



# Full wwPDB EM Validation Report ⓘ

Nov 9, 2022 – 04:34 AM JST

PDB ID : 6IGM  
EMDB ID : EMD-9668  
Title : Cryo-EM Structure of Human SRCAP Complex  
Authors : Feng, Y.; Tian, Y.; Wu, Z.; Xu, Y.  
Deposited on : 2018-09-25  
Resolution : 4.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

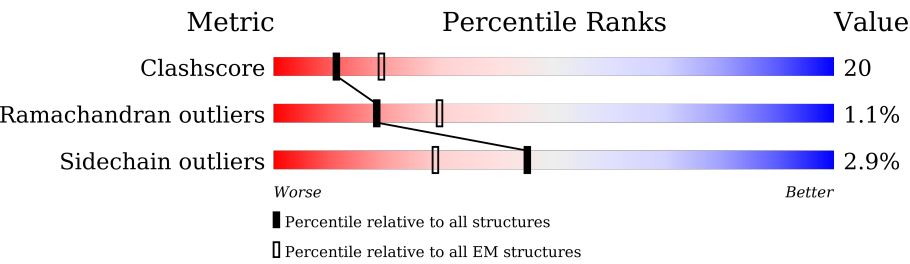
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	456	<div><div>12%</div><div>65%</div><div>21%</div><div>•</div><div>11%</div></div>
1	C	456	<div><div>16%</div><div>66%</div><div>14%</div><div>•</div><div>19%</div></div>
1	E	456	<div><div>14%</div><div>68%</div><div>16%</div><div></div><div>17%</div></div>
2	B	463	<div><div>16%</div><div>69%</div><div>16%</div><div>•</div><div>14%</div></div>
2	D	463	<div><div>17%</div><div>72%</div><div>12%</div><div>•</div><div>14%</div></div>
2	F	463	<div><div>15%</div><div>65%</div><div>13%</div><div>•</div><div>21%</div></div>
3	G	396	<div><div>32%</div><div>67%</div><div>19%</div><div>• •</div><div>8%</div></div>
4	H	3230	<div><div>8%</div><div>8%</div><div>• •</div><div>88%</div></div>

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Mol	Chain	Length	Quality of chain
5	X	62	<div><div></div><div>23%</div><div>65%</div><div>35%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24257 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 RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	405	Total	C	N	O	S	0	0
			3123	1970	536	604	13		
1	C	370	Total	C	N	O	S	0	0
			2852	1801	495	544	12		
1	E	380	Total	C	N	O	S	0	0
			2935	1857	503	564	11		

- Molecule 2 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	398	Total	C	N	O	S	0	0
			3090	1931	540	604	15		
2	D	396	Total	C	N	O	S	0	0
			3078	1927	540	597	14		
2	F	366	Total	C	N	O	S	0	0
			2852	1785	501	553	13		

- Molecule 3 is a protein called Actin-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	366	Total	C	N	O	S	0	0
			2987	1913	489	569	16		

- Molecule 4 is a protein called Helicase SRCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	373	Total	C	N	O	S	0	0
			3030	1925	559	525	21		

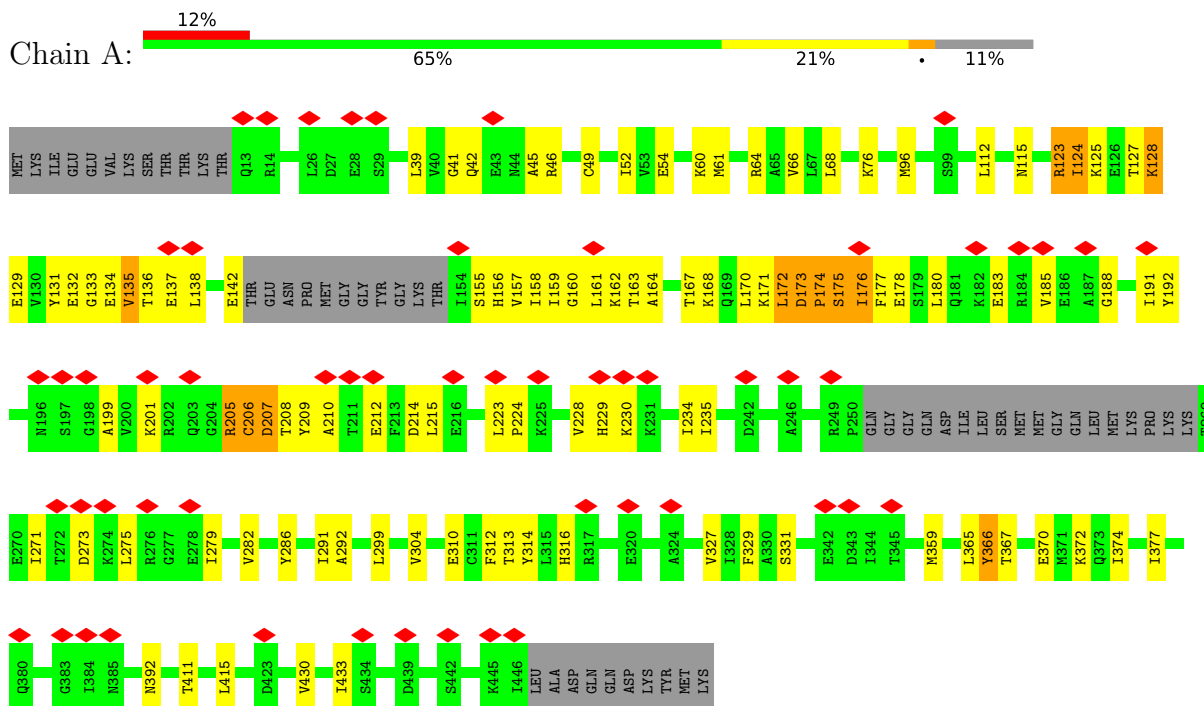
- Molecule 5 is a protein called unknown subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	X	62	Total	C	N	O	0	0
			310	186	62	62		

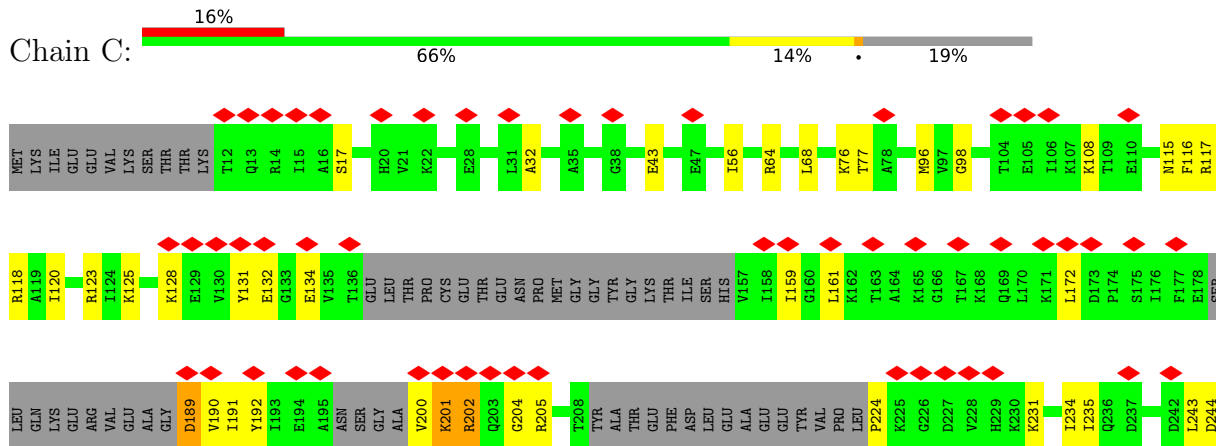
### 3 Residue-property plots

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: RuvB-like 1

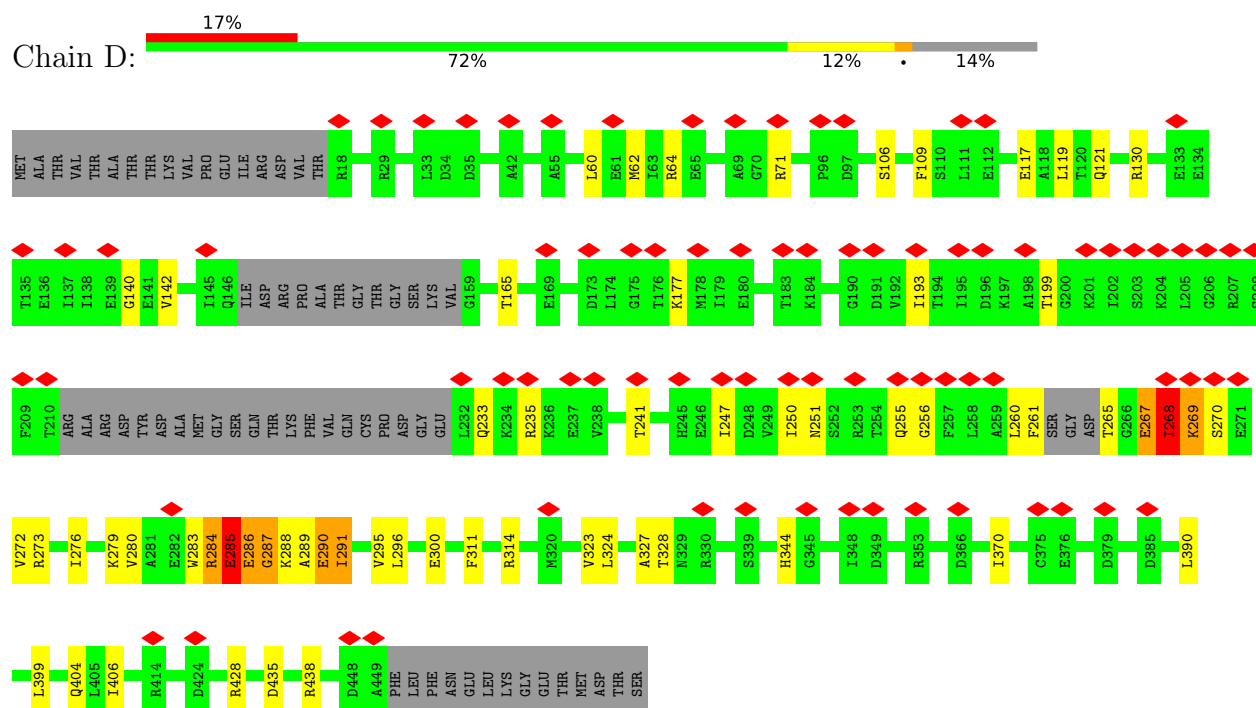


#### • Molecule 1: RuvB-like 1

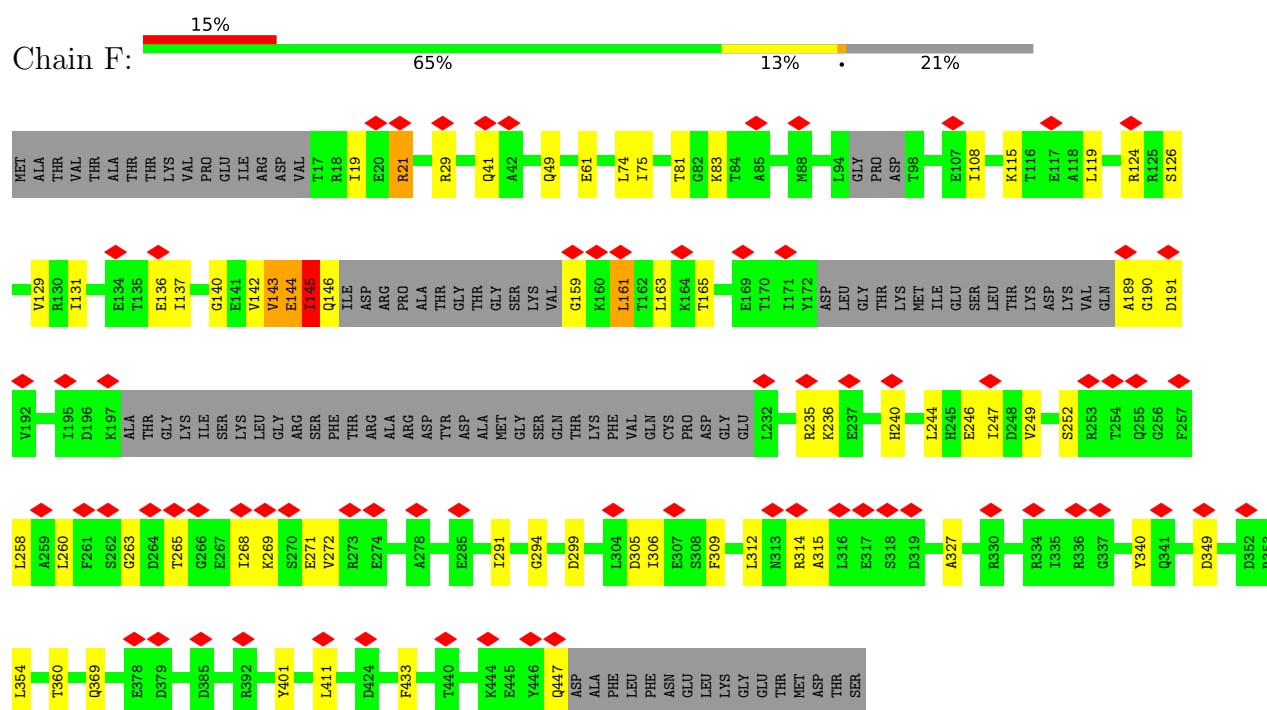




- Molecule 2: RuvB-like 2



- Molecule 2: RuvB-like 2

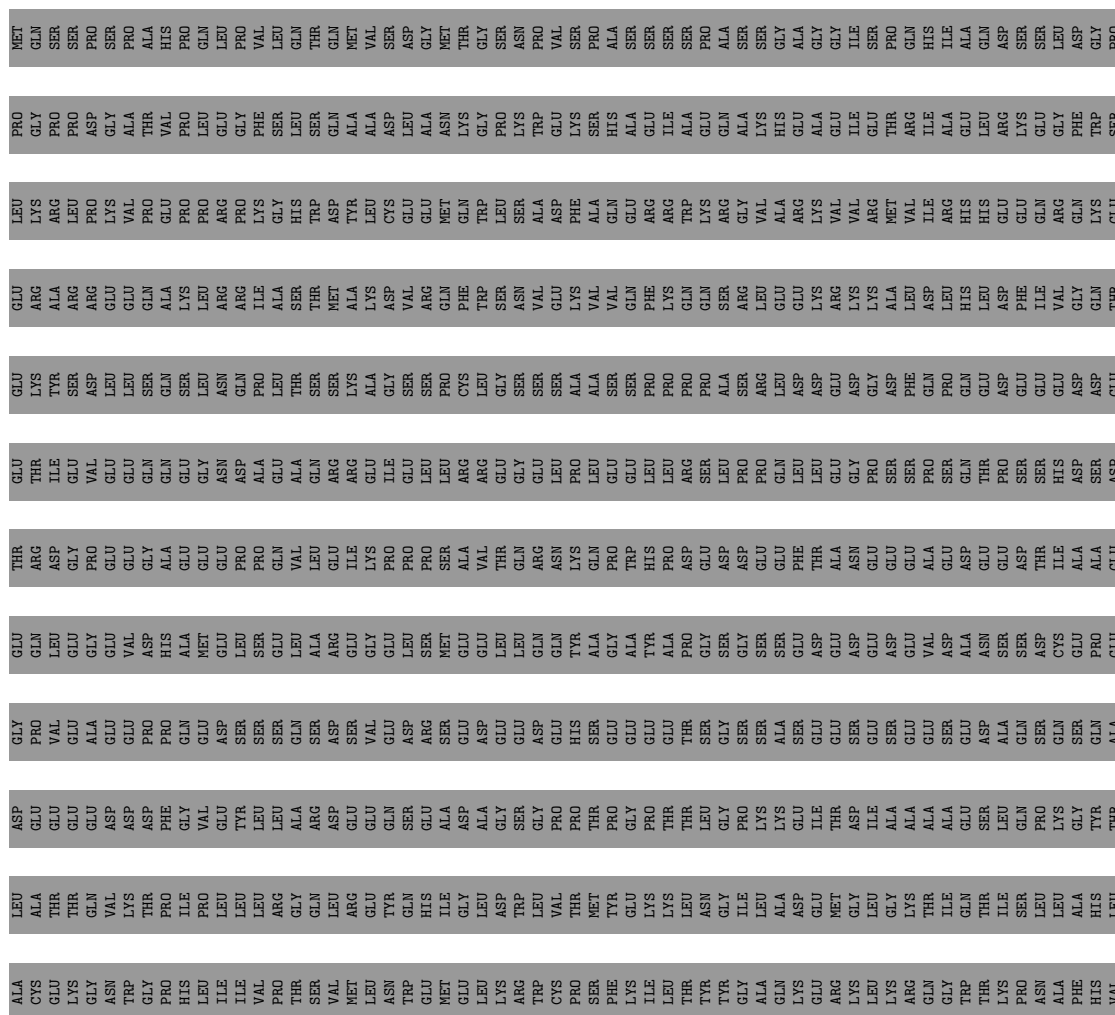


- Molecule 3: Actin-related protein 6



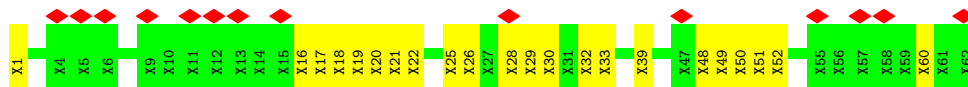


- Molecule 4: Helicase SRCAP









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.5625	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.269	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.058	Depositor
Map size ( $\text{\AA}$ )	432.0, 432.0, 432.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.35, 1.35, 1.35	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.28	1/3163 (0.0%)	0.54	2/4266 (0.0%)
1	C	0.25	0/2883	0.48	0/3878
1	E	0.25	0/2972	0.51	1/4008 (0.0%)
2	B	0.25	0/3122	0.51	1/4203 (0.0%)
2	D	0.25	0/3109	0.49	0/4180
2	F	0.25	0/2880	0.51	1/3873 (0.0%)
3	G	0.32	1/3055 (0.0%)	0.57	4/4141 (0.1%)
4	H	0.26	0/3098	0.50	2/4191 (0.0%)
All	All	0.26	2/24282 (0.0%)	0.51	11/32740 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	PRO	N-CD	5.03	1.54	1.47
3	G	306	PRO	N-CD	5.03	1.54	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	50	ASP	C-N-CD	6.29	141.61	128.40
1	A	173	ASP	C-N-CD	5.81	140.59	128.40
3	G	305	LEU	C-N-CD	5.78	140.54	128.40
2	F	161	LEU	CA-CB-CG	5.60	128.17	115.30
2	B	146	GLN	CA-CB-CG	5.29	125.04	113.40
4	H	871	ASP	CB-CG-OD2	5.17	122.95	118.30
4	H	870	ASP	CB-CG-OD2	5.17	122.95	118.30
3	G	143	LEU	CA-CB-CG	5.15	127.14	115.30
3	G	370	ASP	CB-CG-OD1	5.07	122.87	118.30
1	A	366	TYR	C-N-CA	5.04	134.31	121.70
1	E	138	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3123	0	3214	205	0
1	C	2852	0	2968	95	0
1	E	2935	0	3043	70	0
2	B	3090	0	3163	104	0
2	D	3078	0	3159	65	0
2	F	2852	0	2922	60	0
3	G	2987	0	2905	250	0
4	H	3030	0	3058	247	0
5	X	310	0	74	51	0
All	All	24257	0	24506	989	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (989) 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)
2:B:198:ALA:HB1	4:H:1998:TRP:CE2	1.35	1.57
3:G:306:PRO:CA	3:G:309:MET:HB2	1.25	1.55
1:A:124:ILE:CG2	1:A:292:ALA:CA	1.87	1.49
3:G:30:PHE:HB2	3:G:47:GLU:CG	1.02	1.48
3:G:30:PHE:HB2	3:G:47:GLU:CD	1.20	1.48
1:A:124:ILE:CG2	1:A:292:ALA:HA	1.44	1.46
2:B:135:THR:CG2	4:H:1999:LEU:HD13	1.42	1.46
3:G:30:PHE:CB	3:G:47:GLU:CG	1.91	1.46
5:X:21:UNK:CA	5:X:25:UNK:HA	1.46	1.45
1:E:126:GLU:CB	4:H:1964:GLN:HE22	1.31	1.44
2:B:232:LEU:CD1	2:B:233:GLN:HE22	1.28	1.42
2:B:198:ALA:CB	4:H:1998:TRP:CE2	2.01	1.41
3:G:120:GLN:O	3:G:378:THR:CB	1.69	1.37
3:G:30:PHE:CD1	3:G:56:TYR:HB3	1.57	1.37
1:E:126:GLU:CG	4:H:1964:GLN:NE2	1.84	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:21:UNK:HA	5:X:25:UNK:CA	1.54	1.37
3:G:306:PRO:O	3:G:310:GLN:N	1.58	1.36
1:A:124:ILE:HG23	1:A:292:ALA:CB	1.53	1.36
1:C:192:TYR:CD1	1:C:200:VAL:N	1.94	1.35
3:G:30:PHE:CE2	3:G:56:TYR:HD2	1.44	1.34
2:D:267:GLU:OE2	2:D:273:ARG:NH2	1.59	1.34
3:G:33:LYS:N	3:G:54:LEU:HD21	1.36	1.34
4:H:910:ARG:HH12	4:H:2037:LEU:CG	1.41	1.34
3:G:306:PRO:HA	3:G:309:MET:CB	1.60	1.32
2:B:198:ALA:HB1	4:H:1998:TRP:NE1	1.01	1.32
1:A:124:ILE:CG2	1:A:292:ALA:CB	2.04	1.31
2:B:232:LEU:HD12	2:B:233:GLN:NE2	0.99	1.31
3:G:306:PRO:CB	3:G:309:MET:HB2	1.59	1.30
3:G:306:PRO:HB3	3:G:309:MET:CB	1.59	1.30
1:A:142:GLU:OE1	1:A:156:HIS:N	1.62	1.30
2:D:290:GLU:O	2:D:291:ILE:CG1	1.79	1.30
4:H:2003:GLN:OE1	4:H:2007:GLN:NE2	1.64	1.30
3:G:30:PHE:CB	3:G:47:GLU:CD	1.95	1.29
3:G:306:PRO:CA	3:G:309:MET:CB	2.11	1.28
4:H:928:LEU:CD1	4:H:2000:ALA:HB2	1.61	1.28
3:G:120:GLN:O	3:G:378:THR:HB	1.23	1.28
3:G:306:PRO:CB	3:G:309:MET:CB	2.09	1.27
3:G:30:PHE:CG	3:G:47:GLU:HG2	1.67	1.27
2:B:134:GLU:OE2	2:B:235:ARG:HD3	1.30	1.27
2:B:232:LEU:CD1	2:B:233:GLN:NE2	1.91	1.27
3:G:33:LYS:H	3:G:54:LEU:CD2	1.46	1.26
1:C:247:ASN:HD21	1:C:274:LYS:CE	1.47	1.26
2:D:267:GLU:OE2	2:D:273:ARG:CZ	1.82	1.26
4:H:2000:ALA:HB1	4:H:2001:PRO:CD	1.66	1.25
2:B:198:ALA:CB	4:H:1998:TRP:NE1	1.94	1.25
1:E:126:GLU:CB	4:H:1964:GLN:NE2	1.96	1.24
2:D:267:GLU:OE2	2:D:273:ARG:NH1	1.71	1.23
3:G:30:PHE:CD1	3:G:56:TYR:CB	2.20	1.23
1:A:124:ILE:CG2	1:A:292:ALA:HB2	1.66	1.23
3:G:30:PHE:CG	3:G:56:TYR:HB3	1.74	1.22
4:H:910:ARG:NH1	4:H:2037:LEU:HG	1.54	1.22
4:H:2003:GLN:OE1	4:H:2007:GLN:CD	1.78	1.22
4:H:910:ARG:NH1	4:H:2037:LEU:CD1	2.03	1.21
4:H:2032:PHE:CD1	4:H:2033:PRO:HD2	1.76	1.20
3:G:294:ILE:H	3:G:295:PRO:CD	1.55	1.20
3:G:270:LEU:HD21	3:G:273:GLU:OE2	1.02	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:GLU:HB2	4:H:1964:GLN:NE2	1.55	1.19
1:C:247:ASN:ND2	1:C:274:LYS:HE2	1.53	1.19
4:H:1980:MET:HG3	4:H:1981:PRO:CD	1.70	1.18
1:A:124:ILE:HG22	1:A:292:ALA:CA	1.60	1.18
4:H:1980:MET:CG	4:H:1981:PRO:HD3	1.72	1.18
1:C:189:ASP:OD2	1:C:204:GLY:C	1.79	1.18
3:G:270:LEU:HD23	3:G:271:ALA:H	1.07	1.18
1:A:134:GLU:CB	1:A:161:LEU:HA	1.74	1.16
3:G:30:PHE:CZ	3:G:56:TYR:HD2	1.62	1.15
2:B:198:ALA:HA	4:H:1998:TRP:CZ2	1.80	1.15
1:A:134:GLU:HB2	1:A:160:GLY:O	1.46	1.15
1:A:134:GLU:HG3	1:A:161:LEU:C	1.67	1.14
4:H:910:ARG:HH12	4:H:2037:LEU:CD1	1.60	1.14
3:G:30:PHE:CZ	3:G:56:TYR:CD2	2.35	1.14
4:H:949:ILE:O	4:H:1932:VAL:HG11	1.41	1.13
1:A:210:ALA:CA	5:X:17:UNK:HA	1.77	1.13
1:C:247:ASN:ND2	1:C:274:LYS:CE	2.11	1.12
3:G:30:PHE:CB	3:G:47:GLU:HG2	1.62	1.12
1:A:159:ILE:HD12	1:A:172:LEU:CD1	1.79	1.12
4:H:936:HIS:HB2	4:H:937:PRO:HD2	1.29	1.12
1:A:212:GLU:OE2	5:X:20:UNK:CB	1.97	1.11
3:G:30:PHE:CE2	3:G:56:TYR:CD2	2.37	1.11
1:A:124:ILE:HG21	1:A:292:ALA:HB2	1.21	1.11
3:G:270:LEU:CD2	3:G:273:GLU:OE2	1.99	1.11
3:G:270:LEU:CD2	3:G:271:ALA:H	1.62	1.11
4:H:910:ARG:HH12	4:H:2037:LEU:HG	0.99	1.11
1:A:134:GLU:OE1	1:A:160:GLY:CA	1.99	1.10
4:H:1981:PRO:CG	4:H:1982:PRO:HD3	1.82	1.10
1:A:124:ILE:HG23	1:A:292:ALA:CA	1.61	1.10
1:A:210:ALA:HA	5:X:17:UNK:CA	1.79	1.10
4:H:1981:PRO:HG2	4:H:1982:PRO:HD3	1.27	1.10
2:D:250:ILE:HG13	2:D:276:ILE:HD11	1.19	1.10
4:H:928:LEU:HD13	4:H:2000:ALA:CB	1.79	1.10
3:G:30:PHE:CD2	3:G:47:GLU:HG2	1.86	1.10
3:G:306:PRO:HB3	3:G:309:MET:C	1.70	1.09
1:A:234:ILE:HD12	4:H:939:GLN:OE1	1.52	1.09
1:E:126:GLU:HG3	4:H:1964:GLN:NE2	1.65	1.09
3:G:306:PRO:HB3	3:G:309:MET:HB3	1.36	1.08
3:G:306:PRO:C	3:G:309:MET:H	1.55	1.08
1:C:189:ASP:OD2	1:C:204:GLY:CA	2.01	1.08
3:G:236:TYR:H	3:G:267:ILE:HG12	0.93	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:GLU:HB2	4:H:1964:GLN:HE22	1.11	1.07
1:A:137:GLU:HG2	1:A:160:GLY:N	1.67	1.07
1:A:159:ILE:HD12	1:A:172:LEU:HD11	1.08	1.07
2:B:135:THR:CG2	4:H:1999:LEU:CD1	2.32	1.06
3:G:306:PRO:CB	3:G:309:MET:C	2.24	1.06
2:B:135:THR:HG22	4:H:1999:LEU:HD13	1.26	1.06
1:A:134:GLU:OE1	1:A:160:GLY:HA3	1.56	1.05
3:G:30:PHE:CB	3:G:47:GLU:OE2	2.02	1.05
3:G:30:PHE:HB2	3:G:47:GLU:HG3	1.38	1.05
5:X:50:UNK:O	5:X:52:UNK:N	1.89	1.05
2:B:135:THR:HG22	4:H:1999:LEU:CD1	1.85	1.04
1:E:126:GLU:OE1	4:H:1964:GLN:CD	1.94	1.04
1:A:212:GLU:HG2	5:X:28:UNK:CB	1.88	1.04
1:A:212:GLU:CD	5:X:20:UNK:CB	2.26	1.04
3:G:270:LEU:HD21	3:G:273:GLU:CD	1.77	1.04
2:B:170:THR:HG22	5:X:30:UNK:HA	1.39	1.04
2:D:290:GLU:O	2:D:291:ILE:HG13	0.86	1.03
3:G:269:ARG:HA	3:G:269:ARG:HH11	1.22	1.03
4:H:2000:ALA:CB	4:H:2001:PRO:CD	2.36	1.03
1:E:236:GLN:CD	4:H:1960:LEU:HG	1.72	1.03
3:G:120:GLN:O	3:G:378:THR:CG2	2.04	1.03
4:H:2000:ALA:HB1	4:H:2001:PRO:HD3	1.37	1.03
3:G:236:TYR:CE1	3:G:267:ILE:HD13	1.94	1.03
1:C:192:TYR:HD1	1:C:200:VAL:N	1.38	1.02
1:A:134:GLU:HB2	1:A:161:LEU:HA	1.37	1.02
1:A:134:GLU:HB2	1:A:160:GLY:C	1.80	1.01
3:G:30:PHE:CE1	3:G:56:TYR:CB	2.43	1.01
1:A:124:ILE:HG22	1:A:292:ALA:N	1.76	1.01
2:B:135:THR:HG21	4:H:1999:LEU:HD13	1.38	1.01
1:A:210:ALA:O	5:X:17:UNK:O	1.78	1.01
2:B:198:ALA:CA	4:H:1998:TRP:CZ2	2.44	1.01
4:H:951:LEU:HD13	4:H:958:TYR:HE2	1.24	1.01
2:D:268:ILE:O	2:D:272:VAL:CG2	2.08	1.01
3:G:294:ILE:H	3:G:295:PRO:HD3	1.22	1.01
4:H:2000:ALA:HB1	4:H:2001:PRO:HD2	1.43	1.00
3:G:236:TYR:N	3:G:267:ILE:HG12	1.77	1.00
3:G:238:LEU:HD12	3:G:268:LEU:CD2	1.92	1.00
1:A:286:TYR:OH	4:H:943:MET:HG2	1.62	0.99
3:G:292:MET:SD	5:X:16:UNK:CB	2.50	0.99
3:G:33:LYS:H	3:G:54:LEU:HD21	0.86	0.99
1:A:124:ILE:HG22	1:A:292:ALA:HA	1.12	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:143:VAL:HG21	2:F:163:LEU:O	1.61	0.99
3:G:30:PHE:CE1	3:G:56:TYR:HB2	1.96	0.99
1:C:189:ASP:OD2	1:C:204:GLY:HA3	1.60	0.99
5:X:33:UNK:CB	5:X:39:UNK:HA	1.92	0.99
1:E:126:GLU:HB2	4:H:1964:GLN:CD	1.81	0.98
2:B:134:GLU:OE2	2:B:235:ARG:CD	2.10	0.98
1:C:190:VAL:O	1:C:201:LYS:O	1.82	0.98
1:E:236:GLN:OE1	4:H:1960:LEU:HB2	1.63	0.98
3:G:379:ARG:O	3:G:381:ASP:N	1.96	0.97
1:A:210:ALA:O	5:X:17:UNK:C	2.12	0.97
2:B:198:ALA:HB1	4:H:1998:TRP:CD1	1.98	0.97
1:E:126:GLU:CD	4:H:1964:GLN:NE2	2.17	0.97
2:B:232:LEU:HD12	2:B:233:GLN:HE21	1.29	0.97
1:A:137:GLU:CG	1:A:160:GLY:H	1.78	0.97
2:B:137:ILE:HD12	2:B:236:LYS:HD3	1.47	0.97
2:D:286:GLU:O	2:D:288:LYS:N	1.96	0.97
3:G:306:PRO:HB3	3:G:309:MET:O	1.64	0.96
4:H:951:LEU:HD13	4:H:958:TYR:CE2	2.00	0.96
2:F:260:LEU:HD21	4:H:946:PHE:HE1	1.29	0.96
4:H:2000:ALA:CB	4:H:2001:PRO:HD2	1.96	0.96
1:A:134:GLU:N	1:A:161:LEU:HD23	1.80	0.96
2:F:260:LEU:HD21	4:H:946:PHE:CE1	2.00	0.95
1:A:234:ILE:HB	4:H:939:GLN:OE1	1.65	0.95
3:G:306:PRO:HB3	3:G:309:MET:CA	1.95	0.95
4:H:928:LEU:HD13	4:H:2000:ALA:HB2	0.98	0.95
1:C:247:ASN:HD21	1:C:274:LYS:HE2	0.80	0.94
1:A:234:ILE:HB	4:H:939:GLN:NE2	1.81	0.94
1:A:175:SER:O	1:A:178:GLU:N	2.01	0.94
3:G:304:ASN:HB2	3:G:306:PRO:CD	1.98	0.93
1:A:124:ILE:HG23	1:A:292:ALA:HA	1.25	0.93
1:A:124:ILE:HG22	1:A:291:ILE:C	1.86	0.93
1:A:234:ILE:HB	4:H:939:GLN:CD	1.89	0.93
3:G:236:TYR:OH	3:G:268:LEU:O	1.85	0.93
4:H:1981:PRO:CD	4:H:1982:PRO:CD	2.47	0.93
1:A:134:GLU:CA	1:A:161:LEU:HA	1.99	0.93
3:G:30:PHE:HB2	3:G:47:GLU:HG2	1.16	0.93
3:G:306:PRO:HA	3:G:309:MET:HB2	0.93	0.93
4:H:2027:ASN:CG	4:H:2029:ARG:HH22	1.69	0.93
3:G:30:PHE:CA	3:G:47:GLU:CD	2.31	0.92
4:H:910:ARG:NH1	4:H:2037:LEU:CG	2.11	0.92
4:H:1981:PRO:HD2	4:H:1982:PRO:CD	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:305:LEU:HB2	3:G:309:MET:CE	2.00	0.92
2:B:170:THR:CG2	5:X:30:UNK:HA	1.99	0.92
2:D:285:GLU:O	2:D:287:GLY:N	2.02	0.92
3:G:236:TYR:C	3:G:267:ILE:HG21	1.89	0.92
1:A:134:GLU:CB	1:A:161:LEU:CA	2.47	0.92
3:G:46:ASP:OD1	3:G:47:GLU:N	2.02	0.92
4:H:928:LEU:HD22	4:H:2000:ALA:CB	2.00	0.92
3:G:49:LYS:NZ	3:G:49:LYS:HA	1.85	0.91
3:G:238:LEU:HD12	3:G:268:LEU:HD21	1.48	0.91
4:H:913:THR:OG1	4:H:2032:PHE:CE1	2.22	0.91
4:H:913:THR:OG1	4:H:2032:PHE:HE1	1.52	0.91
4:H:2032:PHE:HD1	4:H:2033:PRO:HD2	1.26	0.91
1:A:134:GLU:HB2	1:A:161:LEU:CA	2.00	0.91
1:A:134:GLU:OE1	1:A:160:GLY:C	2.09	0.91
1:A:175:SER:O	1:A:177:PHE:N	2.03	0.91
3:G:50:ASP:HB3	3:G:51:PRO:HD3	1.52	0.91
3:G:378:THR:OG1	3:G:380:GLU:OE2	1.87	0.91
4:H:940:ARG:HG3	4:H:940:ARG:HH11	1.35	0.91
4:H:1981:PRO:CD	4:H:1982:PRO:HD3	1.99	0.90
3:G:304:ASN:HB2	3:G:306:PRO:HD3	1.53	0.90
3:G:45:ILE:HB	3:G:49:LYS:CE	2.01	0.90
3:G:270:LEU:HD23	3:G:271:ALA:N	1.85	0.90
3:G:270:LEU:CD2	3:G:271:ALA:N	2.35	0.90
1:A:234:ILE:CD1	4:H:939:GLN:OE1	2.20	0.90
2:D:250:ILE:CG1	2:D:276:ILE:HD11	2.02	0.90
1:A:137:GLU:CG	1:A:159:ILE:HA	2.02	0.90
4:H:2003:GLN:OE1	4:H:2007:GLN:CG	2.20	0.90
3:G:30:PHE:CD1	3:G:56:TYR:HB2	2.04	0.89
4:H:910:ARG:CZ	4:H:2037:LEU:HG	2.01	0.89
4:H:936:HIS:HB2	4:H:937:PRO:CD	2.03	0.89
4:H:1981:PRO:HD2	4:H:1982:PRO:HD2	1.52	0.88
3:G:294:ILE:N	3:G:295:PRO:CD	2.26	0.88
1:A:134:GLU:HG3	1:A:161:LEU:CA	2.03	0.88
4:H:928:LEU:CG	4:H:2000:ALA:HB2	2.02	0.88
3:G:30:PHE:CD2	3:G:47:GLU:CG	2.55	0.88
1:A:134:GLU:HG3	1:A:162:LYS:N	1.89	0.88
1:C:189:ASP:HB2	1:C:204:GLY:HA3	1.52	0.88
2:D:290:GLU:C	2:D:291:ILE:HG13	1.93	0.87
3:G:294:ILE:H	3:G:295:PRO:HD2	1.39	0.87
2:B:198:ALA:HB1	4:H:1998:TRP:HE1	1.34	0.87
1:A:134:GLU:O	1:A:205:ARG:NH1	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ILE:CG2	1:A:292:ALA:N	2.36	0.87
2:B:260:LEU:O	1:C:271:ILE:HB	1.73	0.87
1:A:286:TYR:OH	4:H:943:MET:CG	2.23	0.87
3:G:45:ILE:HB	3:G:49:LYS:HE2	1.57	0.86
4:H:869:TYR:HA	4:H:872:PHE:HD2	1.40	0.86
3:G:192:GLN:OE1	3:G:268:LEU:HD13	1.75	0.86
1:A:142:GLU:OE1	1:A:155:SER:C	2.14	0.86
3:G:306:PRO:C	3:G:309:MET:N	2.29	0.85
1:E:126:GLU:HB2	4:H:1964:GLN:OE1	1.75	0.85
4:H:2002:ARG:HG2	4:H:2002:ARG:HH11	1.41	0.85
1:A:133:GLY:C	1:A:161:LEU:CD2	2.44	0.85
4:H:910:ARG:NH1	4:H:2037:LEU:HD12	1.89	0.85
2:B:198:ALA:CB	4:H:1998:TRP:CD1	2.59	0.85
2:B:170:THR:HG22	5:X:30:UNK:CA	2.07	0.85
1:A:137:GLU:HG2	1:A:160:GLY:H	1.31	0.85
3:G:233:MET:HB2	3:G:269:ARG:HD2	1.59	0.85
1:A:128:LYS:HZ2	4:H:938:LEU:H	1.25	0.84
4:H:951:LEU:CD1	4:H:958:TYR:CE2	2.60	0.84
1:A:124:ILE:HD12	1:A:124:ILE:H	1.43	0.84
4:H:928:LEU:HD22	4:H:2000:ALA:HB3	1.58	0.84
3:G:120:GLN:O	3:G:378:THR:HG21	1.77	0.83
3:G:306:PRO:CA	3:G:309:MET:CA	2.56	0.83
1:E:236:GLN:OE1	4:H:1960:LEU:CG	2.27	0.83
3:G:379:ARG:C	3:G:381:ASP:H	1.82	0.83
2:D:279:LYS:HG3	4:H:1984:GLU:HG2	1.58	0.83
1:A:234:ILE:HB	4:H:939:GLN:HE22	1.43	0.82
2:F:144:GLU:OE2	2:F:161:LEU:CA	2.27	0.82
3:G:379:ARG:O	3:G:382:TYR:N	2.11	0.82
4:H:2003:GLN:CD	4:H:2007:GLN:NE2	2.32	0.82
5:X:21:UNK:CB	5:X:25:UNK:CB	2.56	0.82
2:D:268:ILE:O	2:D:272:VAL:HG23	1.79	0.82
1:E:236:GLN:OE1	4:H:1960:LEU:CB	2.27	0.82
1:A:124:ILE:HG22	1:A:291:ILE:O	1.80	0.82
3:G:238:LEU:HD12	3:G:268:LEU:CG	2.08	0.82
2:D:268:ILE:HB	2:D:272:VAL:HG21	1.62	0.82
1:A:134:GLU:CG	1:A:161:LEU:CA	2.58	0.81
2:B:134:GLU:HA	2:B:236:LYS:O	1.79	0.81
1:A:137:GLU:CB	1:A:160:GLY:H	1.94	0.81
1:C:117:ARG:NH1	1:C:276:ARG:HD3	1.96	0.81
1:C:134:GLU:HB3	1:C:205:ARG:HH12	1.45	0.81
2:B:261:PHE:HA	1:C:271:ILE:CB	2.06	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:GLU:CD	4:H:1964:GLN:CD	2.40	0.80
2:B:198:ALA:HB2	4:H:1998:TRP:CE2	2.13	0.80
1:E:126:GLU:HG3	4:H:1964:GLN:HE21	1.45	0.80
3:G:306:PRO:CB	3:G:309:MET:CA	2.55	0.80
2:D:247:ILE:HG23	2:D:272:VAL:HG12	1.63	0.80
2:D:268:ILE:O	2:D:272:VAL:HG21	1.82	0.80
1:A:209:TYR:O	5:X:17:UNK:O	2.00	0.80
3:G:50:ASP:HB3	3:G:51:PRO:CD	2.11	0.80
1:A:128:LYS:HZ2	4:H:938:LEU:N	1.80	0.80
3:G:220:MET:CE	5:X:25:UNK:O	2.30	0.80
1:A:134:GLU:CB	1:A:160:GLY:O	2.30	0.79
1:A:171:LYS:C	1:A:172:LEU:HD23	2.03	0.79
2:B:261:PHE:HA	1:C:271:ILE:HB	1.64	0.79
2:F:145:ILE:O	2:F:159:GLY:N	2.15	0.79
3:G:305:LEU:HD23	3:G:305:LEU:H	1.47	0.79
2:B:235:ARG:HG3	2:B:235:ARG:HH11	1.47	0.79
4:H:949:ILE:O	4:H:1932:VAL:CG1	2.27	0.79
1:C:189:ASP:CB	1:C:204:GLY:HA3	2.11	0.79
1:C:244:ASP:OD2	1:C:275:LEU:CD1	2.31	0.78
3:G:282:PHE:O	3:G:293:GLY:HA2	1.83	0.78
1:A:210:ALA:C	5:X:17:UNK:O	2.20	0.78
1:A:137:GLU:HG2	1:A:159:ILE:CA	2.14	0.78
3:G:41:THR:O	3:G:46:ASP:HA	1.84	0.78
1:A:234:ILE:CB	4:H:939:GLN:OE1	2.31	0.78
3:G:306:PRO:O	3:G:309:MET:C	2.22	0.78
4:H:950:GLY:HA3	4:H:1936:ILE:HG23	1.65	0.78
4:H:2003:GLN:OE1	4:H:2007:GLN:HG3	1.84	0.78
1:C:247:ASN:ND2	1:C:274:LYS:HE3	1.97	0.77
3:G:269:ARG:HA	3:G:269:ARG:NH1	1.99	0.77
2:F:144:GLU:OE2	2:F:161:LEU:HA	1.84	0.77
3:G:306:PRO:O	3:G:309:MET:N	2.16	0.77
1:E:236:GLN:OE1	4:H:1960:LEU:HG	1.84	0.77
1:C:192:TYR:CE1	1:C:200:VAL:HG23	2.19	0.77
4:H:928:LEU:HD21	4:H:1999:LEU:HG	1.67	0.77
1:A:137:GLU:HG2	1:A:159:ILE:C	2.04	0.77
1:A:128:LYS:HD3	4:H:939:GLN:HB2	1.66	0.77
2:B:198:ALA:CA	4:H:1998:TRP:CE2	2.66	0.76
3:G:45:ILE:HD12	3:G:45:ILE:H	1.50	0.76
4:H:2027:ASN:O	4:H:2029:ARG:N	2.17	0.76
5:X:50:UNK:C	5:X:52:UNK:N	2.46	0.76
4:H:910:ARG:NH1	4:H:2037:LEU:HD11	1.97	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:GLU:CG	4:H:1964:GLN:HE22	1.67	0.76
3:G:33:LYS:N	3:G:54:LEU:CD2	2.19	0.75
1:A:168:LYS:HD2	1:A:228:VAL:HG11	1.69	0.75
5:X:21:UNK:CB	5:X:25:UNK:HA	2.16	0.75
1:A:279:ILE:HG23	4:H:945:ARG:HH12	1.50	0.75
3:G:237:VAL:N	3:G:267:ILE:HG21	2.00	0.75
2:B:198:ALA:CB	4:H:1998:TRP:CZ2	2.64	0.75
2:D:267:GLU:CD	2:D:273:ARG:NH2	2.40	0.75
3:G:294:ILE:CG2	3:G:295:PRO:HD3	2.17	0.75
4:H:951:LEU:N	4:H:951:LEU:HD23	2.01	0.74
2:D:251:ASN:ND2	2:D:268:ILE:N	2.34	0.74
1:E:126:GLU:CA	4:H:1964:GLN:HE22	1.99	0.74
4:H:869:TYR:HA	4:H:872:PHE:CD2	2.21	0.74
5:X:48:UNK:O	5:X:50:UNK:N	2.20	0.74
3:G:238:LEU:HD12	3:G:268:LEU:HG	1.69	0.74
1:A:159:ILE:CD1	1:A:172:LEU:HD11	2.04	0.74
4:H:2032:PHE:HD1	4:H:2033:PRO:CD	2.00	0.74
1:C:134:GLU:HB3	1:C:205:ARG:NH1	2.02	0.74
3:G:41:THR:O	3:G:46:ASP:CA	2.35	0.74
3:G:304:ASN:HB2	3:G:306:PRO:HD2	1.68	0.73
1:A:172:LEU:HD23	1:A:172:LEU:N	2.03	0.73
1:C:244:ASP:OD1	1:C:279:ILE:HD13	1.88	0.73
4:H:2027:ASN:CG	4:H:2029:ARG:NH2	2.23	0.73
2:B:198:ALA:CB	4:H:1998:TRP:CD2	2.69	0.73
1:A:137:GLU:HB3	1:A:159:ILE:HA	1.70	0.73
1:A:175:SER:O	1:A:176:ILE:C	2.26	0.73
4:H:940:ARG:HG3	4:H:940:ARG:NH1	2.01	0.73
2:D:283:TRP:HB3	2:D:289:ALA:HB3	1.71	0.73
1:A:124:ILE:HG23	1:A:292:ALA:HB1	1.65	0.73
3:G:307:GLU:HA	3:G:307:GLU:OE1	1.89	0.73
4:H:865:GLN:O	4:H:869:TYR:CD2	2.42	0.73
4:H:1980:MET:H	4:H:1981:PRO:HD2	1.53	0.73
2:F:145:ILE:N	2:F:145:ILE:HD12	2.03	0.72
3:G:304:ASN:ND2	3:G:313:PHE:CE2	2.57	0.72
1:A:134:GLU:HB2	1:A:161:LEU:N	2.03	0.72
1:A:137:GLU:HG3	1:A:158:ILE:O	1.88	0.72
4:H:941:ILE:HD13	4:H:941:ILE:H	1.55	0.72
1:A:123:ARG:HB2	1:A:123:ARG:NH1	2.04	0.72
4:H:2032:PHE:CD1	4:H:2033:PRO:CD	2.65	0.72
2:B:170:THR:HG22	5:X:30:UNK:CB	2.19	0.72
3:G:306:PRO:HA	3:G:309:MET:CA	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:2037:LEU:N	4:H:2037:LEU:HD23	2.04	0.72
1:C:189:ASP:CG	1:C:204:GLY:HA3	2.10	0.71
1:A:134:GLU:CB	1:A:160:GLY:C	2.58	0.71
3:G:32:SER:C	3:G:54:LEU:HD21	2.09	0.71
3:G:235:ASP:HB2	3:G:267:ILE:HG13	1.73	0.71
3:G:237:VAL:HA	3:G:267:ILE:CG2	2.19	0.71
3:G:49:LYS:HA	3:G:49:LYS:HZ3	1.56	0.71
4:H:928:LEU:CD2	4:H:2000:ALA:HB2	2.21	0.71
4:H:910:ARG:NH2	4:H:2037:LEU:HG	2.04	0.71
2:B:135:THR:HG23	4:H:1999:LEU:HD13	1.66	0.71
4:H:938:LEU:O	4:H:940:ARG:HD3	1.91	0.71
3:G:43:ASN:C	3:G:46:ASP:OD2	2.26	0.70
3:G:306:PRO:CB	3:G:309:MET:O	2.32	0.70
5:X:22:UNK:CB	5:X:32:UNK:O	2.38	0.70
1:A:142:GLU:OE1	1:A:155:SER:CA	2.38	0.70
2:B:198:ALA:HB2	4:H:1998:TRP:CD2	2.26	0.70
4:H:2002:ARG:HG2	4:H:2002:ARG:NH1	2.03	0.70
2:B:133:GLU:O	2:B:237:GLU:HA	1.91	0.70
1:A:212:GLU:CG	5:X:28:UNK:CB	2.66	0.69
1:C:192:TYR:CE1	1:C:200:VAL:N	2.57	0.69
1:A:209:TYR:C	5:X:17:UNK:CB	2.60	0.69
1:A:137:GLU:CB	1:A:159:ILE:HA	2.21	0.69
1:A:175:SER:OG	1:A:176:ILE:N	2.25	0.69
1:A:133:GLY:CA	1:A:161:LEU:CD2	2.71	0.69
3:G:49:LYS:HA	3:G:49:LYS:HZ2	1.58	0.69
2:B:262:SER:HB2	1:C:271:ILE:HG12	1.73	0.69
4:H:865:GLN:O	4:H:869:TYR:HD2	1.76	0.69
4:H:910:ARG:HH11	4:H:2037:LEU:CD1	2.04	0.69
4:H:928:LEU:CD2	4:H:2000:ALA:CB	2.71	0.69
3:G:45:ILE:HD12	3:G:45:ILE:N	2.07	0.69
4:H:1981:PRO:CG	4:H:1982:PRO:CD	2.67	0.69
3:G:306:PRO:HB2	3:G:313:PHE:CD2	2.25	0.68
1:A:124:ILE:HG21	1:A:292:ALA:CB	1.93	0.68
3:G:30:PHE:CB	3:G:47:GLU:HG3	2.03	0.68
3:G:47:GLU:O	3:G:48:ILE:HG23	1.93	0.68
3:G:282:PHE:O	3:G:293:GLY:CA	2.42	0.68
1:C:243:LEU:HD23	1:C:279:ILE:HG23	1.74	0.68
3:G:30:PHE:CG	3:G:47:GLU:CG	2.48	0.68
3:G:270:LEU:HD22	3:G:271:ALA:N	2.09	0.68
1:A:133:GLY:C	1:A:161:LEU:HD22	2.15	0.67
3:G:294:ILE:N	3:G:295:PRO:HD2	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:377:VAL:HG13	3:G:389:VAL:HG22	1.77	0.67
4:H:868:LEU:O	4:H:872:PHE:CD2	2.47	0.67
4:H:934:ASP:O	4:H:935:VAL:HG13	1.94	0.67
1:A:131:TYR:OH	1:A:170:LEU:HB3	1.95	0.67
1:A:134:GLU:HA	1:A:161:LEU:HA	1.74	0.67
2:B:136:GLU:OE2	2:B:235:ARG:NH1	2.27	0.67
1:C:288:ASP:OD1	1:C:288:ASP:N	2.27	0.67
4:H:1981:PRO:CD	4:H:1982:PRO:HD2	2.17	0.67
1:A:134:GLU:CG	1:A:161:LEU:N	2.58	0.66
1:C:286:TYR:C	1:C:288:ASP:OD1	2.34	0.66
2:D:251:ASN:HD22	2:D:267:GLU:C	1.99	0.66
3:G:28:CYS:SG	3:G:57:ILE:O	2.53	0.66
3:G:269:ARG:HH11	3:G:269:ARG:CA	2.03	0.66
1:C:244:ASP:OD2	1:C:275:LEU:HD11	1.94	0.66
1:C:284:ASN:O	1:C:288:ASP:N	2.27	0.66
1:A:128:LYS:NZ	4:H:938:LEU:H	1.92	0.66
1:A:137:GLU:HG2	1:A:159:ILE:HA	1.75	0.66
2:B:198:ALA:HA	4:H:1998:TRP:CH2	2.30	0.66
1:C:287:ILE:O	1:C:289:GLN:N	2.28	0.66
1:C:287:ILE:HD11	1:C:294:LEU:HB2	1.77	0.66
2:D:268:ILE:HB	2:D:272:VAL:CG2	2.25	0.66
4:H:2027:ASN:C	4:H:2029:ARG:H	1.98	0.66
2:B:135:THR:HG22	4:H:1999:LEU:HD12	1.77	0.66
3:G:306:PRO:CA	3:G:309:MET:H	2.08	0.66
3:G:238:LEU:HD23	3:G:238:LEU:C	2.15	0.66
3:G:237:VAL:HA	3:G:267:ILE:HG22	1.78	0.65
4:H:934:ASP:C	4:H:935:VAL:HG22	2.16	0.65
5:X:21:UNK:HA	5:X:25:UNK:C	2.25	0.65
4:H:934:ASP:N	4:H:934:ASP:OD1	2.26	0.65
4:H:1961:PHE:HB2	4:H:1962:PRO:CD	2.26	0.65
5:X:18:UNK:O	5:X:19:UNK:C	2.45	0.65
2:B:198:ALA:HB2	4:H:1998:TRP:O	1.96	0.65
2:F:144:GLU:O	2:F:145:ILE:HG23	1.96	0.65
5:X:33:UNK:CB	5:X:39:UNK:CA	2.73	0.65
1:A:209:TYR:O	5:X:17:UNK:CB	2.45	0.65
2:D:280:VAL:HG13	2:D:291:ILE:HD11	1.77	0.65
1:E:126:GLU:OE1	4:H:1964:GLN:CG	2.44	0.65
2:F:260:LEU:CD2	4:H:946:PHE:CE1	2.73	0.65
4:H:1961:PHE:N	4:H:1962:PRO:HD2	2.11	0.64
1:A:282:VAL:HG21	4:H:945:ARG:NE	2.13	0.64
1:A:164:ALA:CB	1:A:223:LEU:HD21	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:LYS:HE2	2:B:179:ILE:HG12	1.79	0.64
3:G:267:ILE:HD12	3:G:267:ILE:C	2.18	0.64
3:G:306:PRO:CG	3:G:309:MET:HB2	2.27	0.64
1:C:274:LYS:NZ	4:H:921:ILE:HD13	2.12	0.64
3:G:220:MET:HE1	5:X:25:UNK:O	1.97	0.64
4:H:1980:MET:H	4:H:1981:PRO:CD	2.10	0.64
1:A:210:ALA:HA	5:X:17:UNK:HA	0.85	0.64
3:G:306:PRO:HB2	3:G:309:MET:C	2.16	0.64
1:A:133:GLY:C	1:A:161:LEU:HD23	2.14	0.64
2:B:134:GLU:CD	2:B:235:ARG:HD3	2.17	0.64
4:H:951:LEU:HD23	4:H:951:LEU:H	1.63	0.64
2:B:233:GLN:HE21	2:B:233:GLN:N	1.95	0.64
1:A:128:LYS:O	1:A:128:LYS:HG3	1.98	0.63
1:A:164:ALA:HB2	1:A:223:LEU:CD2	2.28	0.63
1:A:168:LYS:HD2	1:A:228:VAL:HG21	1.81	0.63
3:G:285:SER:OG	5:X:18:UNK:HA	1.98	0.63
3:G:47:GLU:C	3:G:48:ILE:HG12	2.19	0.63
3:G:306:PRO:CA	3:G:309:MET:N	2.61	0.63
2:B:250:ILE:HD13	4:H:934:ASP:CG	2.19	0.62
2:D:250:ILE:HG13	2:D:276:ILE:CD1	2.12	0.62
1:A:134:GLU:CD	1:A:160:GLY:C	2.58	0.62
4:H:2037:LEU:HD23	4:H:2037:LEU:H	1.62	0.62
1:A:164:ALA:HB2	1:A:223:LEU:HD21	1.80	0.62
1:C:243:LEU:CD2	1:C:279:ILE:HG23	2.29	0.62
2:F:49:GLN:HE22	2:F:360:THR:H	1.47	0.62
3:G:30:PHE:HB2	3:G:47:GLU:OE2	1.72	0.62
1:A:123:ARG:HG3	1:A:123:ARG:HH11	1.65	0.61
1:C:289:GLN:N	1:C:289:GLN:OE1	2.33	0.61
5:X:21:UNK:CB	5:X:25:UNK:CA	2.76	0.61
1:C:117:ARG:HH11	1:C:276:ARG:HD3	1.63	0.61
3:G:48:ILE:O	3:G:49:LYS:HE2	2.00	0.61
3:G:377:VAL:CG1	3:G:389:VAL:HG22	2.30	0.61
1:C:243:LEU:HD23	1:C:279:ILE:CG2	2.30	0.61
3:G:30:PHE:N	3:G:47:GLU:CD	2.53	0.61
1:A:174:PRO:O	1:A:177:PHE:HB3	2.01	0.61
4:H:1979:VAL:HG13	4:H:1979:VAL:O	2.01	0.61
1:A:123:ARG:HH11	1:A:123:ARG:CG	2.13	0.60
1:C:200:VAL:HG12	1:C:200:VAL:O	2.01	0.60
2:D:286:GLU:O	2:D:286:GLU:HG2	1.99	0.60
2:B:262:SER:CB	1:C:271:ILE:HG12	2.30	0.60
2:F:143:VAL:HG12	2:F:143:VAL:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:270:LEU:HD22	3:G:271:ALA:H	1.59	0.60
3:G:237:VAL:CA	3:G:267:ILE:HG21	2.31	0.60
4:H:910:ARG:HH22	4:H:2037:LEU:HG	1.67	0.60
2:F:144:GLU:O	2:F:145:ILE:HG13	1.99	0.60
3:G:294:ILE:N	3:G:295:PRO:HD3	1.97	0.60
2:B:135:THR:N	2:B:236:LYS:O	2.33	0.60
1:A:142:GLU:OE1	1:A:155:SER:N	2.34	0.60
1:E:419:ILE:HD11	2:F:61:GLU:HG2	1.84	0.60
3:G:294:ILE:HG22	3:G:295:PRO:HD3	1.84	0.60
2:F:143:VAL:CG2	2:F:163:LEU:O	2.43	0.60
1:C:274:LYS:NZ	4:H:921:ILE:HG21	2.16	0.59
3:G:306:PRO:HA	3:G:309:MET:CG	2.31	0.59
4:H:2000:ALA:HB3	4:H:2001:PRO:HD2	1.82	0.59
1:A:127:THR:O	1:A:128:LYS:HB3	2.02	0.59
2:B:235:ARG:HH11	2:B:235:ARG:CG	2.15	0.59
3:G:236:TYR:O	3:G:267:ILE:HG21	2.01	0.59
4:H:1959:VAL:HG13	4:H:1959:VAL:O	2.00	0.59
3:G:304:ASN:CB	3:G:306:PRO:HD2	2.33	0.59
3:G:305:LEU:HB2	3:G:309:MET:HE1	1.83	0.59
3:G:305:LEU:HB2	3:G:309:MET:HE3	1.84	0.59
3:G:238:LEU:HB2	3:G:268:LEU:HG	1.85	0.59
3:G:155:THR:HB	3:G:173:ILE:HB	1.85	0.59
1:C:244:ASP:OD1	1:C:279:ILE:CD1	2.51	0.59
2:D:265:THR:O	2:D:265:THR:OG1	2.17	0.59
3:G:306:PRO:HA	3:G:309:MET:N	2.16	0.59
4:H:936:HIS:CB	4:H:937:PRO:CD	2.72	0.59
1:A:128:LYS:NZ	4:H:937:PRO:HB2	2.18	0.58
1:A:134:GLU:HA	1:A:162:LYS:H	1.66	0.58
1:C:189:ASP:OD2	1:C:205:ARG:N	2.33	0.58
3:G:45:ILE:CG2	3:G:49:LYS:HE3	2.33	0.58
3:G:237:VAL:HA	3:G:267:ILE:HG21	1.84	0.58
4:H:2027:ASN:CB	4:H:2029:ARG:NH2	2.66	0.58
1:A:137:GLU:CG	1:A:160:GLY:N	2.43	0.58
2:D:130:ARG:HG2	2:D:241:THR:HG22	1.84	0.58
4:H:951:LEU:CD1	4:H:958:TYR:HE2	2.01	0.58
1:A:155:SER:HA	1:A:174:PRO:HD3	1.85	0.58
1:A:365:LEU:HD11	2:F:447:GLN:HE22	1.68	0.58
4:H:1961:PHE:HB2	4:H:1962:PRO:HD3	1.84	0.58
2:B:249:VAL:HG13	2:B:250:ILE:HG13	1.85	0.58
1:C:96:MET:SD	1:C:115:ASN:ND2	2.76	0.58
1:E:302:ASP:HA	1:E:330:ALA:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:THR:CG2	5:X:30:UNK:CA	2.76	0.58
3:G:30:PHE:HB3	3:G:47:GLU:OE2	2.00	0.58
1:A:96:MET:SD	1:A:115:ASN:ND2	2.77	0.58
3:G:380:GLU:OE1	3:G:381:ASP:N	2.37	0.58
3:G:270:LEU:CD2	3:G:273:GLU:CD	2.57	0.57
2:B:129:VAL:HG22	2:B:291:ILE:HG22	1.86	0.57
3:G:33:LYS:HB2	3:G:55:PHE:CE1	2.39	0.57
1:A:137:GLU:CG	1:A:159:ILE:CA	2.73	0.57
3:G:30:PHE:N	3:G:47:GLU:OE1	2.35	0.57
3:G:56:TYR:CD1	3:G:56:TYR:N	2.73	0.57
4:H:1963:GLN:HA	4:H:1963:GLN:OE1	2.04	0.57
1:C:98:GLY:H	1:C:303:GLU:HB3	1.69	0.57
1:E:430:VAL:HA	1:E:433:ILE:HG12	1.87	0.57
1:E:67:LEU:HD23	1:E:360:ILE:HG12	1.87	0.57
3:G:120:GLN:O	3:G:378:THR:OG1	2.21	0.57
3:G:233:MET:CB	3:G:269:ARG:HD2	2.32	0.57
3:G:236:TYR:CD1	3:G:237:VAL:N	2.73	0.57
3:G:30:PHE:HD2	3:G:47:GLU:CG	2.16	0.57
1:E:362:ARG:NH2	1:E:364:MET:SD	2.76	0.57
3:G:235:ASP:HA	3:G:267:ILE:HD11	1.86	0.57
2:F:75:ILE:HD12	2:F:83:LYS:HD2	1.87	0.57
4:H:1972:ILE:O	4:H:1975:ARG:NH1	2.38	0.57
2:F:137:ILE:HD12	2:F:236:LYS:HD2	1.87	0.56
1:A:164:ALA:HB2	1:A:223:LEU:HG	1.88	0.56
2:B:199:THR:H	4:H:1998:TRP:HE1	1.51	0.56
2:D:435:ASP:H	2:D:438:ARG:HB2	1.71	0.56
3:G:308:GLU:O	3:G:308:GLU:HG2	2.05	0.56
1:C:291:ILE:HG22	1:C:292:ALA:N	2.20	0.56
2:D:247:ILE:CG2	2:D:272:VAL:HG12	2.33	0.56
1:A:191:ILE:HA	1:A:201:LYS:HG2	1.87	0.56
3:G:306:PRO:CB	3:G:309:MET:HB3	2.07	0.56
1:A:137:GLU:HB2	1:A:160:GLY:H	1.70	0.56
3:G:238:LEU:CD1	3:G:268:LEU:HD21	2.29	0.56
3:G:305:LEU:HD23	3:G:305:LEU:N	2.18	0.56
3:G:305:LEU:C	3:G:307:GLU:H	2.09	0.56
1:C:312:PHE:O	1:C:316:HIS:ND1	2.35	0.56
2:D:62:MET:SD	2:D:71:ARG:NH2	2.79	0.56
3:G:220:MET:HE2	5:X:25:UNK:O	2.04	0.56
1:C:244:ASP:CG	1:C:275:LEU:CD1	2.75	0.56
1:A:175:SER:C	1:A:177:PHE:N	2.60	0.56
3:G:236:TYR:HD1	3:G:237:VAL:N	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:GLU:OE1	4:H:1999:LEU:HD21	2.05	0.56
1:E:97:VAL:HG12	1:E:302:ASP:HB3	1.88	0.56
1:A:133:GLY:CA	1:A:161:LEU:HD21	2.36	0.55
1:C:116:PHE:HD1	1:C:325:PRO:HD2	1.71	0.55
3:G:55:PHE:CG	3:G:56:TYR:N	2.73	0.55
1:A:134:GLU:CD	1:A:161:LEU:N	2.59	0.55
1:C:125:LYS:HG2	1:C:235:ILE:HG12	1.86	0.55
1:C:205:ARG:HD3	1:C:224:PRO:HG3	1.88	0.55
2:D:117:GLU:OE2	2:D:121:GLN:NE2	2.39	0.55
3:G:46:ASP:C	3:G:48:ILE:H	2.09	0.55
3:G:30:PHE:CE1	3:G:56:TYR:HB3	2.17	0.55
2:B:137:ILE:HD12	2:B:236:LYS:CD	2.30	0.55
2:B:416:ARG:NH1	2:B:420:GLU:O	2.40	0.55
1:A:128:LYS:HZ2	4:H:937:PRO:HB2	1.72	0.55
2:F:49:GLN:NE2	2:F:360:THR:O	2.40	0.55
1:E:25:GLY:HA3	1:E:36:ALA:HB1	1.89	0.55
3:G:157:ILE:HB	3:G:171:ILE:HB	1.88	0.55
3:G:267:ILE:HD11	3:G:269:ARG:HH12	1.71	0.55
4:H:966:ARG:NH2	4:H:1924:ASP:OD2	2.39	0.55
4:H:917:ILE:HG22	4:H:919:PRO:HD3	1.89	0.55
4:H:933:THR:OG1	4:H:934:ASP:OD1	2.21	0.55
1:A:299:LEU:HB2	1:A:327:VAL:HG22	1.89	0.54
1:A:42:GLN:HB3	1:A:45:ALA:HB3	1.89	0.54
1:A:164:ALA:HB2	1:A:223:LEU:CG	2.37	0.54
1:E:113:MET:SD	1:E:314:TYR:OH	2.66	0.54
3:G:267:ILE:HD12	3:G:268:LEU:N	2.22	0.54
5:X:21:UNK:HA	5:X:25:UNK:HA	0.63	0.54
1:A:135:VAL:HG22	1:A:136:THR:HG23	1.88	0.54
1:C:353:ASP:O	1:C:357:ARG:NH1	2.41	0.54
3:G:30:PHE:H	3:G:47:GLU:CD	2.08	0.54
1:A:123:ARG:HB2	1:A:123:ARG:CZ	2.38	0.54
1:A:234:ILE:CG1	4:H:939:GLN:OE1	2.55	0.54
1:E:162:LYS:HG2	1:E:167:THR:HG22	1.89	0.54
2:F:268:ILE:HG22	2:F:271:GLU:H	1.72	0.54
4:H:936:HIS:CD2	4:H:936:HIS:N	2.73	0.54
1:A:134:GLU:CD	1:A:160:GLY:HA3	2.25	0.54
4:H:1983:VAL:HG11	4:H:2029:ARG:HH21	1.72	0.54
4:H:1981:PRO:HD2	4:H:1982:PRO:HD3	1.69	0.54
1:A:134:GLU:CG	1:A:162:LYS:N	2.68	0.53
2:D:267:GLU:OE1	2:D:267:GLU:N	2.40	0.53
4:H:2063:LEU:HD12	4:H:2133:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:2028:MET:O	4:H:2030:THR:N	2.41	0.53
2:B:138:ILE:HG23	2:B:232:LEU:HB2	1.89	0.53
1:E:159:ILE:HG13	1:E:172:LEU:HD12	1.90	0.53
2:F:129:VAL:HG22	2:F:291:ILE:HG22	1.90	0.53
2:F:144:GLU:CD	2:F:161:LEU:HA	2.28	0.53
3:G:305:LEU:O	3:G:307:GLU:N	2.41	0.53
1:C:128:LYS:O	1:C:231:LYS:HA	2.09	0.53
1:C:274:LYS:HZ2	4:H:921:ILE:HD13	1.73	0.53
3:G:45:ILE:HB	3:G:49:LYS:HE3	1.90	0.53
1:A:286:TYR:OH	4:H:943:MET:SD	2.66	0.53
1:C:56:ILE:HG12	1:C:326:ILE:HG21	1.91	0.53
2:D:261:PHE:HD1	1:E:269:THR:O	1.92	0.53
4:H:905:ASN:ND2	4:H:2071:MET:SD	2.79	0.53
4:H:936:HIS:O	4:H:937:PRO:C	2.47	0.53
2:D:60:LEU:HG	2:D:64:ARG:HE	1.73	0.53
1:E:126:GLU:OE1	4:H:1964:GLN:OE1	2.27	0.53
3:G:306:PRO:O	3:G:309:MET:CA	2.57	0.53
2:B:132:LYS:HG2	2:B:239:VAL:HG22	1.91	0.53
3:G:294:ILE:HG23	3:G:295:PRO:HD3	1.90	0.53
1:A:188:GLY:O	1:A:205:ARG:N	2.42	0.53
1:A:209:TYR:O	5:X:17:UNK:C	2.57	0.53
1:A:234:ILE:CB	4:H:939:GLN:HE22	2.20	0.53
2:B:238:VAL:HG23	2:B:238:VAL:O	2.09	0.53
3:G:46:ASP:O	3:G:48:ILE:N	2.41	0.53
1:A:134:GLU:N	1:A:161:LEU:CD2	2.58	0.52
3:G:235:ASP:HB2	3:G:267:ILE:CG1	2.39	0.52
3:G:267:ILE:HD11	3:G:269:ARG:NH1	2.24	0.52
3:G:50:ASP:CB	3:G:51:PRO:CD	2.85	0.52
3:G:299:VAL:O	3:G:303:GLN:NE2	2.43	0.52
4:H:1961:PHE:N	4:H:1961:PHE:CD1	2.72	0.52
1:C:299:LEU:HB3	1:C:327:VAL:HG22	1.92	0.52
3:G:379:ARG:NH1	3:G:383:GLU:OE2	2.42	0.52
1:A:124:ILE:HD12	1:A:124:ILE:N	2.13	0.52
1:A:124:ILE:HD13	1:A:124:ILE:O	2.09	0.52
1:A:282:VAL:HG21	4:H:945:ARG:CZ	2.40	0.52
2:B:233:GLN:NE2	2:B:233:GLN:CA	2.72	0.52
2:F:246:GLU:OE1	4:H:1939:ARG:NH2	2.41	0.52
1:A:60:LYS:HG3	1:A:61:MET:HG2	1.90	0.52
3:G:237:VAL:CA	3:G:267:ILE:CG2	2.86	0.52
2:B:305:ASP:OD1	2:B:336:ARG:NH2	2.43	0.52
1:E:394:LEU:HD13	1:E:397:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:GLU:O	2:D:291:ILE:CB	2.53	0.52
4:H:934:ASP:O	4:H:935:VAL:HG22	2.10	0.52
3:G:267:ILE:CD1	3:G:268:LEU:N	2.73	0.52
4:H:969:LEU:HD23	4:H:972:ARG:HD2	1.92	0.52
1:E:312:PHE:O	1:E:316:HIS:ND1	2.43	0.51
2:F:115:LYS:NZ	2:F:305:ASP:OD2	2.40	0.51
4:H:1980:MET:HG3	4:H:1981:PRO:HD3	0.77	0.51
2:F:81:THR:OG1	2:F:83:LYS:NZ	2.43	0.51
3:G:102:PHE:HD2	3:G:105:ILE:HD12	1.74	0.51
4:H:2027:ASN:HB2	4:H:2029:ARG:NH2	2.25	0.51
1:A:129:GLU:OE2	1:A:230:LYS:O	2.28	0.51
2:B:198:ALA:HB1	4:H:1998:TRP:CZ2	2.23	0.51
1:C:275:LEU:HA	1:C:279:ILE:HD12	1.91	0.51
4:H:1981:PRO:N	4:H:1982:PRO:CD	2.72	0.51
1:C:77:THR:OG1	2:D:314:ARG:NH1	2.43	0.51
2:B:49:GLN:HB3	2:B:52:ALA:HB3	1.92	0.51
1:E:40:VAL:HG11	1:E:373:GLN:HB3	1.91	0.51
4:H:943:MET:HE3	4:H:943:MET:O	2.11	0.51
4:H:950:GLY:HA2	4:H:1936:ILE:HG12	1.91	0.51
1:A:64:ARG:NH2	1:A:359:MET:SD	2.84	0.51
1:A:131:TYR:CE1	1:A:170:LEU:HD22	2.46	0.51
2:B:235:ARG:NH1	2:B:235:ARG:CG	2.73	0.51
5:X:49:UNK:C	5:X:51:UNK:N	2.73	0.51
1:A:123:ARG:HD3	1:A:235:ILE:CG2	2.41	0.51
2:B:60:LEU:HG	2:B:64:ARG:HE	1.76	0.51
3:G:233:MET:HB2	3:G:269:ARG:CD	2.35	0.51
3:G:305:LEU:H	3:G:305:LEU:CD2	2.12	0.51
1:E:117:ARG:HH21	1:E:240:LEU:HD13	1.76	0.51
2:F:136:GLU:HG2	2:F:235:ARG:HG2	1.92	0.51
3:G:173:ILE:HG22	3:G:175:VAL:H	1.75	0.51
1:A:157:VAL:HG21	1:A:177:PHE:HB2	1.93	0.50
2:D:247:ILE:HD13	2:D:273:ARG:NE	2.27	0.50
2:D:260:LEU:HB3	1:E:274:LYS:HD3	1.93	0.50
3:G:304:ASN:OD1	3:G:304:ASN:N	2.44	0.50
1:C:108:LYS:NZ	1:C:308:ASP:OD2	2.42	0.50
2:F:131:ILE:HB	2:F:240:HIS:HB2	1.93	0.50
4:H:910:ARG:HH11	4:H:2037:LEU:HD12	1.68	0.50
1:A:138:LEU:HD21	1:A:185:VAL:HB	1.92	0.50
1:E:299:LEU:HB2	1:E:327:VAL:HG22	1.94	0.50
2:D:119:LEU:HD23	2:D:311:PHE:HD2	1.76	0.50
1:E:100:GLU:OE2	2:F:314:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:299:ASP:HA	2:F:327:ALA:HB3	1.94	0.50
2:B:164:LYS:HA	2:B:169:GLU:HG2	1.94	0.50
2:B:166:THR:OG1	2:B:229:ASP:OD2	2.30	0.50
3:G:220:MET:SD	5:X:26:UNK:CB	3.00	0.50
1:C:159:ILE:HD12	1:C:172:LEU:HG	1.94	0.50
1:C:287:ILE:O	1:C:288:ASP:C	2.50	0.50
2:F:19:ILE:O	2:F:21:ARG:NH2	2.45	0.50
3:G:283:ASN:OD1	3:G:292:MET:HA	2.12	0.50
4:H:2069:THR:HA	4:H:2072:LEU:HD12	1.93	0.50
1:C:192:TYR:H	1:C:200:VAL:N	2.10	0.50
2:F:142:VAL:CG2	2:F:190:GLY:H	2.25	0.50
2:B:135:THR:O	2:B:236:LYS:N	2.31	0.50
2:B:139:GLU:HG2	2:B:194:THR:HG22	1.94	0.50
1:E:336:CYS:SG	2:F:340:TYR:OH	2.68	0.50
3:G:61:GLN:NE2	5:X:60:UNK:O	2.45	0.50
4:H:910:ARG:HH12	4:H:2037:LEU:HD11	1.57	0.50
1:A:123:ARG:NH1	1:A:123:ARG:CB	2.73	0.49
2:F:247:ILE:HD13	2:F:272:VAL:HG13	1.94	0.49
4:H:951:LEU:N	4:H:951:LEU:CD2	2.73	0.49
5:X:21:UNK:CA	5:X:25:UNK:CA	2.39	0.49
1:A:207:ASP:N	1:A:207:ASP:OD1	2.45	0.49
1:A:367:THR:OG1	1:A:370:GLU:OE1	2.30	0.49
1:C:244:ASP:CG	1:C:275:LEU:HD13	2.33	0.49
2:F:145:ILE:HD13	2:F:146:GLN:H	1.78	0.49
1:A:132:GLU:OE1	1:A:163:THR:HG22	2.12	0.49
1:A:167:THR:HG23	3:G:339:CYS:O	2.12	0.49
3:G:30:PHE:CD2	3:G:56:TYR:HB3	2.40	0.49
3:G:282:PHE:C	3:G:293:GLY:HA2	2.32	0.49
4:H:935:VAL:C	4:H:936:HIS:CD2	2.86	0.49
2:B:250:ILE:CD1	4:H:934:ASP:CG	2.81	0.49
1:A:310:GLU:HA	1:A:313:THR:HG22	1.95	0.49
1:A:123:ARG:CZ	1:A:123:ARG:CB	2.87	0.49
1:C:284:ASN:O	1:C:288:ASP:CB	2.60	0.49
2:B:300:GLU:HG3	1:C:313:THR:HG23	1.95	0.49
4:H:935:VAL:C	4:H:936:HIS:CG	2.85	0.49
1:A:210:ALA:C	5:X:17:UNK:C	2.79	0.49
2:B:250:ILE:HG21	4:H:934:ASP:OD2	2.13	0.49
2:B:370:ILE:HG21	2:B:399:LEU:HD21	1.95	0.49
1:C:205:ARG:HG2	1:C:205:ARG:HH11	1.77	0.49
1:E:336:CYS:HG	2:F:340:TYR:HH	1.57	0.49
1:A:49:CYS:HA	1:A:52:ILE:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:261:PHE:CD1	2:D:261:PHE:C	2.85	0.48
3:G:149:ASP:HB3	3:G:156:HIS:HB2	1.95	0.48
4:H:2062:VAL:O	4:H:2113:CYS:HA	2.13	0.48
2:F:124:ARG:HB3	2:F:244:LEU:HD23	1.95	0.48
2:F:144:GLU:C	2:F:145:ILE:HG13	2.33	0.48
3:G:175:VAL:HA	3:G:179:LEU:HD12	1.95	0.48
1:A:161:LEU:O	1:A:167:THR:HA	2.12	0.48
2:B:279:LYS:HD3	4:H:933:THR:HB	1.95	0.48
2:B:199:THR:N	4:H:1998:TRP:CZ2	2.82	0.48
3:G:66:VAL:HG22	5:X:1:UNK:O	2.13	0.48
4:H:1961:PHE:CB	4:H:1962:PRO:CD	2.90	0.48
1:E:332:ASN:ND2	2:F:349:ASP:OD1	2.46	0.48
4:H:936:HIS:O	4:H:940:ARG:NH2	2.46	0.48
1:A:133:GLY:HA2	1:A:161:LEU:HD21	1.96	0.48
2:B:351:LEU:HD22	2:B:356:ILE:HD11	1.95	0.48
4:H:1980:MET:N	4:H:1981:PRO:CD	2.75	0.48
4:H:973:VAL:HG11	4:H:1913:ALA:HB2	1.96	0.48
4:H:2012:SER:HA	4:H:2015:TRP:HD1	1.79	0.48
4:H:951:LEU:HA	4:H:954:ARG:NE	2.29	0.47
1:C:134:GLU:CB	1:C:205:ARG:HH12	2.24	0.47
1:C:286:TYR:CA	1:C:288:ASP:OD1	2.55	0.47
2:F:41:GLN:O	2:F:369:GLN:NE2	2.47	0.47
1:A:129:GLU:OE1	1:A:229:HIS:NE2	2.47	0.47
1:A:135:VAL:HG12	1:A:162:LYS:HD2	1.96	0.47
1:A:123:ARG:NH1	1:A:123:ARG:CG	2.73	0.47
1:A:210:ALA:CA	5:X:17:UNK:CA	2.63	0.47
1:E:309:ILE:HA	1:E:312:PHE:HD2	1.79	0.47
2:B:232:LEU:C	2:B:234:LYS:H	2.17	0.47
3:G:294:ILE:O	3:G:294:ILE:HG12	2.15	0.47
1:A:66:VAL:O	1:A:329:PHE:N	2.46	0.47
1:A:411:THR:HG21	2:B:68:ILE:HD13	1.95	0.47
1:C:132:GLU:HG2	1:C:190:VAL:HG12	1.95	0.47
1:E:42:GLN:HE22	1:E:364:MET:H	1.62	0.47
3:G:283:ASN:OD1	3:G:292:MET:CA	2.63	0.47
2:B:170:THR:HB	5:X:29:UNK:O	2.14	0.47
2:D:177:LYS:HE3	2:D:199:THR:HG21	1.97	0.47
4:H:937:PRO:C	4:H:938:LEU:HG	2.35	0.47
4:H:951:LEU:HD12	4:H:958:TYR:CE2	2.49	0.47
1:C:115:ASN:HA	1:C:118:ARG:HG2	1.96	0.47
3:G:30:PHE:CD2	3:G:47:GLU:HG3	2.45	0.47
4:H:852:LYS:HE2	4:H:2160:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:2032:PHE:CE1	4:H:2033:PRO:HD2	2.41	0.47
1:C:68:LEU:HD13	1:C:76:LYS:HB2	1.97	0.47
1:E:336:CYS:SG	1:E:337:VAL:N	2.88	0.47
3:G:96:THR:HB	3:G:127:ALA:HB2	1.97	0.47
3:G:306:PRO:CG	3:G:309:MET:CB	2.84	0.47
4:H:943:MET:H	4:H:943:MET:HE2	1.79	0.47
1:C:32:ALA:HB3	1:C:43:GLU:HG3	1.96	0.46
2:F:140:GLY:HA3	2:F:163:LEU:HD11	1.97	0.46
4:H:941:ILE:HD13	4:H:941:ILE:N	2.28	0.46
1:C:123:ARG:O	1:C:292:ALA:HA	2.16	0.46
3:G:238:LEU:CD1	3:G:268:LEU:HG	2.41	0.46
4:H:2024:ILE:HG22	4:H:2024:ILE:O	2.15	0.46
4:H:2022:HIS:CE1	4:H:2024:ILE:HD11	2.50	0.46
2:B:407:THR:OG1	1:C:64:ARG:NH2	2.48	0.46
2:D:251:ASN:ND2	2:D:267:GLU:C	2.66	0.46
3:G:20:GLU:HG3	3:G:21:ASN:H	1.80	0.46
1:C:120:ILE:HD11	1:C:325:PRO:HD3	1.98	0.46
2:B:108:ILE:HD11	2:B:304:LEU:HD11	1.97	0.46
2:B:233:GLN:NE2	2:B:233:GLN:N	2.60	0.46
1:C:274:LYS:HD2	1:C:278:GLU:HB3	1.98	0.46
1:A:312:PHE:O	1:A:316:HIS:ND1	2.49	0.46
1:A:134:GLU:CA	1:A:161:LEU:HD23	2.44	0.46
1:C:191:ILE:HG22	1:C:202:ARG:HH21	1.80	0.46
3:G:210:CYS:HA	3:G:274:ARG:HB2	1.97	0.46
4:H:2027:ASN:C	4:H:2029:ARG:N	2.64	0.46
1:C:247:ASN:ND2	1:C:274:LYS:HG2	2.31	0.46
3:G:379:ARG:C	3:G:381:ASP:N	2.50	0.46
4:H:1963:GLN:NE2	4:H:1967:ASP:OD2	2.48	0.46
1:A:135:VAL:CG1	1:A:162:LYS:HD2	2.46	0.46
2:B:137:ILE:CD1	2:B:236:LYS:HD3	2.29	0.46
1:C:128:LYS:NZ	4:H:915:PRO:O	2.48	0.46
1:A:223:LEU:HD12	1:A:224:PRO:HD2	1.98	0.45
1:A:304:VAL:HG21	1:A:329:PHE:HB3	1.98	0.45
3:G:12:ASN:HD22	3:G:14:LYS:HE3	1.81	0.45
3:G:306:PRO:C	3:G:309:MET:CA	2.82	0.45
2:B:142:VAL:HG21	2:B:193:ILE:HD12	1.98	0.45
1:C:191:ILE:HB	1:C:200:VAL:HA	1.98	0.45
1:A:134:GLU:CB	1:A:161:LEU:N	2.69	0.45
2:D:296:LEU:O	2:D:324:LEU:HA	2.16	0.45
1:E:120:ILE:HD11	1:E:325:PRO:HD3	1.98	0.45
2:F:306:ILE:HA	2:F:309:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLU:CD	1:A:156:HIS:CB	2.85	0.45
1:A:159:ILE:HD12	1:A:172:LEU:HD12	1.89	0.45
2:D:280:VAL:CG1	2:D:291:ILE:HD11	2.45	0.45
1:E:66:VAL:O	1:E:329:PHE:N	2.45	0.45
2:F:126:SER:HB3	2:F:294:GLY:HA3	1.99	0.45
2:F:142:VAL:HG23	2:F:189:ALA:HA	1.98	0.45
1:A:123:ARG:HD3	1:A:235:ILE:HG23	1.97	0.45
1:A:212:GLU:OE1	5:X:20:UNK:HA	2.16	0.45
2:B:198:ALA:CB	4:H:1998:TRP:CG	2.99	0.45
2:B:382:MET:HG2	2:B:421:VAL:HB	1.99	0.45
1:C:247:ASN:ND2	1:C:274:LYS:CG	2.80	0.45
1:C:274:LYS:HZ2	4:H:921:ILE:HG21	1.81	0.45
2:D:142:VAL:HG11	2:D:193:ILE:HD12	1.97	0.45
2:D:428:ARG:NH1	1:E:47:GLU:OE1	2.50	0.45
3:G:66:VAL:CG2	5:X:1:UNK:O	2.65	0.45
1:A:183:GLU:HB3	1:A:201:LYS:HE2	1.99	0.45
4:H:2028:MET:H	4:H:2028:MET:HG2	1.49	0.45
2:B:199:THR:N	4:H:1998:TRP:HZ2	2.14	0.45
2:B:301:VAL:HG21	2:B:326:MET:HB2	1.98	0.45
1:C:282:VAL:HG11	4:H:921:ILE:HG23	1.99	0.45
1:A:68:LEU:HD13	1:A:76:LYS:HB2	1.99	0.45
3:G:45:ILE:HD12	3:G:46:ASP:N	2.31	0.45
4:H:935:VAL:O	4:H:936:HIS:CG	2.70	0.45
1:A:124:ILE:CG2	1:A:291:ILE:C	2.73	0.45
1:A:430:VAL:HA	1:A:433:ILE:HG22	1.98	0.45
1:C:134:GLU:CB	1:C:205:ARG:NH1	2.76	0.45
2:D:247:ILE:CG2	2:D:272:VAL:CG1	2.95	0.45
2:F:258:LEU:HD22	2:F:263:GLY:HA2	1.99	0.45
2:F:401:TYR:OH	2:F:433:PHE:O	2.34	0.45
1:A:282:VAL:HG21	4:H:945:ARG:HE	1.82	0.44
1:E:33:LYS:O	1:E:46:ARG:NH2	2.39	0.44
3:G:29:GLN:HG2	3:G:74:VAL:HG22	1.97	0.44
4:H:2027:ASN:O	4:H:2027:ASN:ND2	2.50	0.44
2:D:328:THR:HG21	2:D:344:HIS:HB3	1.99	0.44
2:D:390:LEU:HD21	2:D:406:ILE:HD11	1.97	0.44
2:F:246:GLU:HA	2:F:249:VAL:HG12	1.98	0.44
1:A:137:GLU:HB3	1:A:159:ILE:HG23	2.00	0.44
2:B:136:GLU:HA	2:B:234:LYS:O	2.17	0.44
2:D:255:GLN:OE1	4:H:1979:VAL:HB	2.16	0.44
3:G:30:PHE:CE1	3:G:56:TYR:CG	3.03	0.44
1:A:164:ALA:CB	1:A:223:LEU:CD2	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:ASP:HB3	1:E:33:LYS:HZ3	1.83	0.44
1:C:191:ILE:CG2	1:C:202:ARG:NH2	2.80	0.44
2:D:256:GLY:HA3	4:H:1975:ARG:HE	1.82	0.44
1:E:126:GLU:CB	4:H:1964:GLN:CD	2.59	0.44
3:G:55:PHE:CD2	3:G:56:TYR:O	2.70	0.44
3:G:304:ASN:C	3:G:306:PRO:CD	2.85	0.44
3:G:45:ILE:CB	3:G:49:LYS:CE	2.86	0.44
2:D:106:SER:HA	2:D:109:PHE:HD2	1.83	0.44
1:E:126:GLU:OE1	4:H:1964:GLN:HG3	2.17	0.44
3:G:30:PHE:CE1	3:G:56:TYR:CD2	2.99	0.44
3:G:232:VAL:HG13	3:G:274:ARG:HH22	1.83	0.44
1:A:39:LEU:O	1:A:46:ARG:NH2	2.51	0.44
1:C:346:SER:OG	1:C:350:ILE:O	2.35	0.44
3:G:238:LEU:H	3:G:267:ILE:HG22	1.82	0.44
3:G:267:ILE:C	3:G:267:ILE:CD1	2.86	0.44
3:G:292:MET:CG	5:X:16:UNK:CB	2.95	0.44
4:H:942:ASP:OD1	4:H:942:ASP:N	2.51	0.44
1:A:159:ILE:HD11	1:A:180:LEU:HD11	2.00	0.43
1:E:161:LEU:HD12	1:E:228:VAL:HG12	2.00	0.43
2:F:144:GLU:C	2:F:145:ILE:CG1	2.85	0.43
3:G:193:LEU:HB3	3:G:195:VAL:HG22	1.99	0.43
3:G:235:ASP:CB	3:G:267:ILE:HG13	2.47	0.43
4:H:934:ASP:C	4:H:935:VAL:CG2	2.85	0.43
1:A:159:ILE:CD1	1:A:172:LEU:CD1	2.72	0.43
2:D:140:GLY:HA3	2:D:165:THR:HG22	2.01	0.43
2:D:247:ILE:HG21	2:D:273:ARG:HD2	1.99	0.43
1:E:105:GLU:HG2	2:F:265:THR:HG21	2.00	0.43
2:F:252:SER:HB2	2:F:258:LEU:HD12	1.99	0.43
4:H:1999:LEU:HD12	4:H:1999:LEU:O	2.18	0.43
1:A:134:GLU:C	1:A:205:ARG:HH11	2.21	0.43
1:C:247:ASN:HD21	1:C:274:LYS:CD	2.24	0.43
3:G:55:PHE:CE2	3:G:56:TYR:O	2.71	0.43
3:G:283:ASN:HA	3:G:292:MET:C	2.38	0.43
5:X:49:UNK:O	5:X:51:UNK:N	2.51	0.43
2:B:247:ILE:O	2:B:251:ASN:HB2	2.19	0.43
3:G:33:LYS:H	3:G:54:LEU:HD22	1.60	0.43
1:A:282:VAL:CG2	4:H:945:ARG:NH1	2.82	0.43
2:B:283:TRP:HE1	4:H:933:THR:HG22	1.83	0.43
3:G:45:ILE:CB	3:G:49:LYS:HE3	2.48	0.43
2:B:134:GLU:CA	2:B:236:LYS:O	2.59	0.43
2:B:246:GLU:OE2	4:H:933:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:304:ASN:ND2	3:G:313:PHE:CZ	2.86	0.43
1:A:275:LEU:HD13	2:F:260:LEU:HD22	2.00	0.43
1:C:131:TYR:HB3	1:C:161:LEU:HD13	2.01	0.43
4:H:965:PRO:HA	4:H:968:ARG:HB2	2.00	0.43
1:A:131:TYR:CE1	1:A:170:LEU:CD2	3.01	0.43
1:A:374:ILE:HA	1:A:377:ILE:HD12	2.00	0.43
2:F:108:ILE:HD13	2:F:119:LEU:HD13	2.01	0.43
3:G:45:ILE:HG21	3:G:49:LYS:HE3	2.00	0.43
4:H:852:LYS:HB2	4:H:2153:HIS:HE1	1.83	0.43
3:G:133:HIS:HB3	3:G:366:ILE:HD11	2.00	0.43
1:A:142:GLU:CD	1:A:156:HIS:HB2	2.39	0.43
1:A:214:ASP:HB3	1:A:215:LEU:H	1.68	0.42
1:E:118:ARG:HH22	2:F:269:LYS:HE3	1.84	0.42
1:E:313:THR:HA	1:E:316:HIS:CE1	2.54	0.42
3:G:267:ILE:HD12	3:G:269:ARG:N	2.33	0.42
2:D:370:ILE:HG21	2:D:399:LEU:HD21	1.99	0.42
3:G:42:ALA:HB1	3:G:47:GLU:OE1	2.19	0.42
3:G:354:ASN:O	3:G:356:ILE:N	2.48	0.42
1:A:415:LEU:HD23	2:B:58:VAL:HG13	2.01	0.42
2:D:235:ARG:HH21	4:H:2053:ARG:HH11	1.66	0.42
3:G:51:PRO:O	3:G:52:SER:OG	2.34	0.42
1:A:183:GLU:HG2	1:A:201:LYS:HB2	2.01	0.42
1:A:313:THR:HA	1:A:316:HIS:CE1	2.54	0.42
1:E:124:ILE:HD12	1:E:238:VAL:HG21	2.00	0.42
3:G:295:PRO:HB3	3:G:336:GLU:HB3	2.01	0.42
2:B:160:LYS:HA	2:B:173:ASP:HA	2.02	0.42
2:D:269:LYS:HD2	2:D:273:ARG:HD3	2.02	0.42
1:C:287:ILE:N	1:C:288:ASP:OD1	2.53	0.42
2:F:142:VAL:HG23	2:F:190:GLY:H	1.84	0.42
2:F:312:LEU:HA	2:F:315:ALA:HB3	2.01	0.42
3:G:30:PHE:HB3	3:G:55:PHE:O	2.20	0.42
3:G:236:TYR:O	3:G:237:VAL:HG23	2.19	0.42
4:H:919:PRO:HG2	4:H:1991:HIS:CE1	2.55	0.42
4:H:2173:GLU:HA	4:H:2176:ILE:HD12	2.02	0.42
5:X:48:UNK:C	5:X:50:UNK:N	2.82	0.42
1:E:240:LEU:HD23	1:E:243:LEU:HD12	2.01	0.42
3:G:30:PHE:CD2	3:G:56:TYR:CD2	3.01	0.42
4:H:2037:LEU:N	4:H:2037:LEU:CD2	2.73	0.42
1:A:168:LYS:CD	1:A:228:VAL:HG21	2.48	0.42
1:A:192:TYR:O	1:A:199:ALA:HA	2.20	0.42
1:A:271:ILE:HG22	1:A:273:ASP:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LYS:HD2	1:C:234:ILE:HD12	2.01	0.42
2:B:250:ILE:CD1	4:H:934:ASP:OD1	2.68	0.42
1:E:122:LEU:HB2	1:E:238:VAL:HB	2.01	0.42
2:F:142:VAL:HG13	2:F:191:ASP:O	2.20	0.42
2:B:365:LYS:HA	2:B:368:LYS:HE2	2.02	0.41
1:C:117:ARG:HH12	1:C:276:ARG:HD3	1.82	0.41
4:H:1961:PHE:H	4:H:1961:PHE:HD1	1.61	0.41
1:A:142:GLU:OE1	1:A:156:HIS:CB	2.68	0.41
2:D:284:ARG:NH1	2:D:290:GLU:O	2.52	0.41
1:E:134:GLU:HG2	1:E:162:LYS:HB2	2.02	0.41
3:G:5:VAL:HG11	3:G:360:TRP:HA	2.01	0.41
3:G:166:LYS:NZ	3:G:305:LEU:HG	2.35	0.41
3:G:236:TYR:CZ	3:G:268:LEU:O	2.70	0.41
3:G:238:LEU:CG	3:G:268:LEU:HG	2.50	0.41
4:H:1998:TRP:O	4:H:1998:TRP:CG	2.73	0.41
1:A:76:LYS:NZ	1:A:331:SER:O	2.53	0.41
1:C:191:ILE:CG2	1:C:202:ARG:HH21	2.33	0.41
2:F:145:ILE:N	2:F:145:ILE:CD1	2.73	0.41
3:G:282:PHE:O	3:G:293:GLY:HA3	2.17	0.41
2:B:99:PRO:HG2	2:B:128:GLY:HA3	2.02	0.41
2:B:262:SER:OG	2:B:263:GLY:N	2.53	0.41
2:D:284:ARG:NH2	2:D:291:ILE:HG21	2.35	0.41
1:A:54:GLU:HG2	2:F:411:LEU:HD22	2.02	0.41
2:B:63:ILE:HD13	2:B:295:VAL:HG22	2.02	0.41
2:D:300:GLU:H	2:D:327:ALA:HB3	1.85	0.41
2:D:404:GLN:HA	1:E:64:ARG:HH12	1.86	0.41
1:E:118:ARG:HH12	2:F:269:LYS:HB2	1.84	0.41
3:G:238:LEU:CB	3:G:268:LEU:HG	2.49	0.41
4:H:854:GLU:HG2	4:H:2163:ILE:HB	2.01	0.41
4:H:910:ARG:HH22	4:H:2037:LEU:H	1.68	0.41
1:A:162:LYS:HG2	1:A:167:THR:HG22	2.03	0.41
2:B:61:GLU:OE1	2:B:64:ARG:NH1	2.54	0.41
2:B:262:SER:H	1:C:271:ILE:HG13	0.91	0.41
2:B:148:ASP:HB3	2:B:149:ARG:H	1.68	0.41
1:E:186:GLU:HB3	1:E:189:ASP:HB3	2.03	0.41
1:E:372:LYS:HA	1:E:375:ILE:HG22	2.02	0.41
1:E:386:ILE:HG12	1:E:425:ILE:HD12	2.02	0.41
1:E:389:GLU:HB3	1:E:427:LYS:HD2	2.03	0.41
2:F:74:LEU:HD22	2:F:354:LEU:HD13	2.03	0.41
1:C:287:ILE:C	1:C:289:GLN:N	2.73	0.41
2:D:247:ILE:HG21	2:D:273:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLU:CB	1:A:160:GLY:N	2.72	0.41
1:A:188:GLY:O	1:A:205:ARG:CG	2.69	0.41
1:A:372:LYS:HD3	1:A:392:ASN:HA	2.02	0.41
2:D:261:PHE:HA	1:E:271:ILE:H	1.86	0.41
2:F:163:LEU:HB3	2:F:165:THR:HB	2.03	0.41
3:G:30:PHE:HD2	3:G:47:GLU:HG3	1.85	0.41
3:G:361:GLU:HA	3:G:364:LYS:HE2	2.03	0.41
4:H:950:GLY:CA	4:H:1936:ILE:HG12	2.51	0.41
1:A:41:GLY:HA3	1:A:366:TYR:HE1	1.85	0.41
1:E:26:LEU:HB3	1:E:30:GLY:HA2	2.03	0.41
3:G:236:TYR:CD1	3:G:267:ILE:CG1	3.03	0.41
4:H:928:LEU:CD1	4:H:2000:ALA:CB	2.56	0.41
4:H:1984:GLU:HG3	4:H:1985:ALA:H	1.85	0.41
1:C:202:ARG:NE	1:C:202:ARG:HA	2.36	0.40
1:E:33:LYS:HB3	1:E:36:ALA:HB2	2.03	0.40
3:G:46:ASP:C	3:G:48:ILE:N	2.73	0.40
3:G:47:GLU:O	3:G:48:ILE:HG12	2.21	0.40
2:B:310:SER:HA	2:B:313:ASN:HD22	1.86	0.40
2:D:288:LYS:O	2:D:288:LYS:HG2	2.21	0.40
4:H:2076:GLU:OE2	4:H:2088:ARG:NE	2.54	0.40
2:D:285:GLU:C	2:D:287:GLY:N	2.73	0.40
2:D:295:VAL:HA	2:D:323:VAL:HG23	2.04	0.40
1:E:130:VAL:HB	1:E:230:LYS:HB2	2.04	0.40
2:F:143:VAL:HG21	2:F:163:LEU:C	2.35	0.40
3:G:236:TYR:CD1	3:G:267:ILE:HD13	2.48	0.40
1:A:112:LEU:HD23	1:A:314:TYR:HD2	1.86	0.40
1:A:134:GLU:CG	1:A:162:LYS:HG3	2.51	0.40
3:G:236:TYR:N	3:G:236:TYR:CD1	2.88	0.40
3:G:305:LEU:C	3:G:307:GLU:N	2.73	0.40
1:A:279:ILE:HD12	4:H:945:ARG:HH12	1.55	0.40
1:C:244:ASP:OD2	1:C:275:LEU:HD13	2.18	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/456 (88%)	365 (92%)	29 (7%)	5 (1%)	12	48
1	C	358/456 (78%)	330 (92%)	25 (7%)	3 (1%)	19	58
1	E	372/456 (82%)	346 (93%)	26 (7%)	0	100	100
2	B	390/463 (84%)	370 (95%)	20 (5%)	0	100	100
2	D	388/463 (84%)	370 (95%)	13 (3%)	5 (1%)	12	48
2	F	356/463 (77%)	330 (93%)	24 (7%)	2 (1%)	25	63
3	G	362/396 (91%)	311 (86%)	42 (12%)	9 (2%)	5	35
4	H	363/3230 (11%)	316 (87%)	38 (10%)	9 (2%)	5	35
All	All	2988/6383 (47%)	2738 (92%)	217 (7%)	33 (1%)	18	51

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	SER
1	A	176	ILE
1	C	288	ASP
1	C	291	ILE
2	D	286	GLU
2	D	287	GLY
2	D	291	ILE
2	F	145	ILE
3	G	47	GLU
3	G	48	ILE
3	G	50	ASP
3	G	380	GLU
4	H	937	PRO
4	H	1962	PRO
4	H	2000	ALA
4	H	2028	MET
1	A	128	LYS
3	G	379	ARG
4	H	935	VAL
4	H	2029	ARG
1	A	206	CYS
2	F	143	VAL
3	G	51	PRO
4	H	2004	ALA

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Mol	Chain	Res	Type
2	D	268	ILE
2	D	285	GLU
3	G	294	ILE
4	H	1980	MET
3	G	52	SER
1	C	290	GLY
3	G	237	VAL
4	H	1963	GLN
1	A	135	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/387 (89%)	334 (97%)	9 (3%)	46	67
1	C	314/387 (81%)	308 (98%)	6 (2%)	57	75
1	E	325/387 (84%)	325 (100%)	0	100	100
2	B	337/390 (86%)	334 (99%)	3 (1%)	78	88
2	D	334/390 (86%)	326 (98%)	8 (2%)	49	69
2	F	309/390 (79%)	305 (99%)	4 (1%)	69	82
3	G	334/361 (92%)	316 (95%)	18 (5%)	22	50
4	H	333/2721 (12%)	304 (91%)	29 (9%)	10	35
All	All	2629/5413 (49%)	2552 (97%)	77 (3%)	45	65

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	124	ILE
1	A	125	LYS
1	A	172	LEU
1	A	173	ASP
1	A	205	ARG

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Mol	Chain	Res	Type
1	A	206	CYS
1	A	207	ASP
1	A	208	THR
2	B	233	GLN
2	B	234	LYS
2	B	235	ARG
1	C	17	SER
1	C	189	ASP
1	C	201	LYS
1	C	202	ARG
1	C	288	ASP
1	C	289	GLN
2	D	233	GLN
2	D	267	GLU
2	D	268	ILE
2	D	269	LYS
2	D	270	SER
2	D	284	ARG
2	D	285	GLU
2	D	290	GLU
2	F	21	ARG
2	F	29	ARG
2	F	144	GLU
2	F	145	ILE
3	G	21	ASN
3	G	45	ILE
3	G	48	ILE
3	G	49	LYS
3	G	54	LEU
3	G	56	TYR
3	G	165	LYS
3	G	236	TYR
3	G	238	LEU
3	G	269	ARG
3	G	270	LEU
3	G	290	GLN
3	G	291	GLU
3	G	292	MET
3	G	294	ILE
3	G	304	ASN
3	G	305	LEU
3	G	380	GLU

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Mol	Chain	Res	Type
4	H	934	ASP
4	H	935	VAL
4	H	936	HIS
4	H	938	LEU
4	H	940	ARG
4	H	941	ILE
4	H	942	ASP
4	H	943	MET
4	H	945	ARG
4	H	946	PHE
4	H	948	LEU
4	H	949	ILE
4	H	951	LEU
4	H	952	GLU
4	H	1939	ARG
4	H	1961	PHE
4	H	1963	GLN
4	H	1978	PHE
4	H	1999	LEU
4	H	2002	ARG
4	H	2003	GLN
4	H	2006	PHE
4	H	2023	ARG
4	H	2025	VAL
4	H	2026	CYS
4	H	2027	ASN
4	H	2028	MET
4	H	2032	PHE
4	H	2037	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	233	GLN
2	B	275	GLN
2	B	313	ASN
2	B	344	HIS
1	C	247	ASN
2	D	245	HIS
1	E	42	GLN
1	E	229	HIS
2	F	49	GLN

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Mol	Chain	Res	Type
2	F	146	GLN
2	F	447	GLN
3	G	21	ASN
3	G	156	HIS
4	H	865	GLN
4	H	903	HIS
4	H	936	HIS
4	H	1964	GLN
4	H	1991	HIS
4	H	2022	HIS
4	H	2153	HIS

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

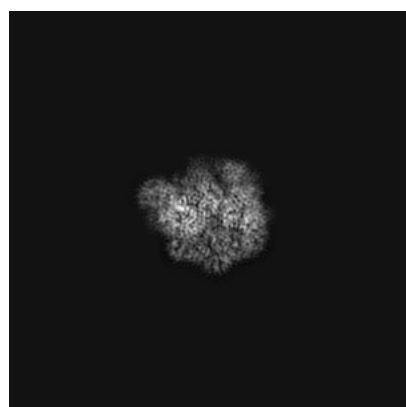
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9668. These allow visual inspection of the internal detail of the map and identification of artifacts.

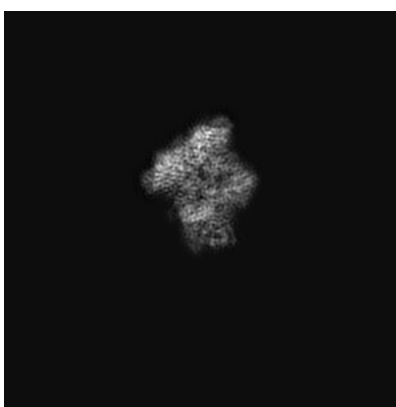
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

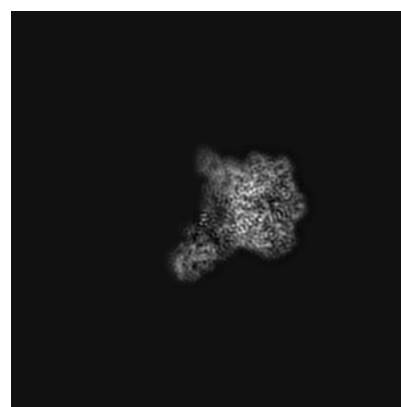
#### 6.1.1 Primary map



X



Y

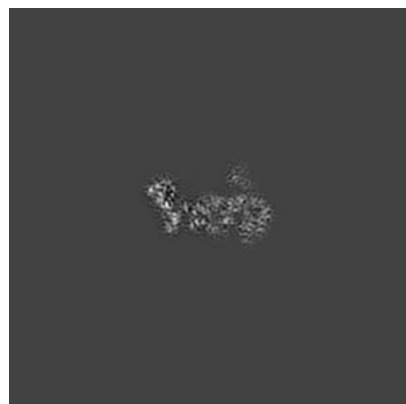


Z

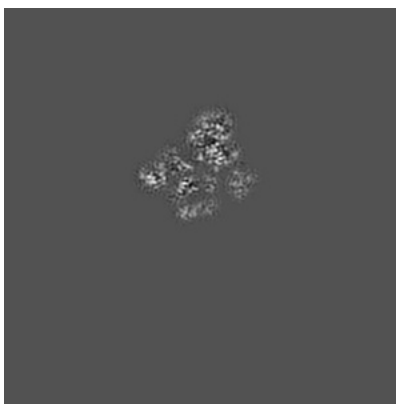
The images above show the map projected in three orthogonal directions.

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

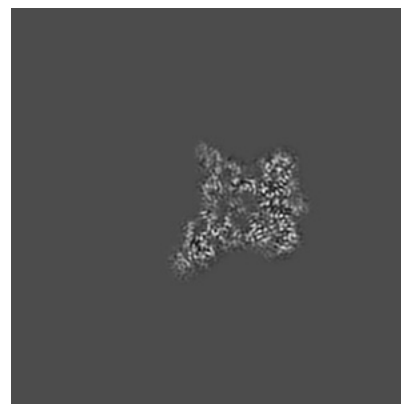
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

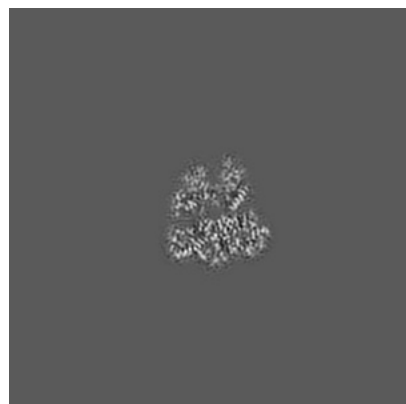


Z Index: 160

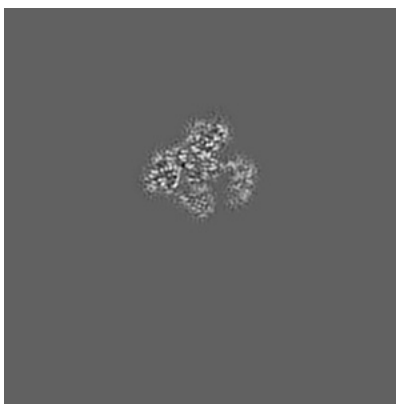
The images above show central slices of the map in three orthogonal directions.

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

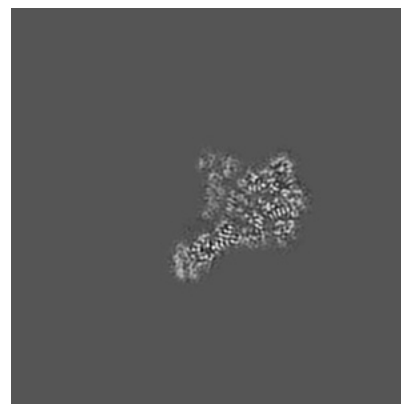
### 6.3.1 Primary map



X Index: 193



Y Index: 175

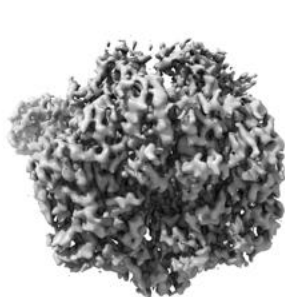


Z Index: 166

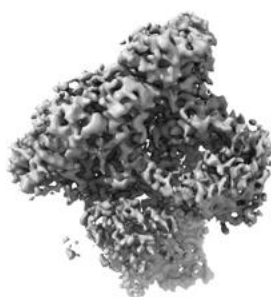
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.058. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

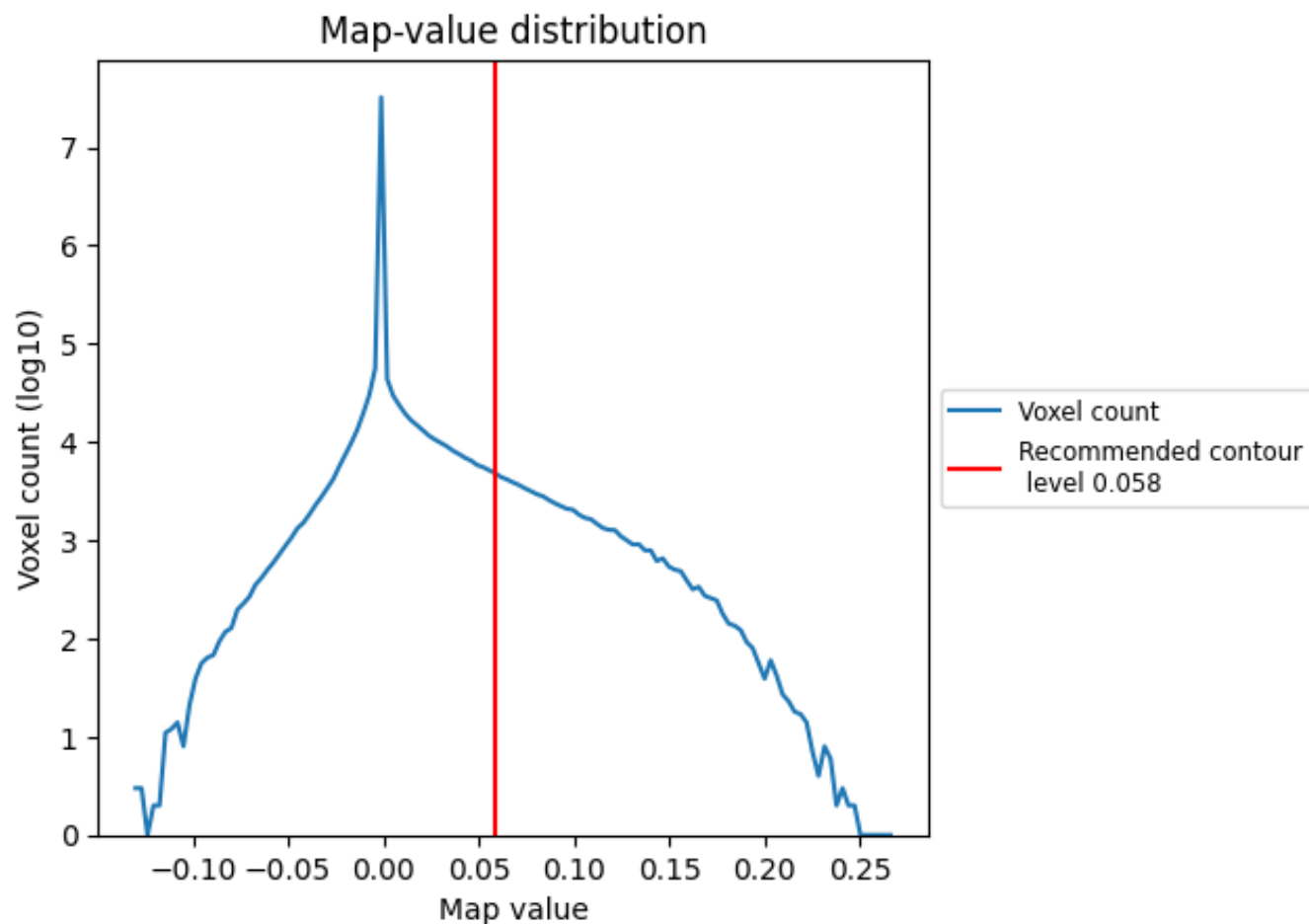
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

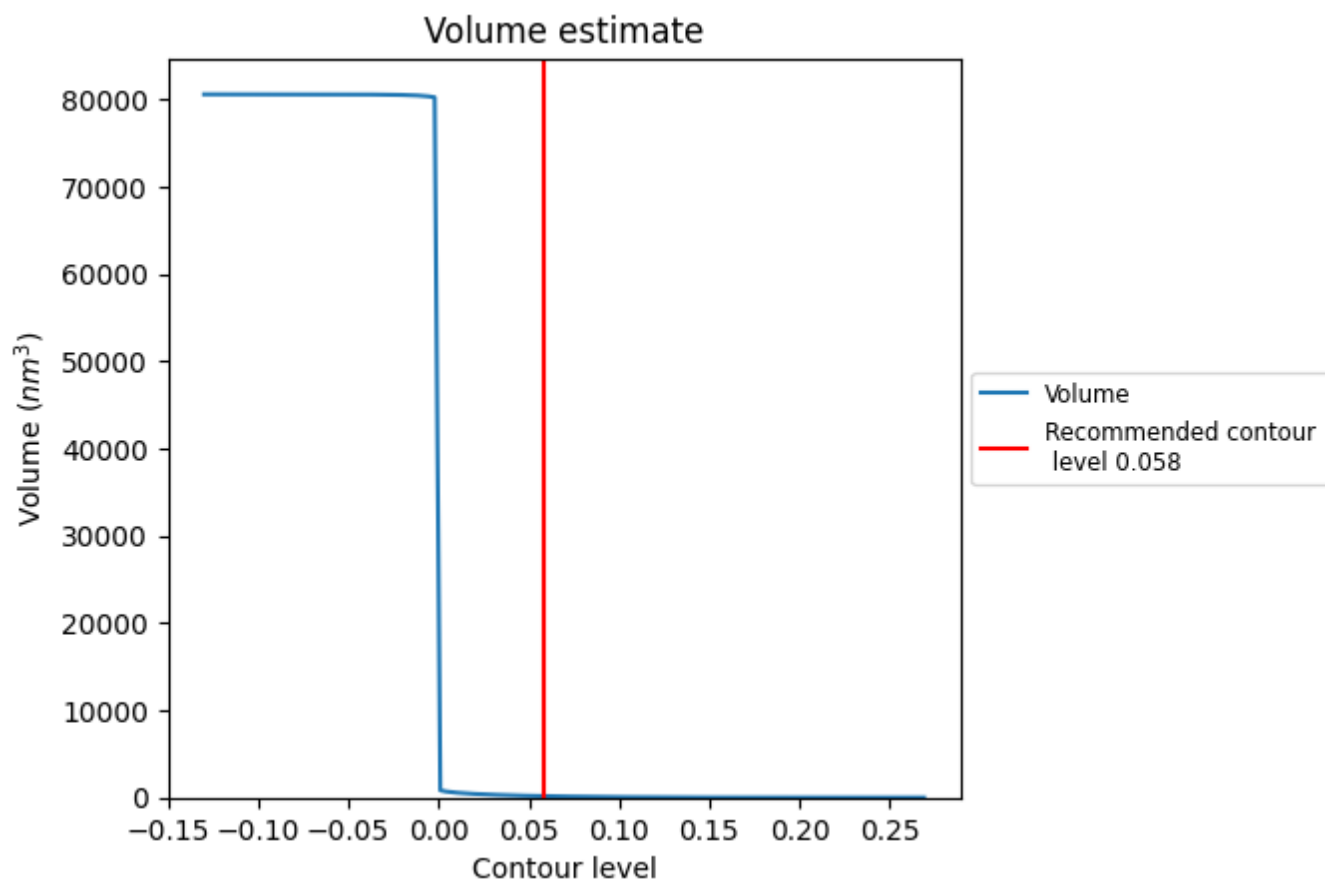
### 7.1 Map-value distribution [i](#)



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



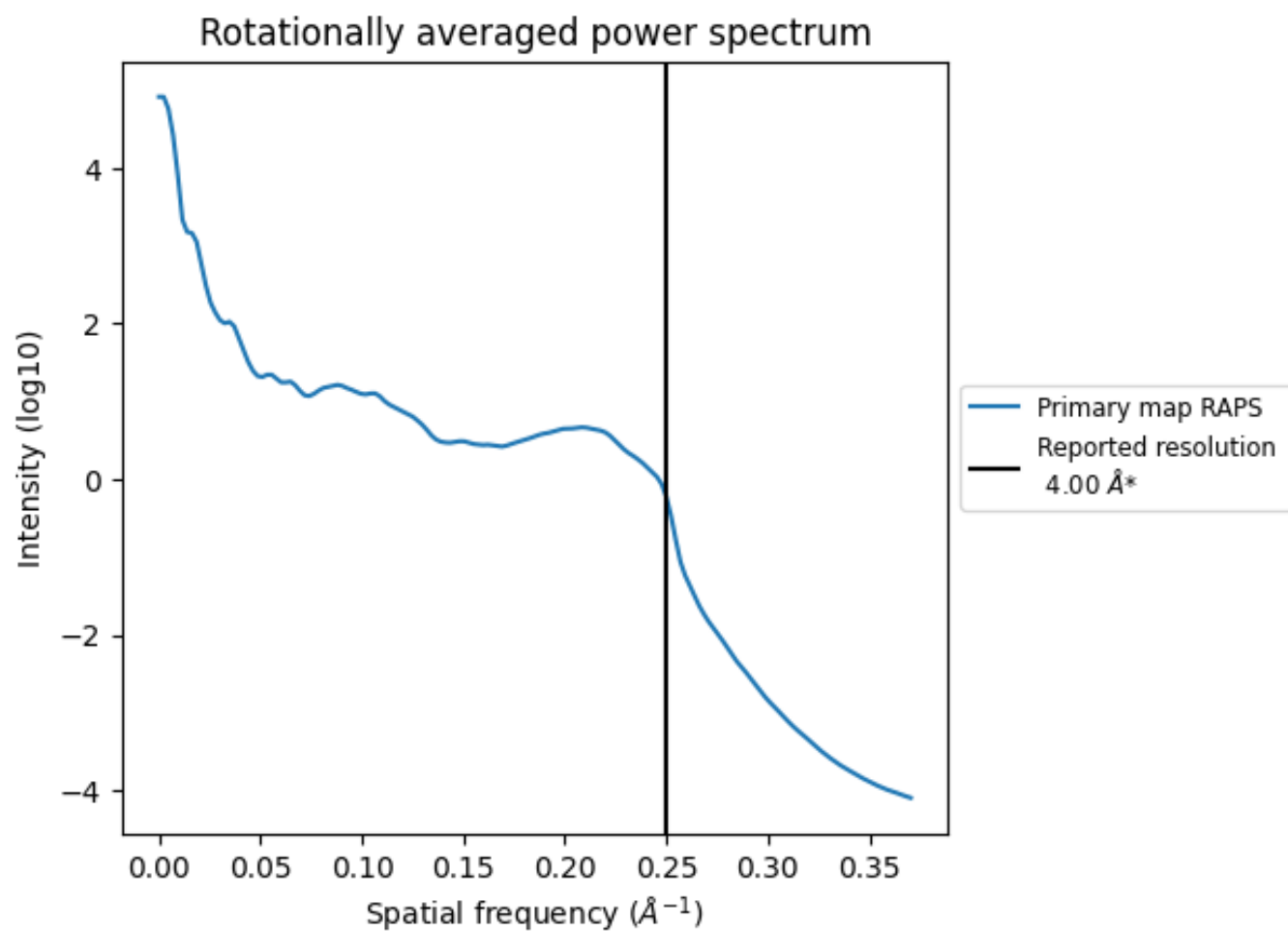
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165  $\text{nm}^3$ ; this corresponds to an approximate mass of 149 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 0.250 Å<sup>-1</sup>

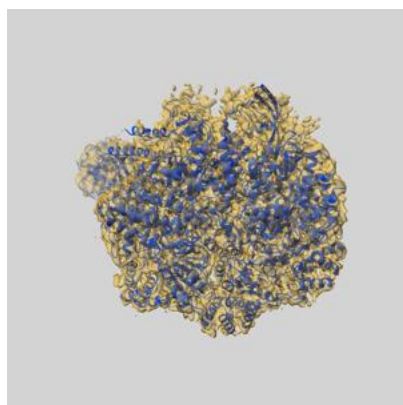
## 8 Fourier-Shell correlation

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

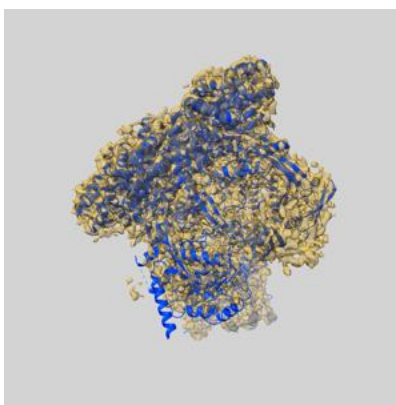
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9668 and PDB model 6IGM. Per-residue inclusion information can be found in section 3 on page 6.

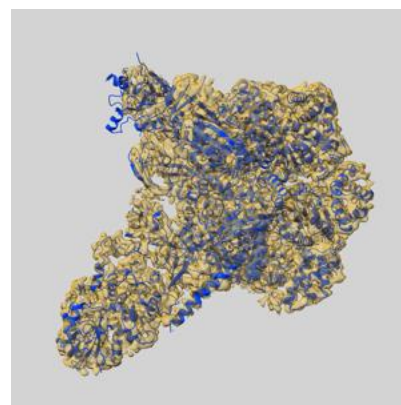
### 9.1 Map-model overlay [i](#)



X



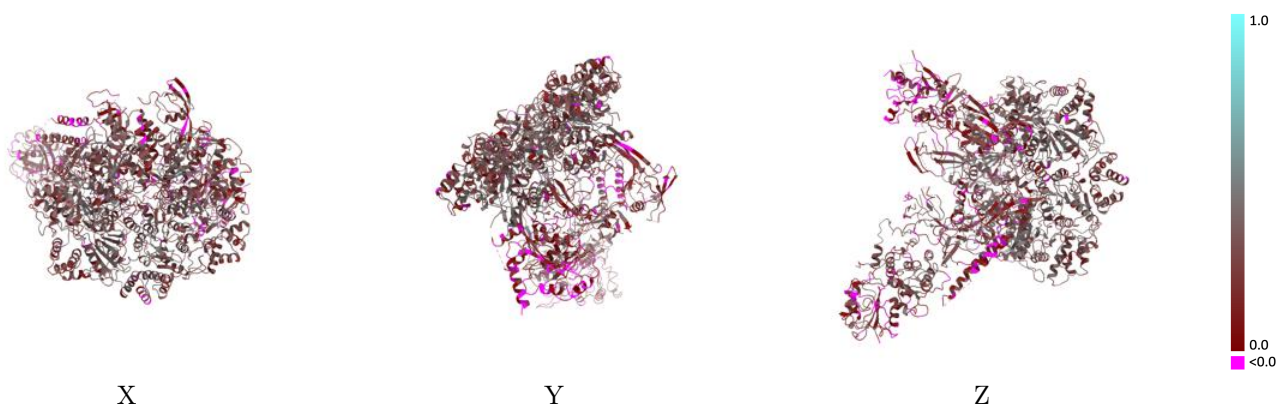
Y



Z

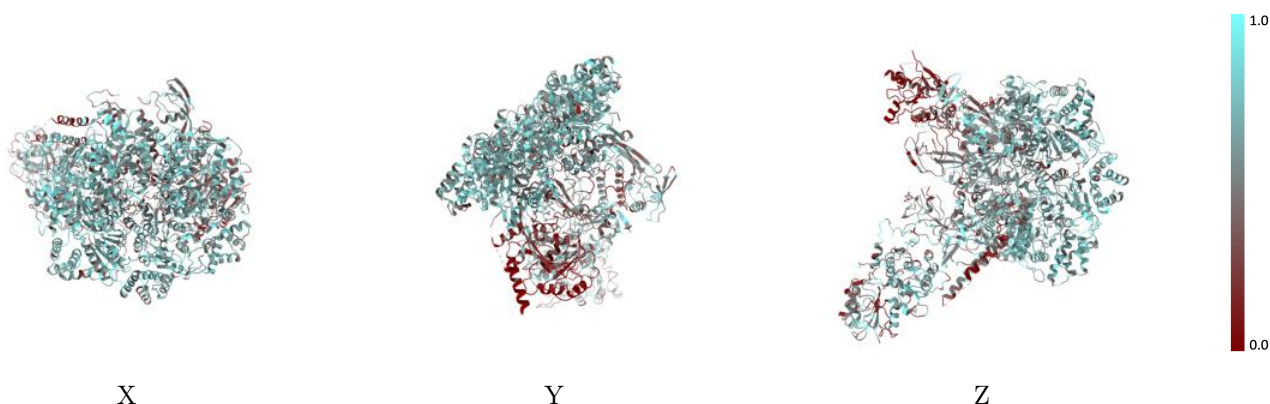
The images above show the 3D surface view of the map at the recommended contour level 0.058 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



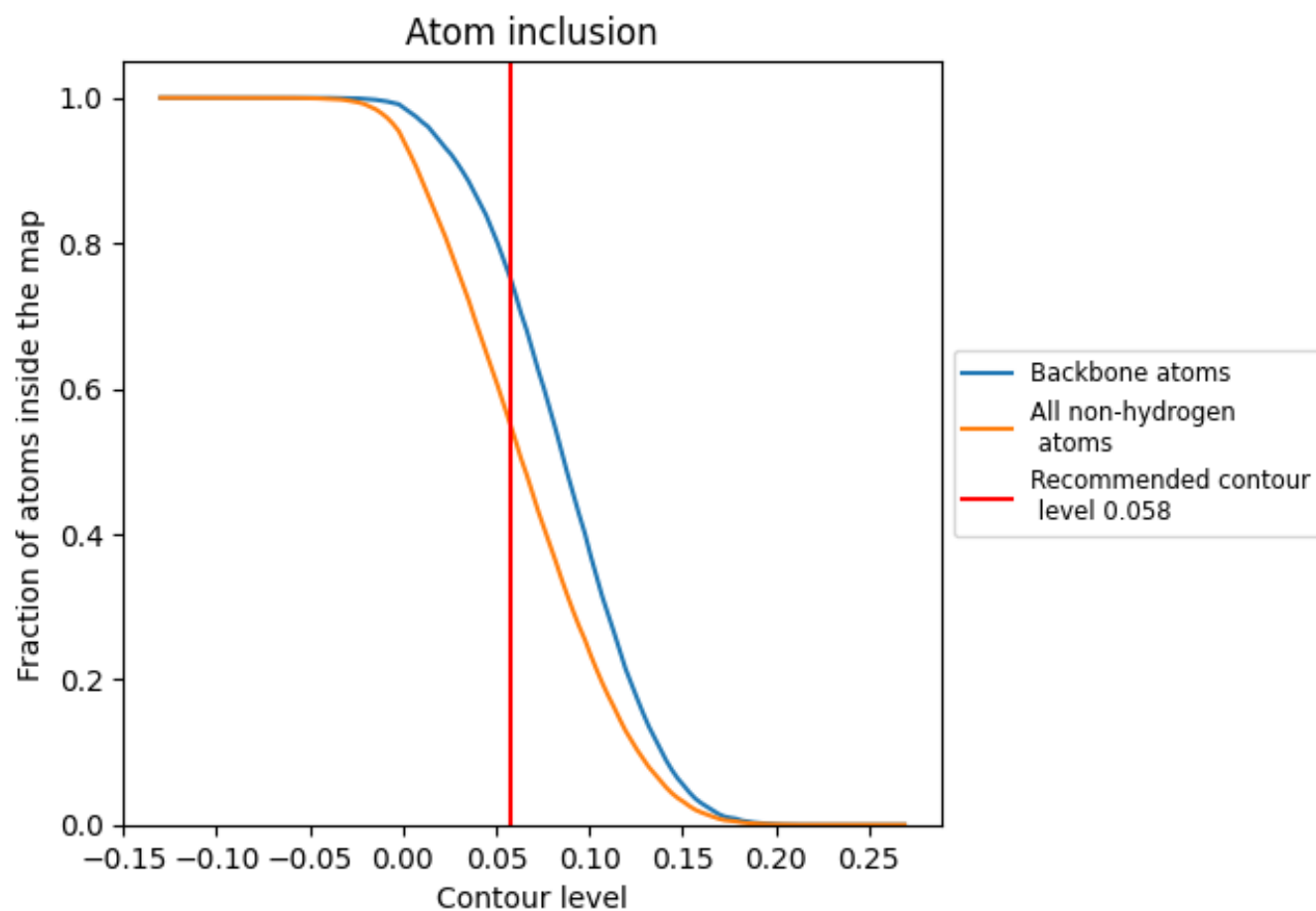
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.058).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 55% 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 (0.058) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.5478</div>	<div><div></div>0.2530</div>
A	<div><div></div>0.6250</div>	<div><div></div>0.2990</div>
B	<div><div></div>0.5964</div>	<div><div></div>0.2870</div>
C	<div><div></div>0.5836</div>	<div><div></div>0.2840</div>
D	<div><div></div>0.5852</div>	<div><div></div>0.2860</div>
E	<div><div></div>0.6044</div>	<div><div></div>0.2760</div>
F	<div><div></div>0.6132</div>	<div><div></div>0.2770</div>
G	<div><div></div>0.4932</div>	<div><div></div>0.1930</div>
H	<div><div></div>0.2667</div>	<div><div></div>0.1140</div>
X	<div><div></div>0.6903</div>	<div><div></div>0.3310</div>

1.0

0.0

<0.0