



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:10 AM UTC

PDB ID : 7FB0 / pdb_00007fb0
EMDB ID : EMD-31511
Title : SARS-CoV-2 spike protein in closed state
Authors : Zhu, Y.; Tai, L.H.; Sun, F.
Deposited on : 2021-07-08
Resolution : 3.40 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

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

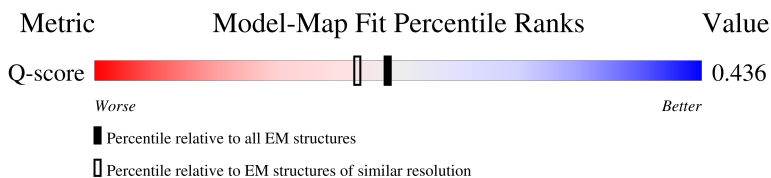
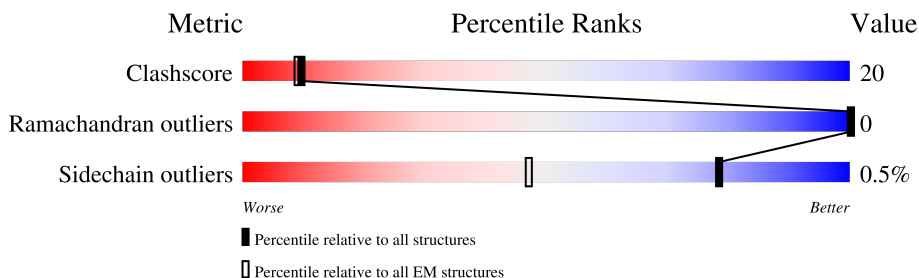
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	1247	 46% 32% 22%
1	B	1247	 48% 30% 22%
1	C	1247	 47% 31% 22%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22876 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	976	Total	C	N	O	S	0	0
			7628	4876	1266	1453	33		
1	B	975	Total	C	N	O	S	0	0
			7624	4874	1265	1452	33		
1	C	975	Total	C	N	O	S	0	0
			7624	4874	1265	1452	33		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	ALA	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	LEU	-	expression tag	UNP P0DTC2
A	1210	VAL	-	expression tag	UNP P0DTC2
A	1211	PRO	-	expression tag	UNP P0DTC2
A	1212	ARG	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	TYR	-	expression tag	UNP P0DTC2
A	1217	ILE	-	expression tag	UNP P0DTC2
A	1218	PRO	-	expression tag	UNP P0DTC2
A	1219	GLU	-	expression tag	UNP P0DTC2
A	1220	ALA	-	expression tag	UNP P0DTC2
A	1221	PRO	-	expression tag	UNP P0DTC2
A	1222	ARG	-	expression tag	UNP P0DTC2
A	1223	ASP	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLN	-	expression tag	UNP P0DTC2
A	1226	ALA	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	VAL	-	expression tag	UNP P0DTC2
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	LYS	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLU	-	expression tag	UNP P0DTC2
A	1234	TRP	-	expression tag	UNP P0DTC2
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	THR	-	expression tag	UNP P0DTC2
A	1240	PHE	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	ALA	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	LEU	-	expression tag	UNP P0DTC2
B	1210	VAL	-	expression tag	UNP P0DTC2
B	1211	PRO	-	expression tag	UNP P0DTC2
B	1212	ARG	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	TYR	-	expression tag	UNP P0DTC2
B	1217	ILE	-	expression tag	UNP P0DTC2
B	1218	PRO	-	expression tag	UNP P0DTC2
B	1219	GLU	-	expression tag	UNP P0DTC2
B	1220	ALA	-	expression tag	UNP P0DTC2
B	1221	PRO	-	expression tag	UNP P0DTC2
B	1222	ARG	-	expression tag	UNP P0DTC2
B	1223	ASP	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1226	ALA	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	VAL	-	expression tag	UNP P0DTC2
B	1229	ARG	-	expression tag	UNP P0DTC2
B	1230	LYS	-	expression tag	UNP P0DTC2
B	1231	ASP	-	expression tag	UNP P0DTC2
B	1232	GLY	-	expression tag	UNP P0DTC2
B	1233	GLU	-	expression tag	UNP P0DTC2
B	1234	TRP	-	expression tag	UNP P0DTC2
B	1235	VAL	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	THR	-	expression tag	UNP P0DTC2
B	1240	PHE	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	ALA	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	LEU	-	expression tag	UNP P0DTC2
C	1210	VAL	-	expression tag	UNP P0DTC2
C	1211	PRO	-	expression tag	UNP P0DTC2
C	1212	ARG	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	TYR	-	expression tag	UNP P0DTC2
C	1217	ILE	-	expression tag	UNP P0DTC2
C	1218	PRO	-	expression tag	UNP P0DTC2
C	1219	GLU	-	expression tag	UNP P0DTC2
C	1220	ALA	-	expression tag	UNP P0DTC2
C	1221	PRO	-	expression tag	UNP P0DTC2
C	1222	ARG	-	expression tag	UNP P0DTC2
C	1223	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLN	-	expression tag	UNP P0DTC2
C	1226	ALA	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	VAL	-	expression tag	UNP P0DTC2
C	1229	ARG	-	expression tag	UNP P0DTC2
C	1230	LYS	-	expression tag	UNP P0DTC2
C	1231	ASP	-	expression tag	UNP P0DTC2
C	1232	GLY	-	expression tag	UNP P0DTC2
C	1233	GLU	-	expression tag	UNP P0DTC2
C	1234	TRP	-	expression tag	UNP P0DTC2
C	1235	VAL	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	THR	-	expression tag	UNP P0DTC2
C	1240	PHE	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2

HIS	ARG	F1103	E988	T881	F797	ALA	Q607	Q506	VAL	S375
HIS	LEU	V1104	I996	I882	G798	S689	V608	P507	GLY	T376
HIS	ASN	Q1106	I996	S884	G799	Q690	L611	Y508	C447	F377
	VAL	D1118	Q1002	A890	N801	Y695	N616	V510	N448	K378
	LYS	V1122	T1006	L894	F802	S698	T618	V511	Y449	C379
	ASN	S1123	V1007	L907	S803	L699	E619	V512	M450	V382
	ASN	G1124	T1009	M900	Q804	N703	V622	S514	P384	S383
	GLU	N1125	I1013	Y904	I805	S704	ALA	F515	R454	T385
	SER	C1126	I1013	R905	L806	Y707	ILE	E516	LEU	K386
	LEU	I1132	T1027	R906	P807	Y707	HIS	L517	PHE	L387
	ILE		M1028	F906	P809	P715	ASP	L518	ARG	
	ASP		K1029	N907	K810	T716	ALA	L519	LYS	C391
	LEU		G1030	G908	S812	N717	GLN	G526	SER	F392
	GLN		S1031	N914	S813	S721	LEU	G527	ASN	T393
	GLU		E1031	V915	K814	V722	THR	P527	N394	N394
	LEU		R1039	L916	R815	T723	PRO	K528	S399	S399
	GLY		L1141	Y917	S816	T724	THR		I402	I402
	LYS		L1145	L922	F817	E725	GLY		R403	R403
	TYR		D1146	I923	T827	T734	THR		G404	G404
	GLU		S1147	Q926	LEU	S735	ASP		D405	D405
	GLN		PHE	Q935	ALA	C738	THR		E406	E406
	LEU		LYS	Q949	ASP	T739	GLY		V407	V407
	VAL		GLU	D950	ALA	M740	S640		R408	R408
	PRO		GLU	V951	ILE	Y741	Q644		Q409	Q409
	ARG		LYS	V952	LYS	I742	T645		I410	I410
	GLY		TYR	N953	GLN	C743	G648		G413	G413
	TYR		PHE	Q954	LYS	C749	L650		Q414	Q414
	ILE		ASN	N955	TYR	C749	I651		T415	T415
	PRO		GLU	A958	ASP	Y756	H655		G416	G416
	GLU		ALA	L959	CYS	Y756	V656		K417	K417
	ALA		THR	T961	LEU	F759	E661		I418	I418
	THR		SER	V963	ARG	L767	I666		A419	A419
	PRO		PRO	Q965	ASP	I770	G669		D420	D420
	ARG		ARG	S974	LEU	Q774	I670		Y421	Y421
	ASP		VAL	S975	ILE	N777	T676		M422	M422
	LYS		ILE	V976	CYS	Q774	GLN		Y423	Y423
	GLY		ASN	L977	ALA	N777	THR		K424	K424
	TRP		ALA	N978	GLN	V781	ASN		L425	L425
	VAL		SER	D979	K854	V781	SER		P426	P426
	LEU		VAL	I980	I870	K786	PRO		D427	D427
	LEU		VAL	L981	Y873	Q787	GLY		D428	D428
	SER		ASN	S982	T874	K790	ALA		T430	T430
	THR		ILE	R983	L878	T791	ALA		G431	G431
	PHE		GLN	L984	P792	P792	SER		C432	C432
	LEU		LYS	P985	L878	P792	ALA		V433	V433
	HIS		ASP	P987	G880	I794	SER		I434	I434
	HIS		ILE				VAL		Q496	Q496
	HIS		ASP						Q498	Q498
									P499	P499
									T500	T500
									N501	N501
									GLY	M440
									V503	V503
									G504	G504
									Y505	Y505
										K444

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55933	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 ($e^-/\text{\AA}^2$)	3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.524	Depositor
Minimum map value	-1.742	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	348.16, 348.16, 348.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/7798	0.52	0/10610
1	B	0.46	0/7793	0.52	0/10602
1	C	0.46	0/7793	0.52	0/10602
All	All	0.46	0/23384	0.52	0/31814

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7628	0	7455	328	0
1	B	7624	0	7451	313	0
1	C	7624	0	7451	310	0
All	All	22876	0	22357	896	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 20.

All (896) 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:379:CYS:HA	1:C:432:CYS:HB3	1.35	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:CYS:HB2	1:C:525:CYS:HA	1.52	0.89
1:B:104:TRP:HB3	1:B:106:PHE:HE1	1.37	0.88
1:B:290:ASP:O	1:B:297:SER:OG	1.93	0.85
1:B:391:CYS:HB2	1:B:525:CYS:HA	1.58	0.84
1:B:676:THR:HG22	1:B:690:GLN:HE21	1.43	0.84
1:A:200:TYR:OH	1:C:394:ASN:ND2	2.11	0.83
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.62	0.81
1:A:676:THR:HG22	1:A:690:GLN:HE21	1.46	0.81
1:A:780:GLU:O	1:A:784:GLN:NE2	2.12	0.81
1:B:103:GLY:HA3	1:B:241:LEU:HB3	1.61	0.81
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.14	0.81
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.14	0.80
1:B:780:GLU:O	1:B:784:GLN:NE2	2.14	0.80
1:C:328:ARG:NH1	1:C:578:ASP:OD2	2.14	0.80
1:C:290:ASP:O	1:C:297:SER:OG	2.00	0.79
1:C:103:GLY:HA3	1:C:241:LEU:HB3	1.65	0.79
1:B:214:ARG:HE	1:B:215:ASP:HB2	1.49	0.78
1:A:328:ARG:NH1	1:A:578:ASP:OD2	2.17	0.78
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.16	0.78
1:C:1086:LYS:HA	1:C:1125:ASN:HA	1.67	0.77
1:A:91:TYR:OH	1:A:191:GLU:OE2	2.01	0.77
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.16	0.77
1:C:424:LYS:HB2	1:C:463:PRO:HA	1.67	0.77
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.66	0.76
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.19	0.75
1:A:391:CYS:HB2	1:A:525:CYS:HA	1.69	0.74
1:A:1086:LYS:HA	1:A:1125:ASN:HA	1.69	0.74
1:A:103:GLY:HA3	1:A:241:LEU:HB3	1.69	0.74
1:A:437:ASN:ND2	1:A:507:PRO:O	2.22	0.73
1:B:216:LEU:H	1:B:216:LEU:HD12	1.54	0.73
1:B:557:LYS:NZ	1:B:574:ASP:O	2.21	0.73
1:C:280:ASN:ND2	1:C:284:THR:OG1	2.21	0.72
1:B:802:PHE:HD2	1:B:805:ILE:HD11	1.54	0.72
1:A:327:VAL:HG11	1:A:528:LYS:HE3	1.71	0.72
1:A:644:GLN:NE2	1:A:645:THR:O	2.22	0.72
1:C:676:THR:HG22	1:C:690:GLN:HE21	1.54	0.72
1:A:802:PHE:HD2	1:A:805:ILE:HD11	1.53	0.72
1:B:369:TYR:HE2	1:B:384:PRO:HB2	1.52	0.72
1:A:81:ASN:O	1:A:239:GLN:NE2	2.21	0.72
1:B:424:LYS:HB2	1:B:463:PRO:HA	1.71	0.71
1:A:557:LYS:NZ	1:A:574:ASP:OD2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:CYS:HA	1:B:432:CYS:HB3	1.72	0.70
1:B:437:ASN:HA	1:B:508:TYR:HA	1.72	0.70
1:B:1045:LYS:NZ	1:C:890:ALA:O	2.24	0.70
1:A:95:THR:HG22	1:A:186:PHE:HB2	1.73	0.70
1:A:1091:ARG:NH1	1:A:1118:ASP:O	2.24	0.70
1:B:656:VAL:HG12	1:B:658:ASN:H	1.57	0.70
1:B:390:LEU:HD11	1:C:983:ARG:HG2	1.71	0.70
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.73	0.70
1:B:918:GLU:O	1:B:919:ASN:ND2	2.24	0.69
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.25	0.69
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.25	0.69
1:C:553:THR:HG23	1:C:586:ASP:HB3	1.73	0.69
1:A:740:MET:SD	1:C:319:ARG:NH1	2.59	0.69
1:A:564:GLN:OE1	1:A:577:ARG:NH2	2.25	0.69
1:B:319:ARG:NH1	1:C:740:MET:SD	2.57	0.69
1:C:557:LYS:NZ	1:C:574:ASP:OD2	2.24	0.69
1:B:379:CYS:HA	1:B:432:CYS:CB	2.23	0.69
1:C:108:THR:O	1:C:237:ARG:NH1	2.26	0.69
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.26	0.68
1:A:723:THR:HG22	1:A:724:THR:H	1.58	0.68
1:A:661:GLU:O	1:A:695:TYR:OH	2.09	0.68
1:B:280:ASN:ND2	1:B:284:THR:OG1	2.26	0.68
1:A:280:ASN:ND2	1:A:284:THR:OG1	2.27	0.68
1:C:214:ARG:HE	1:C:215:ASP:HB2	1.58	0.68
1:A:738:CYS:SG	1:A:739:THR:N	2.67	0.67
1:C:433:VAL:HA	1:C:512:VAL:HA	1.76	0.67
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.28	0.67
1:B:557:LYS:NZ	1:B:574:ASP:OD2	2.22	0.67
1:A:1045:LYS:NZ	1:B:890:ALA:O	2.27	0.66
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.76	0.66
1:B:290:ASP:OD1	1:B:291:CYS:N	2.28	0.66
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.77	0.66
1:C:402:ILE:HD12	1:C:406:GLU:HB2	1.78	0.66
1:B:402:ILE:HD12	1:B:406:GLU:HB2	1.76	0.66
1:B:205:SER:OG	1:B:206:LYS:N	2.26	0.66
1:B:108:THR:HG22	1:B:109:THR:HG23	1.77	0.66
1:C:661:GLU:O	1:C:695:TYR:OH	2.12	0.66
1:C:437:ASN:HA	1:C:508:TYR:HA	1.77	0.66
1:A:557:LYS:NZ	1:A:574:ASP:O	2.29	0.66
1:B:676:THR:HA	1:B:690:GLN:HG2	1.75	0.66
1:C:557:LYS:NZ	1:C:574:ASP:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:SER:OG	1:A:817:PHE:N	2.28	0.66
1:B:661:GLU:O	1:B:695:TYR:OH	2.14	0.66
1:A:390:LEU:HD11	1:B:983:ARG:HG2	1.77	0.65
1:B:99:ASN:OD1	1:B:190:ARG:NH1	2.28	0.65
1:A:1085:GLY:O	1:A:1126:CYS:N	2.28	0.65
1:C:1085:GLY:O	1:C:1126:CYS:N	2.29	0.65
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.29	0.65
1:C:290:ASP:OD1	1:C:291:CYS:N	2.30	0.65
1:A:189:LEU:HD21	1:A:191:GLU:HG2	1.79	0.64
1:C:444:LYS:O	1:C:447:GLY:N	2.30	0.64
1:B:382:VAL:HG12	1:C:983:ARG:HB3	1.79	0.64
1:A:711:SER:OG	1:B:895:GLN:NE2	2.21	0.64
1:C:564:GLN:OE1	1:C:577:ARG:NH2	2.30	0.64
1:A:108:THR:OG1	1:A:234:ASN:O	2.12	0.64
1:A:553:THR:O	1:A:586:ASP:N	2.29	0.64
1:B:86:PHE:HA	1:B:90:VAL:HG21	1.79	0.64
1:B:108:THR:O	1:B:237:ARG:NH1	2.30	0.64
1:B:444:LYS:O	1:B:447:GLY:N	2.30	0.64
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.79	0.64
1:A:619:GLU:OE1	1:A:619:GLU:N	2.32	0.63
1:B:96:GLU:HG3	1:B:98:SER:H	1.63	0.63
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.43	0.63
1:A:186:PHE:N	1:A:212:LEU:O	2.31	0.63
1:A:1093:GLY:HA2	1:A:1107:ARG:HG3	1.80	0.63
1:A:645:THR:HG23	1:A:647:ALA:H	1.62	0.63
1:A:1135:ASN:ND2	1:A:1136:THR:O	2.31	0.63
1:C:553:THR:O	1:C:586:ASP:N	2.31	0.63
1:C:723:THR:HG22	1:C:724:THR:H	1.63	0.63
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.79	0.63
1:C:229:LEU:HB3	1:C:231:ILE:HG23	1.81	0.63
1:A:444:LYS:O	1:A:447:GLY:N	2.32	0.63
1:B:96:GLU:HG2	1:B:100:ILE:H	1.64	0.63
1:B:619:GLU:N	1:B:619:GLU:OE1	2.32	0.63
1:A:605:SER:OG	1:A:606:ASN:N	2.32	0.62
1:A:951:VAL:O	1:A:955:ASN:ND2	2.32	0.62
1:A:985:ASP:OD1	1:A:985:ASP:N	2.32	0.62
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.80	0.62
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.32	0.62
1:A:808:ASP:HB3	1:A:811:LYS:HG2	1.80	0.62
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.33	0.62
1:C:108:THR:OG1	1:C:234:ASN:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:SER:N	1:A:819:GLU:OE1	2.21	0.62
1:B:564:GLN:OE1	1:B:577:ARG:NH2	2.33	0.62
1:C:448:ASN:HD21	1:C:451:TYR:HD2	1.48	0.62
1:B:1086:LYS:HA	1:B:1125:ASN:HA	1.82	0.61
1:A:192:PHE:O	1:A:193:VAL:HG23	1.99	0.61
1:A:305:SER:OG	1:A:306:PHE:N	2.33	0.61
1:B:131:CYS:HA	1:B:166:CYS:HB2	1.83	0.61
1:A:1007:TYR:OH	1:A:1011:GLN:NE2	2.33	0.61
1:C:323:THR:HG21	1:C:537:LYS:HD2	1.83	0.61
1:C:336:CYS:HB3	1:C:358:ILE:HG21	1.82	0.61
1:B:369:TYR:HH	1:B:385:THR:HG1	1.48	0.61
1:B:216:LEU:HG	1:B:266:TYR:HE2	1.66	0.60
1:B:816:SER:OG	1:B:817:PHE:N	2.34	0.60
1:C:377:PHE:H	1:C:378:LYS:HZ3	1.47	0.60
1:C:535:LYS:NZ	1:C:554:GLU:OE2	2.34	0.60
1:C:645:THR:OG1	1:C:648:GLY:O	2.18	0.60
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.32	0.60
1:C:816:SER:OG	1:C:817:PHE:N	2.32	0.60
1:C:108:THR:HG22	1:C:109:THR:HG23	1.84	0.60
1:B:108:THR:OG1	1:B:234:ASN:O	2.17	0.60
1:C:216:LEU:HD12	1:C:216:LEU:H	1.67	0.59
1:B:1093:GLY:HA2	1:B:1107:ARG:HG3	1.83	0.59
1:C:192:PHE:O	1:C:193:VAL:HG23	2.01	0.59
1:C:767:LEU:HD23	1:C:770:ILE:HD12	1.85	0.59
1:A:189:LEU:HB2	1:A:210:ILE:HG12	1.83	0.59
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.85	0.59
1:C:95:THR:HG22	1:C:186:PHE:HB3	1.85	0.59
1:B:1094:VAL:HG13	1:B:1107:ARG:HG2	1.84	0.59
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.85	0.59
1:A:205:SER:OG	1:A:206:LYS:N	2.34	0.58
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.85	0.58
1:A:379:CYS:HA	1:A:432:CYS:HA	1.85	0.58
1:A:502:GLY:O	1:A:506:GLN:NE2	2.35	0.58
1:B:738:CYS:SG	1:B:739:THR:N	2.76	0.58
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.35	0.58
1:A:102:ARG:HB2	1:A:141:LEU:HD21	1.84	0.58
1:A:357:ARG:HH12	1:A:359:SER:HB3	1.69	0.58
1:C:676:THR:HA	1:C:690:GLN:HG2	1.85	0.58
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.86	0.57
1:A:553:THR:HG23	1:A:586:ASP:HB2	1.87	0.57
1:A:1089:PHE:CE2	1:B:914:ASN:HA	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:SER:OG	1:B:317:ASN:N	2.36	0.57
1:A:214:ARG:HE	1:A:215:ASP:HB2	1.70	0.57
1:B:281:GLU:OE1	1:B:281:GLU:N	2.32	0.57
1:A:354:ASN:HD21	1:A:399:SER:HB3	1.69	0.57
1:A:576:VAL:HG12	1:A:577:ARG:H	1.69	0.57
1:A:281:GLU:N	1:A:281:GLU:OE1	2.37	0.57
1:A:462:LYS:HE3	1:A:465:GLU:HB2	1.87	0.57
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.87	0.57
1:A:382:VAL:HG12	1:B:983:ARG:HB3	1.87	0.57
1:A:394:ASN:ND2	1:B:200:TYR:OH	2.37	0.57
1:B:802:PHE:CD2	1:B:805:ILE:HD11	2.37	0.57
1:B:1085:GLY:O	1:B:1126:CYS:N	2.36	0.57
1:C:961:THR:O	1:C:965:GLN:HG2	2.04	0.57
1:A:721:SER:OG	1:A:722:VAL:N	2.38	0.57
1:C:1135:ASN:ND2	1:C:1136:THR:O	2.37	0.56
1:C:100:ILE:HG22	1:C:242:LEU:HG	1.87	0.56
1:A:104:TRP:HB2	1:A:119:ILE:HB	1.88	0.56
1:A:130:VAL:HG12	1:A:168:PHE:O	2.05	0.56
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.40	0.56
1:A:214:ARG:NE	1:A:215:ASP:HB2	2.21	0.56
1:B:264:ALA:HB1	1:B:266:TYR:CE1	2.41	0.56
1:B:553:THR:HG23	1:B:586:ASP:HB2	1.86	0.56
1:C:168:PHE:CZ	1:C:170:TYR:HB2	2.40	0.56
1:B:90:VAL:HG11	1:B:238:PHE:CE1	2.40	0.56
1:C:756:TYR:HB3	1:C:759:PHE:HD2	1.71	0.56
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.36	0.56
1:B:734:THR:OG1	1:B:735:SER:N	2.38	0.56
1:B:103:GLY:N	1:B:241:LEU:O	2.38	0.56
1:A:415:THR:HG22	1:A:416:GLY:H	1.70	0.56
1:A:905:ARG:HD3	1:A:1049:LEU:O	2.04	0.56
1:B:531:THR:HG22	1:B:532:ASN:H	1.71	0.56
1:C:804:GLN:O	1:C:816:SER:OG	2.24	0.56
1:A:434:ILE:HB	1:A:511:VAL:HG23	1.86	0.56
1:A:890:ALA:O	1:C:1045:LYS:NZ	2.32	0.56
1:B:721:SER:OG	1:B:722:VAL:N	2.38	0.56
1:B:880:GLY:O	1:B:884:SER:OG	2.21	0.56
1:A:961:THR:O	1:A:965:GLN:HG2	2.06	0.56
1:A:131:CYS:HA	1:A:166:CYS:HB2	1.88	0.55
1:A:1049:LEU:HB2	1:A:1065:VAL:O	2.05	0.55
1:B:951:VAL:O	1:B:955:ASN:ND2	2.38	0.55
1:A:703:ASN:OD1	1:A:704:SER:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:VAL:HG23	1:B:368:LEU:HD12	1.89	0.55
1:B:596:SER:HB3	1:B:611:LEU:HB3	1.87	0.55
1:C:1141:LEU:HD23	1:C:1145:LEU:HD23	1.88	0.55
1:A:983:ARG:HB3	1:C:382:VAL:HG12	1.87	0.55
1:B:448:ASN:HD21	1:B:451:TYR:HD2	1.53	0.55
1:A:979:ASP:HB3	1:A:983:ARG:HE	1.71	0.55
1:B:1141:LEU:HD23	1:B:1145:LEU:HD23	1.88	0.55
1:C:738:CYS:SG	1:C:739:THR:N	2.79	0.55
1:B:379:CYS:SG	1:B:384:PRO:HB3	2.46	0.55
1:C:434:ILE:HB	1:C:511:VAL:HG23	1.88	0.55
1:A:443:SER:HB3	1:A:499:PRO:HD3	1.88	0.55
1:C:205:SER:OG	1:C:206:LYS:N	2.38	0.55
1:C:800:PHE:N	1:C:800:PHE:CD1	2.75	0.55
1:B:958:ALA:O	1:B:961:THR:OG1	2.25	0.55
1:B:1049:LEU:HB2	1:B:1065:VAL:O	2.07	0.55
1:A:93:ALA:O	1:A:94:SER:OG	2.24	0.55
1:A:1043:CYS:HB3	1:A:1048:HIS:CD2	2.42	0.55
1:C:976:VAL:HB	1:C:979:ASP:OD2	2.06	0.55
1:A:904:TYR:OH	1:C:1094:VAL:HB	2.08	0.54
1:B:816:SER:N	1:B:819:GLU:OE1	2.34	0.54
1:A:86:PHE:H	1:A:237:ARG:HA	1.72	0.54
1:A:532:ASN:OD1	1:A:533:LEU:N	2.31	0.54
1:A:900:MET:HA	1:A:917:TYR:OH	2.07	0.54
1:C:281:GLU:N	1:C:281:GLU:OE1	2.40	0.54
1:C:131:CYS:HB3	1:C:133:PHE:CZ	2.41	0.54
1:C:974:SER:OG	1:C:975:SER:N	2.40	0.54
1:A:576:VAL:HG12	1:A:577:ARG:N	2.22	0.54
1:C:204:TYR:N	1:C:204:TYR:CD1	2.76	0.54
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.89	0.54
1:B:264:ALA:HB1	1:B:266:TYR:HE1	1.72	0.54
1:B:534:VAL:HG23	1:B:539:VAL:HG11	1.90	0.54
1:B:86:PHE:HE2	1:B:196:ASN:HD21	1.55	0.54
1:C:611:LEU:HD12	1:C:650:LEU:HD13	1.90	0.54
1:A:290:ASP:O	1:A:297:SER:HB2	2.07	0.54
1:C:212:LEU:HG	1:C:214:ARG:H	1.72	0.54
1:A:131:CYS:HB3	1:A:133:PHE:CE1	2.43	0.54
1:A:336:CYS:HB3	1:A:358:ILE:HG21	1.89	0.54
1:B:280:ASN:OD1	1:B:284:THR:N	2.34	0.54
1:C:605:SER:OG	1:C:606:ASN:N	2.41	0.54
1:C:803:SER:OG	1:C:804:GLN:NE2	2.40	0.54
1:C:906:PHE:HE1	1:C:1049:LEU:HD11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:PHE:HE2	1:B:914:ASN:HA	1.73	0.53
1:B:131:CYS:HB3	1:B:133:PHE:CZ	2.42	0.53
1:B:436:TRP:O	1:B:509:ARG:N	2.40	0.53
1:B:1118:ASP:OD1	1:B:1119:ASN:N	2.41	0.53
1:C:1043:CYS:HB2	1:C:1048:HIS:CD2	2.42	0.53
1:B:225:PRO:O	1:B:226:LEU:HD23	2.09	0.53
1:C:225:PRO:O	1:C:226:LEU:HD23	2.08	0.53
1:C:979:ASP:O	1:C:983:ARG:N	2.40	0.53
1:A:1141:LEU:HD23	1:A:1145:LEU:HD23	1.91	0.53
1:C:112:SER:HB2	1:C:133:PHE:C	2.33	0.53
1:B:192:PHE:HB3	1:B:194:PHE:CE1	2.43	0.53
1:C:102:ARG:HD2	1:C:243:ALA:HB2	1.90	0.53
1:A:64:TRP:HA	1:A:266:TYR:HD1	1.74	0.53
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.42	0.53
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.91	0.53
1:A:777:ASN:O	1:A:781:VAL:HG23	2.09	0.53
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.43	0.53
1:A:676:THR:HA	1:A:690:GLN:HG2	1.89	0.53
1:B:800:PHE:HD2	1:B:927:PHE:CD2	2.25	0.53
1:C:409:GLN:HB3	1:C:419:ALA:HB2	1.90	0.53
1:A:316:SER:OG	1:A:317:ASN:N	2.39	0.53
1:A:341:VAL:HG22	1:A:356:LYS:HZ1	1.73	0.53
1:B:961:THR:O	1:B:965:GLN:HG2	2.08	0.53
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.91	0.53
1:C:81:ASN:ND2	1:C:139:PRO:O	2.41	0.53
1:C:586:ASP:OD1	1:C:587:ILE:N	2.41	0.53
1:C:644:GLN:HE21	1:C:645:THR:N	2.06	0.53
1:C:802:PHE:HD2	1:C:805:ILE:HD11	1.74	0.53
1:B:65:PHE:HD2	1:B:265:TYR:CZ	2.27	0.53
1:C:1043:CYS:HB2	1:C:1048:HIS:HD2	1.73	0.53
1:C:1047:TYR:O	1:C:1066:THR:OG1	2.21	0.53
1:A:383:SER:OG	1:B:983:ARG:O	2.27	0.53
1:A:645:THR:HG22	1:A:648:GLY:O	2.08	0.53
1:A:880:GLY:O	1:A:884:SER:OG	2.26	0.53
1:B:38:TYR:CE1	1:B:285:ILE:HG13	2.44	0.53
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.92	0.53
1:A:86:PHE:N	1:A:237:ARG:HA	2.23	0.52
1:C:87:ASN:OD1	1:C:87:ASN:N	2.43	0.52
1:C:800:PHE:N	1:C:800:PHE:HD1	2.06	0.52
1:B:327:VAL:HG11	1:B:528:LYS:HZ2	1.74	0.52
1:C:721:SER:OG	1:C:722:VAL:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.35	0.52
1:C:949:GLN:O	1:C:953:ASN:ND2	2.41	0.52
1:A:140:PHE:HB2	1:A:244:LEU:HD13	1.91	0.52
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.91	0.52
1:C:1002:GLN:O	1:C:1006:THR:HG23	2.10	0.52
1:B:62:VAL:CG1	1:B:266:TYR:HB3	2.40	0.52
1:C:84:LEU:HD22	1:C:267:VAL:HG21	1.91	0.52
1:A:981:LEU:O	1:C:386:LYS:NZ	2.42	0.52
1:B:336:CYS:HB3	1:B:358:ILE:HG21	1.92	0.52
1:B:65:PHE:HE2	1:B:84:LEU:HD21	1.74	0.52
1:B:661:GLU:N	1:B:661:GLU:OE1	2.43	0.52
1:B:825:LYS:HE3	1:B:938:LEU:O	2.09	0.52
1:C:543:PHE:CD1	1:C:576:VAL:HG21	2.44	0.52
1:B:388:ASN:HD21	1:B:527:PRO:HG2	1.74	0.52
1:C:365:TYR:O	1:C:369:TYR:HB2	2.09	0.52
1:A:1055:SER:OG	1:A:1056:ALA:N	2.42	0.52
1:B:568:ASP:OD1	1:B:569:ILE:N	2.39	0.52
1:C:666:ILE:HB	1:C:670:ILE:O	2.09	0.52
1:C:1092:GLU:OE2	1:C:1092:GLU:N	2.43	0.52
1:A:391:CYS:CB	1:A:525:CYS:HA	2.38	0.51
1:A:917:TYR:HD2	1:C:1089:PHE:CE2	2.28	0.51
1:B:117:LEU:HD23	1:B:118:LEU:N	2.25	0.51
1:B:197:ILE:HB	1:B:202:LYS:HZ3	1.74	0.51
1:C:1027:THR:O	1:C:1031:GLU:HG3	2.11	0.51
1:A:91:TYR:HB2	1:A:270:LEU:HD21	1.92	0.51
1:A:100:ILE:O	1:A:243:ALA:N	2.39	0.51
1:A:388:ASN:HD21	1:A:527:PRO:HG2	1.76	0.51
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.26	0.51
1:A:767:LEU:HD23	1:A:770:ILE:HD12	1.92	0.51
1:C:703:ASN:OD1	1:C:704:SER:N	2.43	0.51
1:C:354:ASN:HD21	1:C:399:SER:HG	1.58	0.51
1:A:43:PHE:O	1:A:44:ARG:HG3	2.10	0.51
1:A:108:THR:HG22	1:A:109:THR:HG23	1.91	0.51
1:A:421:TYR:O	1:A:424:LYS:NZ	2.39	0.51
1:A:1081:ILE:HD12	1:A:1095:PHE:HE2	1.76	0.51
1:C:809:PRO:HA	1:C:814:LYS:HE2	1.91	0.51
1:C:189:LEU:HB2	1:C:210:ILE:HG12	1.92	0.51
1:C:985:ASP:OD1	1:C:985:ASP:N	2.39	0.51
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.41	0.51
1:C:222:ALA:O	1:C:223:LEU:HD12	2.11	0.51
1:A:105:ILE:HG22	1:A:110:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:O	1:B:580:GLN:HG3	2.10	0.51
1:B:448:ASN:HD22	1:B:497:PHE:HD2	1.57	0.51
1:B:984:LEU:HD12	1:B:988:GLU:HB2	1.93	0.51
1:A:143:VAL:HG11	1:A:245:HIS:CG	2.46	0.51
1:A:290:ASP:OD1	1:A:292:ALA:N	2.44	0.51
1:A:291:CYS:O	1:A:298:GLU:HG3	2.10	0.51
1:A:1089:PHE:N	1:A:1089:PHE:CD1	2.79	0.51
1:B:707:TYR:CD2	1:C:883:THR:HG22	2.46	0.51
1:B:1027:THR:O	1:B:1031:GLU:HG3	2.11	0.51
1:C:808:ASP:HB3	1:C:811:LYS:HG2	1.93	0.51
1:A:96:GLU:HG3	1:A:99:ASN:H	1.74	0.51
1:A:704:SER:HB3	1:B:790:LYS:HE2	1.93	0.51
1:B:329:PHE:HE2	1:B:528:LYS:HB3	1.76	0.51
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.93	0.50
1:A:980:ILE:HD12	1:A:980:ILE:H	1.76	0.50
1:C:133:PHE:HB2	1:C:135:PHE:CZ	2.45	0.50
1:C:922:LEU:O	1:C:926:GLN:HG3	2.11	0.50
1:B:62:VAL:HG12	1:B:266:TYR:HB3	1.93	0.50
1:B:532:ASN:OD1	1:B:533:LEU:N	2.32	0.50
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.76	0.50
1:B:197:ILE:HB	1:B:202:LYS:NZ	2.26	0.50
1:A:103:GLY:CA	1:A:241:LEU:HB3	2.39	0.50
1:A:291:CYS:HA	1:A:297:SER:OG	2.12	0.50
1:C:89:GLY:C	1:C:270:LEU:HD12	2.35	0.50
1:C:950:ASP:OD2	1:C:954:GLN:NE2	2.45	0.50
1:A:105:ILE:HD12	1:A:139:PRO:HB3	1.93	0.50
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.47	0.50
1:A:222:ALA:O	1:A:223:LEU:HD12	2.12	0.50
1:A:1093:GLY:HA2	1:A:1107:ARG:HE	1.76	0.50
1:C:103:GLY:CA	1:C:241:LEU:HB3	2.38	0.50
1:C:978:ASN:O	1:C:982:SER:N	2.44	0.50
1:A:117:LEU:HD23	1:A:118:LEU:N	2.26	0.50
1:A:405:ASP:HA	1:A:408:ARG:HH12	1.76	0.50
1:A:869:MET:HE1	1:C:669:GLY:HA3	1.93	0.50
1:C:661:GLU:OE1	1:C:661:GLU:N	2.45	0.50
1:C:880:GLY:O	1:C:884:SER:OG	2.26	0.50
1:A:377:PHE:H	1:A:378:LYS:NZ	2.09	0.50
1:B:443:SER:HB3	1:B:499:PRO:HD3	1.93	0.50
1:C:436:TRP:O	1:C:509:ARG:N	2.45	0.50
1:C:655:HIS:CD2	1:C:656:VAL:H	2.29	0.50
1:A:130:VAL:HG23	1:A:233:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:ASP:OD2	1:A:673:SER:OG	2.29	0.50
1:A:1105:THR:HG23	1:A:1106:GLN:O	2.12	0.50
1:B:204:TYR:N	1:B:204:TYR:CD1	2.80	0.50
1:C:206:LYS:HD3	1:C:208:THR:HG21	1.93	0.50
1:C:568:ASP:OD1	1:C:569:ILE:N	2.42	0.50
1:B:506:GLN:HB2	1:B:508:TYR:HE1	1.77	0.49
1:B:605:SER:OG	1:B:606:ASN:N	2.42	0.49
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.93	0.49
1:C:443:SER:HB3	1:C:499:PRO:HD3	1.93	0.49
1:A:379:CYS:SG	1:A:384:PRO:HB3	2.52	0.49
1:B:45:SER:O	1:B:47:VAL:HG13	2.12	0.49
1:B:305:SER:OG	1:B:306:PHE:N	2.42	0.49
1:B:551:VAL:HG12	1:B:588:THR:O	2.13	0.49
1:B:979:ASP:O	1:B:983:ARG:N	2.45	0.49
1:C:107:GLY:HA2	1:C:235:ILE:HG12	1.94	0.49
1:C:786:LYS:HG3	1:C:787:GLN:HG3	1.93	0.49
1:A:498:GLN:H	1:A:501:ASN:HD21	1.61	0.49
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.94	0.49
1:B:1062:PHE:O	1:B:1063:LEU:HD23	2.13	0.49
1:A:764:ASN:O	1:A:768:THR:HG23	2.12	0.49
1:B:130:VAL:HG22	1:B:168:PHE:O	2.13	0.49
1:B:201:PHE:N	1:B:229:LEU:O	2.46	0.49
1:B:393:THR:HA	1:B:522:ALA:HA	1.94	0.49
1:C:189:LEU:HD12	1:C:210:ILE:HD13	1.94	0.49
1:A:734:THR:OG1	1:A:735:SER:N	2.46	0.49
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.76	0.49
1:B:434:ILE:HB	1:B:511:VAL:HG23	1.94	0.49
1:B:704:SER:HB3	1:C:790:LYS:HE2	1.95	0.49
1:B:1004:LEU:O	1:B:1008:VAL:HG23	2.13	0.49
1:C:309:GLU:OE1	1:C:310:LYS:N	2.45	0.49
1:A:914:ASN:HD22	1:C:1123:SER:CB	2.25	0.49
1:A:64:TRP:C	1:A:64:TRP:CD1	2.90	0.49
1:A:90:VAL:HG21	1:A:238:PHE:CE1	2.48	0.49
1:B:273:ARG:NH1	1:B:292:ALA:HB3	2.28	0.49
1:B:656:VAL:HG12	1:B:658:ASN:N	2.24	0.49
1:B:1089:PHE:CE2	1:C:914:ASN:HA	2.48	0.49
1:A:201:PHE:HE2	1:A:203:ILE:HG13	1.76	0.49
1:B:222:ALA:C	1:B:223:LEU:HD12	2.37	0.49
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.95	0.49
1:B:978:ASN:O	1:B:982:SER:N	2.46	0.49
1:A:62:VAL:HG12	1:A:266:TYR:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:HB3	1:A:223:LEU:HD21	1.95	0.48
1:A:498:GLN:CD	1:A:499:PRO:HD2	2.38	0.48
1:A:978:ASN:O	1:A:982:SER:N	2.46	0.48
1:B:645:THR:OG1	1:B:648:GLY:O	2.21	0.48
1:B:797:PHE:O	1:B:799:GLY:N	2.45	0.48
1:B:803:SER:OG	1:B:804:GLN:NE2	2.42	0.48
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.48	0.48
1:C:951:VAL:O	1:C:955:ASN:ND2	2.46	0.48
1:A:800:PHE:CD1	1:A:800:PHE:N	2.80	0.48
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.95	0.48
1:C:619:GLU:OE1	1:C:619:GLU:N	2.37	0.48
1:C:813:SER:O	1:C:815:ARG:N	2.41	0.48
1:A:405:ASP:OD1	1:A:406:GLU:HG3	2.13	0.48
1:B:666:ILE:HD12	1:B:670:ILE:HG22	1.94	0.48
1:C:117:LEU:HD23	1:C:118:LEU:N	2.28	0.48
1:C:305:SER:OG	1:C:306:PHE:N	2.46	0.48
1:B:870:ILE:O	1:B:874:THR:HG23	2.14	0.48
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.49	0.48
1:A:309:GLU:O	1:A:313:TYR:OH	2.29	0.48
1:A:809:PRO:HA	1:A:814:LYS:HE2	1.95	0.48
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.13	0.48
1:C:202:LYS:HB3	1:C:204:TYR:HE1	1.78	0.48
1:C:449:TYR:O	1:C:494:SER:OG	2.26	0.48
1:A:707:TYR:CD2	1:B:883:THR:HG22	2.48	0.48
1:B:405:ASP:HA	1:B:408:ARG:HH12	1.79	0.48
1:C:1081:ILE:HG23	1:C:1135:ASN:HB3	1.96	0.48
1:A:376:THR:HG22	1:A:435:ALA:HB3	1.95	0.48
1:A:658:ASN:ND2	1:A:660:TYR:OH	2.46	0.48
1:C:291:CYS:HA	1:C:297:SER:OG	2.13	0.48
1:C:462:LYS:HE3	1:C:465:GLU:HB2	1.96	0.48
1:C:870:ILE:O	1:C:874:THR:HG23	2.14	0.48
1:A:204:TYR:N	1:A:204:TYR:CD1	2.79	0.48
1:A:230:PRO:HG3	1:C:357:ARG:NH1	2.28	0.48
1:A:399:SER:HB2	1:A:511:VAL:HG12	1.96	0.48
1:A:420:ASP:C	1:A:424:LYS:HD2	2.39	0.48
1:A:797:PHE:O	1:A:799:GLY:N	2.46	0.48
1:A:1115:ILE:HG22	1:A:1137:VAL:HG13	1.96	0.48
1:B:568:ASP:CG	1:B:569:ILE:H	2.21	0.48
1:B:806:LEU:HD23	1:B:806:LEU:HA	1.59	0.48
1:B:808:ASP:HB3	1:B:811:LYS:HG2	1.96	0.48
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:TYR:CE1	1:C:285:ILE:HG13	2.49	0.48
1:A:365:TYR:OH	1:A:392:PHE:HE2	1.97	0.48
1:A:746:SER:OG	1:A:748:GLU:OE1	2.32	0.48
1:B:62:VAL:HG13	1:B:267:VAL:C	2.38	0.48
1:B:809:PRO:HA	1:B:814:LYS:HE2	1.96	0.48
1:C:339:GLY:O	1:C:343:ASN:N	2.37	0.48
1:C:431:GLY:HA2	1:C:515:PHE:HD2	1.78	0.48
1:B:107:GLY:HA2	1:B:235:ILE:HG12	1.95	0.48
1:B:586:ASP:O	1:B:587:ILE:HG13	2.14	0.48
1:B:930:ALA:O	1:B:934:ILE:HG12	2.13	0.48
1:C:96:GLU:HG2	1:C:97:LYS:H	1.78	0.48
1:C:415:THR:HG1	1:C:420:ASP:CG	2.19	0.48
1:C:531:THR:HG22	1:C:532:ASN:H	1.78	0.48
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.14	0.48
1:A:329:PHE:O	1:A:580:GLN:HG3	2.12	0.47
1:A:578:ASP:HB3	1:A:581:THR:O	2.13	0.47
1:B:64:TRP:CD1	1:B:64:TRP:C	2.91	0.47
1:B:107:GLY:N	1:B:235:ILE:HG23	2.29	0.47
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.96	0.47
1:B:726:ILE:HD13	1:B:945:LEU:HD13	1.96	0.47
1:C:379:CYS:SG	1:C:384:PRO:HB3	2.54	0.47
1:C:410:ILE:HG23	1:C:425:LEU:HD11	1.96	0.47
1:A:103:GLY:HA3	1:A:241:LEU:HD22	1.96	0.47
1:A:189:LEU:HD12	1:A:210:ILE:HD13	1.95	0.47
1:A:365:TYR:O	1:A:369:TYR:HB2	2.14	0.47
1:B:327:VAL:HG21	1:B:528:LYS:HZ1	1.79	0.47
1:B:433:VAL:O	1:B:434:ILE:HD13	2.14	0.47
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.13	0.47
1:B:449:TYR:O	1:B:494:SER:OG	2.27	0.47
1:B:768:THR:O	1:B:772:VAL:HG12	2.15	0.47
1:B:974:SER:OG	1:B:975:SER:N	2.48	0.47
1:B:1089:PHE:N	1:B:1089:PHE:CD1	2.82	0.47
1:A:62:VAL:HG13	1:A:268:GLY:N	2.30	0.47
1:A:280:ASN:OD1	1:A:284:THR:N	2.29	0.47
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.49	0.47
1:C:698:SER:OG	1:C:699:LEU:N	2.47	0.47
1:A:29:THR:HG22	1:A:62:VAL:O	2.14	0.47
1:A:229:LEU:HB3	1:A:231:ILE:HG23	1.97	0.47
1:A:112:SER:O	1:A:112:SER:OG	2.28	0.47
1:A:540:ASN:OD1	1:A:540:ASN:N	2.47	0.47
1:B:107:GLY:H	1:B:235:ILE:HG23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:SER:HB2	1:B:133:PHE:C	2.39	0.47
1:B:133:PHE:HB2	1:B:135:PHE:CZ	2.50	0.47
1:B:698:SER:OG	1:B:699:LEU:N	2.45	0.47
1:B:1003:SER:O	1:B:1006:THR:OG1	2.33	0.47
1:C:222:ALA:C	1:C:223:LEU:HD12	2.40	0.47
1:A:501:ASN:ND2	1:A:505:TYR:O	2.47	0.47
1:A:979:ASP:HB3	1:A:983:ARG:HH21	1.80	0.47
1:A:1090:PRO:HB3	1:A:1095:PHE:CE1	2.50	0.47
1:B:299:THR:HG22	1:B:308:VAL:HG21	1.97	0.47
1:C:131:CYS:SG	1:C:132:GLU:N	2.87	0.47
1:C:802:PHE:CD2	1:C:805:ILE:HD11	2.50	0.47
1:A:91:TYR:HD2	1:A:268:GLY:H	1.62	0.47
1:A:1089:PHE:N	1:A:1089:PHE:HD1	2.12	0.47
1:B:29:THR:HG22	1:B:62:VAL:O	2.15	0.47
1:B:87:ASN:N	1:B:87:ASN:OD1	2.46	0.47
1:B:228:ASP:OD1	1:B:229:LEU:N	2.48	0.47
1:C:92:PHE:HZ	1:C:240:THR:HB	1.79	0.47
1:C:143:VAL:HG12	1:C:243:ALA:HB1	1.97	0.47
1:C:392:PHE:HB3	1:C:517:LEU:HD13	1.97	0.47
1:C:501:ASN:HB3	1:C:505:TYR:HB2	1.97	0.47
1:A:43:PHE:HD1	1:C:563:GLN:NE2	2.13	0.47
1:A:660:TYR:H	1:A:695:TYR:HE2	1.59	0.47
1:B:773:GLU:OE2	1:B:1019:ARG:HD3	2.14	0.47
1:C:977:LEU:HG	1:C:981:LEU:HD12	1.97	0.47
1:A:112:SER:HB2	1:A:133:PHE:C	2.39	0.47
1:A:394:ASN:ND2	1:A:516:GLU:OE2	2.33	0.47
1:A:913:GLN:O	1:A:916:LEU:N	2.48	0.47
1:B:609:ALA:HB2	1:B:692:ILE:HD12	1.96	0.47
1:B:896:ILE:HG13	1:B:897:PRO:HD2	1.96	0.47
1:C:62:VAL:HG13	1:C:267:VAL:C	2.41	0.47
1:A:86:PHE:HA	1:A:90:VAL:CG2	2.45	0.46
1:C:228:ASP:OD1	1:C:229:LEU:N	2.48	0.46
1:A:894:LEU:HD13	1:C:715:PRO:HD3	1.98	0.46
1:A:968:SER:HB2	1:A:970:PHE:CE1	2.50	0.46
1:B:394:ASN:HB3	1:B:516:GLU:OE2	2.15	0.46
1:B:1094:VAL:HG12	1:C:904:TYR:OH	2.14	0.46
1:C:36:VAL:O	1:C:222:ALA:HA	2.16	0.46
1:C:172:SER:O	1:C:172:SER:OG	2.30	0.46
1:C:376:THR:HG22	1:C:435:ALA:HB3	1.96	0.46
1:C:377:PHE:CD1	1:C:434:ILE:HD12	2.51	0.46
1:C:794:ILE:HG13	1:C:794:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:TYR:O	1:A:494:SER:OG	2.27	0.46
1:B:187:LYS:O	1:B:210:ILE:N	2.33	0.46
1:B:578:ASP:HB3	1:B:581:THR:O	2.15	0.46
1:C:86:PHE:HA	1:C:90:VAL:HG21	1.96	0.46
1:A:498:GLN:H	1:A:501:ASN:ND2	2.13	0.46
1:B:93:ALA:O	1:B:94:SER:OG	2.29	0.46
1:B:978:ASN:HA	1:B:981:LEU:HB2	1.96	0.46
1:A:38:TYR:CE1	1:A:285:ILE:HG13	2.51	0.46
1:A:930:ALA:O	1:A:934:ILE:HG12	2.15	0.46
1:B:655:HIS:CD2	1:B:656:VAL:H	2.34	0.46
1:C:119:ILE:HG12	1:C:128:ILE:HD12	1.97	0.46
1:A:666:ILE:HB	1:A:670:ILE:O	2.15	0.46
1:C:131:CYS:HB2	1:C:166:CYS:HB3	1.68	0.46
1:C:429:PHE:HE1	1:C:514:SER:HA	1.80	0.46
1:C:734:THR:OG1	1:C:735:SER:N	2.48	0.46
1:A:337:PRO:O	1:A:341:VAL:HG23	2.16	0.46
1:C:86:PHE:H	1:C:237:ARG:HA	1.81	0.46
1:C:104:TRP:CD1	1:C:194:PHE:HE2	2.34	0.46
1:A:531:THR:HG22	1:A:532:ASN:H	1.81	0.46
1:A:655:HIS:CD2	1:A:656:VAL:H	2.33	0.46
1:A:794:ILE:O	1:A:794:ILE:HG13	2.16	0.46
1:A:804:GLN:O	1:A:816:SER:OG	2.34	0.46
1:C:960:ASN:HA	1:C:963:VAL:HG12	1.98	0.46
1:C:1049:LEU:HB2	1:C:1065:VAL:O	2.14	0.46
1:A:231:ILE:HG13	1:A:232:GLY:N	2.31	0.46
1:A:714:ILE:HD11	1:A:1094:VAL:HG21	1.96	0.46
1:C:949:GLN:HG3	1:C:953:ASN:ND2	2.31	0.46
1:A:393:THR:HA	1:A:522:ALA:HA	1.97	0.46
1:A:530:SER:OG	1:A:580:GLN:NE2	2.49	0.46
1:C:92:PHE:HE2	1:C:238:PHE:HE2	1.62	0.46
1:C:212:LEU:HD22	1:C:217:PRO:HB3	1.98	0.46
1:B:302:THR:HG23	1:B:303:LEU:HD23	1.98	0.45
1:C:797:PHE:O	1:C:799:GLY:N	2.49	0.45
1:A:92:PHE:HZ	1:A:240:THR:HB	1.81	0.45
1:A:770:ILE:O	1:A:774:GLN:HG2	2.16	0.45
1:A:1027:THR:O	1:A:1031:GLU:HG3	2.17	0.45
1:B:201:PHE:HE2	1:B:203:ILE:HG13	1.81	0.45
1:B:1115:ILE:HG22	1:B:1137:VAL:HG13	1.96	0.45
1:C:332:ILE:HD12	1:C:332:ILE:HA	1.81	0.45
1:C:532:ASN:OD1	1:C:533:LEU:N	2.34	0.45
1:C:770:ILE:O	1:C:774:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1060:VAL:HG22	1:C:1061:VAL:H	1.80	0.45
1:A:392:PHE:CD1	1:A:515:PHE:HB3	2.50	0.45
1:A:754:LEU:HD23	1:A:754:LEU:HA	1.83	0.45
1:B:377:PHE:C	1:B:378:LYS:HD2	2.41	0.45
1:B:530:SER:OG	1:B:580:GLN:NE2	2.49	0.45
1:B:767:LEU:HD23	1:B:770:ILE:HD12	1.97	0.45
1:B:900:MET:HB3	1:B:900:MET:HE2	1.70	0.45
1:C:1029:MET:HE2	1:C:1029:MET:HB2	1.82	0.45
1:A:1082:CYS:HB2	1:A:1126:CYS:HB2	1.93	0.45
1:A:1093:GLY:H	1:A:1107:ARG:NH2	2.15	0.45
1:B:337:PRO:O	1:B:341:VAL:HG23	2.16	0.45
1:B:747:THR:OG1	1:B:748:GLU:N	2.48	0.45
1:C:405:ASP:HA	1:C:408:ARG:HH22	1.82	0.45
1:A:900:MET:HE1	1:C:1094:VAL:HG23	1.99	0.45
1:A:949:GLN:HE21	1:A:953:ASN:HD21	1.63	0.45
1:B:86:PHE:H	1:B:237:ARG:HA	1.81	0.45
1:B:200:TYR:CD2	1:B:230:PRO:HB3	2.52	0.45
1:C:63:THR:O	1:C:63:THR:OG1	2.17	0.45
1:C:118:LEU:HB3	1:C:129:LYS:HB2	1.99	0.45
1:A:107:GLY:HA2	1:A:235:ILE:HG12	1.97	0.45
1:A:403:ARG:HD3	1:A:505:TYR:HA	1.99	0.45
1:A:715:PRO:HD3	1:B:894:LEU:HD13	1.99	0.45
1:B:391:CYS:CB	1:B:525:CYS:HA	2.39	0.45
1:B:611:LEU:HD22	1:B:666:ILE:HG23	1.99	0.45
1:C:407:VAL:HG22	1:C:408:ARG:HH11	1.82	0.45
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.67	0.45
1:B:357:ARG:CZ	1:C:230:PRO:HG3	2.46	0.45
1:B:357:ARG:NH1	1:C:230:PRO:HG3	2.31	0.45
1:B:433:VAL:HG23	1:B:512:VAL:HG22	1.99	0.45
1:C:189:LEU:HD23	1:C:191:GLU:H	1.81	0.45
1:C:506:GLN:HB2	1:C:508:TYR:HE1	1.81	0.45
1:A:137:ASN:OD1	1:A:138:ASP:N	2.49	0.45
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.73	0.45
1:A:748:GLU:H	1:A:748:GLU:CD	2.21	0.45
1:A:896:ILE:HG13	1:A:897:PRO:HD2	1.99	0.45
1:A:914:ASN:OD1	1:A:915:VAL:N	2.49	0.45
1:C:906:PHE:O	1:C:908:GLY:N	2.49	0.45
1:A:351:TYR:CE1	1:A:452:LEU:HB2	2.52	0.45
1:B:91:TYR:HB2	1:B:270:LEU:HD21	1.98	0.45
1:B:273:ARG:HD3	1:B:273:ARG:HA	1.75	0.45
1:B:392:PHE:CD1	1:B:515:PHE:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ILE:HD11	1:B:407:VAL:HG12	1.98	0.45
1:C:94:SER:OG	1:C:95:THR:N	2.50	0.45
1:C:197:ILE:HB	1:C:202:LYS:NZ	2.31	0.45
1:C:958:ALA:O	1:C:961:THR:OG1	2.31	0.45
1:A:34:ARG:NH1	1:A:189:LEU:HD11	2.32	0.45
1:B:214:ARG:NE	1:B:215:ASP:HB2	2.25	0.45
1:B:979:ASP:HB3	1:B:983:ARG:HE	1.81	0.45
1:C:231:ILE:HG13	1:C:232:GLY:N	2.31	0.45
1:C:271:GLN:HB2	1:C:272:PRO:HD2	1.98	0.45
1:B:109:THR:OG1	1:B:111:ASP:OD1	2.35	0.44
1:B:403:ARG:HH21	1:B:495:TYR:HD1	1.64	0.44
1:B:949:GLN:HG3	1:B:953:ASN:HD21	1.83	0.44
1:B:979:ASP:HB3	1:B:983:ARG:NE	2.32	0.44
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.76	0.44
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.75	0.44
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.52	0.44
1:A:419:ALA:HA	1:A:423:TYR:O	2.17	0.44
1:C:379:CYS:HB2	1:C:384:PRO:HD3	1.99	0.44
1:A:189:LEU:HB2	1:A:210:ILE:CG1	2.47	0.44
1:A:273:ARG:NH1	1:A:292:ALA:HB3	2.33	0.44
1:A:737:ASP:OD2	1:C:319:ARG:NH2	2.51	0.44
1:A:797:PHE:C	1:A:799:GLY:H	2.25	0.44
1:B:189:LEU:O	1:B:189:LEU:HD23	2.17	0.44
1:B:200:TYR:CE2	1:B:230:PRO:HB3	2.52	0.44
1:B:222:ALA:O	1:B:223:LEU:HD12	2.17	0.44
1:C:66:HIS:ND1	1:C:66:HIS:O	2.51	0.44
1:A:568:ASP:OD1	1:A:569:ILE:N	2.44	0.44
1:B:106:PHE:HZ	1:B:194:PHE:CE2	2.35	0.44
1:B:1089:PHE:N	1:B:1089:PHE:HD1	2.15	0.44
1:B:1129:VAL:CG2	1:C:917:TYR:HB3	2.48	0.44
1:C:341:VAL:HG22	1:C:356:LYS:HE3	1.99	0.44
1:C:949:GLN:HG3	1:C:953:ASN:HD21	1.81	0.44
1:A:212:LEU:HD22	1:A:217:PRO:HB3	1.99	0.44
1:A:411:ALA:N	1:A:425:LEU:HD12	2.33	0.44
1:B:191:GLU:HB3	1:B:223:LEU:HD21	1.99	0.44
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.99	0.44
1:C:568:ASP:CG	1:C:569:ILE:H	2.23	0.44
1:C:979:ASP:HB3	1:C:983:ARG:NE	2.32	0.44
1:C:1009:THR:O	1:C:1013:ILE:HG13	2.17	0.44
1:B:406:GLU:CD	1:B:418:ILE:HG13	2.43	0.44
1:B:794:ILE:HG13	1:B:794:ILE:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ASN:OD1	1:C:121:ASN:N	2.51	0.44
1:A:92:PHE:CZ	1:A:240:THR:HB	2.52	0.44
1:A:277:LEU:H	1:A:277:LEU:HG	1.65	0.44
1:A:768:THR:O	1:A:772:VAL:HG12	2.18	0.44
1:B:277:LEU:H	1:B:277:LEU:HG	1.49	0.44
1:B:673:SER:OG	1:B:674:TYR:N	2.50	0.44
1:B:877:LEU:HD23	1:B:877:LEU:HA	1.85	0.44
1:B:1090:PRO:HB3	1:B:1095:PHE:CE1	2.52	0.44
1:C:37:TYR:OH	1:C:195:LYS:NZ	2.26	0.44
1:C:1062:PHE:O	1:C:1063:LEU:HD23	2.17	0.44
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.53	0.44
1:B:379:CYS:HA	1:B:432:CYS:HB2	1.99	0.44
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.53	0.44
1:A:748:GLU:OE1	1:A:748:GLU:N	2.36	0.44
1:B:137:ASN:OD1	1:B:138:ASP:N	2.51	0.44
1:A:51:THR:O	1:A:274:THR:HG23	2.18	0.43
1:A:201:PHE:CE2	1:A:203:ILE:HG13	2.52	0.43
1:A:228:ASP:OD1	1:A:229:LEU:N	2.51	0.43
1:B:383:SER:HB3	1:C:985:ASP:H	1.82	0.43
1:C:277:LEU:HD12	1:C:277:LEU:O	2.18	0.43
1:C:756:TYR:N	1:C:756:TYR:CD1	2.86	0.43
1:A:526:GLY:O	1:A:528:LYS:N	2.50	0.43
1:A:913:GLN:NE2	1:C:1090:PRO:HD2	2.34	0.43
1:B:112:SER:OG	1:B:112:SER:O	2.34	0.43
1:C:45:SER:O	1:C:47:VAL:HG13	2.19	0.43
1:C:384:PRO:HA	1:C:387:LEU:HG	2.00	0.43
1:A:443:SER:OG	1:A:497:PHE:HB3	2.18	0.43
1:B:350:VAL:HG12	1:B:402:ILE:HG22	2.00	0.43
1:B:383:SER:N	1:C:983:ARG:O	2.30	0.43
1:B:770:ILE:O	1:B:774:GLN:HG2	2.18	0.43
1:B:103:GLY:CA	1:B:241:LEU:HB3	2.41	0.43
1:B:229:LEU:HB3	1:B:231:ILE:HG12	2.00	0.43
1:B:405:ASP:OD1	1:B:406:GLU:HG3	2.18	0.43
1:B:800:PHE:H	1:B:800:PHE:HD1	1.64	0.43
1:C:105:ILE:HD12	1:C:139:PRO:HB3	2.01	0.43
1:C:806:LEU:HA	1:C:806:LEU:HD23	1.62	0.43
1:B:332:ILE:HG12	1:B:334:ASN:H	1.82	0.43
1:B:737:ASP:OD1	1:B:737:ASP:N	2.51	0.43
1:C:202:LYS:HB3	1:C:204:TYR:CE1	2.53	0.43
1:C:900:MET:HA	1:C:917:TYR:OH	2.18	0.43
1:A:323:THR:HG22	1:A:324:GLU:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:PHE:CZ	1:A:587:ILE:HD13	2.53	0.43
1:A:741:TYR:CZ	1:A:966:LEU:HD21	2.54	0.43
1:A:1089:PHE:HB3	1:A:1090:PRO:HD2	2.00	0.43
1:A:1090:PRO:HD2	1:B:913:GLN:NE2	2.34	0.43
1:B:189:LEU:HB3	1:B:208:THR:HG23	2.00	0.43
1:B:914:ASN:OD1	1:B:915:VAL:N	2.51	0.43
1:C:90:VAL:HG11	1:C:238:PHE:CZ	2.53	0.43
1:A:107:GLY:N	1:A:235:ILE:HG23	2.33	0.43
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.99	0.43
1:B:555:SER:OG	1:B:584:ILE:HG22	2.18	0.43
1:B:576:VAL:HG12	1:B:577:ARG:H	1.83	0.43
1:C:215:ASP:HA	1:C:266:TYR:OH	2.18	0.43
1:A:89:GLY:O	1:A:270:LEU:HD12	2.19	0.43
1:A:110:LEU:HD22	1:A:237:ARG:HH12	1.84	0.43
1:A:429:PHE:HE1	1:A:514:SER:HA	1.82	0.43
1:B:607:GLN:O	1:B:692:ILE:HD11	2.19	0.43
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.53	0.43
1:C:526:GLY:O	1:C:528:LYS:N	2.50	0.43
1:A:81:ASN:OD1	1:A:81:ASN:N	2.52	0.43
1:A:326:ILE:HG13	1:A:534:VAL:HG22	2.01	0.43
1:A:403:ARG:HH21	1:A:495:TYR:HD1	1.65	0.43
1:B:393:THR:HG22	1:B:516:GLU:O	2.19	0.43
1:B:741:TYR:CD1	1:B:741:TYR:C	2.97	0.43
1:C:354:ASN:ND2	1:C:399:SER:OG	2.32	0.43
1:C:433:VAL:C	1:C:434:ILE:HD13	2.44	0.43
1:C:870:ILE:H	1:C:870:ILE:HG12	1.67	0.43
1:A:204:TYR:N	1:A:204:TYR:HD1	2.16	0.43
1:A:776:LYS:O	1:A:780:GLU:HG3	2.19	0.43
1:A:903:ALA:HB1	1:A:913:GLN:HB2	2.00	0.43
1:C:64:TRP:HD1	1:C:266:TYR:CE1	2.37	0.43
1:C:105:ILE:HG22	1:C:110:LEU:HG	2.01	0.43
1:C:291:CYS:HB3	1:C:301:CYS:HB2	1.40	0.43
1:C:426:PRO:HB2	1:C:429:PHE:HB2	2.00	0.43
1:C:777:ASN:O	1:C:781:VAL:HG23	2.19	0.43
1:A:107:GLY:O	1:A:236:THR:N	2.47	0.42
1:A:551:VAL:HG22	1:A:588:THR:O	2.19	0.42
1:A:1031:GLU:OE2	1:C:1039:ARG:HB3	2.19	0.42
1:B:576:VAL:HG12	1:B:577:ARG:N	2.34	0.42
1:B:756:TYR:CD1	1:B:756:TYR:N	2.87	0.42
1:B:756:TYR:HB3	1:B:759:PHE:HD2	1.84	0.42
1:A:103:GLY:N	1:A:241:LEU:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TRP:CD1	1:A:194:PHE:HE2	2.37	0.42
1:A:290:ASP:OD1	1:A:291:CYS:N	2.52	0.42
1:A:669:GLY:HA3	1:B:869:MET:HE1	1.99	0.42
1:B:870:ILE:H	1:B:870:ILE:HG12	1.70	0.42
1:C:878:LEU:HD12	1:C:882:ILE:HD11	2.00	0.42
1:A:86:PHE:HA	1:A:90:VAL:HG23	2.01	0.42
1:A:87:ASN:OD1	1:A:87:ASN:N	2.51	0.42
1:A:332:ILE:HG12	1:A:334:ASN:H	1.85	0.42
1:A:718:PHE:HA	1:A:1069:PRO:HA	2.02	0.42
1:A:900:MET:HE2	1:A:900:MET:HB3	1.69	0.42
1:A:917:TYR:CE2	1:C:1079:PRO:HB2	2.54	0.42
1:B:193:VAL:C	1:B:194:PHE:HD1	2.28	0.42
1:B:418:ILE:HD11	1:B:495:TYR:OH	2.19	0.42
1:B:1107:ARG:HD3	1:C:904:TYR:CE2	2.55	0.42
1:C:186:PHE:HB2	1:C:213:VAL:HA	2.01	0.42
1:A:28:TYR:HD2	1:A:61:ASN:HB3	1.84	0.42
1:A:86:PHE:HE2	1:A:196:ASN:HD21	1.66	0.42
1:A:104:TRP:HD1	1:A:106:PHE:CZ	2.37	0.42
1:A:386:LYS:NZ	1:B:982:SER:HA	2.35	0.42
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.85	0.42
1:B:977:LEU:HG	1:B:981:LEU:HD12	2.02	0.42
1:C:92:PHE:CZ	1:C:240:THR:HB	2.54	0.42
1:C:264:ALA:HB1	1:C:266:TYR:CE1	2.54	0.42
1:A:106:PHE:CD1	1:A:106:PHE:N	2.87	0.42
1:A:547:THR:HG22	1:A:548:GLY:N	2.35	0.42
1:A:1043:CYS:HB3	1:A:1048:HIS:HD2	1.83	0.42
1:C:113:LYS:HA	1:C:113:LYS:HD2	1.83	0.42
1:B:277:LEU:HD12	1:B:277:LEU:O	2.20	0.42
1:B:805:ILE:HB	1:B:1054:GLN:HE22	1.83	0.42
1:B:1029:MET:HA	1:B:1033:VAL:HG23	2.02	0.42
1:C:91:TYR:HE2	1:C:93:ALA:HB2	1.84	0.42
1:C:334:ASN:O	1:C:362:VAL:HG22	2.19	0.42
1:C:797:PHE:C	1:C:799:GLY:H	2.27	0.42
1:A:1093:GLY:H	1:A:1107:ARG:HH21	1.65	0.42
1:B:92:PHE:HE1	1:B:238:PHE:HE2	1.67	0.42
1:C:616:ASN:OD1	1:C:617:CYS:N	2.52	0.42
1:A:225:PRO:O	1:A:226:LEU:HD22	2.19	0.42
1:A:334:ASN:HB3	1:A:361:CYS:HA	2.02	0.42
1:A:916:LEU:HD12	1:A:923:ILE:HD12	2.01	0.42
1:A:957:GLN:O	1:A:961:THR:HG22	2.20	0.42
1:A:985:ASP:H	1:C:383:SER:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:HD2	1:B:243:ALA:HB2	2.02	0.42
1:B:403:ARG:HD3	1:B:505:TYR:HA	2.01	0.42
1:B:512:VAL:O	1:B:513:LEU:HD23	2.19	0.42
1:C:90:VAL:HG11	1:C:238:PHE:CE1	2.54	0.42
1:C:578:ASP:HB3	1:C:581:THR:O	2.19	0.42
1:C:979:ASP:O	1:C:982:SER:N	2.51	0.42
1:A:890:ALA:HA	1:C:1046:GLY:HA2	2.01	0.42
1:A:1060:VAL:HG22	1:A:1061:VAL:H	1.83	0.42
1:A:1062:PHE:O	1:A:1063:LEU:HD23	2.20	0.42
1:B:86:PHE:HB2	1:B:238:PHE:HD1	1.85	0.42
1:B:987:PRO:HB2	1:B:988:GLU:OE1	2.19	0.42
1:C:143:VAL:HG11	1:C:245:HIS:CE1	2.54	0.42
1:C:797:PHE:C	1:C:799:GLY:N	2.77	0.42
1:A:319:ARG:HH12	1:B:740:MET:HB2	1.85	0.42
1:A:506:GLN:HB2	1:A:508:TYR:HE1	1.84	0.42
1:A:560:LEU:O	1:A:562:PHE:N	2.53	0.42
1:A:1094:VAL:HG12	1:B:904:TYR:OH	2.18	0.42
1:B:537:LYS:O	1:B:539:VAL:HG13	2.20	0.42
1:B:800:PHE:CD1	1:B:800:PHE:N	2.88	0.42
1:B:960:ASN:HA	1:B:963:VAL:HG12	2.00	0.42
1:C:204:TYR:N	1:C:204:TYR:HD1	2.17	0.42
1:C:266:TYR:CD1	1:C:266:TYR:N	2.85	0.42
1:C:273:ARG:NH1	1:C:292:ALA:HB3	2.34	0.42
1:C:584:ILE:HD13	1:C:584:ILE:HA	1.83	0.42
1:A:323:THR:HG21	1:A:537:LYS:HD2	2.02	0.41
1:A:350:VAL:O	1:A:353:TRP:HD1	2.03	0.41
1:A:430:THR:O	1:A:430:THR:OG1	2.37	0.41
1:A:741:TYR:C	1:A:741:TYR:CD1	2.98	0.41
1:A:979:ASP:O	1:A:983:ARG:N	2.53	0.41
1:B:906:PHE:C	1:B:908:GLY:N	2.76	0.41
1:C:332:ILE:HG13	1:C:334:ASN:HD22	1.85	0.41
1:C:873:TYR:HD1	1:C:873:TYR:HA	1.73	0.41
1:B:437:ASN:HD22	1:B:439:ASN:H	1.68	0.41
1:B:598:ILE:HB	1:B:609:ALA:HB3	2.02	0.41
1:C:191:GLU:OE1	1:C:223:LEU:HD11	2.19	0.41
1:C:350:VAL:HG12	1:C:402:ILE:HG22	2.01	0.41
1:A:37:TYR:OH	1:A:54:LEU:O	2.26	0.41
1:A:101:ILE:HG12	1:A:242:LEU:HD11	2.02	0.41
1:A:403:ARG:HH22	1:A:496:GLY:H	1.68	0.41
1:A:913:GLN:HE21	1:C:1090:PRO:HD2	1.84	0.41
1:A:949:GLN:O	1:A:953:ASN:ND2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:HD23	1:B:425:LEU:HA	1.84	0.41
1:B:462:LYS:HE3	1:B:465:GLU:OE1	2.20	0.41
1:C:336:CYS:O	1:C:338:PHE:N	2.53	0.41
1:C:541:PHE:HB3	1:C:552:LEU:HD11	2.02	0.41
1:C:1097:SER:HB2	1:C:1102:TRP:HA	2.01	0.41
1:A:143:VAL:HG11	1:A:245:HIS:CD2	2.55	0.41
1:C:427:ASP:OD1	1:C:428:ASP:N	2.52	0.41
1:C:443:SER:OG	1:C:497:PHE:HB3	2.20	0.41
1:A:796:ASP:OD1	1:A:796:ASP:N	2.52	0.41
1:A:802:PHE:CD2	1:A:805:ILE:HD11	2.44	0.41
1:A:805:ILE:HB	1:A:1054:GLN:NE2	2.35	0.41
1:A:1029:MET:HE2	1:A:1029:MET:HB2	1.86	0.41
1:B:804:GLN:O	1:B:816:SER:OG	2.39	0.41
1:B:949:GLN:HG3	1:B:953:ASN:ND2	2.35	0.41
1:A:797:PHE:C	1:A:799:GLY:N	2.77	0.41
1:A:1049:LEU:HD23	1:A:1049:LEU:HA	1.77	0.41
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.30	0.41
1:C:462:LYS:HE3	1:C:465:GLU:OE2	2.20	0.41
1:A:543:PHE:CD1	1:A:576:VAL:HG11	2.56	0.41
1:B:131:CYS:HA	1:B:166:CYS:CB	2.49	0.41
1:B:328:ARG:HH11	1:B:533:LEU:HB2	1.84	0.41
1:B:906:PHE:O	1:B:908:GLY:N	2.52	0.41
1:C:434:ILE:N	1:C:511:VAL:O	2.28	0.41
1:C:741:TYR:CD1	1:C:741:TYR:C	2.98	0.41
1:B:81:ASN:ND2	1:B:139:PRO:O	2.53	0.41
1:B:716:THR:N	1:B:1071:GLN:O	2.45	0.41
1:B:1018:ILE:O	1:B:1021:SER:OG	2.32	0.41
1:C:399:SER:HB3	1:C:511:VAL:HG12	2.03	0.41
1:C:717:ASN:O	1:C:1070:ALA:N	2.52	0.41
1:A:501:ASN:CG	1:A:505:TYR:HB2	2.46	0.41
1:A:987:PRO:HB2	1:A:988:GLU:OE1	2.21	0.41
1:A:1116:THR:HB	1:A:1140:PRO:HG3	2.02	0.41
1:B:28:TYR:HD2	1:B:61:ASN:HB3	1.86	0.41
1:B:117:LEU:HD23	1:B:118:LEU:H	1.86	0.41
1:B:266:TYR:N	1:B:266:TYR:CD1	2.89	0.41
1:B:386:LYS:NZ	1:C:982:SER:HA	2.36	0.41
1:B:443:SER:OG	1:B:497:PHE:HB3	2.21	0.41
1:B:733:LYS:HE3	1:B:771:ALA:HB1	2.03	0.41
1:B:1050:MET:O	1:B:1051:SER:OG	2.35	0.41
1:C:95:THR:HG22	1:C:186:PHE:C	2.46	0.41
1:C:242:LEU:HB3	1:C:244:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:HH11	1:C:533:LEU:HB2	1.86	0.41
1:C:763:LEU:HA	1:C:763:LEU:HD23	1.75	0.41
1:C:996:LEU:HA	1:C:996:LEU:HD23	1.78	0.41
1:C:1105:THR:HG23	1:C:1106:GLN:O	2.21	0.41
1:B:754:LEU:HD23	1:B:754:LEU:HA	1.84	0.41
1:C:104:TRP:HB2	1:C:119:ILE:HB	2.03	0.41
1:C:106:PHE:CD1	1:C:106:PHE:N	2.88	0.41
1:C:363:ALA:O	1:C:527:PRO:HD3	2.21	0.41
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	2.02	0.41
1:A:302:THR:HG23	1:A:303:LEU:HD23	2.03	0.40
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.87	0.40
1:A:1092:GLU:OE1	1:A:1092:GLU:N	2.54	0.40
1:B:331:ASN:HD22	1:B:580:GLN:HG2	1.86	0.40
1:B:341:VAL:HG22	1:B:356:LYS:HZ1	1.86	0.40
1:B:900:MET:HA	1:B:917:TYR:OH	2.21	0.40
1:B:922:LEU:CD2	1:B:926:GLN:HE21	2.34	0.40
1:B:1038:LYS:HE2	1:B:1038:LYS:HB3	1.79	0.40
1:C:189:LEU:HB2	1:C:210:ILE:CG1	2.51	0.40
1:C:916:LEU:HD12	1:C:923:ILE:HD13	2.03	0.40
1:C:1082:CYS:HB2	1:C:1126:CYS:HB2	2.03	0.40
1:A:359:SER:OG	1:A:360:ASN:ND2	2.55	0.40
1:A:707:TYR:CD1	1:A:707:TYR:C	2.99	0.40
1:B:415:THR:C	1:B:419:ALA:HB3	2.47	0.40
1:C:393:THR:HG21	1:C:518:LEU:HB2	2.04	0.40
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.83	0.40
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.51	0.40
1:C:978:ASN:HA	1:C:981:LEU:HB2	2.03	0.40
1:C:377:PHE:H	1:C:378:LYS:NZ	2.16	0.40
1:C:402:ILE:HD11	1:C:407:VAL:HG12	2.03	0.40
1:C:987:PRO:HB2	1:C:988:GLU:OE1	2.20	0.40
1:A:409:GLN:CD	1:A:416:GLY:HA3	2.46	0.40
1:B:327:VAL:HG21	1:B:528:LYS:NZ	2.37	0.40
1:B:393:THR:HG21	1:B:518:LEU:HD12	2.03	0.40
1:C:900:MET:HE2	1:C:900:MET:HB3	1.75	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	954/1247 (76%)	849 (89%)	105 (11%)	0	100	100
1	B	951/1247 (76%)	845 (89%)	106 (11%)	0	100	100
1	C	951/1247 (76%)	834 (88%)	117 (12%)	0	100	100
All	All	2856/3741 (76%)	2528 (88%)	328 (12%)	0	100	100

There are no Ramachandran outliers to report.

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	855/1085 (79%)	852 (100%)	3 (0%)	84	83
1	B	855/1085 (79%)	853 (100%)	2 (0%)	87	85
1	C	855/1085 (79%)	848 (99%)	7 (1%)	73	77
All	All	2565/3255 (79%)	2553 (100%)	12 (0%)	78	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	LEU
1	A	800	PHE
1	A	1089	PHE
1	B	277	LEU
1	B	1089	PHE

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Mol	Chain	Res	Type
1	C	277	LEU
1	C	587	ILE
1	C	651	ILE
1	C	800	PHE
1	C	873	TYR
1	C	1094	VAL
1	C	1104	VAL

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

Mol	Chain	Res	Type
1	A	196	ASN
1	A	360	ASN
1	A	388	ASN
1	A	394	ASN
1	A	501	ASN
1	A	506	GLN
1	A	644	GLN
1	A	655	HIS
1	A	658	ASN
1	A	690	GLN
1	A	779	GLN
1	A	926	GLN
1	A	928	ASN
1	A	953	ASN
1	A	965	GLN
1	A	1005	GLN
1	A	1011	GLN
1	A	1088	HIS
1	B	196	ASN
1	B	211	ASN
1	B	331	ASN
1	B	354	ASN
1	B	388	ASN
1	B	437	ASN
1	B	439	ASN
1	B	448	ASN
1	B	493	GLN
1	B	501	ASN
1	B	644	GLN
1	B	655	HIS
1	B	658	ASN

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Mol	Chain	Res	Type
1	B	690	GLN
1	B	919	ASN
1	B	926	GLN
1	B	953	ASN
1	B	965	GLN
1	B	1088	HIS
1	B	1142	GLN
1	C	137	ASN
1	C	211	ASN
1	C	317	ASN
1	C	334	ASN
1	C	394	ASN
1	C	437	ASN
1	C	448	ASN
1	C	644	GLN
1	C	655	HIS
1	C	690	GLN
1	C	953	ASN
1	C	1058	HIS
1	C	1108	ASN
1	C	1134	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.

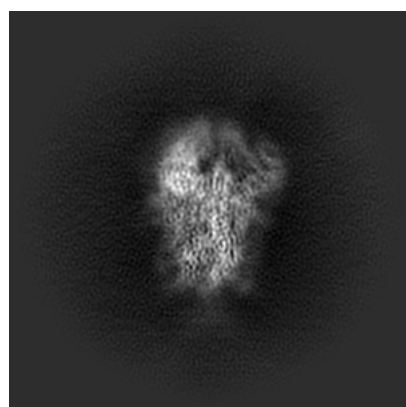
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31511. These allow visual inspection of the internal detail of the map and identification of artifacts.

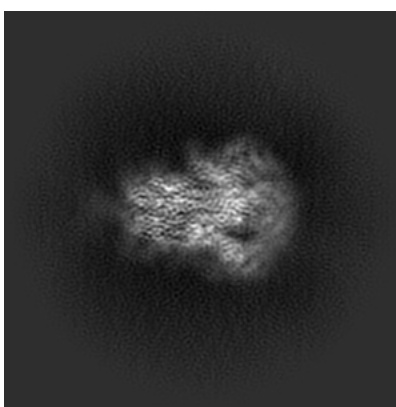
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

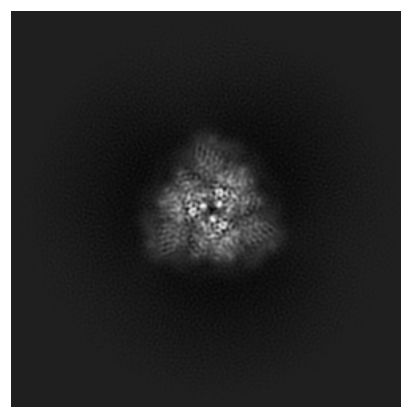
6.1.1 Primary map



X



Y

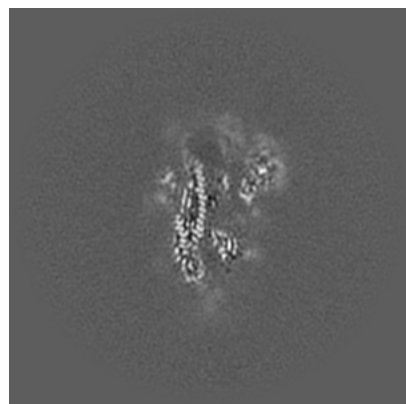


Z

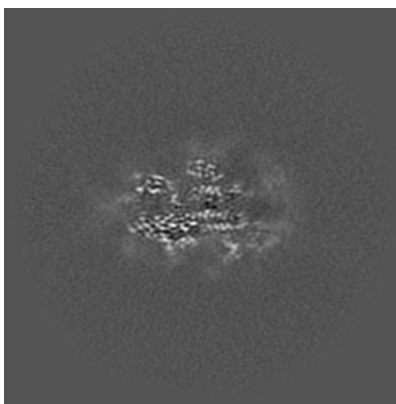
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

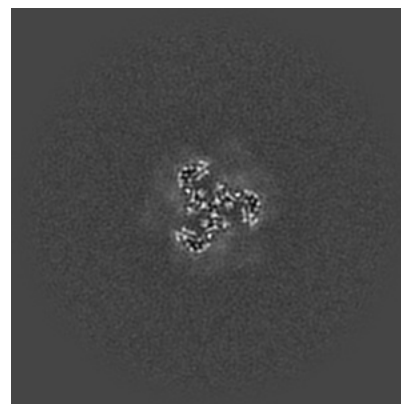
6.2.1 Primary map



X Index: 128



Y Index: 128

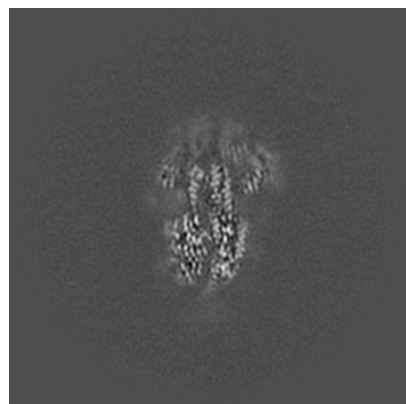


Z Index: 128

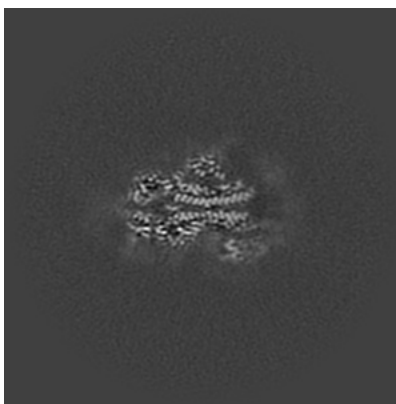
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

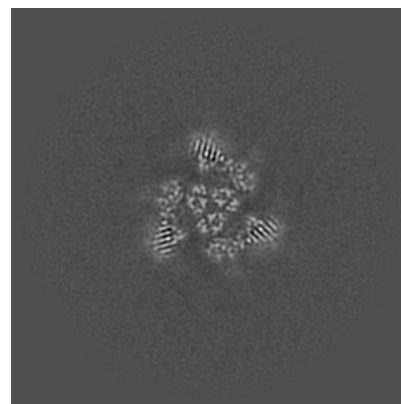
6.3.1 Primary map



X Index: 134



Y Index: 131

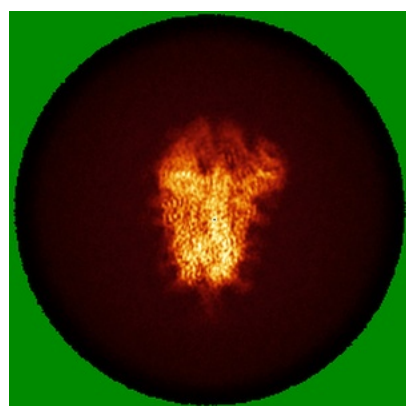


Z Index: 150

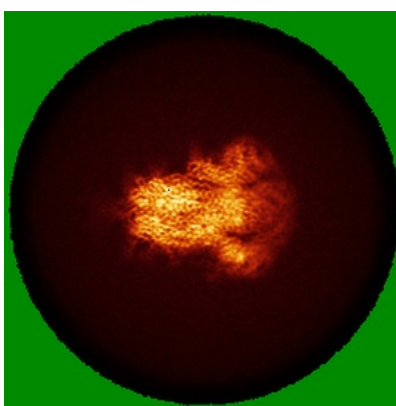
The images above show the largest variance slices of the map in three orthogonal directions.

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

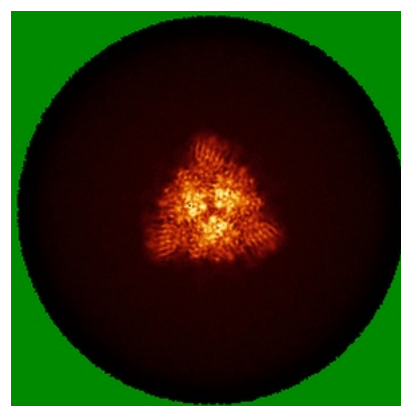
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

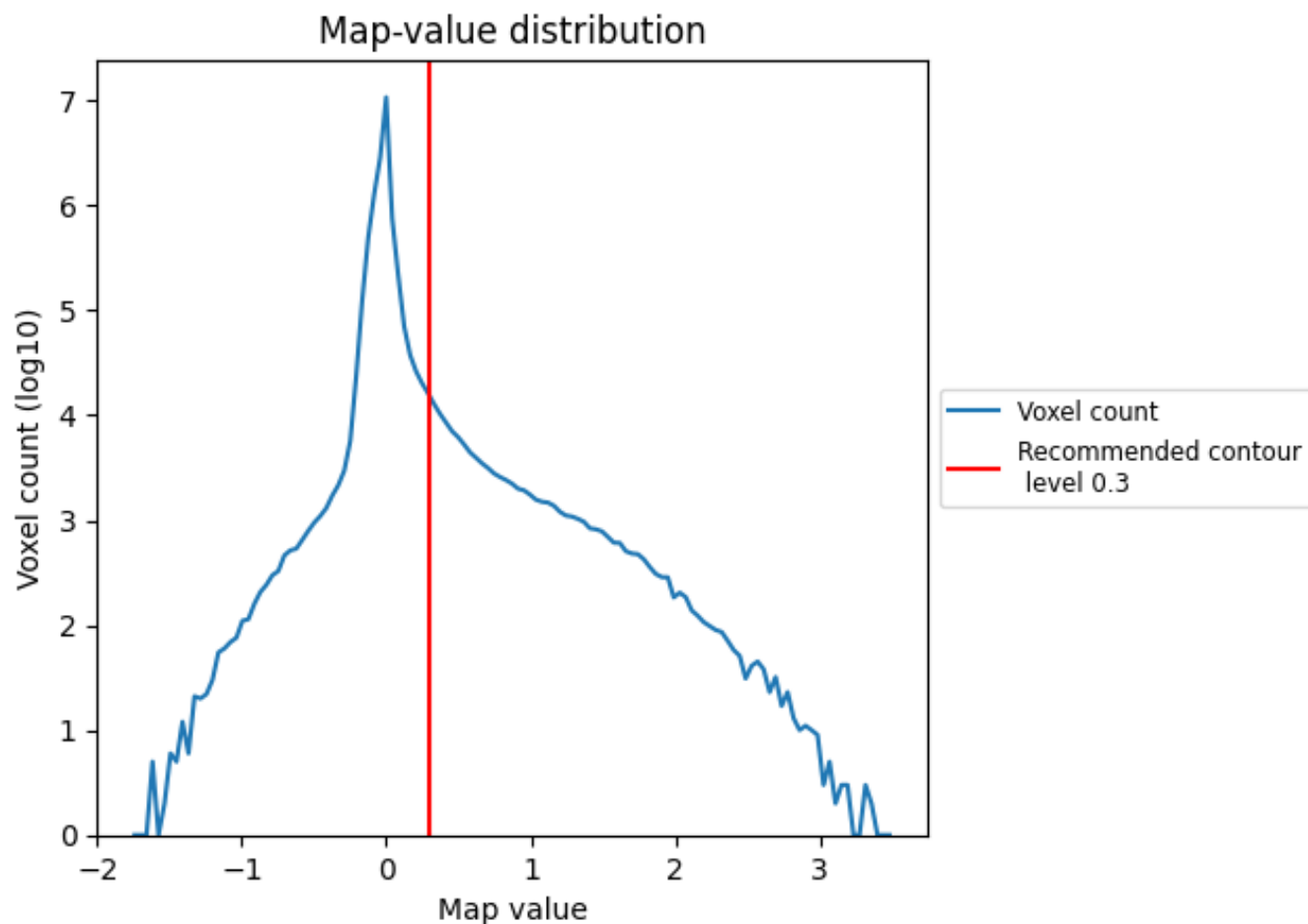
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

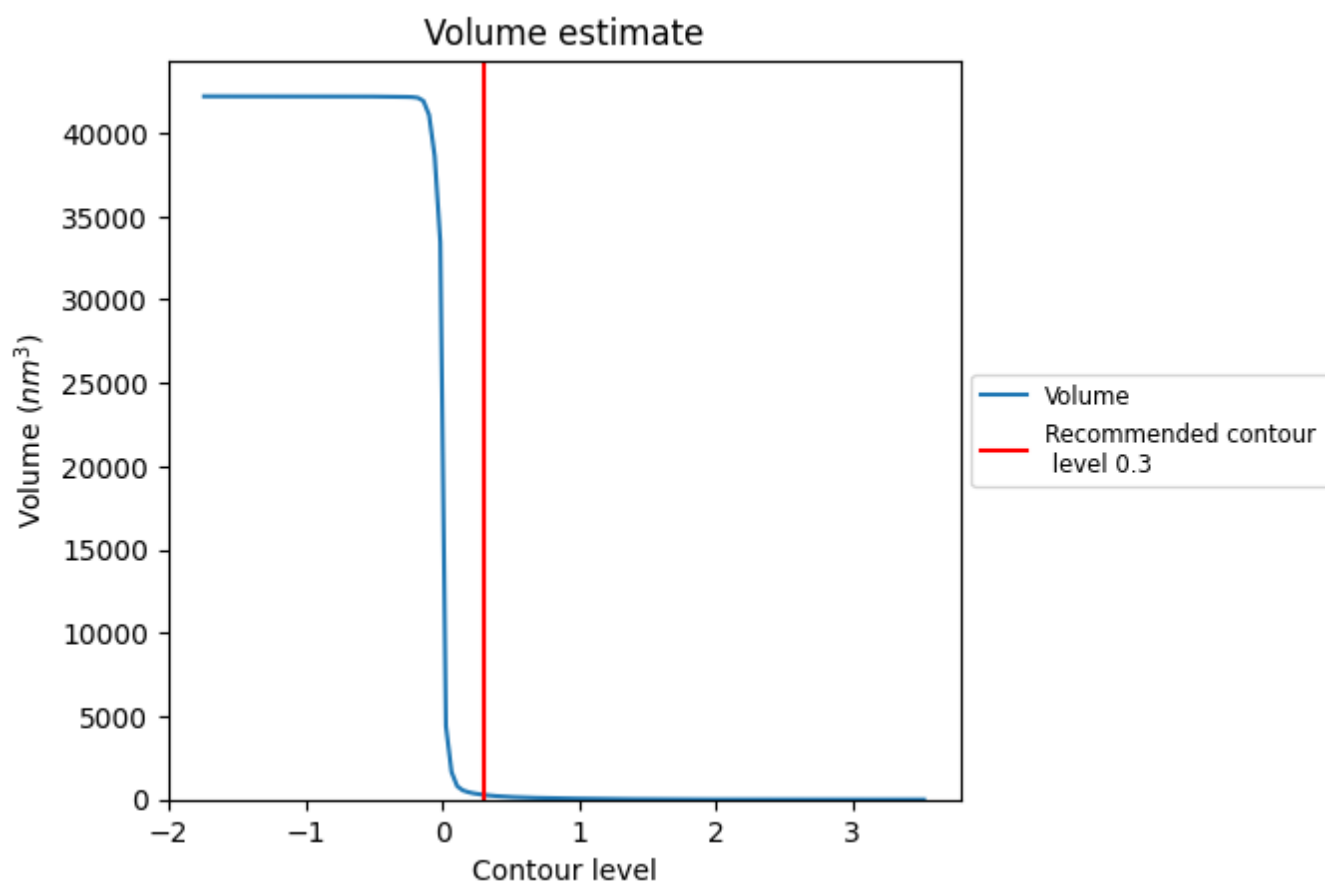
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

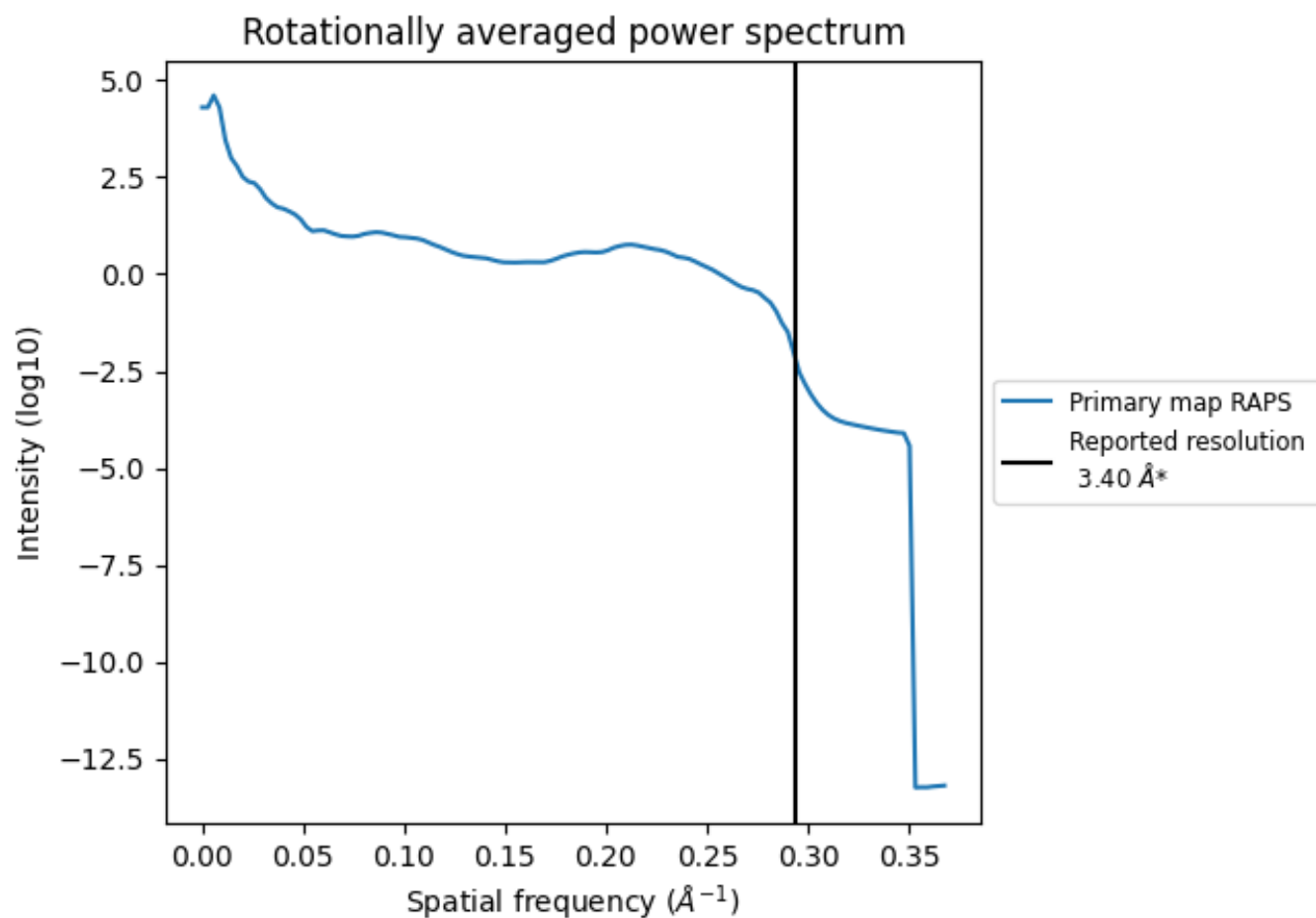
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 285 nm³; this corresponds to an approximate mass of 258 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 ⓘ

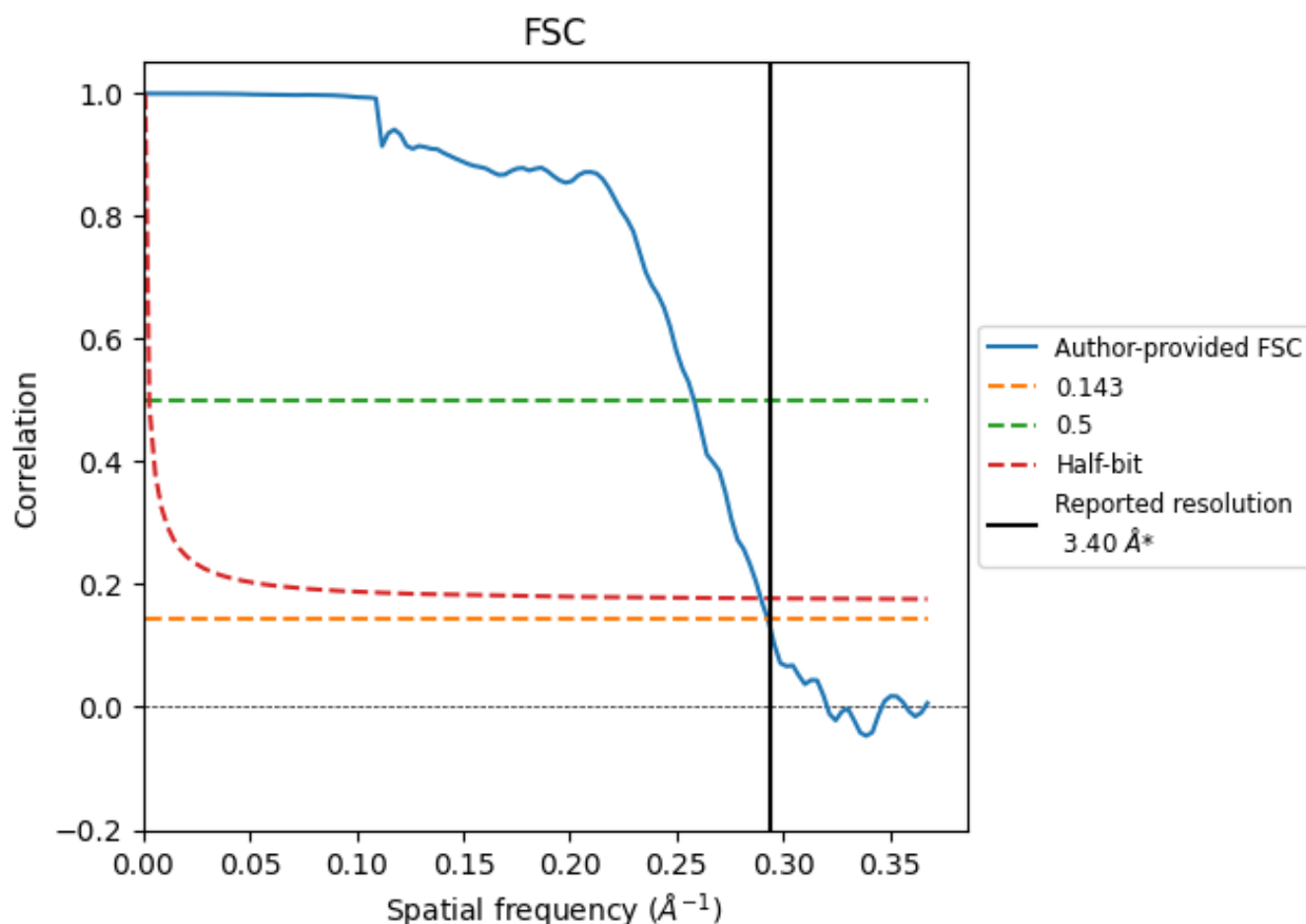


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

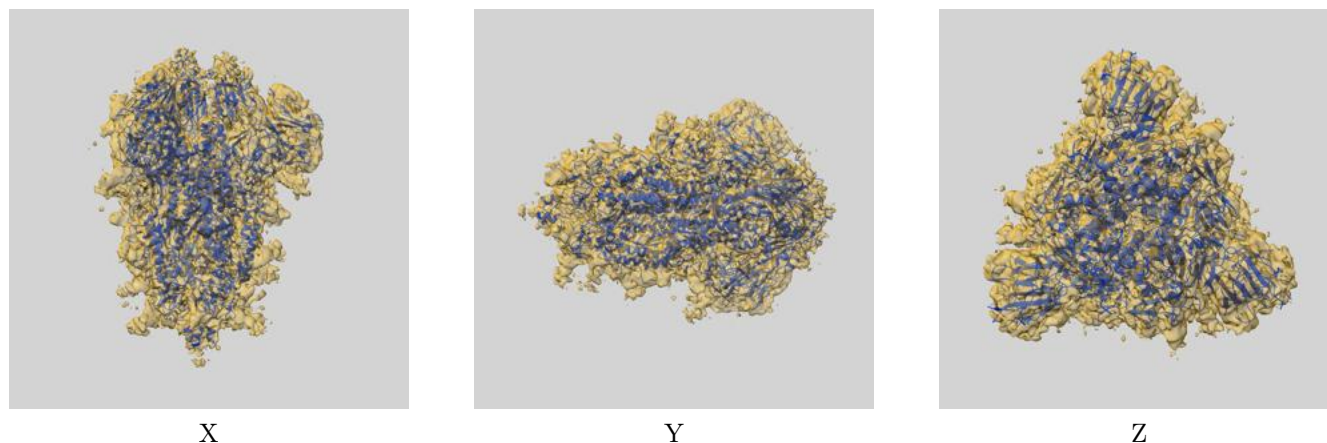
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.41	3.87	3.45
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

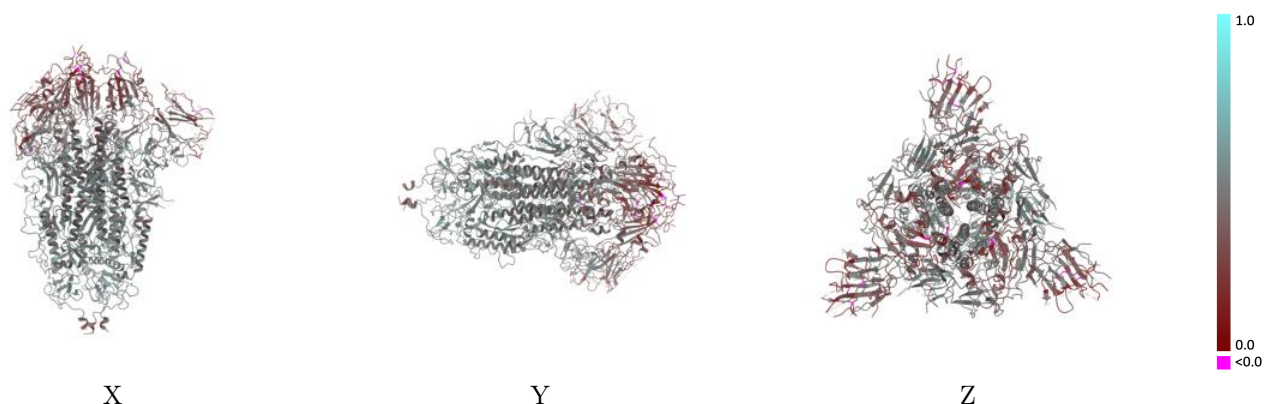
This section contains information regarding the fit between EMDB map EMD-31511 and PDB model 7FB0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



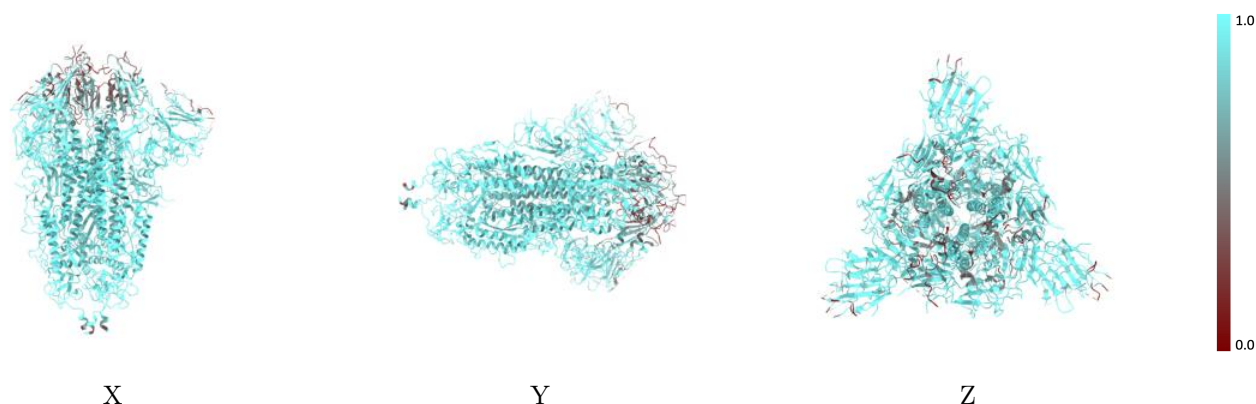
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



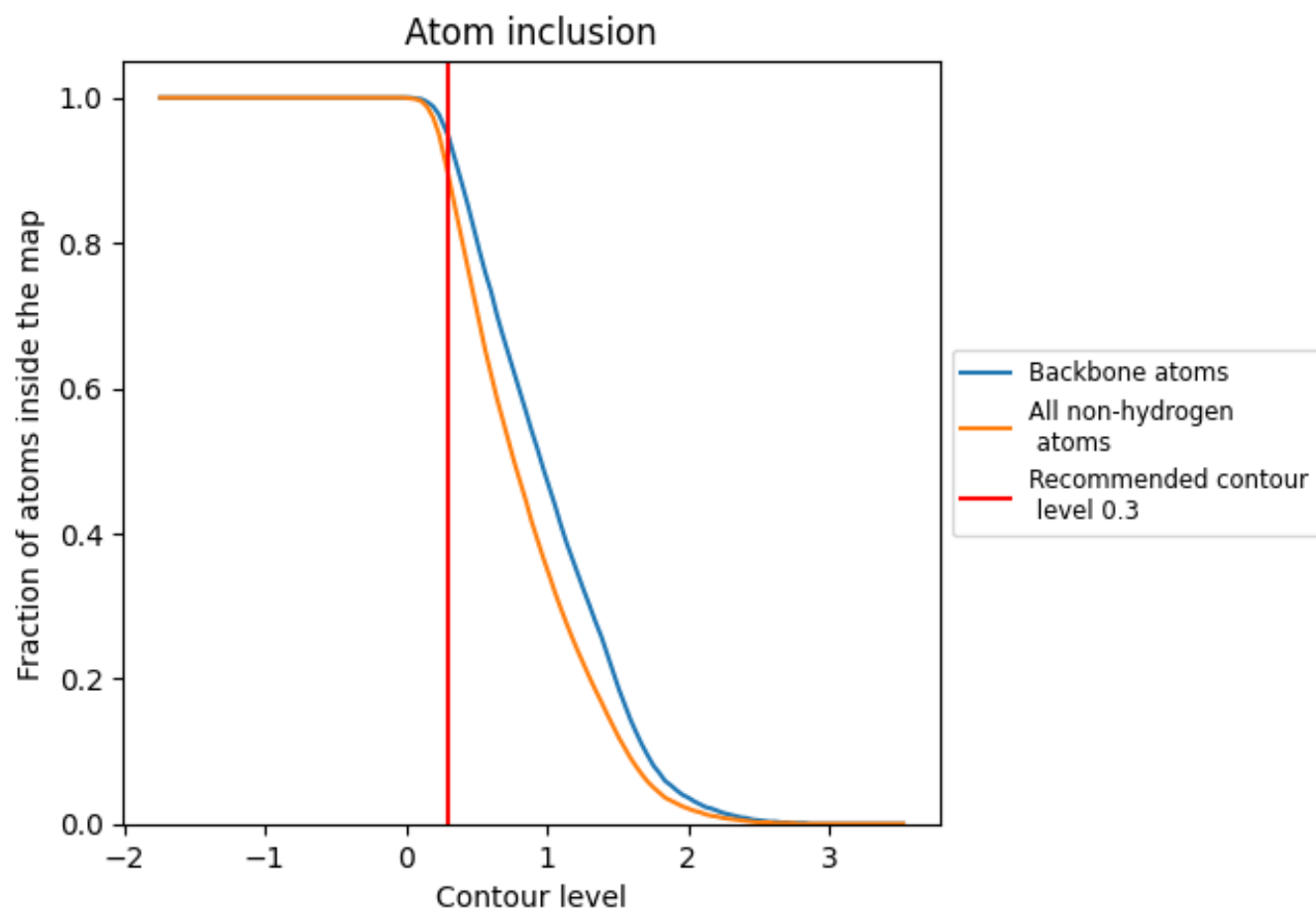
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8930	0.4360
A	0.8930	0.4350
B	0.8930	0.4360
C	0.8950	0.4360

