



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 08:40 PM UTC

PDB ID : 6ACK / pdb_00006ack
EMDB ID : EMD-9594
Title : Trypsin-cleaved and low pH-treated SARS-CoV spike glycoprotein and ACE2 complex, ACE2-bound conformation 3
Authors : Gui, M.; Song, W.
Deposited on : 2018-07-26
Resolution : 4.50 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

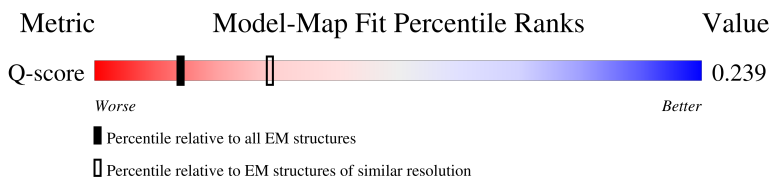
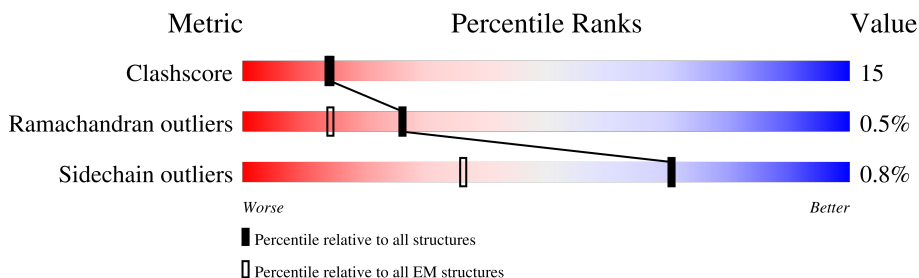
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

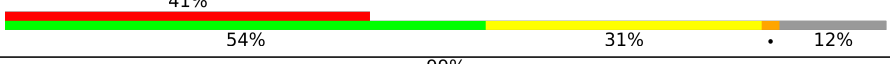
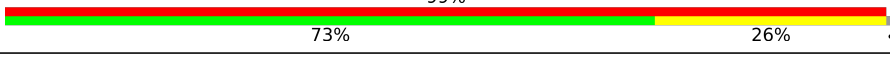
The reported resolution of this entry is 4.50 Å.

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	2937 (4.00 - 5.00)

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		

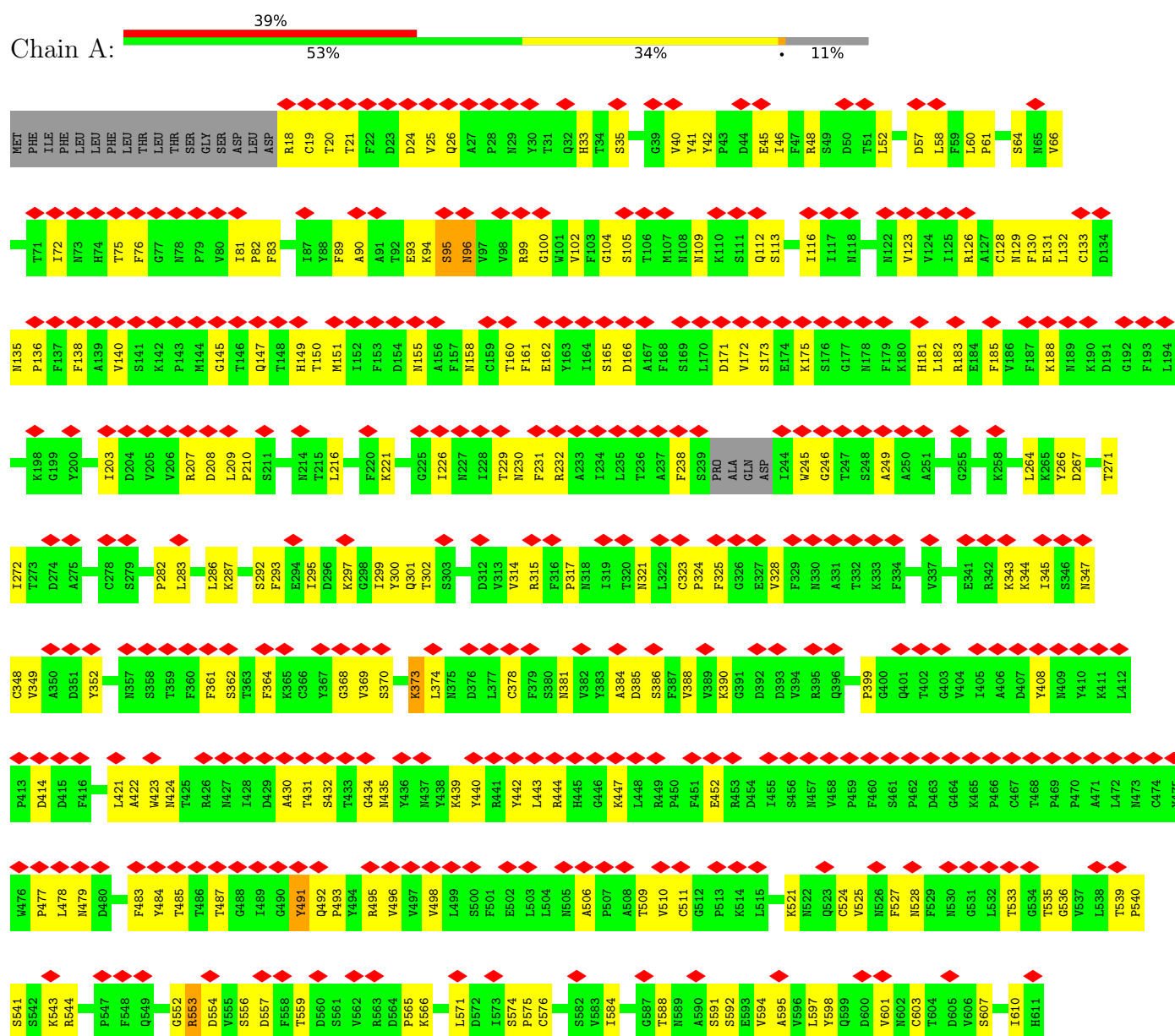
There are 6 discrepancies between the modelled and reference sequences:

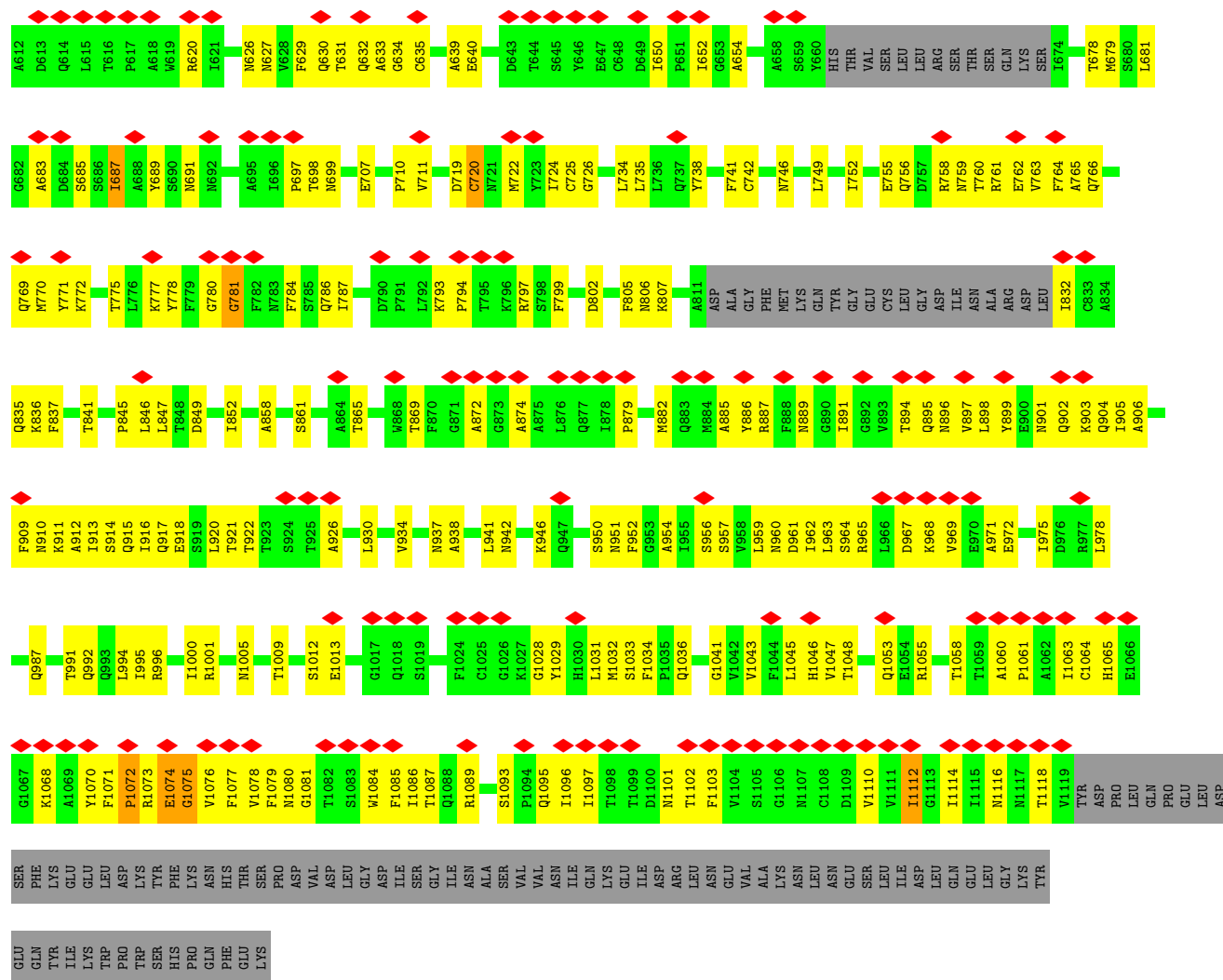
Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1

3 Residue-property plots

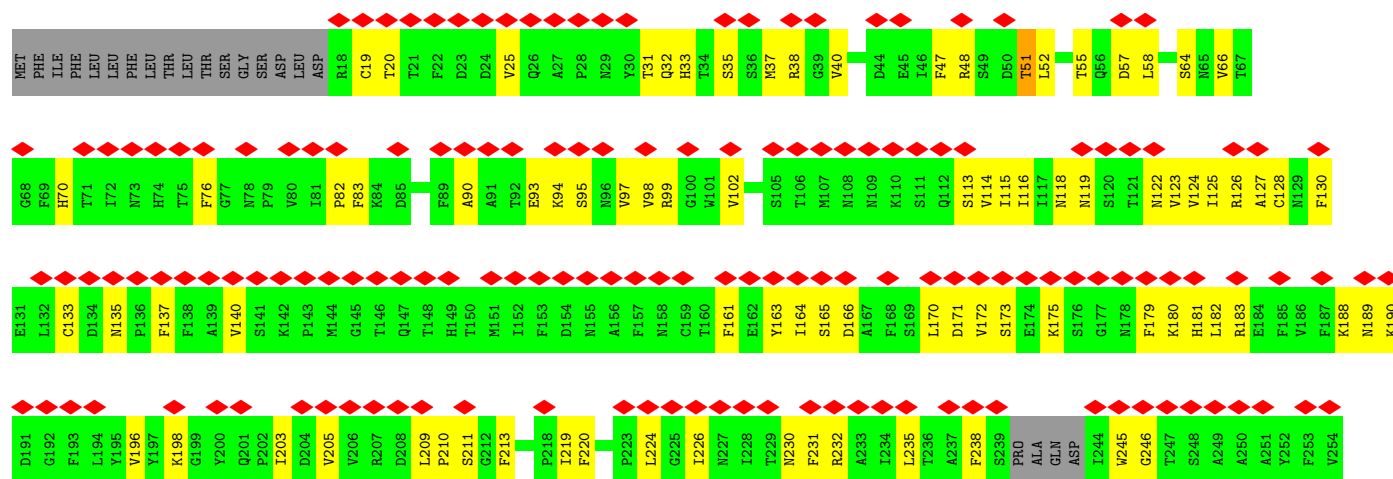
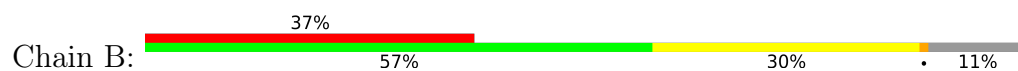
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

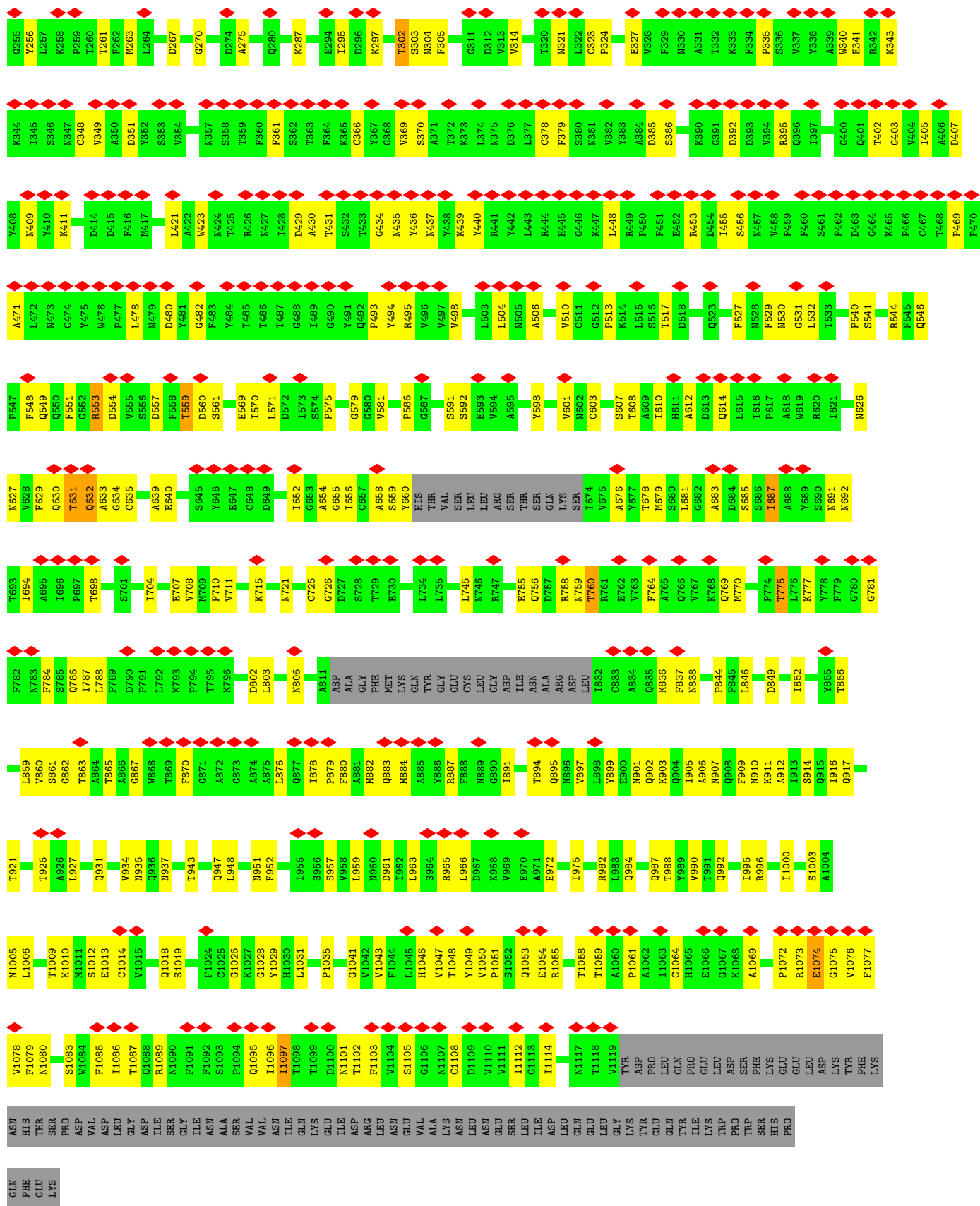
• Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein





- Molecule 1: Spike glycoprotein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56553	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	29.588	Depositor
Minimum map value	-14.552	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.908	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	0.52	0/8499	0.83	15/11568 (0.1%)
1	B	0.52	0/8499	0.84	5/11568 (0.0%)
1	C	0.60	8/8435 (0.1%)	0.87	18/11477 (0.2%)
2	D	0.29	0/5007	0.65	0/6803
All	All	0.51	8/30440 (0.0%)	0.82	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	13
1	B	0	14
1	C	0	18
All	All	0	45

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	676	ALA	C-O	-10.12	1.11	1.24
1	C	677	TYR	CA-C	-9.37	1.40	1.52
1	C	645	SER	CA-C	-8.21	1.41	1.52
1	C	677	TYR	CA-CB	-6.59	1.42	1.53
1	C	645	SER	N-CA	-6.47	1.37	1.46
1	C	675	VAL	CA-CB	-6.45	1.45	1.54
1	C	677	TYR	C-O	-5.71	1.16	1.24
1	C	675	VAL	C-O	-5.67	1.17	1.24

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1112	ILE	N-CA-C	-11.22	102.43	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	646	TYR	CA-C-N	-8.43	109.06	122.79
1	C	646	TYR	C-N-CA	-8.43	109.06	122.79
1	C	644	THR	O-C-N	7.85	132.25	122.91
1	A	891	ILE	N-CA-C	-7.14	106.04	112.90
1	A	553	ARG	CA-C-N	6.99	134.88	121.54
1	A	553	ARG	C-N-CA	6.99	134.88	121.54
1	C	634	GLY	N-CA-C	6.70	120.49	110.97
1	A	491	TYR	CA-C-N	6.40	129.28	120.39
1	A	491	TYR	C-N-CA	6.40	129.28	120.39
1	C	674	ILE	CB-CA-C	-6.36	98.89	111.60
1	A	96	ASN	N-CA-C	6.30	118.28	110.91
1	C	1070	TYR	CA-C-N	-6.22	112.96	121.61
1	C	1070	TYR	C-N-CA	-6.22	112.96	121.61
1	C	724	ILE	N-CA-C	-6.10	103.32	110.21
1	B	554	ASP	N-CA-C	5.96	118.29	111.02
1	C	647	GLU	CA-C-N	5.68	132.40	121.54
1	C	647	GLU	C-N-CA	5.68	132.40	121.54
1	A	926	ALA	CA-C-N	5.62	128.83	120.17
1	A	926	ALA	C-N-CA	5.62	128.83	120.17
1	A	1076	VAL	CA-C-N	5.57	132.18	121.54
1	A	1076	VAL	C-N-CA	5.57	132.18	121.54
1	A	556	SER	CA-C-N	5.52	132.09	121.54
1	A	556	SER	C-N-CA	5.52	132.09	121.54
1	B	559	THR	CA-C-N	5.50	132.04	121.54
1	B	559	THR	C-N-CA	5.50	132.04	121.54
1	C	1076	VAL	CA-C-N	5.50	132.03	121.54
1	C	1076	VAL	C-N-CA	5.50	132.03	121.54
1	C	926	ALA	CA-C-N	5.26	129.71	121.08
1	C	926	ALA	C-N-CA	5.26	129.71	121.08
1	C	370	SER	CA-C-N	5.26	131.58	121.54
1	C	370	SER	C-N-CA	5.26	131.58	121.54
1	B	579	GLY	CA-C-N	-5.24	118.51	122.33
1	B	579	GLY	C-N-CA	-5.24	118.51	122.33
1	C	1116	ASN	CA-C-N	5.19	131.45	121.54
1	C	1116	ASN	C-N-CA	5.19	131.45	121.54
1	A	1116	ASN	CA-C-N	5.17	131.41	121.54
1	A	1116	ASN	C-N-CA	5.17	131.41	121.54

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1074	GLU	Peptide
1	A	1075	GLY	Peptide
1	A	506	ALA	Peptide
1	A	629	PHE	Peptide
1	A	632	GLN	Peptide
1	A	633	ALA	Peptide
1	A	726	GLY	Peptide
1	A	781	GLY	Peptide
1	A	836	LYS	Peptide
1	A	845	PRO	Peptide
1	A	865	THR	Peptide
1	A	922	THR	Peptide
1	A	95	SER	Peptide
1	B	1074	GLU	Peptide
1	B	1075	GLY	Peptide
1	B	1077	PHE	Peptide
1	B	506	ALA	Peptide
1	B	51	THR	Peptide
1	B	527	PHE	Peptide
1	B	548	PHE	Peptide
1	B	553	ARG	Peptide
1	B	629	PHE	Peptide
1	B	631	THR	Peptide
1	B	726	GLY	Peptide
1	B	775	THR	Peptide
1	B	870	PHE	Peptide
1	B	884	MET	Peptide
1	C	1052	SER	Peptide
1	C	1074	GLU	Peptide
1	C	1077	PHE	Peptide
1	C	323	CYS	Peptide
1	C	370	SER	Peptide
1	C	527	PHE	Peptide
1	C	556	SER	Peptide
1	C	574	SER	Peptide
1	C	575	PRO	Peptide
1	C	629	PHE	Peptide
1	C	631	THR	Peptide
1	C	633	ALA	Peptide
1	C	724	ILE	Peptide
1	C	837	PHE	Peptide
1	C	923	THR	Peptide
1	C	95	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	967	ASP	Peptide
1	C	97	VAL	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	293	0
1	B	8302	0	8082	260	0
1	C	8241	0	8009	299	0
2	D	4870	0	4643	100	0
All	All	29715	0	28816	899	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 15.

All (899) 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	1.47	1.48
1:C:646:TYR:CB	1:C:677:TYR:CE2	2.02	1.41
1:C:646:TYR:O	1:C:680:SER:OG	1.62	1.15
1:C:646:TYR:HB2	1:C:677:TYR:CD2	1.84	1.11
1:C:646:TYR:CA	1:C:677:TYR:CE2	2.36	1.07
1:C:646:TYR:CA	1:C:677:TYR:HE2	1.68	1.05
1:C:646:TYR:CB	1:C:677:TYR:CZ	2.41	1.03
1:C:418:GLY:HA3	1:C:499:LEU:O	1.60	1.00
1:C:646:TYR:N	1:C:677:TYR:CE2	2.32	0.98
1:B:93:GLU:O	1:B:181:HIS:HB2	1.63	0.98
1:C:100:GLY:HA2	1:C:116:ILE:O	1.63	0.98
1:C:646:TYR:HB2	1:C:677:TYR:CZ	1.99	0.98
1:B:102:VAL:O	1:B:231:PHE:HA	1.66	0.95
1:B:704:ILE:HA	1:B:1046:HIS:O	1.64	0.94
1:A:93:GLU:O	1:A:181:HIS:HB2	1.69	0.93
1:A:100:GLY:HA2	1:A:116:ILE:O	1.70	0.91
1:A:140:VAL:O	1:A:238:PHE:HA	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:415:PRO:O	2:D:419:LYS:HB2	1.74	0.87
1:C:646:TYR:HB3	1:C:677:TYR:CZ	2.09	0.87
1:A:760:THR:O	1:A:764:PHE:HB2	1.73	0.86
1:C:646:TYR:N	1:C:677:TYR:HE2	1.72	0.86
1:B:90:ALA:HA	1:B:183:ARG:O	1.77	0.85
1:C:422:ALA:HA	1:C:495:ARG:O	1.77	0.85
1:C:598:TYR:O	1:C:634:GLY:HA3	1.77	0.84
1:B:760:THR:O	1:B:764:PHE:HB2	1.77	0.84
1:A:909:PHE:O	1:A:912:ALA:HB3	1.79	0.83
1:C:93:GLU:O	1:C:181:HIS:HB2	1.79	0.83
1:B:914:SER:O	1:B:917:GLN:HB2	1.80	0.81
1:A:913:ILE:O	1:A:916:ILE:HB	1.82	0.78
1:C:646:TYR:N	1:C:677:TYR:CD2	2.53	0.76
2:D:406:GLU:HG3	2:D:518:ARG:HD3	1.70	0.73
1:C:323:CYS:HB2	1:C:345:ILE:HG23	1.69	0.72
1:C:655:GLY:O	1:C:678:THR:O	2.08	0.71
1:C:674:ILE:HD12	1:C:674:ILE:N	2.05	0.71
1:C:677:TYR:HD1	1:C:677:TYR:H	1.39	0.71
1:A:1079:PHE:HB2	1:A:1087:THR:HG23	1.74	0.69
1:C:194:LEU:O	1:C:221:LYS:HA	1.92	0.69
1:B:906:ALA:O	1:B:909:PHE:HB3	1.93	0.69
1:C:25:VAL:HA	1:C:76:PHE:HB3	1.73	0.69
1:A:889:ASN:HD21	1:A:895:GLN:HE21	1.40	0.69
1:B:887:ARG:NH1	1:B:1031:LEU:O	2.26	0.69
1:A:109:ASN:HA	1:A:131:GLU:HA	1.76	0.68
1:C:1063:ILE:HB	1:C:1070:TYR:HB2	1.75	0.68
1:B:996:ARG:O	1:B:1000:ILE:HB	1.92	0.68
1:A:536:GLY:HA3	1:A:574:SER:HA	1.74	0.68
1:B:135:ASN:HA	1:B:232:ARG:HH22	1.59	0.68
1:A:584:ILE:HB	1:A:595:ALA:HB3	1.75	0.67
1:C:678:THR:OG1	1:C:679:MET:N	2.14	0.67
1:C:644:THR:O	1:C:645:SER:O	2.12	0.67
1:C:704:ILE:HA	1:C:1046:HIS:O	1.94	0.67
1:A:759:ASN:O	1:A:763:VAL:HB	1.94	0.67
1:A:707:GLU:OE1	1:A:1046:HIS:NE2	2.28	0.66
1:A:385:ASP:HB2	1:A:498:VAL:HB	1.77	0.66
1:A:484:TYR:HB2	1:A:487:THR:HB	1.76	0.66
1:A:378:CYS:HA	1:A:511:CYS:HA	1.77	0.66
1:B:348:CYS:SG	1:B:349:VAL:N	2.69	0.66
1:B:626:ASN:ND2	1:B:640:GLU:OE2	2.25	0.66
1:C:99:ARG:NH2	1:C:171:ASP:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:HG13	1:A:145:GLY:HA2	1.78	0.66
1:B:1086:ILE:O	1:B:1095:GLN:NE2	2.29	0.66
2:D:524:GLN:HG2	2:D:583:PRO:HG2	1.76	0.66
1:B:1079:PHE:H	1:B:1086:ILE:HA	1.61	0.65
1:C:937:ASN:O	1:C:941:LEU:HB2	1.96	0.65
2:D:50:TYR:HA	2:D:58:ASN:HB3	1.78	0.65
1:C:133:CYS:HB2	1:C:136:PRO:HD3	1.78	0.65
1:A:102:VAL:O	1:A:231:PHE:HA	1.95	0.65
1:B:385:ASP:HB2	1:B:498:VAL:HB	1.78	0.65
1:B:784:PHE:HA	1:B:787:ILE:HD12	1.77	0.65
1:A:95:SER:H	1:A:181:HIS:HD2	1.45	0.65
1:C:1096:ILE:O	1:C:1101:ASN:ND2	2.30	0.65
1:C:388:VAL:HG22	1:C:495:ARG:HG2	1.78	0.65
1:C:1063:ILE:HG23	1:C:1115:ILE:HB	1.78	0.65
1:A:96:ASN:HA	1:A:183:ARG:HH12	1.61	0.64
1:A:887:ARG:NH1	1:A:1031:LEU:O	2.29	0.64
1:C:113:SER:O	1:C:127:ALA:HA	1.98	0.64
1:C:421:LEU:O	1:C:496:VAL:HA	1.98	0.64
1:A:901:ASN:O	1:A:904:GLN:HB3	1.98	0.64
1:B:127:ALA:HB3	1:B:161:PHE:HB3	1.79	0.64
1:C:38:ARG:NH1	1:C:184:GLU:OE2	2.31	0.64
1:C:341:GLU:O	1:C:385:ASP:HA	1.97	0.64
1:C:383:TYR:HB2	1:C:500:SER:HB2	1.80	0.64
1:B:116:ILE:HG12	1:B:125:ILE:HG12	1.81	0.63
1:A:128:CYS:SG	1:A:129:ASN:N	2.72	0.63
1:A:959:LEU:HD23	1:A:962:ILE:HD11	1.80	0.63
1:C:626:ASN:ND2	1:C:640:GLU:OE2	2.31	0.63
1:C:953:GLY:O	1:C:977:ARG:NH1	2.30	0.63
1:C:784:PHE:HA	1:C:787:ILE:HD12	1.80	0.63
1:B:786:GLN:OE1	1:B:917:GLN:NE2	2.32	0.63
1:C:686:SER:OG	1:C:687:ILE:N	2.32	0.63
1:C:58:LEU:HB2	1:C:188:LYS:HE3	1.80	0.63
2:D:30:ASP:O	2:D:34:HIS:ND1	2.32	0.63
1:C:554:ASP:OD1	1:C:554:ASP:N	2.31	0.63
1:A:575:PRO:HD3	1:C:837:PHE:HB3	1.81	0.63
2:D:177:ARG:NH1	2:D:470:LYS:O	2.32	0.63
1:A:786:GLN:HB3	1:A:799:PHE:HB3	1.81	0.63
1:B:123:VAL:HB	1:B:165:SER:HB3	1.81	0.63
2:D:261:CYS:HB2	2:D:488:VAL:HG13	1.81	0.63
1:B:99:ARG:HH12	1:B:172:VAL:HA	1.64	0.62
1:B:188:LYS:HG2	1:B:190:LYS:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:ASN:HD22	1:C:304:ASN:HD22	1.47	0.62
1:C:56:GLN:NE2	1:C:259:PRO:O	2.32	0.62
2:D:580:ASN:HD21	2:D:582:ARG:HH11	1.47	0.62
1:A:575:PRO:O	1:C:835:GLN:NE2	2.32	0.62
1:B:94:LYS:HB3	1:B:175:LYS:HB2	1.81	0.62
1:B:711:VAL:H	1:B:1041:GLY:HA2	1.64	0.62
1:A:992:GLN:HA	1:A:995:ILE:HD12	1.81	0.62
2:D:244:VAL:HG11	2:D:444:LEU:HD11	1.82	0.62
2:D:320:LEU:HD13	2:D:380:GLN:HG2	1.80	0.62
1:B:38:ARG:NH2	1:B:210:PRO:O	2.28	0.62
1:B:423:TRP:O	1:B:494:TYR:HA	2.00	0.62
1:A:90:ALA:HA	1:A:183:ARG:O	1.99	0.62
1:C:315:ARG:HE	1:C:519:LEU:HG	1.64	0.62
1:C:141:SER:HB3	1:C:145:GLY:H	1.65	0.61
1:C:651:PRO:HA	1:C:657:CYS:HA	1.81	0.61
1:A:960:ASN:HA	1:A:963:LEU:HB2	1.82	0.61
1:A:1073:ARG:NH2	1:A:1101:ASN:O	2.33	0.61
1:A:1093:SER:O	1:A:1095:GLN:NE2	2.33	0.61
1:A:35:SER:HB2	1:A:60:LEU:HD21	1.83	0.61
1:C:301:GLN:NE2	1:C:302:THR:O	2.34	0.61
2:D:152:MET:HE1	2:D:265:HIS:HA	1.81	0.61
1:B:710:PRO:HB2	1:B:1000:ILE:HD11	1.82	0.61
1:C:304:ASN:HA	1:C:580:GLY:HA2	1.81	0.61
1:A:626:ASN:ND2	1:A:640:GLU:OE2	2.34	0.61
1:A:903:LYS:O	1:A:906:ALA:HB3	2.00	0.61
1:B:366:CYS:HB3	1:B:369:VAL:HG23	1.81	0.61
1:C:422:ALA:HB1	1:C:494:TYR:HB3	1.82	0.61
1:C:335:PRO:HG3	1:C:341:GLU:HG2	1.83	0.61
1:B:867:GLY:HA3	1:B:876:LEU:H	1.66	0.61
2:D:209:VAL:HG21	2:D:565:PRO:HB3	1.82	0.60
1:B:882:MET:SD	1:B:899:TYR:OH	2.59	0.60
1:C:30:TYR:HB3	1:C:67:THR:HG23	1.84	0.60
1:A:1077:PHE:O	1:A:1087:THR:OG1	2.19	0.60
1:B:544:ARG:O	1:B:546:GLN:NE2	2.34	0.60
1:C:54:LEU:HD21	1:C:288:CYS:HB2	1.82	0.60
1:C:128:CYS:SG	1:C:129:ASN:N	2.74	0.60
1:A:369:VAL:HA	1:C:965:ARG:HG3	1.83	0.60
1:A:996:ARG:O	1:A:1000:ILE:HB	2.02	0.60
1:B:323:CYS:N	1:B:348:CYS:SG	2.74	0.60
1:B:1097:ILE:HA	1:B:1101:ASN:HD22	1.66	0.60
1:C:867:GLY:HA3	1:C:876:LEU:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:ASN:HB3	1:B:911:LYS:HE3	1.84	0.60
1:B:1096:ILE:O	1:B:1101:ASN:ND2	2.35	0.60
1:A:835:GLN:NE2	1:B:575:PRO:O	2.35	0.59
1:C:127:ALA:HB3	1:C:161:PHE:HB3	1.83	0.59
1:A:761:ARG:O	1:A:765:ALA:N	2.29	0.59
1:A:24:ASP:HB3	1:A:245:TRP:HE1	1.65	0.59
1:B:411:LYS:NZ	1:B:448:LEU:O	2.34	0.59
1:C:960:ASN:HA	1:C:963:LEU:HB2	1.84	0.59
1:A:82:PRO:HA	1:A:230:ASN:HA	1.84	0.59
1:B:540:PRO:HA	1:B:570:ILE:HA	1.85	0.59
1:B:987:GLN:NE2	1:C:988:THR:OG1	2.36	0.59
1:C:396:GLN:HB3	1:C:406:ALA:HB2	1.85	0.59
1:B:302:THR:OG1	1:B:303:SER:N	2.35	0.59
1:B:867:GLY:HA2	1:B:878:ILE:HG12	1.84	0.59
1:C:473:ASN:ND2	2:D:83:TYR:OH	2.34	0.59
1:B:659:SER:OG	1:B:660:TYR:N	2.31	0.59
1:A:99:ARG:HH22	1:A:172:VAL:HA	1.66	0.59
1:A:872:ALA:HB2	1:B:1028:GLY:HA2	1.85	0.59
1:B:198:LYS:HD3	1:B:219:ILE:HG13	1.85	0.58
1:C:992:GLN:HA	1:C:995:ILE:HD12	1.84	0.58
1:A:46:ILE:HD13	1:B:553:ARG:HE	1.67	0.58
1:B:302:THR:HG23	1:B:581:VAL:HG23	1.85	0.58
1:C:340:TRP:O	1:C:453:ARG:NE	2.33	0.58
2:D:462:MET:O	2:D:467:GLU:N	2.37	0.58
1:A:123:VAL:HB	1:A:165:SER:HB3	1.86	0.58
1:A:685:SER:HB2	1:C:769:GLN:HE21	1.68	0.58
1:A:720:CYS:SG	1:A:746:ASN:ND2	2.77	0.58
1:C:315:ARG:NH2	1:C:518:ASP:OD1	2.37	0.58
2:D:245:ARG:NH1	2:D:603:PHE:O	2.37	0.58
1:C:756:GLN:HA	1:C:759:ASN:HD22	1.68	0.58
1:B:626:ASN:ND2	1:B:639:ALA:O	2.37	0.58
1:C:777:LYS:NZ	1:C:790:ASP:OD1	2.35	0.58
2:D:236:LEU:HD21	2:D:588:PHE:HD2	1.68	0.58
1:A:348:CYS:SG	1:A:349:VAL:N	2.77	0.58
1:B:961:ASP:OD1	1:B:965:ARG:NH2	2.37	0.58
1:C:99:ARG:HD3	1:C:118:ASN:HB2	1.84	0.58
1:C:1003:SER:HA	1:C:1006:LEU:HD12	1.86	0.58
1:C:444:ARG:NH1	1:C:447:LYS:O	2.37	0.58
1:A:541:SER:HA	1:A:571:LEU:HG	1.86	0.57
1:A:698:THR:H	1:A:1053:GLN:HB2	1.69	0.57
1:A:711:VAL:HG22	1:A:1041:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:ILE:HA	1:A:978:LEU:HD12	1.86	0.57
1:B:341:GLU:HB3	1:B:386:SER:HB3	1.85	0.57
1:B:707:GLU:OE1	1:B:1046:HIS:NE2	2.37	0.57
2:D:90:ASN:HB3	2:D:93:VAL:HG22	1.85	0.57
1:B:692:ASN:HA	1:B:1059:THR:HG22	1.86	0.57
1:C:1086:ILE:O	1:C:1095:GLN:N	2.31	0.57
1:A:149:HIS:NE2	1:A:151:MET:SD	2.77	0.57
1:A:301:GLN:NE2	1:A:302:THR:O	2.37	0.57
1:C:707:GLU:OE1	1:C:1046:HIS:NE2	2.37	0.57
1:A:45:GLU:OE2	1:A:221:LYS:NZ	2.35	0.57
1:A:94:LYS:NZ	1:A:249:ALA:O	2.38	0.57
1:B:504:LEU:HD22	1:B:531:GLY:HA3	1.87	0.57
1:A:21:THR:HA	1:A:135:ASN:HB3	1.86	0.57
1:B:867:GLY:O	1:B:883:GLN:NE2	2.37	0.57
1:C:609:ALA:HA	1:C:614:GLN:HB2	1.87	0.57
1:C:647:GLU:N	1:C:677:TYR:OH	2.37	0.57
1:B:546:GLN:HB2	1:B:549:GLN:HB2	1.86	0.57
1:B:861:SER:O	1:B:865:THR:OG1	2.23	0.57
1:B:957:SER:O	1:B:982:ARG:NH2	2.38	0.57
1:C:775:THR:HA	1:C:777:LYS:HE3	1.85	0.57
2:D:439:LEU:HB3	2:D:591:LEU:HD22	1.86	0.57
1:A:18:ARG:HB3	1:A:151:MET:HE1	1.87	0.56
1:A:41:TYR:OH	1:A:188:LYS:NZ	2.33	0.56
1:B:1078:VAL:HA	1:B:1086:ILE:HG23	1.86	0.56
1:C:89:PHE:HB3	1:C:185:PHE:HB2	1.87	0.56
1:A:631:THR:O	1:A:634:GLY:N	2.35	0.56
1:A:687:ILE:HD11	1:C:772:LYS:H	1.70	0.56
1:B:1029:TYR:H	1:B:1049:TYR:H	1.53	0.56
1:C:758:ARG:NH2	1:C:762:GLU:OE2	2.39	0.56
1:C:1060:ALA:HB3	1:C:1080:ASN:HD22	1.70	0.56
1:A:539:THR:HG23	1:A:571:LEU:HB2	1.87	0.56
1:A:894:THR:OG1	1:A:895:GLN:N	2.38	0.56
1:B:51:THR:OG1	1:B:52:LEU:N	2.39	0.56
1:C:1012:SER:HA	1:C:1016:LEU:HD12	1.88	0.56
1:A:885:ALA:HB2	1:A:898:LEU:HD22	1.88	0.56
1:A:784:PHE:HA	1:A:787:ILE:HD12	1.88	0.56
1:B:31:THR:HG21	1:B:70:HIS:HD2	1.69	0.56
1:B:402:THR:HB	1:B:407:ASP:HB2	1.87	0.56
1:B:1078:VAL:HG13	1:B:1086:ILE:HG12	1.88	0.56
2:D:190:MET:SD	2:D:194:ASN:ND2	2.79	0.56
1:A:348:CYS:H	1:A:510:VAL:HG22	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASN:ND2	1:A:492:GLN:OE1	2.37	0.56
1:B:115:ILE:O	1:B:125:ILE:HA	2.06	0.56
1:C:646:TYR:HB3	1:C:677:TYR:OH	2.05	0.56
1:A:444:ARG:NH2	1:A:452:GLU:OE2	2.39	0.55
1:B:392:ASP:OD1	1:B:395:ARG:NH2	2.40	0.55
1:B:903:LYS:O	1:B:906:ALA:HB3	2.06	0.55
1:C:527:PHE:HZ	1:C:538:LEU:HD21	1.71	0.55
1:C:1098:THR:H	1:C:1101:ASN:HB2	1.71	0.55
1:B:303:SER:OG	1:B:304:ASN:N	2.39	0.55
1:C:1005:ASN:O	1:C:1009:THR:OG1	2.21	0.55
1:A:435:ASN:HB3	1:A:483:PHE:HB2	1.87	0.55
1:A:1058:THR:OG1	1:A:1080:ASN:O	2.19	0.55
1:C:979:ILE:O	1:C:983:LEU:HB2	2.07	0.55
1:A:315:ARG:HH22	1:A:566:LYS:HD2	1.71	0.55
1:A:553:ARG:HD3	1:A:559:THR:HA	1.88	0.55
1:B:114:VAL:HA	1:B:126:ARG:O	2.07	0.55
1:C:700:PHE:HA	1:C:1052:SER:H	1.69	0.55
2:D:46:ALA:HB1	2:D:62:MET:HA	1.88	0.55
2:D:588:PHE:O	2:D:592:PHE:N	2.39	0.55
1:A:19:CYS:HA	1:A:133:CYS:HB3	1.87	0.55
1:A:756:GLN:HA	1:A:759:ASN:HD22	1.71	0.55
1:B:1005:ASN:O	1:B:1009:THR:OG1	2.21	0.55
1:B:802:ASP:O	1:B:806:ASN:ND2	2.40	0.55
1:C:631:THR:O	1:C:633:ALA:N	2.38	0.55
1:B:118:ASN:HB3	1:B:170:LEU:HD21	1.89	0.55
1:C:126:ARG:NH2	1:C:162:GLU:OE2	2.39	0.55
1:C:331:ALA:O	1:C:495:ARG:NH1	2.40	0.55
1:A:440:TYR:O	1:A:478:LEU:HA	2.07	0.55
1:A:691:ASN:HA	1:C:879:PRO:HB3	1.87	0.55
1:A:1005:ASN:O	1:A:1009:THR:OG1	2.18	0.55
1:B:715:LYS:HZ1	1:B:846:LEU:HB2	1.71	0.55
1:B:756:GLN:O	1:B:760:THR:OG1	2.24	0.55
1:B:631:THR:O	1:B:633:ALA:N	2.40	0.55
1:C:838:ASN:HB3	1:C:840:LEU:HG	1.87	0.55
1:A:105:SER:O	1:A:229:THR:OG1	2.23	0.55
1:B:48:ARG:HB3	1:C:553:ARG:HB2	1.88	0.55
1:B:992:GLN:HA	1:B:995:ILE:HD12	1.89	0.55
1:C:26:GLN:HB2	1:C:75:THR:HA	1.89	0.55
2:D:499:ASP:HA	2:D:502:SER:HB3	1.89	0.55
1:C:56:GLN:OE1	1:C:261:THR:OG1	2.24	0.54
1:C:706:THR:OG1	1:C:707:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLU:HB2	1:A:155:ASN:HD22	1.72	0.54
1:B:435:ASN:OD1	1:B:437:ASN:ND2	2.40	0.54
1:C:1078:VAL:HA	1:C:1086:ILE:HG12	1.90	0.54
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.87	0.54
1:B:856:THR:HA	1:B:859:LEU:HD12	1.89	0.54
1:C:644:THR:C	1:C:645:SER:O	2.49	0.54
1:C:798:SER:N	1:C:801:GLU:OE1	2.40	0.54
1:A:328:VAL:HA	1:A:343:LYS:HE3	1.90	0.54
1:A:911:LYS:O	1:A:915:GLN:N	2.39	0.54
1:A:48:ARG:HB2	1:A:266:TYR:HD2	1.71	0.54
1:A:209:LEU:HD12	1:A:210:PRO:HD2	1.90	0.54
1:A:283:LEU:HD21	1:A:588:THR:HG22	1.90	0.54
1:B:1031:LEU:N	1:B:1047:VAL:O	2.39	0.54
1:B:114:VAL:HG11	1:B:224:LEU:HD13	1.88	0.54
1:C:951:ASN:ND2	1:C:954:ALA:O	2.40	0.54
1:C:24:ASP:HB3	1:C:245:TRP:HE1	1.73	0.54
1:C:59:PHE:O	1:C:257:LEU:HA	2.08	0.54
1:C:305:PHE:HB2	1:C:615:LEU:HD22	1.90	0.54
1:A:104:GLY:HA2	1:A:113:SER:HA	1.89	0.54
1:B:1003:SER:HA	1:B:1006:LEU:HD12	1.90	0.54
1:C:1085:PHE:HD1	1:C:1096:ILE:HA	1.72	0.54
1:A:525:VAL:O	1:A:535:THR:HA	2.08	0.53
1:B:553:ARG:HA	1:B:559:THR:H	1.73	0.53
1:B:770:MET:N	1:C:683:ALA:O	2.41	0.53
1:B:1058:THR:OG1	1:B:1080:ASN:O	2.20	0.53
2:D:245:ARG:NE	2:D:258:PRO:O	2.41	0.53
1:A:105:SER:O	1:A:230:ASN:ND2	2.41	0.53
1:A:314:VAL:HA	1:A:528:ASN:HB3	1.89	0.53
1:A:937:ASN:O	1:A:941:LEU:HB2	2.07	0.53
1:B:1085:PHE:HB3	1:B:1095:GLN:H	1.74	0.53
1:C:281:ASN:H	1:C:284:ALA:HB3	1.74	0.53
1:C:385:ASP:OD2	1:C:500:SER:OG	2.24	0.53
1:C:848:THR:HB	1:C:851:MET:HB2	1.90	0.53
2:D:263:PRO:HB3	2:D:490:PRO:HG3	1.89	0.53
1:A:165:SER:OG	1:A:166:ASP:N	2.39	0.53
1:B:561:SER:HB3	1:B:571:LEU:HD23	1.89	0.53
1:C:303:SER:OG	1:C:304:ASN:N	2.41	0.53
2:D:285:PHE:H	2:D:437:ASN:HD21	1.56	0.53
1:C:105:SER:O	1:C:229:THR:OG1	2.24	0.53
1:C:197:TYR:HB3	1:C:216:LEU:HB3	1.89	0.53
1:C:1093:SER:O	1:C:1095:GLN:NE2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:SER:OG	1:A:293:PHE:N	2.42	0.53
1:A:323:CYS:N	1:A:348:CYS:SG	2.81	0.53
1:A:1028:GLY:HA2	1:C:872:ALA:HB2	1.90	0.53
1:B:379:PHE:O	1:B:510:VAL:N	2.38	0.53
1:C:96:ASN:HB3	1:C:183:ARG:HH22	1.74	0.53
2:D:247:LYS:HD3	2:D:250:ASN:HD22	1.73	0.53
1:B:631:THR:HB	1:B:654:ALA:HB3	1.91	0.53
1:B:775:THR:HA	1:B:777:LYS:HE3	1.90	0.53
1:C:294:GLU:HG3	1:C:589:ASN:HD21	1.73	0.53
1:A:541:SER:HB3	1:A:543:LYS:HG2	1.91	0.53
1:A:956:SER:HB3	1:A:962:ILE:HG23	1.91	0.53
1:B:601:VAL:HG23	1:B:634:GLY:HA3	1.90	0.53
1:B:1013:GLU:HB3	1:B:1019:SER:HB2	1.89	0.53
1:C:19:CYS:HA	1:C:133:CYS:HB3	1.91	0.53
2:D:365:THR:HG22	2:D:367:ASP:H	1.74	0.53
1:A:432:SER:HA	1:A:485:THR:H	1.73	0.53
1:A:914:SER:O	1:A:918:GLU:N	2.41	0.53
1:C:200:TYR:O	1:C:214:ASN:ND2	2.41	0.53
1:A:399:PRO:HB3	1:A:414:ASP:HA	1.90	0.52
1:A:735:LEU:HD21	1:A:742:CYS:HB2	1.89	0.52
1:A:1063:ILE:HD11	1:A:1078:VAL:HG11	1.92	0.52
1:A:1096:ILE:O	1:A:1101:ASN:ND2	2.28	0.52
1:C:399:PRO:HD3	1:C:417:MET:HG2	1.92	0.52
1:A:872:ALA:HB1	1:B:1050:VAL:HA	1.90	0.52
1:A:951:ASN:ND2	1:A:954:ALA:O	2.30	0.52
1:B:745:LEU:HD22	1:B:990:VAL:HG21	1.92	0.52
2:D:539:LEU:HB3	2:D:587:TYR:HD1	1.75	0.52
1:A:832:ILE:O	1:B:632:GLN:NE2	2.31	0.52
1:C:102:VAL:HA	1:C:114:VAL:O	2.09	0.52
2:D:378:HIS:HE1	2:D:402:GLU:HA	1.74	0.52
2:D:503:LEU:HD22	2:D:506:VAL:HG23	1.92	0.52
1:A:81:ILE:O	1:A:231:PHE:N	2.36	0.52
1:A:207:ARG:NH1	1:A:208:ASP:OD1	2.43	0.52
1:B:559:THR:O	1:B:561:SER:N	2.42	0.52
1:B:603:CYS:HB3	1:B:627:ASN:HD21	1.74	0.52
1:C:125:ILE:HB	1:C:163:TYR:HB3	1.90	0.52
1:C:645:SER:HB3	1:C:680:SER:CA	2.40	0.52
1:C:848:THR:O	1:C:852:ILE:N	2.34	0.52
1:A:1063:ILE:HB	1:A:1070:TYR:HB2	1.92	0.52
1:C:412:LEU:HD11	1:C:498:VAL:HG11	1.90	0.52
1:C:652:ILE:N	1:C:656:ILE:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:NH2	1:B:171:ASP:O	2.34	0.52
1:B:897:VAL:O	1:B:901:ASN:ND2	2.39	0.52
1:A:961:ASP:O	1:A:964:SER:OG	2.25	0.52
1:B:35:SER:OG	1:B:64:SER:N	2.41	0.52
1:B:321:ASN:HB3	1:B:348:CYS:HA	1.92	0.52
1:B:859:LEU:O	1:B:863:THR:OG1	2.25	0.52
1:B:1061:PRO:HG2	1:B:1112:ILE:HD12	1.91	0.52
1:C:407:ASP:HB3	1:C:447:LYS:HA	1.91	0.52
1:C:1038:ALA:HB2	1:C:1043:VAL:HG23	1.91	0.52
2:D:81:GLN:NE2	2:D:103:ASN:OD1	2.43	0.52
1:A:373:LYS:NZ	1:C:966:LEU:O	2.39	0.52
1:A:1033:SER:HA	1:A:1045:LEU:O	2.09	0.52
1:B:340:TRP:O	1:B:453:ARG:NH1	2.43	0.52
1:C:315:ARG:HD2	1:C:566:LYS:HD2	1.90	0.52
1:C:853:ALA:O	1:C:856:THR:OG1	2.21	0.52
1:B:83:PHE:HE2	1:B:189:ASN:HB2	1.75	0.52
1:B:140:VAL:O	1:B:238:PHE:HA	2.09	0.52
1:B:607:SER:HA	1:B:610:ILE:HD12	1.91	0.52
1:B:948:LEU:O	1:B:957:SER:OG	2.27	0.52
2:D:482:ARG:NH2	2:D:611:SER:OG	2.43	0.52
1:B:32:GLN:HA	1:B:66:VAL:O	2.10	0.51
1:B:125:ILE:HD12	1:B:163:TYR:HD2	1.75	0.51
1:B:469:PRO:HA	1:B:471:ALA:H	1.75	0.51
2:D:184:VAL:O	2:D:188:ASN:ND2	2.42	0.51
1:C:95:SER:H	1:C:181:HIS:CD2	2.28	0.51
1:B:1064:CYS:HB3	1:B:1114:ILE:HA	1.92	0.51
1:C:363:THR:O	1:C:421:LEU:HA	2.11	0.51
1:A:683:ALA:O	1:C:769:GLN:NE2	2.43	0.51
1:A:896:ASN:OD1	1:B:1105:SER:OG	2.26	0.51
1:A:112:GLN:HE22	1:B:456:SER:HB2	1.75	0.51
1:A:386:SER:HA	1:A:496:VAL:O	2.10	0.51
1:A:679:MET:HE2	1:A:681:LEU:HA	1.91	0.51
1:A:1078:VAL:HG13	1:A:1086:ILE:HG12	1.93	0.51
1:B:94:LYS:HD2	1:B:179:PHE:HA	1.93	0.51
1:B:608:THR:O	1:B:612:ALA:N	2.41	0.51
1:B:678:THR:OG1	1:B:679:MET:N	2.42	0.51
1:B:849:ASP:HA	1:B:852:ILE:HD12	1.92	0.51
1:C:425:THR:HB	1:C:428:ILE:HB	1.93	0.51
1:C:961:ASP:O	1:C:965:ARG:NE	2.43	0.51
2:D:247:LYS:HB2	2:D:282:THR:HG22	1.92	0.51
2:D:284:PRO:HD3	2:D:440:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:443:ALA:O	2:D:447:VAL:HB	2.10	0.51
1:C:267:ASP:OD1	1:C:271:THR:N	2.43	0.51
1:C:400:GLY:O	1:C:411:LYS:NZ	2.33	0.51
1:A:99:ARG:NH2	1:A:171:ASP:O	2.43	0.51
1:A:1028:GLY:HA3	1:A:1048:THR:HB	1.93	0.51
1:B:348:CYS:H	1:B:510:VAL:HG22	1.75	0.51
2:D:99:ALA:HB1	2:D:391:LEU:HD22	1.92	0.51
1:A:755:GLU:OE1	1:A:1001:ARG:NH2	2.44	0.51
1:A:1073:ARG:HH22	1:A:1101:ASN:HB3	1.75	0.51
1:C:114:VAL:HA	1:C:126:ARG:O	2.11	0.51
1:A:749:LEU:HA	1:A:752:ILE:HD12	1.92	0.51
1:C:1072:PRO:HA	1:C:1102:THR:HA	1.91	0.51
1:A:897:VAL:O	1:A:901:ASN:ND2	2.43	0.51
1:B:598:TYR:HB2	1:B:635:CYS:HB2	1.92	0.51
1:C:677:TYR:N	1:C:677:TYR:CD1	2.71	0.51
2:D:294:THR:HG23	2:D:365:THR:HA	1.93	0.51
2:D:610:TRP:NE1	2:D:615:ASP:OD2	2.44	0.51
1:A:879:PRO:HB3	1:B:691:ASN:HA	1.93	0.50
1:A:1029:TYR:OH	1:A:1089:ARG:NH2	2.43	0.50
1:B:436:TYR:HE1	1:B:482:GLY:HA2	1.76	0.50
1:C:211:SER:OG	1:C:212:GLY:N	2.44	0.50
1:A:915:GLN:O	1:A:918:GLU:HB2	2.10	0.50
1:B:934:VAL:HA	1:B:937:ASN:HD22	1.77	0.50
1:B:82:PRO:O	1:B:256:TYR:OH	2.23	0.50
1:C:302:THR:OG1	1:C:303:SER:N	2.45	0.50
1:C:1102:THR:OG1	1:C:1103:PHE:N	2.44	0.50
1:A:443:LEU:HB2	1:A:477:PRO:HB3	1.94	0.50
1:B:755:GLU:OE2	1:B:758:ARG:NH1	2.45	0.50
1:B:1073:ARG:HE	1:B:1101:ASN:HA	1.77	0.50
1:C:630:GLN:HB3	1:C:631:THR:HG23	1.91	0.50
1:C:646:TYR:C	1:C:677:TYR:HE2	2.19	0.50
1:A:408:TYR:HE1	1:A:447:LYS:HG2	1.77	0.50
1:A:442:TYR:HE1	1:A:479:ASN:HB2	1.77	0.50
1:A:1074:GLU:HG2	1:C:895:GLN:HG3	1.94	0.50
1:B:37:MET:SD	1:B:211:SER:OG	2.69	0.50
1:B:423:TRP:HE1	1:B:495:ARG:HD2	1.77	0.50
1:A:40:VAL:HG11	1:A:272:ILE:HG21	1.94	0.50
1:B:708:VAL:HG22	1:B:1043:VAL:HG22	1.92	0.50
1:C:419:CYS:HB2	1:C:499:LEU:HB2	1.93	0.50
2:D:169:ARG:NH1	2:D:270:MET:O	2.39	0.50
1:A:286:LEU:HD21	1:A:300:TYR:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:SER:N	1:A:422:ALA:O	2.36	0.50
1:A:678:THR:OG1	1:A:679:MET:N	2.40	0.50
1:B:182:LEU:HD22	1:B:203:ILE:HD13	1.92	0.50
1:B:894:THR:OG1	1:C:1074:GLU:OE2	2.23	0.50
1:C:1062:ALA:HB3	1:C:1111:VAL:HG13	1.93	0.50
1:A:793:LYS:HE3	1:A:794:PRO:HD2	1.93	0.50
1:A:849:ASP:HA	1:A:852:ILE:HD12	1.92	0.50
1:B:931:GLN:O	1:B:935:ASN:HB2	2.12	0.50
1:C:612:ALA:O	1:C:614:GLN:NE2	2.33	0.50
1:B:40:VAL:HB	1:B:213:PHE:HB2	1.94	0.49
1:B:124:VAL:HG22	1:B:164:ILE:HG12	1.94	0.49
2:D:116:LEU:HD11	2:D:187:LYS:HE2	1.93	0.49
1:A:778:TYR:CZ	1:A:781:GLY:HA2	2.47	0.49
1:B:238:PHE:HB2	1:B:246:GLY:HA3	1.94	0.49
1:B:652:ILE:HD11	1:B:658:ALA:HB2	1.93	0.49
1:C:347:ASN:H	1:C:509:THR:HB	1.77	0.49
1:C:486:THR:HB	2:D:357:ARG:HH12	1.77	0.49
1:C:755:GLU:OE2	1:C:758:ARG:NH1	2.45	0.49
1:A:837:PHE:HB3	1:B:575:PRO:HD3	1.94	0.49
1:B:972:GLU:HA	1:B:975:ILE:HD12	1.94	0.49
1:C:178:ASN:HB2	1:C:204:ASP:HA	1.94	0.49
1:C:660:TYR:HB2	1:C:674:ILE:HA	1.95	0.49
1:A:287:LYS:HA	1:A:295:ILE:HD11	1.94	0.49
1:A:1036:GLN:HG2	1:A:1045:LEU:HD11	1.95	0.49
1:C:887:ARG:NH1	1:C:1032:MET:SD	2.85	0.49
2:D:291:ILE:HG13	2:D:438:PHE:HB2	1.94	0.49
1:A:364:PHE:HD1	1:A:421:LEU:HD13	1.76	0.49
1:A:698:THR:OG1	1:A:1053:GLN:OE1	2.24	0.49
1:A:1086:ILE:H	1:A:1095:GLN:H	1.58	0.49
1:B:984:GLN:O	1:B:988:THR:OG1	2.28	0.49
1:B:1031:LEU:HB3	1:B:1047:VAL:HG12	1.95	0.49
1:C:332:THR:O	1:C:495:ARG:NH2	2.44	0.49
1:C:1015:VAL:HA	1:C:1033:SER:HB3	1.94	0.49
1:A:882:MET:SD	1:A:899:TYR:OH	2.70	0.49
1:B:324:PRO:O	1:B:327:GLU:HB3	2.13	0.49
1:A:719:ASP:HB3	1:A:722:MET:HB2	1.95	0.49
1:C:538:LEU:HD22	1:C:570:ILE:HD12	1.95	0.49
1:A:229:THR:OG1	1:A:230:ASN:N	2.45	0.49
1:A:297:LYS:HG2	1:A:650:ILE:HD11	1.93	0.49
1:A:626:ASN:ND2	1:A:639:ALA:O	2.46	0.49
1:B:1054:GLU:O	1:B:1055:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LYS:HZ3	1:C:250:ALA:HB2	1.78	0.49
1:C:972:GLU:HA	1:C:975:ILE:HD12	1.94	0.49
1:A:902:GLN:O	1:A:905:ILE:HB	2.13	0.49
1:A:603:CYS:HB3	1:A:627:ASN:HD21	1.78	0.48
1:C:405:ILE:HG23	1:C:409:ASN:HD22	1.78	0.48
1:C:448:LEU:HB3	1:C:452:GLU:HB3	1.94	0.48
1:C:937:ASN:O	1:C:941:LEU:CB	2.60	0.48
1:C:1030:HIS:CE1	1:C:1033:SER:HB2	2.47	0.48
2:D:237:TYR:OH	2:D:485:VAL:O	2.19	0.48
2:D:272:GLY:HA2	2:D:275:TRP:HE1	1.76	0.48
2:D:388:GLN:O	2:D:393:ARG:NE	2.47	0.48
2:D:557:MET:HE2	2:D:569:ALA:HB1	1.94	0.48
1:A:544:ARG:NE	1:C:269:ASN:OD1	2.46	0.48
1:B:656:ILE:HA	1:B:678:THR:HA	1.95	0.48
1:A:299:ILE:HG12	1:A:584:ILE:HG13	1.94	0.48
1:C:138:PHE:HB3	1:C:140:VAL:HG23	1.95	0.48
1:B:351:ASP:HA	1:B:513:PRO:HD3	1.94	0.48
1:B:439:LYS:HD3	1:B:478:LEU:HB3	1.96	0.48
1:B:891:ILE:HB	1:B:1018:GLN:HE22	1.79	0.48
2:D:226:VAL:HG21	2:D:513:ILE:HD11	1.95	0.48
1:A:33:HIS:HB2	1:A:66:VAL:HB	1.96	0.48
1:A:138:PHE:HB3	1:A:140:VAL:HG23	1.96	0.48
1:B:102:VAL:HA	1:B:115:ILE:HG12	1.93	0.48
1:C:285:GLU:O	1:C:289:SER:OG	2.23	0.48
2:D:63:ASN:O	2:D:67:ASP:N	2.46	0.48
1:A:368:GLY:O	1:C:965:ARG:NH1	2.46	0.48
1:B:267:ASP:OD1	1:B:270:GLY:N	2.47	0.48
1:A:94:LYS:HB3	1:A:175:LYS:HB2	1.95	0.48
1:A:1032:MET:HB2	1:A:1047:VAL:HB	1.96	0.48
1:B:25:VAL:HG22	1:B:76:PHE:HB3	1.94	0.48
1:B:378:CYS:N	1:B:530:ASN:O	2.44	0.48
1:A:769:GLN:HG2	1:A:874:ALA:HB1	1.95	0.48
1:C:82:PRO:HA	1:C:230:ASN:HA	1.96	0.48
1:C:94:LYS:NZ	1:C:249:ALA:O	2.45	0.48
2:D:460:ARG:HD2	2:D:506:VAL:HG22	1.95	0.48
1:A:769:GLN:HA	1:B:683:ALA:HB3	1.95	0.47
1:A:1072:PRO:HB3	1:A:1086:ILE:HD13	1.96	0.47
1:B:98:VAL:HG12	1:B:235:LEU:HG	1.95	0.47
1:B:429:ASP:O	1:B:435:ASN:ND2	2.46	0.47
1:B:846:LEU:HD11	1:C:651:PRO:HB2	1.96	0.47
1:C:165:SER:OG	1:C:166:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:GLY:HA2	1:C:650:ILE:HG21	1.95	0.47
2:D:58:ASN:O	2:D:62:MET:HB2	2.14	0.47
1:A:807:LYS:NZ	1:A:920:LEU:O	2.42	0.47
1:B:758:ARG:HH22	1:C:929:LYS:HE2	1.78	0.47
1:C:363:THR:HB	1:C:422:ALA:H	1.79	0.47
2:D:169:ARG:NH2	2:D:270:MET:SD	2.86	0.47
1:B:756:GLN:HA	1:B:759:ASN:HD22	1.78	0.47
1:B:1009:THR:O	1:B:1012:SER:OG	2.29	0.47
1:C:48:ARG:HB2	1:C:266:TYR:CD2	2.49	0.47
2:D:468:ILE:HG12	2:D:476:LYS:HG2	1.97	0.47
1:A:147:GLN:HB3	1:A:150:THR:HB	1.95	0.47
1:A:521:LYS:HD3	1:A:540:PRO:HD3	1.97	0.47
1:B:541:SER:HA	1:B:571:LEU:HG	1.96	0.47
1:B:781:GLY:O	1:B:910:ASN:ND2	2.41	0.47
1:C:51:THR:OG1	1:C:52:LEU:N	2.48	0.47
1:A:129:ASN:HD22	1:A:158:ASN:HB2	1.79	0.47
1:A:906:ALA:O	1:A:910:ASN:N	2.44	0.47
1:A:968:LYS:HG3	1:A:969:VAL:HG23	1.96	0.47
1:B:122:ASN:OD1	1:B:123:VAL:N	2.48	0.47
1:B:314:VAL:O	1:B:517:THR:N	2.42	0.47
1:B:837:PHE:HB3	1:C:575:PRO:HG3	1.96	0.47
1:B:879:PRO:HG3	1:C:691:ASN:HA	1.96	0.47
1:C:930:LEU:HD22	1:C:1041:GLY:HA3	1.97	0.47
2:D:245:ARG:NH2	2:D:605:GLY:O	2.48	0.47
2:D:347:THR:OG1	2:D:349:TRP:NE1	2.47	0.47
2:D:462:MET:HB3	2:D:468:ILE:HG13	1.95	0.47
1:A:324:PRO:O	1:A:328:VAL:N	2.35	0.47
1:B:694:ILE:HD12	1:B:1059:THR:HB	1.97	0.47
1:A:267:ASP:OD1	1:A:271:THR:N	2.39	0.47
1:A:325:PHE:HA	1:A:328:VAL:HG12	1.96	0.47
1:A:390:LYS:HB3	1:A:491:TYR:HA	1.97	0.47
1:C:313:VAL:HG22	1:C:520:ILE:H	1.80	0.47
1:C:453:ARG:HG2	1:C:455:ILE:HD11	1.96	0.47
1:C:94:LYS:HB2	1:C:94:LYS:HE2	1.72	0.47
1:C:694:ILE:N	1:C:1057:PHE:O	2.44	0.47
2:D:432:ASN:HA	2:D:435:GLU:HB3	1.96	0.47
1:B:113:SER:O	1:B:127:ALA:HA	2.15	0.46
1:C:975:ILE:HA	1:C:978:LEU:HD12	1.97	0.46
1:C:1063:ILE:H	1:C:1070:TYR:H	1.61	0.46
1:A:591:SER:OG	1:A:592:SER:N	2.48	0.46
1:C:646:TYR:O	1:C:680:SER:CB	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:314:PHE:HB3	2:D:373:HIS:HE1	1.79	0.46
1:A:83:PHE:N	1:A:229:THR:O	2.47	0.46
1:A:99:ARG:HH12	1:A:172:VAL:HG13	1.79	0.46
1:A:135:ASN:HA	1:A:232:ARG:HH12	1.79	0.46
1:B:431:THR:OG1	1:B:434:GLY:O	2.33	0.46
1:C:129:ASN:ND2	1:C:157:PHE:O	2.49	0.46
1:C:939:GLN:O	1:C:943:THR:OG1	2.21	0.46
2:D:180:TYR:HA	2:D:183:TYR:HB3	1.97	0.46
1:A:128:CYS:HB3	1:A:130:PHE:CE1	2.51	0.46
1:B:865:THR:O	1:B:883:GLN:NE2	2.48	0.46
1:B:903:LYS:O	1:B:907:ASN:N	2.41	0.46
2:D:278:LEU:O	2:D:282:THR:N	2.48	0.46
1:A:430:ALA:O	1:A:485:THR:OG1	2.27	0.46
1:A:527:PHE:O	1:A:533:THR:OG1	2.29	0.46
1:A:1061:PRO:HG2	1:A:1112:ILE:HB	1.97	0.46
1:B:931:GLN:O	1:B:935:ASN:ND2	2.49	0.46
1:C:869:THR:HB	1:C:876:LEU:HD21	1.97	0.46
2:D:389:PRO:HG2	2:D:392:LEU:HD13	1.98	0.46
1:A:52:LEU:HA	1:A:264:LEU:O	2.15	0.46
1:B:99:ARG:HD3	1:B:118:ASN:HB2	1.98	0.46
1:C:426:ARG:HB2	1:C:485:THR:HG23	1.98	0.46
1:A:711:VAL:HG11	1:A:763:VAL:HG11	1.97	0.46
1:B:612:ALA:O	1:B:614:GLN:NE2	2.44	0.46
2:D:281:LEU:HD12	2:D:282:THR:HG23	1.97	0.46
1:A:786:GLN:OE1	1:A:917:GLN:NE2	2.49	0.46
1:C:209:LEU:HD12	1:C:210:PRO:HD2	1.98	0.46
1:C:679:MET:HE2	1:C:681:LEU:HA	1.98	0.46
2:D:419:LYS:HE3	2:D:428:PHE:HB3	1.98	0.46
2:D:520:LEU:HD22	2:D:579:MET:HB2	1.97	0.46
1:A:317:PRO:HG3	1:A:565:PRO:HB3	1.97	0.46
1:A:835:GLN:HE21	1:B:575:PRO:HB2	1.81	0.46
1:A:1064:CYS:HB3	1:A:1114:ILE:HG23	1.98	0.46
1:B:83:PHE:HD1	1:B:231:PHE:HB3	1.80	0.46
1:A:35:SER:N	1:A:64:SER:O	2.46	0.46
1:A:886:TYR:HA	1:A:889:ASN:ND2	2.30	0.46
1:B:361:PHE:CG	1:B:421:LEU:HD11	2.51	0.46
1:C:678:THR:O	1:C:679:MET:HB2	2.16	0.46
1:C:931:GLN:O	1:C:935:ASN:ND2	2.48	0.46
1:A:100:GLY:CA	1:A:116:ILE:O	2.55	0.45
1:A:344:LYS:HE3	1:A:381:ASN:HB3	1.98	0.45
1:A:1036:GLN:HB2	1:A:1043:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1026:GLY:HA3	1:B:1048:THR:HG22	1.98	0.45
1:B:1080:ASN:HA	1:B:1083:SER:HA	1.98	0.45
1:C:93:GLU:OE1	1:C:97:VAL:N	2.45	0.45
1:C:99:ARG:HG3	1:C:138:PHE:HE2	1.81	0.45
1:C:801:GLU:HA	1:C:804:LEU:HD12	1.98	0.45
1:A:42:TYR:HE1	1:A:272:ILE:HG13	1.81	0.45
1:B:784:PHE:HB3	1:B:788:LEU:HG	1.98	0.45
1:C:722:MET:HA	1:C:726:GLY:HA2	1.98	0.45
1:B:561:SER:HA	1:B:571:LEU:HA	1.98	0.45
1:C:869:THR:H	1:C:876:LEU:HD11	1.81	0.45
1:A:46:ILE:HG12	1:B:551:PHE:HB2	1.98	0.45
1:A:158:ASN:HB3	1:B:455:ILE:HG21	1.98	0.45
1:A:607:SER:HA	1:A:610:ILE:HD12	1.97	0.45
1:A:1031:LEU:HB3	1:A:1047:VAL:HG12	1.98	0.45
1:C:33:HIS:HB2	1:C:66:VAL:HB	1.97	0.45
1:C:346:SER:HA	1:C:509:THR:HB	1.98	0.45
1:C:426:ARG:O	1:C:485:THR:OG1	2.27	0.45
1:C:955:ILE:HG21	1:C:965:ARG:HH12	1.82	0.45
1:C:1044:PHE:HB3	1:C:1046:HIS:CE1	2.51	0.45
1:A:886:TYR:HD1	1:B:1076:VAL:HG13	1.82	0.45
1:A:946:LYS:O	1:A:950:SER:N	2.49	0.45
1:A:1034:PHE:HB2	1:A:1045:LEU:HD12	1.97	0.45
1:A:1065:HIS:HB2	1:A:1118:THR:HB	1.99	0.45
1:C:425:THR:O	1:C:429:ASP:N	2.40	0.45
1:C:443:LEU:HB2	1:C:477:PRO:HA	1.98	0.45
2:D:229:THR:HG21	2:D:579:MET:HE2	1.98	0.45
1:B:55:THR:O	1:B:261:THR:HA	2.17	0.45
1:B:895:GLN:HG3	1:C:1074:GLU:HG2	1.98	0.45
1:C:138:PHE:HD2	1:C:236:THR:HG22	1.82	0.45
1:C:467:CYS:HB3	1:C:474:CYS:HB3	1.76	0.45
1:C:648:CYS:N	1:C:677:TYR:OH	2.47	0.45
1:C:961:ASP:O	1:C:964:SER:OG	2.28	0.45
1:A:858:ALA:O	1:A:861:SER:OG	2.32	0.45
1:C:987:GLN:O	1:C:991:THR:OG1	2.23	0.45
1:B:94:LYS:HG3	1:B:180:LYS:HB3	1.98	0.45
1:A:26:GLN:HB2	1:A:75:THR:HA	1.98	0.45
1:A:749:LEU:HD23	1:A:752:ILE:HD12	1.99	0.45
1:A:1072:PRO:HG3	1:A:1078:VAL:HG22	1.98	0.45
1:C:979:ILE:O	1:C:983:LEU:CB	2.65	0.45
2:D:410:LEU:HD23	2:D:526:GLN:HE21	1.82	0.45
1:A:57:ASP:OD2	1:A:188:LYS:NZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:PRO:HG3	1:B:341:GLU:HB2	1.97	0.45
1:B:756:GLN:HA	1:B:759:ASN:ND2	2.32	0.45
1:C:847:LEU:HD11	1:C:855:TYR:HE2	1.82	0.45
2:D:209:VAL:HG23	2:D:216:ASP:HA	1.99	0.45
2:D:518:ARG:O	2:D:522:GLN:HB2	2.17	0.45
1:A:57:ASP:OD1	1:A:58:LEU:N	2.50	0.44
1:A:687:ILE:HB	1:A:689:TYR:CE2	2.51	0.44
1:A:760:THR:HG22	1:A:847:LEU:HD23	1.99	0.44
1:B:1095:GLN:HB3	1:B:1101:ASN:HD21	1.82	0.44
1:C:369:VAL:HG23	1:C:371:ALA:H	1.82	0.44
1:A:132:LEU:HD23	1:A:132:LEU:HA	1.75	0.44
1:B:19:CYS:HA	1:B:133:CYS:HB3	1.98	0.44
1:B:405:ILE:HG23	1:B:409:ASN:HD22	1.82	0.44
2:D:234:LYS:O	2:D:238:GLU:HB2	2.18	0.44
1:A:72:ILE:HG13	1:A:75:THR:H	1.83	0.44
1:A:1084:TRP:HB3	1:A:1085:PHE:CD2	2.52	0.44
1:B:880:PHE:HA	1:B:883:GLN:HB2	1.99	0.44
1:C:302:THR:HG23	1:C:581:VAL:HG23	1.99	0.44
1:C:1084:TRP:HB3	1:C:1085:PHE:CD2	2.52	0.44
1:A:343:LYS:HB2	1:A:384:ALA:HB3	2.00	0.44
1:A:597:LEU:HD22	1:A:652:ILE:HG23	1.99	0.44
1:A:951:ASN:OD1	1:A:952:PHE:N	2.50	0.44
1:A:1055:ARG:HA	1:A:1055:ARG:HD3	1.70	0.44
1:B:860:VAL:HG22	1:B:1035:PRO:HD2	1.99	0.44
1:C:343:LYS:HB3	1:C:384:ALA:HB3	2.00	0.44
1:C:1012:SER:OG	1:C:1013:GLU:N	2.51	0.44
1:A:802:ASP:O	1:A:806:ASN:ND2	2.51	0.44
1:C:98:VAL:HG12	1:C:235:LEU:HG	1.99	0.44
1:C:997:ALA:HA	1:C:1000:ILE:HG22	1.99	0.44
1:C:1088:GLN:HG2	1:C:1093:SER:HB2	1.99	0.44
2:D:222:LEU:HD21	2:D:513:ILE:HG21	1.99	0.44
1:A:238:PHE:HB2	1:A:246:GLY:HA3	2.00	0.44
1:A:370:SER:HB3	1:C:967:ASP:HB2	1.99	0.44
1:B:82:PRO:HA	1:B:230:ASN:HA	1.99	0.44
1:B:305:PHE:HB3	1:B:581:VAL:HG13	2.00	0.44
1:B:430:ALA:HB2	1:B:493:PRO:HG3	1.99	0.44
1:A:112:GLN:HB3	1:A:226:ILE:HD12	1.99	0.44
1:A:771:TYR:HB3	1:B:687:ILE:HG12	2.00	0.44
1:B:287:LYS:HA	1:B:295:ILE:HD11	1.99	0.44
1:C:646:TYR:H	1:C:677:TYR:HE2	1.40	0.44
1:A:938:ALA:O	1:A:942:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1049:TYR:CE2	1:B:1051:PRO:HG3	2.53	0.44
1:C:316:PHE:CD1	1:C:317:PRO:HD2	2.53	0.44
1:C:334:PHE:HB2	1:C:388:VAL:HG23	1.99	0.44
2:D:554:LEU:O	2:D:558:LEU:HB2	2.18	0.44
2:D:554:LEU:HG	2:D:558:LEU:HD13	2.00	0.44
1:A:89:PHE:HB3	1:A:185:PHE:HB2	1.99	0.44
1:A:770:MET:N	1:B:683:ALA:O	2.51	0.44
1:B:803:LEU:HD22	1:B:921:THR:HG22	1.99	0.44
1:C:362:SER:H	1:C:423:TRP:HA	1.82	0.44
1:C:638:GLY:O	1:C:674:ILE:HD13	2.18	0.44
1:C:690:SER:OG	1:C:691:ASN:N	2.51	0.44
1:C:1064:CYS:HB2	1:C:1111:VAL:HG11	2.00	0.44
2:D:374:HIS:HE1	2:D:406:GLU:HG2	1.83	0.44
1:A:64:SER:HA	1:A:620:ARG:CZ	2.48	0.43
1:A:797:ARG:HD2	1:A:805:PHE:HE2	1.83	0.43
1:A:869:THR:OG1	1:B:1089:ARG:NH1	2.51	0.43
1:B:630:GLN:HG2	1:B:631:THR:H	1.82	0.43
2:D:21:ILE:HD13	2:D:84:PRO:HG2	2.00	0.43
1:A:390:LYS:HG2	1:A:483:PHE:HE1	1.84	0.43
1:A:724:ILE:HG22	1:A:725:CYS:HB2	2.00	0.43
1:A:1065:HIS:HB3	1:A:1070:TYR:HE2	1.82	0.43
1:B:33:HIS:HB2	1:B:66:VAL:HB	1.99	0.43
1:B:963:LEU:HA	1:B:966:LEU:HB3	2.00	0.43
1:C:933:VAL:O	1:C:937:ASN:ND2	2.51	0.43
2:D:19:SER:OG	2:D:20:THR:N	2.52	0.43
1:A:41:TYR:HB3	1:A:216:LEU:HB2	2.01	0.43
1:A:968:LYS:HD3	1:A:968:LYS:HA	1.83	0.43
1:B:943:THR:O	1:B:947:GLN:HG2	2.18	0.43
1:C:530:ASN:OD1	1:C:530:ASN:N	2.50	0.43
1:C:951:ASN:OD1	1:C:952:PHE:N	2.49	0.43
1:C:974:GLN:OE1	1:C:977:ARG:NH1	2.50	0.43
1:A:95:SER:OG	1:A:173:SER:O	2.35	0.43
1:A:282:PRO:HB2	1:A:594:VAL:HG11	1.99	0.43
1:A:431:THR:OG1	1:A:434:GLY:O	2.37	0.43
1:A:710:PRO:HA	1:A:930:LEU:HD21	1.99	0.43
1:A:1102:THR:OG1	1:A:1103:PHE:N	2.51	0.43
1:C:631:THR:HB	1:C:654:ALA:HB3	2.00	0.43
2:D:188:ASN:HD21	2:D:464:PHE:HA	1.83	0.43
1:A:361:PHE:HA	1:A:423:TRP:HB3	2.00	0.43
1:A:439:LYS:HD3	1:A:478:LEU:HD13	1.99	0.43
1:A:630:GLN:HG2	1:A:631:THR:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:ALA:HB2	1:A:1080:ASN:HD22	1.82	0.43
1:B:681:LEU:HD13	1:B:681:LEU:HA	1.87	0.43
2:D:200:GLY:HA2	2:D:203:TRP:CE3	2.53	0.43
1:A:126:ARG:NH2	1:A:162:GLU:OE2	2.51	0.43
1:A:780:GLY:O	1:A:903:LYS:NZ	2.52	0.43
1:A:1071:PHE:HB2	1:A:1103:PHE:CZ	2.54	0.43
1:B:861:SER:OG	1:B:862:GLY:N	2.51	0.43
1:C:427:ASN:OD1	1:C:427:ASN:N	2.42	0.43
2:D:130:GLY:HA3	2:D:172:VAL:HG11	2.00	0.43
2:D:581:VAL:HG22	2:D:585:LEU:HD23	2.00	0.43
1:B:1069:ALA:HB2	1:B:1108:CYS:HA	2.00	0.43
1:C:742:CYS:O	1:C:746:ASN:ND2	2.52	0.43
1:C:756:GLN:O	1:C:760:THR:OG1	2.28	0.43
2:D:528:ALA:HB1	2:D:553:LYS:HE3	2.01	0.43
1:B:1079:PHE:HB2	1:B:1087:THR:HG23	2.00	0.43
1:C:56:GLN:HB2	1:C:261:THR:HG23	2.00	0.43
1:C:283:LEU:H	1:C:594:VAL:HG11	1.84	0.43
1:C:597:LEU:HD22	1:C:652:ILE:HG23	2.01	0.43
1:C:603:CYS:HA	1:C:606:VAL:HB	2.01	0.43
1:C:745:LEU:HD22	1:C:990:VAL:HG21	2.01	0.43
1:A:48:ARG:HB2	1:A:266:TYR:CD2	2.53	0.43
1:A:524:CYS:HB2	1:A:576:CYS:HB3	1.92	0.43
1:B:47:PHE:HE1	1:B:270:GLY:HA3	1.83	0.43
1:B:631:THR:HG21	1:B:656:ILE:HG13	2.01	0.43
1:C:281:ASN:HB3	1:C:283:LEU:HB3	2.01	0.43
1:C:312:ASP:H	1:C:520:ILE:HD13	1.84	0.43
1:C:861:SER:O	1:C:865:THR:N	2.37	0.43
2:D:307:ILE:HG23	2:D:369:PHE:HD1	1.84	0.43
1:A:626:ASN:OD1	1:A:626:ASN:N	2.51	0.43
1:B:57:ASP:OD1	1:B:58:LEU:N	2.51	0.43
1:C:553:ARG:HA	1:C:558:PHE:O	2.19	0.43
1:C:752:ILE:O	1:C:756:GLN:HG3	2.18	0.43
1:A:959:LEU:HA	1:A:962:ILE:HD11	2.00	0.42
1:B:1031:LEU:HD12	1:B:1031:LEU:HA	1.85	0.42
1:C:302:THR:HG21	1:C:583:VAL:HG23	2.00	0.42
2:D:503:LEU:HD23	2:D:505:HIS:H	1.84	0.42
1:A:352:TYR:CE2	1:A:374:LEU:HG	2.54	0.42
1:A:772:LYS:N	1:B:685:SER:O	2.53	0.42
2:D:152:MET:HE3	2:D:152:MET:HB3	1.87	0.42
2:D:524:GLN:HB3	2:D:574:VAL:HG11	2.00	0.42
2:D:578:ASN:OD1	2:D:579:MET:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:PHE:HB2	1:B:532:LEU:HB3	2.00	0.42
1:C:122:ASN:OD1	1:C:123:VAL:N	2.52	0.42
1:C:140:VAL:HB	1:C:236:THR:HB	2.00	0.42
1:C:629:PHE:H	1:C:641:HIS:CE1	2.37	0.42
1:A:1032:MET:HE3	1:A:1032:MET:HB3	1.89	0.42
1:B:93:GLU:O	1:B:181:HIS:CB	2.51	0.42
1:B:836:LYS:HD3	1:B:838:ASN:HD22	1.85	0.42
2:D:288:LYS:HD3	2:D:288:LYS:HA	1.88	0.42
1:A:598:TYR:HB2	1:A:635:CYS:HB2	2.01	0.42
1:B:205:VAL:HG11	1:B:210:PRO:HD3	2.01	0.42
1:A:972:GLU:HA	1:A:975:ILE:HB	2.02	0.42
1:A:1064:CYS:SG	1:A:1068:LYS:N	2.92	0.42
1:A:1110:VAL:HG11	1:C:900:GLU:HA	2.01	0.42
1:B:931:GLN:H	1:B:931:GLN:HG3	1.67	0.42
1:C:196:VAL:HB	1:C:220:PHE:HB2	2.00	0.42
1:C:676:ALA:O	1:C:677:TYR:O	2.38	0.42
1:C:786:GLN:HB3	1:C:799:PHE:HB3	2.01	0.42
1:C:925:THR:C	1:C:927:LEU:H	2.27	0.42
2:D:489:GLU:HA	2:D:490:PRO:HD3	1.89	0.42
1:A:160:THR:OG1	1:A:161:PHE:N	2.53	0.42
1:A:1012:SER:OG	1:A:1013:GLU:N	2.52	0.42
1:B:541:SER:HB2	1:B:569:GLU:HB3	2.01	0.42
1:B:1010:LYS:O	1:B:1014:CYS:N	2.46	0.42
1:C:115:ILE:O	1:C:125:ILE:HA	2.19	0.42
1:C:340:TRP:HH2	1:C:342:ARG:HH21	1.68	0.42
1:C:674:ILE:O	1:C:674:ILE:CD1	2.68	0.42
1:C:718:VAL:HG21	1:C:986:LEU:HD11	2.02	0.42
2:D:145:GLU:HA	2:D:146:PRO:HA	1.94	0.42
1:A:95:SER:H	1:A:181:HIS:CD2	2.31	0.42
1:A:552:GLY:HA2	1:C:47:PHE:HB3	2.01	0.42
1:A:631:THR:HB	1:A:654:ALA:HB3	2.01	0.42
1:B:97:VAL:N	1:B:183:ARG:HH12	2.18	0.42
1:B:715:LYS:NZ	1:B:844:PRO:O	2.46	0.42
1:B:894:THR:OG1	1:B:895:GLN:N	2.53	0.42
1:C:1027:LYS:H	1:C:1048:THR:HG21	1.85	0.42
1:C:1049:TYR:CE2	1:C:1051:PRO:HG3	2.55	0.42
2:D:477:TRP:HD1	2:D:478:TRP:CD1	2.38	0.42
1:A:598:TYR:HB3	1:A:601:VAL:HG11	2.02	0.42
1:A:738:TYR:HB3	1:A:741:PHE:CE2	2.55	0.42
1:A:994:LEU:HG	1:B:995:ILE:HG21	2.01	0.42
1:B:439:LYS:NZ	1:B:480:ASP:OD1	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:PRO:HG3	1:C:633:ALA:HB2	2.01	0.42
1:B:951:ASN:OD1	1:B:952:PHE:N	2.52	0.42
1:C:48:ARG:HB2	1:C:266:TYR:HD2	1.85	0.42
1:C:629:PHE:H	1:C:641:HIS:HE1	1.66	0.42
1:C:912:ALA:O	1:C:916:ILE:HG12	2.20	0.42
1:C:1107:ASN:OD1	1:C:1107:ASN:N	2.42	0.42
2:D:398:GLU:HG3	2:D:514:ARG:HB3	2.02	0.42
1:A:321:ASN:HB3	1:A:348:CYS:HA	2.02	0.41
1:A:934:VAL:HA	1:A:937:ASN:HD22	1.84	0.41
1:B:658:ALA:HA	1:B:676:ALA:HA	2.02	0.41
1:B:775:THR:HA	1:B:777:LYS:HG3	2.01	0.41
1:B:902:GLN:O	1:B:905:ILE:HB	2.20	0.41
1:B:1055:ARG:HD3	1:B:1055:ARG:HA	1.84	0.41
2:D:526:GLN:HG3	2:D:539:LEU:HD11	2.01	0.41
1:A:24:ASP:O	1:A:245:TRP:NE1	2.53	0.41
1:A:896:ASN:HD21	1:B:1103:PHE:HE2	1.66	0.41
1:A:987:GLN:O	1:A:991:THR:OG1	2.35	0.41
1:B:1029:TYR:HB2	1:B:1049:TYR:HB3	2.02	0.41
1:C:122:ASN:ND2	1:C:165:SER:O	2.45	0.41
1:C:603:CYS:SG	1:C:629:PHE:HB2	2.59	0.41
1:C:1065:HIS:HA	1:C:1116:ASN:HA	2.01	0.41
2:D:81:GLN:HG2	2:D:101:GLN:HG2	2.02	0.41
2:D:238:GLU:HG3	2:D:605:GLY:HA2	2.02	0.41
1:B:95:SER:OG	1:B:173:SER:O	2.37	0.41
1:B:119:ASN:OD1	1:B:122:ASN:N	2.53	0.41
1:B:341:GLU:OE2	1:B:343:LYS:NZ	2.47	0.41
1:B:912:ALA:O	1:B:916:ILE:HG12	2.21	0.41
1:C:645:SER:HB3	1:C:680:SER:HA	2.02	0.41
2:D:336:PRO:HB2	2:D:340:GLN:HB3	2.03	0.41
2:D:477:TRP:CE2	2:D:500:PRO:HD3	2.55	0.41
1:A:60:LEU:HD12	1:A:61:PRO:HD2	2.02	0.41
1:C:96:ASN:O	1:C:99:ARG:NH2	2.53	0.41
1:A:967:ASP:HB2	1:B:370:SER:HB3	2.01	0.41
1:B:114:VAL:HG12	1:B:226:ILE:HD11	2.02	0.41
1:B:128:CYS:HB3	1:B:130:PHE:CE1	2.56	0.41
1:B:165:SER:OG	1:B:166:ASP:N	2.52	0.41
1:B:725:CYS:HA	1:B:959:LEU:HD11	2.01	0.41
1:C:93:GLU:O	1:C:181:HIS:CB	2.61	0.41
1:C:361:PHE:HA	1:C:423:TRP:HB3	2.02	0.41
2:D:481:LYS:O	2:D:487:VAL:N	2.42	0.41
1:A:758:ARG:NH1	1:A:1001:ARG:HH12	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:THR:HB	1:B:137:PHE:HE1	1.86	0.41
1:B:591:SER:OG	1:B:592:SER:N	2.54	0.41
1:C:41:TYR:HB3	1:C:216:LEU:HB2	2.01	0.41
1:C:638:GLY:O	1:C:674:ILE:CD1	2.68	0.41
1:C:859:LEU:O	1:C:863:THR:OG1	2.19	0.41
1:A:895:GLN:HG3	1:B:1074:GLU:HG2	2.01	0.41
1:C:527:PHE:HE1	1:C:538:LEU:HD11	1.85	0.41
1:A:347:ASN:H	1:A:509:THR:HB	1.86	0.41
1:A:846:LEU:HD12	1:B:655:GLY:H	1.86	0.41
1:B:769:GLN:HA	1:C:683:ALA:HB3	2.02	0.41
1:B:1086:ILE:HD12	1:B:1101:ASN:HB3	2.02	0.41
1:A:133:CYS:HB2	1:A:136:PRO:HD3	2.02	0.41
1:A:182:LEU:HD22	1:A:203:ILE:HD13	2.02	0.41
1:A:775:THR:HA	1:A:777:LYS:HG3	2.03	0.41
1:B:76:PHE:HB2	1:B:245:TRP:CE2	2.56	0.41
1:B:196:VAL:HB	1:B:220:PHE:HB2	2.03	0.41
1:B:263:MET:O	1:B:275:ALA:HA	2.20	0.41
1:B:402:THR:OG1	1:B:403:GLY:N	2.54	0.41
1:B:409:ASN:HD21	1:B:440:TYR:HB2	1.86	0.41
1:B:1102:THR:OG1	1:B:1103:PHE:N	2.54	0.41
1:C:35:SER:OG	1:C:64:SER:N	2.40	0.41
1:C:591:SER:OG	1:C:592:SER:N	2.54	0.41
1:C:852:ILE:O	1:C:856:THR:HG23	2.21	0.41
2:D:184:VAL:HG12	2:D:464:PHE:HE1	1.86	0.41
2:D:440:LEU:HA	2:D:443:ALA:HB3	2.03	0.41
1:A:112:GLN:HE21	1:B:455:ILE:H	1.69	0.41
1:A:793:LYS:HA	1:A:793:LYS:HD2	1.79	0.41
1:A:1079:PHE:CZ	1:A:1081:GLY:HA3	2.56	0.41
1:B:911:LYS:O	1:B:914:SER:HB2	2.20	0.41
1:B:927:LEU:HD12	1:B:927:LEU:HA	1.90	0.41
1:C:764:PHE:HD1	1:C:1011:MET:HE1	1.86	0.41
1:B:553:ARG:HD3	1:B:557:ASP:HA	2.02	0.40
1:C:38:ARG:HH21	1:C:210:PRO:C	2.28	0.40
2:D:119:ILE:HD13	2:D:119:ILE:HA	1.97	0.40
2:D:289:PRO:HG2	2:D:428:PHE:HE1	1.86	0.40
1:A:57:ASP:CG	1:A:188:LYS:HZ1	2.29	0.40
1:A:553:ARG:HD2	1:A:557:ASP:HA	2.03	0.40
1:A:734:LEU:HA	1:A:734:LEU:HD23	1.85	0.40
1:A:961:ASP:O	1:A:965:ARG:NE	2.53	0.40
1:C:561:SER:HB3	1:C:571:LEU:HD23	2.03	0.40
1:C:1009:THR:O	1:C:1013:GLU:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:THR:HG21	1:A:149:HIS:HE1	1.86	0.40
1:A:483:PHE:CE2	1:A:493:PRO:HB3	2.57	0.40
1:A:536:GLY:HA2	1:A:576:CYS:SG	2.62	0.40
1:A:956:SER:OG	1:A:957:SER:N	2.54	0.40
1:B:209:LEU:HD12	1:B:209:LEU:HA	1.90	0.40
1:B:297:LYS:HG3	1:B:586:PRO:HA	2.03	0.40
1:B:698:THR:H	1:B:1053:GLN:HB2	1.86	0.40
1:C:18:ARG:HB3	1:C:151:MET:HE1	2.04	0.40
1:C:141:SER:H	1:C:145:GLY:HA2	1.86	0.40
1:C:314:VAL:HB	1:C:517:THR:HB	2.03	0.40
1:C:385:ASP:HB2	1:C:498:VAL:HB	2.02	0.40
1:C:800:ILE:O	1:C:804:LEU:HG	2.21	0.40
1:A:324:PRO:HD2	1:A:345:ILE:HG12	2.02	0.40
1:A:697:PRO:HB3	1:A:1053:GLN:H	1.86	0.40
1:A:968:LYS:O	1:A:971:ALA:N	2.36	0.40
1:C:355:LEU:HB3	1:C:421:LEU:HD21	2.03	0.40
1:A:25:VAL:HA	1:A:76:PHE:HB3	2.04	0.40
1:A:72:ILE:HG12	1:A:75:THR:HB	2.02	0.40
1:A:758:ARG:HH21	1:A:762:GLU:CD	2.29	0.40
1:A:763:VAL:O	1:A:766:GLN:NE2	2.54	0.40
1:C:1079:PHE:N	1:C:1085:PHE:O	2.54	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%)	874 (83%)	180 (17%)	3 (0%)	36	71
1	B	1057/1203 (88%)	852 (81%)	201 (19%)	4 (0%)	30	67
1	C	1045/1203 (87%)	843 (81%)	192 (18%)	10 (1%)	12	47
2	D	595/603 (99%)	564 (95%)	31 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3754/4212 (89%)	3133 (84%)	604 (16%)	17 (0%)	26	63

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	ASP
1	B	560	ASP
1	B	1072	PRO
1	C	645	SER
1	B	632	GLN
1	C	632	GLN
1	C	675	VAL
1	C	1072	PRO
1	A	1072	PRO
1	C	677	TYR
1	C	692	ASN
1	C	925	THR
1	C	679	MET
1	B	925	THR
1	A	1075	GLY
1	C	676	ALA
1	C	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%)	915 (99%)	7 (1%)	73	77
1	B	922/1048 (88%)	918 (100%)	4 (0%)	84	82
1	C	914/1048 (87%)	901 (99%)	13 (1%)	59	71
2	D	527/533 (99%)	525 (100%)	2 (0%)	84	82
All	All	3285/3677 (89%)	3259 (99%)	26 (1%)	70	77

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	LYS
1	A	687	ILE
1	A	699	ASN
1	A	720	CYS
1	A	841	THR
1	A	921	THR
1	A	1097	ILE
1	B	302	THR
1	B	687	ILE
1	B	760	THR
1	B	1097	ILE
1	C	302	THR
1	C	316	PHE
1	C	484	TYR
1	C	581	VAL
1	C	642	VAL
1	C	646	TYR
1	C	674	ILE
1	C	677	TYR
1	C	687	ILE
1	C	699	ASN
1	C	921	THR
1	C	1097	ILE
1	C	1110	VAL
2	D	436	ILE
2	D	570	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	109	ASN
1	A	129	ASN
1	A	155	ASN
1	A	181	HIS
1	A	214	ASN
1	A	230	ASN
1	A	347	ASN
1	A	381	ASN
1	A	435	ASN
1	A	437	ASN
1	A	457	ASN
1	A	523	GLN

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Mol	Chain	Res	Type
1	A	528	ASN
1	A	627	ASN
1	A	691	ASN
1	A	699	ASN
1	A	759	ASN
1	A	769	GLN
1	A	806	ASN
1	A	835	GLN
1	A	883	GLN
1	A	895	GLN
1	A	896	ASN
1	A	937	ASN
1	A	1018	GLN
1	A	1095	GLN
1	B	32	GLN
1	B	70	HIS
1	B	129	ASN
1	B	147	GLN
1	B	155	ASN
1	B	201	GLN
1	B	269	ASN
1	B	381	ASN
1	B	437	ASN
1	B	445	HIS
1	B	546	GLN
1	B	692	ASN
1	B	699	ASN
1	B	721	ASN
1	B	733	ASN
1	B	766	GLN
1	B	806	ASN
1	B	838	ASN
1	B	904	GLN
1	B	917	GLN
1	B	937	ASN
1	B	984	GLN
1	B	987	GLN
1	B	993	GLN
1	B	1116	ASN
1	C	149	HIS
1	C	318	ASN
1	C	347	ASN

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Mol	Chain	Res	Type
1	C	435	ASN
1	C	473	ASN
1	C	589	ASN
1	C	692	ASN
1	C	699	ASN
1	C	733	ASN
1	C	746	ASN
1	C	759	ASN
1	C	895	GLN
1	C	896	ASN
1	C	910	ASN
1	C	917	GLN
1	C	935	ASN
1	C	937	ASN
1	C	987	GLN
1	C	1101	ASN
2	D	49	ASN
2	D	250	ASN
2	D	300	GLN
2	D	322	ASN
2	D	388	GLN
2	D	522	GLN
2	D	526	GLN
2	D	552	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

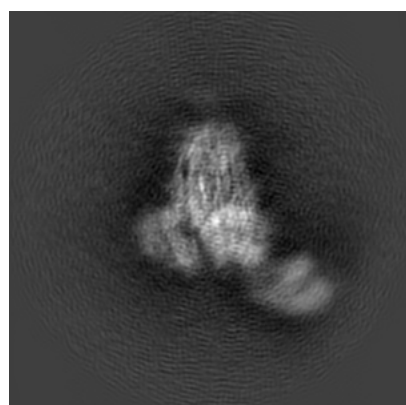
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9594. These allow visual inspection of the internal detail of the map and identification of artifacts.

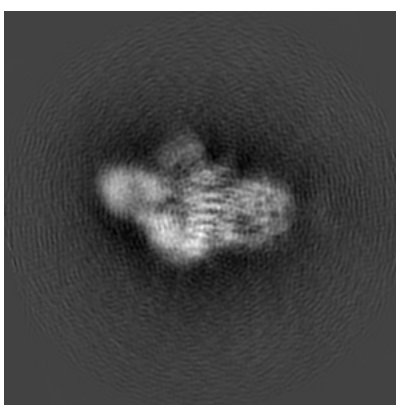
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

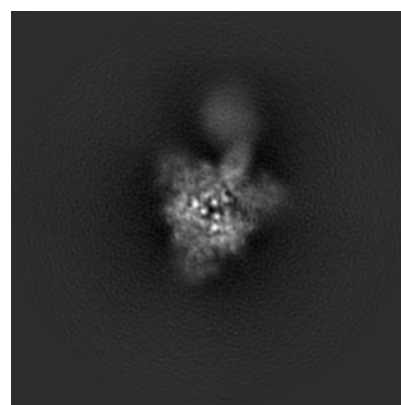
6.1.1 Primary map



X



Y

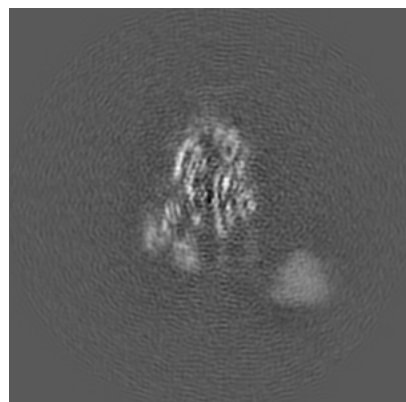


Z

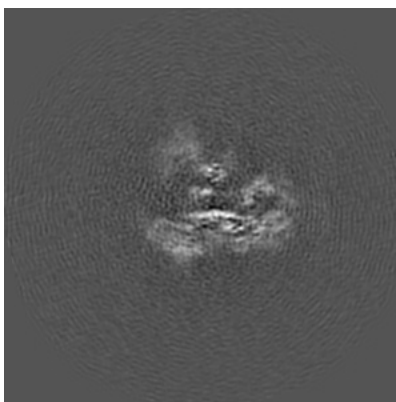
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

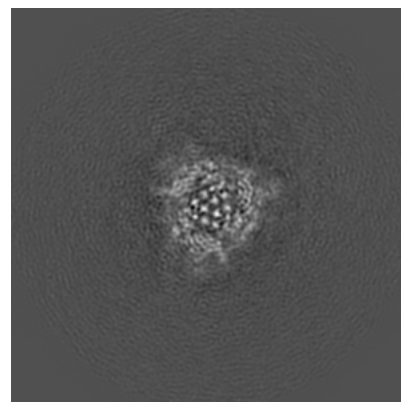
6.2.1 Primary map



X Index: 144



Y Index: 144

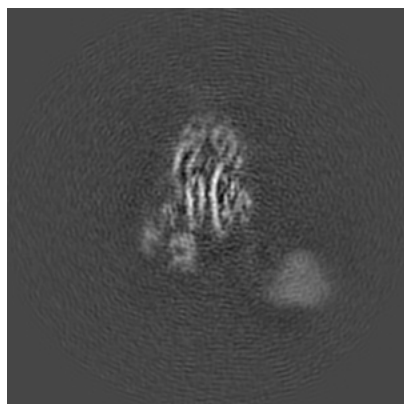


Z Index: 144

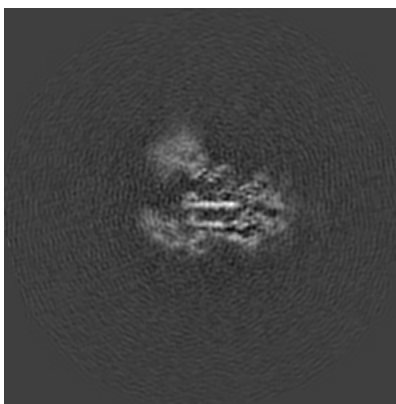
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

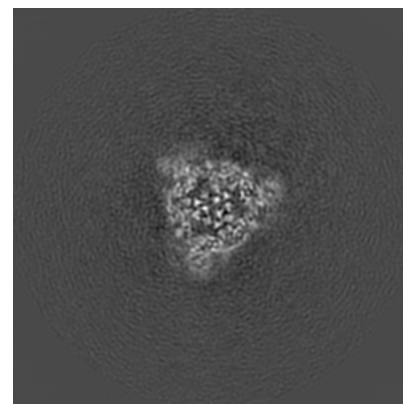
6.3.1 Primary map



X Index: 146



Y Index: 149

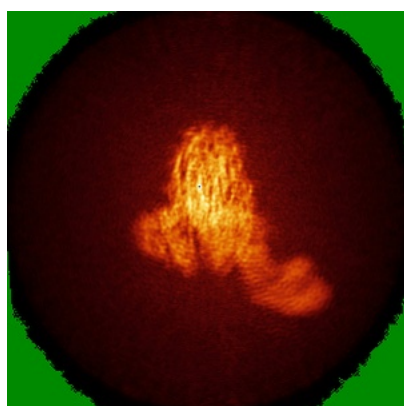


Z Index: 141

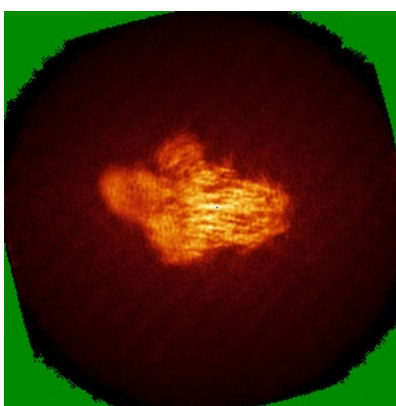
The images above show the largest variance slices of the map in three orthogonal directions.

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

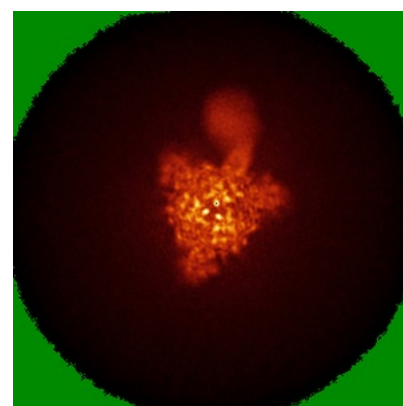
6.4.1 Primary map



X



Y

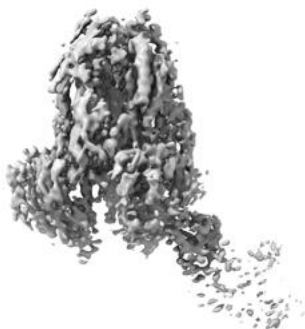


Z

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



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.

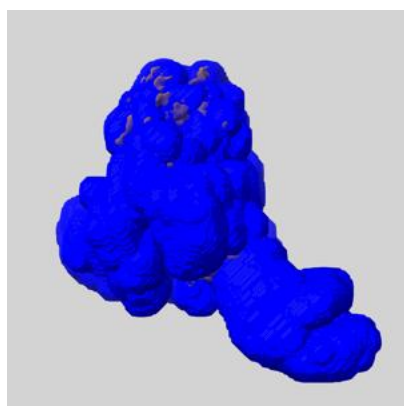
6.6 Mask visualisation [i](#)

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

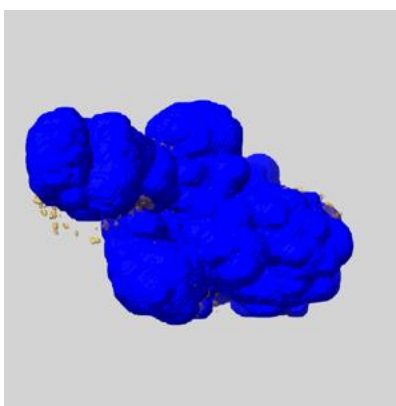
A mask typically either:

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

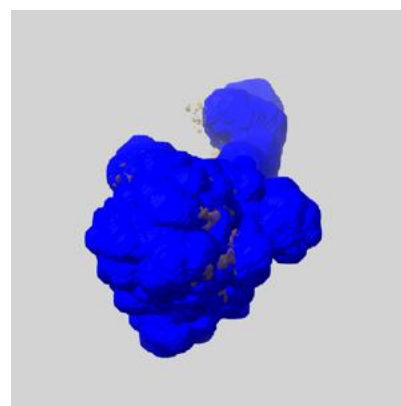
6.6.1 emd_9594_msk_1.map [i](#)



X



Y

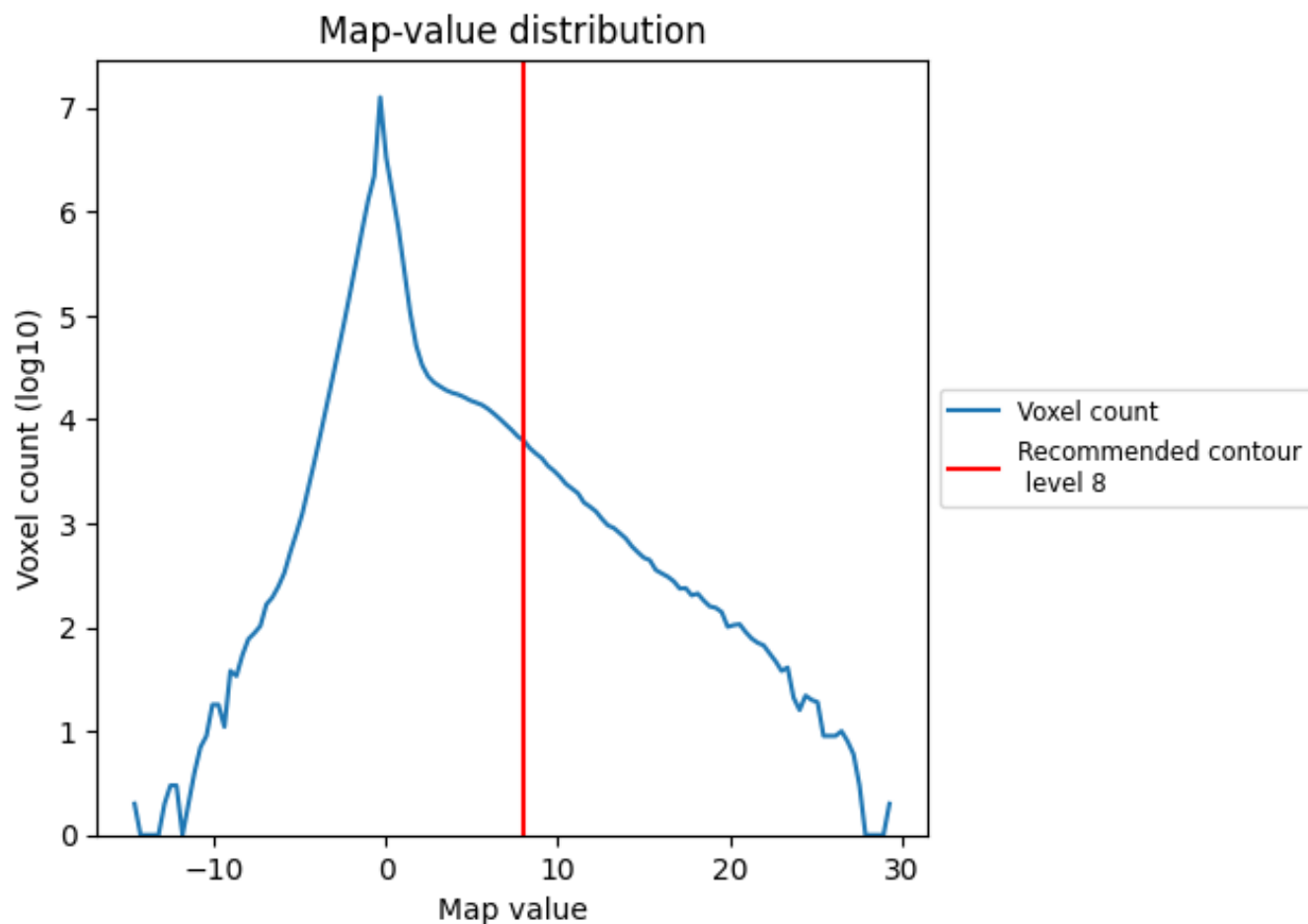


Z

7 Map analysis [i](#)

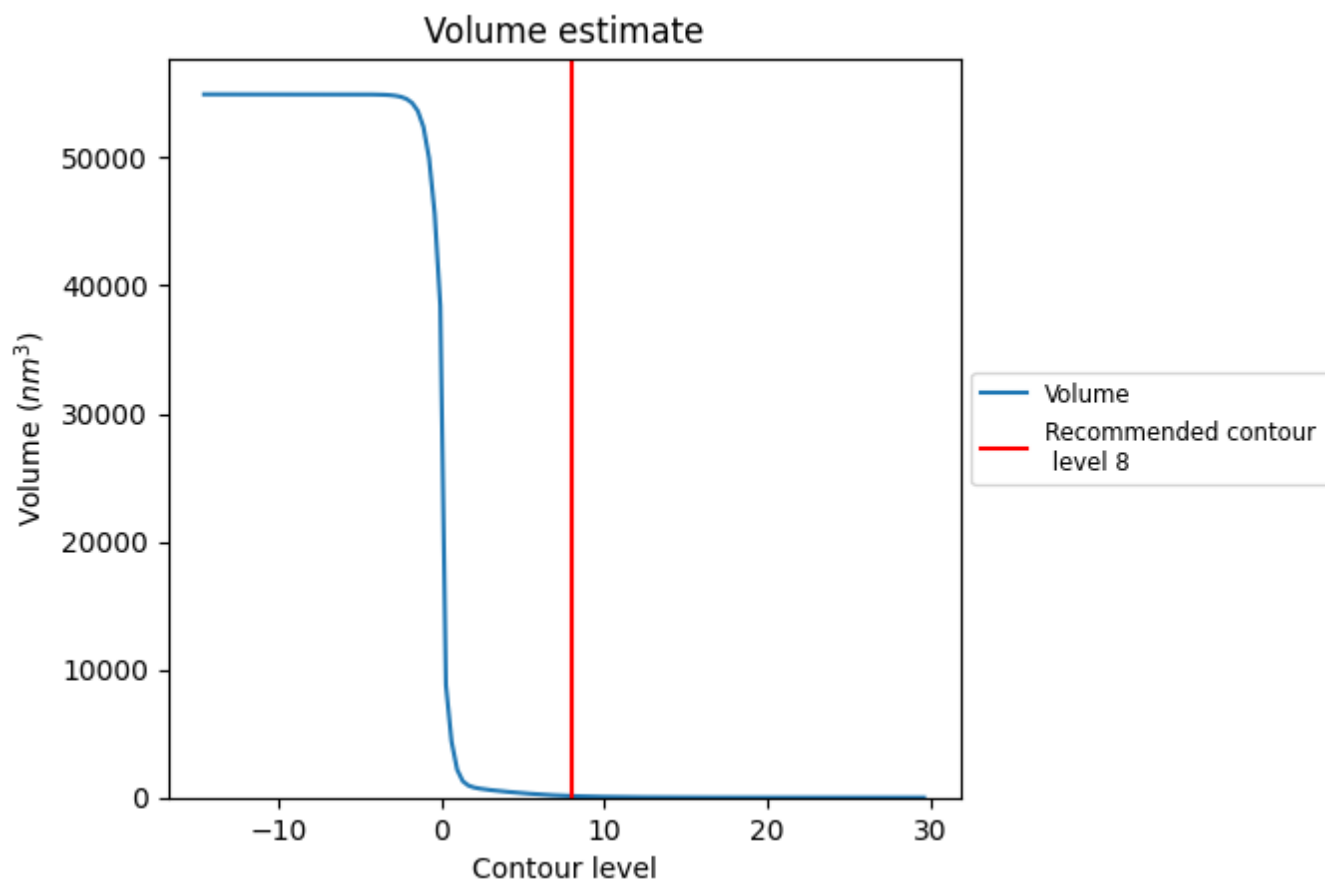
This section contains the results of statistical analysis of the map.

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.

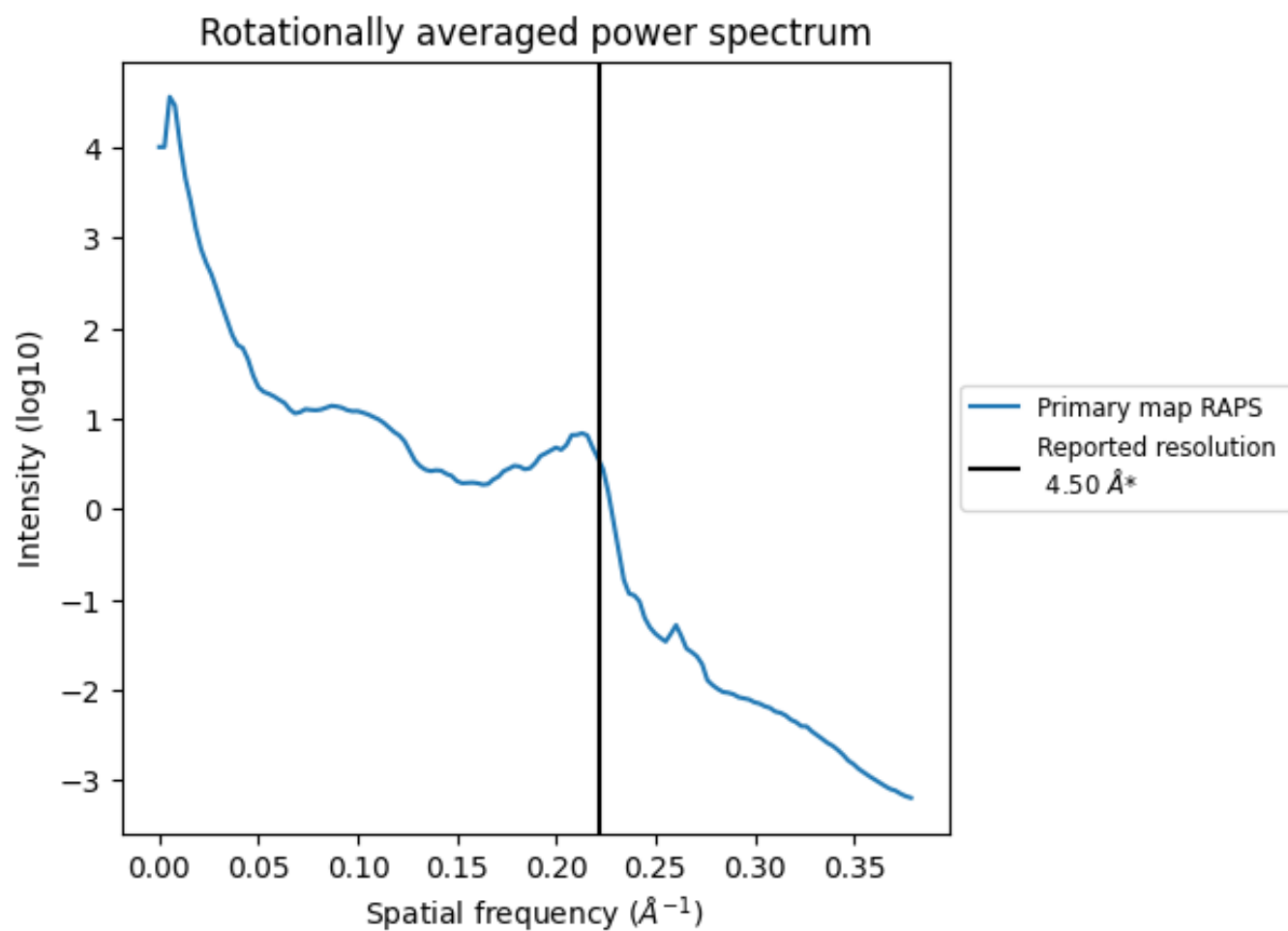
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm^3 ; this corresponds to an approximate mass of 108 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 ⓘ

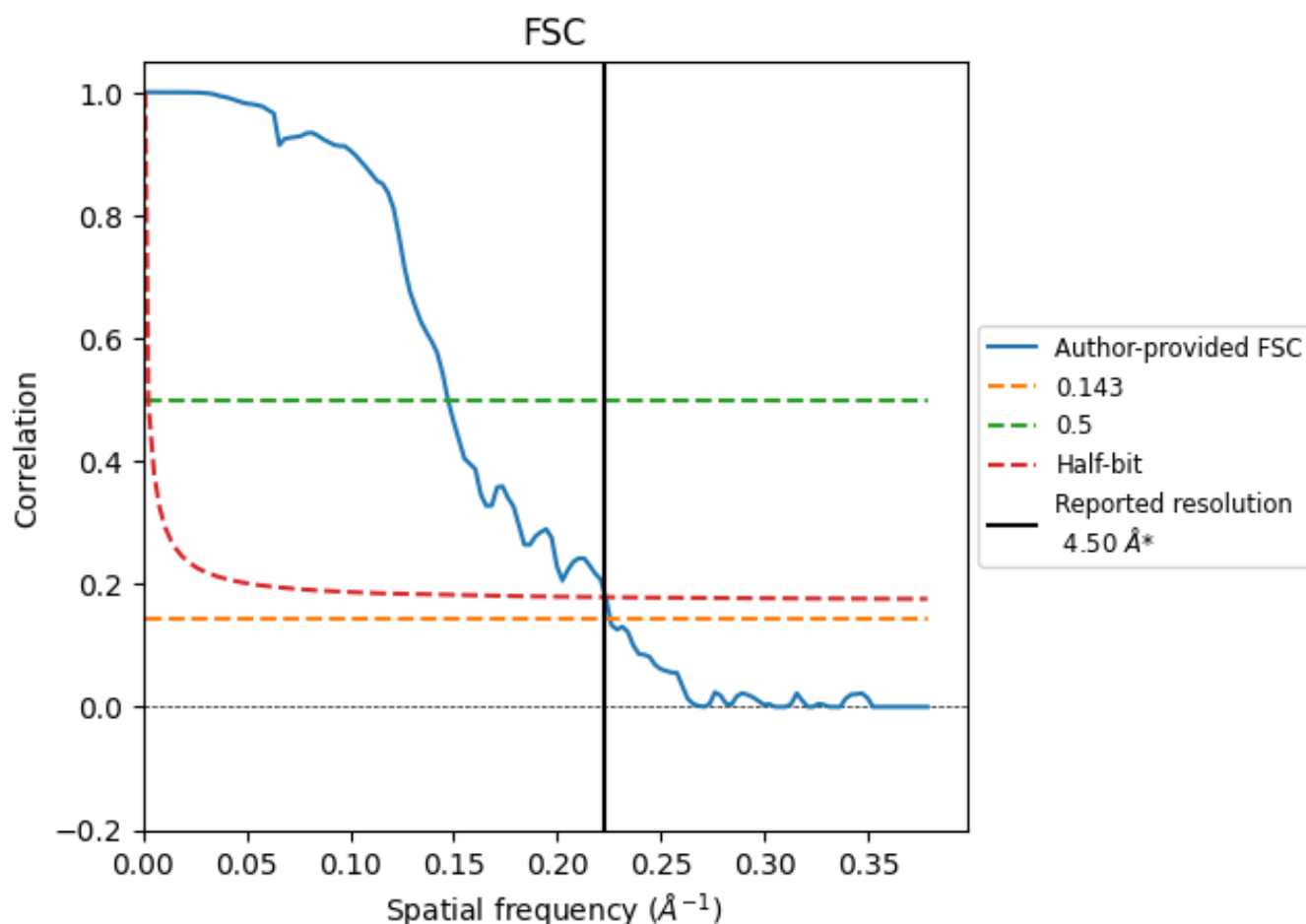


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

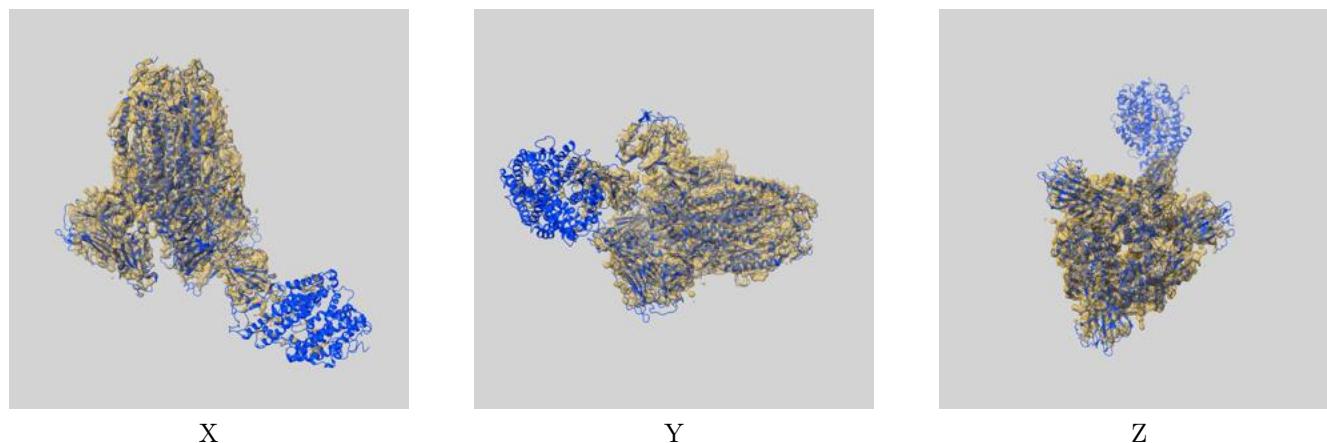
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.43	6.79	4.48
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

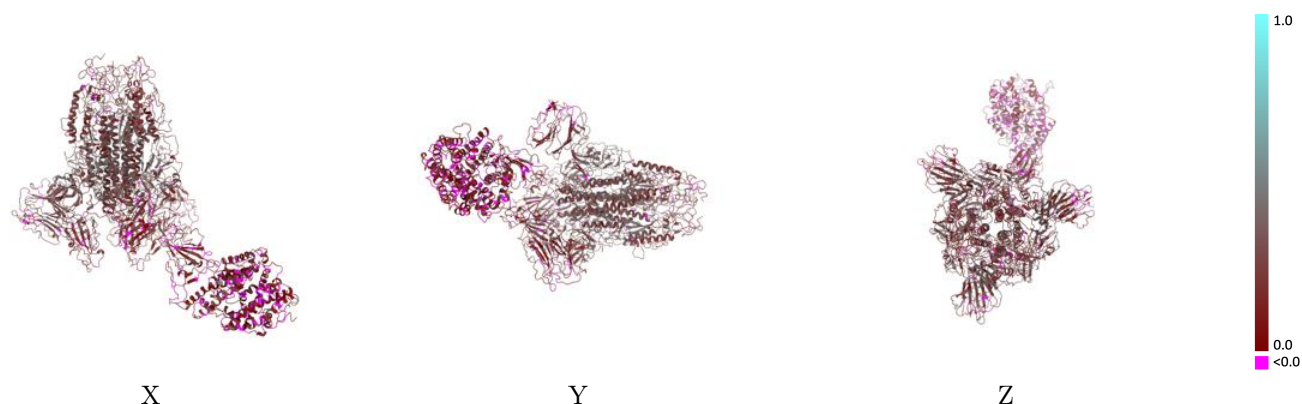
This section contains information regarding the fit between EMDB map EMD-9594 and PDB model 6ACK. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



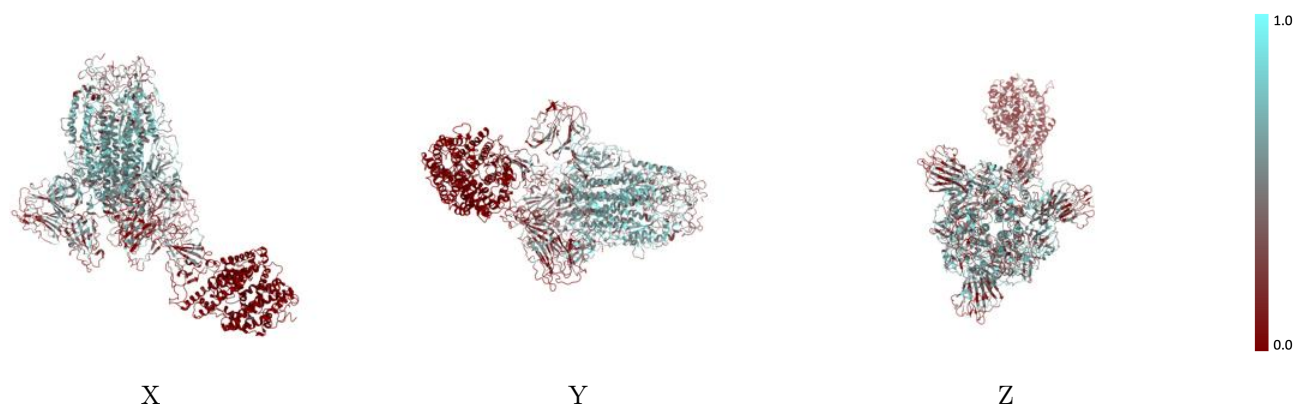
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



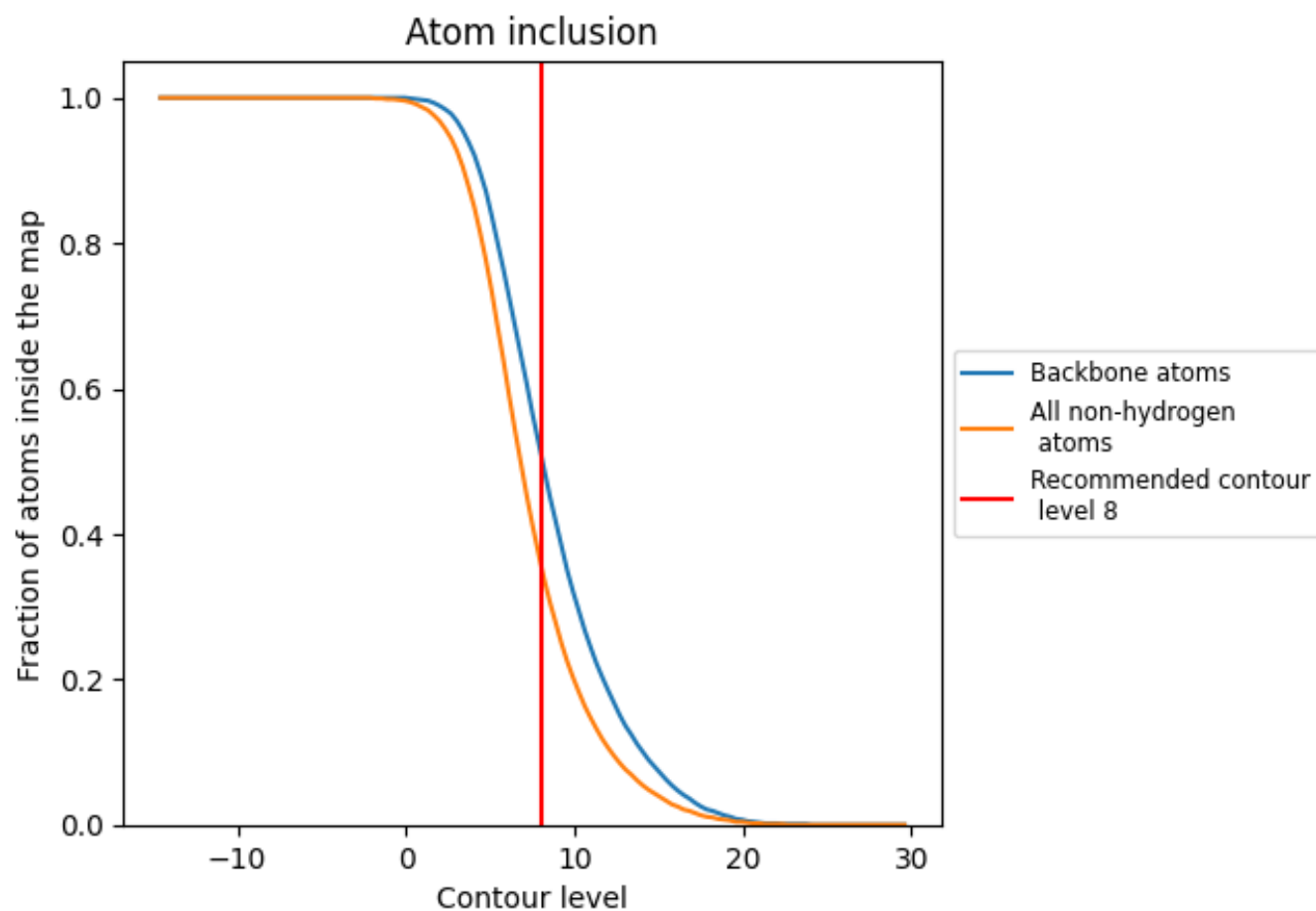
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 51% of all backbone atoms, 36% 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	0.3590	0.2390
A	0.4340	0.2750
B	0.4370	0.2630
C	0.4110	0.2560
D	0.0110	0.1050

