:TYR:HB2	1.81	0.61
1:B:553:ARG:HD3	1:B:557:ASP:HA	1.83	0.61
1:B:960:ASN:H	1:B:963:LEU:HD13	1.66	0.61
1:C:704:ILE:HA	1:C:1046:HIS:O	1.99	0.61
1:A:123:VAL:HB	1:A:165:SER:HB3	1.81	0.61
1:C:651:PRO:HA	1:C:657:CYS:HA	1.81	0.61
1:B:717:SER:OG	1:B:718:VAL:N	2.32	0.61
1:C:801:GLU:OE2	1:C:1037:ALA:N	2.33	0.61
1:C:90:ALA:HB3	1:C:253:PHE:HB2	1.83	0.61
1:C:656:ILE:CG1	1:C:678:THR:HA	2.31	0.61
1:B:405:ILE:HG23	1:B:409:ASN:HD22	1.65	0.61
1:C:603:CYS:N	1:C:635:CYS:SG	2.74	0.61
1:A:99:ARG:NH2	1:A:171:ASP:O	2.33	0.61
1:B:262:PHE:HA	1:B:276:VAL:O	2.01	0.61
1:B:393:ASP:O	1:B:397:ILE:N	2.33	0.61
1:B:769:GLN:HE21	1:C:685:SER:H	1.47	0.61
1:C:38:ARG:NH2	1:C:211:SER:O	2.34	0.61
1:A:869:THR:OG1	1:B:1089:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1036:GLN:HB2	1:B:1043:VAL:HB	1.82	0.60
1:A:127:ALA:HB3	1:A:161:PHE:HB3	1.84	0.60
1:A:1031:LEU:N	1:A:1047:VAL:O	2.34	0.60
1:A:385:ASP:HB2	1:A:498:VAL:HB	1.83	0.60
1:A:749:LEU:HA	1:A:752:ILE:HD12	1.83	0.60
1:B:140:VAL:HG13	1:B:145:GLY:HA2	1.84	0.60
1:C:948:LEU:O	1:C:982:ARG:NH2	2.34	0.60
1:B:190:LYS:NZ	1:B:191:ASP:OD2	2.35	0.60
1:B:544:ARG:O	1:B:546:GLN:NE2	2.34	0.60
1:C:626:ASN:ND2	1:C:640:GLU:OE2	2.34	0.60
1:B:897:VAL:HG12	1:B:905:ILE:HD11	1.83	0.60
1:A:306:ARG:HA	1:A:578:PHE:HA	1.82	0.60
1:C:645:SER:CB	1:C:677:TYR:HD2	2.15	0.60
1:A:698:THR:OG1	1:A:1053:GLN:OE1	2.19	0.60
1:B:536:GLY:HA3	1:B:574:SER:HA	1.82	0.60
1:B:777:LYS:NZ	1:B:790:ASP:OD1	2.33	0.60
1:C:722:MET:HA	1:C:726:GLY:HA2	1.84	0.60
1:B:180:LYS:HG3	1:B:202:PRO:HB3	1.83	0.60
1:C:369:VAL:HG21	1:C:374:LEU:HD13	1.84	0.60
1:C:838:ASN:HB2	1:C:840:LEU:HG	1.83	0.59
1:B:348:CYS:SG	1:B:349:VAL:N	2.75	0.59
1:C:35:SER:HB2	1:C:60:LEU:HD21	1.84	0.59
1:C:444:ARG:NH1	1:C:447:LYS:O	2.35	0.59
2:D:285:PHE:H	2:D:437:ASN:HD21	1.50	0.59
1:C:645:SER:HA	1:C:677:TYR:HD2	1.66	0.59
1:C:1096:ILE:O	1:C:1101:ASN:ND2	2.35	0.59
1:C:686:SER:OG	1:C:687:ILE:N	2.36	0.59
1:A:194:LEU:HB3	1:A:222:LEU:O	2.03	0.59
1:A:432:SER:HA	1:A:485:THR:H	1.68	0.59
1:C:262:PHE:HA	1:C:276:VAL:O	2.03	0.59
1:C:310:SER:HB3	1:C:525:VAL:HG12	1.84	0.59
1:C:645:SER:HB3	1:C:680:SER:N	2.15	0.59
2:D:482:ARG:NH1	2:D:608:THR:O	2.35	0.59
1:A:260:THR:HG23	1:A:262:PHE:HE2	1.68	0.59
1:B:861:SER:O	1:B:865:THR:OG1	2.18	0.59
1:A:301:GLN:OE1	1:A:599:GLN:NE2	2.35	0.59
1:C:263:MET:HB3	1:C:276:VAL:HB	1.85	0.59
1:A:782:PHE:HA	1:A:910:ASN:HD21	1.68	0.59
1:C:586:PRO:HG2	1:C:591:SER:HB3	1.85	0.58
1:A:48:ARG:HB2	1:A:266:TYR:HD2	1.68	0.58
1:B:418:GLY:HA3	1:B:499:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:887:ARG:NH1	1:B:1031:LEU:O	2.35	0.58
1:C:871:GLY:N	1:C:873:GLY:O	2.37	0.58
1:C:1093:SER:O	1:C:1095:GLN:NE2	2.36	0.58
1:A:209:LEU:HD12	1:A:210:PRO:HD2	1.85	0.58
1:B:528:ASN:HA	1:B:533:THR:HA	1.83	0.58
1:A:550:GLN:NE2	1:C:45:GLU:OE1	2.35	0.58
1:B:345:ILE:O	1:B:381:ASN:CA	2.50	0.58
1:C:78:ASN:O	1:C:232:ARG:NH2	2.36	0.58
1:C:1053:GLN:OE1	1:C:1055:ARG:NH2	2.36	0.58
2:D:406:GLU:HG3	2:D:518:ARG:HD3	1.84	0.58
1:B:134:ASP:O	1:B:232:ARG:NH1	2.36	0.58
1:C:646:TYR:HA	1:C:680:SER:HB3	1.86	0.58
2:D:557:MET:HG2	2:D:573:VAL:HG22	1.86	0.58
1:A:316:PHE:HE2	1:A:514:LYS:HB2	1.69	0.58
1:C:968:LYS:HG3	1:C:969:VAL:HG23	1.84	0.58
1:B:440:TYR:HE2	1:B:442:TYR:HB3	1.69	0.58
1:B:553:ARG:HG2	1:B:559:THR:H	1.69	0.58
2:D:291:ILE:HD11	2:D:434:THR:HB	1.86	0.58
1:A:659:SER:O	1:A:674:ILE:HA	2.03	0.58
1:B:601:VAL:HG23	1:B:634:GLY:HA3	1.85	0.58
1:B:941:LEU:HD12	1:B:944:LEU:HD23	1.85	0.57
1:A:45:GLU:OE1	1:B:550:GLN:NE2	2.37	0.57
1:B:444:ARG:NH1	1:B:445:HIS:O	2.37	0.57
1:A:553:ARG:H	1:A:559:THR:HA	1.68	0.57
1:B:591:SER:OG	1:B:592:SER:N	2.37	0.57
1:B:1064:CYS:HB2	1:B:1111:VAL:HG11	1.86	0.57
2:D:209:VAL:HG11	2:D:565:PRO:HB3	1.87	0.57
1:A:193:PHE:HA	1:A:223:PRO:HA	1.85	0.57
1:C:646:TYR:O	1:C:680:SER:OG	2.03	0.57
1:A:631:THR:O	1:A:634:GLY:N	2.37	0.57
1:A:229:THR:OG1	1:A:230:ASN:N	2.37	0.57
1:A:609:ALA:HA	1:A:612:ALA:HB3	1.86	0.57
1:A:1057:PHE:HB3	1:A:1079:PHE:HE1	1.69	0.57
1:C:647:GLU:OE1	1:C:648:CYS:O	2.23	0.57
1:A:129:ASN:ND2	1:A:157:PHE:O	2.38	0.57
1:C:267:ASP:OD1	1:C:271:THR:N	2.34	0.57
1:C:598:TYR:HB3	1:C:601:VAL:HG11	1.87	0.57
2:D:81:GLN:NE2	2:D:101:GLN:O	2.37	0.57
1:A:420:VAL:HG13	1:A:498:VAL:HG22	1.87	0.57
1:A:692:ASN:HB3	1:A:1059:THR:H	1.69	0.57
1:A:956:SER:OG	1:A:957:SER:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:HIS:ND1	1:C:250:ALA:O	2.38	0.57
1:A:720:CYS:HA	1:A:723:TYR:HB3	1.85	0.57
1:A:1096:ILE:O	1:A:1101:ASN:ND2	2.37	0.57
2:D:482:ARG:NH2	2:D:611:SER:OG	2.37	0.57
1:A:1054:GLU:O	1:A:1055:ARG:NH1	2.31	0.57
1:A:626:ASN:ND2	1:A:640:GLU:OE2	2.36	0.56
1:A:969:VAL:O	1:A:973:VAL:N	2.38	0.56
1:B:698:THR:OG1	1:B:1055:ARG:NH2	2.38	0.56
1:C:286:LEU:HD22	1:C:583:VAL:HB	1.87	0.56
1:C:784:PHE:HA	1:C:787:ILE:HD12	1.87	0.56
1:A:1093:SER:O	1:A:1095:GLN:NE2	2.37	0.56
1:C:910:ASN:HA	1:C:913:ILE:HD12	1.86	0.56
2:D:304:ALA:HA	2:D:307:ILE:HD12	1.86	0.56
1:A:95:SER:H	1:A:181:HIS:CD2	2.23	0.56
1:A:880:PHE:HA	1:A:883:GLN:HB2	1.86	0.56
1:B:48:ARG:HB2	1:B:266:TYR:HD2	1.69	0.56
1:B:78:ASN:O	1:B:232:ARG:NH2	2.38	0.56
1:B:698:THR:OG1	1:B:1053:GLN:OE1	2.23	0.56
1:C:105:SER:O	1:C:230:ASN:ND2	2.35	0.56
1:C:767:VAL:HG22	1:C:871:GLY:HA2	1.87	0.56
2:D:54:ILE:HB	2:D:341:LYS:HD3	1.88	0.56
1:A:521:LYS:HA	1:A:538:LEU:HB2	1.87	0.56
1:C:324:PRO:HG2	1:C:345:ILE:HG23	1.87	0.56
1:C:341:GLU:O	1:C:385:ASP:HA	2.06	0.56
1:C:755:GLU:OE2	1:C:758:ARG:NH1	2.39	0.56
1:A:678:THR:OG1	1:A:679:MET:N	2.38	0.56
1:A:832:ILE:O	1:B:632:GLN:NE2	2.33	0.56
2:D:473:TRP:O	2:D:477:TRP:HB2	2.06	0.56
1:A:849:ASP:HA	1:A:852:ILE:HD12	1.88	0.56
1:B:315:ARG:NH1	1:B:517:THR:O	2.39	0.56
1:A:807:LYS:O	1:A:931:GLN:NE2	2.39	0.56
1:A:945:VAL:HA	1:A:948:LEU:HD12	1.88	0.56
1:C:24:ASP:HB3	1:C:245:TRP:HE1	1.69	0.56
1:B:267:ASP:OD1	1:B:271:THR:N	2.38	0.56
1:B:712:SER:O	1:B:1040:HIS:ND1	2.36	0.56
1:C:88:TYR:O	1:C:254:VAL:HA	2.05	0.56
1:A:115:ILE:O	1:A:125:ILE:HA	2.06	0.55
1:B:1099:THR:HA	1:B:1102:THR:HG22	1.88	0.55
1:A:527:PHE:O	1:A:533:THR:HA	2.06	0.55
1:A:719:ASP:OD1	1:B:304:ASN:ND2	2.40	0.55
1:A:544:ARG:NE	1:C:269:ASN:OD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1065:HIS:CE1	1:B:1118:THR:H	2.25	0.55
1:B:1072:PRO:HA	1:B:1102:THR:HA	1.87	0.55
1:A:194:LEU:HB3	1:A:222:LEU:H	1.71	0.55
1:C:300:TYR:O	1:C:582:SER:HA	2.07	0.55
1:A:379:PHE:HB2	1:A:510:VAL:HB	1.89	0.55
1:B:179:PHE:HB2	1:B:204:ASP:HA	1.87	0.55
1:C:961:ASP:OD1	1:C:965:ARG:NH2	2.40	0.55
1:B:1072:PRO:HB3	1:B:1086:ILE:HD13	1.89	0.55
2:D:529:LEU:HD11	2:D:554:LEU:HB2	1.89	0.55
1:A:876:LEU:HA	1:B:695:ALA:HB3	1.89	0.55
1:C:577:SER:OG	1:C:600:ASP:O	2.23	0.55
1:A:35:SER:OG	1:A:64:SER:N	2.38	0.55
1:C:303:SER:OG	1:C:304:ASN:N	2.40	0.55
1:C:563:ARG:HG3	1:C:569:GLU:HG2	1.88	0.55
1:C:650:ILE:HB	1:C:658:ALA:HB3	1.89	0.55
1:A:807:LYS:NZ	1:A:920:LEU:O	2.33	0.55
1:B:429:ASP:OD1	1:B:495:ARG:NH2	2.40	0.55
1:B:656:ILE:HA	1:B:678:THR:HA	1.88	0.55
1:B:960:ASN:HA	1:B:963:LEU:HB2	1.89	0.55
1:C:563:ARG:HH22	1:C:567:THR:HA	1.72	0.55
1:B:631:THR:O	1:B:634:GLY:N	2.39	0.54
1:B:962:ILE:HG13	1:B:963:LEU:HD12	1.88	0.54
1:C:469:PRO:HA	1:C:471:ALA:H	1.72	0.54
2:D:331:SER:HA	2:D:357:ARG:HD3	1.88	0.54
1:B:439:LYS:HD3	1:B:478:LEU:HB3	1.87	0.54
1:A:227:ASN:OD1	1:B:449:ARG:NH2	2.34	0.54
1:C:440:TYR:O	1:C:478:LEU:HA	2.06	0.54
1:C:529:PHE:N	1:C:532:LEU:O	2.31	0.54
1:C:608:THR:O	1:C:612:ALA:N	2.31	0.54
1:A:717:SER:OG	1:A:718:VAL:N	2.40	0.54
1:B:643:ASP:OD1	1:B:643:ASP:N	2.39	0.54
1:C:715:LYS:HA	1:C:756:GLN:HE22	1.71	0.54
1:A:962:ILE:HG13	1:A:963:LEU:HD12	1.89	0.54
1:B:53:TYR:O	1:B:263:MET:HA	2.07	0.54
2:D:375:GLU:HA	2:D:378:HIS:HD2	1.73	0.54
2:D:469:PRO:HD2	2:D:472:GLN:HB2	1.90	0.54
1:A:52:LEU:HA	1:A:264:LEU:O	2.08	0.54
1:A:761:ARG:O	1:A:764:PHE:N	2.41	0.54
1:C:128:CYS:SG	1:C:129:ASN:N	2.76	0.54
1:A:964:SER:OG	1:A:965:ARG:N	2.41	0.54
1:B:306:ARG:HA	1:B:578:PHE:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1029:TYR:HB2	1:B:1049:TYR:HB3	1.90	0.54
1:C:52:LEU:HA	1:C:264:LEU:O	2.07	0.54
1:C:335:PRO:HD2	1:C:341:GLU:HG2	1.89	0.54
2:D:362:THR:HG23	2:D:368:ASP:HB3	1.89	0.54
1:B:140:VAL:HG11	1:B:236:THR:HB	1.89	0.53
1:C:78:ASN:ND2	1:C:233:ALA:O	2.41	0.53
1:A:711:VAL:N	1:A:1040:HIS:O	2.41	0.53
1:A:846:LEU:O	1:B:655:GLY:N	2.40	0.53
1:A:988:THR:OG1	1:C:987:GLN:NE2	2.42	0.53
1:C:1073:ARG:HE	1:C:1101:ASN:HA	1.72	0.53
1:A:134:ASP:O	1:A:232:ARG:NH1	2.41	0.53
1:A:1080:ASN:HA	1:A:1083:SER:HA	1.89	0.53
1:B:99:ARG:NH2	1:B:171:ASP:O	2.42	0.53
1:C:645:SER:HB3	1:C:679:MET:CA	2.37	0.53
2:D:134:ASN:ND2	2:D:140:GLU:OE1	2.41	0.53
2:D:560:LEU:HD22	2:D:569:ALA:HB2	1.89	0.53
1:B:769:GLN:HA	1:C:683:ALA:HB3	1.90	0.53
1:B:982:ARG:O	1:B:986:LEU:HB2	2.07	0.53
1:C:710:PRO:HB2	1:C:1000:ILE:HD11	1.89	0.53
1:C:763:VAL:O	1:C:766:GLN:NE2	2.41	0.53
2:D:183:TYR:OH	2:D:509:ASP:OD1	2.26	0.53
2:D:439:LEU:HB3	2:D:591:LEU:HD22	1.91	0.53
1:A:755:GLU:O	1:A:759:ASN:ND2	2.42	0.53
1:C:93:GLU:HB3	1:C:96:ASN:H	1.73	0.53
1:C:607:SER:HA	1:C:610:ILE:HD12	1.91	0.53
1:A:56:GLN:HA	1:A:261:THR:HA	1.91	0.53
1:A:131:GLU:OE1	1:A:155:ASN:ND2	2.42	0.53
1:C:707:GLU:HB3	1:C:1044:PHE:HB2	1.90	0.53
1:A:92:THR:HB	1:A:179:PHE:HB3	1.90	0.53
1:A:721:ASN:HD22	1:B:304:ASN:HD22	1.56	0.53
1:B:659:SER:OG	1:B:660:TYR:N	2.36	0.53
1:A:719:ASP:O	1:A:723:TYR:N	2.42	0.53
1:B:807:LYS:O	1:B:931:GLN:NE2	2.41	0.53
1:C:887:ARG:NH1	1:C:1032:MET:SD	2.81	0.53
1:A:106:THR:H	1:A:111:SER:HB3	1.73	0.52
1:B:660:TYR:HB2	1:B:675:VAL:HG22	1.91	0.52
1:C:1088:GLN:HG2	1:C:1093:SER:HB2	1.92	0.52
1:A:112:GLN:HA	1:A:128:CYS:O	2.09	0.52
1:A:194:LEU:CB	1:A:222:LEU:O	2.58	0.52
1:A:455:ILE:HD12	1:C:112:GLN:HG2	1.90	0.52
1:B:910:ASN:HA	1:B:913:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:ILE:HD13	1:C:525:VAL:HG11	1.91	0.52
1:A:19:CYS:HA	1:A:133:CYS:HB3	1.92	0.52
1:A:740:SER:OG	1:A:744:GLN:NE2	2.43	0.52
1:A:1059:THR:OG1	1:A:1078:VAL:O	2.24	0.52
1:B:969:VAL:O	1:B:973:VAL:N	2.41	0.52
1:C:376:ASP:OD1	1:C:376:ASP:N	2.41	0.52
1:C:934:VAL:HA	1:C:937:ASN:HD22	1.73	0.52
2:D:370:LEU:HB3	2:D:409:SER:HB2	1.91	0.52
1:B:1009:THR:O	1:B:1012:SER:OG	2.27	0.52
1:C:429:ASP:OD1	1:C:495:ARG:NH2	2.39	0.52
2:D:404:VAL:HG11	2:D:558:LEU:HD11	1.91	0.52
2:D:560:LEU:HD23	2:D:564:GLU:HB2	1.91	0.52
1:A:1108:CYS:HA	1:A:1111:VAL:HG21	1.91	0.52
1:B:397:ILE:HD13	1:B:496:VAL:HG11	1.92	0.52
1:B:896:ASN:OD1	1:C:1105:SER:OG	2.24	0.52
1:C:849:ASP:HA	1:C:852:ILE:HB	1.91	0.52
1:A:282:PRO:HB2	1:A:594:VAL:HG21	1.91	0.52
1:A:601:VAL:HG23	1:A:634:GLY:HA3	1.92	0.52
1:B:1034:PHE:HB2	1:B:1045:LEU:HB2	1.92	0.52
1:C:646:TYR:CA	1:C:680:SER:CB	2.88	0.52
1:A:165:SER:OG	1:A:166:ASP:N	2.37	0.52
1:B:529:PHE:HB2	1:B:532:LEU:HB3	1.91	0.52
2:D:511:SER:HB3	2:D:514:ARG:HE	1.75	0.52
1:A:196:VAL:O	1:A:219:ILE:N	2.41	0.52
1:C:112:GLN:HE21	1:C:129:ASN:HD21	1.58	0.52
1:C:849:ASP:O	1:C:853:ALA:HB2	2.10	0.52
2:D:252:TYR:HB3	2:D:255:TYR:HD2	1.75	0.52
1:C:59:PHE:O	1:C:257:LEU:HA	2.10	0.52
1:C:99:ARG:HG3	1:C:138:PHE:HE2	1.75	0.52
1:C:352:TYR:O	1:C:356:TYR:N	2.42	0.52
1:A:1076:VAL:HG23	1:A:1077:PHE:HB2	1.92	0.51
1:C:642:VAL:CG1	1:C:675:VAL:CG1	2.83	0.51
2:D:116:LEU:HD11	2:D:187:LYS:HE2	1.91	0.51
1:A:361:PHE:HB3	1:A:421:LEU:HD11	1.92	0.51
1:A:804:LEU:HD22	1:A:927:LEU:HD21	1.93	0.51
1:A:992:GLN:HA	1:A:995:ILE:HD12	1.93	0.51
1:B:650:ILE:O	1:B:657:CYS:HA	2.10	0.51
1:C:707:GLU:OE1	1:C:1046:HIS:NE2	2.43	0.51
2:D:585:LEU:O	2:D:589:GLU:HB2	2.10	0.51
1:B:176:SER:OG	1:B:177:GLY:N	2.43	0.51
1:B:1063:ILE:HB	1:B:1070:TYR:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:GLY:CA	1:C:499:LEU:O	2.53	0.51
1:C:698:THR:OG1	1:C:1055:ARG:NH2	2.43	0.51
2:D:589:GLU:HA	2:D:592:PHE:HB3	1.92	0.51
1:C:645:SER:CA	1:C:677:TYR:HD2	2.23	0.51
1:C:655:GLY:O	1:C:678:THR:O	2.29	0.51
2:D:489:GLU:HG3	2:D:492:PRO:HA	1.92	0.51
1:B:1093:SER:O	1:B:1095:GLN:NE2	2.44	0.51
1:C:340:TRP:HH2	1:C:342:ARG:HH21	1.57	0.51
1:A:770:MET:N	1:B:683:ALA:O	2.43	0.51
1:C:1054:GLU:O	1:C:1055:ARG:NH1	2.36	0.51
2:D:356:PHE:HB3	2:D:379:ILE:HD12	1.92	0.51
1:A:51:THR:OG1	1:A:52:LEU:N	2.44	0.51
1:A:267:ASP:OD1	1:A:271:THR:N	2.38	0.51
1:A:707:GLU:OE1	1:A:1046:HIS:NE2	2.44	0.51
1:A:710:PRO:HB2	1:A:1000:ILE:HD11	1.93	0.51
1:B:352:TYR:HA	1:B:355:LEU:HD12	1.93	0.51
1:C:538:LEU:HD22	1:C:570:ILE:HD12	1.93	0.51
1:A:32:GLN:HE22	1:A:67:THR:HG23	1.76	0.51
1:B:539:THR:HG23	1:B:571:LEU:HD12	1.93	0.51
1:B:849:ASP:HA	1:B:852:ILE:HD12	1.93	0.51
1:C:646:TYR:CB	1:C:677:TYR:CE2	2.94	0.51
2:D:580:ASN:HD21	2:D:582:ARG:HD2	1.76	0.51
1:A:553:ARG:HG3	1:C:46:ILE:HG23	1.93	0.51
1:B:867:GLY:HA3	1:B:876:LEU:HB2	1.92	0.51
1:B:1012:SER:HA	1:B:1016:LEU:HD12	1.92	0.51
1:C:1086:ILE:O	1:C:1095:GLN:N	2.32	0.51
1:A:78:ASN:ND2	1:A:233:ALA:O	2.43	0.50
1:A:564:ASP:HB3	1:A:568:SER:H	1.75	0.50
1:A:1012:SER:OG	1:A:1013:GLU:N	2.44	0.50
1:B:658:ALA:HA	1:B:676:ALA:HA	1.92	0.50
1:C:123:VAL:HB	1:C:165:SER:HB3	1.94	0.50
1:C:652:ILE:N	1:C:656:ILE:O	2.44	0.50
1:A:549:GLN:HE22	1:C:47:PHE:HB2	1.76	0.50
1:B:581:VAL:HA	1:B:597:LEU:O	2.12	0.50
1:B:704:ILE:HG12	1:B:1047:VAL:HA	1.94	0.50
1:C:775:THR:HA	1:C:777:LYS:HE3	1.91	0.50
2:D:453:THR:HG21	2:D:516:TYR:HB2	1.93	0.50
1:A:57:ASP:OD2	1:A:188:LYS:NZ	2.45	0.50
1:A:484:TYR:HB2	1:A:487:THR:HB	1.92	0.50
1:A:553:ARG:NH2	1:C:45:GLU:O	2.44	0.50
1:B:203:ILE:HD12	1:B:205:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:PRO:HB2	1:B:319:ILE:HG13	1.93	0.50
1:B:801:GLU:HA	1:B:804:LEU:HD12	1.92	0.50
1:C:367:TYR:HB2	1:C:417:MET:HG2	1.93	0.50
1:C:313:VAL:HA	1:C:518:ASP:HB2	1.94	0.50
1:C:755:GLU:O	1:C:759:ASN:ND2	2.44	0.50
1:B:725:CYS:HA	1:B:959:LEU:HD11	1.93	0.50
1:B:880:PHE:HA	1:B:883:GLN:HB2	1.94	0.50
1:B:1029:TYR:HD2	1:B:1049:TYR:HD2	1.60	0.50
1:C:119:ASN:OD1	1:C:122:ASN:N	2.37	0.50
1:B:93:GLU:HB3	1:B:96:ASN:H	1.77	0.50
1:A:837:PHE:HB3	1:B:575:PRO:HD3	1.94	0.50
1:C:960:ASN:HA	1:C:963:LEU:HD13	1.94	0.50
1:A:128:CYS:SG	1:A:129:ASN:N	2.84	0.50
1:A:894:THR:OG1	1:A:896:ASN:ND2	2.45	0.50
1:B:503:LEU:O	1:B:505:ASN:ND2	2.45	0.50
1:B:1068:LYS:HZ3	1:B:1104:VAL:HG22	1.77	0.50
1:C:645:SER:HG	1:C:677:TYR:HD2	0.60	0.50
1:C:646:TYR:O	1:C:680:SER:N	2.44	0.50
1:C:887:ARG:NH1	1:C:1031:LEU:O	2.37	0.50
1:A:429:ASP:OD1	1:A:495:ARG:NH2	2.44	0.50
1:A:608:THR:O	1:A:612:ALA:N	2.45	0.50
1:B:761:ARG:HH12	1:B:855:TYR:HE2	1.58	0.50
1:B:1005:ASN:O	1:B:1009:THR:OG1	2.22	0.49
1:A:314:VAL:HA	1:A:528:ASN:HB3	1.93	0.49
1:A:580:GLY:H	1:A:599:GLN:HB2	1.77	0.49
1:A:646:TYR:O	1:A:680:SER:N	2.38	0.49
1:B:180:LYS:HA	1:B:202:PRO:HA	1.94	0.49
1:B:610:ILE:O	1:B:622:TYR:OH	2.25	0.49
1:C:42:TYR:HB2	1:C:218:PRO:HD3	1.94	0.49
1:C:235:LEU:HD23	1:C:247:THR:HG21	1.95	0.49
1:C:603:CYS:SG	1:C:627:ASN:ND2	2.85	0.49
1:C:1060:ALA:HB1	1:C:1113:GLY:HA2	1.93	0.49
2:D:90:ASN:HB3	2:D:93:VAL:HG22	1.93	0.49
1:A:959:LEU:HD23	1:A:962:ILE:HD11	1.95	0.49
1:A:1102:THR:OG1	1:A:1103:PHE:N	2.45	0.49
1:B:95:SER:OG	1:B:173:SER:O	2.29	0.49
1:B:399:PRO:HB3	1:B:414:ASP:HA	1.93	0.49
1:B:449:ARG:NH2	1:B:452:GLU:OE2	2.40	0.49
1:B:787:ILE:HA	1:B:800:ILE:HD12	1.94	0.49
1:C:40:VAL:HG21	1:C:213:PHE:HB2	1.94	0.49
1:C:848:THR:HB	1:C:851:MET:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:GLU:OE2	1:A:1037:ALA:N	2.42	0.49
1:A:939:GLN:O	1:A:943:THR:OG1	2.23	0.49
1:B:375:ASN:OD1	1:B:375:ASN:N	2.41	0.49
1:B:424:ASN:OD1	1:B:426:ARG:N	2.45	0.49
2:D:599:ASN:HD22	2:D:602:SER:HB2	1.77	0.49
1:A:1087:THR:HG22	1:A:1094:PRO:HA	1.94	0.49
1:C:867:GLY:HA3	1:C:876:LEU:HD12	1.94	0.49
2:D:188:ASN:HD21	2:D:464:PHE:HA	1.77	0.49
2:D:204:ARG:HG2	2:D:222:LEU:HD23	1.95	0.49
1:A:19:CYS:HB3	1:A:134:ASP:HB2	1.95	0.49
1:C:931:GLN:O	1:C:935:ASN:ND2	2.46	0.49
1:A:343:LYS:HB2	1:A:384:ALA:HB3	1.95	0.49
1:A:551:PHE:O	1:A:553:ARG:NH1	2.46	0.49
1:A:607:SER:HA	1:A:610:ILE:HD12	1.94	0.49
1:A:692:ASN:HD22	1:A:1059:THR:HG23	1.78	0.49
1:B:226:ILE:HG13	1:B:228:ILE:HG13	1.95	0.49
1:B:135:ASN:HA	1:B:232:ARG:HH12	1.78	0.49
1:B:972:GLU:HA	1:B:975:ILE:HB	1.95	0.49
1:C:541:SER:HA	1:C:571:LEU:HG	1.95	0.49
2:D:443:ALA:O	2:D:447:VAL:HB	2.12	0.49
1:A:78:ASN:HB3	1:A:232:ARG:HH21	1.78	0.49
1:A:265:LYS:O	1:A:273:THR:OG1	2.31	0.49
1:B:21:THR:HA	1:B:135:ASN:HB3	1.94	0.49
1:C:1053:GLN:HB3	1:C:1055:ARG:HH12	1.78	0.49
1:A:420:VAL:HG22	1:A:498:VAL:HG13	1.94	0.48
1:A:554:ASP:HB3	1:A:560:ASP:HB2	1.94	0.48
1:C:178:ASN:HB2	1:C:204:ASP:HA	1.94	0.48
1:C:690:SER:OG	1:C:691:ASN:N	2.44	0.48
1:C:954:ALA:HB2	1:C:974:GLN:HB3	1.94	0.48
2:D:184:VAL:HG12	2:D:464:PHE:HE1	1.77	0.48
1:B:48:ARG:HB2	1:B:266:TYR:CD2	2.48	0.48
1:B:323:CYS:N	1:B:348:CYS:SG	2.85	0.48
1:B:352:TYR:HD2	1:B:375:ASN:HA	1.78	0.48
1:B:529:PHE:N	1:B:532:LEU:O	2.41	0.48
1:C:207:ARG:NH1	1:C:208:ASP:OD1	2.46	0.48
1:C:324:PRO:HG2	1:C:345:ILE:HG12	1.94	0.48
1:C:714:ALA:O	1:C:756:GLN:NE2	2.46	0.48
1:C:724:ILE:HD13	1:C:979:ILE:HG23	1.95	0.48
2:D:233:ILE:HD11	2:D:581:VAL:HG21	1.93	0.48
1:A:35:SER:OG	1:A:35:SER:O	2.29	0.48
1:B:138:PHE:HB2	1:B:236:THR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:CYS:SG	1:B:627:ASN:ND2	2.86	0.48
1:B:631:THR:HG21	1:B:652:ILE:HG22	1.95	0.48
1:C:95:SER:OG	1:C:173:SER:O	2.25	0.48
1:C:645:SER:HB3	1:C:679:MET:O	2.11	0.48
1:B:384:ALA:HA	1:B:498:VAL:O	2.13	0.48
1:C:1063:ILE:HD11	1:C:1078:VAL:HG21	1.95	0.48
1:A:57:ASP:OD1	1:A:58:LEU:N	2.46	0.48
1:A:441:ARG:HE	1:A:477:PRO:HB2	1.78	0.48
1:A:642:VAL:HG21	1:A:675:VAL:HB	1.95	0.48
1:B:122:ASN:OD1	1:B:123:VAL:N	2.45	0.48
1:C:397:ILE:HD12	1:C:410:TYR:HD2	1.78	0.48
1:C:431:THR:OG1	1:C:434:GLY:O	2.30	0.48
1:C:853:ALA:O	1:C:856:THR:OG1	2.31	0.48
2:D:247:LYS:HB2	2:D:282:THR:HG22	1.96	0.48
1:A:367:TYR:OH	1:A:397:ILE:O	2.26	0.48
1:A:599:GLN:HA	1:A:633:ALA:HB1	1.96	0.48
1:A:1076:VAL:HG12	1:C:895:GLN:HE22	1.78	0.48
1:C:56:GLN:NE2	1:C:259:PRO:O	2.38	0.48
1:B:707:GLU:HB3	1:B:1044:PHE:HB2	1.95	0.48
1:C:1033:SER:HA	1:C:1045:LEU:O	2.13	0.48
1:A:972:GLU:HA	1:A:975:ILE:HD12	1.95	0.48
1:B:527:PHE:O	1:B:533:THR:HA	2.14	0.48
1:B:1088:GLN:HG3	1:B:1091:PHE:HB3	1.95	0.48
1:C:165:SER:OG	1:C:166:ASP:N	2.45	0.48
1:C:425:THR:HB	1:C:428:ILE:HB	1.96	0.48
1:A:716:THR:HA	1:A:841:THR:O	2.14	0.48
1:A:756:GLN:O	1:A:760:THR:OG1	2.28	0.48
1:B:867:GLY:HA3	1:B:876:LEU:HD12	1.96	0.48
1:B:120:SER:HA	1:B:170:LEU:HD23	1.95	0.48
2:D:123:MET:HB3	2:D:507:SER:HB2	1.96	0.48
2:D:408:MET:O	2:D:412:ALA:CB	2.61	0.48
1:A:1022:VAL:N	1:C:1013:GLU:OE1	2.47	0.47
1:C:332:THR:O	1:C:495:ARG:NH2	2.47	0.47
1:C:612:ALA:O	1:C:614:GLN:NE2	2.31	0.47
1:C:1062:ALA:HB1	1:C:1069:ALA:HB1	1.95	0.47
2:D:346:PRO:HG3	2:D:360:MET:HG3	1.95	0.47
1:A:133:CYS:HB2	1:A:136:PRO:HD3	1.96	0.47
1:A:575:PRO:HB2	1:C:835:GLN:HG2	1.95	0.47
1:A:1069:ALA:HB2	1:A:1111:VAL:HG22	1.96	0.47
1:B:72:ILE:HG13	1:B:75:THR:H	1.79	0.47
1:B:1028:GLY:HA3	1:B:1048:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ARG:HD3	1:C:566:LYS:HD2	1.95	0.47
1:A:374:LEU:HD12	1:A:377:LEU:HD12	1.95	0.47
1:A:694:ILE:H	1:A:1057:PHE:H	1.61	0.47
1:A:803:LEU:HA	1:A:806:ASN:HD22	1.80	0.47
1:B:713:MET:HG3	1:B:756:GLN:NE2	2.28	0.47
1:C:441:ARG:HG3	1:C:477:PRO:HB2	1.95	0.47
2:D:46:ALA:HB1	2:D:61:ASN:HB3	1.97	0.47
1:A:449:ARG:HH22	1:C:228:ILE:H	1.61	0.47
1:A:685:SER:OG	1:A:686:SER:N	2.46	0.47
1:A:782:PHE:HE1	1:A:906:ALA:HA	1.79	0.47
1:B:269:ASN:OD1	1:C:544:ARG:NE	2.48	0.47
1:B:607:SER:HA	1:B:610:ILE:HB	1.95	0.47
2:D:581:VAL:HG22	2:D:584:LEU:HB3	1.96	0.47
1:A:879:PRO:HD3	1:B:694:ILE:HD11	1.95	0.47
1:A:946:LYS:O	1:A:949:SER:OG	2.21	0.47
1:A:366:CYS:HB3	1:A:369:VAL:HG23	1.96	0.47
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.96	0.47
1:A:1088:GLN:HB3	1:A:1090:ASN:H	1.79	0.47
1:B:198:LYS:O	1:B:217:LYS:N	2.34	0.47
1:B:365:LYS:HB3	1:B:367:TYR:HE1	1.79	0.47
1:B:443:LEU:HB2	1:B:477:PRO:HB3	1.97	0.47
1:B:1065:HIS:HB3	1:B:1070:TYR:HE2	1.80	0.47
1:C:371:ALA:HA	1:C:374:LEU:HB2	1.97	0.47
2:D:381:TYR:HB2	2:D:404:VAL:HG11	1.97	0.47
2:D:511:SER:HB3	2:D:514:ARG:HH21	1.80	0.47
1:A:303:SER:OG	1:A:304:ASN:N	2.47	0.47
1:A:315:ARG:HB3	1:A:565:PRO:HD2	1.97	0.47
1:A:797:ARG:HD2	1:A:805:PHE:HE2	1.79	0.47
1:B:196:VAL:O	1:B:219:ILE:N	2.48	0.47
1:B:380:SER:HB2	1:B:508:ALA:HA	1.97	0.47
1:B:578:PHE:O	1:B:600:ASP:HB3	2.15	0.47
1:C:1002:ALA:HA	1:C:1005:ASN:HD22	1.80	0.47
2:D:245:ARG:HA	2:D:262:LEU:HD21	1.97	0.47
2:D:284:PRO:HD3	2:D:440:LEU:HD12	1.97	0.47
1:C:54:LEU:HD21	1:C:288:CYS:HB2	1.97	0.47
2:D:77:SER:O	2:D:81:GLN:N	2.42	0.47
2:D:375:GLU:HA	2:D:378:HIS:CD2	2.49	0.47
1:A:1086:ILE:N	1:A:1095:GLN:O	2.34	0.47
1:B:35:SER:OG	1:B:61:PRO:O	2.33	0.47
1:B:652:ILE:HD12	1:B:656:ILE:HG22	1.97	0.47
1:B:696:ILE:HB	1:B:1055:ARG:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:GLN:O	1:B:935:ASN:ND2	2.48	0.47
2:D:54:ILE:HD12	2:D:341:LYS:HG2	1.96	0.47
1:A:301:GLN:HE22	1:A:581:VAL:H	1.62	0.46
1:A:947:GLN:NE2	1:C:740:SER:OG	2.48	0.46
1:B:287:LYS:HA	1:B:295:ILE:HD11	1.95	0.46
1:B:348:CYS:H	1:B:510:VAL:HG22	1.78	0.46
1:B:884:MET:HA	1:B:887:ARG:HB2	1.97	0.46
1:B:934:VAL:HA	1:B:937:ASN:HD22	1.79	0.46
1:C:26:GLN:H	1:C:75:THR:HA	1.80	0.46
1:C:1079:PHE:CE2	1:C:1084:TRP:HB2	2.50	0.46
1:A:41:TYR:OH	1:A:57:ASP:OD2	2.31	0.46
1:A:502:GLU:HG2	1:A:505:ASN:HD22	1.80	0.46
1:B:108:ASN:O	1:B:111:SER:OG	2.32	0.46
1:B:209:LEU:HD12	1:B:210:PRO:HD2	1.97	0.46
1:B:277:ASP:OD2	1:B:279:SER:OG	2.31	0.46
1:C:342:ARG:HH22	1:C:451:PHE:HB3	1.80	0.46
1:C:720:CYS:HA	1:C:723:TYR:HB3	1.98	0.46
1:C:766:GLN:HE22	1:C:1011:MET:HB3	1.81	0.46
2:D:355:ASP:OD2	2:D:357:ARG:NH1	2.49	0.46
1:A:287:LYS:HA	1:A:295:ILE:HD11	1.98	0.46
1:A:931:GLN:O	1:A:935:ASN:ND2	2.49	0.46
1:B:739:GLY:HA3	1:C:947:GLN:HE22	1.80	0.46
1:B:948:LEU:O	1:B:982:ARG:NH2	2.48	0.46
1:C:441:ARG:HG2	1:C:443:LEU:H	1.81	0.46
1:C:717:SER:OG	1:C:718:VAL:N	2.48	0.46
1:B:487:THR:O	1:B:492:GLN:NE2	2.48	0.46
1:C:617:PRO:HB2	1:C:619:TRP:NE1	2.30	0.46
1:C:677:TYR:CD1	1:C:677:TYR:N	2.71	0.46
2:D:588:PHE:O	2:D:592:PHE:N	2.49	0.46
1:A:196:VAL:HB	1:A:220:PHE:H	1.79	0.46
1:A:467:CYS:HB3	1:A:474:CYS:HB3	1.62	0.46
1:A:840:LEU:HD13	1:A:941:LEU:HD11	1.97	0.46
1:B:301:GLN:NE2	1:B:581:VAL:O	2.48	0.46
1:B:394:VAL:HA	1:B:397:ILE:HD12	1.98	0.46
1:C:344:LYS:NZ	1:C:381:ASN:O	2.39	0.46
1:A:86:GLY:HA3	1:A:257:LEU:HB2	1.98	0.46
1:B:36:SER:OG	1:B:37:MET:N	2.49	0.46
1:B:483:PHE:CD2	1:B:493:PRO:HB3	2.50	0.46
1:B:803:LEU:HA	1:B:806:ASN:HD22	1.81	0.46
1:B:1063:ILE:HD11	1:B:1078:VAL:HG21	1.98	0.46
1:C:631:THR:O	1:C:631:THR:OG1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ASN:O	1:B:99:ARG:NH2	2.49	0.46
1:A:297:LYS:NZ	1:A:649:ASP:OD2	2.44	0.46
1:A:659:SER:OG	1:A:660:TYR:N	2.48	0.46
1:C:87:ILE:HD11	1:C:187:PHE:HD2	1.80	0.46
1:B:552:GLY:N	1:B:559:THR:O	2.46	0.46
1:B:609:ALA:HA	1:B:612:ALA:HB3	1.97	0.46
1:C:337:VAL:HG12	1:C:409:ASN:HB3	1.97	0.46
1:C:550:GLN:OE1	1:C:550:GLN:N	2.49	0.46
1:C:906:ALA:O	1:C:910:ASN:ND2	2.49	0.46
1:C:976:ASP:HA	1:C:979:ILE:HD12	1.97	0.46
1:A:35:SER:O	1:A:63:TYR:N	2.45	0.45
1:A:950:SER:OG	1:A:951:ASN:O	2.34	0.45
1:B:802:ASP:HA	1:B:805:PHE:CD2	2.51	0.45
1:B:835:GLN:NE2	1:C:575:PRO:O	2.42	0.45
1:C:102:VAL:O	1:C:231:PHE:HA	2.15	0.45
1:A:116:ILE:HA	1:A:125:ILE:HG12	1.97	0.45
1:B:951:ASN:ND2	1:B:954:ALA:O	2.40	0.45
1:C:127:ALA:HB3	1:C:161:PHE:HB3	1.97	0.45
1:A:82:PRO:HB2	1:A:84:LYS:HG3	1.98	0.45
1:A:425:THR:HG21	1:A:495:ARG:HD2	1.97	0.45
1:A:696:ILE:HD12	1:A:1057:PHE:HB2	1.99	0.45
1:A:793:LYS:HD3	1:A:793:LYS:HA	1.80	0.45
1:B:67:THR:HB	1:B:254:VAL:HB	1.97	0.45
1:A:190:LYS:HZ1	1:B:416:PHE:HE2	1.64	0.45
1:A:642:VAL:HB	1:A:677:TYR:HB3	1.99	0.45
1:A:786:GLN:HG2	1:A:799:PHE:HD2	1.82	0.45
1:C:779:PHE:HB2	1:C:782:PHE:HB2	1.99	0.45
2:D:271:TRP:O	2:D:481:LYS:NZ	2.50	0.45
2:D:527:GLU:O	2:D:531:GLN:HB2	2.16	0.45
2:D:568:LEU:HD23	2:D:572:ASN:HD21	1.82	0.45
1:A:41:TYR:HB3	1:A:216:LEU:HB2	1.98	0.45
1:B:432:SER:HB3	1:B:485:THR:H	1.82	0.45
1:C:645:SER:CA	1:C:677:TYR:CD2	2.98	0.45
1:C:859:LEU:HD23	1:C:859:LEU:HA	1.75	0.45
1:C:951:ASN:ND2	1:C:954:ALA:O	2.45	0.45
1:B:652:ILE:HD11	1:B:658:ALA:HB2	1.99	0.45
1:B:861:SER:OG	1:B:862:GLY:N	2.49	0.45
1:C:88:TYR:HD1	1:C:186:VAL:HG22	1.81	0.45
1:A:1000:ILE:O	1:A:1003:SER:OG	2.27	0.45
1:B:966:LEU:HB2	1:B:971:ALA:HB2	1.98	0.45
1:C:379:PHE:CD2	1:C:501:PHE:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1034:PHE:HB2	1:A:1045:LEU:HD12	1.98	0.45
1:B:766:GLN:HE22	1:B:1011:MET:HB3	1.82	0.45
1:C:1059:THR:HA	1:C:1080:ASN:H	1.82	0.45
2:D:180:TYR:HA	2:D:183:TYR:HB3	1.99	0.45
1:A:314:VAL:N	1:A:517:THR:OG1	2.36	0.45
1:A:612:ALA:O	1:A:614:GLN:NE2	2.33	0.45
1:A:1011:MET:O	1:A:1015:VAL:HB	2.17	0.45
1:B:174:GLU:HB2	1:B:238:PHE:CE2	2.52	0.45
1:C:38:ARG:NE	1:C:210:PRO:O	2.41	0.45
1:C:323:CYS:HB2	1:C:349:VAL:N	2.29	0.45
1:A:575:PRO:HD3	1:C:837:PHE:HB3	1.99	0.45
1:A:734:LEU:HD11	1:A:972:GLU:HB3	1.99	0.45
1:B:87:ILE:HG22	1:B:256:TYR:HE1	1.81	0.45
1:B:363:THR:HB	1:B:422:ALA:HB3	1.99	0.45
1:B:487:THR:HG23	1:B:492:GLN:HG3	1.99	0.45
1:C:646:TYR:HB3	1:C:677:TYR:OH	2.17	0.45
1:A:194:LEU:HD23	1:A:222:LEU:HB2	1.98	0.44
1:A:525:VAL:O	1:A:535:THR:HA	2.17	0.44
1:B:361:PHE:CG	1:B:421:LEU:HD11	2.52	0.44
1:B:989:TYR:O	1:B:993:GLN:HG2	2.18	0.44
1:B:1069:ALA:HB2	1:B:1111:VAL:HG22	1.99	0.44
1:B:1093:SER:HA	1:B:1094:PRO:HD3	1.83	0.44
1:A:858:ALA:O	1:A:861:SER:OG	2.30	0.44
1:A:961:ASP:O	1:A:965:ARG:NE	2.51	0.44
1:A:1058:THR:OG1	1:A:1080:ASN:O	2.28	0.44
1:A:1089:ARG:HE	1:A:1089:ARG:HB3	1.69	0.44
1:B:440:TYR:O	1:B:478:LEU:HA	2.17	0.44
1:C:76:PHE:HB2	1:C:245:TRP:CZ2	2.53	0.44
1:C:523:GLN:H	1:C:537:VAL:HG13	1.83	0.44
1:C:530:ASN:N	1:C:530:ASN:OD1	2.48	0.44
1:A:41:TYR:HA	1:A:216:LEU:H	1.83	0.44
1:A:182:LEU:HG	1:A:184:GLU:HG3	1.98	0.44
1:A:554:ASP:N	1:A:554:ASP:OD1	2.50	0.44
1:A:976:ASP:HA	1:A:979:ILE:HD12	1.98	0.44
1:B:19:CYS:HB3	1:B:134:ASP:HB2	1.99	0.44
1:B:848:THR:O	1:B:852:ILE:N	2.33	0.44
1:C:24:ASP:OD1	1:C:74:HIS:ND1	2.50	0.44
2:D:408:MET:O	2:D:412:ALA:HB2	2.16	0.44
1:B:964:SER:OG	1:B:965:ARG:N	2.50	0.44
2:D:311:ALA:HA	2:D:373:HIS:CE1	2.52	0.44
1:A:701:SER:N	1:A:1050:VAL:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:HG12	1:B:272:ILE:HD13	1.99	0.44
1:B:81:ILE:O	1:B:231:PHE:N	2.47	0.44
1:B:808:VAL:HG21	1:B:1039:PRO:HG2	1.99	0.44
1:C:19:CYS:HA	1:C:133:CYS:HB3	1.98	0.44
2:D:378:HIS:CE1	2:D:402:GLU:HA	2.43	0.44
1:A:315:ARG:NH2	1:A:566:LYS:HB2	2.32	0.44
1:B:1059:THR:HA	1:B:1080:ASN:H	1.82	0.44
1:C:314:VAL:N	1:C:518:ASP:OD2	2.50	0.44
1:C:675:VAL:HB	1:C:676:ALA:H	1.56	0.44
1:A:897:VAL:HA	1:A:900:GLU:HB2	2.00	0.44
1:B:61:PRO:O	1:B:64:SER:OG	2.34	0.44
1:C:25:VAL:HG13	1:C:76:PHE:HB3	1.99	0.44
1:C:97:VAL:HG13	1:C:236:THR:HG23	1.98	0.44
2:D:50:TYR:CE1	2:D:59:VAL:HB	2.52	0.44
1:B:432:SER:HA	1:B:484:TYR:HA	1.99	0.44
1:C:24:ASP:HB3	1:C:245:TRP:NE1	2.33	0.44
1:C:645:SER:CB	1:C:679:MET:CA	2.95	0.44
1:C:956:SER:HB3	1:C:962:ILE:HG23	2.00	0.44
1:C:1079:PHE:N	1:C:1085:PHE:O	2.51	0.44
1:A:460:PHE:N	1:A:475:TYR:O	2.51	0.44
1:A:951:ASN:ND2	1:A:954:ALA:O	2.38	0.44
1:C:430:ALA:O	1:C:485:THR:OG1	2.35	0.44
1:C:894:THR:OG1	1:C:896:ASN:ND2	2.51	0.44
1:C:1078:VAL:HA	1:C:1086:ILE:HG12	2.00	0.44
2:D:176:LEU:HD23	2:D:179:LEU:HD12	2.00	0.44
1:A:301:GLN:NE2	1:A:302:THR:O	2.40	0.43
1:A:547:PRO:O	1:A:563:ARG:NH2	2.51	0.43
1:A:553:ARG:NH1	1:C:47:PHE:H	2.15	0.43
1:A:679:MET:HB3	1:A:681:LEU:HD13	1.99	0.43
1:A:693:THR:HB	1:A:1058:THR:HG22	1.98	0.43
1:C:95:SER:H	1:C:181:HIS:CD2	2.36	0.43
1:C:1088:GLN:HG3	1:C:1091:PHE:HB3	2.00	0.43
1:A:808:VAL:HG21	1:A:1039:PRO:HG2	1.99	0.43
1:B:891:ILE:HD11	1:B:1029:TYR:HB3	2.00	0.43
1:C:315:ARG:NE	1:C:518:ASP:OD1	2.51	0.43
1:C:362:SER:N	1:C:422:ALA:O	2.50	0.43
1:C:728:SER:HB2	1:C:731:CYS:HB3	2.00	0.43
1:A:630:GLN:HB3	1:A:656:ILE:HD11	2.00	0.43
1:B:126:ARG:HD2	1:B:130:PHE:HZ	1.83	0.43
1:B:429:ASP:OD2	1:B:495:ARG:NE	2.51	0.43
1:B:859:LEU:HD23	1:B:859:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:ASN:HA	1:B:1083:SER:HA	2.00	0.43
1:C:286:LEU:HD21	1:C:300:TYR:HD2	1.84	0.43
1:C:1009:THR:O	1:C:1012:SER:OG	2.29	0.43
1:A:89:PHE:HD2	1:A:185:PHE:HB2	1.82	0.43
1:A:352:TYR:HA	1:A:355:LEU:HD12	2.00	0.43
1:B:79:PRO:HD2	1:B:81:ILE:HD11	2.00	0.43
1:B:724:ILE:HG12	1:B:982:ARG:HB3	1.99	0.43
1:C:260:THR:OG1	1:C:261:THR:N	2.50	0.43
1:C:425:THR:O	1:C:429:ASP:N	2.48	0.43
1:C:564:ASP:HB3	1:C:568:SER:HB3	2.00	0.43
1:C:777:LYS:NZ	1:C:790:ASP:OD1	2.38	0.43
1:C:1005:ASN:O	1:C:1009:THR:OG1	2.22	0.43
2:D:450:LEU:HD21	2:D:519:THR:HG21	1.99	0.43
1:A:998:ALA:O	1:A:1001:ARG:HG2	2.17	0.43
1:C:342:ARG:HD2	1:C:383:TYR:HD1	1.83	0.43
1:C:430:ALA:HB2	1:C:483:PHE:HB3	2.01	0.43
1:C:700:PHE:HA	1:C:1052:SER:N	2.33	0.43
1:C:836:LYS:HB2	1:C:840:LEU:HB2	2.01	0.43
1:A:628:VAL:HG22	1:A:636:LEU:HB3	1.99	0.43
1:A:630:GLN:HG2	1:A:631:THR:H	1.83	0.43
1:B:96:ASN:HB3	1:B:183:ARG:HH21	1.83	0.43
1:B:746:ASN:HA	1:B:749:LEU:HD12	1.99	0.43
1:B:1079:PHE:CE2	1:B:1084:TRP:HB2	2.54	0.43
1:C:440:TYR:HE2	1:C:442:TYR:HB3	1.84	0.43
1:A:473:ASN:HA	1:A:475:TYR:CZ	2.54	0.43
1:B:186:VAL:HB	1:B:197:TYR:HB2	2.00	0.43
1:B:894:THR:OG1	1:B:895:GLN:N	2.52	0.43
1:B:1062:ALA:HB3	1:B:1112:ILE:H	1.84	0.43
1:B:1102:THR:OG1	1:B:1103:PHE:N	2.51	0.43
1:C:301:GLN:HE22	1:C:581:VAL:N	2.17	0.43
1:C:342:ARG:NH2	1:C:451:PHE:HB3	2.33	0.43
1:C:997:ALA:HA	1:C:1000:ILE:HG22	2.01	0.43
2:D:224:GLU:O	2:D:228:HIS:HB2	2.19	0.43
2:D:526:GLN:HG3	2:D:539:LEU:HD11	2.00	0.43
1:A:1028:GLY:HA3	1:A:1048:THR:HB	1.99	0.43
1:B:205:VAL:HG21	1:B:210:PRO:HG3	1.99	0.43
1:C:209:LEU:HD12	1:C:210:PRO:HD2	2.00	0.43
1:C:299:ILE:HG13	1:C:650:ILE:HG22	1.99	0.43
1:A:78:ASN:HD21	1:A:232:ARG:HB3	1.83	0.43
1:A:545:PHE:HE2	1:A:563:ARG:HD2	1.84	0.43
1:B:1060:ALA:HB1	1:B:1113:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LYS:H	1:A:217:LYS:H	1.67	0.43
1:A:807:LYS:HD3	1:A:807:LYS:HA	1.84	0.43
1:A:1036:GLN:HE21	1:A:1045:LEU:HD11	1.84	0.43
1:A:683:ALA:O	1:C:769:GLN:NE2	2.52	0.42
1:A:698:THR:HA	1:A:1092:PHE:HB3	2.00	0.42
1:A:886:TYR:HA	1:A:889:ASN:ND2	2.33	0.42
1:A:1098:THR:H	1:A:1101:ASN:HB2	1.83	0.42
1:B:538:LEU:HB3	1:B:570:ILE:HD12	2.00	0.42
1:B:717:SER:HA	1:B:749:LEU:HD22	2.01	0.42
1:C:646:TYR:H	1:C:680:SER:N	2.03	0.42
1:C:777:LYS:O	1:C:783:ASN:HA	2.19	0.42
1:C:933:VAL:O	1:C:937:ASN:ND2	2.52	0.42
1:A:901:ASN:HB3	1:A:904:GLN:HB3	2.00	0.42
1:B:302:THR:OG1	1:B:303:SER:N	2.52	0.42
1:B:553:ARG:HA	1:B:558:PHE:H	1.84	0.42
1:B:761:ARG:NH2	1:B:765:ALA:HB2	2.33	0.42
1:C:316:PHE:HA	1:C:317:PRO:HD3	1.83	0.42
1:C:331:ALA:O	1:C:495:ARG:NH1	2.52	0.42
1:C:731:CYS:HA	1:C:734:LEU:HD12	2.01	0.42
1:C:1064:CYS:HA	1:C:1069:ALA:HA	2.01	0.42
2:D:50:TYR:HA	2:D:58:ASN:HB3	2.01	0.42
1:B:119:ASN:OD1	1:B:122:ASN:N	2.49	0.42
1:C:945:VAL:HA	1:C:948:LEU:HD12	2.01	0.42
1:C:1034:PHE:HB2	1:C:1045:LEU:HB2	2.01	0.42
2:D:237:TYR:OH	2:D:485:VAL:O	2.25	0.42
1:A:76:PHE:HE1	1:A:235:LEU:HD22	1.84	0.42
1:A:379:PHE:O	1:A:510:VAL:N	2.39	0.42
1:A:396:GLN:HA	1:A:401:GLN:HB3	2.01	0.42
1:A:469:PRO:HA	1:A:471:ALA:H	1.84	0.42
1:B:197:TYR:HD1	1:B:218:PRO:HA	1.85	0.42
1:B:281:ASN:HB2	1:B:621:ILE:HD12	2.00	0.42
1:B:421:LEU:HD12	1:B:421:LEU:HA	1.85	0.42
1:B:685:SER:OG	1:B:686:SER:N	2.53	0.42
1:C:56:GLN:HA	1:C:261:THR:HA	2.01	0.42
1:C:211:SER:OG	1:C:212:GLY:N	2.50	0.42
1:C:646:TYR:CB	1:C:677:TYR:HE2	2.32	0.42
1:C:946:LYS:O	1:C:949:SER:OG	2.23	0.42
2:D:278:LEU:O	2:D:282:THR:N	2.52	0.42
1:A:181:HIS:HA	1:A:200:TYR:HE1	1.85	0.42
1:B:57:ASP:OD1	1:B:58:LEU:N	2.52	0.42
1:B:267:ASP:OD1	1:B:270:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:SER:N	1:B:485:THR:OG1	2.52	0.42
1:B:530:ASN:OD1	1:B:530:ASN:N	2.52	0.42
1:C:786:GLN:HG2	1:C:799:PHE:HB3	2.01	0.42
1:A:149:HIS:NE2	1:A:151:MET:SD	2.93	0.42
1:A:374:LEU:HD11	1:A:379:PHE:HZ	1.83	0.42
1:A:390:LYS:HG2	1:A:483:PHE:HE1	1.85	0.42
1:A:769:GLN:NE2	1:B:683:ALA:O	2.52	0.42
1:A:1076:VAL:HG12	1:C:895:GLN:NE2	2.34	0.42
1:B:60:LEU:HD12	1:B:61:PRO:HD2	2.02	0.42
1:B:532:LEU:HD12	1:B:532:LEU:HA	1.84	0.42
1:C:222:LEU:HA	1:C:223:PRO:HD3	1.92	0.42
1:C:296:ASP:HB3	1:C:297:LYS:H	1.62	0.42
1:C:645:SER:CB	1:C:679:MET:C	2.66	0.42
1:C:1010:LYS:HG2	1:C:1024:PHE:CE2	2.54	0.42
2:D:460:ARG:HD2	2:D:506:VAL:HG22	2.02	0.42
1:B:867:GLY:H	1:B:883:GLN:NE2	2.18	0.42
1:B:1013:GLU:OE2	1:C:1022:VAL:N	2.53	0.42
1:C:315:ARG:HG2	1:C:517:THR:HA	2.01	0.42
1:C:439:LYS:HG2	1:C:480:ASP:HA	2.01	0.42
1:A:749:LEU:HD23	1:A:752:ILE:HD12	2.02	0.42
1:B:35:SER:HB2	1:B:60:LEU:HD21	2.02	0.42
1:B:38:ARG:NH2	1:B:210:PRO:O	2.44	0.42
1:B:51:THR:OG1	1:B:52:LEU:N	2.53	0.42
1:B:138:PHE:HB3	1:B:140:VAL:HG23	2.02	0.42
1:B:756:GLN:O	1:B:760:THR:OG1	2.35	0.42
1:B:951:ASN:OD1	1:B:952:PHE:N	2.50	0.42
1:A:321:ASN:HB3	1:A:348:CYS:HA	2.01	0.42
1:A:859:LEU:HD23	1:A:859:LEU:HA	1.87	0.42
1:B:1071:PHE:HB2	1:B:1103:PHE:CZ	2.55	0.42
1:A:848:THR:HB	1:A:851:MET:HB2	2.02	0.41
1:B:54:LEU:HA	1:B:262:PHE:O	2.20	0.41
1:B:126:ARG:HD2	1:B:130:PHE:CZ	2.55	0.41
1:B:467:CYS:HB2	1:B:474:CYS:HB3	1.93	0.41
1:B:41:TYR:CE2	1:B:43:PRO:HA	2.54	0.41
1:B:438:TYR:HD1	1:B:438:TYR:HA	1.71	0.41
1:B:846:LEU:O	1:C:655:GLY:N	2.52	0.41
1:B:1000:ILE:HD12	1:B:1000:ILE:HA	1.89	0.41
1:B:1031:LEU:N	1:B:1047:VAL:O	2.53	0.41
1:C:701:SER:N	1:C:1050:VAL:O	2.50	0.41
1:C:887:ARG:HG2	1:C:1032:MET:SD	2.60	0.41
1:A:390:LYS:HG2	1:A:483:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:THR:OG1	1:B:679:MET:N	2.53	0.41
1:B:887:ARG:O	1:B:1018:GLN:NE2	2.43	0.41
1:C:51:THR:OG1	1:C:52:LEU:N	2.53	0.41
1:A:140:VAL:HG22	1:A:147:GLN:HG2	2.01	0.41
1:A:197:TYR:HB3	1:A:216:LEU:HB3	2.02	0.41
1:A:859:LEU:O	1:A:863:THR:OG1	2.23	0.41
1:B:1059:THR:OG1	1:B:1060:ALA:N	2.53	0.41
1:C:281:ASN:HB3	1:C:284:ALA:H	1.84	0.41
2:D:108:LEU:HD13	2:D:112:LYS:HB3	2.02	0.41
1:A:190:LYS:NZ	1:A:191:ASP:OD2	2.54	0.41
1:A:530:ASN:OD1	1:A:531:GLY:N	2.50	0.41
1:A:997:ALA:HA	1:A:1000:ILE:HG22	2.02	0.41
1:B:308:VAL:HB	1:B:614:GLN:HB3	2.02	0.41
2:D:131:LYS:HB3	2:D:143:LEU:HG	2.01	0.41
1:A:24:ASP:HB3	1:A:245:TRP:HE1	1.86	0.41
1:A:559:THR:O	1:A:561:SER:N	2.53	0.41
1:A:699:ASN:HD22	1:A:699:ASN:HA	1.66	0.41
1:C:725:CYS:HB2	1:C:728:SER:HB3	2.01	0.41
1:C:1087:THR:OG1	1:C:1088:GLN:O	2.29	0.41
2:D:412:ALA:HA	2:D:417:HIS:CG	2.56	0.41
1:A:47:PHE:CZ	1:A:49:SER:HB2	2.56	0.41
1:A:101:TRP:O	1:A:116:ILE:HB	2.20	0.41
1:A:916:ILE:HD13	1:A:916:ILE:HA	1.89	0.41
1:B:98:VAL:HG12	1:B:235:LEU:HG	2.01	0.41
1:C:101:TRP:HB3	1:C:103:PHE:CE2	2.55	0.41
1:C:342:ARG:HD2	1:C:383:TYR:CD1	2.55	0.41
1:C:698:THR:OG1	1:C:1053:GLN:OE1	2.38	0.41
2:D:288:LYS:HD3	2:D:288:LYS:HA	1.93	0.41
2:D:473:TRP:O	2:D:477:TRP:CB	2.68	0.41
1:B:149:HIS:CD2	1:B:151:MET:HB3	2.56	0.41
1:B:315:ARG:HB3	1:B:565:PRO:HD2	2.02	0.41
1:B:356:TYR:CE1	1:B:371:ALA:HB1	2.56	0.41
1:B:627:ASN:HB3	1:B:629:PHE:HE1	1.86	0.41
1:B:704:ILE:HA	1:B:1046:HIS:O	2.20	0.41
1:B:840:LEU:HD23	1:B:840:LEU:HA	1.82	0.41
1:B:860:VAL:HG22	1:B:1035:PRO:HD2	2.03	0.41
1:B:907:ASN:HA	1:B:910:ASN:HD22	1.85	0.41
2:D:554:LEU:HG	2:D:558:LEU:HD13	2.02	0.41
1:A:69:PHE:O	1:A:251:ALA:HA	2.21	0.41
1:A:100:GLY:HA3	1:A:234:ILE:HB	2.02	0.41
1:A:527:PHE:HB2	1:A:534:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:ARG:HD3	1:A:1055:ARG:HA	1.92	0.41
1:B:112:GLN:HE21	1:B:129:ASN:HD21	1.68	0.41
1:B:332:THR:HG22	1:B:495:ARG:HH22	1.84	0.41
1:B:563:ARG:HA	1:B:568:SER:O	2.21	0.41
1:B:888:PHE:HD1	1:B:888:PHE:HA	1.72	0.41
1:C:315:ARG:HG3	1:C:518:ASP:OD2	2.21	0.41
1:C:440:TYR:CE2	1:C:442:TYR:HB3	2.56	0.41
1:C:784:PHE:HB3	1:C:787:ILE:HB	2.03	0.41
1:C:1000:ILE:HD12	1:C:1000:ILE:HA	1.81	0.41
2:D:407:ILE:HD13	2:D:407:ILE:HA	1.81	0.41
2:D:611:SER:HB2	2:D:614:ALA:HB3	2.03	0.41
1:A:769:GLN:HA	1:B:683:ALA:HB3	2.03	0.41
1:B:743:THR:HA	1:B:746:ASN:HD22	1.85	0.41
1:C:40:VAL:O	1:C:216:LEU:N	2.47	0.41
1:C:804:LEU:HD13	1:C:1043:VAL:HG21	2.03	0.41
1:C:840:LEU:HA	1:C:840:LEU:HD23	1.83	0.41
1:C:869:THR:HB	1:C:876:LEU:HD11	2.02	0.41
1:C:888:PHE:CE2	1:C:898:LEU:HB2	2.55	0.41
1:C:961:ASP:O	1:C:965:ARG:NE	2.53	0.41
1:C:1078:VAL:HG22	1:C:1086:ILE:HG12	2.02	0.41
1:A:881:ALA:O	1:A:885:ALA:HB2	2.21	0.40
1:B:390:LYS:HG2	1:B:483:PHE:HE1	1.85	0.40
1:C:723:TYR:HD2	1:C:724:ILE:HG13	1.85	0.40
2:D:177:ARG:HD3	2:D:498:CYS:HB2	2.04	0.40
1:A:347:ASN:H	1:A:509:THR:HB	1.85	0.40
1:A:575:PRO:O	1:C:835:GLN:NE2	2.54	0.40
1:A:713:MET:HG3	1:A:756:GLN:NE2	2.36	0.40
1:A:786:GLN:HG2	1:A:799:PHE:CD2	2.56	0.40
1:B:20:THR:HB	1:B:136:PRO:HA	2.02	0.40
1:B:866:ALA:O	1:B:876:LEU:N	2.55	0.40
1:B:956:SER:HG	1:B:958:VAL:H	1.67	0.40
1:C:58:LEU:HB2	1:C:188:LYS:HE3	2.02	0.40
1:C:70:HIS:CE1	1:C:251:ALA:HB2	2.56	0.40
1:C:193:PHE:CD1	1:C:223:PRO:HA	2.56	0.40
1:C:782:PHE:HD1	1:C:782:PHE:HA	1.80	0.40
2:D:524:GLN:NE2	2:D:580:ASN:H	2.19	0.40
1:A:301:GLN:HA	1:A:582:SER:HA	2.03	0.40
1:A:648:CYS:HB2	1:A:679:MET:HG3	2.03	0.40
1:A:930:LEU:HD21	1:A:1041:GLY:HA3	2.04	0.40
1:A:1064:CYS:HB2	1:A:1111:VAL:HG11	2.01	0.40
1:B:1085:PHE:HB3	1:B:1095:GLN:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ASP:O	1:C:232:ARG:NH1	2.40	0.40
1:C:711:VAL:HG22	1:C:1040:HIS:C	2.42	0.40
1:C:1031:LEU:HD12	1:C:1031:LEU:HA	1.85	0.40
1:A:123:VAL:HG23	1:A:168:PHE:HE1	1.85	0.40
1:B:25:VAL:HA	1:B:76:PHE:HB3	2.02	0.40
1:B:90:ALA:HB3	1:B:253:PHE:HB2	2.03	0.40
1:B:784:PHE:HD1	1:B:787:ILE:HG21	1.85	0.40
1:C:647:GLU:CD	1:C:647:GLU:C	2.79	0.40
2:D:236:LEU:HD21	2:D:588:PHE:HD2	1.85	0.40
1:A:99:ARG:HH12	1:A:172:VAL:HG13	1.86	0.40
1:A:267:ASP:OD1	1:A:267:ASP:N	2.55	0.40
1:A:777:LYS:NZ	1:A:790:ASP:OD1	2.40	0.40
1:B:35:SER:OG	1:B:35:SER:O	2.39	0.40
1:B:554:ASP:OD1	1:B:554:ASP:N	2.53	0.40
1:C:314:VAL:HA	1:C:528:ASN:O	2.22	0.40
1:C:395:ARG:HG3	1:C:396:GLN:HG3	2.03	0.40
1:C:847:LEU:HG	1:C:852:ILE:HG13	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	850 (80%)	203 (19%)	4 (0%)	30	68
1	B	1057/1203 (88%)	836 (79%)	213 (20%)	8 (1%)	16	54
1	C	1045/1203 (87%)	834 (80%)	201 (19%)	10 (1%)	13	49
2	D	595/603 (99%)	565 (95%)	30 (5%)	0	100	100
All	All	3754/4212 (89%)	3085 (82%)	647 (17%)	22 (1%)	24	60

All (22) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	C	645	SER
1	C	648	CYS
1	C	675	VAL
1	C	676	ALA
1	C	679	MET
1	C	692	ASN
1	C	1072	PRO
1	A	1072	PRO
1	B	632	GLN
1	B	925	THR
1	C	557	ASP
1	C	560	ASP
1	C	691	ASN
1	B	576	CYS
1	B	631	THR
1	B	1072	PRO
1	A	554	ASP
1	A	560	ASP
1	B	1075	GLY
1	B	969	VAL
1	B	1076	VAL
1	A	1076	VAL

### 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%)	914 (99%)	8 (1%)	75	83
1	B	922/1048 (88%)	914 (99%)	8 (1%)	75	83
1	C	914/1048 (87%)	903 (99%)	11 (1%)	67	79
2	D	527/533 (99%)	522 (99%)	5 (1%)	75	83
All	All	3285/3677 (89%)	3253 (99%)	32 (1%)	71	81

All (32) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	260	THR
1	A	395	ARG
1	A	553	ARG
1	A	558	PHE
1	A	699	ASN
1	A	807	LYS
1	A	921	THR
1	A	965	ARG
1	B	373	LYS
1	B	601	VAL
1	B	699	ASN
1	B	720	CYS
1	B	760	THR
1	B	807	LYS
1	B	841	THR
1	B	965	ARG
1	C	333	LYS
1	C	553	ARG
1	C	645	SER
1	C	646	TYR
1	C	647	GLU
1	C	677	TYR
1	C	678	THR
1	C	699	ASN
1	C	720	CYS
1	C	738	TYR
1	C	965	ARG
2	D	53	ASN
2	D	114	LYS
2	D	273	ARG
2	D	341	LYS
2	D	436	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	181	HIS
1	A	505	ASN
1	A	526	ASN
1	A	641	HIS
1	A	692	ASN
1	A	699	ASN

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Mol	Chain	Res	Type
1	A	733	ASN
1	A	744	GLN
1	A	759	ASN
1	A	769	GLN
1	A	806	ASN
1	A	835	GLN
1	A	838	ASN
1	A	877	GLN
1	A	889	ASN
1	A	895	GLN
1	A	896	ASN
1	A	910	ASN
1	A	931	GLN
1	A	935	ASN
1	A	937	ASN
1	A	947	GLN
1	A	993	GLN
1	A	1005	ASN
1	A	1095	GLN
1	A	1101	ASN
1	B	112	GLN
1	B	149	HIS
1	B	158	ASN
1	B	181	HIS
1	B	304	ASN
1	B	381	ASN
1	B	505	ASN
1	B	699	ASN
1	B	733	ASN
1	B	759	ASN
1	B	769	GLN
1	B	806	ASN
1	B	883	GLN
1	B	901	ASN
1	B	935	ASN
1	B	937	ASN
1	B	984	GLN
1	B	1005	ASN
1	C	112	GLN
1	C	304	ASN
1	C	409	ASN
1	C	523	GLN

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Mol	Chain	Res	Type
1	C	632	GLN
1	C	699	ASN
1	C	733	ASN
1	C	759	ASN
1	C	769	GLN
1	C	838	ASN
1	C	895	GLN
1	C	896	ASN
1	C	904	GLN
1	C	907	ASN
1	C	935	ASN
1	C	937	ASN
1	C	947	GLN
1	C	987	GLN
1	C	1005	ASN
2	D	33	ASN
2	D	53	ASN
2	D	81	GLN
2	D	417	HIS
2	D	437	ASN
2	D	522	GLN
2	D	526	GLN
2	D	572	ASN
2	D	599	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.

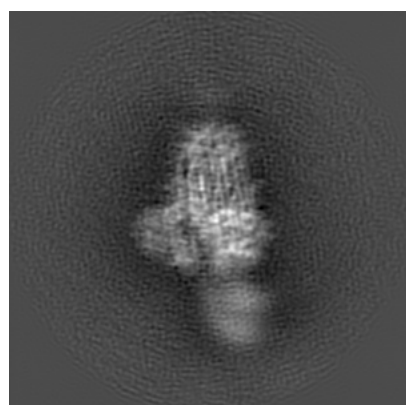
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9591. These allow visual inspection of the internal detail of the map and identification of artifacts.

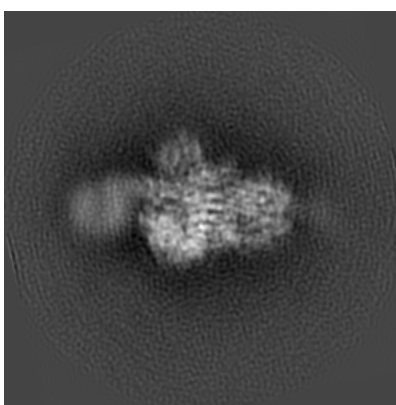
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

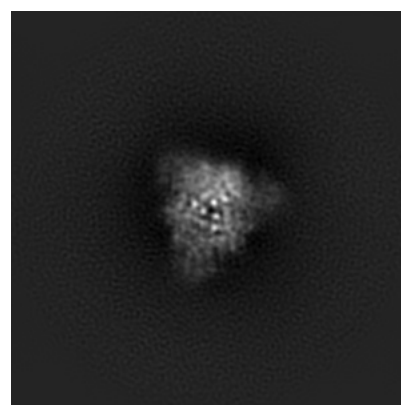
#### 6.1.1 Primary map



X



Y

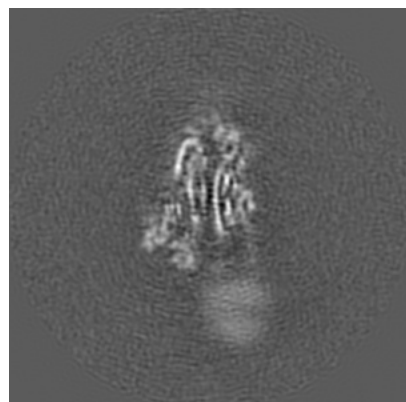


Z

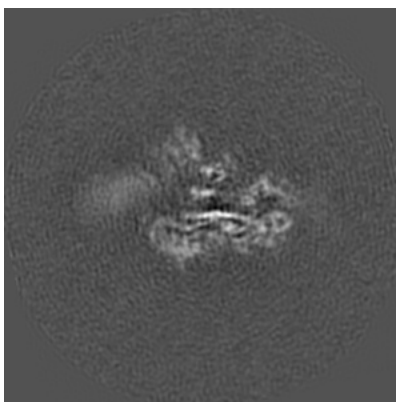
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

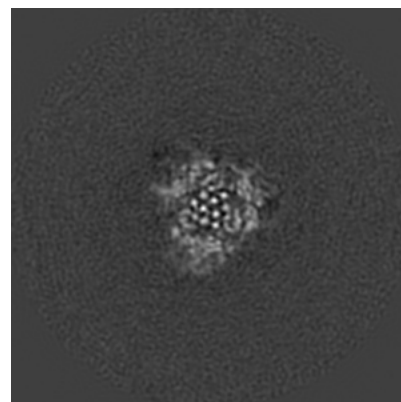
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

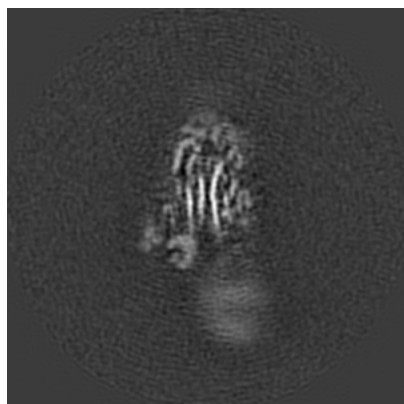


Z Index: 144

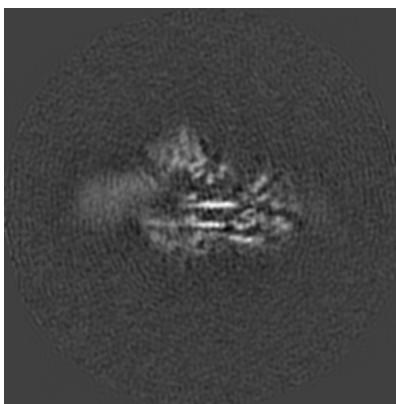
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

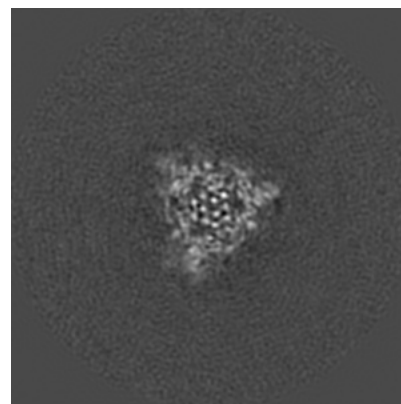
### 6.3.1 Primary map



X Index: 146



Y Index: 148

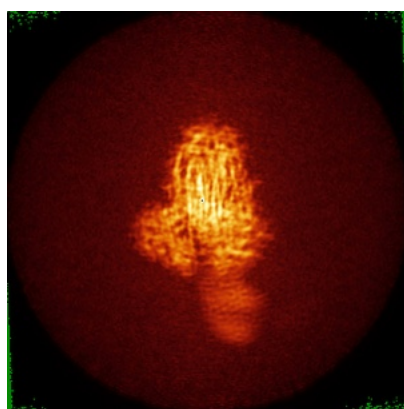


Z Index: 142

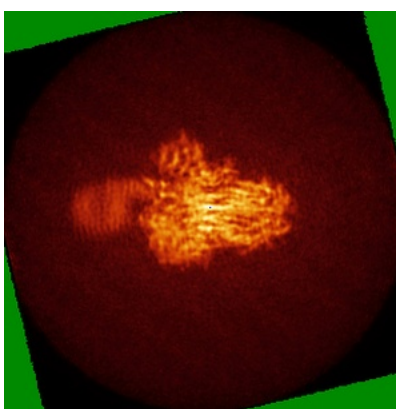
The images above show the largest variance slices of the map in three orthogonal directions.

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

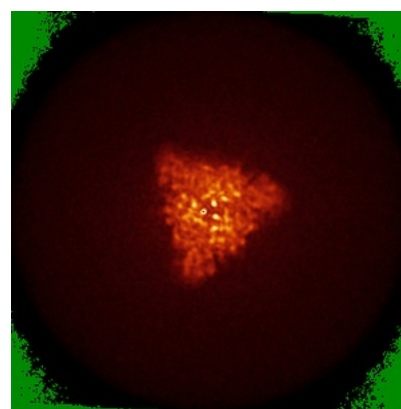
### 6.4.1 Primary map



X



Y



Z

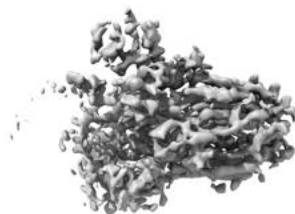
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

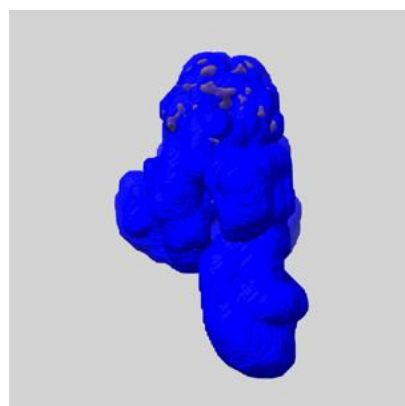
## 6.6 Mask visualisation [i](#)

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

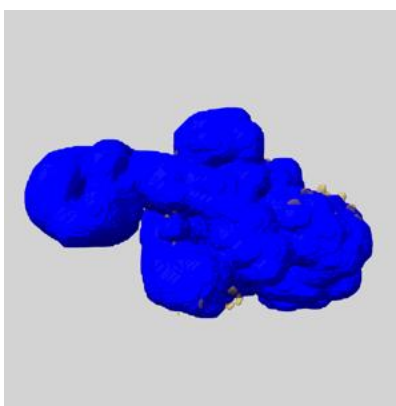
A mask typically either:

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

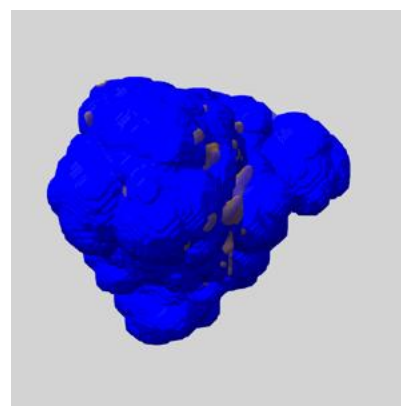
### 6.6.1 emd\_9591\_msk\_1.map [i](#)



X



Y



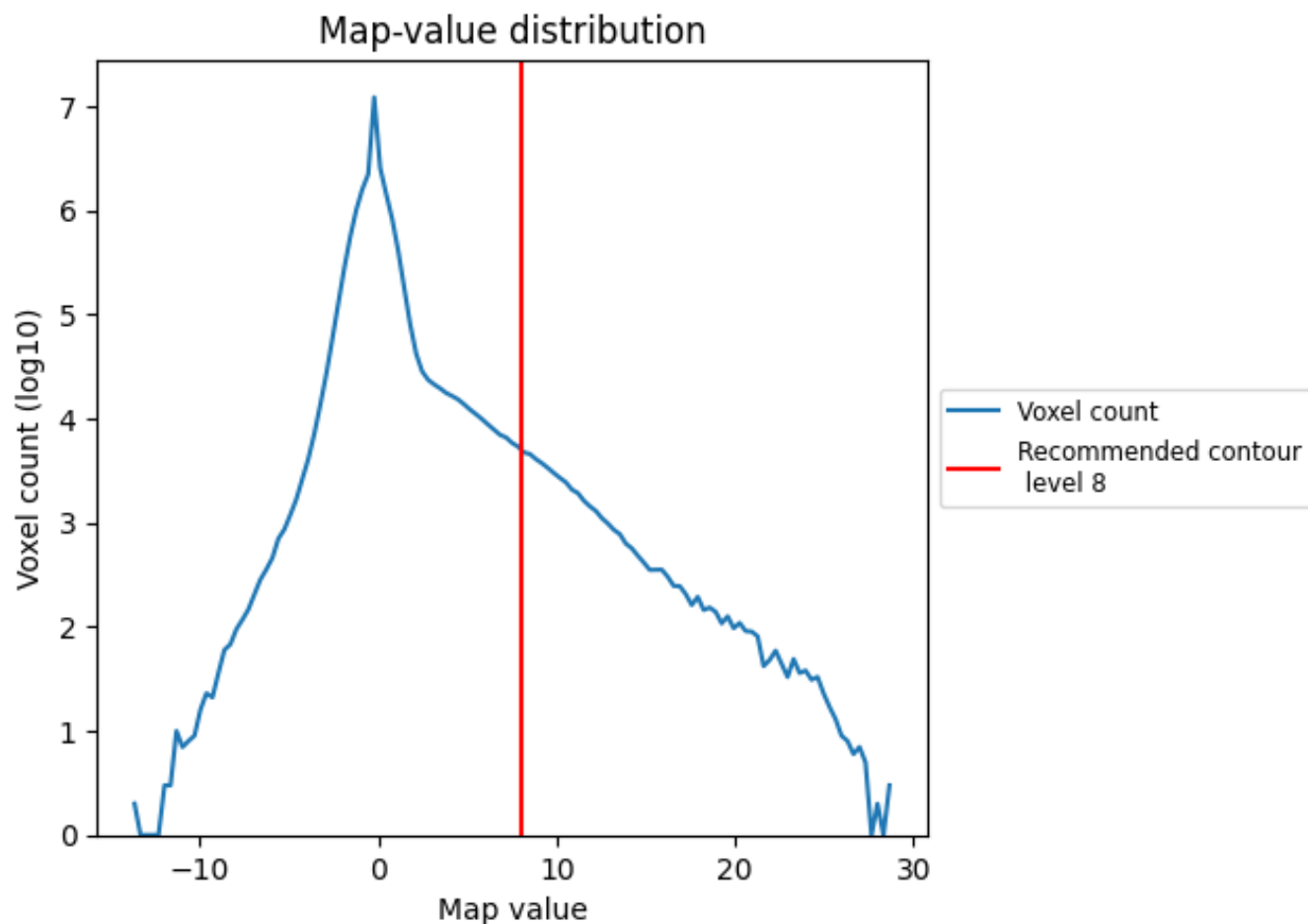
Z



## 7 Map analysis [i](#)

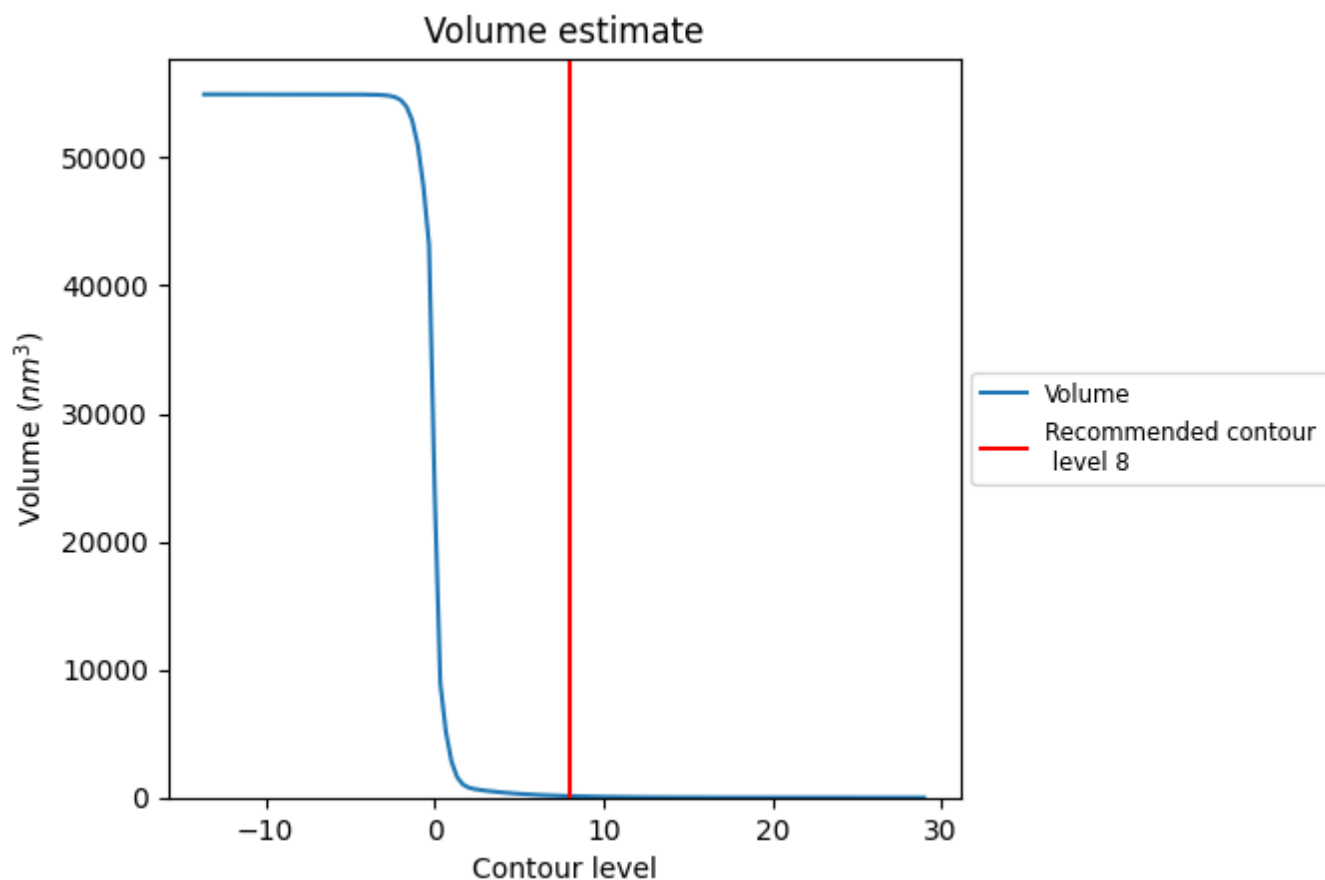
This section contains the results of statistical analysis of the map.

### 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.

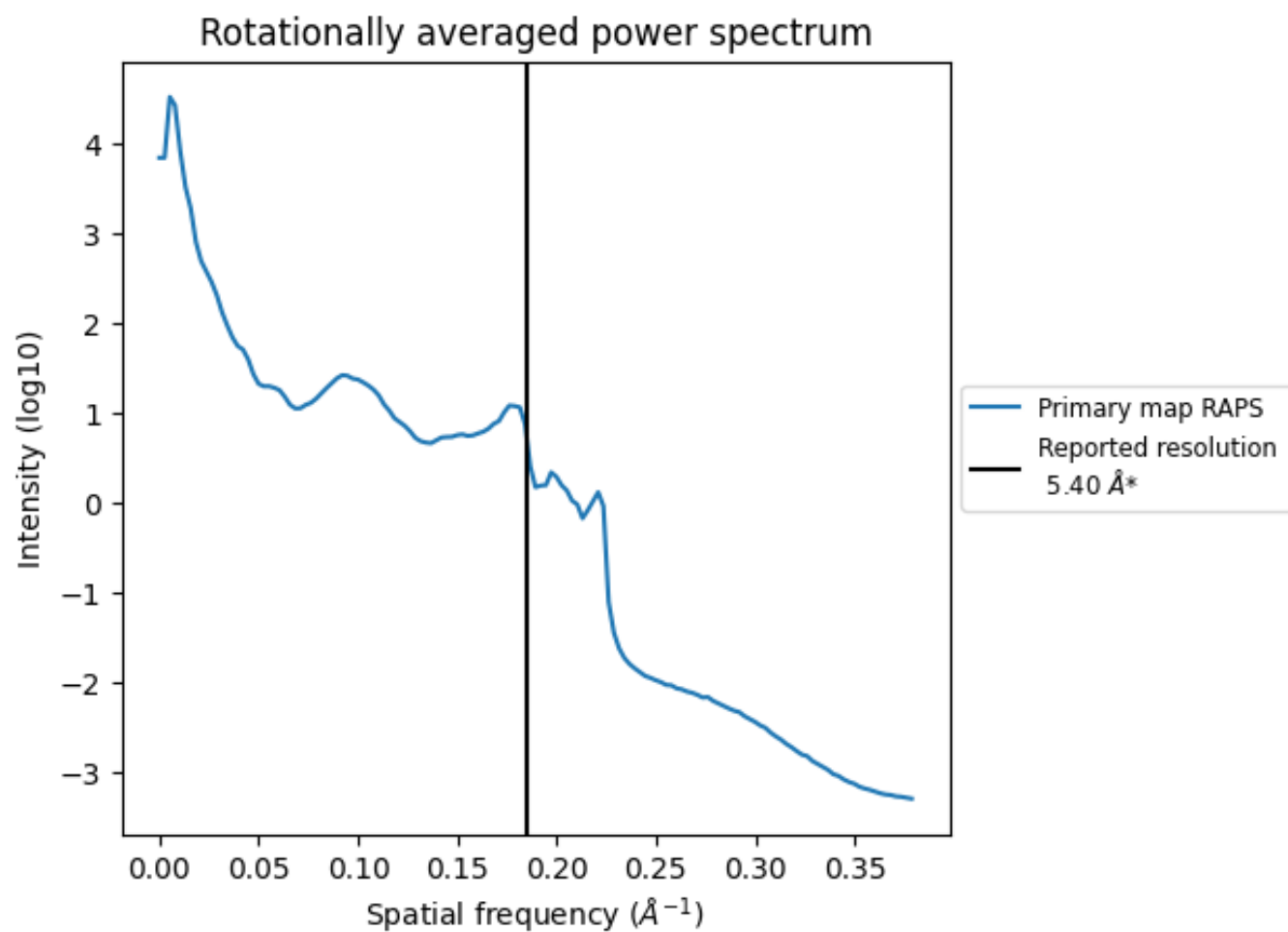
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm<sup>3</sup>; this corresponds to an approximate mass of 103 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 ⓘ

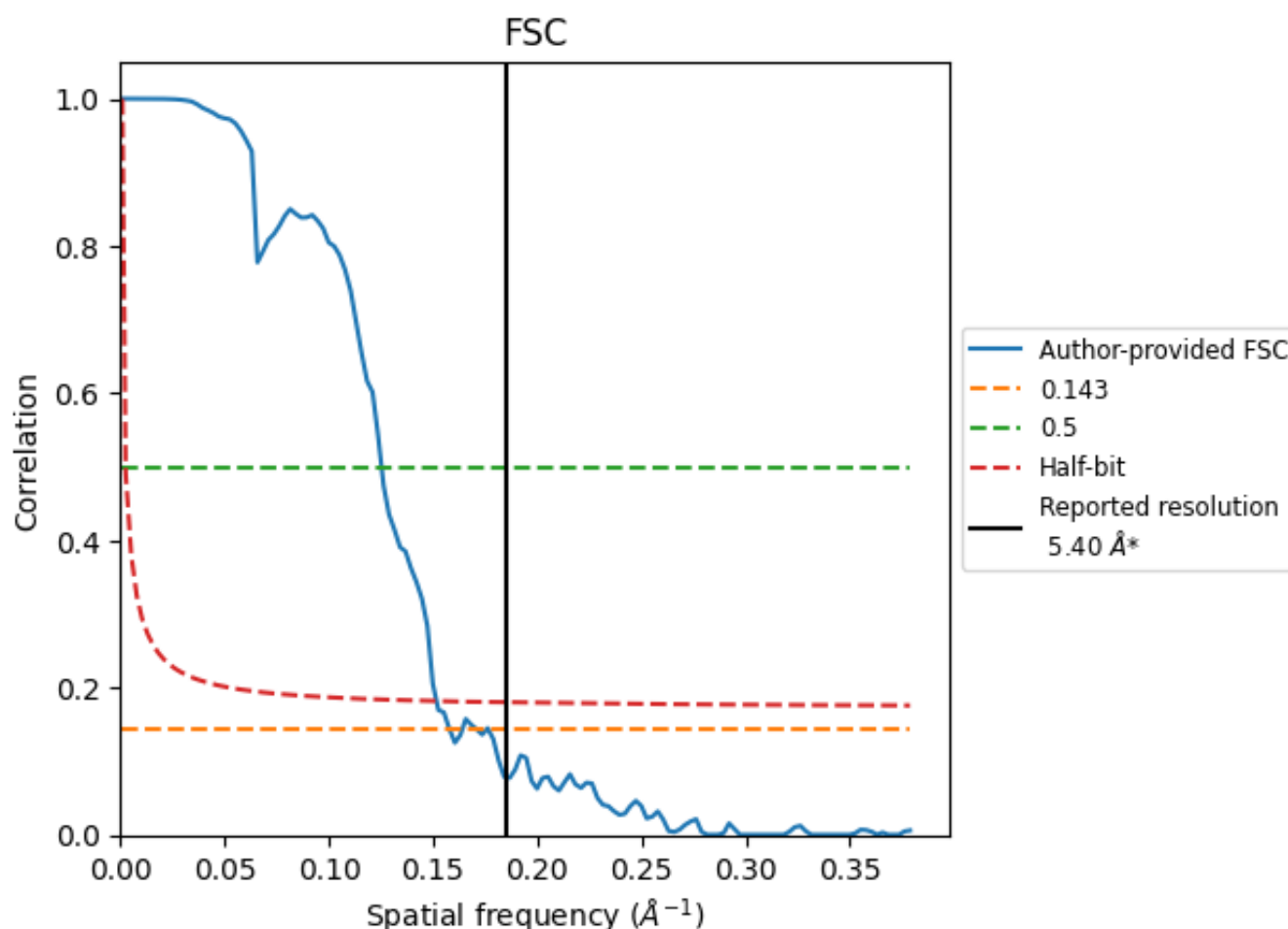


\*Reported resolution corresponds to spatial frequency of 0.185 Å<sup>-1</sup>

## 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 0.185  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

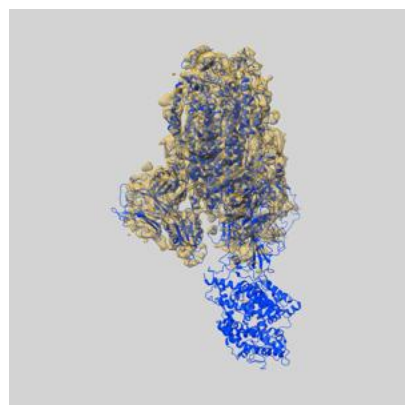
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	6.33	7.98	6.59
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.33 differs from the reported value 5.4 by more than 10 %

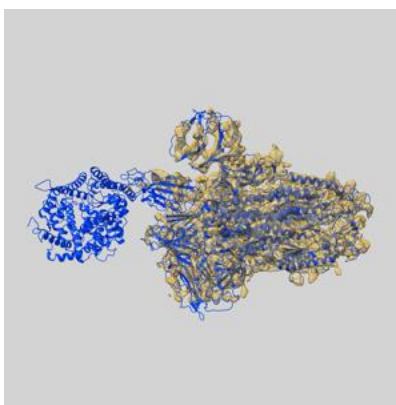
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9591 and PDB model 6ACG. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

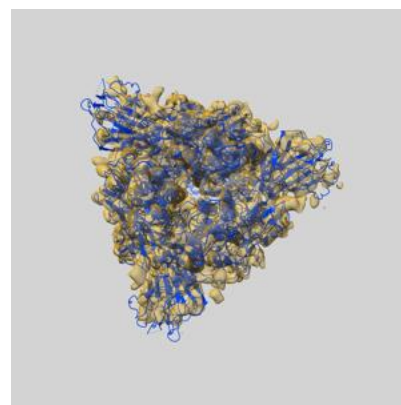
### 9.1 Map-model overlay [i](#)



X



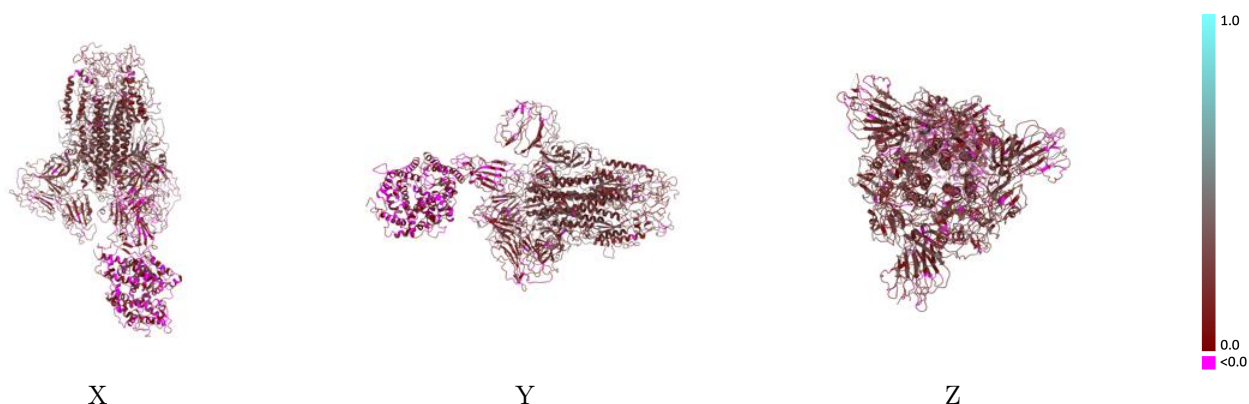
Y



Z

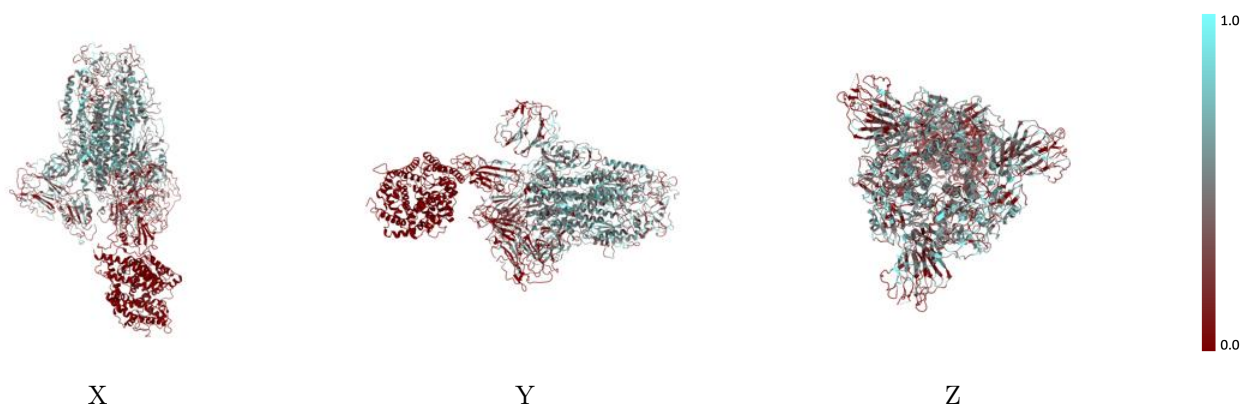
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



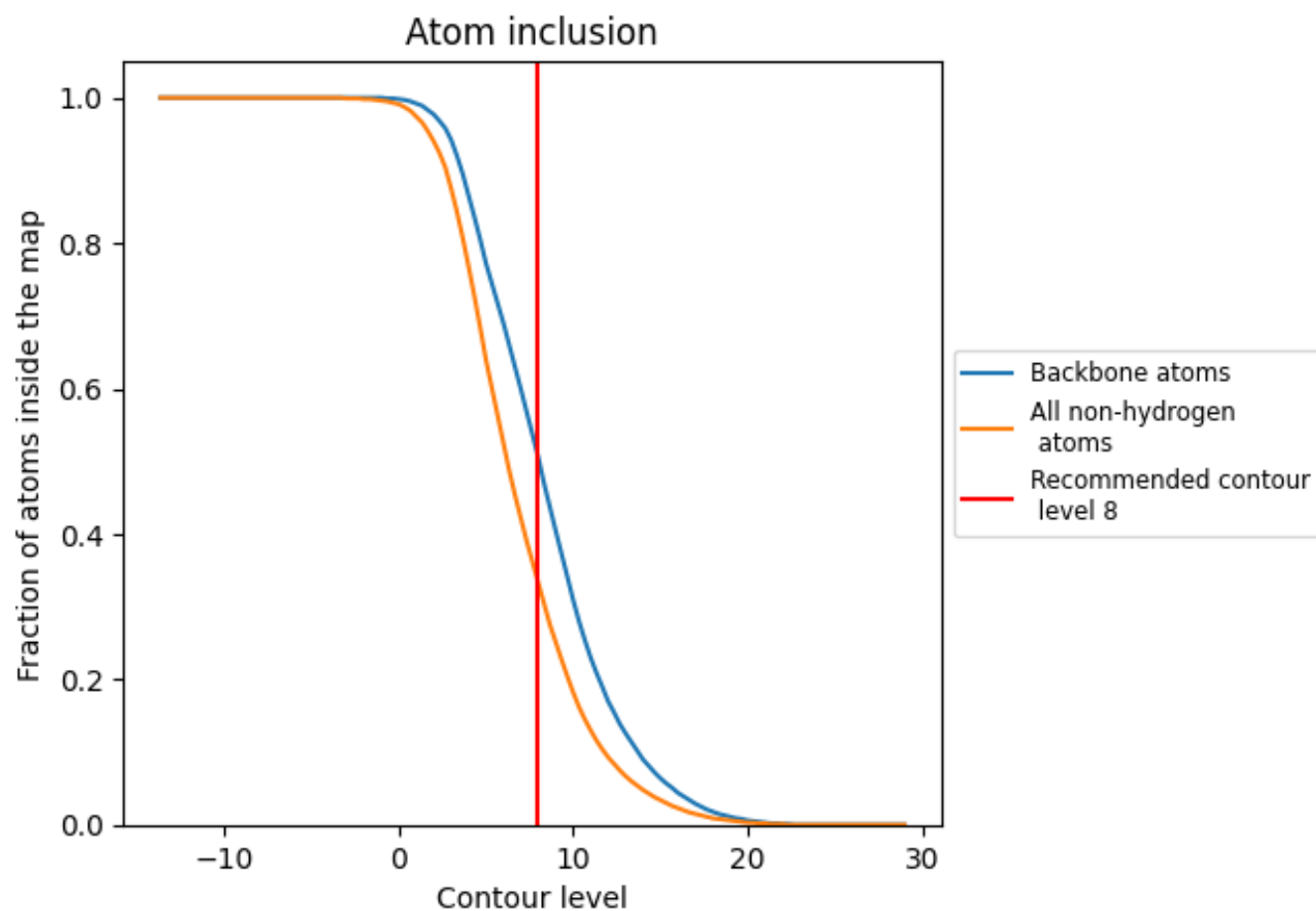
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 50% of all backbone atoms, 33% 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	<div></div> 0.3320	<div></div> 0.2020
A	<div></div> 0.3870	<div></div> 0.2280
B	<div></div> 0.4300	<div></div> 0.2360
C	<div></div> 0.3730	<div></div> 0.2150
D	<div></div> 0.0000	<div></div> 0.0800

