



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 12:59 PM JST

PDB ID : 7V3L
EMDB ID : EMD-31683
Title : MERS S ectodomain trimer in complex with neutralizing antibody 6516
Authors : Wang, X.; Zhao, J.; Wang, Z.; Wang, Y.; Zeng, J.
Deposited on : 2021-08-10
Resolution : 3.47 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

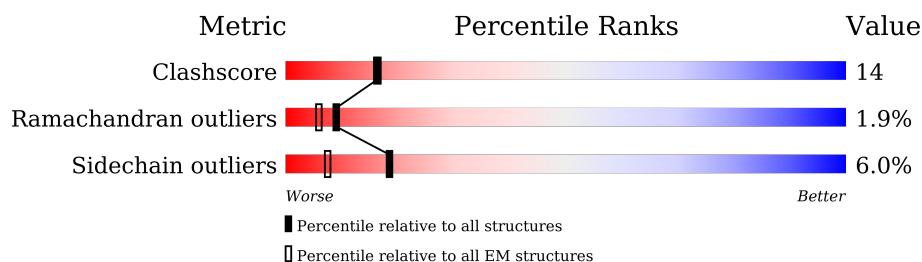
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.47 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1290	
1	B	1290	
1	C	1290	
2	D	226	
2	F	226	
2	H	226	
3	E	215	
3	G	215	

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Mol	Chain	Length	Quality of chain
3	I	215	<div><div></div><div>79%</div><div>18%</div><div>..</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36238 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	1131	Total	C	N	O	S	1	0
			8737	5550	1441	1695	51		
1	B	1135	Total	C	N	O	S	1	0
			8785	5579	1453	1702	51		
1	C	1126	Total	C	N	O	S	1	0
			8719	5536	1442	1690	51		

- Molecule 2 is a protein called antibody H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	226	Total	C	N	O	S	0	0
			1688	1063	279	337	9		
2	F	226	Total	C	N	O	S	0	0
			1688	1063	279	337	9		
2	H	226	Total	C	N	O	S	0	0
			1681	1057	279	336	9		

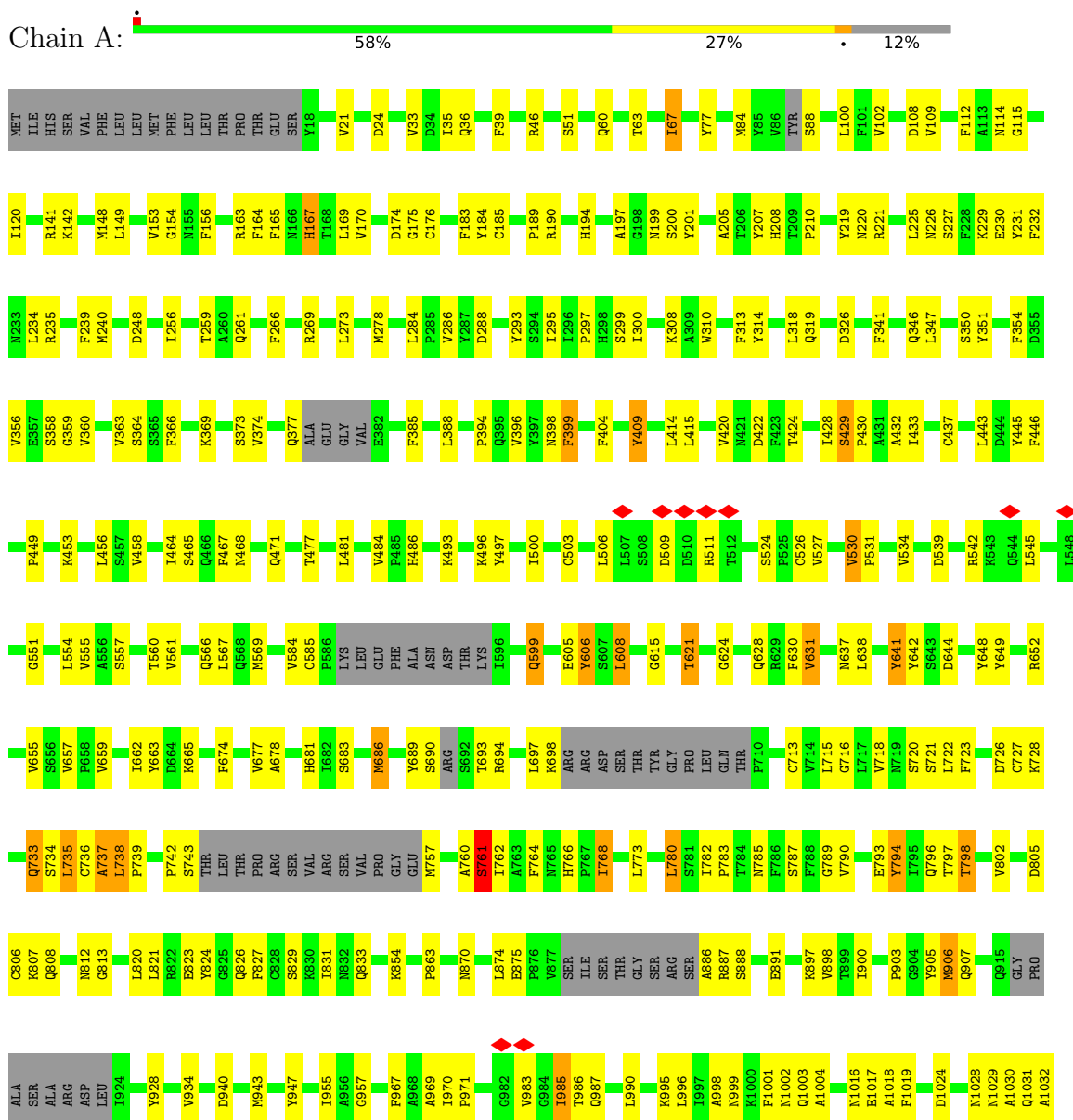
- Molecule 3 is a protein called antibody L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	214	Total	C	N	O	S	0	0
			1651	1037	277	332	5		
3	G	214	Total	C	N	O	S	0	0
			1651	1037	277	332	5		
3	I	212	Total	C	N	O	S	0	0
			1638	1030	275	328	5		

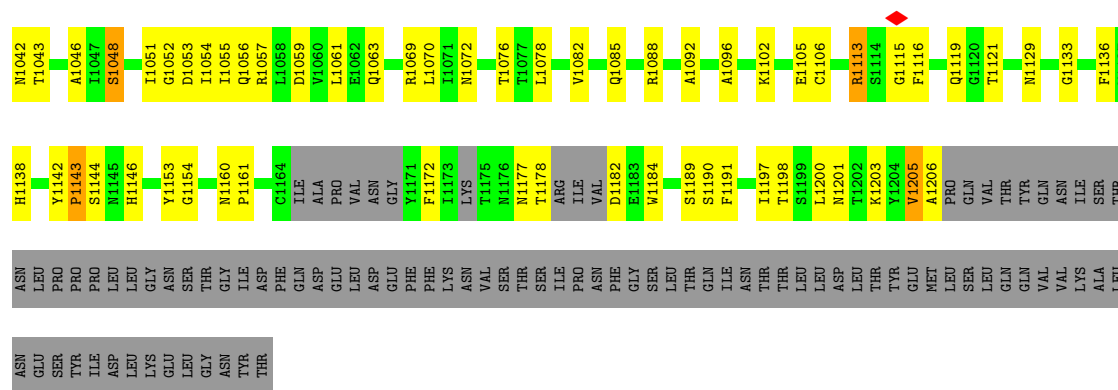
3 Residue-property plots

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.

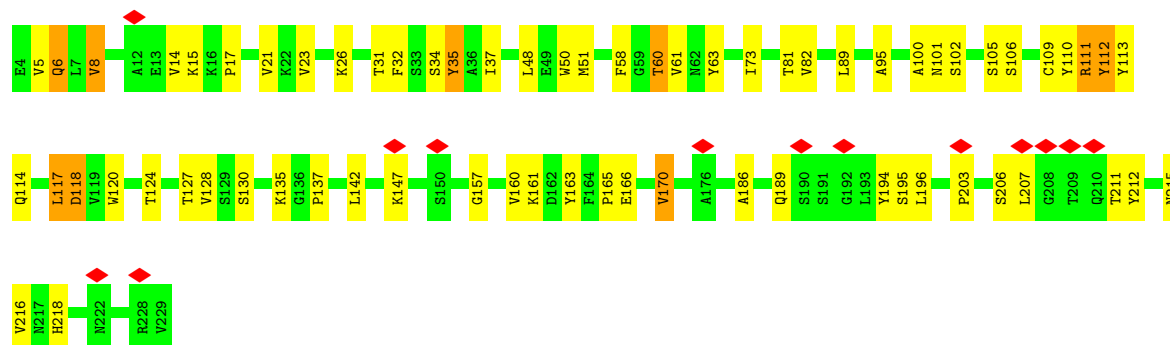
• Molecule 1: Spike glycoprotein



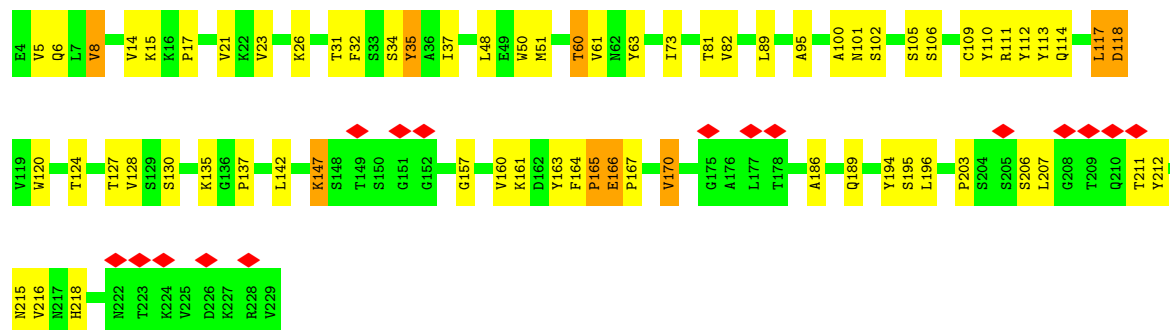




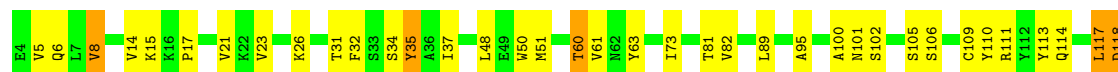
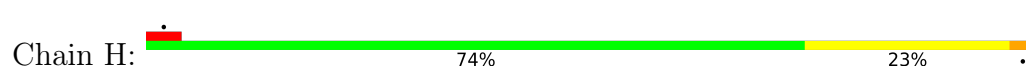
• Molecule 2: antibody H

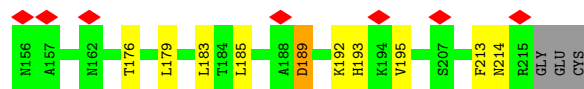


• Molecule 2: antibody H



• Molecule 2: antibody H





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1289518	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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 K3 (6k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.003	Depositor
Map size (\AA)	343.74402, 343.74402, 343.74402	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0742, 1.0742, 1.0742	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	0.60	0/8931	0.69	2/12136 (0.0%)
1	B	0.59	0/8981	0.70	3/12206 (0.0%)
1	C	0.59	0/8912	0.69	3/12105 (0.0%)
2	D	0.68	1/1729 (0.1%)	0.71	1/2357 (0.0%)
2	F	0.66	0/1729	0.70	1/2357 (0.0%)
2	H	0.66	0/1721	0.69	0/2346
3	E	0.65	0/1687	0.70	0/2291
3	G	0.65	0/1687	0.70	0/2291
3	I	0.65	0/1674	0.70	0/2274
All	All	0.61	1/37051 (0.0%)	0.69	10/50363 (0.0%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	111	ARG	C-N	6.06	1.48	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	761	SER	N-CA-C	6.42	128.33	111.00
1	C	788	PHE	CB-CA-C	-6.16	98.08	110.40
1	A	641	TYR	CB-CA-C	-5.65	99.09	110.40
2	D	111	ARG	O-C-N	5.61	131.67	122.70
1	C	642	TYR	CB-CA-C	5.15	120.70	110.40
2	F	165	PRO	N-CA-C	5.15	125.48	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1167	PRO	N-CA-C	5.13	125.44	112.10
1	B	1186	TYR	CB-CA-C	-5.11	100.18	110.40
1	C	906	MET	CA-CB-CG	5.11	121.98	113.30
1	B	617	PHE	CB-CA-C	-5.06	100.28	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51[A]	SER	Mainchain
1	A	51[B]	SER	Mainchain

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	8737	0	8422	264	0
1	B	8785	0	8501	302	0
1	C	8719	0	8414	311	0
2	D	1688	0	1636	39	0
2	F	1688	0	1636	39	0
2	H	1681	0	1629	35	0
3	E	1651	0	1615	26	0
3	G	1651	0	1615	24	0
3	I	1638	0	1606	23	0
All	All	36238	0	35074	999	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 14.

All (999) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ILE:H	1:A:1181:VAL:HG21	1.50	0.77
1:B:189:PRO:HB2	1:B:197:ALA:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:SER:H	1:A:686:MET:HG2	1.50	0.77
1:C:990:LEU:HD21	1:C:1184:TRP:HB2	1.67	0.76
1:B:1040:LEU:HD22	1:B:1077:THR:HB	1.67	0.76
1:A:738:LEU:HG	1:B:940:ASP:HB2	1.67	0.75
1:C:27:LYS:O	1:C:190:ARG:NH2	2.18	0.75
1:C:35:ILE:HD11	1:C:202:THR:HB	1.69	0.75
1:C:797:THR:HB	1:C:1133:GLY:HA2	1.68	0.74
1:A:422:ASP:HB2	1:A:481:LEU:HB2	1.68	0.74
1:C:1172:PHE:HB2	1:C:1177:ASN:HB2	1.69	0.74
1:B:206:THR:HG23	1:B:298:HIS:ND1	2.02	0.73
1:B:1123:ILE:HG22	1:B:1124:VAL:HG23	1.70	0.73
1:B:204:PHE:HD1	1:B:296:ILE:HG23	1.53	0.73
1:A:738:LEU:HD13	1:A:762:ILE:HG12	1.70	0.73
1:C:722:LEU:CD1	1:C:724:VAL:HG22	2.20	0.72
1:C:893:LEU:HD11	1:C:897:LYS:HE3	1.71	0.72
1:C:789:GLY:HA3	1:C:1004:ALA:HB1	1.71	0.72
1:A:928:TYR:HB3	1:C:653:ALA:HB3	1.70	0.71
1:A:524:SER:HB3	1:A:527:VAL:HG13	1.73	0.71
1:A:77:TYR:HD1	1:A:319:GLN:HE22	1.38	0.71
1:C:196:PRO:HG2	1:C:232:PHE:CZ	2.25	0.71
1:B:422:ASP:HB2	1:B:481:LEU:HB2	1.72	0.70
1:C:524:SER:HB3	1:C:527:VAL:HG13	1.73	0.70
1:A:100:LEU:HD23	1:A:299:SER:HB3	1.74	0.70
1:A:184:TYR:OH	1:A:288:ASP:OD2	2.08	0.70
1:C:100:LEU:HD22	1:C:299:SER:HB3	1.73	0.70
1:A:437:CYS:HB2	1:A:585:CYS:HA	1.74	0.69
1:B:174:ASP:OD1	1:B:175:GLY:N	2.26	0.69
1:C:174:ASP:OD1	1:C:175:GLY:N	2.26	0.69
1:B:1058:LEU:HB3	1:B:1062:GLU:HG2	1.73	0.69
1:C:632:TYR:HA	1:C:638:LEU:HA	1.74	0.69
1:A:189:PRO:HG2	1:A:197:ALA:HB2	1.73	0.69
1:A:194:HIS:N	1:A:199:ASN:O	2.25	0.69
1:B:437:CYS:HB2	1:B:585:CYS:HA	1.74	0.69
1:B:148:MET:HG3	1:B:170:VAL:HG22	1.74	0.69
1:B:524:SER:HB3	1:B:527:VAL:HG13	1.73	0.69
1:A:240:MET:SD	1:A:240:MET:N	2.67	0.68
1:A:1160:ASN:HB2	1:A:1198:THR:HG21	1.75	0.68
1:A:599:GLN:HE21	1:A:649:TYR:HD2	1.42	0.68
1:B:205:ALA:HB2	1:B:297:PRO:HG2	1.76	0.68
1:C:212:THR:O	1:C:215:SER:OG	2.11	0.68
1:C:437:CYS:HB2	1:C:585:CYS:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1085:GLN:OE1	1:C:1088:ARG:NH2	2.27	0.68
1:B:1165:ILE:HB	1:B:1192:TYR:HE1	1.58	0.68
1:C:101:PHE:HE2	1:C:131:ILE:HG22	1.58	0.68
2:F:14:VAL:HG12	2:F:127:THR:HB	1.76	0.68
1:C:642:TYR:C	1:C:644:ASP:H	1.96	0.67
1:B:58:TYR:OH	1:B:331:GLY:O	2.11	0.67
1:B:1168:VAL:HG13	1:C:962:ALA:HA	1.76	0.67
1:C:429:SER:HB3	1:C:432:ALA:HB2	1.75	0.67
1:B:631:VAL:HG22	1:B:640:GLY:HA2	1.76	0.67
1:A:789:GLY:HA3	1:A:1004:ALA:HB1	1.74	0.67
1:B:765:ASN:HD22	1:C:946:ALA:CB	2.07	0.67
1:C:58:TYR:OH	1:C:331:GLY:O	2.10	0.67
1:B:765:ASN:HD21	1:C:946:ALA:C	1.98	0.67
1:A:727:CYS:HA	1:A:761:SER:HB2	1.77	0.67
1:C:366:PHE:HB3	1:C:689:TYR:HB3	1.77	0.67
1:A:295:ILE:HD11	1:A:313:PHE:CZ	2.30	0.67
2:H:14:VAL:HG12	2:H:127:THR:HB	1.76	0.67
1:A:415:LEU:HD23	1:A:420:VAL:HG11	1.77	0.66
2:D:14:VAL:HG12	2:D:127:THR:HB	1.76	0.66
1:B:415:LEU:HD23	1:B:420:VAL:HG11	1.77	0.66
1:B:605:GLU:HA	1:B:614:ARG:HA	1.78	0.66
1:C:622:ALA:HA	1:C:626:ARG:HH12	1.61	0.66
3:E:50:LEU:HB3	3:E:51:ILE:HD12	1.78	0.66
1:C:690:SER:O	1:C:694:ARG:HG3	1.94	0.66
1:A:1181:VAL:HG13	1:A:1182:ASP:H	1.60	0.66
1:B:620:CYS:HB2	1:B:648:TYR:CE2	2.31	0.66
3:E:51:ILE:HG13	3:E:57:LEU:HD13	1.78	0.65
1:A:67:ILE:HG13	1:C:634:ALA:HB2	1.78	0.65
1:B:496:LYS:HE3	1:B:560:THR:HG22	1.79	0.65
1:A:399:PHE:HA	1:A:446:PHE:HB3	1.78	0.65
1:A:990:LEU:HD11	1:A:1183:GLU:HB2	1.76	0.65
1:C:91:HIS:O	1:C:98:GLN:N	2.23	0.65
3:I:51:ILE:HG13	3:I:57:LEU:HD13	1.78	0.65
1:C:183:PHE:HB3	1:C:240:MET:HG2	1.79	0.65
1:A:190:ARG:NE	1:A:230:GLU:O	2.30	0.65
1:B:797:THR:HB	1:B:1133:GLY:HA2	1.78	0.65
1:B:809:TYR:OH	1:B:1040:LEU:HD23	1.97	0.65
1:C:257:THR:HG22	1:C:266:PHE:HE2	1.63	0.64
1:C:415:LEU:HD23	1:C:420:VAL:HG11	1.77	0.64
1:A:449:PRO:HG3	1:A:561:VAL:HG11	1.79	0.64
1:C:722:LEU:CD1	1:C:724:VAL:CG2	2.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:50:TRP:CZ3	3:G:99:GLN:HA	2.33	0.64
1:A:1072:ASN:O	1:A:1076:THR:HG23	1.98	0.64
1:C:399:PHE:HA	1:C:446:PHE:HB3	1.79	0.64
1:C:804:VAL:HA	1:C:932:TYR:HA	1.78	0.64
1:A:1201:ASN:ND2	1:A:1206:ALA:O	2.31	0.64
1:C:496:LYS:HE3	1:C:560:THR:HG22	1.79	0.64
1:B:399:PHE:HA	1:B:446:PHE:HB3	1.78	0.64
1:B:620:CYS:HB2	1:B:648:TYR:HE2	1.61	0.64
1:C:449:PRO:HG3	1:C:561:VAL:HG11	1.79	0.64
2:H:26:LYS:HG2	2:H:81:THR:HG22	1.80	0.64
1:A:1199:SER:H	1:A:1205:VAL:HG22	1.62	0.64
1:B:449:PRO:HG3	1:B:561:VAL:HG11	1.79	0.64
2:D:50:TRP:CZ3	3:E:99:GLN:HA	2.33	0.64
1:A:295:ILE:HD11	1:A:313:PHE:HZ	1.63	0.63
1:C:722:LEU:HD13	1:C:724:VAL:HG22	1.80	0.63
1:C:798:THR:HA	1:C:1092:ALA:HB1	1.80	0.63
3:G:51:ILE:HG13	3:G:57:LEU:HD13	1.79	0.63
1:A:808:GLN:NE2	1:C:365:SER:H	1.96	0.63
1:A:1115:GLY:HA3	1:B:1104:ASN:HD22	1.62	0.63
1:B:854:LYS:HD2	1:B:855:SER:N	2.13	0.63
1:A:176:CYS:HB2	1:A:219:TYR:HD2	1.64	0.63
1:A:493:LYS:HB3	1:A:567:LEU:HD21	1.81	0.63
1:A:1160:ASN:N	1:A:1161:PRO:HD3	2.14	0.63
1:A:496:LYS:HE3	1:A:560:THR:HG22	1.79	0.63
1:B:185:CYS:HB3	1:B:237:CYS:HA	1.81	0.63
2:D:26:LYS:HG2	2:D:81:THR:HG22	1.80	0.63
2:H:50:TRP:CZ3	3:I:99:GLN:HA	2.33	0.63
1:C:1160:ASN:HB3	1:C:1198:THR:HG21	1.80	0.62
1:A:782:ILE:HD11	1:A:1180:ILE:HA	1.80	0.62
1:B:346:GLN:HE21	1:B:694:ARG:HD3	1.64	0.62
1:B:420:VAL:HG22	2:F:60:THR:HG21	1.81	0.62
1:C:364:SER:HB2	1:C:691:ARG:HH21	1.63	0.62
1:C:493:LYS:HB3	1:C:567:LEU:HD21	1.81	0.62
1:B:33:VAL:HG22	1:B:100:LEU:HB2	1.80	0.62
1:B:493:LYS:HB3	1:B:567:LEU:HD21	1.81	0.62
1:B:638:LEU:C	1:B:640:GLY:H	2.02	0.62
1:C:679:CYS:HA	1:C:717:LEU:HD13	1.80	0.62
1:A:205:ALA:H	1:A:231:TYR:HE2	1.46	0.62
1:B:735:LEU:HB2	1:B:741:THR:HG22	1.81	0.62
1:A:985:ILE:HB	1:A:1181:VAL:HG11	1.81	0.62
1:C:50:VAL:HG22	1:C:78:GLN:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:PHE:HA	1:B:231:TYR:CE1	2.35	0.62
1:B:652:ARG:NH1	1:C:915:GLN:O	2.33	0.62
1:A:797:THR:HB	1:A:1133:GLY:HA2	1.82	0.61
1:C:192:GLY:O	1:C:198:GLY:HA3	1.99	0.61
1:C:906:MET:SD	1:C:907:GLN:HG3	2.39	0.61
1:C:430:PRO:HD2	2:H:105:SER:HB3	1.81	0.61
1:B:738:LEU:HD13	1:B:762:ILE:HG23	1.82	0.61
1:B:887:ARG:HD2	1:B:891:GLU:HG2	1.81	0.61
1:C:27:LYS:HD2	1:C:230:GLU:HG2	1.83	0.61
2:F:8:VAL:HG13	2:F:26:LYS:HB2	1.83	0.61
2:F:26:LYS:HG2	2:F:81:THR:HG22	1.80	0.61
1:A:1154:GLY:HA3	1:A:1205:VAL:HG12	1.81	0.61
3:G:195:VAL:HG23	3:G:214:ASN:HB3	1.83	0.61
1:B:1164:CYS:O	1:B:1165:ILE:HG13	2.01	0.61
2:H:8:VAL:HG13	2:H:26:LYS:HB2	1.83	0.61
1:C:912:CYS:HB2	1:C:928:TYR:OH	2.00	0.61
1:C:429:SER:CB	2:H:106:SER:HA	2.31	0.60
1:B:46:ARG:HH22	1:B:123:ALA:HB2	1.66	0.60
1:B:1201:ASN:HB2	1:B:1206:ALA:HB3	1.82	0.60
1:B:190:ARG:NH1	1:B:233:ASN:OD1	2.33	0.60
1:B:205:ALA:HA	1:B:296:ILE:HG22	1.83	0.60
1:C:420:VAL:HG22	2:H:60:THR:HG21	1.81	0.60
3:I:195:VAL:HG23	3:I:214:ASN:HB3	1.83	0.60
1:A:437:CYS:HB2	1:A:584:VAL:O	2.01	0.60
1:A:112:PHE:CE1	1:A:115:GLY:HA2	2.37	0.60
1:B:97:PRO:HB3	1:B:301:ARG:HB3	1.83	0.60
1:B:437:CYS:HB2	1:B:584:VAL:O	2.01	0.60
3:E:117:PRO:HB3	3:E:143:PHE:HB3	1.83	0.60
1:A:657:VAL:CG1	1:A:677:VAL:HG11	2.32	0.60
3:I:117:PRO:HB3	3:I:143:PHE:HB3	1.83	0.60
1:A:621:THR:HA	1:A:648:TYR:CD2	2.36	0.59
1:B:205:ALA:N	1:B:231:TYR:OH	2.31	0.59
1:C:140:ILE:HA	1:C:309:ALA:HB3	1.85	0.59
1:C:207:TYR:HA	1:C:298:HIS:CD2	2.38	0.59
2:D:8:VAL:HG13	2:D:26:LYS:HB2	1.83	0.59
1:B:1040:LEU:CD2	1:B:1077:THR:HB	2.31	0.59
1:C:155:ASN:HB2	1:C:159:GLY:HA2	1.83	0.59
1:C:196:PRO:HA	1:C:201:TYR:CD1	2.37	0.59
3:G:117:PRO:HB3	3:G:143:PHE:HB3	1.83	0.59
1:B:188:GLU:HB3	1:B:233:ASN:HB2	1.84	0.59
1:C:437:CYS:HB2	1:C:584:VAL:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:195:VAL:HG23	3:E:214:ASN:HB3	1.83	0.59
1:A:1115:GLY:HA3	1:B:1104:ASN:ND2	2.17	0.59
1:B:741:THR:HA	1:B:759:LEU:HA	1.85	0.59
1:C:181:ARG:HD2	1:C:225:LEU:HD13	1.83	0.59
1:C:987:GLN:H	1:C:990:LEU:HD12	1.68	0.59
2:H:186:ALA:HB1	2:H:194:TYR:HB3	1.85	0.59
1:A:793:GLU:HA	1:A:1018:ALA:HB2	1.84	0.59
1:A:678:ALA:HB3	1:A:681:HIS:HB2	1.84	0.58
1:A:906:MET:HB2	1:C:713:CYS:O	2.02	0.58
1:A:239:PHE:CE1	1:A:284:LEU:HB3	2.39	0.58
1:B:106:SER:HB2	1:B:107:GLN:NE2	2.19	0.58
1:B:188:GLU:OE2	1:B:235:ARG:NH2	2.36	0.58
1:B:678:ALA:C	1:B:680:GLU:H	2.07	0.58
1:C:618:GLN:O	1:C:649:TYR:HA	2.03	0.58
1:A:780:LEU:HD11	1:A:1172:PHE:HE1	1.69	0.58
1:C:954:SER:HA	1:C:967:PHE:CE2	2.38	0.58
1:B:87:TYR:OH	1:B:145:PRO:HA	2.03	0.58
1:B:1165:ILE:HB	1:B:1192:TYR:CE1	2.37	0.58
1:C:366:PHE:HB3	1:C:689:TYR:CB	2.33	0.58
2:H:17:PRO:HD2	2:H:130:SER:HA	1.85	0.58
1:B:826:GLN:O	1:B:830:LYS:HG2	2.04	0.58
1:C:998:ALA:O	1:C:1002:ASN:ND2	2.37	0.58
1:C:1054:ILE:HD12	1:C:1057:ARG:HH22	1.67	0.58
2:D:17:PRO:HD2	2:D:130:SER:HA	1.86	0.58
1:A:420:VAL:HG22	2:D:60:THR:HG21	1.85	0.57
1:A:621:THR:HA	1:A:648:TYR:HD2	1.69	0.57
1:B:102:VAL:HG21	1:B:203:SER:HB3	1.85	0.57
1:B:304:GLN:HG2	1:B:307:ARG:HH11	1.68	0.57
1:C:234:LEU:O	1:C:235:ARG:NH1	2.32	0.57
1:A:599:GLN:HB3	1:A:649:TYR:HE2	1.69	0.57
2:F:166:GLU:HB2	2:F:194:TYR:CD2	2.40	0.57
1:B:1029:ASN:OD1	1:B:1030:ALA:N	2.37	0.57
1:A:903:PRO:HG2	1:A:934:VAL:HG11	1.87	0.57
2:F:17:PRO:HD2	2:F:130:SER:HA	1.86	0.57
1:A:154:GLY:HA3	1:A:165:PHE:HE2	1.69	0.57
1:B:204:PHE:CE1	1:B:296:ILE:HG12	2.39	0.57
1:C:130:VAL:HB	1:C:136:THR:HB	1.85	0.57
1:B:652:ARG:NH2	1:C:913:MET:SD	2.77	0.57
1:B:765:ASN:ND2	1:C:946:ALA:CB	2.68	0.57
1:C:259:THR:OG1	1:C:264:HIS:NE2	2.24	0.57
1:C:357:GLU:HA	1:C:665:LYS:HD2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:189:ASP:HA	3:E:192:LYS:HD3	1.87	0.57
1:A:346:GLN:NE2	1:A:694:ARG:HH12	2.03	0.56
1:A:359:GLY:HA2	1:A:733:GLN:HB2	1.87	0.56
1:A:1143:PRO:HG3	1:B:965:SER:HB3	1.86	0.56
1:C:192:GLY:O	1:C:195:CYS:HB2	2.05	0.56
1:B:23:PRO:O	1:B:229:LYS:NZ	2.30	0.56
1:C:37:GLN:N	1:C:37:GLN:OE1	2.34	0.56
1:C:388:LEU:HD22	1:C:443:LEU:HD21	1.87	0.56
1:C:996:LEU:C	1:C:998:ALA:N	2.58	0.56
1:B:324:LEU:HD12	1:B:349:CYS:HA	1.86	0.56
1:C:471:GLN:HB3	1:C:477:THR:HG21	1.87	0.56
1:C:1053:ASP:H	1:C:1057:ARG:HH21	1.53	0.56
1:A:176:CYS:HB2	1:A:219:TYR:CD2	2.41	0.56
1:A:715:LEU:HD11	1:B:936:PRO:HG2	1.87	0.56
1:B:732:GLY:C	1:B:734:SER:N	2.57	0.56
1:B:1053:ASP:HB3	1:B:1063:GLN:HG3	1.88	0.56
1:C:409:TYR:CE2	1:C:584:VAL:HG12	2.41	0.56
1:A:388:LEU:HD22	1:A:443:LEU:HD21	1.87	0.56
1:A:471:GLN:HB3	1:A:477:THR:HG21	1.87	0.56
1:B:985:ILE:HG12	1:B:1168:VAL:CG2	2.35	0.56
1:B:43:THR:HG22	1:B:45:PRO:HD3	1.88	0.56
1:B:471:GLN:HB3	1:B:477:THR:HG21	1.87	0.56
1:C:64:TYR:CD2	1:C:67:ILE:HD11	2.41	0.56
1:C:722:LEU:HB3	1:C:758:ARG:HA	1.87	0.56
1:A:308:LYS:O	1:A:310:TRP:NE1	2.39	0.56
1:B:204:PHE:CD1	1:B:296:ILE:HG23	2.38	0.56
1:B:409:TYR:CE2	1:B:584:VAL:HG12	2.41	0.56
1:B:618:GLN:O	1:B:649:TYR:HA	2.05	0.56
1:C:189:PRO:HB2	1:C:197:ALA:HB2	1.88	0.56
1:C:229:LYS:HE2	1:C:234:LEU:HD12	1.88	0.56
1:A:409:TYR:CE2	1:A:584:VAL:HG12	2.41	0.56
1:B:875:GLU:HG3	1:B:886:ALA:HB3	1.87	0.56
1:A:429:SER:HB3	1:A:432:ALA:HB2	1.87	0.56
1:B:388:LEU:HD22	1:B:443:LEU:HD21	1.87	0.56
1:A:189:PRO:HA	1:A:232:PHE:HA	1.88	0.55
1:C:373:SER:HA	1:C:605:GLU:O	2.05	0.55
1:C:648:TYR:HE2	1:C:650:CYS:HB3	1.69	0.55
3:I:189:ASP:HA	3:I:192:LYS:HD3	1.87	0.55
1:A:969:ALA:HB1	1:C:772:GLN:HA	1.88	0.55
1:C:207:TYR:OH	1:C:230:GLU:OE2	2.24	0.55
1:C:374:VAL:HG22	1:C:598:SER:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:CYS:HB2	1:A:234:LEU:HD22	1.88	0.55
1:A:655:VAL:HG22	1:B:909:TYR:CE2	2.41	0.55
1:B:605:GLU:HG3	1:B:614:ARG:HG2	1.89	0.55
1:C:740:ASP:HB3	1:C:761:SER:HB3	1.88	0.55
1:A:404:PHE:HE2	1:A:443:LEU:HB3	1.72	0.55
1:B:765:ASN:HD22	1:C:946:ALA:HB1	1.71	0.55
1:C:631:VAL:HG12	1:C:640:GLY:O	2.07	0.55
1:C:1113:ARG:HE	1:C:1115:GLY:H	1.53	0.55
3:G:189:ASP:HA	3:G:192:LYS:HD3	1.87	0.55
1:A:780:LEU:HD23	1:A:1151:SER:OG	2.06	0.55
1:A:999:ASN:O	1:A:1003:GLN:HG3	2.07	0.55
2:D:37:ILE:HG13	2:D:82:VAL:HG21	1.89	0.55
1:C:697:LEU:HG	1:C:698:LYS:H	1.72	0.55
1:C:957:GLY:HA3	1:C:967:PHE:CD2	2.42	0.55
2:F:37:ILE:HG13	2:F:82:VAL:HG21	1.89	0.55
1:A:1016:ASN:HB3	1:A:1019:PHE:HB3	1.88	0.55
1:B:429:SER:HB3	1:B:432:ALA:HB2	1.89	0.55
1:B:679:CYS:HA	1:B:717:LEU:HD22	1.89	0.55
1:C:92:ALA:HA	1:C:97:PRO:HA	1.89	0.55
3:E:9:GLN:HE21	3:E:24:ILE:HD11	1.72	0.55
1:A:141:ARG:HH21	1:A:310:TRP:HH2	1.55	0.54
1:A:987:GLN:HE21	1:A:1192:TYR:HE1	1.53	0.54
1:B:91:HIS:HB2	1:B:98:GLN:HB2	1.88	0.54
1:C:404:PHE:HE2	1:C:443:LEU:HB3	1.72	0.54
3:I:9:GLN:HE21	3:I:24:ILE:HD11	1.72	0.54
1:C:642:TYR:C	1:C:644:ASP:N	2.60	0.54
2:F:111:ARG:C	2:F:113:TYR:H	2.11	0.54
3:I:51:ILE:HD12	3:I:51:ILE:H	1.71	0.54
1:A:358:SER:HB3	1:A:665:LYS:HG2	1.89	0.54
1:A:428:ILE:HG13	1:A:432:ALA:HB3	1.90	0.54
1:A:736:CYS:HB3	1:B:936:PRO:HB2	1.89	0.54
1:C:818:GLU:O	1:C:822:ARG:HG3	2.07	0.54
1:C:1048:SER:HB3	1:C:1070:LEU:HD12	1.89	0.54
1:B:850:PHE:CD1	1:B:947:TYR:HD2	2.26	0.54
1:C:189:PRO:HA	1:C:232:PHE:HD1	1.73	0.54
2:H:37:ILE:HG13	2:H:82:VAL:HG21	1.89	0.54
1:B:233:ASN:HB3	1:B:235:ARG:NH2	2.23	0.54
1:B:343:ASP:OD1	1:B:344:LEU:N	2.40	0.54
1:C:937:PRO:O	1:C:939:MET:N	2.38	0.54
1:A:259:THR:HG23	1:A:261:GLN:H	1.73	0.54
1:A:1035:LYS:O	1:A:1039:GLU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:LEU:HD12	1:B:290:ILE:HG21	1.88	0.54
1:B:1050:SER:O	1:B:1051:ILE:HG12	2.08	0.54
1:C:206:THR:HG22	1:C:228:PHE:HB2	1.90	0.54
2:D:34:SER:HB3	2:D:105:SER:H	1.73	0.54
3:G:9:GLN:HE21	3:G:24:ILE:HD11	1.72	0.54
1:B:89:ALA:HB3	1:B:132:ILE:CG2	2.38	0.54
1:B:1165:ILE:HG21	1:B:1170:GLY:HA2	1.89	0.54
1:A:205:ALA:N	1:A:231:TYR:HE2	2.06	0.53
1:C:168:THR:N	1:C:185:CYS:O	2.34	0.53
1:C:720:SER:HB3	1:C:759:LEU:HD11	1.91	0.53
1:B:92:ALA:HB1	1:B:303:ILE:HA	1.90	0.53
1:C:866:GLY:HA3	1:C:869:PHE:HD2	1.73	0.53
2:H:161:LYS:HE3	3:I:185:LEU:HD22	1.90	0.53
2:H:34:SER:HB3	2:H:105:SER:H	1.73	0.53
1:C:428:ILE:HG13	1:C:432:ALA:HB3	1.90	0.53
1:A:226:ASN:O	1:A:230:GLU:HG3	2.09	0.53
1:C:190:ARG:NE	1:C:230:GLU:O	2.41	0.53
1:C:430:PRO:HD2	2:H:105:SER:CB	2.37	0.53
2:D:189:GLN:HE22	2:D:195:SER:HB3	1.73	0.53
2:F:161:LYS:HE3	3:G:185:LEU:HD22	1.90	0.53
2:F:189:GLN:HE22	2:F:195:SER:HB3	1.73	0.53
1:A:657:VAL:HG13	1:A:677:VAL:HG11	1.91	0.53
1:B:1167:PRO:HB2	1:B:1180:ILE:HD11	1.90	0.53
1:C:678:ALA:HB3	1:C:681:HIS:HB2	1.89	0.53
1:C:691:ARG:HB3	1:C:694:ARG:HA	1.91	0.53
1:B:143:ILE:HD11	1:B:298:HIS:CD2	2.43	0.53
1:B:404:PHE:HE2	1:B:443:LEU:HB3	1.72	0.53
1:A:374:VAL:H	1:A:606:TYR:HA	1.73	0.53
1:A:854:LYS:HG2	1:A:947:TYR:HE1	1.74	0.53
1:A:1157:ASP:HB2	1:A:1161:PRO:HD2	1.91	0.53
1:B:207:TYR:HA	1:B:298:HIS:CE1	2.44	0.53
1:B:428:ILE:HG13	1:B:432:ALA:HB3	1.90	0.53
1:C:220:ASN:OD1	1:C:221:ARG:N	2.42	0.53
1:B:765:ASN:ND2	1:C:946:ALA:HB1	2.24	0.52
1:C:678:ALA:HB3	1:C:681:HIS:CB	2.39	0.52
3:E:51:ILE:HD11	3:E:65:PHE:HB3	1.89	0.52
1:A:971:PRO:HD3	1:C:778:PHE:CZ	2.44	0.52
1:B:905:TYR:O	1:B:906:MET:HG2	2.09	0.52
1:C:1054:ILE:HD12	1:C:1057:ARG:NH2	2.24	0.52
1:A:156:PHE:HD2	1:A:201:TYR:CE2	2.27	0.52
1:A:366:PHE:HB3	1:A:689:TYR:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:ASP:HA	1:A:1057:ARG:HB2	1.92	0.52
1:B:149:LEU:HB2	1:B:169:LEU:HB3	1.91	0.52
1:C:1178:THR:HG21	1:C:1189:SER:HB3	1.89	0.52
1:B:140:ILE:HA	1:B:309:ALA:O	2.08	0.52
1:B:641:TYR:HB2	1:B:649:TYR:H	1.75	0.52
1:B:765:ASN:HD22	1:C:946:ALA:HB3	1.74	0.52
1:C:970:ILE:HG12	1:C:971:PRO:HD2	1.90	0.52
1:A:891:GLU:HG2	1:A:1128:VAL:HB	1.91	0.52
1:B:148:MET:SD	1:B:296:ILE:HD11	2.49	0.52
2:F:34:SER:HB3	2:F:105:SER:H	1.73	0.52
3:I:24:ILE:HG23	3:I:76:LEU:HB3	1.91	0.52
1:A:599:GLN:HB3	1:A:649:TYR:CE2	2.44	0.52
1:B:619:ASN:HA	1:B:648:TYR:O	2.09	0.52
1:C:181:ARG:NH1	1:C:225:LEU:HD22	2.25	0.52
1:C:45:PRO:HA	1:C:81:HIS:NE2	2.24	0.52
1:C:180:LEU:HB2	1:C:245:ILE:HD11	1.91	0.52
1:C:632:TYR:CD1	1:C:638:LEU:HB3	2.45	0.52
3:G:51:ILE:HD11	3:G:65:PHE:HB3	1.92	0.52
1:B:208:HIS:CE1	1:B:298:HIS:HE2	2.28	0.52
1:B:300:ILE:HD13	1:B:310:TRP:CD1	2.45	0.52
2:D:161:LYS:HE3	3:E:185:LEU:HD22	1.90	0.52
1:C:101:PHE:CZ	1:C:132:ILE:HA	2.45	0.52
1:C:188:GLU:HB3	1:C:233:ASN:HB2	1.91	0.52
2:H:213:ILE:HG22	2:H:228:ARG:HA	1.91	0.52
1:B:429:SER:CB	2:F:106:SER:HA	2.39	0.52
1:C:172:LEU:HD21	1:C:225:LEU:HA	1.92	0.52
1:A:183:PHE:HD2	1:A:185:CYS:SG	2.33	0.51
1:B:89:ALA:HB3	1:B:132:ILE:HG21	1.92	0.51
1:A:46:ARG:HB2	1:A:314:TYR:HE2	1.75	0.51
1:A:1169:ASN:HB2	1:A:1180:ILE:HG21	1.92	0.51
1:C:84:MET:SD	1:C:86:VAL:HG13	2.51	0.51
1:C:210:PRO:HG2	1:C:302:SER:HB3	1.92	0.51
1:A:360:VAL:HG22	1:A:662:ILE:HG12	1.92	0.51
1:C:340:GLY:O	1:C:695:SER:HB3	2.11	0.51
1:A:785:ASN:HB2	1:A:1144:SER:HB3	1.91	0.51
1:A:1028:ASN:O	1:A:1031:GLN:HG3	2.10	0.51
1:B:1164:CYS:SG	1:B:1196:PRO:HG3	2.50	0.51
1:C:899:THR:H	1:C:1023:GLN:HE22	1.59	0.51
1:A:807:LYS:NZ	1:C:692:SER:HB2	2.26	0.51
1:A:875:GLU:OE2	1:A:887:ARG:N	2.44	0.51
3:G:24:ILE:HG23	3:G:76:LEU:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:MET:HG2	1:A:314:TYR:CE1	2.45	0.51
1:B:132:ILE:O	1:B:134:PRO:HD3	2.10	0.51
1:B:420:VAL:CG2	2:F:60:THR:HG21	2.40	0.51
1:C:545:LEU:HD22	1:C:554:LEU:HB2	1.93	0.51
1:A:84:MET:HG2	1:A:314:TYR:CD1	2.45	0.51
1:C:605:GLU:HA	1:C:614:ARG:HA	1.93	0.51
1:C:620:CYS:HB2	1:C:648:TYR:CE2	2.45	0.51
1:A:1024:ASP:O	1:A:1028:ASN:HB2	2.11	0.51
1:C:30:CYS:SG	1:C:231:TYR:CD2	3.04	0.51
1:C:190:ARG:HD3	1:C:231:TYR:C	2.31	0.51
2:F:207:LEU:HA	2:F:212:TYR:HE2	1.76	0.51
1:A:429:SER:CB	2:D:106:SER:HA	2.41	0.51
1:B:19:VAL:HB	1:B:237:CYS:HB3	1.93	0.51
1:B:142:LYS:NZ	1:B:250:ILE:O	2.43	0.51
1:B:1051:ILE:O	1:B:1054:ILE:HG13	2.10	0.51
1:C:831:ILE:HG23	1:C:1082:VAL:HG21	1.92	0.51
1:B:1164:CYS:HB3	1:B:1196:PRO:HG3	1.93	0.51
1:C:337:ILE:HG22	1:C:339:CYS:H	1.75	0.51
3:E:24:ILE:HG23	3:E:76:LEU:HB3	1.91	0.51
1:A:100:LEU:HD21	1:A:207:TYR:HB3	1.93	0.50
1:A:120:ILE:HD13	1:A:313:PHE:HB2	1.93	0.50
1:B:735:LEU:HB2	1:B:741:THR:CG2	2.41	0.50
1:B:806:CYS:HB3	1:B:828:CYS:HB3	1.94	0.50
1:B:810:VAL:HG21	1:B:1075:LEU:HD12	1.92	0.50
1:C:420:VAL:CG2	2:H:60:THR:HG21	2.40	0.50
2:D:207:LEU:HA	2:D:212:TYR:HE2	1.76	0.50
1:B:25:SER:HB2	1:B:229:LYS:HB3	1.92	0.50
1:B:234:LEU:O	1:B:235:ARG:NH1	2.37	0.50
1:C:123:ALA:HB3	1:C:140:ILE:HG21	1.94	0.50
1:B:429:SER:HB2	2:F:106:SER:HA	1.92	0.50
1:C:641:TYR:HA	1:C:649:TYR:H	1.75	0.50
1:A:424:THR:HA	2:D:110:TYR:O	2.11	0.50
1:C:726:ASP:O	1:C:727:CYS:C	2.50	0.50
1:C:849:LEU:HD12	1:C:1096:ALA:HB1	1.94	0.50
1:A:1154:GLY:HA3	1:A:1205:VAL:CG1	2.42	0.50
1:B:105:TYR:HB2	1:B:297:PRO:HD3	1.92	0.50
1:B:251:LEU:HD12	1:B:252:GLU:H	1.76	0.50
1:A:655:VAL:HG22	1:B:909:TYR:CZ	2.47	0.50
1:A:827:PHE:O	1:A:831:ILE:HG13	2.12	0.50
1:C:30:CYS:N	1:C:193:ASN:O	2.45	0.50
1:A:266:PHE:HB3	1:A:278:MET:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ILE:HG23	1:A:733:GLN:HG3	1.94	0.50
1:A:806:CYS:O	1:A:807:LYS:HB3	2.11	0.50
1:B:656:SER:HB2	1:C:930:ALA:HB2	1.93	0.50
1:C:715:LEU:HD21	1:C:736:CYS:HB2	1.93	0.50
3:I:143:PHE:HZ	3:I:179:LEU:HB2	1.77	0.50
1:A:437:CYS:CB	1:A:585:CYS:HA	2.42	0.50
1:B:123:ALA:HB3	1:B:140:ILE:HG21	1.93	0.50
3:I:51:ILE:HD11	3:I:65:PHE:HB3	1.94	0.50
1:B:484:VAL:HG12	1:B:569:MET:HE1	1.94	0.49
1:B:545:LEU:HD22	1:B:554:LEU:HB2	1.93	0.49
1:C:1046:ALA:HB3	1:C:1069:ARG:NH2	2.27	0.49
3:I:142:ASN:HA	3:I:176:THR:HB	1.94	0.49
3:G:142:ASN:HA	3:G:176:THR:HB	1.94	0.49
1:A:326:ASP:HB2	1:A:354:PHE:CE2	2.46	0.49
1:A:420:VAL:CG2	2:D:60:THR:HG21	2.42	0.49
1:A:545:LEU:HD22	1:A:554:LEU:HB2	1.93	0.49
1:B:87:TYR:CG	1:B:298:HIS:HB3	2.47	0.49
1:B:107:GLN:HA	1:B:161:MET:HB2	1.94	0.49
1:B:738:LEU:HD21	1:C:943:MET:CE	2.42	0.49
1:C:142:LYS:NZ	1:C:250:ILE:O	2.45	0.49
1:C:374:VAL:H	1:C:606:TYR:HA	1.76	0.49
1:C:394:PRO:HB2	1:C:398:ASN:HB2	1.95	0.49
1:A:36:GLN:HB3	1:A:39:PHE:HB2	1.94	0.49
1:B:497:TYR:HB2	1:B:561:VAL:HB	1.95	0.49
1:B:602:ASN:HB3	1:B:617:PHE:O	2.12	0.49
1:C:464:ILE:HG13	1:C:465:SER:N	2.28	0.49
2:D:100:ALA:HB2	2:D:120:TRP:CE3	2.47	0.49
2:F:100:ALA:HB2	2:F:120:TRP:CE3	2.47	0.49
2:H:100:ALA:HB2	2:H:120:TRP:CE3	2.47	0.49
1:A:484:VAL:HG12	1:A:569:MET:HE1	1.95	0.49
1:A:628:GLN:HB2	1:B:63:THR:HG23	1.93	0.49
1:A:821:LEU:O	1:A:824:TYR:N	2.46	0.49
1:B:32:GLU:O	1:B:99:LYS:HD2	2.11	0.49
1:B:1051:ILE:CG2	1:B:1054:ILE:HA	2.42	0.49
1:C:1072:ASN:O	1:C:1076:THR:HG23	2.11	0.49
3:E:143:PHE:HZ	3:E:179:LEU:HB2	1.77	0.49
1:B:623:VAL:O	1:B:648:TYR:HE1	1.94	0.49
2:F:166:GLU:HB2	2:F:194:TYR:CE2	2.48	0.49
1:B:985:ILE:HG12	1:B:1168:VAL:HG21	1.95	0.49
1:C:388:LEU:HD21	1:C:414:LEU:HD13	1.95	0.49
3:E:38:TRP:O	3:E:50:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:GLU:OE1	1:A:886:ALA:N	2.46	0.49
1:C:141:ARG:N	1:C:309:ALA:O	2.27	0.49
1:C:599:GLN:NE2	1:C:644:ASP:HB2	2.28	0.49
3:I:6:ARG:H	3:I:29:SER:HB3	1.77	0.49
1:A:109:VAL:HG11	1:A:153:VAL:HG21	1.95	0.49
1:A:194:HIS:HA	1:A:200:SER:O	2.13	0.49
1:C:1056:GLN:HG2	1:C:1057:ARG:HD3	1.95	0.49
2:D:32:PHE:HA	2:D:35:TYR:CE2	2.48	0.49
3:G:6:ARG:H	3:G:29:SER:HB3	1.77	0.49
1:A:175:GLY:HA2	1:A:220:ASN:O	2.13	0.49
1:A:1162:THR:HG23	1:A:1198:THR:HG22	1.94	0.49
1:B:233:ASN:HB3	1:B:235:ARG:HH22	1.78	0.49
1:A:347:LEU:HG	1:A:356:VAL:HG11	1.93	0.48
1:A:1047:ILE:HD13	1:A:1066:GLN:NE2	2.27	0.48
1:A:1172:PHE:HD2	1:A:1177:ASN:HB2	1.76	0.48
1:B:388:LEU:HD21	1:B:414:LEU:HD13	1.95	0.48
1:B:1154:GLY:HA3	1:B:1205:VAL:HG12	1.95	0.48
1:C:783:PRO:HB3	1:C:1143:PRO:HB3	1.94	0.48
2:H:21:VAL:HG22	2:H:89:LEU:HD11	1.94	0.48
1:B:196:PRO:HG2	1:B:232:PHE:HE1	1.78	0.48
1:B:773:LEU:HD23	1:B:774:ASN:N	2.28	0.48
1:B:799:ILE:HG23	1:B:1092:ALA:HB2	1.94	0.48
1:C:497:TYR:HB2	1:C:561:VAL:HB	1.95	0.48
1:C:545:LEU:HD23	1:C:551:GLY:O	2.13	0.48
1:C:804:VAL:HG21	1:C:1078:LEU:HD11	1.95	0.48
2:F:32:PHE:HA	2:F:35:TYR:CE2	2.48	0.48
1:B:266:PHE:HB3	1:B:278:MET:HG2	1.95	0.48
1:B:394:PRO:HB2	1:B:398:ASN:HB2	1.95	0.48
1:B:821:LEU:O	1:B:824:TYR:N	2.39	0.48
1:C:101:PHE:CD1	1:C:132:ILE:HG13	2.49	0.48
1:C:429:SER:HB2	2:H:106:SER:HA	1.95	0.48
2:D:111:ARG:C	2:D:113:TYR:H	2.17	0.48
3:E:6:ARG:H	3:E:29:SER:HB3	1.77	0.48
1:A:394:PRO:HB2	1:A:398:ASN:HB2	1.95	0.48
1:A:409:TYR:HE2	1:A:584:VAL:HG12	1.78	0.48
1:A:733:GLN:N	1:A:733:GLN:HE21	2.11	0.48
1:A:957:GLY:HA3	1:A:967:PHE:CE1	2.48	0.48
1:B:70:THR:HA	1:B:324:LEU:HA	1.94	0.48
1:B:409:TYR:HE2	1:B:584:VAL:HG12	1.78	0.48
1:B:785:ASN:HB2	1:B:1144:SER:OG	2.14	0.48
1:B:1113:ARG:HG2	1:B:1115:GLY:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LEU:HD23	1:C:170:VAL:N	2.29	0.48
1:C:711:VAL:HG21	1:C:721:SER:HA	1.94	0.48
2:H:32:PHE:HA	2:H:35:TYR:CE2	2.48	0.48
1:A:35:ILE:HA	1:A:102:VAL:O	2.14	0.48
1:C:1059:ASP:O	1:C:1063:GLN:HB3	2.14	0.48
1:A:369:LYS:HD2	1:A:690:SER:HB2	1.96	0.48
1:A:429:SER:HB2	2:D:106:SER:HA	1.96	0.48
1:A:497:TYR:HB2	1:A:561:VAL:HB	1.95	0.48
1:A:787:SER:HB2	1:A:1142:TYR:HB2	1.95	0.48
1:C:875:GLU:H	1:C:875:GLU:CD	2.17	0.48
3:G:51:ILE:HG13	3:G:57:LEU:CD1	2.44	0.48
3:G:143:PHE:HZ	3:G:179:LEU:HB2	1.77	0.48
1:A:464:ILE:HG13	1:A:465:SER:N	2.28	0.48
1:A:655:VAL:HG11	1:B:913:MET:SD	2.54	0.48
1:B:628:GLN:HB2	1:C:63:THR:HG22	1.96	0.48
3:E:142:ASN:HA	3:E:176:THR:HB	1.94	0.48
1:A:824:TYR:HB3	1:A:827:PHE:CD2	2.49	0.48
1:B:464:ILE:HG13	1:B:465:SER:N	2.28	0.48
1:B:854:LYS:O	1:B:855:SER:C	2.52	0.48
1:C:21:VAL:HG21	1:C:240:MET:SD	2.54	0.48
2:H:137:PRO:HA	2:H:163:TYR:HB3	1.96	0.48
1:B:37:GLN:CG	1:B:104:ASN:HB2	2.44	0.48
1:B:849:LEU:O	1:B:853:VAL:HG23	2.14	0.48
1:C:786:PHE:HB3	1:C:788:PHE:CE1	2.48	0.48
1:C:957:GLY:HA3	1:C:967:PHE:CE2	2.49	0.48
2:D:21:VAL:HG22	2:D:89:LEU:HD11	1.94	0.48
1:A:388:LEU:HD21	1:A:414:LEU:HD13	1.95	0.47
1:A:484:VAL:HG22	1:A:486:HIS:H	1.79	0.47
1:A:826:GLN:OE1	1:A:826:GLN:N	2.36	0.47
1:B:1031:GLN:NE2	1:B:1035:LYS:HG2	2.29	0.47
1:C:88:SER:HA	1:C:310:TRP:CD1	2.49	0.47
1:C:954:SER:HA	1:C:967:PHE:HE2	1.79	0.47
2:F:21:VAL:HG22	2:F:89:LEU:HD11	1.94	0.47
1:A:167:HIS:HB2	1:A:184:TYR:CZ	2.49	0.47
1:B:806:CYS:O	1:B:807:LYS:HB3	2.14	0.47
1:C:603:CYS:HA	1:C:616:VAL:HG23	1.95	0.47
1:A:545:LEU:HD23	1:A:551:GLY:O	2.13	0.47
1:A:831:ILE:HG23	1:A:1082:VAL:HG21	1.96	0.47
1:B:545:LEU:HD23	1:B:551:GLY:O	2.13	0.47
1:C:205:ALA:HB3	1:C:231:TYR:OH	2.14	0.47
1:C:369:LYS:O	1:C:604:VAL:HG11	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:792:GLN:HG3	1:C:1138:HIS:HB2	1.97	0.47
2:H:156:LEU:HD12	2:H:207:LEU:HD11	1.94	0.47
1:B:765:ASN:ND2	1:C:946:ALA:C	2.67	0.47
1:C:85:TYR:HD1	1:C:105:TYR:CD1	2.33	0.47
1:C:1053:ASP:HA	1:C:1057:ARG:HB2	1.97	0.47
1:A:169:LEU:HA	1:A:169:LEU:HD23	1.72	0.47
1:A:404:PHE:CE2	1:A:443:LEU:HB3	2.49	0.47
1:A:789:GLY:HA3	1:A:1004:ALA:CB	2.43	0.47
1:B:204:PHE:HZ	1:B:294:SER:HB2	1.78	0.47
1:C:1205:VAL:O	1:C:1206:ALA:C	2.52	0.47
1:B:245:ILE:HD12	1:B:269:ARG:NH2	2.30	0.47
1:B:484:VAL:HG22	1:B:486:HIS:H	1.79	0.47
1:C:633:ASP:OD1	1:C:633:ASP:N	2.47	0.47
1:C:875:GLU:OE2	1:C:875:GLU:N	2.46	0.47
2:F:137:PRO:HA	2:F:163:TYR:HB3	1.96	0.47
2:F:142:LEU:HB2	2:F:157:GLY:O	2.15	0.47
1:A:148:MET:HG2	1:A:170:VAL:HG22	1.95	0.47
1:A:798:THR:O	1:A:1132:ASN:HB3	2.15	0.47
1:B:42:LYS:HG3	1:B:44:TRP:CH2	2.50	0.47
1:B:437:CYS:CB	1:B:585:CYS:HA	2.42	0.47
1:C:59:PRO:HB3	1:C:71:TYR:CZ	2.50	0.47
1:C:782:ILE:HG13	1:C:1182:ASP:O	2.15	0.47
1:C:785:ASN:HB2	1:C:1144:SER:OG	2.15	0.47
1:C:954:SER:O	1:C:958:VAL:HG12	2.14	0.47
1:B:267:SER:OG	1:B:268:SER:N	2.47	0.47
3:E:51:ILE:HG13	3:E:57:LEU:CD1	2.44	0.47
1:A:1104:ASN:O	1:A:1108:LYS:HB2	2.14	0.47
1:C:912:CYS:HB2	1:C:928:TYR:CZ	2.50	0.47
2:D:15:LYS:HD2	2:D:21:VAL:HG12	1.97	0.47
2:D:35:TYR:HB2	2:D:101:ASN:HB2	1.96	0.47
2:D:142:LEU:HB2	2:D:157:GLY:O	2.15	0.47
1:B:616:VAL:HB	1:B:652:ARG:HE	1.79	0.47
1:C:56:ILE:O	1:C:278:MET:HG2	2.15	0.47
2:D:137:PRO:HA	2:D:163:TYR:HB3	1.96	0.47
1:B:324:LEU:HD22	1:B:354:PHE:CE1	2.51	0.46
1:B:1199:SER:HB2	1:B:1205:VAL:O	2.15	0.46
1:C:484:VAL:HG22	1:C:486:HIS:H	1.79	0.46
2:F:165:PRO:HD2	2:F:218:HIS:HE1	1.80	0.46
2:H:35:TYR:HB2	2:H:101:ASN:HB2	1.96	0.46
1:A:24:ASP:OD2	1:A:235:ARG:NH2	2.24	0.46
1:A:782:ILE:HD11	1:A:1180:ILE:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:ILE:CD1	1:A:1180:ILE:HA	2.45	0.46
1:A:829:SER:O	1:A:833:GLN:HG3	2.15	0.46
1:C:640:GLY:CA	1:C:651:LEU:HD13	2.45	0.46
1:C:1105:GLU:HG2	1:C:1116:PHE:HB2	1.96	0.46
1:A:957:GLY:HA3	1:A:967:PHE:CZ	2.51	0.46
1:B:783:PRO:HD2	1:B:1181:VAL:HG13	1.97	0.46
2:F:35:TYR:HB2	2:F:101:ASN:HB2	1.96	0.46
1:A:738:LEU:HA	1:A:738:LEU:HD23	1.76	0.46
1:A:826:GLN:H	1:A:826:GLN:CD	2.17	0.46
1:B:932:TYR:HB2	1:B:1033:LEU:HD11	1.97	0.46
1:B:1160:ASN:N	1:B:1161:PRO:HD2	2.30	0.46
1:C:88:SER:HA	1:C:310:TRP:HD1	1.80	0.46
1:C:633:ASP:O	1:C:635:TYR:N	2.49	0.46
1:A:300:ILE:HD13	1:A:310:TRP:CD1	2.49	0.46
1:B:404:PHE:CE2	1:B:443:LEU:HB3	2.49	0.46
1:C:126:SER:O	1:C:140:ILE:N	2.31	0.46
1:C:437:CYS:CB	1:C:585:CYS:HA	2.42	0.46
2:D:165:PRO:HB2	2:D:218:HIS:CE1	2.50	0.46
2:H:15:LYS:HD2	2:H:21:VAL:HG12	1.97	0.46
2:H:142:LEU:HB2	2:H:157:GLY:O	2.15	0.46
1:A:373:SER:HB3	1:A:605:GLU:CD	2.36	0.46
1:A:644:ASP:HB2	1:A:649:TYR:CE2	2.51	0.46
1:B:144:TYR:OH	1:B:252:GLU:OE1	2.18	0.46
1:B:718:VAL:HG11	1:B:759:LEU:HD21	1.97	0.46
1:B:802:VAL:HG21	1:B:1033:LEU:HD13	1.97	0.46
1:C:725:GLU:HG3	1:C:758:ARG:HD2	1.98	0.46
3:E:33:SER:HA	3:E:71:GLY:HA2	1.97	0.46
1:A:102:VAL:HB	1:A:297:PRO:HB2	1.97	0.46
1:A:998:ALA:HA	1:A:1001:PHE:HB3	1.98	0.46
1:B:175:GLY:HA2	1:B:220:ASN:O	2.16	0.46
1:B:308:LYS:HE2	1:B:310:TRP:CZ2	2.51	0.46
1:B:641:TYR:HA	1:B:649:TYR:O	2.16	0.46
1:C:404:PHE:CE2	1:C:443:LEU:HB3	2.49	0.46
1:A:998:ALA:HB1	1:A:1002:ASN:HD21	1.80	0.46
1:B:298:HIS:HD2	1:B:300:ILE:HD11	1.81	0.46
1:B:648:TYR:HE2	1:B:650:CYS:HB3	1.81	0.46
1:B:1179:ARG:HG2	1:B:1186:TYR:HB2	1.98	0.46
1:C:814:PHE:CD2	1:C:1051:ILE:HG13	2.51	0.46
3:I:136:VAL:H	3:I:183:LEU:HB2	1.81	0.46
1:A:220:ASN:OD1	1:A:221:ARG:N	2.49	0.46
1:A:735:LEU:HD22	1:A:739:PRO:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ALA:HB1	1:C:308:LYS:HE3	1.97	0.46
1:C:363:VAL:HB	1:C:659:VAL:HG13	1.98	0.46
3:G:33:SER:HA	3:G:71:GLY:HA2	1.97	0.46
1:A:388:LEU:HA	1:A:445:TYR:CZ	2.51	0.45
1:B:652:ARG:NH1	1:C:913:MET:O	2.48	0.45
1:B:738:LEU:CD1	1:B:762:ILE:HG23	2.45	0.45
1:B:783:PRO:HB3	1:B:1143:PRO:HB3	1.97	0.45
1:B:860:PRO:O	1:B:862:ILE:HG13	2.15	0.45
1:C:190:ARG:HB2	1:C:231:TYR:O	2.16	0.45
1:C:631:VAL:O	1:C:639:VAL:N	2.50	0.45
2:D:6:GLN:HE21	2:D:6:GLN:HB2	1.50	0.45
1:A:1070:LEU:HD21	1:A:1074:ARG:CZ	2.46	0.45
1:B:85:TYR:CG	1:B:295:ILE:HG21	2.51	0.45
1:C:190:ARG:HD3	1:C:232:PHE:N	2.31	0.45
1:C:291:LYS:HG3	1:C:292:TYR:CE2	2.50	0.45
1:C:640:GLY:HA3	1:C:651:LEU:HD13	1.97	0.45
1:C:792:GLN:HB2	1:C:1136:PHE:O	2.16	0.45
3:I:33:SER:HA	3:I:71:GLY:HA2	1.97	0.45
1:B:809:TYR:OH	1:B:1040:LEU:HB3	2.16	0.45
1:B:967:PHE:HB2	1:B:968:ALA:H	1.60	0.45
1:C:32:GLU:HB3	1:C:99:LYS:HG2	1.97	0.45
1:C:409:TYR:HE2	1:C:584:VAL:HG12	1.78	0.45
1:A:363:VAL:HG23	1:A:659:VAL:HG13	1.98	0.45
1:A:608:LEU:HD12	1:A:608:LEU:HA	1.75	0.45
1:A:1111:SER:HB3	1:A:1122:HIS:HB3	1.98	0.45
2:D:102:SER:HA	2:D:118:ASP:H	1.82	0.45
3:E:57:LEU:HD11	3:E:65:PHE:HB2	1.98	0.45
2:F:165:PRO:C	2:F:167:PRO:HD3	2.36	0.45
1:A:996:LEU:HD13	1:A:996:LEU:HA	1.84	0.45
1:B:376:GLU:O	1:B:377:GLN:HG3	2.16	0.45
1:B:738:LEU:HD21	1:C:943:MET:HE2	1.98	0.45
1:C:1061:LEU:HD23	1:C:1061:LEU:H	1.82	0.45
1:B:388:LEU:HA	1:B:445:TYR:CZ	2.51	0.45
1:C:95:THR:O	1:C:97:PRO:HD3	2.16	0.45
1:C:141:ARG:O	1:C:310:TRP:HA	2.16	0.45
1:C:1154:GLY:HA3	1:C:1205:VAL:HB	1.98	0.45
2:F:15:LYS:HD2	2:F:21:VAL:HG12	1.97	0.45
3:I:57:LEU:HD11	3:I:65:PHE:HB2	1.98	0.45
1:A:149:LEU:O	1:A:169:LEU:N	2.49	0.45
1:A:1029:ASN:OD1	1:A:1030:ALA:N	2.50	0.45
1:B:206:THR:O	1:B:298:HIS:ND1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:673:LEU:HD11	1:C:715:LEU:HD23	1.99	0.45
3:G:57:LEU:HD11	3:G:65:PHE:HB2	1.98	0.45
1:A:820:LEU:O	1:A:823:GLU:HB2	2.16	0.45
1:C:35:ILE:HG22	1:C:37:GLN:OE1	2.17	0.45
1:C:786:PHE:HB2	1:C:1000:LYS:HD3	1.99	0.45
2:F:89:LEU:HD23	2:F:128:VAL:HG22	1.99	0.45
2:F:160:VAL:HB	2:F:196:LEU:HD23	1.99	0.45
1:A:156:PHE:HE1	1:A:163:ARG:HG3	1.82	0.45
1:A:983:VAL:HG12	1:A:1121:THR:HB	1.98	0.45
1:B:167:HIS:HB3	1:B:184:TYR:CZ	2.52	0.45
1:B:810:VAL:HA	1:B:1074:ARG:HG2	1.98	0.45
1:C:388:LEU:HA	1:C:445:TYR:CZ	2.51	0.45
1:C:509:ASP:HB2	1:C:511:ARG:HD3	1.99	0.45
1:C:796:GLN:O	1:C:797:THR:C	2.55	0.45
1:C:891:GLU:OE2	1:C:1129:ASN:HB2	2.17	0.45
1:C:894:LEU:O	1:C:898:VAL:HG23	2.17	0.45
3:E:136:VAL:H	3:E:183:LEU:HB2	1.81	0.45
1:A:164:PHE:HZ	1:A:293:TYR:HA	1.82	0.45
1:A:780:LEU:HD11	1:A:1172:PHE:CE1	2.51	0.45
1:A:1171:TYR:HB3	1:A:1176:ASN:HA	1.97	0.45
1:C:189:PRO:HA	1:C:232:PHE:CD1	2.51	0.45
1:A:456:LEU:HD23	1:A:481:LEU:HD21	1.99	0.44
1:B:810:VAL:HG13	1:B:1074:ARG:HB3	1.99	0.44
1:C:905:TYR:C	1:C:907:GLN:N	2.70	0.44
2:H:102:SER:HA	2:H:118:ASP:H	1.82	0.44
1:B:424:THR:HA	2:F:110:TYR:O	2.17	0.44
1:B:464:ILE:HA	1:B:468:ASN:HD22	1.82	0.44
1:B:791:THR:HG21	1:B:1118:GLY:HA2	1.98	0.44
2:H:111:ARG:C	2:H:113:TYR:H	2.20	0.44
1:B:146:ALA:CB	1:B:296:ILE:HD12	2.47	0.44
1:B:509:ASP:HB2	1:B:511:ARG:HD3	1.99	0.44
1:B:872:THR:HB	1:B:890:ILE:HD11	2.00	0.44
1:C:429:SER:OG	2:H:106:SER:HA	2.17	0.44
1:C:794:TYR:CG	1:C:1022:VAL:HG22	2.52	0.44
1:A:141:ARG:O	1:A:310:TRP:HA	2.17	0.44
1:B:323:PHE:CD1	1:B:338:ASP:HA	2.53	0.44
1:C:424:THR:HA	2:H:110:TYR:O	2.17	0.44
1:C:618:GLN:HB2	1:C:650:CYS:SG	2.58	0.44
1:C:1119:GLN:HB2	1:C:1142:TYR:OH	2.17	0.44
2:F:102:SER:HA	2:F:118:ASP:H	1.82	0.44
3:G:136:VAL:H	3:G:183:LEU:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HD3	1:B:308:LYS:HD2	1.99	0.44
1:B:697:LEU:HG	1:B:698:LYS:H	1.82	0.44
1:B:985:ILE:HG21	1:B:1168:VAL:HG21	2.00	0.44
2:F:170:VAL:HA	2:F:215:ASN:O	2.18	0.44
1:A:207:TYR:H	1:A:227:SER:CB	2.30	0.44
1:A:346:GLN:HE21	1:A:694:ARG:HH12	1.64	0.44
1:A:733:GLN:HE21	1:A:733:GLN:H	1.65	0.44
1:A:986:THR:HG22	1:A:1182:ASP:HB2	1.99	0.44
1:B:47:PRO:HA	1:B:81:HIS:HA	1.99	0.44
1:C:631:VAL:HG13	1:C:639:VAL:HB	2.00	0.44
2:D:160:VAL:HB	2:D:196:LEU:HD23	1.99	0.44
2:H:147:LYS:HE3	2:H:147:LYS:HB3	1.86	0.44
1:A:486:HIS:HB2	1:A:566:GLN:HE22	1.83	0.44
1:A:674:PHE:O	1:A:716:GLY:HA3	2.17	0.44
1:A:794:TYR:CZ	1:A:796:GLN:HA	2.52	0.44
1:B:119:ARG:HD3	1:B:122:ALA:HB2	2.00	0.44
1:B:464:ILE:HA	1:B:468:ASN:HB2	2.00	0.44
1:B:985:ILE:HG12	1:B:1168:VAL:HG23	1.98	0.44
1:C:464:ILE:HA	1:C:468:ASN:HB2	2.00	0.44
2:D:89:LEU:HD23	2:D:128:VAL:HG22	1.99	0.44
3:I:51:ILE:HD13	3:I:76:LEU:HD13	2.00	0.44
1:A:985:ILE:CB	1:A:1181:VAL:HG11	2.48	0.44
1:B:732:GLY:C	1:B:734:SER:H	2.22	0.44
1:C:366:PHE:O	1:C:656:SER:HA	2.17	0.44
1:A:464:ILE:HA	1:A:468:ASN:HB2	2.00	0.44
1:A:500:ILE:HG23	1:A:557:SER:O	2.18	0.44
1:A:1112:LYS:HD2	1:A:1112:LYS:HA	1.81	0.44
1:B:791:THR:CG2	1:B:1138:HIS:HB2	2.48	0.44
1:C:464:ILE:HA	1:C:468:ASN:HD22	1.82	0.44
1:C:500:ILE:HG23	1:C:557:SER:O	2.18	0.44
2:D:203:PRO:HG2	2:D:206:SER:HB3	2.00	0.44
1:A:385:PHE:HB2	1:A:388:LEU:HD23	2.00	0.43
1:A:986:THR:CG2	1:A:1182:ASP:HB2	2.48	0.43
2:F:109:CYS:HA	2:F:114:GLN:NE2	2.33	0.43
1:A:624:GLY:HA3	1:A:642:TYR:HE2	1.83	0.43
1:A:998:ALA:O	1:A:999:ASN:C	2.56	0.43
1:B:87:TYR:CD2	1:B:298:HIS:HB3	2.53	0.43
1:B:786:PHE:HA	1:B:1141:TYR:CE1	2.52	0.43
1:C:101:PHE:CE2	1:C:132:ILE:HA	2.53	0.43
1:C:215:SER:HB2	1:C:218:ASN:O	2.17	0.43
3:E:52:TYR:C	3:E:54:ALA:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:19:GLY:H	3:G:81:LEU:HB3	1.83	0.43
3:I:19:GLY:H	3:I:81:LEU:HB3	1.83	0.43
1:A:194:HIS:H	1:A:200:SER:HB2	1.83	0.43
1:A:1152:ALA:O	1:A:1154:GLY:N	2.51	0.43
1:B:398:ASN:O	1:B:399:PHE:C	2.57	0.43
1:A:453:LYS:HB3	1:A:453:LYS:HE2	1.80	0.43
1:A:509:ASP:HB2	1:A:511:ARG:HD3	1.99	0.43
1:A:782:ILE:HG23	1:A:1182:ASP:O	2.17	0.43
1:A:1189:SER:O	1:A:1190:SER:HB3	2.17	0.43
1:B:385:PHE:HB2	1:B:388:LEU:HD23	2.00	0.43
1:B:486:HIS:HB2	1:B:566:GLN:HE22	1.83	0.43
1:B:638:LEU:C	1:B:640:GLY:N	2.69	0.43
1:B:865:PHE:HD1	1:B:865:PHE:HA	1.74	0.43
1:C:302:SER:HB2	1:C:306:ASP:HB2	2.00	0.43
1:C:486:HIS:HB2	1:C:566:GLN:HE22	1.83	0.43
1:A:149:LEU:HD22	1:A:256:ILE:HD13	2.01	0.43
1:A:350:SER:O	1:A:351:TYR:HB2	2.18	0.43
1:B:363:VAL:HG21	1:B:661:VAL:HG23	2.00	0.43
1:B:795:ILE:HG13	1:B:1136:PHE:CE1	2.53	0.43
1:B:1008:MET:HE2	1:B:1008:MET:HB3	1.92	0.43
1:C:905:TYR:C	1:C:907:GLN:H	2.22	0.43
1:C:1203:LYS:HD2	1:C:1203:LYS:HA	1.78	0.43
2:D:109:CYS:HA	2:D:114:GLN:NE2	2.33	0.43
3:I:52:TYR:C	3:I:54:ALA:H	2.22	0.43
1:A:464:ILE:HA	1:A:468:ASN:HD22	1.82	0.43
1:C:44:TRP:HZ3	1:C:86:VAL:HG11	1.83	0.43
1:C:120:ILE:HD12	1:C:145:PRO:HD3	2.01	0.43
1:C:819:GLN:HA	1:C:822:ARG:HD3	2.00	0.43
1:C:1053:ASP:HA	1:C:1057:ARG:NE	2.33	0.43
2:D:170:VAL:HA	2:D:215:ASN:O	2.18	0.43
2:F:186:ALA:HB1	2:F:194:TYR:HB3	2.00	0.43
3:G:51:ILE:HD13	3:G:76:LEU:HD13	2.00	0.43
2:H:109:CYS:HA	2:H:114:GLN:NE2	2.33	0.43
1:A:768:ILE:O	1:B:857:GLN:HA	2.17	0.43
1:A:1113:ARG:HB3	1:A:1116:PHE:HE1	1.83	0.43
1:B:608:LEU:HD11	1:B:642:TYR:HA	2.00	0.43
1:B:691:ARG:C	1:B:693:THR:H	2.21	0.43
1:B:983:VAL:HG21	1:B:1112:LYS:HA	2.00	0.43
1:C:629:ARG:HB3	1:C:642:TYR:HD2	1.83	0.43
1:C:792:GLN:HE21	1:C:1138:HIS:HD2	1.66	0.43
3:E:19:GLY:H	3:E:81:LEU:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:ALA:O	1:A:1036:LEU:HB2	2.18	0.43
1:B:172:LEU:HD23	1:B:173:PRO:O	2.18	0.43
1:C:34:ASP:OD1	1:C:35:ILE:N	2.52	0.43
1:A:985:ILE:N	1:A:1181:VAL:HG21	2.28	0.43
1:A:1049:ALA:C	1:A:1051:ILE:H	2.22	0.43
1:A:1167:PRO:O	1:B:961:THR:HB	2.18	0.43
1:B:791:THR:HG23	1:B:792:GLN:H	1.84	0.43
1:C:40:PHE:HD2	1:C:86:VAL:HG23	1.84	0.43
1:C:291:LYS:HG3	1:C:292:TYR:CD2	2.54	0.43
1:C:364:SER:HB2	1:C:691:ARG:NH2	2.32	0.43
1:C:614:ARG:HG3	1:C:614:ARG:HH11	1.83	0.43
1:C:996:LEU:C	1:C:998:ALA:H	2.22	0.43
1:A:174:ASP:OD1	1:A:175:GLY:N	2.42	0.43
1:A:870:ASN:N	1:A:1002:ASN:OD1	2.48	0.43
1:B:496:LYS:HE3	1:B:560:THR:CG2	2.49	0.43
1:B:500:ILE:HG23	1:B:557:SER:O	2.18	0.43
1:B:628:GLN:HB2	1:C:63:THR:CG2	2.49	0.43
1:B:648:TYR:CE2	1:B:650:CYS:HB3	2.54	0.43
1:B:872:THR:HG22	1:B:889:ALA:HB3	2.01	0.43
1:C:1055:ILE:HG13	1:C:1056:GLN:N	2.34	0.43
3:G:52:TYR:C	3:G:54:ALA:H	2.22	0.43
1:A:374:VAL:HG11	1:A:599:GLN:HA	1.99	0.42
1:B:228:PHE:HA	1:B:231:TYR:HD2	1.84	0.42
1:B:304:GLN:CG	1:B:307:ARG:HH11	2.31	0.42
1:B:794:TYR:HB3	1:B:1021:LYS:HD2	2.01	0.42
1:C:272:ASP:OD2	1:C:334:ARG:NH2	2.52	0.42
1:C:376:GLU:HG3	1:C:643:SER:O	2.19	0.42
1:C:385:PHE:HB2	1:C:388:LEU:HD23	2.00	0.42
3:E:51:ILE:HD13	3:E:76:LEU:HD13	2.00	0.42
1:A:356:VAL:HG23	1:A:663:TYR:CD2	2.54	0.42
1:B:34:ASP:N	1:B:100:LEU:O	2.46	0.42
1:B:990:LEU:HD22	1:B:990:LEU:HA	1.78	0.42
1:B:1078:LEU:HD12	1:B:1078:LEU:HA	1.82	0.42
1:C:30:CYS:HB2	1:C:194:HIS:HB2	2.01	0.42
1:C:496:LYS:HE3	1:C:560:THR:CG2	2.49	0.42
1:C:872:THR:HG22	1:C:889:ALA:HB3	2.01	0.42
2:D:58:PHE:HE2	2:D:112:TYR:HE1	1.67	0.42
3:I:12:VAL:HA	3:I:106:THR:HG23	2.01	0.42
1:A:805:ASP:HB2	1:A:808:GLN:HE21	1.84	0.42
1:A:1202:THR:C	1:A:1204:TYR:H	2.21	0.42
1:B:87:TYR:CE1	1:B:297:PRO:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:SER:HA	1:C:805:ASP:OD2	2.19	0.42
1:B:1116:PHE:O	1:B:1117:CYS:C	2.58	0.42
1:C:227:SER:O	1:C:230:GLU:HB2	2.19	0.42
1:C:456:LEU:HA	1:C:464:ILE:HD11	2.02	0.42
1:C:924:ILE:HG13	1:C:925:CYS:N	2.34	0.42
2:H:89:LEU:HD23	2:H:128:VAL:HG22	1.99	0.42
1:A:456:LEU:HA	1:A:464:ILE:HD11	2.02	0.42
1:A:905:TYR:C	1:A:907:GLN:H	2.22	0.42
1:B:111:GLN:HE22	1:B:291:LYS:HB3	1.83	0.42
1:B:632:TYR:HB2	1:C:64:TYR:CE2	2.54	0.42
1:C:267:SER:OG	1:C:269:ARG:HG3	2.19	0.42
2:D:166:GLU:HG2	2:D:194:TYR:CE2	2.55	0.42
3:E:95:ASP:O	3:E:96:ASN:C	2.57	0.42
1:A:398:ASN:O	1:A:399:PHE:C	2.57	0.42
1:A:820:LEU:HD23	1:A:820:LEU:HA	1.88	0.42
1:A:1166:ALA:N	1:A:1167:PRO:HD2	2.34	0.42
1:B:106:SER:HA	1:B:204:PHE:CZ	2.54	0.42
1:B:937:PRO:O	1:B:939:MET:N	2.52	0.42
1:B:1179:ARG:HD2	1:B:1183:GLU:O	2.19	0.42
1:C:138:ALA:HB3	1:C:309:ALA:HB2	2.02	0.42
1:C:1142:TYR:HA	1:C:1143:PRO:HD3	1.85	0.42
2:H:207:LEU:HA	2:H:212:TYR:HE2	1.84	0.42
3:I:51:ILE:HG13	3:I:57:LEU:CD1	2.47	0.42
1:A:190:ARG:HD3	1:A:231:TYR:C	2.38	0.42
1:A:225:LEU:O	1:A:229:LYS:HG2	2.19	0.42
1:A:359:GLY:CA	1:A:733:GLN:HB2	2.49	0.42
1:A:615:GLY:HA2	1:A:652:ARG:O	2.19	0.42
1:B:59:PRO:HB3	1:B:71:TYR:CZ	2.55	0.42
1:B:248:ASP:OD2	1:B:250:ILE:HB	2.20	0.42
1:B:1199:SER:N	1:B:1205:VAL:HG23	2.34	0.42
1:C:713:CYS:O	1:C:714:VAL:C	2.58	0.42
1:A:542:ARG:HG3	1:A:555:VAL:HG12	2.02	0.42
1:A:783:PRO:HB3	1:A:1143:PRO:HB3	2.01	0.42
1:A:1162:THR:O	1:A:1195:GLU:HA	2.19	0.42
1:B:358:SER:HB2	1:B:664:ASP:HA	2.01	0.42
1:C:110:LYS:HB2	1:C:293:TYR:CE1	2.55	0.42
2:F:203:PRO:HG2	2:F:206:SER:HB3	2.00	0.42
1:B:526:CYS:O	1:B:530:VAL:HG13	2.20	0.42
1:B:1027:ASN:O	1:B:1031:GLN:HB2	2.20	0.42
1:C:620:CYS:HB2	1:C:648:TYR:HE2	1.83	0.42
1:C:1200:LEU:HG	1:C:1201:ASN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:ALA:HB1	2:D:194:TYR:HB3	2.00	0.42
2:F:63:TYR:HE1	2:F:73:ILE:HG13	1.85	0.42
3:G:95:ASP:O	3:G:96:ASN:C	2.57	0.42
3:I:95:ASP:O	3:I:96:ASN:C	2.57	0.42
1:A:467:PHE:CD1	1:A:503:CYS:HB3	2.55	0.42
1:A:526:CYS:O	1:A:530:VAL:HG13	2.20	0.42
1:A:998:ALA:HB1	1:A:1002:ASN:ND2	2.33	0.42
1:A:1111:SER:HB2	1:A:1112:LYS:H	1.56	0.42
1:C:204:PHE:HE1	1:C:296:ILE:HA	1.84	0.42
1:C:467:PHE:CD1	1:C:503:CYS:HB3	2.55	0.42
1:C:526:CYS:O	1:C:530:VAL:HG13	2.20	0.42
1:C:741:THR:HG23	1:C:759:LEU:HD23	2.01	0.42
1:A:631:VAL:CG1	1:A:641:TYR:H	2.33	0.42
1:A:642:TYR:HE1	1:A:648:TYR:HE1	1.68	0.42
1:B:220:ASN:ND2	1:B:223:ALA:HB2	2.35	0.42
1:B:467:PHE:CD1	1:B:503:CYS:HB3	2.55	0.42
1:B:1051:ILE:HB	1:B:1054:ILE:HA	2.01	0.42
1:C:21:VAL:HG11	1:C:240:MET:HB2	2.02	0.42
1:C:129:THR:HA	1:C:137:SER:HA	2.02	0.42
3:E:12:VAL:HA	3:E:106:THR:HG23	2.01	0.42
1:A:208:HIS:O	1:A:210:PRO:HD3	2.20	0.41
1:A:567:LEU:HD13	1:A:567:LEU:HA	1.87	0.41
1:A:898:VAL:HG12	1:A:900:ILE:HG12	2.02	0.41
1:B:545:LEU:HD12	1:B:545:LEU:HA	1.93	0.41
1:B:773:LEU:HD23	1:B:775:SER:H	1.84	0.41
1:C:534:VAL:HG13	1:C:539:ASP:HB2	2.02	0.41
1:C:1197:ILE:HG22	1:C:1198:THR:H	1.85	0.41
2:D:63:TYR:HE1	2:D:73:ILE:HG13	1.85	0.41
3:G:12:VAL:HA	3:G:106:THR:HG23	2.01	0.41
1:B:800:GLN:HB2	1:B:1029:ASN:ND2	2.36	0.41
1:C:1143:PRO:HB2	1:C:1146:HIS:CE1	2.54	0.41
3:E:50:LEU:HG	3:E:65:PHE:CD2	2.55	0.41
1:B:304:GLN:HA	1:B:307:ARG:HE	1.85	0.41
1:B:433:ILE:H	1:B:433:ILE:HG13	1.67	0.41
1:B:1063:GLN:HG2	1:B:1067:ILE:HD12	2.02	0.41
1:C:34:ASP:OD1	1:C:36:GLN:HG2	2.20	0.41
3:G:50:LEU:HB3	3:G:51:ILE:HD12	2.01	0.41
1:A:88:SER:O	1:A:299:SER:OG	2.17	0.41
1:A:430:PRO:HB3	2:D:112:TYR:CD1	2.55	0.41
1:A:1044:PHE:H	1:A:1048:SER:HB2	1.85	0.41
1:B:181:ARG:HD3	1:B:240:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:VAL:HG13	1:B:539:ASP:HB2	2.02	0.41
1:B:595:LYS:HB3	1:B:596:ILE:H	1.50	0.41
1:B:608:LEU:HD12	1:B:608:LEU:HA	1.97	0.41
1:B:887:ARG:HE	1:B:941:VAL:CG1	2.34	0.41
1:B:907:GLN:HA	1:B:907:GLN:OE1	2.21	0.41
1:B:1130:ALA:HB2	1:B:1135:TYR:HB2	2.02	0.41
1:C:1153:TYR:HD2	1:C:1206:ALA:HA	1.84	0.41
1:A:728:LYS:HG3	1:A:742:PRO:HG3	2.01	0.41
1:B:257:THR:HG22	1:B:266:PHE:HE1	1.86	0.41
1:C:358:SER:HB2	1:C:664:ASP:HA	2.03	0.41
1:C:542:ARG:HG3	1:C:555:VAL:HG12	2.02	0.41
1:C:912:CYS:HB2	1:C:928:TYR:CE2	2.56	0.41
2:F:135:LYS:HB2	2:F:163:TYR:HA	2.03	0.41
2:H:63:TYR:HE1	2:H:73:ILE:HG13	1.85	0.41
1:A:534:VAL:HG13	1:A:539:ASP:HB2	2.02	0.41
1:B:214:CYS:HA	1:B:219:TYR:CE1	2.55	0.41
1:C:181:ARG:CZ	1:C:225:LEU:HD22	2.50	0.41
1:C:190:ARG:O	1:C:197:ALA:HB3	2.21	0.41
1:C:207:TYR:HA	1:C:298:HIS:HD2	1.85	0.41
1:C:249:GLU:OE1	1:C:249:GLU:HA	2.20	0.41
1:C:694:ARG:O	1:C:695:SER:C	2.59	0.41
1:A:453:LYS:HD2	3:E:95:ASP:OD2	2.21	0.41
1:B:456:LEU:HA	1:B:464:ILE:HD11	2.02	0.41
1:B:1124:VAL:HG12	1:B:1125:SER:N	2.35	0.41
1:C:100:LEU:HB3	1:C:299:SER:HB3	2.03	0.41
1:C:888:SER:OG	1:C:889:ALA:N	2.54	0.41
1:A:114:ASN:HB2	1:A:318:LEU:O	2.20	0.41
1:B:206:THR:O	1:B:298:HIS:HA	2.21	0.41
1:B:278:MET:HE2	1:B:278:MET:HB2	1.87	0.41
1:B:374:VAL:HG13	1:B:597:ALA:O	2.19	0.41
1:B:854:LYS:HD2	1:B:855:SER:H	1.82	0.41
1:B:1016:ASN:HB2	1:B:1019:PHE:HB3	2.03	0.41
1:C:722:LEU:HD12	1:C:724:VAL:CG2	2.51	0.41
1:A:326:ASP:HB2	1:A:354:PHE:HE2	1.83	0.41
1:A:430:PRO:HD2	2:D:105:SER:HB3	2.03	0.41
1:A:863:PRO:HA	1:A:874:LEU:HD13	2.02	0.41
1:B:46:ARG:HB2	1:B:314:TYR:CE2	2.56	0.41
1:B:542:ARG:HG3	1:B:555:VAL:HG12	2.02	0.41
1:B:715:LEU:HD13	1:B:715:LEU:HA	1.77	0.41
1:C:165:PHE:HB3	1:C:166:ASN:H	1.69	0.41
1:C:339:CYS:O	1:C:346:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:PHE:O	1:C:696:MET:HB3	2.20	0.41
1:C:524:SER:O	1:C:527:VAL:HG22	2.21	0.41
1:C:937:PRO:C	1:C:939:MET:H	2.22	0.41
2:D:135:LYS:HB2	2:D:163:TYR:HA	2.03	0.41
3:E:57:LEU:HD13	3:E:57:LEU:HA	1.90	0.41
2:F:147:LYS:HB3	2:F:147:LYS:HE3	1.86	0.41
3:G:164:GLN:HE21	3:G:164:GLN:HB3	1.71	0.41
3:I:40:GLN:HB2	3:I:50:LEU:HD11	2.03	0.41
1:A:377:GLN:OE1	1:A:377:GLN:HA	2.21	0.41
1:A:733:GLN:HG2	1:A:734:SER:O	2.21	0.41
1:B:56:ILE:HG23	1:B:75:PHE:CE1	2.56	0.41
1:C:150:GLY:HA3	1:C:164:PHE:HD2	1.86	0.41
1:C:453:LYS:HB3	1:C:453:LYS:HE2	1.80	0.41
3:G:40:GLN:HB2	3:G:50:LEU:HD11	2.02	0.41
1:A:396:VAL:HG22	1:A:468:ASN:HB3	2.03	0.40
1:A:662:ILE:CG2	1:A:733:GLN:HG3	2.51	0.40
1:A:808:GLN:O	1:A:812:ASN:HA	2.21	0.40
1:A:1073:GLY:O	1:A:1077:THR:HG23	2.20	0.40
1:B:91:HIS:O	1:B:98:GLN:N	2.54	0.40
1:C:62:ARG:HB3	1:C:64:TYR:CE1	2.56	0.40
2:H:160:VAL:HB	2:H:196:LEU:HD23	2.03	0.40
1:A:239:PHE:CZ	1:A:286:VAL:HG23	2.56	0.40
1:A:697:LEU:O	1:A:698:LYS:HB3	2.21	0.40
1:B:239:PHE:CD2	1:B:241:TYR:CE1	3.10	0.40
1:B:524:SER:O	1:B:527:VAL:HG22	2.21	0.40
1:B:782:ILE:HD11	1:B:1181:VAL:HA	2.03	0.40
1:C:396:VAL:HG22	1:C:468:ASN:HB3	2.03	0.40
1:C:490:THR:HG23	1:C:491:ILE:HG13	2.04	0.40
1:C:595:LYS:HB3	1:C:596:ILE:H	1.56	0.40
2:F:37:ILE:HD13	2:F:101:ASN:HB3	2.04	0.40
2:F:170:VAL:HB	2:F:216:VAL:HG12	2.02	0.40
1:A:736:CYS:O	1:A:737:ALA:C	2.58	0.40
1:B:104:ASN:HA	1:B:107:GLN:OE1	2.21	0.40
1:B:208:HIS:CE1	1:B:298:HIS:NE2	2.89	0.40
1:B:835:LEU:HD23	1:B:835:LEU:HA	1.86	0.40
1:C:89:ALA:O	1:C:101:PHE:HB3	2.21	0.40
1:C:420:VAL:HA	1:C:482:ALA:HA	2.03	0.40
2:D:170:VAL:HB	2:D:216:VAL:HG12	2.02	0.40
1:A:142:LYS:HE2	1:A:248:ASP:O	2.21	0.40
1:B:205:ALA:HA	1:B:296:ILE:CG2	2.51	0.40
1:B:678:ALA:C	1:B:680:GLU:N	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:ARG:HB2	1:B:695:SER:H	1.59	0.40
1:B:824:TYR:O	1:B:826:GLN:N	2.54	0.40
1:C:146:ALA:HB3	1:C:296:ILE:HB	2.02	0.40
1:C:220:ASN:OD1	1:C:222:ASN:N	2.32	0.40
1:C:484:VAL:HG12	1:C:569:MET:HE1	2.02	0.40
1:A:269:ARG:HA	1:A:273:LEU:HD13	2.03	0.40
1:A:364:SER:HB2	1:A:694:ARG:NH2	2.37	0.40
1:B:148:MET:O	1:B:293:TYR:HA	2.21	0.40
1:B:204:PHE:O	1:B:297:PRO:HD2	2.21	0.40
1:B:868:ASP:O	1:B:998:ALA:HB1	2.22	0.40
1:B:1204:TYR:C	1:B:1206:ALA:H	2.24	0.40
1:C:842:GLN:O	1:C:846:VAL:HG23	2.21	0.40
2:H:37:ILE:HD13	2:H:101:ASN:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1108/1290 (86%)	977 (88%)	117 (11%)	14 (1%)	10	41
1	B	1118/1290 (87%)	957 (86%)	132 (12%)	29 (3%)	4	28
1	C	1103/1290 (86%)	938 (85%)	135 (12%)	30 (3%)	4	28
2	D	224/226 (99%)	203 (91%)	18 (8%)	3 (1%)	10	41
2	F	224/226 (99%)	202 (90%)	18 (8%)	4 (2%)	7	35
2	H	224/226 (99%)	206 (92%)	15 (7%)	3 (1%)	10	41
3	E	212/215 (99%)	198 (93%)	13 (6%)	1 (0%)	25	59
3	G	212/215 (99%)	198 (93%)	13 (6%)	1 (0%)	25	59
3	I	210/215 (98%)	196 (93%)	12 (6%)	2 (1%)	13	46
All	All	4635/5193 (89%)	4075 (88%)	473 (10%)	87 (2%)	9	34

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	737	ALA
1	A	995	LYS
1	A	1153	TYR
1	A	1181	VAL
1	B	731	LEU
1	B	790	VAL
1	B	1055	ILE
1	B	1058	LEU
1	B	1108	LYS
1	C	695	SER
1	C	714	VAL
1	C	737	ALA
1	C	797	THR
1	C	865	PHE
1	C	966	SER
2	F	166	GLU
1	A	531	PRO
1	A	760	ALA
1	A	1055	ILE
1	B	41	ASP
1	B	855	SER
1	B	1119	GLN
1	B	1167	PRO
1	B	1182	ASP
1	B	1185	SER
1	C	60	GLN
1	C	622	ALA
1	C	727	CYS
1	C	732	GLY
1	C	767	PRO
1	C	906	MET
1	C	1161	PRO
2	D	117	LEU
2	D	118	ASP
2	F	117	LEU
2	F	118	ASP
2	H	117	LEU
2	H	118	ASP
1	A	1159	ALA
1	B	531	PRO
1	B	679	CYS
1	B	724	VAL

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Mol	Chain	Res	Type
1	B	767	PRO
1	B	865	PHE
1	B	903	PRO
1	B	994	GLN
1	C	167	HIS
1	C	399	PHE
1	C	531	PRO
1	C	813	GLY
1	C	888	SER
1	C	969	ALA
1	C	1052	GLY
1	C	1190	SER
1	A	399	PHE
1	A	1017	GLU
1	B	399	PHE
1	B	695	SER
1	B	1117	CYS
1	B	1165	ILE
1	C	66	ASN
1	C	641	TYR
1	C	648	TYR
1	C	902	ASP
1	C	962	ALA
3	I	100	LEU
1	A	888	SER
1	B	605	GLU
1	B	888	SER
1	B	1196	PRO
2	D	95	ALA
2	F	95	ALA
3	G	95	ASP
2	H	95	ALA
1	A	813	GLY
1	B	902	ASP
3	E	95	ASP
3	I	95	ASP
1	A	738	LEU
1	B	1131	PRO
1	C	604	VAL
1	C	724	VAL
1	B	861	ILE
1	A	766	HIS

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Mol	Chain	Res	Type
1	C	1143	PRO
1	B	1160	ASN
1	C	861	ILE

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	970/1118 (87%)	908 (94%)	62 (6%)	14	42
1	B	978/1118 (88%)	924 (94%)	54 (6%)	18	46
1	C	969/1118 (87%)	928 (96%)	41 (4%)	25	54
2	D	191/191 (100%)	175 (92%)	16 (8%)	9	32
2	F	191/191 (100%)	174 (91%)	17 (9%)	8	31
2	H	190/191 (100%)	174 (92%)	16 (8%)	9	32
3	E	188/189 (100%)	175 (93%)	13 (7%)	13	39
3	G	188/189 (100%)	176 (94%)	12 (6%)	14	42
3	I	187/189 (99%)	175 (94%)	12 (6%)	14	42
All	All	4052/4494 (90%)	3809 (94%)	243 (6%)	18	43

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	33	VAL
1	A	60	GLN
1	A	63	THR
1	A	67	ILE
1	A	108	ASP
1	A	167	HIS
1	A	341	PHE
1	A	409	TYR
1	A	429	SER
1	A	433	ILE

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Mol	Chain	Res	Type
1	A	458	VAL
1	A	506	LEU
1	A	530	VAL
1	A	599	GLN
1	A	606	TYR
1	A	608	LEU
1	A	621	THR
1	A	630	PHE
1	A	631	VAL
1	A	637	ASN
1	A	638	LEU
1	A	686	MET
1	A	693	THR
1	A	713	CYS
1	A	718	VAL
1	A	720	SER
1	A	721	SER
1	A	722	LEU
1	A	723	PHE
1	A	726	ASP
1	A	733	GLN
1	A	735	LEU
1	A	743	SER
1	A	757	MET
1	A	761	SER
1	A	764	PHE
1	A	768	ILE
1	A	773	LEU
1	A	780	LEU
1	A	790	VAL
1	A	794	TYR
1	A	798	THR
1	A	802	VAL
1	A	897	LYS
1	A	906	MET
1	A	940	ASP
1	A	943	MET
1	A	955	ILE
1	A	970	ILE
1	A	985	ILE
1	A	1039	GLU
1	A	1041	SER

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Mol	Chain	Res	Type
1	A	1059	ASP
1	A	1106	CYS
1	A	1111	SER
1	A	1121	THR
1	A	1124	VAL
1	A	1125	SER
1	A	1149	VAL
1	A	1153	TYR
1	A	1205	VAL
1	B	40	PHE
1	B	110	LYS
1	B	114	ASN
1	B	185	CYS
1	B	409	TYR
1	B	429	SER
1	B	430	PRO
1	B	433	ILE
1	B	458	VAL
1	B	506	LEU
1	B	530	VAL
1	B	611	VAL
1	B	621	THR
1	B	626	ARG
1	B	629	ARG
1	B	630	PHE
1	B	638	LEU
1	B	644	ASP
1	B	686	MET
1	B	687	SER
1	B	688	GLN
1	B	691	ARG
1	B	694	ARG
1	B	711	VAL
1	B	718	VAL
1	B	721	SER
1	B	722	LEU
1	B	723	PHE
1	B	724	VAL
1	B	729	LEU
1	B	731	LEU
1	B	738	LEU
1	B	764	PHE

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Mol	Chain	Res	Type
1	B	781	SER
1	B	791	THR
1	B	795	ILE
1	B	798	THR
1	B	802	VAL
1	B	854	LYS
1	B	865	PHE
1	B	967	PHE
1	B	990	LEU
1	B	996	LEU
1	B	997	ILE
1	B	1056	GLN
1	B	1057	ARG
1	B	1062	GLU
1	B	1110	GLN
1	B	1121	THR
1	B	1153	TYR
1	B	1165	ILE
1	B	1179	ARG
1	B	1184	TRP
1	B	1186	TYR
1	C	46	ARG
1	C	62	ARG
1	C	63	THR
1	C	183	PHE
1	C	409	TYR
1	C	433	ILE
1	C	458	VAL
1	C	480	ILE
1	C	506	LEU
1	C	530	VAL
1	C	604	VAL
1	C	638	LEU
1	C	641	TYR
1	C	691	ARG
1	C	718	VAL
1	C	722	LEU
1	C	723	PHE
1	C	728	LYS
1	C	735	LEU
1	C	780	LEU
1	C	784	THR

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Mol	Chain	Res	Type
1	C	790	VAL
1	C	796	GLN
1	C	802	VAL
1	C	808	GLN
1	C	810	VAL
1	C	853	VAL
1	C	862	ILE
1	C	865	PHE
1	C	960	TRP
1	C	970	ILE
1	C	1033	LEU
1	C	1042	ASN
1	C	1043	THR
1	C	1048	SER
1	C	1102	LYS
1	C	1106	CYS
1	C	1113	ARG
1	C	1121	THR
1	C	1191	PHE
1	C	1205	VAL
2	D	5	VAL
2	D	6	GLN
2	D	8	VAL
2	D	23	VAL
2	D	31	THR
2	D	35	TYR
2	D	48	LEU
2	D	51	MET
2	D	60	THR
2	D	61	VAL
2	D	112	TYR
2	D	117	LEU
2	D	124	THR
2	D	147	LYS
2	D	170	VAL
2	D	211	THR
3	E	9	GLN
3	E	10	SER
3	E	18	VAL
3	E	24	ILE
3	E	36	LEU
3	E	50	LEU

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Mol	Chain	Res	Type
3	E	97	TYR
3	E	128	GLN
3	E	139	LEU
3	E	153	LYS
3	E	189	ASP
3	E	193	HIS
3	E	213	PHE
2	F	5	VAL
2	F	6	GLN
2	F	8	VAL
2	F	23	VAL
2	F	31	THR
2	F	35	TYR
2	F	48	LEU
2	F	51	MET
2	F	60	THR
2	F	61	VAL
2	F	112	TYR
2	F	117	LEU
2	F	124	THR
2	F	147	LYS
2	F	164	PHE
2	F	170	VAL
2	F	211	THR
3	G	9	GLN
3	G	10	SER
3	G	18	VAL
3	G	24	ILE
3	G	36	LEU
3	G	97	TYR
3	G	128	GLN
3	G	139	LEU
3	G	153	LYS
3	G	189	ASP
3	G	193	HIS
3	G	213	PHE
2	H	5	VAL
2	H	6	GLN
2	H	8	VAL
2	H	23	VAL
2	H	31	THR
2	H	35	TYR

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Mol	Chain	Res	Type
2	H	48	LEU
2	H	51	MET
2	H	60	THR
2	H	61	VAL
2	H	117	LEU
2	H	124	THR
2	H	147	LYS
2	H	196	LEU
2	H	200	VAL
2	H	202	VAL
3	I	9	GLN
3	I	10	SER
3	I	18	VAL
3	I	24	ILE
3	I	36	LEU
3	I	97	TYR
3	I	128	GLN
3	I	139	LEU
3	I	153	LYS
3	I	189	ASP
3	I	193	HIS
3	I	213	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	280	GLN
1	A	346	GLN
1	A	408	ASN
1	A	599	GLN
1	A	733	GLN
1	A	808	GLN
1	A	812	ASN
1	A	839	ASN
1	A	987	GLN
1	A	993	ASN
1	A	999	ASN
1	A	1056	GLN
1	A	1176	ASN
1	B	107	GLN
1	B	111	GLN

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Mol	Chain	Res	Type
1	B	166	ASN
1	B	208	HIS
1	B	346	GLN
1	B	408	ASN
1	B	765	ASN
1	B	842	GLN
1	B	1016	ASN
1	B	1072	ASN
1	B	1104	ASN
1	B	1110	GLN
1	B	1132	ASN
1	C	298	HIS
1	C	346	GLN
1	C	408	ASN
1	C	647	ASN
1	C	719	ASN
1	C	792	GLN
1	C	812	ASN
1	C	842	GLN
1	C	1023	GLN
1	C	1042	ASN
1	C	1084	GLN
1	C	1119	GLN
1	C	1176	ASN
2	D	6	GLN
2	D	114	GLN
3	E	93	GLN
3	E	96	ASN
3	E	142	ASN
3	E	164	GLN
2	F	6	GLN
2	F	114	GLN
3	G	93	GLN
3	G	96	ASN
3	G	142	ASN
3	G	164	GLN
2	H	6	GLN
2	H	114	GLN
2	H	210	GLN
3	I	93	GLN
3	I	96	ASN
3	I	142	ASN

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Mol	Chain	Res	Type
3	I	164	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

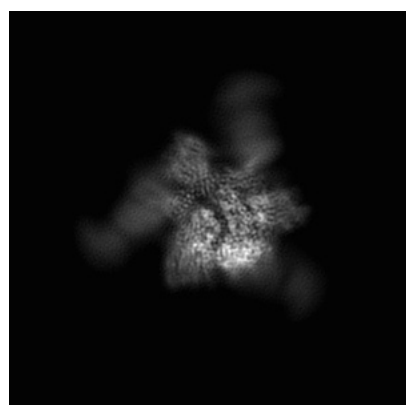
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31683. These allow visual inspection of the internal detail of the map and identification of artifacts.

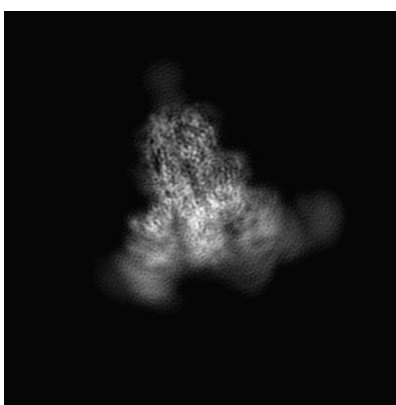
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

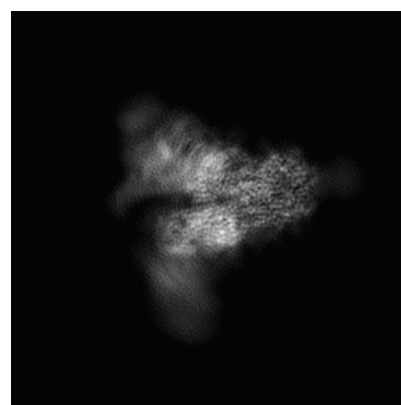
6.1.1 Primary map



X



Y

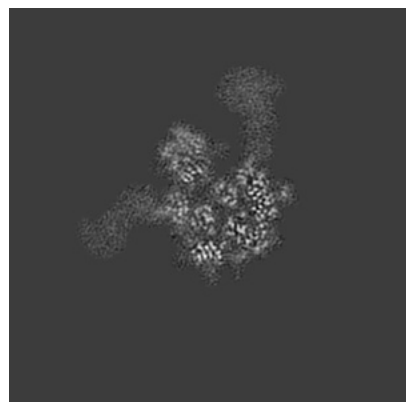


Z

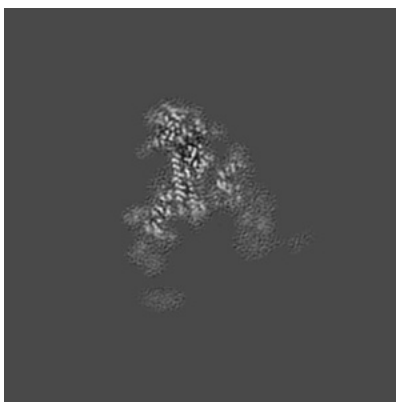
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

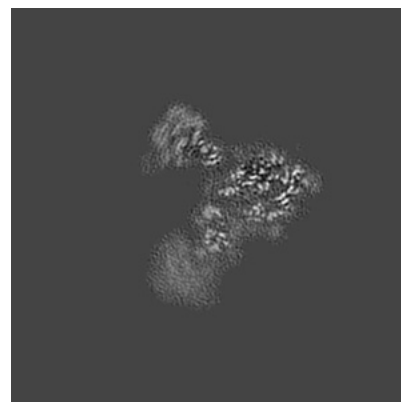
6.2.1 Primary map



X Index: 160



Y Index: 160

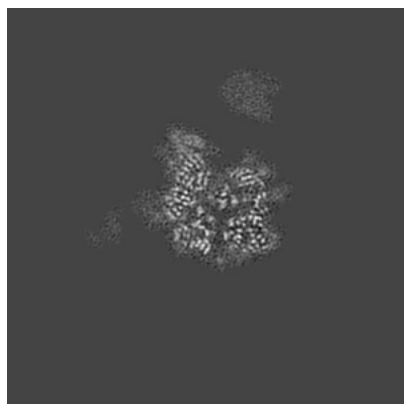


Z Index: 160

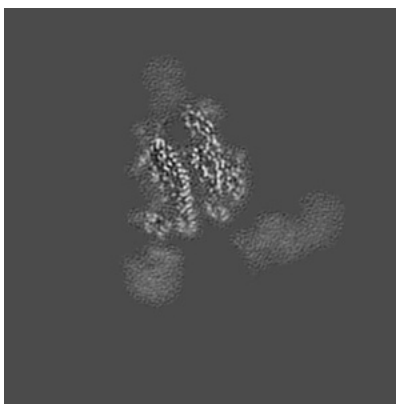
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

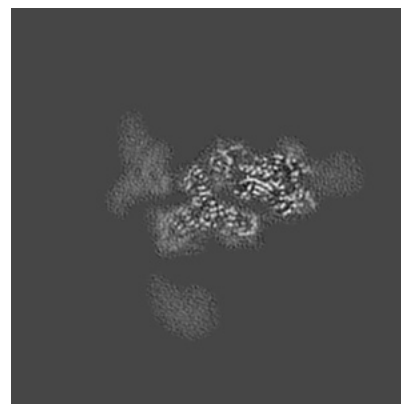
6.3.1 Primary map



X Index: 167



Y Index: 179

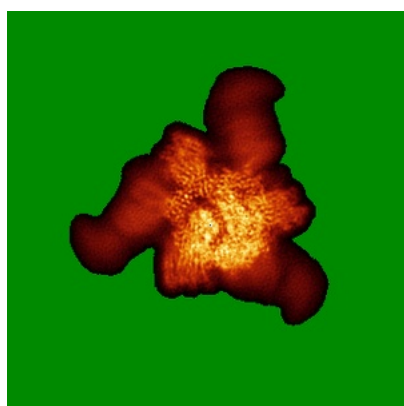


Z Index: 127

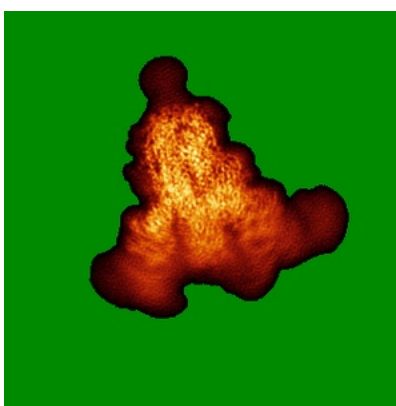
The images above show the largest variance slices of the map in three orthogonal directions.

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

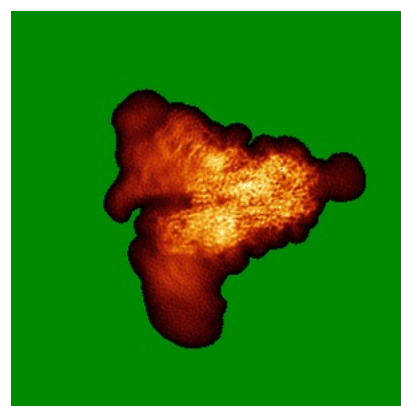
6.4.1 Primary map



X



Y

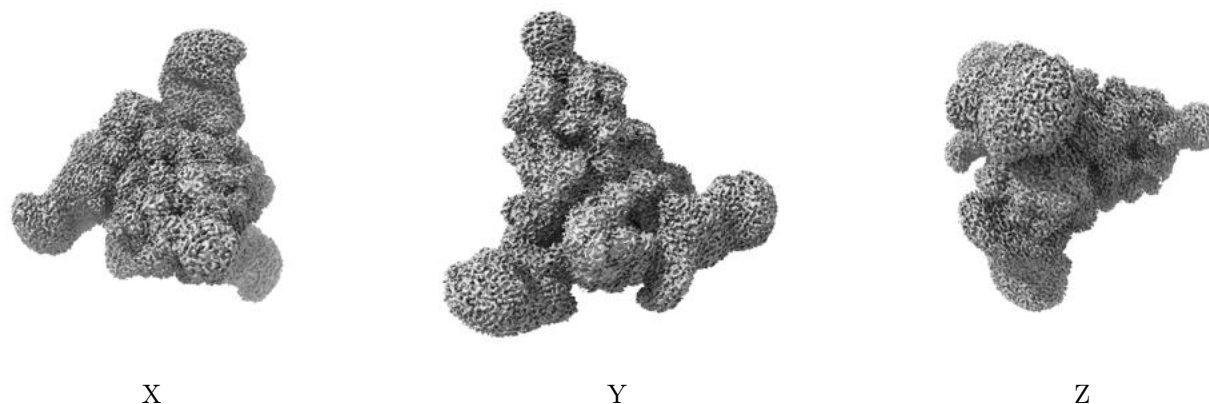


Z

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

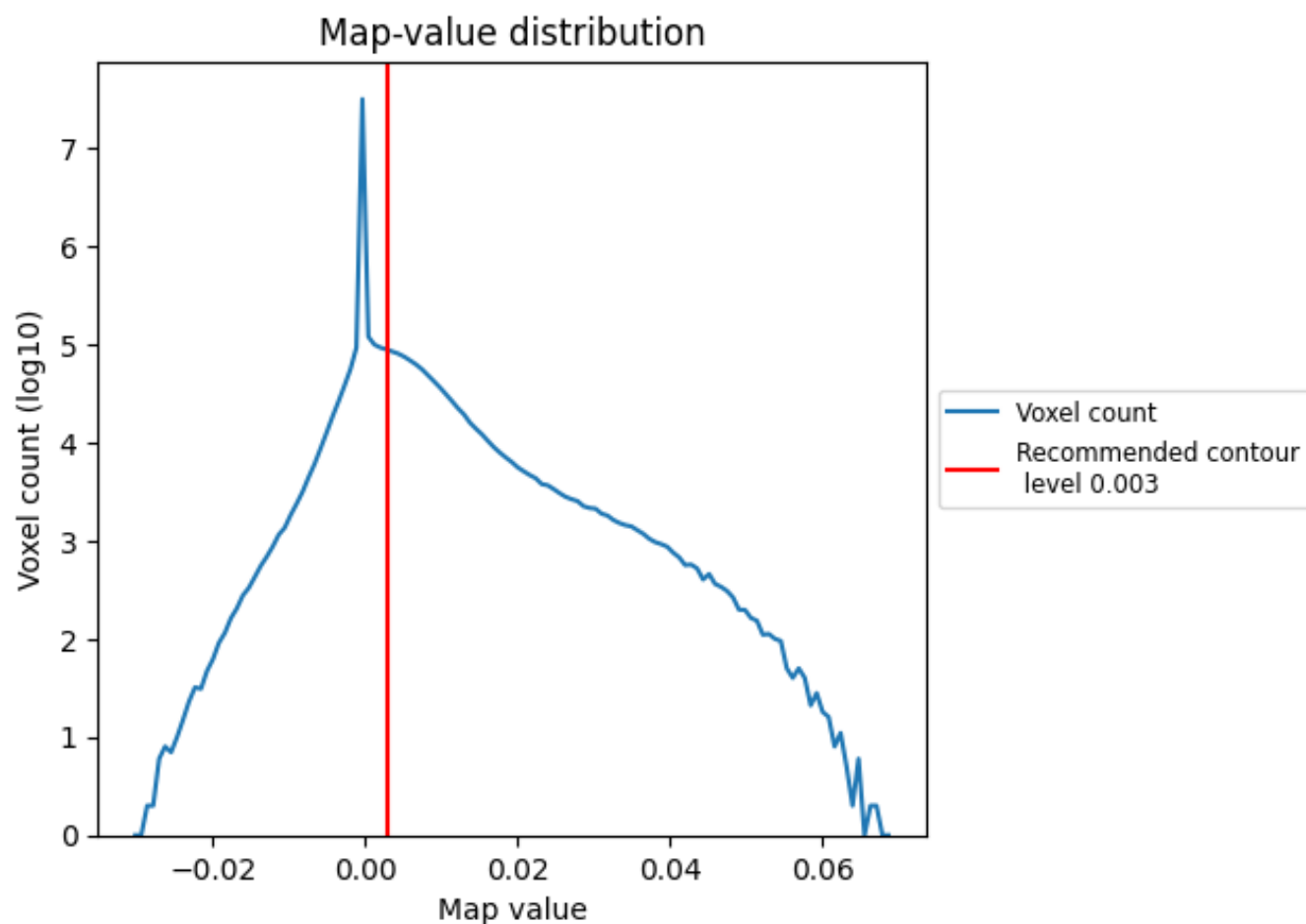
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

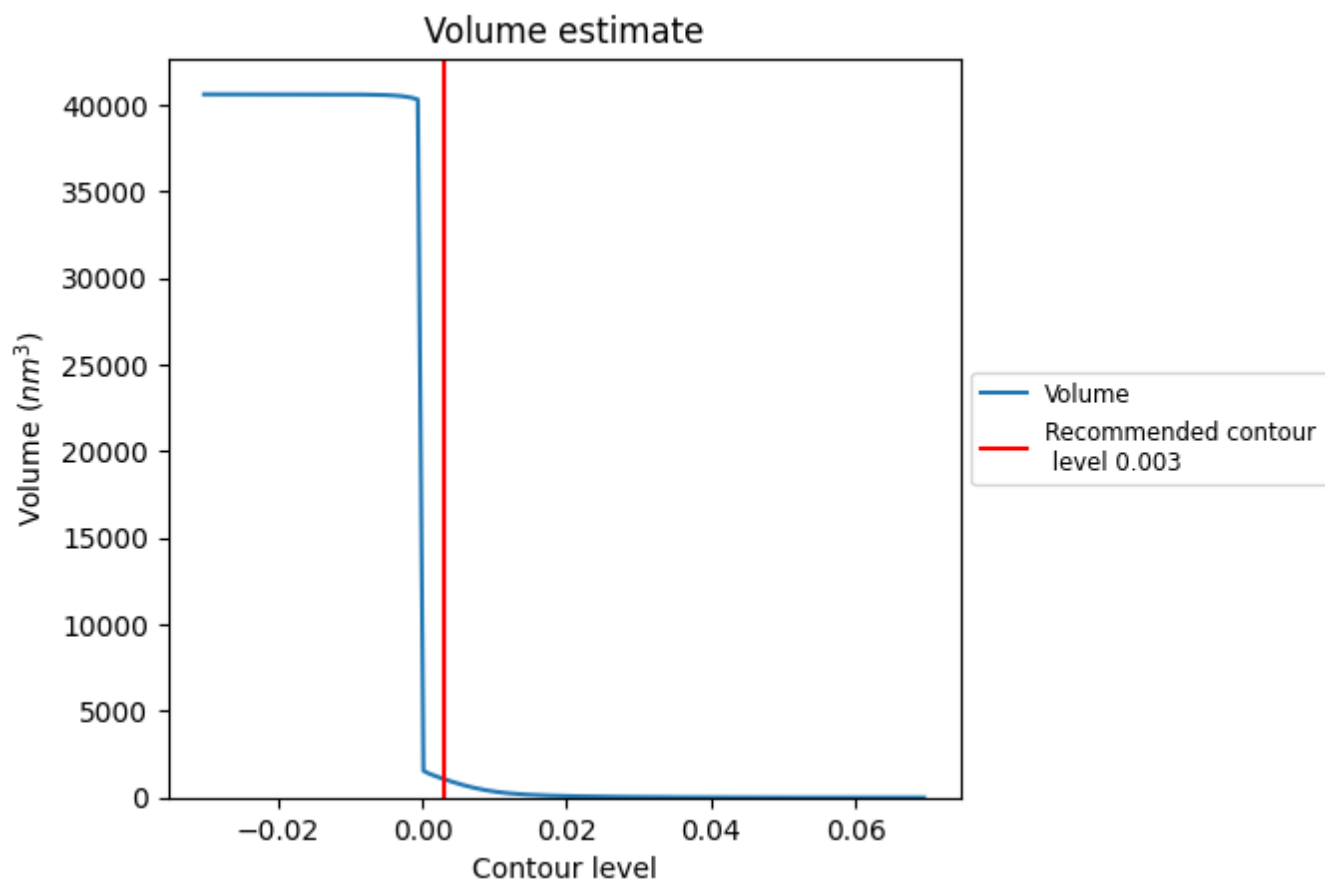
This section contains the results of statistical analysis of the map.

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.

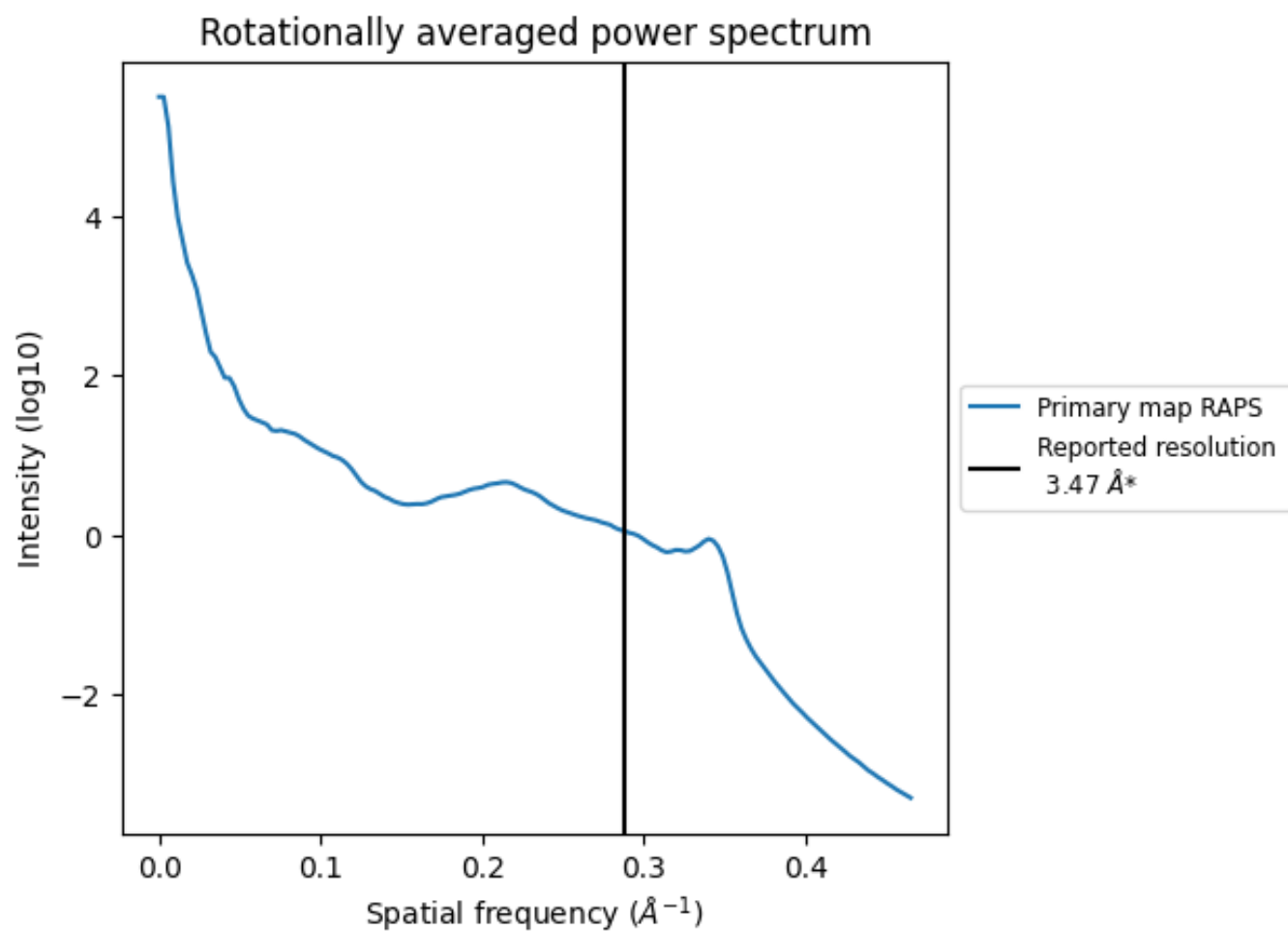
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1070 nm³; this corresponds to an approximate mass of 967 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 0.288 Å⁻¹

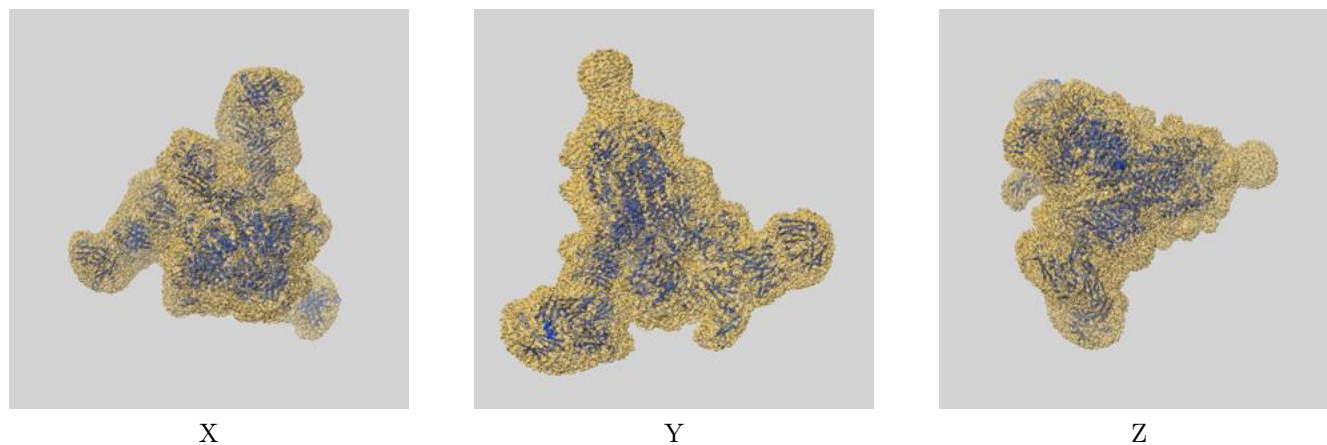
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

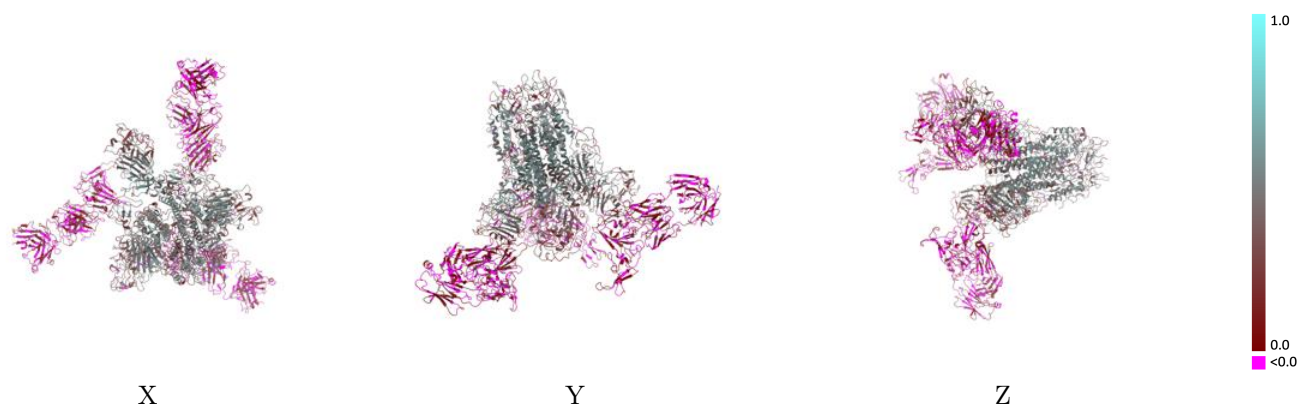
This section contains information regarding the fit between EMDB map EMD-31683 and PDB model 7V3L. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



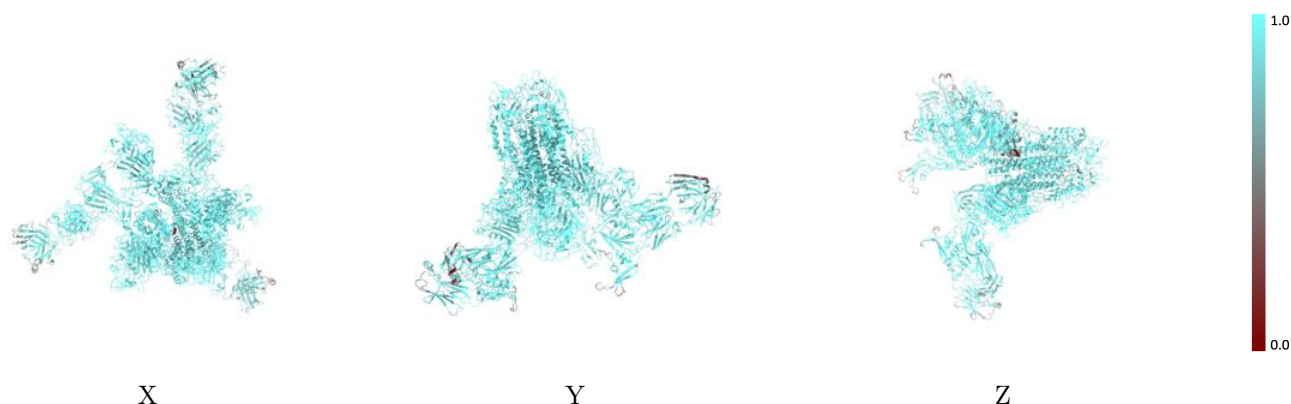
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



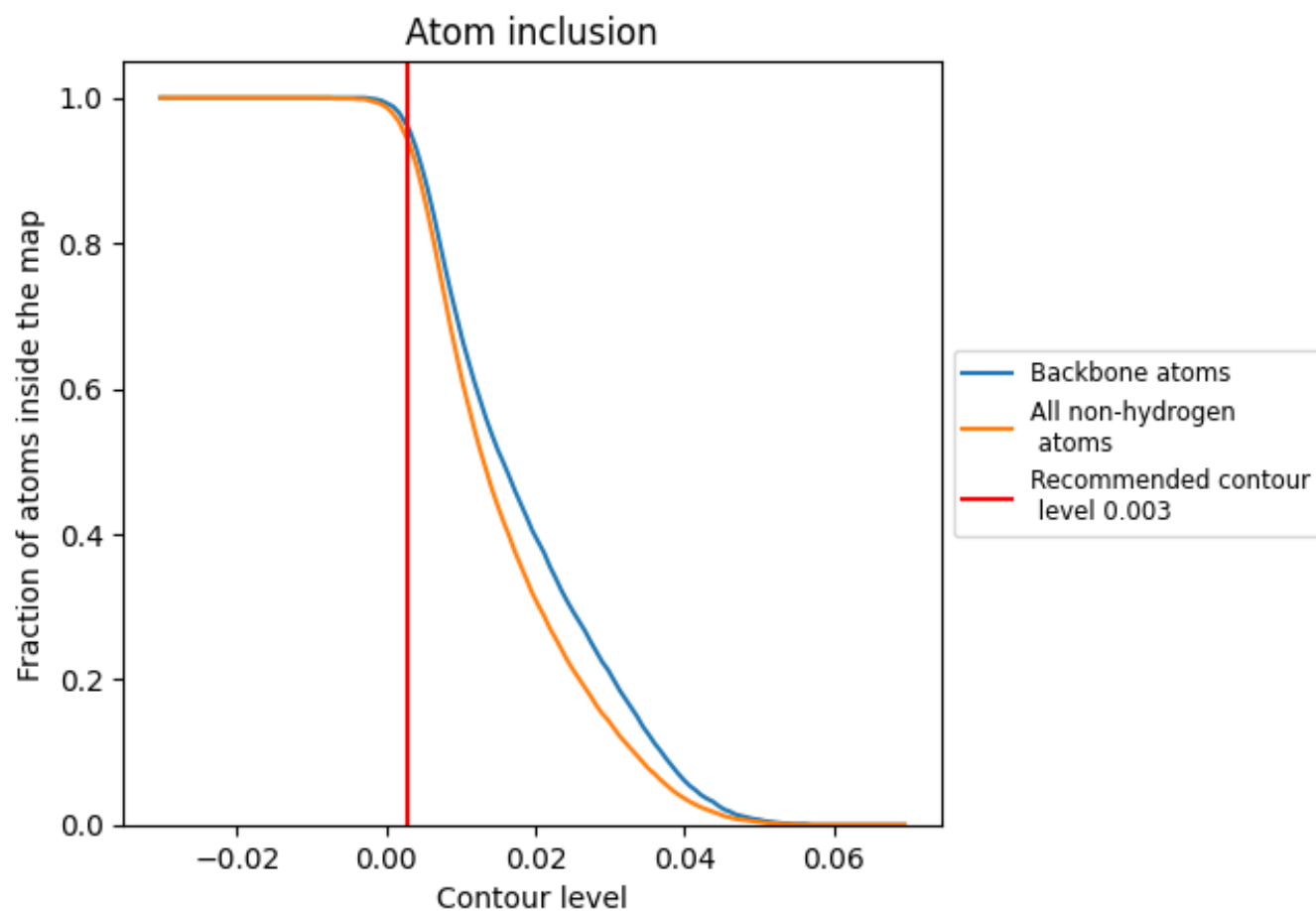
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9400</div>	<div><div></div>0.2560</div>
A	<div><div></div>0.9640</div>	<div><div></div>0.3380</div>
B	<div><div></div>0.9630</div>	<div><div></div>0.3520</div>
C	<div><div></div>0.9680</div>	<div><div></div>0.3390</div>
D	<div><div></div>0.8610</div>	<div><div></div>0.0170</div>
E	<div><div></div>0.8950</div>	<div><div></div>0.0350</div>
F	<div><div></div>0.8510</div>	<div><div></div>0.0400</div>
G	<div><div></div>0.8600</div>	<div><div></div>0.0300</div>
H	<div><div></div>0.9060</div>	<div><div></div>0.0200</div>
I	<div><div></div>0.8800</div>	<div><div></div>0.0120</div>

1.0

0.0

<0.0