



Full wwPDB EM Validation Report ⓘ

Sep 17, 2026 – 10:23 am BST

PDB ID : 9SLF / pdb_00009slf
EMDB ID : EMD-54988
Title : Open conformation dome complex including the Sec-translocon (SecYEG-SecA-SecDF) in untreated Mycoplasma pneumoniae cells
Authors : Jensen, R.K.; Xue, L.; Mahamid, J.
Deposited on : 2025-09-03
Resolution : 17.00 Å(reported)
Based on initial model : .

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:

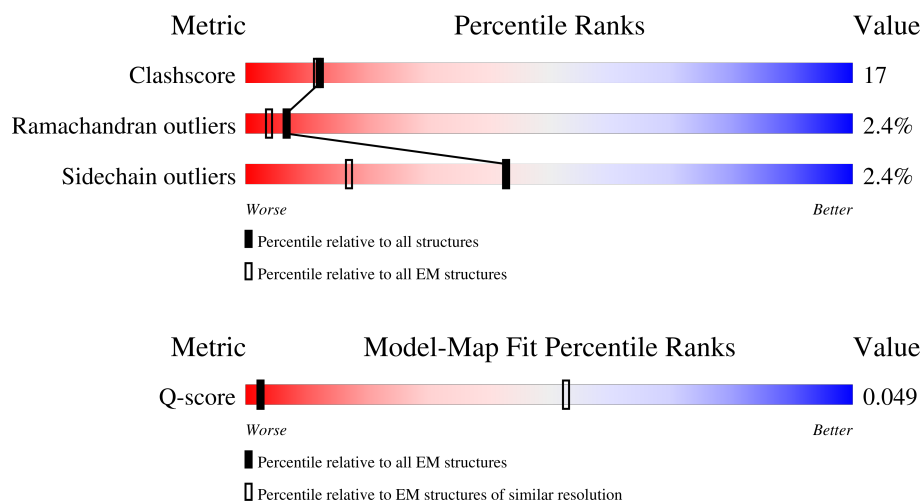
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 17.00 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	38 (16.50 - 17.50)

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	D	971	
2	E	125	
3	G	76	
4	Y	477	

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Mol	Chain	Length	Quality of chain
5	C	1298	 16% 77% 22% .
6	F	1274	 14% 70% 28% .
7	B	1217	 7% 76% 23% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 41483 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 SecDF.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	938	Total	C	N	O	S	0	0
			7388	4804	1218	1356	10		

- Molecule 2 is a protein called SecE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	71	Total	C	N	O	S	0	0
			573	393	89	90	1		

- Molecule 3 is a protein called Probable protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	76	Total	C	N	O	S	0	0
			585	391	93	96	5		

- Molecule 4 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Y	435	Total	C	N	O	S	0	0
			3338	2200	539	591	8		

- Molecule 5 is a protein called Uncharacterized lipoprotein MG309 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	1297	Total	C	N	O	S	0	0
			10101	6304	1723	2068	6		

- Molecule 6 is a protein called Uncharacterized lipoprotein MG338 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	1273	Total	C	N	O	S	0	0
			9894	6200	1706	1977	11		

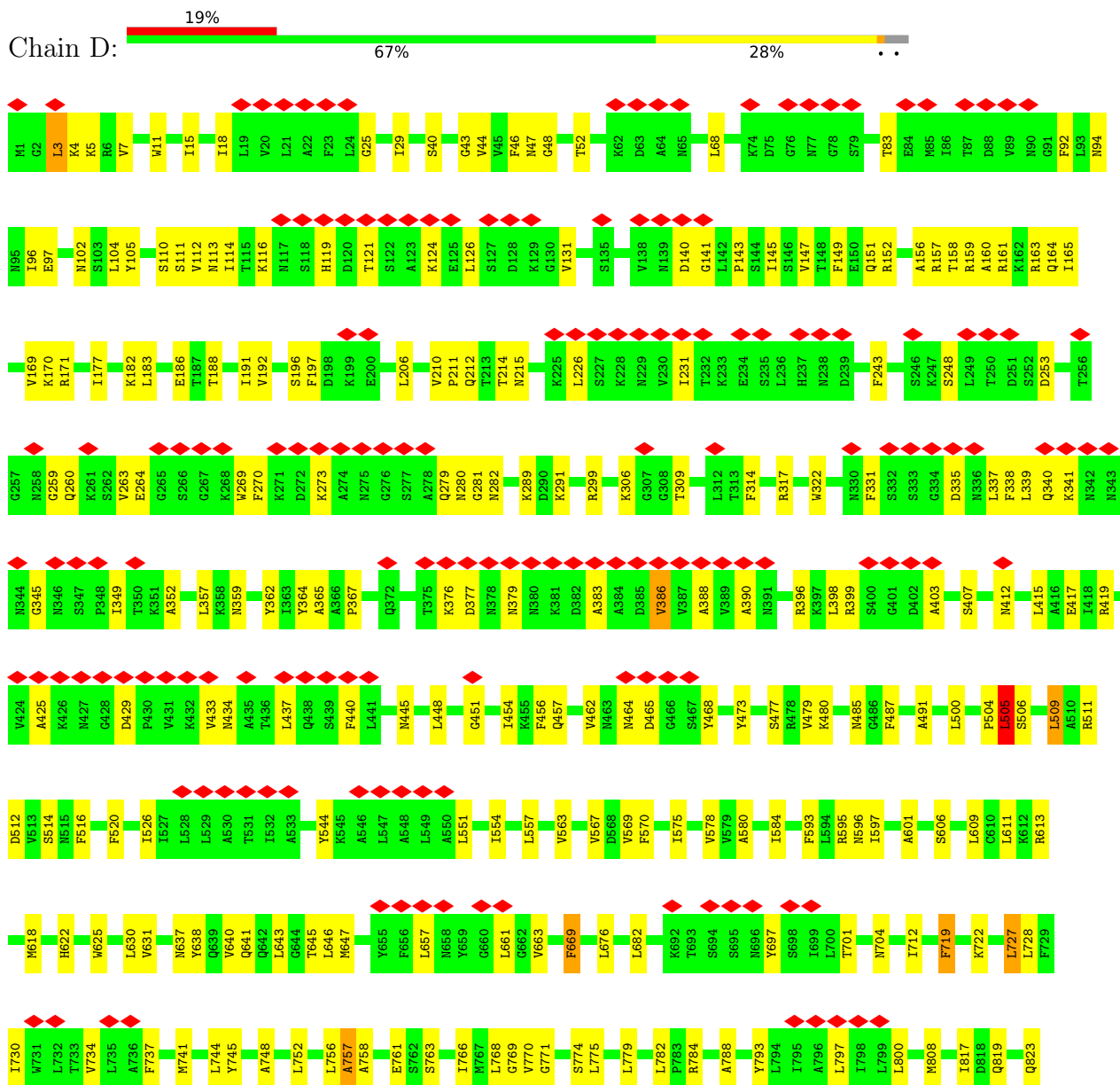
- Molecule 7 is a protein called Uncharacterized lipoprotein MG307 homolog.

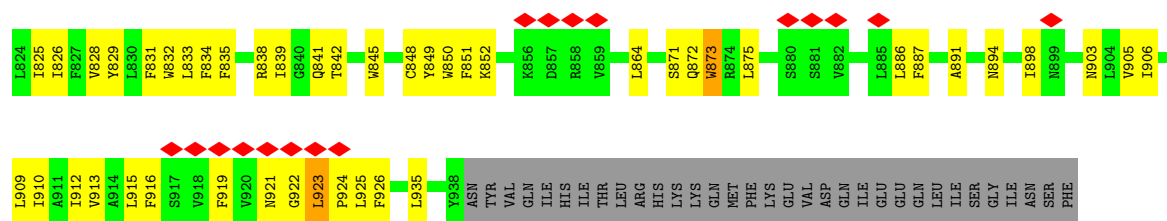
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	1216	9604	6055	1627	1915	7	0	0

3 Residue-property plots

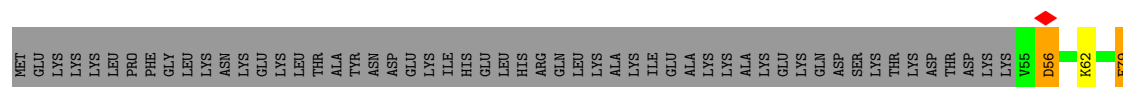
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

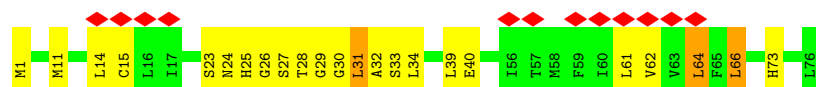




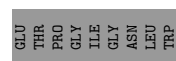
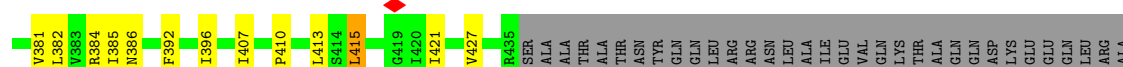
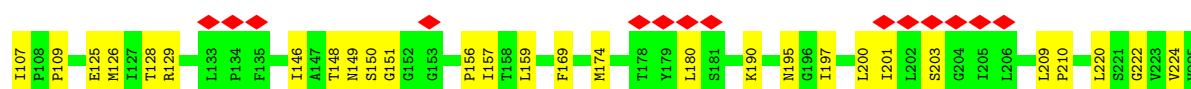
- Molecule 2: SecE



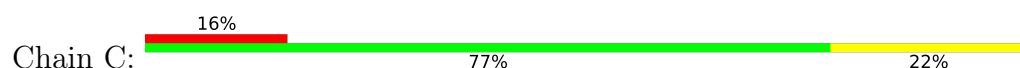
- Molecule 3: Probable protein-export membrane protein SecG

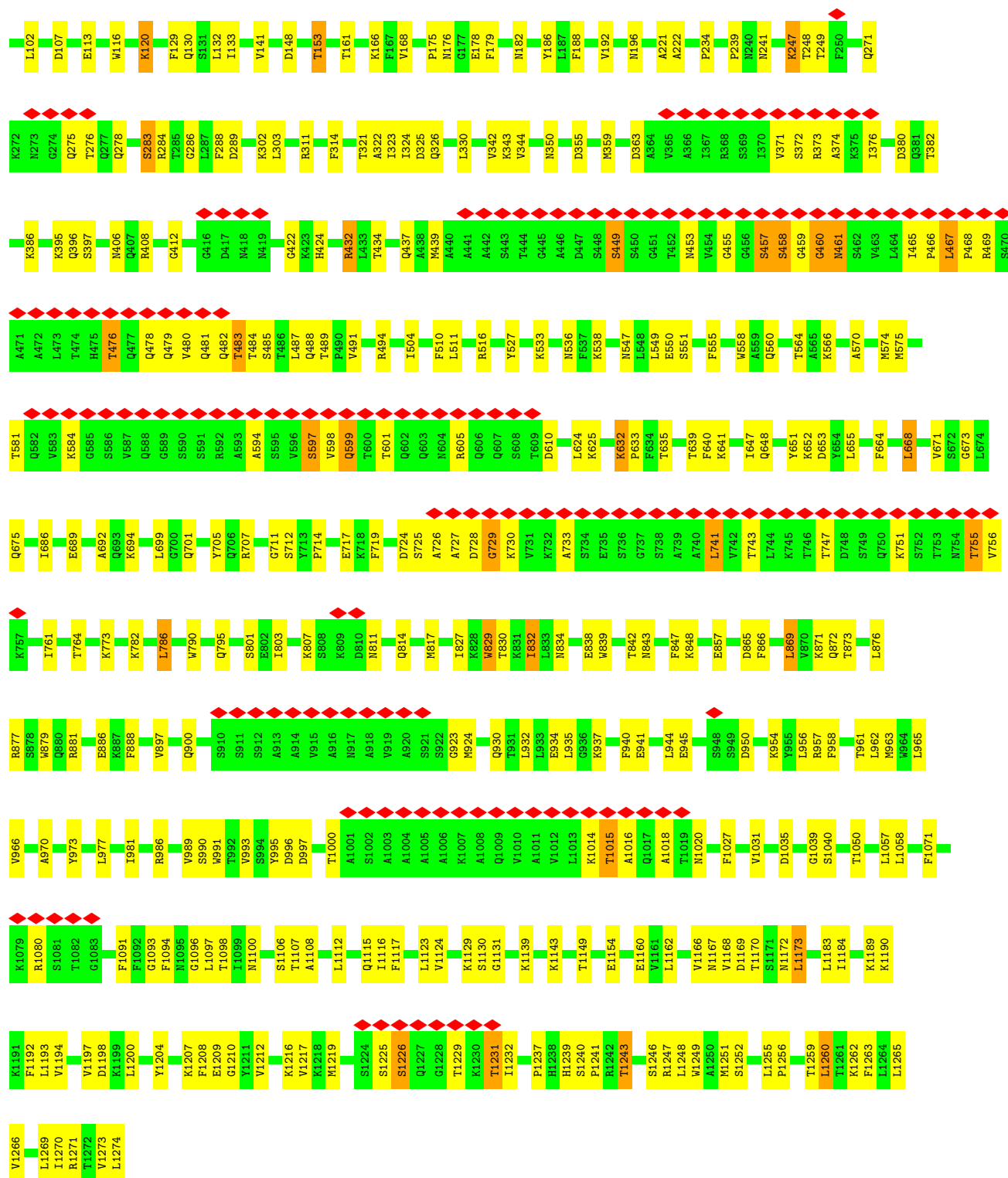


- Molecule 4: Protein translocase subunit SecY

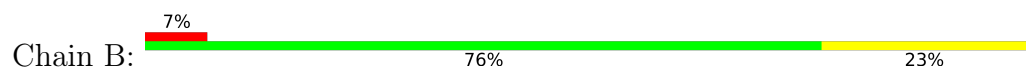


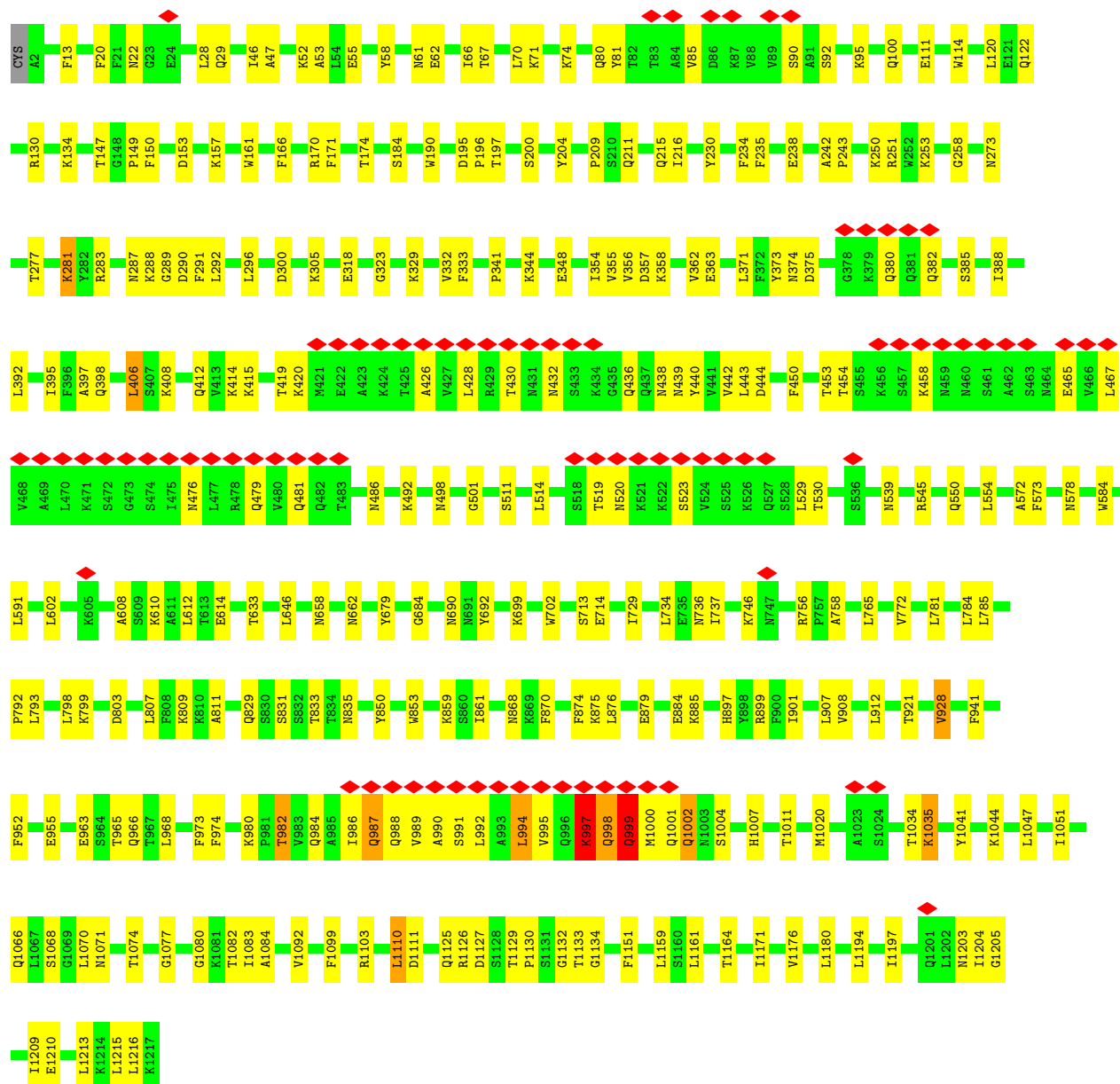
- Molecule 5: Uncharacterized lipoprotein MG309 homolog





- Molecule 7: Uncharacterized lipoprotein MG307 homolog





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	1001	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	115	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.837	Depositor
Minimum map value	-0.866	Depositor
Average map value	0.031	Depositor
Map value standard deviation	0.290	Depositor
Recommended contour level	0.354	Depositor
Map size (Å)	297.69598, 297.69598, 297.69598	wwPDB
Map dimensions	56, 56, 56	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	5.3159995, 5.3159995, 5.3159995	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	D	0.67	0/7549	1.07	1/10241 (0.0%)
2	E	0.68	0/587	1.14	0/791
3	G	0.68	0/592	1.08	0/795
4	Y	0.70	0/3406	1.10	2/4634 (0.0%)
5	C	0.88	9/10260 (0.1%)	1.06	4/13850 (0.0%)
6	F	0.91	9/10076 (0.1%)	1.10	9/13621 (0.1%)
7	B	0.85	4/9772 (0.0%)	1.05	3/13211 (0.0%)
All	All	0.83	22/42242 (0.1%)	1.07	19/57143 (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
2	E	0	1
4	Y	0	2
5	C	0	1
6	F	0	16
7	B	0	6
All	All	0	26

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1031	LYS	CE-NZ	-17.75	0.96	1.49
7	B	1035	LYS	CE-NZ	-17.35	0.97	1.49
6	F	1015	THR	CB-OG1	-16.77	1.17	1.43
6	F	694	LYS	CE-NZ	-16.11	1.01	1.49
5	C	149	LYS	CE-NZ	-15.78	1.02	1.49
6	F	120	LYS	CE-NZ	-15.30	1.03	1.49
5	C	226	LYS	CE-NZ	-14.49	1.05	1.49
6	F	395	LYS	CE-NZ	-13.56	1.08	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	247	LYS	CE-NZ	-13.48	1.08	1.49
5	C	1124	LYS	CE-NZ	-13.07	1.10	1.49
5	C	860	LYS	CE-NZ	-12.87	1.10	1.49
7	B	281	LYS	CE-NZ	-12.72	1.11	1.49
7	B	250	LYS	CE-NZ	-12.41	1.12	1.49
5	C	385	LYS	CE-NZ	-12.40	1.12	1.49
7	B	71	LYS	CE-NZ	-11.11	1.16	1.49
6	F	1015	THR	CB-CG2	-10.40	1.18	1.52
6	F	632	LYS	CE-NZ	-9.72	1.20	1.49
6	F	1015	THR	N-CA	-7.71	1.36	1.46
6	F	632	LYS	C-O	-6.42	1.18	1.24
5	C	1124	LYS	C-N	-5.90	1.25	1.33
5	C	860	LYS	C-O	-5.26	1.18	1.24
5	C	1123	ASN	C-N	-5.17	1.25	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	461	ASN	N-CA-C	7.29	121.93	112.89
5	C	369	ASP	N-CA-C	7.22	119.83	111.02
5	C	507	ASP	CA-CB-CG	7.16	119.76	112.60
7	B	1035	LYS	CD-CE-NZ	6.19	131.70	111.90
6	F	458	SER	N-CA-C	6.14	120.94	112.90
6	F	597	SER	N-CA-C	6.13	117.79	110.19
6	F	1015	THR	CA-CB-OG1	5.75	118.22	109.60
6	F	460	GLY	CA-C-N	5.53	130.82	121.14
6	F	460	GLY	C-N-CA	5.53	130.82	121.14
5	C	368	SER	CA-C-N	5.49	128.42	120.79
5	C	368	SER	C-N-CA	5.49	128.42	120.79
6	F	459	GLY	N-CA-C	5.43	119.52	112.25
7	B	520	ASN	CA-C-N	5.31	129.10	120.60
7	B	520	ASN	C-N-CA	5.31	129.10	120.60
6	F	457	SER	N-CA-C	5.24	116.68	110.19
4	Y	289	VAL	CA-C-N	5.23	123.54	120.24
4	Y	289	VAL	C-N-CA	5.23	123.54	120.24
1	D	722	LYS	N-CA-C	5.14	117.63	111.71
6	F	599	GLN	N-CA-C	5.08	117.26	110.35

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	B	458	LYS	Peptide
7	B	987	GLN	Peptide
7	B	994	LEU	Peptide
7	B	997	LYS	Peptide
7	B	998	GLN	Peptide
7	B	999	GLN	Peptide
5	C	369	ASP	Peptide
2	E	122	PHE	Sidechain
6	F	1225	SER	Peptide
6	F	1226	SER	Peptide
6	F	275	GLN	Peptide
6	F	432	ARG	Sidechain
6	F	449	SER	Peptide
6	F	453	ASN	Peptide
6	F	455	GLY	Peptide
6	F	457	SER	Peptide
6	F	458	SER	Peptide
6	F	460	GLY	Peptide
6	F	461	ASN	Peptide
6	F	467	LEU	Peptide
6	F	594	ALA	Peptide
6	F	597	SER	Peptide
6	F	598	VAL	Peptide
6	F	599	GLN	Peptide
4	Y	58	THR	Peptide
4	Y	68	PHE	Sidechain

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	D	7388	0	7428	410	0
2	E	573	0	627	17	0
3	G	585	0	646	27	0
4	Y	3338	0	3524	142	0
5	C	10101	0	9905	305	0
6	F	9894	0	9754	499	0
7	B	9604	0	9523	347	0
All	All	41483	0	41407	1421	0

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

All (1421) 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)
5:C:148:THR:HB	7:B:1084:ALA:CB	1.33	1.56
6:F:1169:ASP:CB	7:B:147:THR:HB	1.36	1.55
7:B:984:GLN:NE2	7:B:1133:THR:CG2	1.70	1.54
6:F:1169:ASP:HB3	7:B:147:THR:CB	1.41	1.50
1:D:161:ARG:HB3	6:F:88:ASP:CB	1.45	1.46
7:B:984:GLN:CG	7:B:1133:THR:H	1.15	1.42
1:D:160:ALA:CB	6:F:82:GLU:O	1.72	1.35
5:C:609:GLN:CD	6:F:248:THR:HG21	1.53	1.33
6:F:1167:ASN:O	7:B:149:PRO:HA	1.24	1.32
6:F:1071:PHE:HD2	6:F:1247:ARG:CZ	1.40	1.32
1:D:157:ARG:CB	6:F:91:GLN:OE1	1.76	1.32
1:D:164:GLN:HG3	6:F:85:ASN:ND2	1.45	1.32
1:D:161:ARG:CB	6:F:88:ASP:HB2	1.56	1.31
1:D:44:VAL:HG13	1:D:567:VAL:O	1.28	1.31
5:C:156:GLU:OE2	7:B:1125:GLN:CD	1.74	1.30
1:D:110:SER:O	4:Y:227:ILE:HG23	1.32	1.30
6:F:1071:PHE:CD2	6:F:1247:ARG:CZ	2.14	1.30
1:D:158:THR:C	6:F:84:ASP:O	1.72	1.30
5:C:154:LEU:CD1	7:B:1074:THR:CG2	2.10	1.30
6:F:1167:ASN:O	7:B:149:PRO:CA	1.80	1.28
1:D:873:TRP:NE1	1:D:926:PHE:CE2	2.01	1.28
1:D:160:ALA:HA	6:F:81:ASP:O	1.35	1.26
5:C:148:THR:CB	7:B:1084:ALA:HB1	1.66	1.26
1:D:160:ALA:HB2	6:F:82:GLU:O	1.27	1.26
5:C:148:THR:CB	7:B:1084:ALA:CB	2.12	1.25
5:C:152:LYS:HB3	7:B:1071:ASN:ND2	1.47	1.25
1:D:264:GLU:OE1	1:D:269:TRP:CB	1.85	1.25
5:C:151:THR:HB	7:B:1071:ASN:OD1	1.34	1.25
1:D:164:GLN:N	6:F:85:ASN:HD21	1.33	1.24
1:D:396:ARG:O	1:D:419:ARG:NH1	1.68	1.23
7:B:984:GLN:NE2	7:B:1133:THR:HG23	0.91	1.23
1:D:873:TRP:CD1	1:D:926:PHE:HE2	1.56	1.21
5:C:156:GLU:CD	7:B:1125:GLN:OE1	1.82	1.21
1:D:264:GLU:OE1	1:D:269:TRP:HB2	1.05	1.21
6:F:1169:ASP:HB2	7:B:147:THR:O	1.08	1.20
6:F:877:ARG:NH1	6:F:1270:ILE:HG22	1.54	1.20
5:C:144:VAL:HG21	7:B:1080:GLY:HA3	1.20	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ARG:C	6:F:85:ASN:OD1	1.85	1.17
1:D:156:ALA:HB1	6:F:88:ASP:OD2	1.04	1.17
6:F:1169:ASP:CB	7:B:147:THR:O	1.91	1.16
5:C:149:LYS:HD3	7:B:1083:ILE:CG2	1.76	1.16
5:C:148:THR:C	7:B:1084:ALA:CB	2.19	1.15
1:D:156:ALA:CB	6:F:88:ASP:OD2	1.93	1.15
5:C:154:LEU:HG	7:B:1074:THR:HG21	1.23	1.15
6:F:900:GLN:NE2	6:F:934:GLU:HG2	1.61	1.15
5:C:1096:ILE:O	5:C:1130:LYS:NZ	1.78	1.14
6:F:962:LEU:HA	6:F:1269:LEU:HD11	1.24	1.14
6:F:1071:PHE:CD2	6:F:1247:ARG:NE	2.15	1.14
7:B:986:ILE:HD12	7:B:1130:PRO:HB3	1.21	1.13
1:D:270:PHE:HB3	1:D:396:ARG:NH2	1.63	1.12
5:C:154:LEU:HD11	7:B:1074:THR:HG22	1.22	1.12
7:B:984:GLN:CG	7:B:1133:THR:N	1.81	1.12
1:D:43:GLY:O	1:D:520:PHE:HE2	1.32	1.12
5:C:147:LEU:HD22	7:B:1082:THR:CG2	1.79	1.12
5:C:144:VAL:HG11	7:B:1080:GLY:O	1.49	1.12
5:C:154:LEU:CG	7:B:1074:THR:HG21	1.80	1.12
6:F:900:GLN:HE21	6:F:934:GLU:CG	1.62	1.12
7:B:984:GLN:HG3	7:B:1133:THR:H	0.97	1.11
1:D:161:ARG:CA	6:F:85:ASN:OD1	1.98	1.10
1:D:280:ASN:O	1:D:396:ARG:NH1	1.82	1.10
7:B:984:GLN:CD	7:B:1133:THR:N	2.08	1.10
5:C:144:VAL:CG2	7:B:1080:GLY:HA3	1.80	1.09
6:F:900:GLN:NE2	6:F:934:GLU:CG	2.15	1.09
1:D:873:TRP:CD1	1:D:926:PHE:CE2	2.39	1.09
5:C:144:VAL:HG21	7:B:1080:GLY:CA	1.82	1.09
5:C:262:ASN:OD1	7:B:988:GLN:NE2	1.84	1.09
6:F:343:LYS:HE2	6:F:439:MET:HB2	1.12	1.09
1:D:563:VAL:HG11	4:Y:231:LEU:HB2	1.26	1.09
6:F:130:GLN:HE22	6:F:560:GLN:HG2	1.11	1.08
6:F:997:ASP:HB2	6:F:1241:PRO:HB3	1.36	1.08
6:F:1071:PHE:HB2	6:F:1247:ARG:NH2	1.69	1.08
5:C:609:GLN:NE2	6:F:248:THR:HG21	1.68	1.08
1:D:163:ARG:NH2	6:F:80:GLU:HB2	1.69	1.07
6:F:1172:ASN:ND2	7:B:171:PHE:HD2	1.52	1.07
1:D:161:ARG:CB	6:F:88:ASP:CB	2.22	1.06
1:D:270:PHE:HB3	1:D:396:ARG:HH21	1.15	1.06
6:F:877:ARG:CZ	6:F:1270:ILE:HG22	1.85	1.06
6:F:707:ARG:NH2	6:F:886:GLU:O	1.89	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:LYS:HE3	1:D:197:PHE:HD2	1.20	1.06
1:D:44:VAL:CG1	1:D:567:VAL:O	2.03	1.05
1:D:338:PHE:HE2	1:D:359:ASN:HB3	1.21	1.05
5:C:149:LYS:N	7:B:1084:ALA:HB2	1.70	1.05
5:C:154:LEU:HD11	7:B:1074:THR:CG2	1.78	1.05
7:B:785:LEU:HD21	7:B:793:LEU:HD12	1.37	1.04
5:C:806:VAL:HG13	5:C:818:GLY:HA2	1.37	1.04
6:F:962:LEU:HA	6:F:1269:LEU:CD1	1.87	1.04
5:C:607:ASN:C	6:F:247:LYS:HB2	1.81	1.04
7:B:986:ILE:CD1	7:B:1130:PRO:HB3	1.86	1.04
6:F:343:LYS:CE	6:F:439:MET:HB2	1.87	1.03
6:F:692:ALA:HB2	7:B:243:PRO:HD2	1.39	1.03
6:F:961:THR:HB	6:F:1269:LEU:CD2	1.88	1.03
6:F:866:PHE:CE1	6:F:1262:LYS:HG2	1.93	1.03
7:B:283:ARG:CD	7:B:290:ASP:OD1	2.06	1.03
7:B:283:ARG:HD3	7:B:290:ASP:OD1	1.58	1.03
1:D:110:SER:O	4:Y:227:ILE:CG2	2.06	1.02
1:D:157:ARG:HB3	6:F:91:GLN:CD	1.84	1.02
7:B:1099:PHE:HE1	7:B:1103:ARG:NH2	1.58	1.02
1:D:264:GLU:CD	1:D:269:TRP:HB2	1.85	1.01
1:D:645:THR:HG23	4:Y:231:LEU:HD22	1.36	1.01
1:D:157:ARG:HB3	6:F:91:GLN:OE1	0.84	1.01
5:C:149:LYS:HD3	7:B:1083:ILE:HG23	1.40	1.01
1:D:509:LEU:HB2	1:D:823:GLN:NE2	1.75	1.01
7:B:756:ARG:NH2	7:B:1205:GLY:O	1.93	1.01
5:C:147:LEU:HD22	7:B:1082:THR:HG21	1.39	1.01
6:F:22:PHE:CE1	6:F:827:ILE:HD11	1.97	1.00
5:C:152:LYS:CB	7:B:1071:ASN:ND2	2.23	1.00
5:C:607:ASN:HA	6:F:247:LYS:CB	1.91	1.00
5:C:152:LYS:CA	7:B:1071:ASN:HD21	1.73	1.00
6:F:396:GLN:NE2	6:F:412:GLY:HA2	1.77	0.99
5:C:609:GLN:CG	6:F:248:THR:HG21	1.92	0.99
1:D:160:ALA:HB1	6:F:82:GLU:O	1.57	0.99
1:D:164:GLN:H	6:F:85:ASN:ND2	1.59	0.99
5:C:152:LYS:N	7:B:1071:ASN:OD1	1.95	0.99
5:C:148:THR:HB	7:B:1084:ALA:HB3	1.01	0.99
5:C:149:LYS:CB	7:B:1084:ALA:HB2	1.92	0.99
4:Y:67:PHE:CZ	4:Y:71:PHE:HE2	1.79	0.98
5:C:152:LYS:CB	7:B:1071:ASN:HD21	1.77	0.98
1:D:338:PHE:CE2	1:D:359:ASN:HB3	1.99	0.98
1:D:291:LYS:HE3	1:D:357:LEU:HD22	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:807:LYS:HE3	6:F:811:ASN:OD1	1.62	0.98
1:D:164:GLN:N	6:F:85:ASN:ND2	2.11	0.98
5:C:148:THR:HB	7:B:1084:ALA:HB1	1.29	0.98
5:C:149:LYS:N	7:B:1084:ALA:CB	2.26	0.98
1:D:630:LEU:CD2	4:Y:235:ILE:HG21	1.94	0.97
7:B:984:GLN:CD	7:B:1133:THR:HG23	1.89	0.97
5:C:148:THR:CG2	7:B:1084:ALA:HB1	1.94	0.97
5:C:153:SER:H	7:B:1071:ASN:ND2	1.61	0.97
7:B:283:ARG:HH22	7:B:492:LYS:HB2	1.30	0.96
1:D:601:ALA:HB2	1:D:850:TRP:HZ3	1.31	0.96
5:C:149:LYS:NZ	7:B:1068:SER:CB	2.24	0.96
6:F:222:ALA:HA	7:B:211:GLN:HA	1.45	0.96
6:F:1237:PRO:HG2	6:F:1239:HIS:NE2	1.81	0.96
6:F:900:GLN:HE21	6:F:934:GLU:HG2	1.19	0.96
6:F:130:GLN:NE2	6:F:560:GLN:HG2	1.80	0.96
7:B:1099:PHE:CE1	7:B:1103:ARG:NH2	2.32	0.96
1:D:18:ILE:HD13	1:D:669:PHE:HD2	1.29	0.96
1:D:113:ASN:HB2	1:D:505:LEU:HD21	1.48	0.96
7:B:318:GLU:OE2	7:B:498:ASN:HB2	1.65	0.96
5:C:151:THR:CB	7:B:1071:ASN:OD1	2.12	0.95
5:C:745:GLN:O	5:C:751:LYS:HE3	1.66	0.95
1:D:113:ASN:CB	1:D:505:LEU:HD21	1.96	0.95
5:C:149:LYS:HB2	7:B:1084:ALA:HB2	1.48	0.95
5:C:148:THR:C	7:B:1084:ALA:HB1	1.89	0.95
6:F:877:ARG:NH1	6:F:1270:ILE:CG2	2.28	0.94
1:D:43:GLY:O	1:D:520:PHE:CE2	2.18	0.94
7:B:734:LEU:CD1	7:B:885:LYS:O	2.16	0.94
6:F:1167:ASN:O	7:B:149:PRO:CB	2.15	0.94
5:C:149:LYS:NZ	7:B:1068:SER:HB2	1.83	0.94
6:F:877:ARG:HD2	6:F:1270:ILE:HG21	1.47	0.93
7:B:1099:PHE:HE1	7:B:1103:ARG:HH21	0.99	0.93
1:D:161:ARG:HB3	6:F:88:ASP:HB2	0.95	0.93
1:D:563:VAL:CG1	4:Y:231:LEU:HB2	1.97	0.93
1:D:188:THR:HB	1:D:260:GLN:HE22	1.30	0.93
6:F:343:LYS:HE2	6:F:439:MET:CB	1.98	0.93
5:C:1183:ARG:NH1	5:C:1243:ASN:HB2	1.84	0.93
6:F:1167:ASN:C	7:B:149:PRO:HB3	1.93	0.92
1:D:157:ARG:CD	6:F:91:GLN:HB3	1.98	0.92
1:D:264:GLU:CD	1:D:269:TRP:CB	2.40	0.92
3:G:28:THR:HA	4:Y:125:GLU:OE2	1.67	0.92
6:F:1071:PHE:HB2	6:F:1247:ARG:HH22	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:VAL:HG23	1:D:516:PHE:HB3	1.52	0.92
5:C:607:ASN:HA	6:F:247:LYS:HB3	1.50	0.92
1:D:188:THR:HB	1:D:260:GLN:NE2	1.83	0.92
1:D:509:LEU:HB2	1:D:823:GLN:HE22	1.32	0.92
5:C:152:LYS:HB3	7:B:1071:ASN:HD21	1.31	0.92
1:D:113:ASN:HB2	1:D:505:LEU:CD2	1.99	0.91
7:B:662:ASN:O	7:B:966:GLN:NE2	2.03	0.91
1:D:7:VAL:HG13	1:D:11:TRP:CE3	2.06	0.91
1:D:164:GLN:CG	6:F:85:ASN:ND2	2.33	0.91
5:C:316:LYS:CE	5:C:454:GLN:NE2	2.32	0.91
1:D:269:TRP:HZ3	1:D:386:VAL:CG1	1.82	0.91
7:B:290:ASP:HB2	7:B:511:SER:OG	1.70	0.91
1:D:161:ARG:HB3	6:F:88:ASP:HB3	1.53	0.91
1:D:282:ASN:HD21	1:D:364:TYR:HE1	1.03	0.91
5:C:154:LEU:HD12	7:B:1074:THR:CG2	1.99	0.90
6:F:1071:PHE:CD2	6:F:1247:ARG:NH2	2.39	0.90
6:F:1071:PHE:CE2	6:F:1247:ARG:NE	2.40	0.90
6:F:54:GLU:HG2	6:F:814:GLN:NE2	1.87	0.90
7:B:699:LYS:NZ	7:B:714:GLU:OE1	2.06	0.89
1:D:157:ARG:N	6:F:88:ASP:OD1	1.90	0.89
1:D:364:TYR:O	1:D:399:ARG:NH2	2.05	0.89
5:C:148:THR:CB	7:B:1084:ALA:HB3	1.87	0.89
6:F:995:TYR:O	6:F:1241:PRO:O	1.91	0.89
6:F:71:ARG:NH1	6:F:132:LEU:HD21	1.86	0.89
1:D:317:ARG:NE	1:D:403:ALA:O	2.06	0.88
5:C:144:VAL:HG21	7:B:1080:GLY:C	1.97	0.88
5:C:154:LEU:CD1	7:B:1074:THR:HG21	1.99	0.88
6:F:1169:ASP:HB2	7:B:147:THR:C	1.98	0.88
5:C:147:LEU:HD22	7:B:1082:THR:HG23	1.53	0.88
1:D:161:ARG:HD3	6:F:88:ASP:HB3	1.54	0.88
5:C:153:SER:N	7:B:1071:ASN:HD21	1.71	0.88
6:F:807:LYS:HE3	6:F:811:ASN:CG	1.97	0.88
6:F:986:ARG:NH2	6:F:1131:GLY:O	2.06	0.88
1:D:158:THR:CB	6:F:84:ASP:O	2.21	0.88
5:C:144:VAL:CG1	7:B:1080:GLY:O	2.22	0.88
6:F:958:PHE:CE2	6:F:1270:ILE:HG13	2.07	0.88
5:C:154:LEU:HD12	7:B:1074:THR:HG23	1.54	0.88
6:F:1172:ASN:HD22	7:B:171:PHE:HD2	0.90	0.87
6:F:958:PHE:HE2	6:F:1270:ILE:HG13	1.35	0.87
6:F:343:LYS:CE	6:F:439:MET:CB	2.52	0.87
6:F:958:PHE:N	6:F:1273:VAL:HG11	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1139:LYS:HE3	6:F:1197:VAL:O	1.74	0.87
1:D:210:VAL:HG11	4:Y:410:PRO:HD3	1.56	0.86
1:D:158:THR:C	6:F:84:ASP:C	2.38	0.86
7:B:290:ASP:CB	7:B:511:SER:OG	2.23	0.86
3:G:30:GLY:HA3	4:Y:96:GLN:HE22	1.40	0.86
5:C:153:SER:N	7:B:1071:ASN:ND2	2.21	0.86
5:C:609:GLN:NE2	6:F:248:THR:CG2	2.38	0.86
7:B:216:ILE:HG21	7:B:406:LEU:HD23	1.54	0.86
6:F:1143:LYS:HE3	6:F:1194:VAL:HG13	1.58	0.86
7:B:283:ARG:CG	7:B:290:ASP:OD1	2.23	0.85
5:C:638:LYS:HE3	5:C:668:GLU:OE2	1.75	0.85
6:F:961:THR:CB	6:F:1269:LEU:CD2	2.55	0.85
6:F:1169:ASP:CG	7:B:147:THR:HB	1.99	0.85
5:C:745:GLN:O	5:C:751:LYS:CE	2.25	0.85
7:B:734:LEU:HD13	7:B:885:LYS:O	1.76	0.85
1:D:18:ILE:HD13	1:D:669:PHE:CD2	2.11	0.85
6:F:1071:PHE:CB	6:F:1247:ARG:NH2	2.39	0.85
1:D:160:ALA:CA	6:F:81:ASP:O	2.22	0.84
1:D:270:PHE:CB	1:D:396:ARG:HH21	1.90	0.84
6:F:1091:PHE:CZ	6:F:1247:ARG:HD2	2.12	0.84
1:D:161:ARG:NH1	6:F:92:GLN:CB	2.40	0.84
1:D:741:MET:HE2	1:D:771:GLY:CA	2.08	0.84
5:C:152:LYS:C	7:B:1071:ASN:HD21	1.85	0.84
1:D:160:ALA:HB2	6:F:82:GLU:C	2.01	0.84
1:D:509:LEU:CB	1:D:823:GLN:NE2	2.41	0.84
1:D:158:THR:O	6:F:84:ASP:O	1.95	0.84
6:F:1209:GLU:OE1	6:F:1249:TRP:NE1	2.10	0.84
6:F:877:ARG:CD	6:F:1270:ILE:HG21	2.07	0.84
1:D:264:GLU:OE2	1:D:269:TRP:HB3	1.78	0.83
6:F:900:GLN:NE2	6:F:934:GLU:HG3	1.91	0.83
1:D:741:MET:HE2	1:D:771:GLY:HA3	1.59	0.83
1:D:161:ARG:HB2	6:F:88:ASP:HB2	1.57	0.83
5:C:144:VAL:HG21	7:B:1080:GLY:O	1.77	0.83
1:D:46:PHE:CE2	1:D:504:PRO:HA	2.13	0.83
4:Y:224:VAL:HG11	4:Y:232:THR:HB	1.61	0.83
5:C:154:LEU:CD1	7:B:1074:THR:HG22	1.91	0.82
7:B:984:GLN:NE2	7:B:1133:THR:HG22	1.90	0.82
7:B:358:LYS:NZ	7:B:374:ASN:O	2.12	0.82
5:C:154:LEU:CD1	7:B:1074:THR:HG23	2.09	0.82
6:F:178:GLU:OE2	6:F:632:LYS:NZ	2.10	0.82
1:D:158:THR:HA	6:F:87:LEU:HD23	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:961:THR:C	6:F:1269:LEU:HD21	2.03	0.82
1:D:164:GLN:H	6:F:85:ASN:CG	1.87	0.82
6:F:1172:ASN:ND2	7:B:171:PHE:CD2	2.42	0.82
1:D:188:THR:CB	1:D:260:GLN:NE2	2.43	0.81
5:C:209:VAL:HG23	5:C:467:HIS:ND1	1.95	0.81
6:F:877:ARG:CD	6:F:1270:ILE:CG2	2.58	0.81
1:D:157:ARG:HD3	6:F:91:GLN:HB3	1.61	0.81
6:F:838:GLU:HG2	6:F:956:LEU:HD12	1.62	0.81
6:F:965:LEU:HB3	6:F:1265:LEU:CD2	2.11	0.81
6:F:82:GLU:OE2	6:F:120:LYS:HE2	1.80	0.81
3:G:31:LEU:HD11	4:Y:93:ILE:HG23	1.63	0.81
6:F:1209:GLU:HG2	6:F:1249:TRP:CD1	2.15	0.81
5:C:607:ASN:O	6:F:248:THR:HG23	1.81	0.81
7:B:811:ALA:HB1	7:B:901:ILE:HG22	1.62	0.81
1:D:158:THR:HA	6:F:87:LEU:HB3	1.62	0.80
5:C:68:ARG:NH1	5:C:126:ASP:OD1	2.13	0.80
5:C:148:THR:HG22	7:B:1084:ALA:HB1	1.63	0.80
1:D:625:TRP:CD1	1:D:833:LEU:HD11	2.16	0.80
6:F:1167:ASN:O	7:B:149:PRO:HB3	1.80	0.80
7:B:1194:LEU:HD23	7:B:1197:ILE:HD11	1.62	0.80
1:D:182:LYS:HE3	1:D:197:PHE:CD2	2.12	0.80
5:C:316:LYS:HE3	5:C:454:GLN:HE21	1.47	0.80
1:D:44:VAL:HG23	1:D:516:PHE:CB	2.11	0.80
5:C:154:LEU:CG	7:B:1074:THR:CG2	2.50	0.80
6:F:877:ARG:CZ	6:F:1270:ILE:CG2	2.58	0.80
1:D:601:ALA:HB2	1:D:850:TRP:CZ3	2.17	0.80
1:D:774:SER:HB3	1:D:797:LEU:HD11	1.64	0.80
1:D:163:ARG:NH2	6:F:80:GLU:CB	2.45	0.80
6:F:847:PHE:CD2	6:F:963:MET:HE1	2.17	0.80
6:F:1219:MET:HE2	6:F:1247:ARG:HH21	1.45	0.80
5:C:607:ASN:CA	6:F:247:LYS:HB2	2.12	0.80
1:D:164:GLN:H	6:F:85:ASN:HD21	1.09	0.79
1:D:376:LYS:NZ	1:D:383:ALA:O	2.14	0.79
1:D:158:THR:CA	6:F:87:LEU:HB3	1.82	0.79
6:F:839:TRP:NE1	6:F:843:ASN:ND2	2.30	0.79
1:D:253:ASP:OD2	1:D:282:ASN:N	2.14	0.79
1:D:697:TYR:CD1	1:D:852:LYS:NZ	2.50	0.79
5:C:148:THR:CA	7:B:1084:ALA:CB	2.60	0.79
6:F:396:GLN:HE21	6:F:412:GLY:HA2	1.42	0.79
6:F:434:THR:HG22	6:F:489:THR:HG21	1.62	0.79
6:F:343:LYS:HE3	6:F:439:MET:SD	2.23	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:962:LEU:CA	6:F:1269:LEU:CD1	2.60	0.79
6:F:1251:MET:SD	6:F:1256:PRO:HD3	2.23	0.79
4:Y:263:ILE:HD11	4:Y:280:LEU:HB2	1.65	0.79
6:F:1184:ILE:HD11	7:B:171:PHE:CZ	2.18	0.79
1:D:669:PHE:CD1	1:D:676:LEU:HD11	2.18	0.78
5:C:154:LEU:HG	7:B:1074:THR:CG2	2.09	0.78
6:F:33:VAL:HA	6:F:832:ILE:CD1	2.13	0.78
5:C:52:VAL:CG2	5:C:563:ILE:HD12	2.14	0.78
1:D:158:THR:OG1	6:F:84:ASP:O	2.00	0.78
1:D:161:ARG:HA	6:F:85:ASN:OD1	1.81	0.78
5:C:607:ASN:HA	6:F:247:LYS:HB2	1.62	0.78
1:D:630:LEU:HD22	4:Y:235:ILE:HG21	1.62	0.78
4:Y:259:ARG:HD3	4:Y:385:ILE:HD11	1.66	0.78
5:C:609:GLN:HG3	6:F:248:THR:HG21	1.64	0.78
6:F:1208:PHE:CD2	6:F:1216:LYS:HE3	2.19	0.77
6:F:954:LYS:HB3	6:F:1274:LEU:HD23	1.65	0.77
5:C:46:ALA:HB2	5:C:527:ILE:HD13	1.65	0.77
5:C:151:THR:C	7:B:1071:ASN:OD1	2.27	0.77
1:D:514:SER:CB	1:D:898:ILE:HG13	2.14	0.77
6:F:707:ARG:HE	6:F:711:GLY:HA2	1.48	0.77
6:F:1167:ASN:HB3	7:B:149:PRO:CB	2.15	0.77
6:F:326:GLN:OE1	6:F:432:ARG:NH1	2.17	0.76
1:D:161:ARG:NH1	6:F:92:GLN:HB2	2.01	0.76
4:Y:148:THR:HG22	4:Y:159:LEU:HD12	1.67	0.76
6:F:847:PHE:CD2	6:F:963:MET:CE	2.69	0.76
7:B:986:ILE:HG13	7:B:1130:PRO:HB2	1.66	0.76
4:Y:67:PHE:CZ	4:Y:71:PHE:CE2	2.69	0.76
6:F:961:THR:HB	6:F:1269:LEU:HD22	1.66	0.76
7:B:868:ASN:HD22	7:B:1002:GLN:HE21	1.33	0.76
1:D:335:ASP:O	1:D:340:GLN:OE1	2.03	0.76
6:F:68:ILE:HD12	6:F:176:ASN:ND2	2.01	0.76
6:F:965:LEU:HD12	6:F:1269:LEU:HG	1.67	0.76
6:F:1166:VAL:O	7:B:149:PRO:HB3	1.86	0.76
1:D:7:VAL:CG1	1:D:11:TRP:CE3	2.69	0.75
6:F:839:TRP:CE2	6:F:843:ASN:ND2	2.54	0.75
1:D:157:ARG:HD2	6:F:91:GLN:HB3	1.67	0.75
1:D:160:ALA:CB	6:F:82:GLU:C	2.57	0.75
5:C:316:LYS:HE2	5:C:454:GLN:NE2	2.00	0.75
6:F:961:THR:HG22	6:F:1269:LEU:HD21	1.66	0.75
7:B:195:ASP:OD2	7:B:329:LYS:NZ	2.19	0.75
5:C:152:LYS:CA	7:B:1071:ASN:ND2	2.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:958:PHE:CA	6:F:1273:VAL:HG11	2.17	0.75
1:D:280:ASN:C	1:D:396:ARG:NH1	2.44	0.74
5:C:149:LYS:CD	7:B:1083:ILE:HG23	2.17	0.74
1:D:570:PHE:CZ	1:D:823:GLN:HG2	2.22	0.74
5:C:1124:LYS:HB3	5:C:1128:GLU:OE2	1.87	0.74
5:C:148:THR:CA	7:B:1084:ALA:HB1	2.17	0.74
5:C:209:VAL:CG2	5:C:467:HIS:CE1	2.70	0.74
3:G:62:VAL:HG12	4:Y:41:LEU:HD21	1.70	0.74
5:C:609:GLN:CD	6:F:248:THR:CG2	2.48	0.74
5:C:677:LYS:NZ	5:C:834:GLU:O	2.19	0.74
6:F:930:GLN:OE1	6:F:935:LEU:HD21	1.86	0.74
6:F:962:LEU:CA	6:F:1269:LEU:HD11	2.12	0.74
6:F:1166:VAL:HG23	6:F:1168:VAL:HG23	1.70	0.74
5:C:152:LYS:HB3	7:B:1071:ASN:HD22	1.52	0.73
1:D:164:GLN:HG3	6:F:85:ASN:HD22	1.51	0.73
6:F:1207:LYS:HE2	6:F:1252:SER:CB	2.18	0.73
6:F:1208:PHE:CE2	6:F:1216:LYS:HE2	2.23	0.73
7:B:702:TRP:HE1	7:B:736:ASN:HD22	1.36	0.73
1:D:171:ARG:HH12	1:D:314:PHE:HD1	1.35	0.73
1:D:47:ASN:HB3	1:D:152:ARG:HA	1.70	0.73
1:D:730:ILE:HG21	1:D:782:LEU:HD13	1.70	0.73
5:C:531:PHE:HZ	5:C:563:ILE:HG21	1.54	0.73
1:D:161:ARG:CB	6:F:88:ASP:HB3	2.10	0.73
1:D:163:ARG:HH21	6:F:80:GLU:HB2	1.51	0.73
7:B:1204:ILE:CD1	7:B:1213:LEU:HD11	2.19	0.73
1:D:630:LEU:HD21	4:Y:235:ILE:HG21	1.69	0.73
3:G:11:MET:HE1	3:G:64:LEU:HB3	1.69	0.73
1:D:838:ARG:HH22	1:D:875:LEU:HB3	1.53	0.73
5:C:149:LYS:CA	7:B:1084:ALA:HB2	2.18	0.73
5:C:934:GLN:OE1	5:C:1004:LYS:HD3	1.88	0.73
6:F:958:PHE:HZ	6:F:1266:VAL:HG13	1.54	0.73
1:D:279:GLN:C	1:D:396:ARG:HH12	1.96	0.72
6:F:54:GLU:HG2	6:F:814:GLN:HE22	1.55	0.72
6:F:1172:ASN:CB	7:B:171:PHE:CD2	2.72	0.72
7:B:984:GLN:CD	7:B:1133:THR:CA	2.62	0.72
4:Y:107:ILE:HG22	4:Y:109:PRO:HD2	1.71	0.72
4:Y:97:ILE:CG2	4:Y:294:PHE:CZ	2.73	0.72
6:F:1219:MET:HE2	6:F:1247:ARG:NH2	2.04	0.72
5:C:316:LYS:CG	5:C:454:GLN:NE2	2.51	0.72
1:D:273:LYS:HE3	1:D:388:ALA:HB3	1.71	0.72
1:D:158:THR:CA	6:F:84:ASP:O	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ARG:CD	6:F:88:ASP:HB3	2.19	0.72
6:F:148:ASP:OD1	6:F:166:LYS:NZ	2.21	0.72
6:F:989:VAL:HG11	6:F:1260:LEU:HD21	1.71	0.72
7:B:20:PHE:HB3	7:B:1209:ILE:HD11	1.70	0.71
1:D:157:ARG:N	6:F:88:ASP:CG	2.47	0.71
1:D:160:ALA:HB2	6:F:83:HIS:C	2.15	0.71
1:D:113:ASN:HB3	1:D:505:LEU:HD21	1.71	0.71
2:E:122:PHE:CE2	4:Y:47:ILE:HG23	2.25	0.71
6:F:962:LEU:HB2	6:F:1269:LEU:HD13	1.70	0.71
6:F:284:ARG:NH1	6:F:527:TYR:CD2	2.59	0.71
1:D:613:ARG:HB3	1:D:848:CYS:SG	2.31	0.71
4:Y:349:ILE:HD12	4:Y:382:LEU:CD1	2.21	0.71
5:C:166:LEU:HD21	5:C:515:PHE:CZ	2.26	0.71
6:F:129:PHE:CE1	6:F:133:ILE:HD11	2.26	0.71
6:F:996:ASP:HB2	6:F:1057:LEU:CD1	2.20	0.71
1:D:625:TRP:NE1	1:D:833:LEU:HD11	2.05	0.71
6:F:961:THR:CB	6:F:1269:LEU:HD21	2.21	0.71
1:D:164:GLN:HG3	6:F:85:ASN:CG	2.15	0.71
5:C:563:ILE:HG23	5:C:567:LEU:HD12	1.71	0.71
1:D:215:ASN:ND2	4:Y:58:THR:HA	2.06	0.71
5:C:313:ALA:HB1	5:C:455:PRO:HG2	1.73	0.71
6:F:1183:LEU:HD21	7:B:171:PHE:HB3	1.71	0.71
5:C:1280:LYS:HE3	5:C:1296:ARG:NH2	2.05	0.70
6:F:1071:PHE:CG	6:F:1247:ARG:NH2	2.58	0.70
6:F:1173:LEU:O	6:F:1189:LYS:HE2	1.90	0.70
1:D:253:ASP:OD2	1:D:281:GLY:C	2.34	0.70
1:D:282:ASN:ND2	1:D:364:TYR:HE1	1.85	0.70
6:F:33:VAL:HA	6:F:832:ILE:HD12	1.73	0.70
4:Y:104:THR:HG21	4:Y:347:ILE:HG23	1.73	0.70
4:Y:82:LEU:HD23	4:Y:174:MET:CE	2.21	0.70
5:C:971:TYR:HE2	5:C:973:LYS:HE3	1.56	0.70
1:D:838:ARG:HG2	1:D:925:LEU:HD13	1.72	0.70
1:D:891:ALA:CB	1:D:910:ILE:HD11	2.21	0.70
6:F:222:ALA:HA	7:B:211:GLN:CA	2.21	0.70
7:B:195:ASP:HA	7:B:545:ARG:NH1	2.06	0.70
1:D:156:ALA:C	6:F:88:ASP:OD1	2.33	0.70
6:F:20:ILE:HG23	6:F:24:GLU:HA	1.72	0.70
5:C:609:GLN:HG3	6:F:248:THR:CG2	2.21	0.70
5:C:316:LYS:HG2	5:C:454:GLN:NE2	2.07	0.70
6:F:186:TYR:CE1	6:F:570:ALA:HA	2.27	0.70
1:D:712:ILE:HG21	1:D:784:ARG:NH1	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:835:PHE:CZ	1:D:839:ILE:HD11	2.27	0.70
6:F:981:ILE:HD11	6:F:1097:LEU:HD21	1.74	0.70
6:F:1167:ASN:HB3	7:B:149:PRO:HB2	1.74	0.69
6:F:1207:LYS:HE2	6:F:1252:SER:HB3	1.73	0.69
1:D:159:ARG:N	6:F:84:ASP:O	2.25	0.69
4:Y:97:ILE:CG2	4:Y:294:PHE:HZ	2.05	0.69
5:C:209:VAL:HG23	5:C:467:HIS:CE1	2.28	0.69
6:F:900:GLN:HE21	6:F:934:GLU:HG3	1.46	0.69
6:F:1169:ASP:CB	7:B:147:THR:CB	2.26	0.69
5:C:316:LYS:HE3	5:C:454:GLN:NE2	2.03	0.69
6:F:961:THR:CG2	6:F:1269:LEU:CD2	2.70	0.69
7:B:984:GLN:HG3	7:B:1133:THR:OG1	1.92	0.69
1:D:105:TYR:CE1	4:Y:227:ILE:HG12	2.26	0.69
6:F:877:ARG:HH11	6:F:1270:ILE:CG2	2.03	0.69
7:B:53:ALA:O	7:B:612:LEU:HD12	1.92	0.69
7:B:984:GLN:HG3	7:B:1133:THR:N	1.77	0.69
1:D:161:ARG:HB3	6:F:88:ASP:CG	2.17	0.69
5:C:609:GLN:NE2	6:F:248:THR:CB	2.55	0.69
6:F:958:PHE:HA	6:F:1273:VAL:HG21	1.73	0.69
5:C:806:VAL:HG13	5:C:818:GLY:CA	2.19	0.68
7:B:799:LYS:NZ	7:B:884:GLU:OE2	2.26	0.68
7:B:997:LYS:HB3	7:B:999:GLN:HG3	1.75	0.68
5:C:242:LYS:NZ	5:C:396:GLU:OE1	2.25	0.68
6:F:865:ASP:HB3	6:F:1262:LYS:NZ	2.08	0.68
7:B:209:PRO:HD3	7:B:234:PHE:CD1	2.27	0.68
1:D:509:LEU:HB2	1:D:823:GLN:CD	2.17	0.68
5:C:975:SER:HB3	5:C:1003:ALA:HA	1.75	0.68
6:F:1169:ASP:CB	7:B:147:THR:C	2.63	0.68
5:C:1183:ARG:NH1	5:C:1243:ASN:CB	2.57	0.68
6:F:961:THR:CG2	6:F:1269:LEU:HD21	2.23	0.68
6:F:1149:THR:CG2	6:F:1154:GLU:OE2	2.41	0.68
1:D:158:THR:O	6:F:88:ASP:CG	2.36	0.67
1:D:226:LEU:CD1	1:D:454:ILE:HD12	2.24	0.67
1:D:226:LEU:HD12	1:D:454:ILE:HD12	1.75	0.67
1:D:269:TRP:CZ3	1:D:386:VAL:CG1	2.72	0.67
7:B:344:LYS:HE3	7:B:363:GLU:HG3	1.75	0.67
1:D:226:LEU:HD12	1:D:454:ILE:CD1	2.25	0.67
6:F:222:ALA:CB	7:B:211:GLN:HG2	2.24	0.67
6:F:434:THR:HG22	6:F:489:THR:CG2	2.24	0.67
7:B:397:ALA:O	7:B:414:LYS:NZ	2.25	0.67
5:C:144:VAL:CG2	7:B:1080:GLY:O	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:197:ILE:HD13	5:C:489:LYS:HA	1.77	0.67
7:B:984:GLN:HE22	7:B:1133:THR:CG2	2.00	0.67
5:C:495:ARG:HD2	5:C:510:TYR:OH	1.95	0.67
6:F:900:GLN:HE22	6:F:934:GLU:HA	1.60	0.67
4:Y:67:PHE:CE1	4:Y:71:PHE:HE2	2.12	0.67
6:F:467:LEU:HD23	6:F:468:PRO:HD3	1.75	0.67
6:F:962:LEU:CB	6:F:1269:LEU:HD13	2.24	0.67
1:D:264:GLU:CD	1:D:269:TRP:HB3	2.14	0.67
1:D:757:ALA:H	1:D:819:GLN:HB3	1.60	0.67
4:Y:53:ILE:HG23	4:Y:157:ILE:HG23	1.75	0.67
5:C:144:VAL:CG2	7:B:1080:GLY:CA	2.55	0.67
5:C:316:LYS:CE	5:C:454:GLN:HE22	2.06	0.67
1:D:121:THR:HG21	1:D:143:PRO:HD3	1.77	0.67
4:Y:47:ILE:HA	4:Y:81:GLN:OE1	1.95	0.67
6:F:839:TRP:CD1	6:F:843:ASN:ND2	2.63	0.67
5:C:153:SER:H	7:B:1071:ASN:CG	2.03	0.66
6:F:1091:PHE:HZ	6:F:1247:ARG:HD2	1.60	0.66
6:F:1071:PHE:CE1	6:F:1209:GLU:HB3	2.30	0.66
6:F:1149:THR:HG23	6:F:1154:GLU:OE2	1.95	0.66
1:D:157:ARG:HH12	6:F:95:PRO:HB3	1.61	0.66
5:C:68:ARG:HD2	5:C:130:ARG:NH2	2.11	0.66
6:F:71:ARG:HH12	6:F:132:LEU:HD21	1.60	0.66
6:F:192:VAL:O	6:F:516:ARG:NH2	2.29	0.66
7:B:356:VAL:HG21	7:B:362:VAL:HG21	1.76	0.66
4:Y:220:LEU:HD21	4:Y:407:ILE:CG2	2.26	0.66
5:C:65:ILE:HG12	5:C:130:ARG:NH1	2.11	0.66
5:C:152:LYS:NZ	7:B:1125:GLN:HB2	2.11	0.66
1:D:289:LYS:HE3	1:D:412:ASN:O	1.95	0.66
5:C:151:THR:CA	7:B:1071:ASN:OD1	2.43	0.66
6:F:1208:PHE:CE2	6:F:1216:LYS:CE	2.79	0.66
7:B:81:TYR:CZ	7:B:111:GLU:HG3	2.31	0.66
6:F:865:ASP:HB3	6:F:1262:LYS:HZ3	1.60	0.66
1:D:161:ARG:O	6:F:85:ASN:OD1	2.13	0.66
5:C:152:LYS:N	7:B:1071:ASN:CG	2.53	0.66
5:C:806:VAL:CG1	5:C:818:GLY:HA2	2.21	0.66
7:B:986:ILE:HG13	7:B:1130:PRO:CB	2.26	0.65
7:B:1047:LEU:HD23	7:B:1110:LEU:HD21	1.79	0.65
1:D:509:LEU:CB	1:D:823:GLN:HE22	2.07	0.65
6:F:1143:LYS:HE3	6:F:1194:VAL:CG1	2.26	0.65
1:D:158:THR:N	6:F:88:ASP:CA	2.58	0.65
6:F:330:LEU:HD21	6:F:488:GLN:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:GLN:CA	6:F:85:ASN:HD21	2.09	0.65
5:C:148:THR:C	7:B:1084:ALA:HB2	2.01	0.65
6:F:1170:THR:HB	6:F:1173:LEU:HD12	1.78	0.65
1:D:215:ASN:ND2	4:Y:58:THR:O	2.30	0.65
1:D:630:LEU:CD2	4:Y:235:ILE:CG2	2.74	0.65
4:Y:220:LEU:HD21	4:Y:407:ILE:HG21	1.79	0.65
6:F:873:THR:HG22	6:F:1270:ILE:CD1	2.27	0.65
7:B:66:ILE:HG12	7:B:130:ARG:NH1	2.12	0.65
1:D:269:TRP:HZ3	1:D:386:VAL:HG11	1.61	0.65
1:D:730:ILE:CG2	1:D:782:LEU:HD13	2.27	0.65
5:C:730:LEU:HA	5:C:735:LEU:HD22	1.79	0.64
7:B:1194:LEU:HD23	7:B:1197:ILE:CD1	2.27	0.64
5:C:148:THR:HB	7:B:1084:ALA:CA	2.22	0.64
6:F:962:LEU:CA	6:F:1269:LEU:HD13	2.26	0.64
7:B:1044:LYS:NZ	7:B:1111:ASP:OD1	2.28	0.64
5:C:863:LYS:HE3	5:C:1224:GLU:HA	1.79	0.64
7:B:355:VAL:HG21	7:B:406:LEU:HD12	1.79	0.64
1:D:113:ASN:CB	1:D:505:LEU:CD2	2.66	0.64
1:D:338:PHE:HE2	1:D:359:ASN:CB	2.03	0.64
7:B:997:LYS:C	7:B:999:GLN:H	2.05	0.64
7:B:1204:ILE:HD11	7:B:1213:LEU:HD11	1.78	0.64
1:D:570:PHE:HZ	1:D:823:GLN:HG2	1.61	0.64
1:D:163:ARG:NH1	6:F:80:GLU:N	2.45	0.64
4:Y:289:VAL:HG22	4:Y:421:ILE:HG22	1.80	0.63
5:C:316:LYS:CE	5:C:454:GLN:HE21	2.03	0.63
5:C:316:LYS:HE2	5:C:454:GLN:HE22	1.60	0.63
5:C:1028:ARG:NH1	5:C:1032:GLN:O	2.28	0.63
6:F:965:LEU:HD12	6:F:1269:LEU:CG	2.28	0.63
1:D:331:PHE:CE2	1:D:339:LEU:HB2	2.33	0.63
1:D:514:SER:OG	1:D:898:ILE:HG13	1.98	0.63
5:C:764:GLN:HE21	5:C:776:ASN:HB2	1.63	0.63
6:F:1208:PHE:CD2	6:F:1216:LYS:CE	2.81	0.63
1:D:645:THR:HG23	4:Y:231:LEU:CD2	2.23	0.63
4:Y:349:ILE:HD12	4:Y:382:LEU:HD13	1.79	0.63
4:Y:354:LEU:HD23	4:Y:378:ILE:HD13	1.78	0.63
7:B:47:ALA:HB1	7:B:120:LEU:CD2	2.29	0.63
7:B:765:LEU:CD1	7:B:781:LEU:HD11	2.28	0.63
7:B:899:ARG:HG2	7:B:1194:LEU:HD11	1.80	0.63
1:D:630:LEU:HD21	4:Y:235:ILE:CG2	2.28	0.63
7:B:897:HIS:NE2	7:B:901:ILE:HD11	2.13	0.63
7:B:1194:LEU:CD2	7:B:1197:ILE:HD11	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:842:THR:HG23	1:D:872:GLN:NE2	2.13	0.63
6:F:1270:ILE:HG23	6:F:1274:LEU:HD12	1.80	0.62
1:D:845:TRP:CZ2	1:D:871:SER:HB3	2.35	0.62
6:F:888:PHE:HB3	6:F:935:LEU:HD22	1.82	0.62
1:D:741:MET:HE2	1:D:771:GLY:HA2	1.81	0.62
4:Y:60:LEU:HD11	4:Y:157:ILE:CD1	2.29	0.62
5:C:173:LYS:HA	5:C:550:TYR:CD1	2.34	0.62
6:F:1071:PHE:HE1	6:F:1209:GLU:HB3	1.64	0.62
5:C:1090:LYS:NZ	5:C:1138:ASP:OD1	2.28	0.62
6:F:168:VAL:HG13	6:F:625:LYS:HE3	1.80	0.62
6:F:221:ALA:O	7:B:211:GLN:O	2.18	0.62
4:Y:82:LEU:HD12	4:Y:157:ILE:HD12	1.81	0.62
5:C:247:SER:O	5:C:254:ASN:ND2	2.32	0.62
7:B:195:ASP:HA	7:B:545:ARG:HH12	1.62	0.62
1:D:264:GLU:OE1	1:D:269:TRP:N	2.31	0.62
1:D:367:PRO:HB3	1:D:399:ARG:NH1	2.14	0.62
1:D:595:ARG:NH1	1:D:849:TYR:CZ	2.68	0.62
6:F:839:TRP:NE1	6:F:843:ASN:HD21	1.97	0.62
7:B:868:ASN:HD22	7:B:1002:GLN:NE2	1.97	0.62
1:D:7:VAL:CG1	1:D:11:TRP:HE3	2.13	0.62
1:D:289:LYS:CE	1:D:412:ASN:O	2.48	0.62
1:D:473:TYR:CD1	4:Y:222:GLY:HA3	2.34	0.62
1:D:873:TRP:HD1	1:D:926:PHE:HE2	1.35	0.62
4:Y:97:ILE:HG21	4:Y:294:PHE:CZ	2.34	0.62
5:C:263:LEU:HD21	5:C:468:LEU:HD21	1.81	0.62
1:D:44:VAL:HG21	1:D:516:PHE:CG	2.35	0.61
1:D:788:ALA:HB1	1:D:935:LEU:HD13	1.81	0.61
5:C:1280:LYS:HE3	5:C:1296:ARG:HH21	1.63	0.61
6:F:965:LEU:CD1	6:F:1269:LEU:HG	2.30	0.61
5:C:608:ASN:ND2	6:F:247:LYS:HG3	2.15	0.61
1:D:163:ARG:NH2	6:F:80:GLU:CA	2.62	0.61
1:D:669:PHE:HE1	1:D:676:LEU:HD21	1.65	0.61
6:F:322:ALA:HB1	6:F:491:VAL:HG11	1.80	0.61
6:F:558:TRP:O	6:F:566:LYS:NZ	2.33	0.61
7:B:997:LYS:C	7:B:999:GLN:N	2.59	0.61
3:G:62:VAL:CG1	4:Y:41:LEU:HD21	2.30	0.61
6:F:71:ARG:HH11	6:F:132:LEU:HD21	1.64	0.61
1:D:163:ARG:NH1	6:F:79:VAL:C	2.59	0.61
7:B:53:ALA:C	7:B:612:LEU:HD12	2.26	0.61
7:B:61:ASN:HA	7:B:608:ALA:HB2	1.83	0.61
4:Y:60:LEU:HA	4:Y:156:PRO:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:VAL:CG2	1:D:516:PHE:CG	2.84	0.61
1:D:514:SER:CB	1:D:898:ILE:CG1	2.78	0.61
5:C:68:ARG:HD2	5:C:130:ARG:HH21	1.66	0.61
5:C:144:VAL:CG2	7:B:1080:GLY:C	2.72	0.61
5:C:608:ASN:HD22	6:F:247:LYS:H	1.49	0.61
6:F:961:THR:HG22	6:F:1269:LEU:CD2	2.29	0.61
6:F:1116:ILE:HG21	6:F:1248:LEU:HD11	1.83	0.61
1:D:745:TYR:CE2	1:D:768:LEU:HD12	2.36	0.61
5:C:260:ALA:HA	5:C:263:LEU:HD12	1.82	0.61
1:D:156:ALA:C	6:F:88:ASP:CG	2.69	0.60
1:D:157:ARG:CA	6:F:91:GLN:OE1	2.46	0.60
6:F:1035:ASP:HB2	6:F:1058:LEU:O	2.01	0.60
7:B:765:LEU:HD11	7:B:781:LEU:HD11	1.83	0.60
1:D:253:ASP:CG	1:D:281:GLY:HA3	2.27	0.60
1:D:260:GLN:OE1	1:D:365:ALA:HB2	2.01	0.60
1:D:158:THR:HA	6:F:87:LEU:CD2	2.30	0.60
6:F:1172:ASN:HB2	7:B:171:PHE:CD2	2.37	0.60
1:D:212:GLN:HB3	4:Y:61:ASP:HB3	1.83	0.60
6:F:900:GLN:HE22	6:F:934:GLU:CG	2.14	0.60
1:D:752:LEU:O	1:D:756:LEU:O	2.20	0.60
5:C:391:ASP:OD2	5:C:398:LYS:NZ	2.34	0.60
4:Y:60:LEU:N	4:Y:156:PRO:HB3	2.16	0.60
1:D:526:ILE:HG21	1:D:886:LEU:HD22	1.84	0.60
1:D:557:LEU:HD21	1:D:575:ILE:CD1	2.32	0.60
6:F:1237:PRO:HG2	6:F:1239:HIS:CD2	2.37	0.60
4:Y:67:PHE:CE2	4:Y:71:PHE:HE2	2.19	0.60
5:C:16:SER:HB3	5:C:1282:GLY:HA3	1.82	0.60
5:C:101:THR:CG2	5:C:703:GLN:HE21	2.14	0.59
6:F:286:GLY:HA2	6:F:487:LEU:HD22	1.83	0.59
7:B:238:GLU:OE1	7:B:253:LYS:HD2	2.01	0.59
1:D:331:PHE:CE2	1:D:339:LEU:CB	2.85	0.59
4:Y:82:LEU:HD12	4:Y:157:ILE:CD1	2.32	0.59
5:C:605:GLU:HG2	5:C:961:ARG:NH2	2.17	0.59
6:F:222:ALA:HB2	7:B:211:GLN:HG2	1.85	0.59
6:F:239:PRO:HG2	6:F:350:ASN:OD1	2.01	0.59
6:F:1173:LEU:HD23	6:F:1189:LYS:HG2	1.83	0.59
1:D:124:LYS:NZ	1:D:141:GLY:HA3	2.18	0.59
7:B:62:GLU:HB2	7:B:174:THR:HG21	1.83	0.59
7:B:166:PHE:HB2	7:B:184:SER:HB2	1.83	0.59
7:B:986:ILE:CG1	7:B:1130:PRO:CB	2.80	0.59
5:C:22:ARG:NE	5:C:746:GLU:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:152:LYS:CE	7:B:1125:GLN:HB2	2.32	0.59
6:F:325:ASP:OD1	6:F:432:ARG:NH2	2.36	0.59
6:F:1071:PHE:CE2	6:F:1247:ARG:CD	2.86	0.59
6:F:1166:VAL:O	7:B:149:PRO:CB	2.50	0.59
5:C:191:LYS:HG3	5:C:537:LEU:HG	1.83	0.59
5:C:200:GLU:OE2	5:C:291:LYS:HB3	2.03	0.59
1:D:737:PHE:CZ	1:D:797:LEU:HD22	2.37	0.59
2:E:86:VAL:HG21	4:Y:256:GLN:HB3	1.85	0.59
4:Y:93:ILE:HD11	4:Y:201:ILE:HD11	1.84	0.59
5:C:316:LYS:HG2	5:C:454:GLN:HE22	1.67	0.59
6:F:671:VAL:HG13	6:F:717:GLU:HG2	1.84	0.59
2:E:79:GLU:HG3	4:Y:259:ARG:NH1	2.17	0.59
6:F:675:GLN:NE2	6:F:711:GLY:O	2.35	0.59
6:F:991:TRP:CZ2	6:F:1260:LEU:HD11	2.37	0.59
1:D:253:ASP:OD1	1:D:281:GLY:HA3	2.02	0.59
3:G:31:LEU:HD23	3:G:34:LEU:HD12	1.85	0.59
1:D:44:VAL:CG2	1:D:516:PHE:HB3	2.29	0.58
6:F:1014:LYS:NZ	7:B:465:GLU:OE1	2.36	0.58
4:Y:97:ILE:HG23	4:Y:294:PHE:HZ	1.66	0.58
2:E:122:PHE:CZ	4:Y:47:ILE:HG23	2.39	0.58
5:C:753:ILE:HG21	5:C:782:TRP:CZ2	2.38	0.58
4:Y:244:PHE:HD2	4:Y:415:LEU:HD22	1.67	0.58
5:C:397:TYR:CE2	5:C:615:LEU:HD11	2.39	0.58
5:C:1183:ARG:HH21	5:C:1222:ASP:CG	2.11	0.58
5:C:1218:VAL:HG13	5:C:1242:LEU:HD22	1.85	0.58
1:D:157:ARG:O	6:F:87:LEU:HD23	2.03	0.58
1:D:509:LEU:H	1:D:823:GLN:HE22	1.51	0.58
5:C:148:THR:CA	7:B:1084:ALA:HB3	2.32	0.58
6:F:954:LYS:HB3	6:F:1274:LEU:CD2	2.34	0.58
6:F:1169:ASP:HB3	7:B:147:THR:HB	0.61	0.58
1:D:800:LEU:HD22	1:D:835:PHE:CD1	2.39	0.58
5:C:343:ASN:OD1	5:C:440:ALA:HB2	2.03	0.58
6:F:1108:ALA:HB1	6:F:1112:LEU:HD23	1.85	0.58
6:F:1169:ASP:CB	7:B:147:THR:CA	2.80	0.58
7:B:20:PHE:HB3	7:B:1209:ILE:CD1	2.33	0.58
7:B:235:PHE:HE2	7:B:354:ILE:HD11	1.69	0.58
7:B:984:GLN:CD	7:B:1132:GLY:C	2.70	0.58
6:F:692:ALA:CB	7:B:242:ALA:HA	2.34	0.58
1:D:417:GLU:HB2	1:D:468:TYR:OH	2.03	0.58
1:D:526:ILE:CG2	1:D:886:LEU:CD2	2.82	0.58
1:D:891:ALA:HB2	1:D:910:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:505:ASP:C	7:B:1126:ARG:HH11	2.12	0.58
6:F:1143:LYS:CE	6:F:1194:VAL:HG13	2.32	0.58
6:F:1167:ASN:ND2	7:B:150:PHE:O	2.37	0.58
1:D:317:ARG:NH1	1:D:464:ASN:O	2.30	0.58
1:D:766:ILE:HD12	1:D:825:ILE:HG22	1.85	0.58
5:C:80:PHE:HB2	5:C:114:TRP:CZ3	2.39	0.58
6:F:153:THR:O	6:F:536:ASN:ND2	2.37	0.58
6:F:1139:LYS:HE2	6:F:1198:ASP:HA	1.86	0.58
7:B:986:ILE:CD1	7:B:1130:PRO:CB	2.73	0.58
1:D:894:ASN:HB3	1:D:906:ILE:HD11	1.86	0.57
7:B:277:THR:OG1	7:B:450:PHE:HE2	1.87	0.57
1:D:188:THR:OG1	1:D:260:GLN:NE2	2.36	0.57
7:B:52:LYS:HD2	7:B:772:VAL:HG21	1.85	0.57
4:Y:82:LEU:CD2	4:Y:174:MET:HE1	2.34	0.57
6:F:4:LEU:HD11	6:F:99:PRO:HD2	1.87	0.57
6:F:40:GLU:CD	6:F:829:TRP:HZ2	2.12	0.57
7:B:251:ARG:NH1	7:B:300:ASP:HA	2.18	0.57
7:B:1035:LYS:C	7:B:1070:LEU:HD23	2.29	0.57
1:D:851:PHE:HE1	1:D:864:LEU:HD22	1.70	0.57
5:C:607:ASN:CA	6:F:247:LYS:CB	2.71	0.57
6:F:872:GLN:HG3	6:F:897:VAL:HG21	1.86	0.57
1:D:509:LEU:O	1:D:905:VAL:HG11	2.04	0.57
1:D:752:LEU:HD13	1:D:763:SER:HB2	1.86	0.57
5:C:38:ARG:NH2	5:C:578:ALA:HA	2.19	0.57
5:C:858:ASN:CG	5:C:1228:THR:HG23	2.29	0.57
6:F:881:ARG:HH22	6:F:1274:LEU:HB3	1.69	0.57
7:B:290:ASP:HB3	7:B:511:SER:OG	2.01	0.57
7:B:415:LYS:NZ	7:B:436:GLN:OE1	2.38	0.57
7:B:602:LEU:CD1	7:B:612:LEU:HD23	2.35	0.57
6:F:1124:VAL:HG13	6:F:1129:LYS:HA	1.87	0.57
2:E:106:ILE:HG23	4:Y:210:PRO:HG3	1.86	0.57
6:F:1169:ASP:HB3	7:B:147:THR:CA	2.28	0.57
6:F:1115:GLN:HG3	6:F:1123:LEU:HD11	1.86	0.57
3:G:26:GLY:HA3	4:Y:129:ARG:NH2	2.20	0.57
5:C:87:LEU:HD11	5:C:103:ILE:HD12	1.86	0.57
1:D:161:ARG:CA	6:F:85:ASN:CG	2.71	0.56
1:D:737:PHE:HD1	1:D:775:LEU:HD12	1.69	0.56
4:Y:67:PHE:CE1	4:Y:71:PHE:CE2	2.93	0.56
5:C:52:VAL:HG23	5:C:563:ILE:HD12	1.87	0.56
1:D:838:ARG:HH22	1:D:875:LEU:CB	2.17	0.56
1:D:894:ASN:HB3	1:D:906:ILE:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:345:SER:OG	4:Y:386:ASN:ND2	2.38	0.56
5:C:209:VAL:HG21	5:C:467:HIS:CE1	2.39	0.56
6:F:958:PHE:CE2	6:F:1270:ILE:CG1	2.86	0.56
7:B:986:ILE:CG1	7:B:1130:PRO:HB3	2.34	0.56
1:D:151:GLN:OE1	1:D:169:VAL:HG13	2.05	0.56
5:C:58:GLU:O	5:C:66:LYS:HE3	2.05	0.56
5:C:849:TYR:CE1	5:C:1270:LEU:HB2	2.41	0.56
5:C:1043:VAL:HG21	5:C:1073:ASN:OD1	2.05	0.56
6:F:1167:ASN:CA	7:B:149:PRO:HB3	2.35	0.56
7:B:373:TYR:HE1	7:B:375:ASP:OD1	1.87	0.56
7:B:982:THR:O	7:B:1134:GLY:HA3	2.04	0.56
7:B:984:GLN:OE1	7:B:1132:GLY:C	2.49	0.56
1:D:645:THR:HG21	4:Y:228:ASN:HD22	1.70	0.56
4:Y:68:PHE:CZ	4:Y:146:ILE:HD12	2.40	0.56
1:D:157:ARG:HB2	6:F:91:GLN:HB2	1.87	0.56
1:D:171:ARG:NH1	1:D:314:PHE:CD1	2.73	0.56
7:B:984:GLN:CD	7:B:1133:THR:CG2	2.64	0.56
5:C:156:GLU:OE2	7:B:1125:GLN:OE1	0.61	0.56
6:F:386:LYS:HE3	6:F:424:HIS:CG	2.39	0.56
6:F:396:GLN:HE22	6:F:412:GLY:HA2	1.67	0.56
6:F:1210:GLY:HA2	6:F:1219:MET:HG2	1.87	0.56
7:B:22:ASN:ND2	7:B:1203:ASN:HD22	2.04	0.56
1:D:433:VAL:HG13	1:D:437:LEU:HD23	1.87	0.56
4:Y:97:ILE:HG23	4:Y:294:PHE:CZ	2.41	0.56
7:B:332:VAL:HG12	7:B:514:LEU:HD13	1.86	0.56
1:D:512:ASP:O	1:D:903:ASN:ND2	2.39	0.56
5:C:205:VAL:HG21	5:C:290:LEU:HD13	1.88	0.56
5:C:931:ASP:HA	5:C:1198:TYR:CZ	2.41	0.56
6:F:321:THR:HB	6:F:705:TYR:CE2	2.40	0.56
7:B:980:LYS:HB2	7:B:1007:HIS:NE2	2.20	0.56
1:D:149:PHE:HE1	1:D:177:ILE:HD11	1.70	0.55
1:D:341:LYS:HD3	1:D:345:GLY:O	2.05	0.55
1:D:645:THR:HG21	4:Y:228:ASN:ND2	2.21	0.55
2:E:122:PHE:CE2	4:Y:47:ILE:CG2	2.88	0.55
4:Y:244:PHE:CD2	4:Y:415:LEU:HD22	2.42	0.55
6:F:961:THR:CG2	6:F:1269:LEU:HD23	2.36	0.55
1:D:526:ILE:HG23	1:D:886:LEU:CD2	2.36	0.55
1:D:643:LEU:HD22	1:D:826:ILE:HG23	1.87	0.55
5:C:1096:ILE:O	5:C:1130:LYS:CE	2.54	0.55
6:F:689:GLU:OE2	6:F:1040:SER:OG	2.20	0.55
7:B:211:GLN:OE1	7:B:215:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:42:PHE:CG	4:Y:200:LEU:HD22	2.42	0.55
5:C:152:LYS:H	7:B:1071:ASN:CG	2.14	0.55
6:F:141:VAL:HG21	6:F:549:LEU:CD1	2.36	0.55
7:B:238:GLU:OE1	7:B:253:LYS:CD	2.54	0.55
1:D:842:THR:HG23	1:D:872:GLN:HE22	1.71	0.55
4:Y:289:VAL:HG22	4:Y:421:ILE:CG2	2.37	0.55
1:D:92:PHE:CZ	1:D:96:ILE:HD11	2.42	0.55
1:D:163:ARG:NH2	6:F:80:GLU:N	2.55	0.55
1:D:851:PHE:HE1	1:D:864:LEU:CD2	2.20	0.55
5:C:246:GLN:NE2	7:B:963:GLU:OE2	2.39	0.55
5:C:606:ARG:HA	6:F:247:LYS:NZ	2.21	0.55
7:B:398:GLN:HA	7:B:414:LYS:HZ3	1.70	0.55
5:C:152:LYS:NZ	5:C:505:ASP:OD1	2.37	0.55
5:C:152:LYS:HE2	7:B:1125:GLN:HB2	1.87	0.55
6:F:234:PRO:HD2	6:F:699:LEU:HD12	1.86	0.55
6:F:707:ARG:NE	6:F:711:GLY:HA2	2.19	0.55
7:B:190:TRP:CZ2	7:B:196:PRO:HB3	2.41	0.55
1:D:669:PHE:CE1	1:D:676:LEU:HD21	2.41	0.55
1:D:887:PHE:CD2	1:D:913:VAL:HG11	2.42	0.55
5:C:858:ASN:ND2	5:C:1228:THR:HG23	2.22	0.55
6:F:692:ALA:HB2	7:B:243:PRO:CD	2.26	0.55
1:D:850:TRP:CE2	1:D:852:LYS:HE3	2.42	0.55
7:B:1068:SER:HA	7:B:1083:ILE:HG21	1.89	0.55
1:D:112:VAL:O	1:D:638:TYR:CD1	2.60	0.55
1:D:734:VAL:HG11	1:D:779:LEU:HD21	1.89	0.55
5:C:316:LYS:CG	5:C:454:GLN:HE22	2.20	0.55
6:F:873:THR:CG2	6:F:1270:ILE:CD1	2.84	0.55
6:F:966:VAL:HG22	6:F:1265:LEU:HD13	1.88	0.55
6:F:995:TYR:CE1	6:F:997:ASP:OD1	2.59	0.55
7:B:868:ASN:ND2	7:B:1002:GLN:HE21	2.02	0.55
1:D:264:GLU:OE1	1:D:269:TRP:CA	2.53	0.55
5:C:22:ARG:HD2	5:C:746:GLU:OE1	2.07	0.55
6:F:22:PHE:CD1	6:F:827:ILE:HD11	2.41	0.55
6:F:363:ASP:OD2	6:F:424:HIS:CD2	2.60	0.55
7:B:912:LEU:CD2	7:B:1180:LEU:HD11	2.37	0.55
1:D:367:PRO:HB3	1:D:399:ARG:CZ	2.37	0.54
6:F:877:ARG:NE	6:F:1270:ILE:CG2	2.69	0.54
1:D:770:VAL:HG13	1:D:832:TRP:CD1	2.42	0.54
2:E:109:TYR:OH	4:Y:203:SER:HB2	2.07	0.54
1:D:124:LYS:HZ2	1:D:141:GLY:HA3	1.73	0.54
5:C:173:LYS:HA	5:C:550:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:607:ASN:HB3	6:F:248:THR:CG2	2.36	0.54
5:C:870:LEU:HD12	5:C:1223:VAL:HG21	1.89	0.54
7:B:197:THR:OG1	7:B:329:LYS:HE3	2.07	0.54
1:D:188:THR:CB	1:D:260:GLN:HE21	2.14	0.54
6:F:59:TRP:HB2	6:F:640:PHE:CD2	2.42	0.54
6:F:786:LEU:HD23	6:F:790:TRP:CH2	2.43	0.54
7:B:1194:LEU:CD2	7:B:1197:ILE:CD1	2.85	0.54
1:D:156:ALA:CA	6:F:88:ASP:OD2	2.53	0.54
1:D:161:ARG:HH11	6:F:92:GLN:HB2	1.73	0.54
6:F:961:THR:C	6:F:1269:LEU:CD2	2.80	0.54
6:F:1167:ASN:HB3	7:B:149:PRO:HB3	1.89	0.54
4:Y:254:ILE:HD12	4:Y:396:ILE:HD11	1.89	0.54
5:C:148:THR:HG21	7:B:1084:ALA:O	2.08	0.54
6:F:1217:VAL:HG21	6:F:1237:PRO:HA	1.90	0.54
1:D:114:ILE:HG23	1:D:145:ILE:CG2	2.38	0.54
1:D:126:LEU:HD23	1:D:131:VAL:HA	1.89	0.54
6:F:33:VAL:HA	6:F:832:ILE:HD11	1.88	0.54
1:D:719:PHE:O	1:D:727:LEU:CD1	2.55	0.53
5:C:152:LYS:N	7:B:1071:ASN:ND2	2.56	0.53
5:C:609:GLN:HE21	6:F:248:THR:CB	2.21	0.53
6:F:83:HIS:NE2	6:F:113:GLU:HG3	2.23	0.53
6:F:877:ARG:HH11	6:F:1270:ILE:HG21	1.72	0.53
6:F:1149:THR:HG21	6:F:1154:GLU:CB	2.39	0.53
7:B:344:LYS:CE	7:B:363:GLU:HG3	2.37	0.53
2:E:79:GLU:OE1	4:Y:259:ARG:NH2	2.41	0.53
6:F:434:THR:CG2	6:F:489:THR:HG21	2.37	0.53
6:F:467:LEU:CD2	6:F:468:PRO:HD3	2.39	0.53
7:B:355:VAL:CG2	7:B:406:LEU:HD12	2.39	0.53
1:D:509:LEU:HG	1:D:905:VAL:HG13	1.91	0.53
1:D:516:PHE:HE1	1:D:569:VAL:HG23	1.73	0.53
6:F:83:HIS:HB2	6:F:116:TRP:CZ3	2.43	0.53
6:F:1237:PRO:HG2	6:F:1239:HIS:CE1	2.43	0.53
1:D:163:ARG:CZ	6:F:80:GLU:N	2.72	0.53
1:D:171:ARG:NH1	1:D:314:PHE:CE1	2.76	0.53
5:C:345:THR:HG23	5:C:380:LYS:NZ	2.23	0.53
6:F:65:ASP:HB2	6:F:175:PRO:HG2	1.89	0.53
4:Y:50:LEU:HB2	4:Y:53:ILE:HD12	1.89	0.53
7:B:196:PRO:HG2	7:B:554:LEU:HD11	1.90	0.53
7:B:702:TRP:HE1	7:B:736:ASN:ND2	2.03	0.53
1:D:317:ARG:HH22	1:D:465:ASP:HA	1.73	0.53
2:E:79:GLU:CG	4:Y:259:ARG:NH1	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ILE:CD1	1:D:669:PHE:CD2	2.90	0.53
1:D:425:ALA:HB1	1:D:429:ASP:O	2.08	0.53
4:Y:92:TYR:HE1	4:Y:197:ILE:HD13	1.73	0.53
6:F:1097:LEU:HD13	6:F:1251:MET:HE2	1.90	0.53
6:F:1107:THR:HG23	6:F:1271:ARG:NH2	2.24	0.53
1:D:593:PHE:CZ	1:D:597:ILE:HD11	2.44	0.53
1:D:894:ASN:HB2	1:D:906:ILE:HD13	1.91	0.53
2:E:98:ILE:HA	4:Y:427:VAL:HG11	1.91	0.53
6:F:1071:PHE:HE2	6:F:1247:ARG:CD	2.21	0.52
7:B:1151:PHE:CD2	7:B:1171:ILE:HD11	2.44	0.52
1:D:259:GLY:HA3	1:D:270:PHE:CD2	2.44	0.52
4:Y:368:ILE:HD13	4:Y:377:HIS:CG	2.44	0.52
5:C:34:SER:O	5:C:40:SER:HB2	2.10	0.52
5:C:149:LYS:HD3	7:B:1083:ILE:HG22	1.82	0.52
6:F:995:TYR:HE1	6:F:997:ASP:OD1	1.92	0.52
1:D:11:TRP:CZ2	1:D:15:ILE:CD1	2.92	0.52
1:D:44:VAL:HG21	1:D:516:PHE:CD1	2.45	0.52
1:D:253:ASP:OD2	1:D:281:GLY:HA3	2.08	0.52
4:Y:280:LEU:CD2	4:Y:354:LEU:HD21	2.40	0.52
5:C:296:PHE:CE2	5:C:590:VAL:HG22	2.45	0.52
1:D:817:ILE:HD11	1:D:912:ILE:HD11	1.91	0.52
6:F:271:GLN:HB2	6:F:437:GLN:OE1	2.09	0.52
6:F:494:ARG:HH11	6:F:701:GLN:NE2	2.07	0.52
6:F:648:GLN:O	6:F:652:LYS:HB2	2.08	0.52
6:F:839:TRP:CD1	6:F:843:ASN:HD21	2.26	0.52
6:F:1031:VAL:HG21	6:F:1058:LEU:HD11	1.90	0.52
6:F:1098:THR:HG23	6:F:1106:SER:OG	2.10	0.52
7:B:1035:LYS:O	7:B:1070:LEU:HD23	2.09	0.52
1:D:119:HIS:CD2	1:D:140:ASP:O	2.62	0.52
6:F:324:ILE:HG23	6:F:719:PHE:HB2	1.91	0.52
7:B:875:LYS:HE2	7:B:879:GLU:OE1	2.09	0.52
7:B:899:ARG:NH1	7:B:1215:LEU:O	2.38	0.52
1:D:29:ILE:HG23	1:D:554:ILE:HD13	1.91	0.52
6:F:51:ASN:HB3	6:F:647:ILE:HG12	1.90	0.52
7:B:811:ALA:CB	7:B:901:ILE:HG22	2.37	0.52
4:Y:259:ARG:NH1	4:Y:381:VAL:HG13	2.24	0.52
1:D:206:LEU:O	1:D:480:LYS:HE3	2.10	0.52
1:D:448:LEU:C	4:Y:311:GLN:OE1	2.52	0.52
3:G:15:CYS:SG	4:Y:180:LEU:HD13	2.50	0.52
5:C:730:LEU:HA	5:C:735:LEU:CD2	2.40	0.52
5:C:730:LEU:HD22	5:C:1286:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:869:LEU:HD22	6:F:1262:LYS:HB3	1.92	0.52
1:D:68:LEU:CD1	1:D:83:THR:HG22	2.40	0.52
1:D:282:ASN:ND2	1:D:364:TYR:CE1	2.59	0.52
6:F:1149:THR:HG21	6:F:1154:GLU:HB3	1.92	0.52
1:D:337:LEU:HD13	1:D:386:VAL:HG21	1.93	0.51
7:B:46:ILE:HD12	7:B:591:LEU:HD23	1.92	0.51
7:B:253:LYS:HE3	7:B:348:GLU:OE2	2.10	0.51
4:Y:60:LEU:H	4:Y:156:PRO:HB3	1.75	0.51
4:Y:349:ILE:HD12	4:Y:382:LEU:HD11	1.90	0.51
7:B:388:ILE:HG23	7:B:952:PHE:CE1	2.46	0.51
1:D:317:ARG:CZ	1:D:403:ALA:O	2.59	0.51
5:C:606:ARG:HA	6:F:247:LYS:HZ2	1.75	0.51
6:F:965:LEU:HD12	6:F:1269:LEU:CD1	2.40	0.51
6:F:1097:LEU:CD1	6:F:1251:MET:HG3	2.41	0.51
7:B:356:VAL:HG21	7:B:443:LEU:HD11	1.92	0.51
7:B:897:HIS:CE1	7:B:901:ILE:HD11	2.45	0.51
1:D:831:PHE:CE2	1:D:916:PHE:HB3	2.44	0.51
3:G:27:SER:O	4:Y:125:GLU:OE1	2.27	0.51
4:Y:104:THR:CG2	4:Y:347:ILE:HG23	2.39	0.51
5:C:1078:GLY:HA2	5:C:1182:SER:O	2.11	0.51
6:F:1212:VAL:CG2	6:F:1248:LEU:HD12	2.40	0.51
1:D:704:ASN:HD22	1:D:850:TRP:CD1	2.28	0.51
1:D:891:ALA:HA	1:D:906:ILE:HG21	1.92	0.51
5:C:1188:ILE:HG12	5:C:1192:LYS:HG3	1.92	0.51
6:F:397:SER:HB3	6:F:408:ARG:NH1	2.26	0.51
7:B:803:ASP:O	7:B:809:LYS:HE3	2.11	0.51
1:D:186:GLU:OE1	1:D:192:VAL:HG22	2.10	0.51
1:D:273:LYS:HD2	1:D:390:ALA:HA	1.92	0.51
4:Y:82:LEU:CD1	4:Y:157:ILE:CD1	2.89	0.51
6:F:221:ALA:C	7:B:211:GLN:O	2.54	0.51
6:F:977:LEU:HD12	6:F:1255:LEU:HD21	1.92	0.51
6:F:1139:LYS:CE	6:F:1197:VAL:O	2.53	0.51
7:B:29:GLN:NE2	7:B:746:LYS:HB2	2.25	0.51
1:D:52:THR:HB	1:D:177:ILE:CD1	2.41	0.51
5:C:147:LEU:CD2	7:B:1082:THR:HG21	2.28	0.51
5:C:242:LYS:NZ	5:C:396:GLU:CD	2.68	0.51
6:F:575:MET:SD	6:F:641:LYS:HG3	2.51	0.51
6:F:965:LEU:HB3	6:F:1265:LEU:HD21	1.89	0.51
6:F:1130:SER:O	6:F:1216:LYS:NZ	2.37	0.51
6:F:1184:ILE:CD1	7:B:171:PHE:CZ	2.94	0.51
6:F:1207:LYS:HE2	6:F:1252:SER:OG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:LEU:CD2	1:D:663:VAL:HG22	2.41	0.51
6:F:311:ARG:NH1	6:F:673:GLY:HA3	2.26	0.51
6:F:714:PRO:HG2	6:F:761:ILE:HG22	1.92	0.51
7:B:329:LYS:HD2	7:B:692:TYR:CE2	2.46	0.51
3:G:11:MET:HE3	3:G:61:LEU:HD23	1.94	0.50
5:C:152:LYS:HZ3	7:B:1125:GLN:HB2	1.76	0.50
7:B:81:TYR:HB2	7:B:114:TRP:CZ3	2.46	0.50
7:B:784:LEU:HD11	7:B:792:PRO:HG2	1.93	0.50
1:D:578:VAL:HG22	1:D:625:TRP:HZ2	1.77	0.50
5:C:745:GLN:O	5:C:751:LYS:NZ	2.44	0.50
6:F:1219:MET:CE	6:F:1247:ARG:HH21	2.19	0.50
7:B:798:LEU:HD23	7:B:1216:LEU:CD1	2.41	0.50
5:C:753:ILE:CG2	5:C:782:TRP:CE2	2.94	0.50
6:F:1116:ILE:CG2	6:F:1248:LEU:HD11	2.41	0.50
1:D:509:LEU:CD1	1:D:823:GLN:OE1	2.60	0.50
5:C:242:LYS:HE2	5:C:396:GLU:OE2	2.12	0.50
6:F:866:PHE:HE1	6:F:1262:LYS:HG2	1.69	0.50
1:D:46:PHE:CE1	1:D:48:GLY:HA2	2.47	0.50
1:D:161:ARG:CG	6:F:88:ASP:HB3	2.40	0.50
4:Y:68:PHE:CZ	4:Y:146:ILE:CD1	2.95	0.50
6:F:161:THR:HG21	6:F:283:SER:OG	2.12	0.50
1:D:44:VAL:CG2	1:D:516:PHE:CB	2.87	0.50
1:D:253:ASP:OD2	1:D:281:GLY:CA	2.60	0.50
1:D:793:TYR:CD2	1:D:839:ILE:HD13	2.46	0.50
5:C:677:LYS:HE2	5:C:681:GLU:OE1	2.10	0.50
6:F:857:GLU:OE1	6:F:871:LYS:NZ	2.23	0.50
6:F:973:TYR:CE1	6:F:977:LEU:HD11	2.47	0.50
6:F:1172:ASN:HB2	7:B:171:PHE:CE2	2.47	0.50
7:B:984:GLN:NE2	7:B:1133:THR:CB	2.66	0.50
7:B:1151:PHE:CE2	7:B:1171:ILE:CD1	2.95	0.50
1:D:831:PHE:CE2	1:D:916:PHE:CB	2.95	0.50
6:F:1209:GLU:CG	6:F:1249:TRP:CD1	2.93	0.50
1:D:97:GLU:CD	1:D:116:LYS:HE2	2.37	0.50
1:D:415:LEU:HD11	1:D:479:VAL:HG11	1.92	0.50
2:E:79:GLU:CD	4:Y:259:ARG:HH12	2.20	0.50
5:C:1184:PHE:CZ	5:C:1192:LYS:HG2	2.46	0.50
6:F:1071:PHE:HD2	6:F:1247:ARG:NH1	2.00	0.50
6:F:1131:GLY:HA3	6:F:1208:PHE:HB2	1.94	0.50
7:B:984:GLN:HG3	7:B:1133:THR:CB	2.41	0.50
4:Y:60:LEU:HD11	4:Y:157:ILE:HD11	1.93	0.50
5:C:149:LYS:HB2	7:B:1084:ALA:CB	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:868:ASN:ND2	7:B:1002:GLN:NE2	2.60	0.50
1:D:158:THR:O	6:F:88:ASP:OD2	2.29	0.49
1:D:299:ARG:HG2	1:D:352:ALA:O	2.11	0.49
1:D:697:TYR:CE1	1:D:852:LYS:NZ	2.72	0.49
4:Y:82:LEU:CD1	4:Y:157:ILE:HD12	2.42	0.49
6:F:991:TRP:HA	6:F:1093:GLY:O	2.12	0.49
7:B:80:GLN:HE22	7:B:122:GLN:NE2	2.09	0.49
7:B:134:LYS:C	7:B:578:ASN:HD21	2.20	0.49
7:B:633:THR:HG23	7:B:737:ILE:HD13	1.94	0.49
1:D:158:THR:O	6:F:84:ASP:C	2.51	0.49
4:Y:53:ILE:HG23	4:Y:157:ILE:CG2	2.41	0.49
6:F:141:VAL:HG21	6:F:549:LEU:HD11	1.95	0.49
1:D:156:ALA:HB2	1:D:165:ILE:HD12	1.94	0.49
2:E:122:PHE:HE2	4:Y:47:ILE:CG2	2.24	0.49
3:G:24:ASN:OD1	4:Y:126:MET:SD	2.70	0.49
5:C:51:PRO:HB3	5:C:714:THR:HG21	1.95	0.49
7:B:58:TYR:HB3	7:B:70:LEU:HB2	1.94	0.49
1:D:263:VAL:HG12	1:D:362:TYR:HD2	1.78	0.49
4:Y:53:ILE:HD13	4:Y:82:LEU:HB3	1.93	0.49
6:F:494:ARG:NH1	6:F:701:GLN:NE2	2.60	0.49
6:F:1173:LEU:O	6:F:1189:LYS:CE	2.60	0.49
1:D:111:SER:OG	1:D:505:LEU:HD13	2.12	0.49
1:D:338:PHE:CZ	1:D:349:ILE:HD11	2.48	0.49
6:F:1172:ASN:CG	7:B:171:PHE:CD2	2.90	0.49
1:D:516:PHE:HE1	1:D:569:VAL:CG2	2.25	0.49
4:Y:82:LEU:HD23	4:Y:174:MET:HE1	1.92	0.49
6:F:1149:THR:HG22	6:F:1154:GLU:OE2	2.13	0.49
5:C:323:SER:HB2	5:C:448:LYS:HE3	1.93	0.49
6:F:717:GLU:OE2	6:F:764:THR:OG1	2.15	0.49
6:F:888:PHE:CB	6:F:935:LEU:HD22	2.42	0.49
6:F:1091:PHE:CZ	6:F:1247:ARG:CD	2.89	0.49
6:F:343:LYS:CE	6:F:439:MET:HB3	2.41	0.49
6:F:993:VAL:HG22	6:F:1027:PHE:CE1	2.48	0.49
7:B:928:VAL:HG21	7:B:1034:THR:CG2	2.42	0.49
1:D:331:PHE:HE2	1:D:339:LEU:HB3	1.77	0.49
1:D:578:VAL:HG22	1:D:625:TRP:CZ2	2.47	0.49
5:C:872:ARG:HG2	5:C:1220:LEU:HD12	1.95	0.49
6:F:343:LYS:HE3	6:F:439:MET:CB	2.39	0.49
6:F:1139:LYS:NZ	6:F:1200:LEU:O	2.23	0.49
5:C:311:TYR:CE2	5:C:478:LEU:HD21	2.47	0.48
6:F:1149:THR:CG2	6:F:1154:GLU:CB	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1183:LEU:HD21	7:B:171:PHE:CB	2.40	0.48
7:B:161:TRP:HH2	7:B:291:PHE:CE1	2.31	0.48
7:B:296:LEU:HD11	7:B:572:ALA:O	2.13	0.48
1:D:526:ILE:HG21	1:D:886:LEU:CD2	2.43	0.48
6:F:44:THR:HG23	6:F:655:LEU:CD2	2.43	0.48
6:F:168:VAL:CG1	6:F:625:LYS:HE3	2.43	0.48
7:B:29:GLN:HE22	7:B:746:LYS:HD2	1.79	0.48
1:D:29:ILE:HG23	1:D:554:ILE:CD1	2.43	0.48
1:D:212:GLN:CB	4:Y:61:ASP:HB3	2.42	0.48
1:D:643:LEU:CD2	1:D:826:ILE:HG23	2.43	0.48
1:D:919:PHE:O	1:D:924:PRO:CD	2.62	0.48
5:C:700:LEU:HD23	5:C:701:TYR:CE2	2.48	0.48
6:F:547:ASN:OD1	6:F:550:GLU:HB2	2.13	0.48
1:D:445:ASN:ND2	1:D:457:GLN:OE1	2.46	0.48
7:B:13:PHE:HE2	7:B:1210:GLU:OE1	1.95	0.48
7:B:216:ILE:HD12	7:B:234:PHE:CE2	2.49	0.48
1:D:756:LEU:C	1:D:758:ALA:H	2.20	0.48
6:F:196:ASN:HA	6:F:516:ARG:NH2	2.28	0.48
6:F:795:GLN:CD	6:F:807:LYS:HB2	2.39	0.48
6:F:1149:THR:CG2	6:F:1154:GLU:HB2	2.44	0.48
5:C:208:VAL:HG13	5:C:281:SER:HA	1.96	0.48
5:C:381:THR:OG1	5:C:618:LYS:HG2	2.14	0.48
5:C:386:ILE:HG12	5:C:948:VAL:HG12	1.96	0.48
1:D:191:ILE:HD13	1:D:248:SER:HA	1.95	0.48
1:D:850:TRP:CZ2	1:D:852:LYS:HE3	2.48	0.48
4:Y:107:ILE:CG2	4:Y:109:PRO:HD2	2.42	0.48
5:C:152:LYS:HE2	5:C:156:GLU:OE1	2.13	0.48
1:D:669:PHE:HD1	1:D:676:LEU:HD11	1.77	0.48
6:F:961:THR:HB	6:F:1269:LEU:HD23	1.89	0.48
7:B:323:GLY:HA3	7:B:679:TYR:CE2	2.49	0.48
7:B:684:GLY:HA3	7:B:861:ILE:O	2.14	0.48
4:Y:254:ILE:CD1	4:Y:392:PHE:HB3	2.44	0.48
5:C:505:ASP:O	7:B:1126:ARG:NH1	2.47	0.48
6:F:94:GLU:O	6:F:98:TRP:HB3	2.14	0.48
1:D:210:VAL:CG1	4:Y:410:PRO:HD3	2.38	0.47
1:D:337:LEU:HD22	1:D:362:TYR:OH	2.14	0.47
1:D:851:PHE:CE1	1:D:864:LEU:CD2	2.97	0.47
3:G:25:HIS:O	4:Y:190:LYS:NZ	2.45	0.47
5:C:87:LEU:HD11	5:C:103:ILE:CD1	2.43	0.47
5:C:148:THR:HB	7:B:1084:ALA:C	2.39	0.47
5:C:316:LYS:HD2	5:C:480:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:607:ASN:HB3	6:F:248:THR:HG22	1.96	0.47
7:B:870:PHE:HB3	7:B:874:PHE:CE2	2.49	0.47
7:B:907:LEU:O	7:B:912:LEU:HA	2.13	0.47
7:B:1151:PHE:HE2	7:B:1171:ILE:CD1	2.27	0.47
5:C:22:ARG:CD	5:C:746:GLU:OE1	2.62	0.47
6:F:372:SER:C	6:F:374:ALA:H	2.23	0.47
7:B:658:ASN:ND2	7:B:955:GLU:OE1	2.48	0.47
1:D:584:ILE:HG22	1:D:841:GLN:OE1	2.14	0.47
5:C:609:GLN:NE2	6:F:248:THR:HB	2.28	0.47
5:C:775:ASN:ND2	5:C:1228:THR:O	2.46	0.47
5:C:853:TRP:CE2	5:C:861:ASN:ND2	2.82	0.47
7:B:332:VAL:HG12	7:B:514:LEU:CD1	2.44	0.47
7:B:1041:TYR:CE2	7:B:1066:GLN:OE1	2.67	0.47
4:Y:60:LEU:HG	4:Y:156:PRO:CG	2.44	0.47
5:C:849:TYR:CE2	5:C:1270:LEU:HD13	2.49	0.47
6:F:286:GLY:HA2	6:F:487:LEU:CD2	2.44	0.47
6:F:727:ALA:C	6:F:729:GLY:H	2.22	0.47
6:F:872:GLN:HG3	6:F:897:VAL:CG2	2.44	0.47
1:D:52:THR:HB	1:D:177:ILE:HD13	1.96	0.47
4:Y:280:LEU:HD21	4:Y:354:LEU:HD21	1.97	0.47
6:F:725:SER:C	6:F:727:ALA:H	2.22	0.47
4:Y:67:PHE:CE2	4:Y:71:PHE:CE2	3.00	0.47
5:C:168:PRO:HG3	5:C:183:ALA:HA	1.96	0.47
5:C:579:VAL:HG11	5:C:644:VAL:HG21	1.97	0.47
6:F:50:VAL:HG13	6:F:817:MET:CE	2.45	0.47
1:D:509:LEU:H	1:D:823:GLN:NE2	2.12	0.47
1:D:637:ASN:ND2	1:D:761:GLU:OE2	2.47	0.47
4:Y:97:ILE:HG21	4:Y:294:PHE:CE1	2.50	0.47
5:C:152:LYS:NZ	5:C:505:ASP:OD2	2.47	0.47
5:C:295:MET:CE	5:C:308:ILE:HD11	2.44	0.47
5:C:295:MET:HE3	5:C:296:PHE:CE2	2.50	0.47
5:C:1193:VAL:HG11	5:C:1197:ASN:O	2.14	0.47
6:F:965:LEU:O	6:F:970:ALA:HA	2.13	0.47
6:F:1014:LYS:O	6:F:1016:ALA:N	2.48	0.47
7:B:283:ARG:HD3	7:B:290:ASP:CG	2.35	0.47
3:G:62:VAL:CG1	4:Y:41:LEU:CD2	2.92	0.47
6:F:98:TRP:CG	6:F:99:PRO:HD3	2.50	0.47
7:B:253:LYS:HE3	7:B:348:GLU:CD	2.40	0.47
1:D:170:LYS:HE3	1:D:500:LEU:HD12	1.97	0.47
3:G:66:LEU:HD11	4:Y:44:VAL:CG1	2.45	0.47
5:C:1090:LYS:NZ	5:C:1138:ASP:CG	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:SER:HB2	6:F:96:ILE:HD13	1.96	0.47
6:F:87:LEU:HD12	6:F:102:LEU:CD2	2.45	0.47
1:D:160:ALA:CB	6:F:83:HIS:C	2.87	0.47
1:D:509:LEU:HB3	1:D:823:GLN:NE2	2.30	0.47
1:D:631:VAL:HG11	1:D:769:GLY:HA2	1.97	0.47
5:C:340:PHE:HD2	5:C:400:GLN:OE1	1.98	0.47
5:C:607:ASN:O	6:F:247:LYS:HB2	2.11	0.47
5:C:1183:ARG:NH2	5:C:1222:ASP:OD1	2.47	0.47
7:B:204:TYR:O	7:B:501:GLY:HA3	2.15	0.47
1:D:11:TRP:CZ2	1:D:15:ILE:HD11	2.49	0.46
3:G:28:THR:HA	4:Y:125:GLU:CD	2.39	0.46
6:F:288:PHE:HE2	6:F:488:GLN:NE2	2.13	0.46
6:F:692:ALA:CB	7:B:242:ALA:CB	2.93	0.46
7:B:305:LYS:HD2	7:B:573:PHE:CG	2.50	0.46
7:B:912:LEU:HD22	7:B:1180:LEU:HD11	1.96	0.46
1:D:741:MET:CE	1:D:771:GLY:HA3	2.38	0.46
4:Y:343:PHE:CZ	4:Y:347:ILE:HD11	2.50	0.46
6:F:87:LEU:HD12	6:F:102:LEU:HD22	1.97	0.46
7:B:853:TRP:CH2	7:B:859:LYS:HD3	2.50	0.46
1:D:164:GLN:CB	6:F:85:ASN:ND2	2.79	0.46
3:G:32:ALA:CB	3:G:39:LEU:HD12	2.45	0.46
5:C:531:PHE:CZ	5:C:563:ILE:HG21	2.42	0.46
6:F:692:ALA:HB3	7:B:242:ALA:CB	2.46	0.46
4:Y:60:LEU:CA	4:Y:156:PRO:HG3	2.45	0.46
4:Y:96:GLN:HG2	4:Y:128:THR:HG21	1.98	0.46
5:C:217:ASP:HB2	5:C:221:ASN:HD22	1.80	0.46
5:C:789:TYR:HB2	5:C:847:TYR:CE1	2.50	0.46
7:B:1161:LEU:HD21	7:B:1180:LEU:HD12	1.98	0.46
1:D:618:MET:HE3	1:D:622:HIS:HE1	1.81	0.46
5:C:309:GLN:NE2	5:C:318:SER:HB2	2.30	0.46
5:C:386:ILE:HD13	5:C:949:TYR:CE1	2.50	0.46
5:C:1014:THR:H	5:C:1017:THR:HG1	1.63	0.46
6:F:1212:VAL:HG21	6:F:1248:LEU:HD12	1.97	0.46
1:D:94:ASN:OD1	1:D:116:LYS:NZ	2.35	0.46
1:D:419:ARG:O	1:D:434:ASN:HB3	2.16	0.46
3:G:66:LEU:HD11	4:Y:44:VAL:HG11	1.98	0.46
5:C:313:ALA:HB1	5:C:455:PRO:CG	2.45	0.46
5:C:923:GLY:C	5:C:925:GLY:H	2.23	0.46
6:F:60:TYR:HB3	6:F:72:LEU:HB2	1.97	0.46
6:F:937:LYS:HE2	6:F:941:GLU:OE1	2.15	0.46
1:D:102:ASN:HB3	1:D:485:ASN:HD22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:PRO:HD3	1:D:473:TYR:CD2	2.51	0.46
1:D:894:ASN:CB	1:D:906:ILE:HD13	2.46	0.46
4:Y:60:LEU:HD11	4:Y:157:ILE:HD12	1.98	0.46
5:C:197:ILE:O	5:C:483:ARG:NH2	2.48	0.46
1:D:851:PHE:CE1	1:D:864:LEU:HD21	2.51	0.46
2:E:109:TYR:CZ	4:Y:203:SER:HB2	2.51	0.46
6:F:692:ALA:HB1	7:B:242:ALA:HA	1.98	0.46
6:F:773:LYS:HE2	6:F:945:GLU:OE2	2.16	0.46
6:F:879:TRP:CD2	6:F:932:LEU:HD11	2.51	0.46
1:D:309:THR:CG2	6:F:82:GLU:HG3	2.46	0.46
1:D:894:ASN:CB	1:D:906:ILE:CD1	2.94	0.46
5:C:1281:VAL:HG11	5:C:1286:ILE:HB	1.98	0.46
1:D:25:GLY:HA2	1:D:551:LEU:HD13	1.97	0.45
1:D:157:ARG:CB	6:F:91:GLN:CB	2.94	0.45
1:D:834:PHE:HE1	1:D:921:ASN:OD1	2.00	0.45
4:Y:68:PHE:CE2	4:Y:146:ILE:CD1	2.99	0.45
4:Y:271:VAL:HB	4:Y:277:LEU:HD21	1.97	0.45
5:C:138:GLU:OE1	5:C:169:LYS:HE3	2.17	0.45
5:C:753:ILE:HG21	5:C:782:TRP:CE2	2.51	0.45
5:C:1136:PHE:CD2	5:C:1140:ASN:ND2	2.84	0.45
6:F:363:ASP:CG	6:F:424:HIS:HD2	2.24	0.45
7:B:230:TYR:OH	7:B:444:ASP:OD2	2.28	0.45
7:B:912:LEU:HD21	7:B:1180:LEU:HD11	1.99	0.45
1:D:544:TYR:OH	1:D:669:PHE:CE2	2.63	0.45
1:D:669:PHE:CD1	1:D:676:LEU:CD1	2.96	0.45
7:B:1051:ILE:HD12	7:B:1110:LEU:HD11	1.98	0.45
1:D:161:ARG:HA	6:F:85:ASN:CG	2.38	0.45
4:Y:149:ASN:C	4:Y:151:GLY:H	2.23	0.45
6:F:355:ASP:CG	6:F:406:ASN:HD22	2.24	0.45
6:F:397:SER:HB3	6:F:408:ARG:CZ	2.46	0.45
6:F:1031:VAL:HG11	6:F:1058:LEU:HD12	1.97	0.45
7:B:941:PHE:HB2	7:B:973:PHE:CE1	2.51	0.45
1:D:763:SER:HB3	1:D:825:ILE:HD13	1.99	0.45
4:Y:254:ILE:HD12	4:Y:396:ILE:CD1	2.45	0.45
6:F:686:ILE:HD13	6:F:1039:GLY:HA2	1.98	0.45
1:D:163:ARG:HB2	6:F:81:ASP:O	2.16	0.45
1:D:212:GLN:HB3	4:Y:61:ASP:CB	2.47	0.45
1:D:306:LYS:HB2	1:D:322:TRP:CH2	2.51	0.45
1:D:487:PHE:CE1	1:D:491:ALA:HB3	2.52	0.45
1:D:850:TRP:CZ2	1:D:852:LYS:CE	2.99	0.45
4:Y:72:ASN:OD1	4:Y:77:GLY:HA2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:197:THR:OG1	7:B:329:LYS:CE	2.64	0.45
1:D:158:THR:HB	6:F:84:ASP:O	2.13	0.45
1:D:744:LEU:O	1:D:748:ALA:HB2	2.16	0.45
3:G:23:SER:HA	4:Y:129:ARG:HD2	1.97	0.45
5:C:149:LYS:N	7:B:1084:ALA:HB3	2.26	0.45
5:C:1141:PHE:HB3	5:C:1181:PHE:HE2	1.81	0.45
5:C:1229:ASP:OD2	5:C:1240:LYS:NZ	2.49	0.45
7:B:81:TYR:CE1	7:B:111:GLU:HG3	2.52	0.45
1:D:570:PHE:CE1	1:D:823:GLN:HG2	2.52	0.45
1:D:923:LEU:HB3	1:D:924:PRO:HD3	1.98	0.45
2:E:121:VAL:HA	3:G:73:HIS:NE2	2.31	0.45
3:G:33:SER:HB3	4:Y:195:ASN:HD22	1.81	0.45
4:Y:82:LEU:HD21	4:Y:174:MET:HE1	1.98	0.45
5:C:855:LEU:HD23	5:C:859:LEU:HD21	1.98	0.45
6:F:82:GLU:OE2	6:F:120:LYS:CE	2.59	0.45
7:B:200:SER:HB2	7:B:292:LEU:HD23	1.98	0.45
1:D:46:PHE:CZ	1:D:48:GLY:HA2	2.52	0.45
1:D:97:GLU:OE2	1:D:116:LYS:HE2	2.16	0.45
1:D:793:TYR:CE2	1:D:839:ILE:HD13	2.52	0.45
5:C:152:LYS:NZ	5:C:505:ASP:CG	2.75	0.45
5:C:345:THR:HG23	5:C:380:LYS:HZ1	1.80	0.45
5:C:887:ASN:HB2	5:C:1210:TYR:CE1	2.52	0.45
7:B:408:LYS:HD3	7:B:440:TYR:OH	2.17	0.45
1:D:808:MET:SD	1:D:828:VAL:HG21	2.57	0.45
5:C:59:ASP:OD2	5:C:555:LYS:HD2	2.17	0.45
5:C:290:LEU:HD23	5:C:295:MET:HB2	1.98	0.45
6:F:161:THR:CG2	6:F:283:SER:OG	2.65	0.45
6:F:330:LEU:HD21	6:F:488:GLN:CB	2.46	0.45
6:F:533:LYS:NZ	6:F:550:GLU:OE1	2.43	0.45
6:F:1097:LEU:HD11	6:F:1251:MET:HG3	1.98	0.45
7:B:195:ASP:CA	7:B:545:ARG:NH1	2.77	0.45
7:B:341:PRO:HG3	7:B:443:LEU:HD22	1.99	0.45
1:D:551:LEU:HD23	1:D:657:LEU:HD22	1.99	0.44
3:G:26:GLY:HA3	4:Y:129:ARG:CZ	2.47	0.44
4:Y:92:TYR:CE1	4:Y:197:ILE:HD13	2.51	0.44
4:Y:220:LEU:CD2	4:Y:407:ILE:CG2	2.95	0.44
5:C:52:VAL:HG21	5:C:563:ILE:HD12	1.95	0.44
6:F:991:TRP:O	6:F:1246:SER:HA	2.17	0.44
7:B:287:ASN:C	7:B:289:GLY:H	2.25	0.44
1:D:597:ILE:HD13	1:D:682:LEU:HD11	1.99	0.44
5:C:242:LYS:CE	5:C:396:GLU:OE2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:386:ILE:HG21	5:C:949:TYR:CZ	2.52	0.44
6:F:12:ARG:CZ	6:F:801:SER:O	2.65	0.44
6:F:1207:LYS:CE	6:F:1252:SER:OG	2.65	0.44
7:B:968:LEU:HD22	7:B:973:PHE:CD2	2.53	0.44
1:D:580:ALA:HB2	1:D:886:LEU:HD12	1.99	0.44
3:G:15:CYS:SG	4:Y:180:LEU:CD1	3.06	0.44
5:C:507:ASP:OD1	7:B:1127:ASP:OD2	2.31	0.44
5:C:912:SER:O	5:C:914:VAL:HG23	2.17	0.44
5:C:1028:ARG:NH2	5:C:1038:GLU:OE1	2.50	0.44
6:F:1237:PRO:CG	6:F:1239:HIS:NE2	2.68	0.44
7:B:356:VAL:CG2	7:B:362:VAL:HG21	2.46	0.44
3:G:1:MET:CE	4:Y:169:PHE:HB2	2.48	0.44
5:C:250:THR:O	5:C:280:PHE:HA	2.18	0.44
6:F:314:PHE:CE2	6:F:323:ILE:CD1	3.00	0.44
7:B:211:GLN:OE1	7:B:215:GLN:CD	2.60	0.44
7:B:357:ASP:OD1	7:B:439:ASN:HB3	2.18	0.44
1:D:97:GLU:OE2	1:D:116:LYS:NZ	2.48	0.44
1:D:231:ILE:O	1:D:448:LEU:HD13	2.17	0.44
4:Y:251:THR:HG21	4:Y:421:ILE:HA	2.00	0.44
4:Y:292:VAL:HG13	4:Y:333:TYR:OH	2.17	0.44
4:Y:294:PHE:HE2	4:Y:344:TYR:CE2	2.34	0.44
5:C:507:ASP:OD1	5:C:507:ASP:N	2.51	0.44
5:C:606:ARG:CA	6:F:247:LYS:NZ	2.81	0.44
6:F:1192:PHE:HE2	7:B:170:ARG:HH12	1.65	0.44
6:F:1237:PRO:O	6:F:1239:HIS:N	2.49	0.44
1:D:214:THR:HB	2:E:125:LYS:NZ	2.33	0.44
1:D:157:ARG:CB	6:F:91:GLN:HB2	2.48	0.44
5:C:325:GLU:OE1	5:C:451:SER:HB3	2.18	0.44
5:C:827:TYR:CE2	5:C:832:LEU:HD12	2.53	0.44
6:F:869:LEU:HD21	6:F:1263:PHE:HA	1.99	0.44
1:D:104:LEU:HD11	1:D:147:VAL:HG11	1.99	0.44
1:D:105:TYR:OH	1:D:638:TYR:CD1	2.71	0.44
1:D:126:LEU:HD21	1:D:131:VAL:HG22	2.00	0.44
1:D:516:PHE:CE1	1:D:569:VAL:HG23	2.52	0.44
1:D:640:VAL:HG13	1:D:766:ILE:HD11	1.99	0.44
1:D:306:LYS:HD2	1:D:322:TRP:CZ3	2.53	0.43
1:D:701:THR:HG23	1:D:850:TRP:CZ2	2.52	0.43
6:F:54:GLU:HG2	6:F:814:GLN:HE21	1.76	0.43
6:F:179:PHE:HD2	6:F:633:PRO:HG2	1.82	0.43
6:F:182:ASN:HB3	6:F:574:MET:HE3	2.00	0.43
6:F:222:ALA:HA	7:B:211:GLN:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:977:LEU:CD1	6:F:1255:LEU:HD21	2.47	0.43
7:B:398:GLN:HA	7:B:414:LYS:NZ	2.32	0.43
1:D:164:GLN:CG	6:F:85:ASN:CG	2.85	0.43
5:C:138:GLU:OE2	5:C:501:TYR:OH	2.22	0.43
1:D:157:ARG:C	6:F:91:GLN:OE1	2.60	0.43
1:D:158:THR:N	6:F:88:ASP:HA	2.29	0.43
1:D:669:PHE:HD1	1:D:676:LEU:CD1	2.31	0.43
1:D:835:PHE:CE1	1:D:839:ILE:HD11	2.53	0.43
1:D:922:GLY:O	1:D:926:PHE:HB3	2.19	0.43
5:C:863:LYS:CE	5:C:1224:GLU:HA	2.46	0.43
1:D:68:LEU:HD11	1:D:83:THR:HG22	2.00	0.43
1:D:575:ILE:HG13	1:D:646:LEU:HD21	2.00	0.43
4:Y:60:LEU:N	4:Y:156:PRO:CB	2.80	0.43
5:C:563:ILE:CG2	5:C:567:LEU:HD12	2.46	0.43
7:B:80:GLN:NE2	7:B:122:GLN:HE22	2.17	0.43
7:B:899:ARG:HG2	7:B:1194:LEU:CD1	2.48	0.43
7:B:1011:THR:HB	7:B:1020:MET:SD	2.58	0.43
4:Y:410:PRO:CG	4:Y:413:LEU:HD12	2.48	0.43
5:C:49:LEU:HD21	5:C:530:LEU:HD23	2.01	0.43
6:F:712:SER:HB2	6:F:717:GLU:OE1	2.18	0.43
6:F:714:PRO:HG2	6:F:761:ILE:CG2	2.48	0.43
6:F:996:ASP:HB2	6:F:1057:LEU:HD13	1.99	0.43
6:F:1167:ASN:CB	7:B:149:PRO:HB3	2.48	0.43
7:B:28:LEU:HD22	7:B:765:LEU:HD21	1.99	0.43
1:D:25:GLY:HA2	1:D:551:LEU:CD1	2.48	0.43
5:C:139:TYR:CZ	5:C:154:LEU:HD23	2.54	0.43
6:F:510:PHE:CD2	6:F:511:LEU:HG	2.54	0.43
6:F:664:PHE:CE1	6:F:668:LEU:HD12	2.53	0.43
7:B:371:LEU:HB3	7:B:442:VAL:HB	2.00	0.43
7:B:984:GLN:CG	7:B:1133:THR:CA	2.87	0.43
1:D:160:ALA:HB2	6:F:83:HIS:CA	2.48	0.43
1:D:838:ARG:CG	1:D:925:LEU:HD22	2.48	0.43
5:C:27:LEU:HD11	5:C:707:VAL:HG11	2.00	0.43
5:C:33:LYS:HB3	5:C:729:TYR:CZ	2.54	0.43
5:C:401:ILE:CD1	5:C:615:LEU:HD21	2.49	0.43
5:C:1218:VAL:CG1	5:C:1242:LEU:HD22	2.46	0.43
6:F:1094:PHE:CZ	6:F:1096:GLY:HA2	2.54	0.43
6:F:1169:ASP:CG	7:B:147:THR:CB	2.83	0.43
3:G:29:GLY:HA3	3:G:40:GLU:HG3	2.01	0.43
1:D:97:GLU:OE2	1:D:116:LYS:CE	2.67	0.43
1:D:226:LEU:HD21	1:D:243:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:745:TYR:CD2	1:D:768:LEU:HD12	2.54	0.43
5:C:152:LYS:NZ	7:B:1126:ARG:HG3	2.34	0.43
6:F:51:ASN:ND2	6:F:651:TYR:CE2	2.87	0.43
6:F:807:LYS:CE	6:F:811:ASN:CG	2.81	0.43
6:F:834:ASN:ND2	6:F:950:ASP:HA	2.34	0.43
7:B:90:SER:OG	7:B:95:LYS:HA	2.19	0.43
7:B:988:GLN:C	7:B:990:ALA:H	2.26	0.43
6:F:342:VAL:HG22	6:F:359:MET:HE2	2.01	0.43
7:B:908:VAL:HA	7:B:912:LEU:HD23	2.00	0.43
1:D:462:VAL:HG22	1:D:468:TYR:CE1	2.54	0.42
5:C:158:THR:HG23	5:C:270:GLN:O	2.19	0.42
5:C:1028:ARG:HA	5:C:1032:GLN:HB2	2.01	0.42
6:F:288:PHE:O	6:F:302:LYS:NZ	2.44	0.42
6:F:1219:MET:CE	6:F:1247:ARG:NH2	2.77	0.42
7:B:80:GLN:HE22	7:B:122:GLN:HE22	1.66	0.42
7:B:385:SER:HB2	7:B:420:LYS:HB2	2.01	0.42
7:B:392:LEU:O	7:B:395:ILE:HG12	2.19	0.42
1:D:112:VAL:O	1:D:638:TYR:HD1	2.02	0.42
1:D:338:PHE:CE2	1:D:359:ASN:CB	2.85	0.42
4:Y:59:GLY:H	4:Y:156:PRO:HB3	1.84	0.42
5:C:324:LYS:NZ	5:C:338:ASN:O	2.43	0.42
5:C:607:ASN:HB3	6:F:248:THR:HG23	1.99	0.42
6:F:330:LEU:HD12	6:F:504:ILE:HD12	2.00	0.42
6:F:363:ASP:CG	6:F:424:HIS:CD2	2.97	0.42
2:E:79:GLU:CD	4:Y:259:ARG:NH1	2.77	0.42
5:C:699:PRO:HD3	5:C:706:LEU:HD12	2.01	0.42
5:C:888:LYS:NZ	5:C:1198:TYR:O	2.52	0.42
7:B:928:VAL:HG21	7:B:1034:THR:HG23	2.01	0.42
1:D:367:PRO:HD3	1:D:399:ARG:NH2	2.35	0.42
6:F:178:GLU:CD	6:F:632:LYS:HD3	2.44	0.42
6:F:842:THR:O	6:F:848:LYS:HD2	2.20	0.42
6:F:940:PHE:CE1	6:F:944:LEU:HD11	2.54	0.42
1:D:331:PHE:CE2	1:D:339:LEU:HB3	2.53	0.42
1:D:509:LEU:CD2	1:D:909:LEU:HD12	2.49	0.42
4:Y:68:PHE:CE2	4:Y:146:ILE:HD13	2.54	0.42
6:F:1129:LYS:HD3	6:F:1204:TYR:CE2	2.54	0.42
6:F:1208:PHE:CE2	6:F:1216:LYS:HE3	2.49	0.42
7:B:765:LEU:HD12	7:B:781:LEU:HD11	2.01	0.42
1:D:647:MET:HG3	1:D:829:TYR:HE1	1.85	0.42
5:C:619:LEU:O	5:C:953:ASN:ND2	2.50	0.42
5:C:877:PHE:CE1	5:C:1217:GLN:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1031:VAL:HG21	6:F:1058:LEU:CD1	2.50	0.42
7:B:85:VAL:HG12	7:B:95:LYS:HE2	2.02	0.42
1:D:270:PHE:HD1	1:D:396:ARG:HE	1.67	0.42
1:D:596:ASN:HB2	1:D:606:SER:OG	2.19	0.42
1:D:641:GLN:HE22	4:Y:226:THR:HB	1.84	0.42
5:C:201:ASN:HA	5:C:483:ARG:NH2	2.34	0.42
5:C:531:PHE:HZ	5:C:563:ILE:CG2	2.25	0.42
6:F:314:PHE:CE2	6:F:323:ILE:HD12	2.55	0.42
1:D:183:LEU:HB3	1:D:196:SER:HB3	2.02	0.42
1:D:611:LEU:HD21	1:D:663:VAL:HG22	2.02	0.42
1:D:657:LEU:O	1:D:661:LEU:HB3	2.20	0.42
5:C:139:TYR:HB2	5:C:497:LEU:HD21	2.02	0.42
5:C:295:MET:HE3	5:C:296:PHE:HE2	1.83	0.42
5:C:587:GLU:HG3	5:C:665:PHE:CD1	2.55	0.42
5:C:608:ASN:N	6:F:247:LYS:HD2	2.35	0.42
6:F:68:ILE:HD12	6:F:176:ASN:HD22	1.82	0.42
6:F:289:ASP:OD2	6:F:538:LYS:HD2	2.19	0.42
1:D:44:VAL:HG23	1:D:516:PHE:CG	2.51	0.42
1:D:161:ARG:HB2	6:F:85:ASN:O	2.19	0.42
1:D:509:LEU:HB2	1:D:823:GLN:OE1	2.20	0.42
1:D:514:SER:HB3	1:D:898:ILE:HG13	1.97	0.42
3:G:11:MET:CE	3:G:64:LEU:HB3	2.47	0.42
6:F:107:ASP:HB3	6:F:803:ILE:CD1	2.50	0.42
6:F:881:ARG:NH2	6:F:1274:LEU:HB3	2.33	0.42
6:F:940:PHE:CZ	6:F:944:LEU:HD11	2.55	0.42
7:B:412:GLN:HG3	7:B:438:ASN:OD1	2.20	0.42
7:B:646:LEU:HD23	7:B:690:ASN:OD1	2.20	0.42
7:B:1002:GLN:C	7:B:1004:SER:H	2.27	0.42
1:D:514:SER:HB2	1:D:898:ILE:CG1	2.50	0.42
2:E:79:GLU:OE2	4:Y:384:ARG:HD3	2.20	0.42
5:C:878:LEU:HD13	5:C:1244:LEU:HD11	2.00	0.42
6:F:653:ASP:HB3	6:F:782:LYS:HD2	2.00	0.42
6:F:1100:ASN:HB2	6:F:1117:PHE:CE1	2.55	0.42
7:B:1159:LEU:HD22	7:B:1176:VAL:HG22	2.02	0.42
5:C:295:MET:HE1	5:C:308:ILE:HD11	2.00	0.41
5:C:806:VAL:HG23	5:C:944:PHE:CE2	2.55	0.41
5:C:1183:ARG:HH12	5:C:1243:ASN:HB2	1.80	0.41
6:F:221:ALA:O	7:B:211:GLN:C	2.62	0.41
7:B:713:SER:HA	7:B:729:ILE:HD11	2.01	0.41
1:D:331:PHE:CD1	1:D:386:VAL:CG2	3.04	0.41
6:F:990:SER:HB3	6:F:1248:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1169:ASP:OD2	7:B:147:THR:HG22	2.19	0.41
1:D:121:THR:CG2	1:D:143:PRO:HD3	2.49	0.41
1:D:477:SER:CB	4:Y:222:GLY:O	2.68	0.41
1:D:838:ARG:NH2	1:D:875:LEU:HB3	2.26	0.41
5:C:217:ASP:HB2	5:C:221:ASN:ND2	2.36	0.41
6:F:871:LYS:HB2	6:F:897:VAL:HG11	2.03	0.41
3:G:33:SER:CB	4:Y:195:ASN:HD22	2.33	0.41
6:F:1143:LYS:NZ	6:F:1198:ASP:OD2	2.52	0.41
6:F:1167:ASN:O	7:B:149:PRO:N	2.46	0.41
7:B:55:GLU:OE1	7:B:74:LYS:NZ	2.47	0.41
1:D:309:THR:HG22	6:F:82:GLU:CG	2.51	0.41
6:F:958:PHE:CB	6:F:1273:VAL:HG11	2.51	0.41
7:B:850:TYR:CZ	7:B:974:PHE:HB2	2.55	0.41
1:D:440:PHE:CE1	1:D:456:PHE:CD1	3.08	0.41
1:D:584:ILE:CG2	1:D:841:GLN:OE1	2.69	0.41
5:C:316:LYS:CD	5:C:454:GLN:NE2	2.84	0.41
7:B:216:ILE:CD1	7:B:234:PHE:CE2	3.04	0.41
7:B:1151:PHE:HE2	7:B:1171:ILE:HD12	1.86	0.41
6:F:866:PHE:CZ	6:F:1262:LYS:HG2	2.50	0.41
6:F:957:ARG:HB3	6:F:1273:VAL:HG13	2.02	0.41
6:F:1149:THR:O	6:F:1190:LYS:NZ	2.49	0.41
7:B:100:GLN:HG2	7:B:758:ALA:O	2.21	0.41
7:B:258:GLY:HA3	7:B:281:LYS:HD2	2.03	0.41
1:D:331:PHE:CD2	1:D:339:LEU:O	2.73	0.41
6:F:965:LEU:HD12	6:F:1269:LEU:HD11	2.01	0.41
7:B:984:GLN:HG3	7:B:1133:THR:CA	2.50	0.41
7:B:1041:TYR:HE2	7:B:1066:GLN:OE1	2.02	0.41
1:D:119:HIS:CG	1:D:140:ASP:O	2.74	0.41
1:D:506:SER:HB2	1:D:511:ARG:HA	2.02	0.41
5:C:101:THR:HG22	5:C:703:GLN:HE21	1.83	0.41
5:C:152:LYS:N	7:B:1071:ASN:HD21	2.13	0.41
5:C:753:ILE:HG23	5:C:782:TRP:CE2	2.55	0.41
5:C:850:THR:OG1	5:C:1263:GLN:HA	2.21	0.41
5:C:862:TYR:CZ	5:C:866:LEU:HD11	2.56	0.41
6:F:22:PHE:CE1	6:F:827:ILE:CD1	2.87	0.41
6:F:188:PHE:HA	6:F:555:PHE:CE2	2.56	0.41
6:F:877:ARG:HD3	6:F:1270:ILE:CG2	2.47	0.41
6:F:991:TRP:HZ2	6:F:1260:LEU:HD11	1.85	0.41
6:F:1162:LEU:HD12	6:F:1193:LEU:HD22	2.03	0.41
6:F:1240:SER:O	6:F:1243:THR:OG1	2.26	0.41
7:B:899:ARG:HH11	7:B:1215:LEU:C	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1151:PHE:HD2	7:B:1171:ILE:HD11	1.83	0.41
1:D:161:ARG:HB2	6:F:88:ASP:CB	2.28	0.41
4:Y:261:ILE:HD11	4:Y:381:VAL:HG11	2.03	0.41
5:C:228:ILE:HD11	5:C:392:VAL:HG13	2.03	0.41
7:B:153:ASP:O	7:B:157:LYS:HE3	2.21	0.41
1:D:595:ARG:NH1	1:D:849:TYR:CE2	2.89	0.40
1:D:793:TYR:CZ	1:D:797:LEU:HD12	2.56	0.40
4:Y:254:ILE:HD13	4:Y:392:PHE:HB3	2.02	0.40
5:C:338:ASN:O	5:C:445:ILE:HD11	2.21	0.40
6:F:166:LYS:HD3	6:F:624:LEU:C	2.47	0.40
1:D:509:LEU:HD13	1:D:823:GLN:OE1	2.22	0.40
1:D:557:LEU:CD2	1:D:575:ILE:CD1	3.00	0.40
1:D:630:LEU:HD22	4:Y:235:ILE:CG2	2.40	0.40
5:C:152:LYS:HZ2	5:C:505:ASP:CG	2.25	0.40
5:C:196:PHE:CE1	5:C:202:PRO:HG3	2.56	0.40
5:C:1136:PHE:CE2	5:C:1140:ASN:ND2	2.89	0.40
5:C:1281:VAL:CG1	5:C:1286:ILE:HB	2.51	0.40
7:B:190:TRP:HB2	7:B:584:TRP:CD1	2.57	0.40
7:B:333:PHE:HE1	7:B:514:LEU:HD21	1.86	0.40
7:B:610:LYS:HE2	7:B:614:GLU:OE1	2.22	0.40
5:C:32:GLN:HG2	5:C:685:LYS:HA	2.03	0.40
7:B:1044:LYS:CE	7:B:1111:ASP:OD1	2.69	0.40
1:D:68:LEU:HD21	1:D:131:VAL:HG11	2.03	0.40
6:F:465:ILE:HA	6:F:466:PRO:HD3	1.83	0.40
7:B:161:TRP:HH2	7:B:291:PHE:CZ	2.39	0.40
7:B:545:ARG:HD2	7:B:550:GLN:OE1	2.21	0.40
5:C:138:GLU:CD	5:C:169:LYS:HE3	2.46	0.40
5:C:547:PHE:HA	5:C:550:TYR:CD2	2.57	0.40
6:F:50:VAL:HG13	6:F:817:MET:HE3	2.04	0.40
6:F:343:LYS:CE	6:F:439:MET:SD	3.04	0.40
7:B:1151:PHE:CE2	7:B:1171:ILE:HD11	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	936/971 (96%)	904 (97%)	24 (3%)	8 (1%)	14	51
2	E	69/125 (55%)	62 (90%)	5 (7%)	2 (3%)	3	23
3	G	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
4	Y	433/477 (91%)	414 (96%)	15 (4%)	4 (1%)	14	51
5	C	1295/1298 (100%)	1183 (91%)	76 (6%)	36 (3%)	4	24
6	F	1271/1274 (100%)	1146 (90%)	83 (6%)	42 (3%)	3	21
7	B	1214/1217 (100%)	1119 (92%)	62 (5%)	33 (3%)	4	25
All	All	5292/5438 (97%)	4900 (93%)	267 (5%)	125 (2%)	7	27

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	505	LEU
5	C	651	THR
6	F	241	ASN
6	F	371	VAL
6	F	1226	SER
7	B	998	GLN
7	B	999	GLN
1	D	379	ASN
5	C	430	THR
5	C	654	THR
5	C	659	THR
5	C	1167	LYS
6	F	278	GLN
6	F	373	ARG
6	F	380	ASP
6	F	422	GLY
6	F	478	GLN
6	F	482	GLN
6	F	484	THR
6	F	730	LYS
6	F	923	GLY
6	F	1020	ASN
6	F	1080	ARG
6	F	1229	THR
6	F	1231	THR
7	B	380	GLN

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Mol	Chain	Res	Type
7	B	382	GLN
7	B	426	ALA
7	B	428	LEU
7	B	432	ASN
7	B	479	GLN
7	B	519	THR
7	B	829	GLN
7	B	833	THR
7	B	987	GLN
7	B	992	LEU
7	B	997	LYS
7	B	1001	GLN
1	D	3	LEU
1	D	4	LYS
1	D	5	LYS
4	Y	10	LYS
4	Y	150	SER
4	Y	415	LEU
5	C	364	LEU
5	C	431	GLU
5	C	432	THR
5	C	433	THR
5	C	650	SER
5	C	657	SER
5	C	910	LEU
5	C	916	LEU
5	C	920	GLN
5	C	982	ALA
6	F	276	THR
6	F	449	SER
6	F	469	ARG
6	F	476	THR
6	F	479	GLN
6	F	480	VAL
6	F	481	GLN
6	F	483	THR
6	F	726	ALA
6	F	728	ASP
6	F	741	LEU
6	F	751	LYS
6	F	755	THR
6	F	924	MET

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Mol	Chain	Res	Type
6	F	1015	THR
7	B	288	LYS
7	B	476	ASN
7	B	481	GLN
7	B	539	ASN
7	B	835	ASN
7	B	994	LEU
4	Y	270	LEU
5	C	426	THR
5	C	436	ASN
5	C	775	ASN
5	C	907	LEU
5	C	918	GLN
5	C	985	SER
5	C	988	VAL
5	C	1046	GLN
5	C	1048	LEU
6	F	485	SER
6	F	724	ASP
7	B	273	ASN
7	B	989	VAL
7	B	991	SER
7	B	1000	MET
7	B	1002	GLN
1	D	757	ALA
2	E	62	LYS
5	C	373	THR
5	C	773	GLY
5	C	914	VAL
5	C	983	GLN
5	C	997	GLY
5	C	1000	THR
6	F	584	LYS
6	F	605	ARG
6	F	610	ASP
6	F	1018	ALA
7	B	430	THR
7	B	486	ASN
7	B	523	SER
7	B	529	LEU
7	B	831	SER
2	E	56	ASP

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Mol	Chain	Res	Type
5	C	361	THR
5	C	372	GLY
5	C	924	GLN
5	C	979	THR
5	C	1164	GLN
6	F	376	ILE
6	F	733	ALA
1	D	451	GLY
5	C	980	GLY
7	B	1077	GLY
6	F	1232	ILE
7	B	995	VAL
1	D	386	VAL
6	F	729	GLY
6	F	756	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	802/834 (96%)	787 (98%)	15 (2%)	50	67
2	E	64/113 (57%)	61 (95%)	3 (5%)	23	45
3	G	65/65 (100%)	61 (94%)	4 (6%)	16	38
4	Y	372/406 (92%)	367 (99%)	5 (1%)	61	74
5	C	1128/1129 (100%)	1102 (98%)	26 (2%)	44	64
6	F	1085/1086 (100%)	1047 (96%)	38 (4%)	32	53
7	B	1068/1069 (100%)	1050 (98%)	18 (2%)	53	69
All	All	4584/4702 (98%)	4475 (98%)	109 (2%)	43	64

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	LEU
1	D	40	SER

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Mol	Chain	Res	Type
1	D	377	ASP
1	D	398	LEU
1	D	407	SER
1	D	505	LEU
1	D	509	LEU
1	D	609	LEU
1	D	669	PHE
1	D	719	PHE
1	D	727	LEU
1	D	728	LEU
1	D	873	TRP
1	D	915	LEU
1	D	923	LEU
2	E	56	ASP
2	E	79	GLU
2	E	114	HIS
3	G	14	LEU
3	G	31	LEU
3	G	64	LEU
3	G	66	LEU
4	Y	33	LEU
4	Y	82	LEU
4	Y	90	SER
4	Y	209	LEU
4	Y	270	LEU
5	C	154	LEU
5	C	209	VAL
5	C	345	THR
5	C	361	THR
5	C	374	THR
5	C	377	THR
5	C	430	THR
5	C	432	THR
5	C	443	ASP
5	C	507	ASP
5	C	655	THR
5	C	757	THR
5	C	791	LEU
5	C	898	THR
5	C	907	LEU
5	C	927	ASP
5	C	987	THR

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Mol	Chain	Res	Type
5	C	999	THR
5	C	1000	THR
5	C	1002	THR
5	C	1050	THR
5	C	1058	THR
5	C	1059	LEU
5	C	1162	THR
5	C	1168	THR
5	C	1228	THR
6	F	2	SER
6	F	4	LEU
6	F	19	LEU
6	F	73	THR
6	F	87	LEU
6	F	153	THR
6	F	249	THR
6	F	283	SER
6	F	303	LEU
6	F	344	VAL
6	F	382	THR
6	F	476	THR
6	F	483	THR
6	F	551	SER
6	F	564	THR
6	F	581	THR
6	F	601	THR
6	F	635	THR
6	F	639	THR
6	F	668	LEU
6	F	741	LEU
6	F	743	THR
6	F	747	THR
6	F	755	THR
6	F	786	LEU
6	F	829	TRP
6	F	830	THR
6	F	832	ILE
6	F	869	LEU
6	F	876	LEU
6	F	1000	THR
6	F	1050	THR
6	F	1160	GLU

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Mol	Chain	Res	Type
6	F	1173	LEU
6	F	1231	THR
6	F	1243	THR
6	F	1259	THR
6	F	1260	LEU
7	B	67	THR
7	B	92	SER
7	B	406	LEU
7	B	419	THR
7	B	453	THR
7	B	454	THR
7	B	467	LEU
7	B	530	THR
7	B	807	LEU
7	B	876	LEU
7	B	921	THR
7	B	928	VAL
7	B	965	THR
7	B	982	THR
7	B	1092	VAL
7	B	1110	LEU
7	B	1129	THR
7	B	1164	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	119	HIS
1	D	260	GLN
1	D	485	ASN
1	D	600	ASN
1	D	658	ASN
1	D	823	GLN
1	D	872	GLN
1	D	894	ASN
1	D	899	ASN
3	G	24	ASN
3	G	25	HIS
4	Y	13	GLN
4	Y	62	GLN
4	Y	208	GLN
4	Y	264	GLN

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Mol	Chain	Res	Type
4	Y	348	GLN
4	Y	377	HIS
4	Y	386	ASN
5	C	32	GLN
5	C	111	GLN
5	C	181	ASN
5	C	315	GLN
5	C	454	GLN
5	C	608	ASN
5	C	609	GLN
5	C	676	ASN
5	C	736	GLN
5	C	764	GLN
5	C	941	ASN
5	C	1123	ASN
5	C	1140	ASN
5	C	1143	GLN
5	C	1173	GLN
6	F	13	GLN
6	F	62	ASN
6	F	130	GLN
6	F	136	ASN
6	F	220	GLN
6	F	241	ASN
6	F	295	ASN
6	F	351	GLN
6	F	396	GLN
6	F	406	ASN
6	F	407	GLN
6	F	424	HIS
6	F	428	GLN
6	F	637	ASN
6	F	676	GLN
6	F	693	GLN
6	F	701	GLN
6	F	814	GLN
6	F	834	ASN
6	F	843	ASN
6	F	900	GLN
6	F	1095	ASN
7	B	19	GLN
7	B	22	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	B	29	GLN
7	B	80	GLN
7	B	117	GLN
7	B	122	GLN
7	B	175	ASN
7	B	246	ASN
7	B	254	GLN
7	B	451	ASN
7	B	588	HIS
7	B	604	GLN
7	B	642	GLN
7	B	662	ASN
7	B	736	ASN
7	B	786	GLN
7	B	864	ASN
7	B	905	GLN
7	B	1002	GLN
7	B	1154	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 ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54988. These allow visual inspection of the internal detail of the map and identification of artifacts.

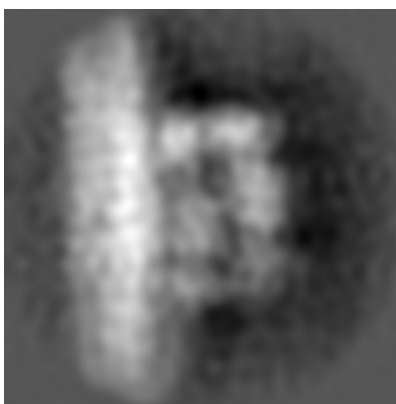
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

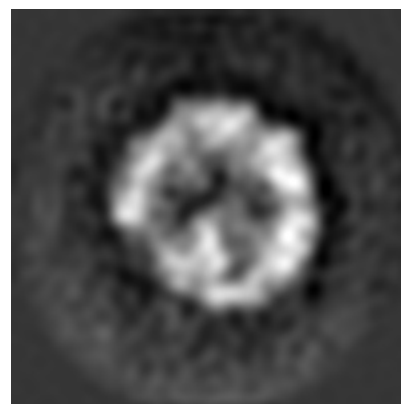
6.1.1 Primary map



X



Y

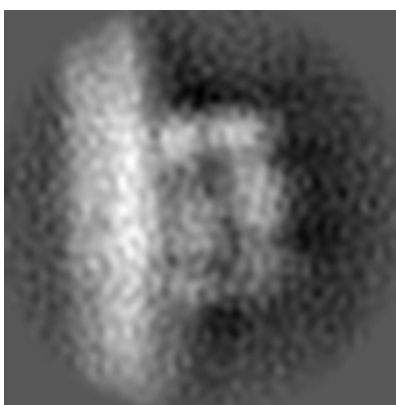


Z

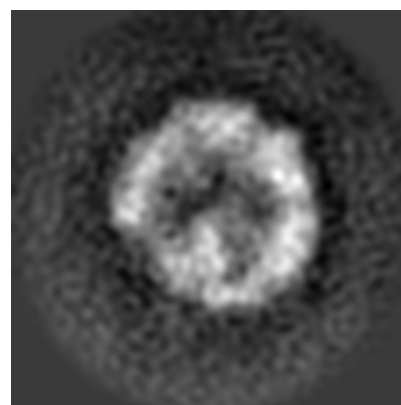
6.1.2 Raw map



X



Y

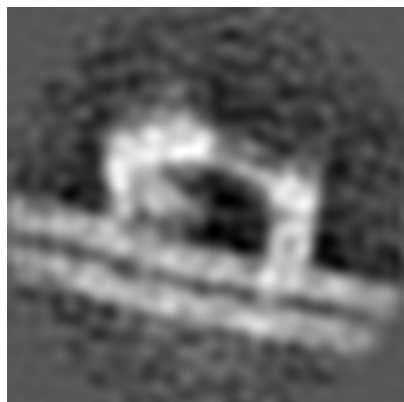


Z

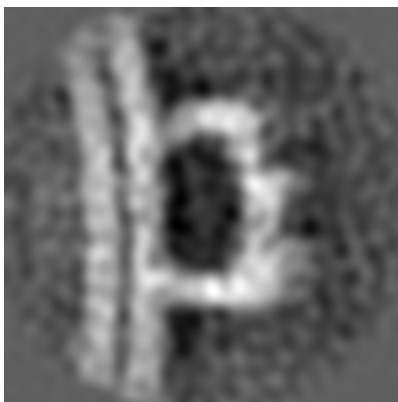
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 28

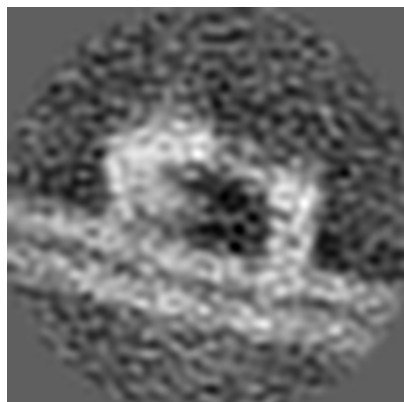


Y Index: 28

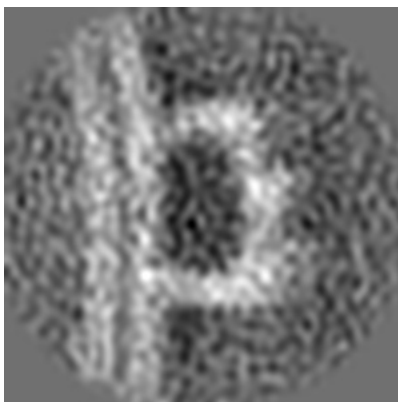


Z Index: 28

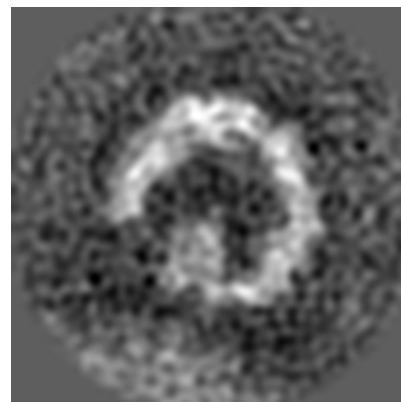
6.2.2 Raw map



X Index: 28



Y Index: 28

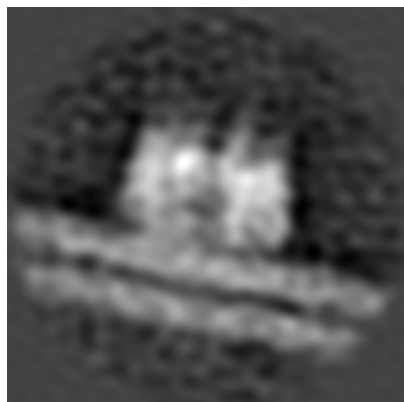


Z Index: 28

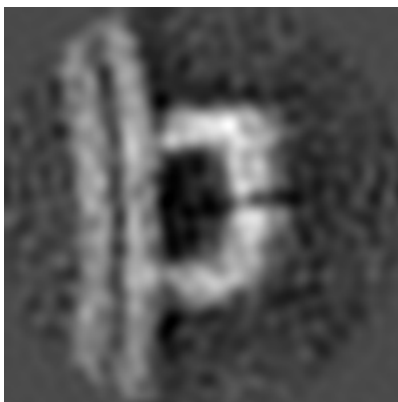
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

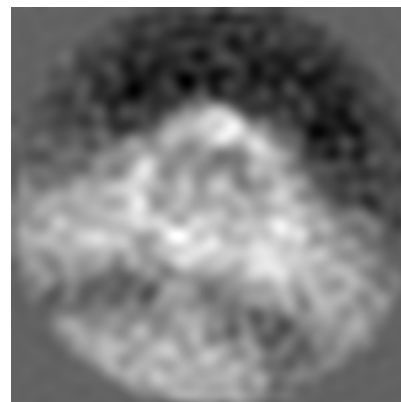
6.3.1 Primary map



X Index: 38

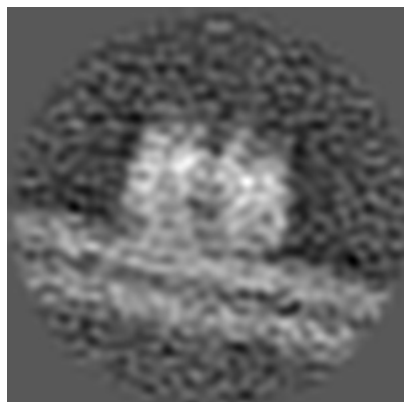


Y Index: 32

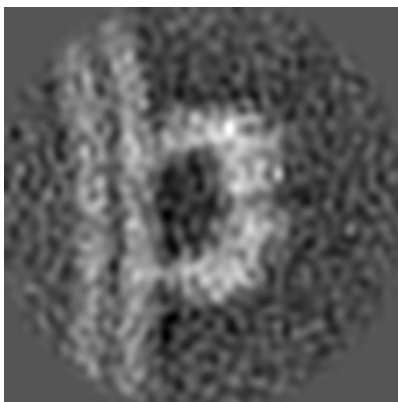


Z Index: 20

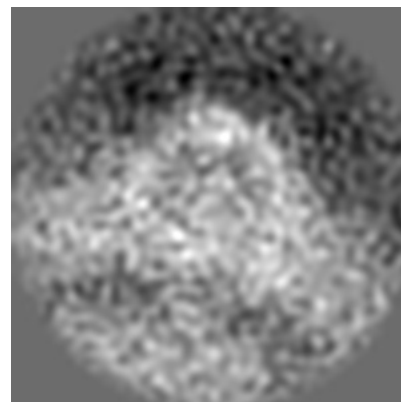
6.3.2 Raw map



X Index: 38



Y Index: 33

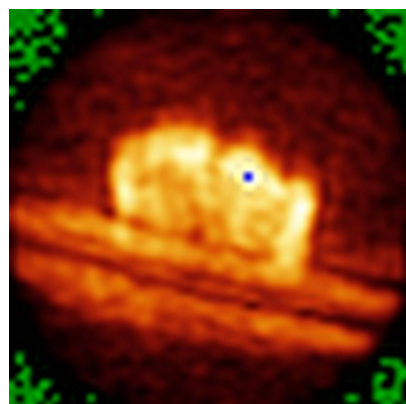


Z Index: 20

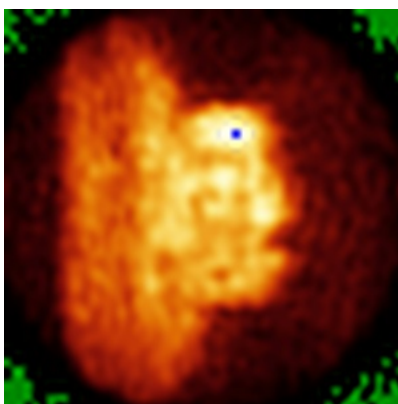
The images above show the largest variance slices of the map in three orthogonal directions.

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

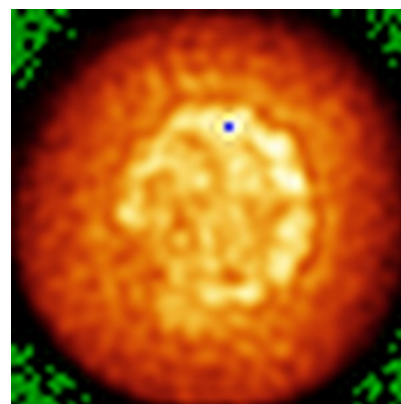
6.4.1 Primary map



X

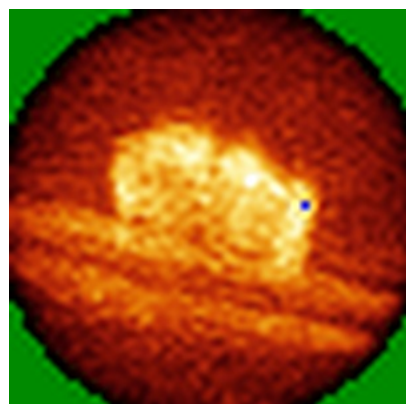


Y

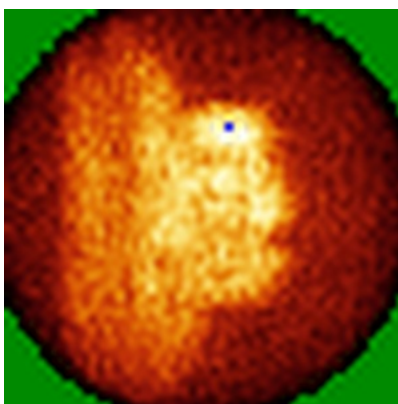


Z

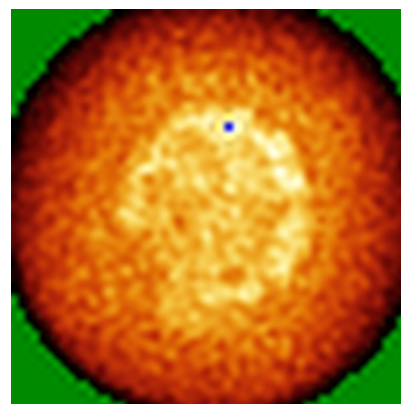
6.4.2 Raw map



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.

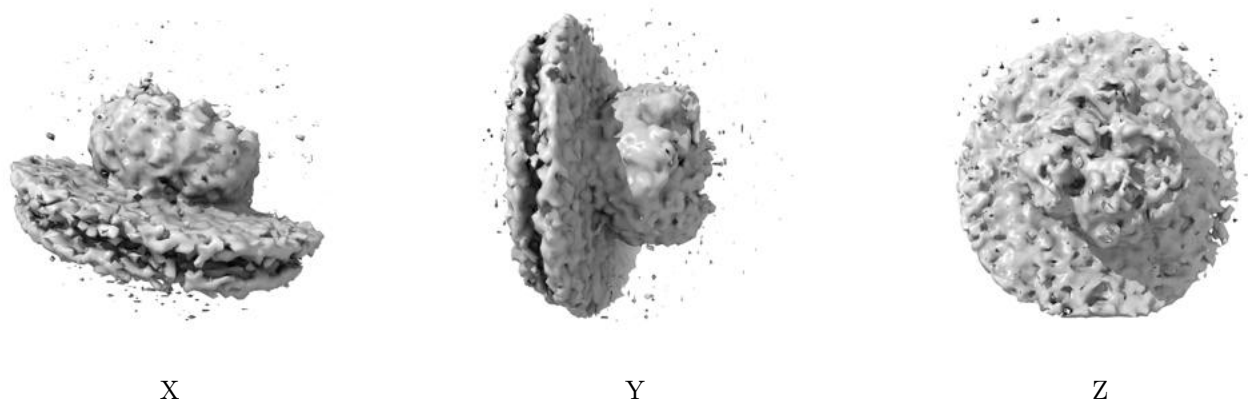
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.354. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

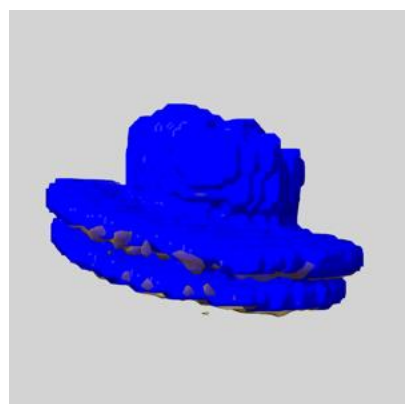
6.6 Mask visualisation [i](#)

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

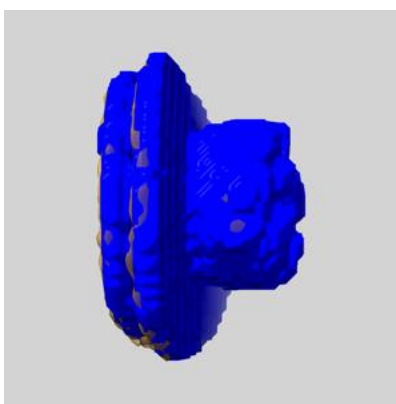
A mask typically either:

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

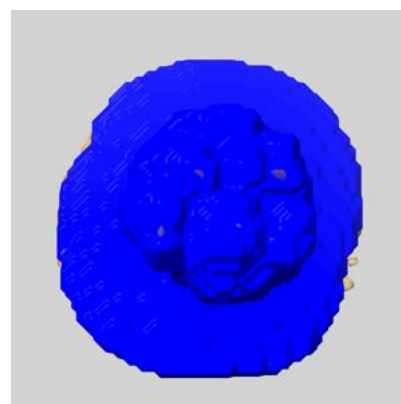
6.6.1 emd_54988_msk_1.map [i](#)



X



Y

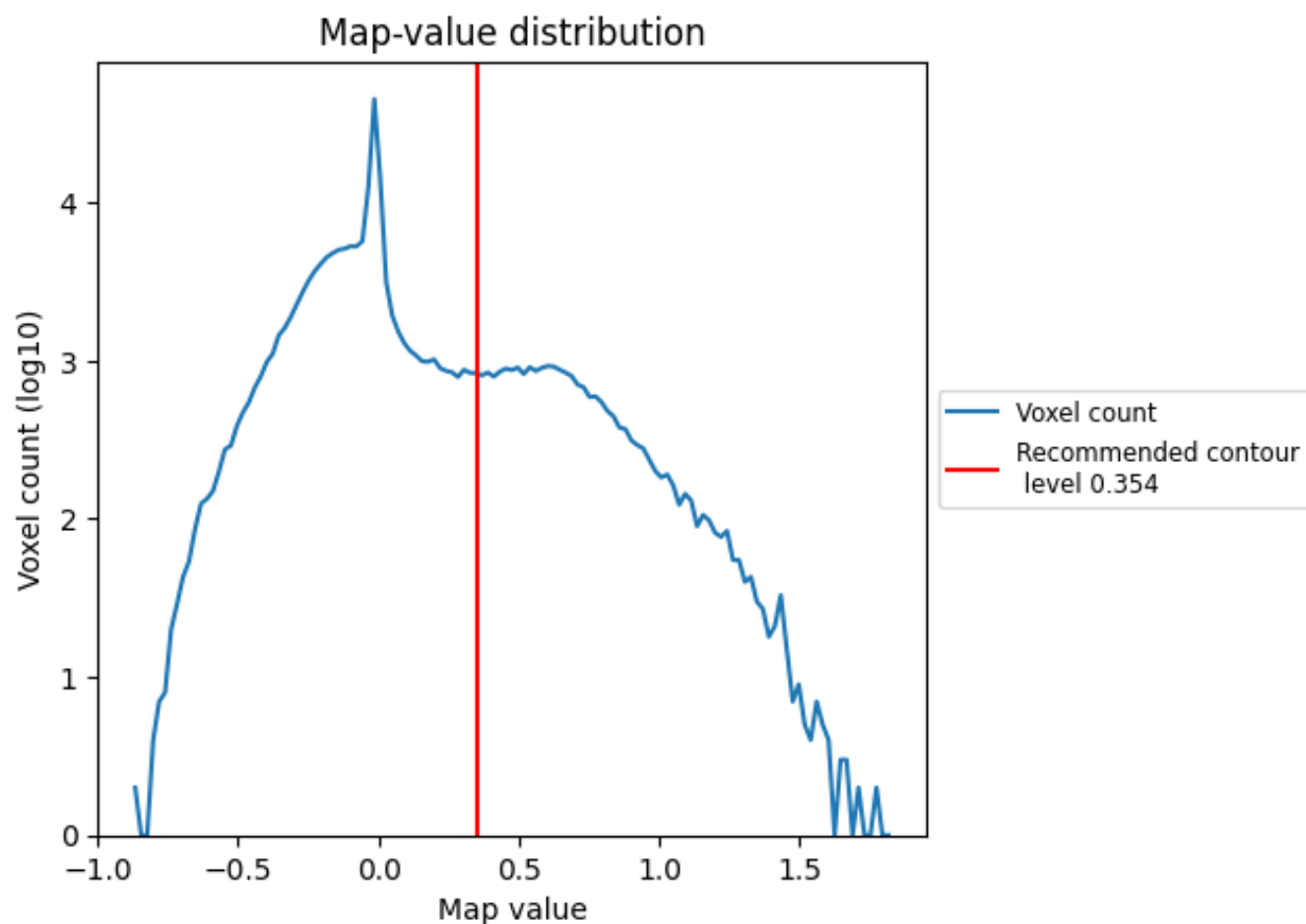


Z

7 Map analysis [i](#)

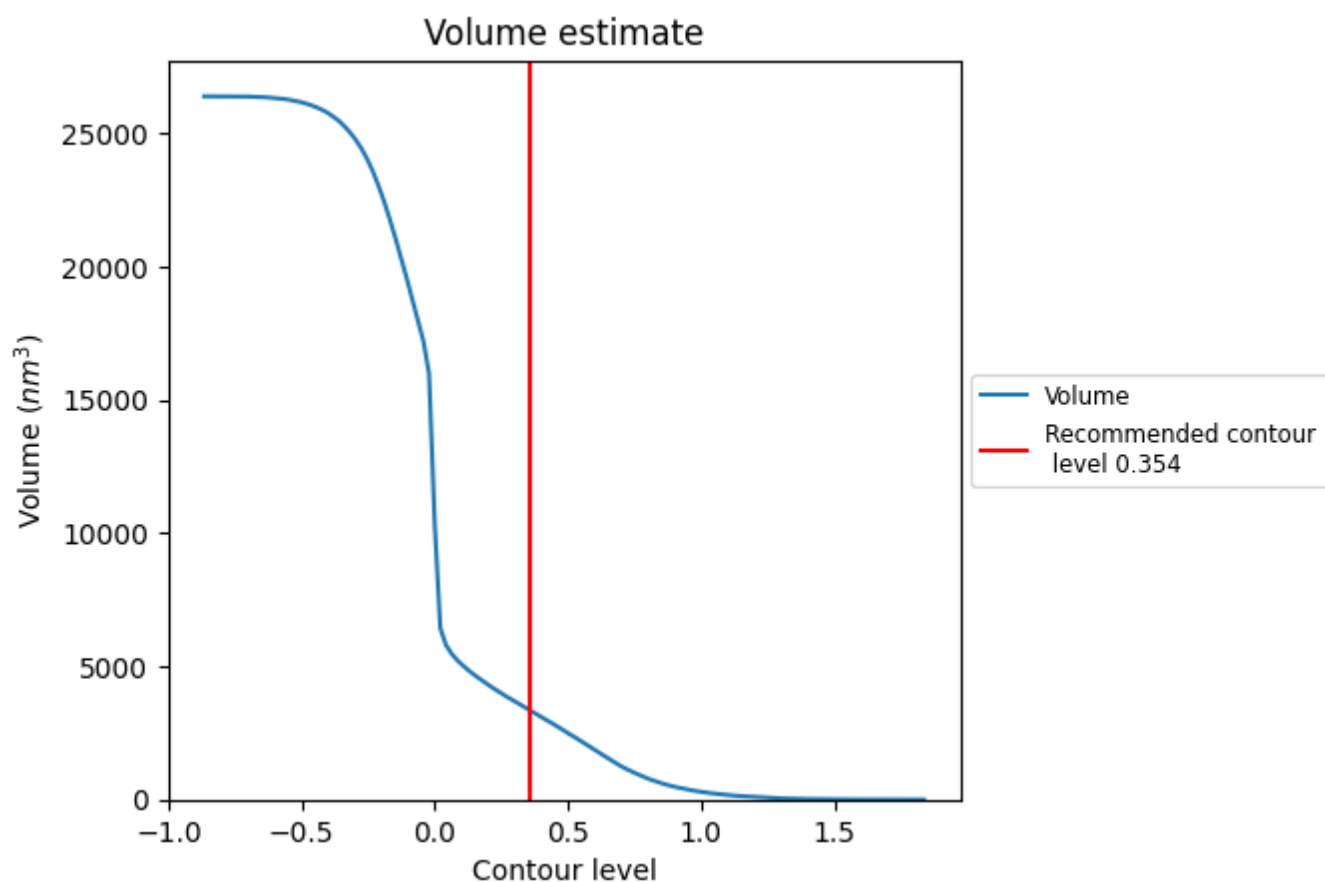
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

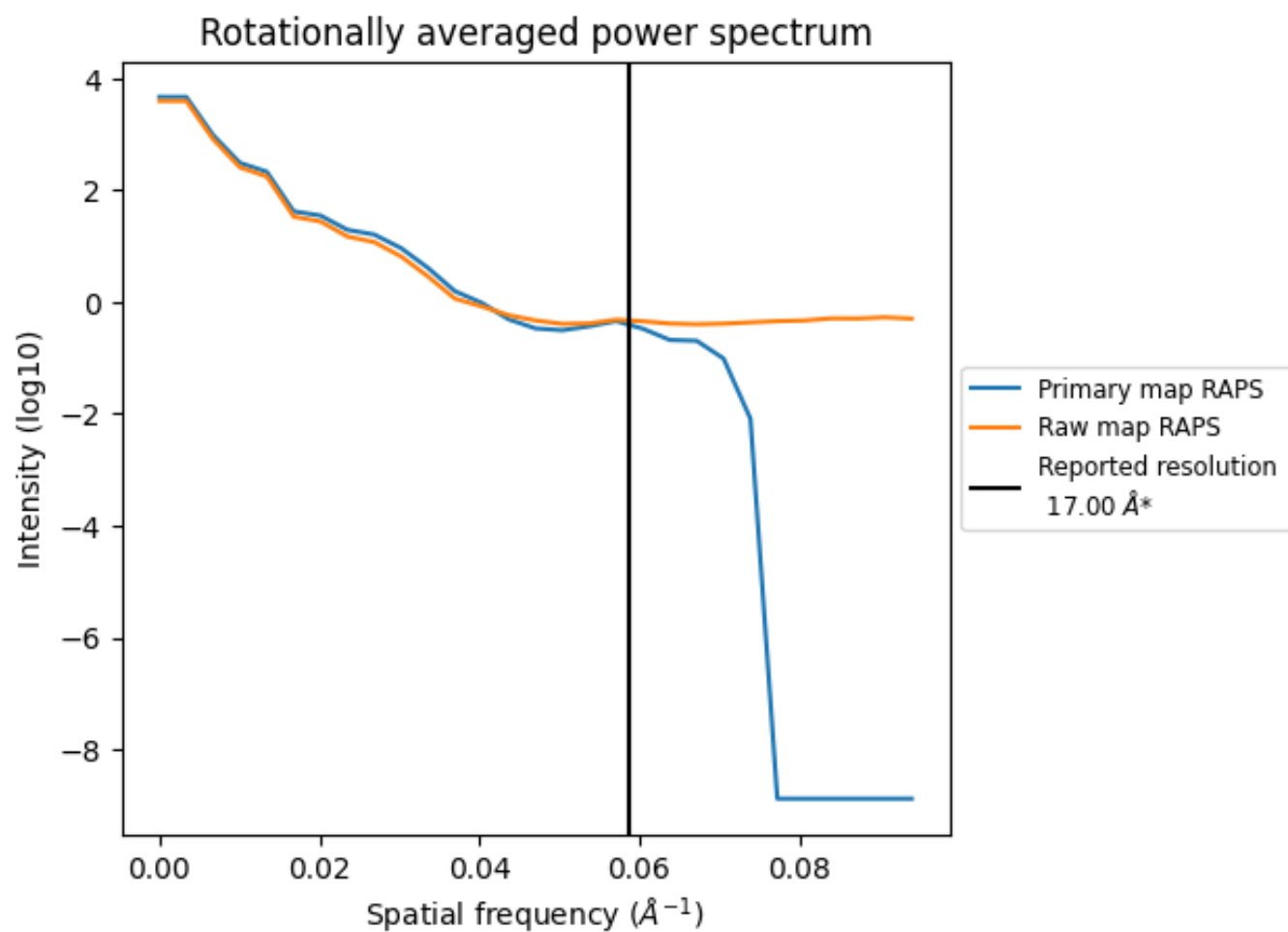
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3366 nm³; this corresponds to an approximate mass of 3040 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 ⓘ

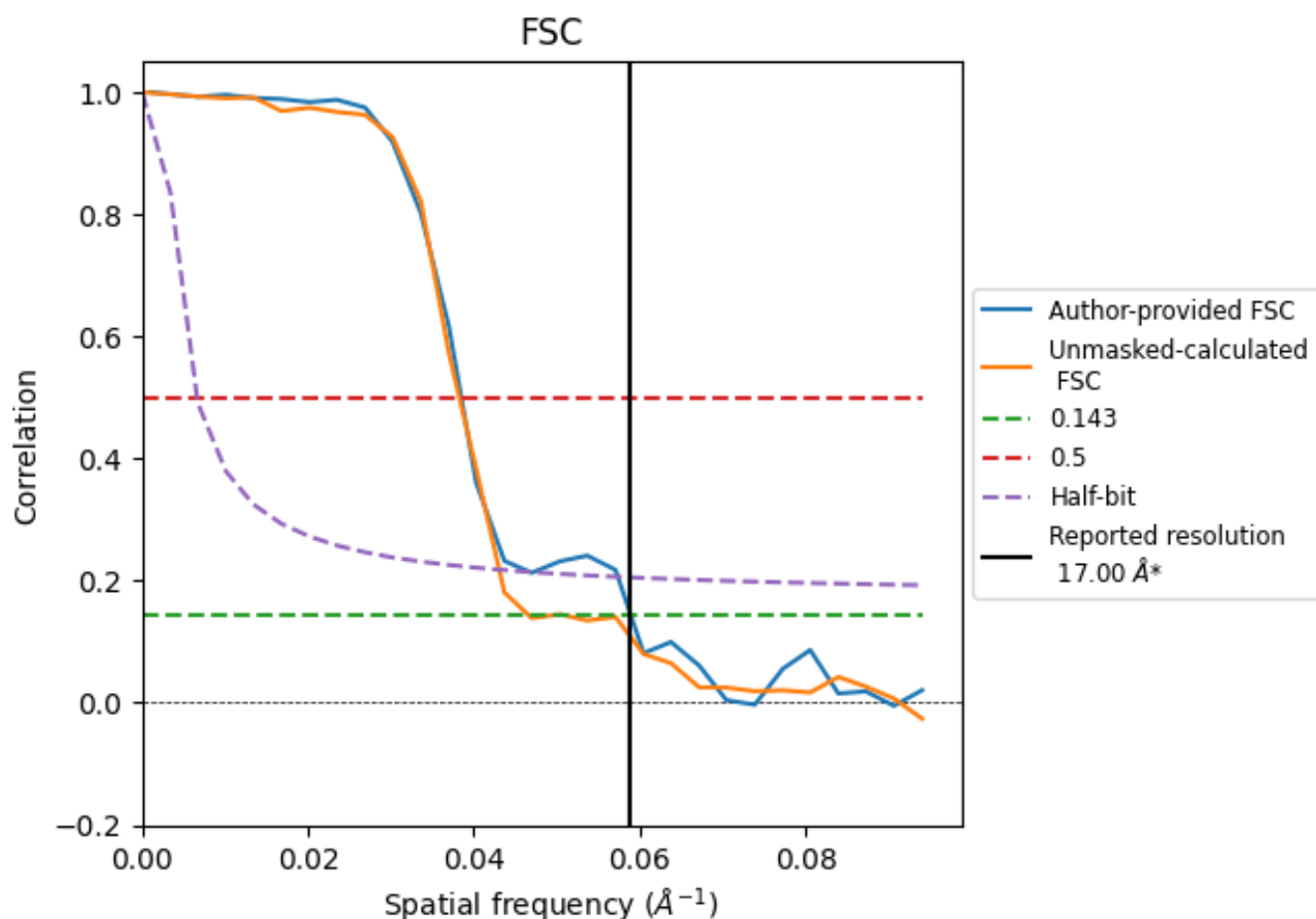


*Reported resolution corresponds to spatial frequency of 0.059 Å⁻¹

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 0.059 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

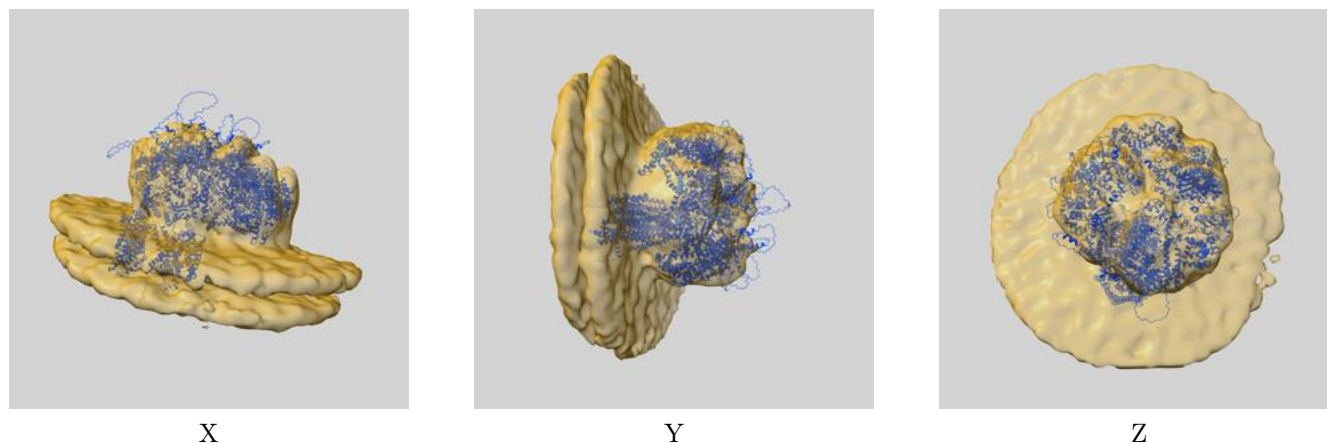
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	17.00	-	-
Author-provided FSC curve	16.98	25.97	17.42
Unmasked-calculated*	21.41	26.18	23.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 21.41 differs from the reported value 17.0 by more than 10 %

9 Map-model fit [i](#)

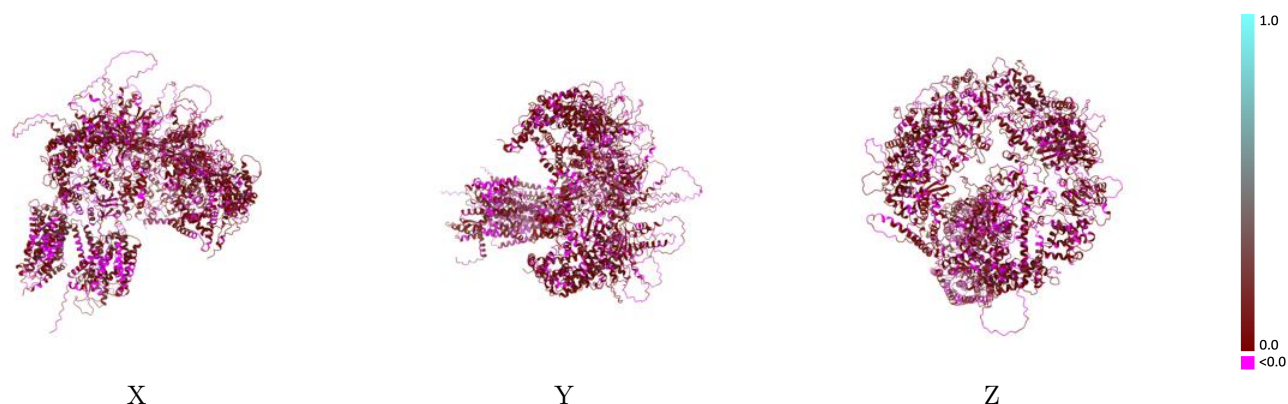
This section contains information regarding the fit between EMDB map EMD-54988 and PDB model 9SLF. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



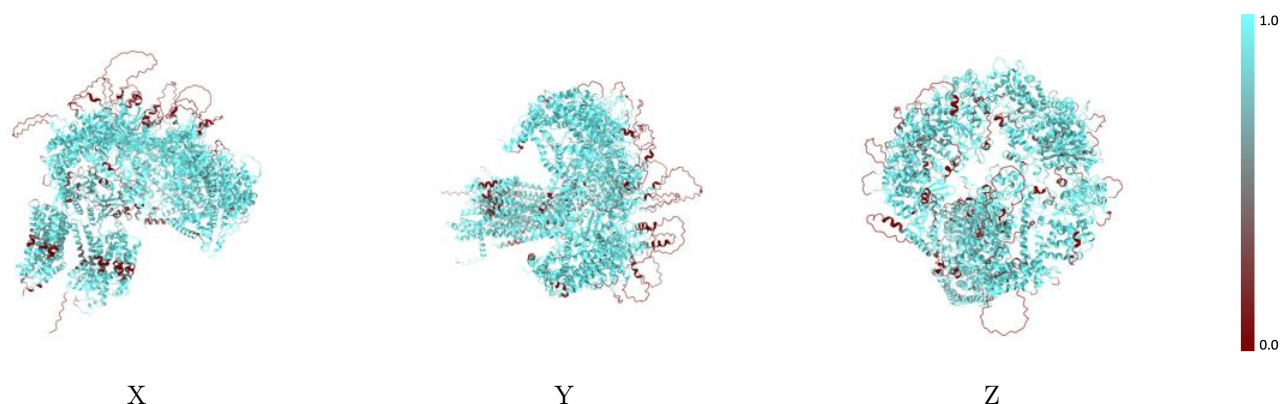
The images above show the 3D surface view of the map at the recommended contour level 0.354 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



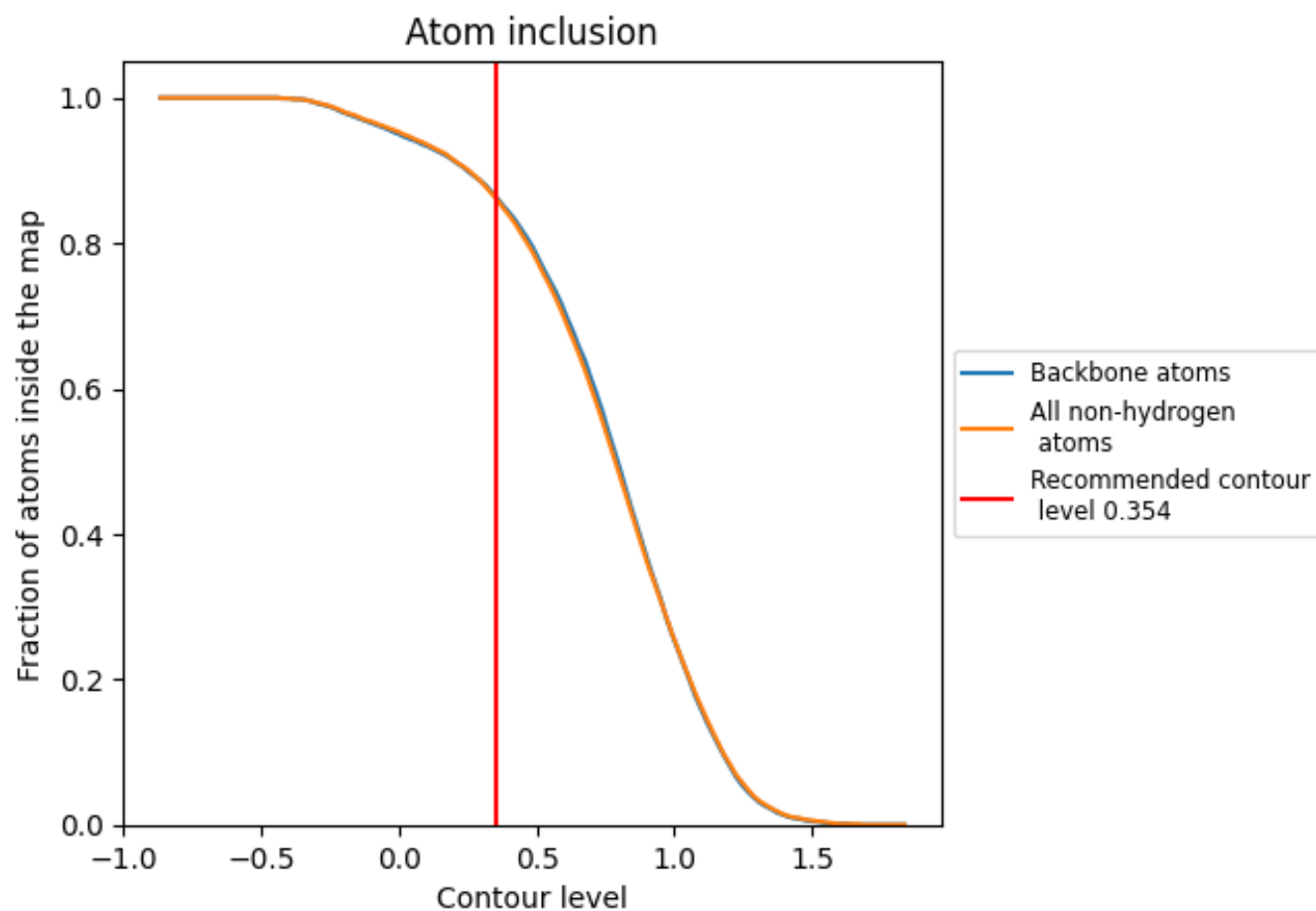
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.354).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.354) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8610	0.0490
B	0.9210	0.0560
C	0.8470	0.0530
D	0.7920	0.0360
E	0.8890	0.0550
F	0.8640	0.0520
G	0.8000	0.0150
Y	0.8810	0.0390

1.0

0.0

<0.0