



Full wwPDB EM Validation Report ⓘ

Feb 27, 2025 – 06:11 PM JST

PDB ID : 8YGF
EMDB ID : EMD-39246
Title : The tetramer Structure of SPR-DSR2 complex
Authors : Gao, X.; Zhu, H.; Cui, S.
Deposited on : 2024-02-26
Resolution : 4.66 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

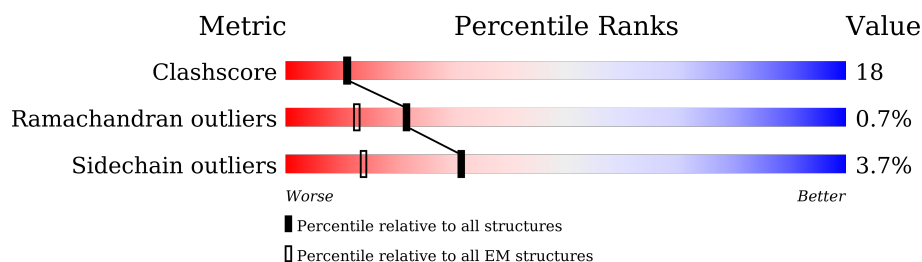
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.66 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1005	<div> <div>8%</div> <div>58%</div> <div>37%</div> <div>..</div> </div>
1	B	1005	<div> <div>8%</div> <div>63%</div> <div>33%</div> <div>..</div> </div>
1	E	1005	<div> <div>8%</div> <div>60%</div> <div>35%</div> <div>..</div> </div>
1	F	1005	<div> <div>8%</div> <div>60%</div> <div>35%</div> <div>..</div> </div>
2	C	264	<div> <div>13%</div> <div>34%</div> <div>21%</div> <div>43%</div> </div>
2	D	264	<div> <div>17%</div> <div>29%</div> <div>26%</div> <div>43%</div> </div>
2	G	264	<div> <div>16%</div> <div>34%</div> <div>21%</div> <div>43%</div> </div>
2	H	264	<div> <div>20%</div> <div>31%</div> <div>23%</div> <div>43%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 37524 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 SIR2-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	983	Total	C	N	O	S	0	0
			8183	5292	1322	1538	31		
1	B	983	Total	C	N	O	S	0	0
			8183	5292	1322	1538	31		
1	E	983	Total	C	N	O	S	0	0
			8183	5292	1322	1538	31		
1	F	983	Total	C	N	O	S	0	0
			8183	5292	1322	1538	31		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	HIS	engineered mutation	UNP D4G637
B	171	ALA	HIS	engineered mutation	UNP D4G637
E	171	ALA	HIS	engineered mutation	UNP D4G637
F	171	ALA	HIS	engineered mutation	UNP D4G637

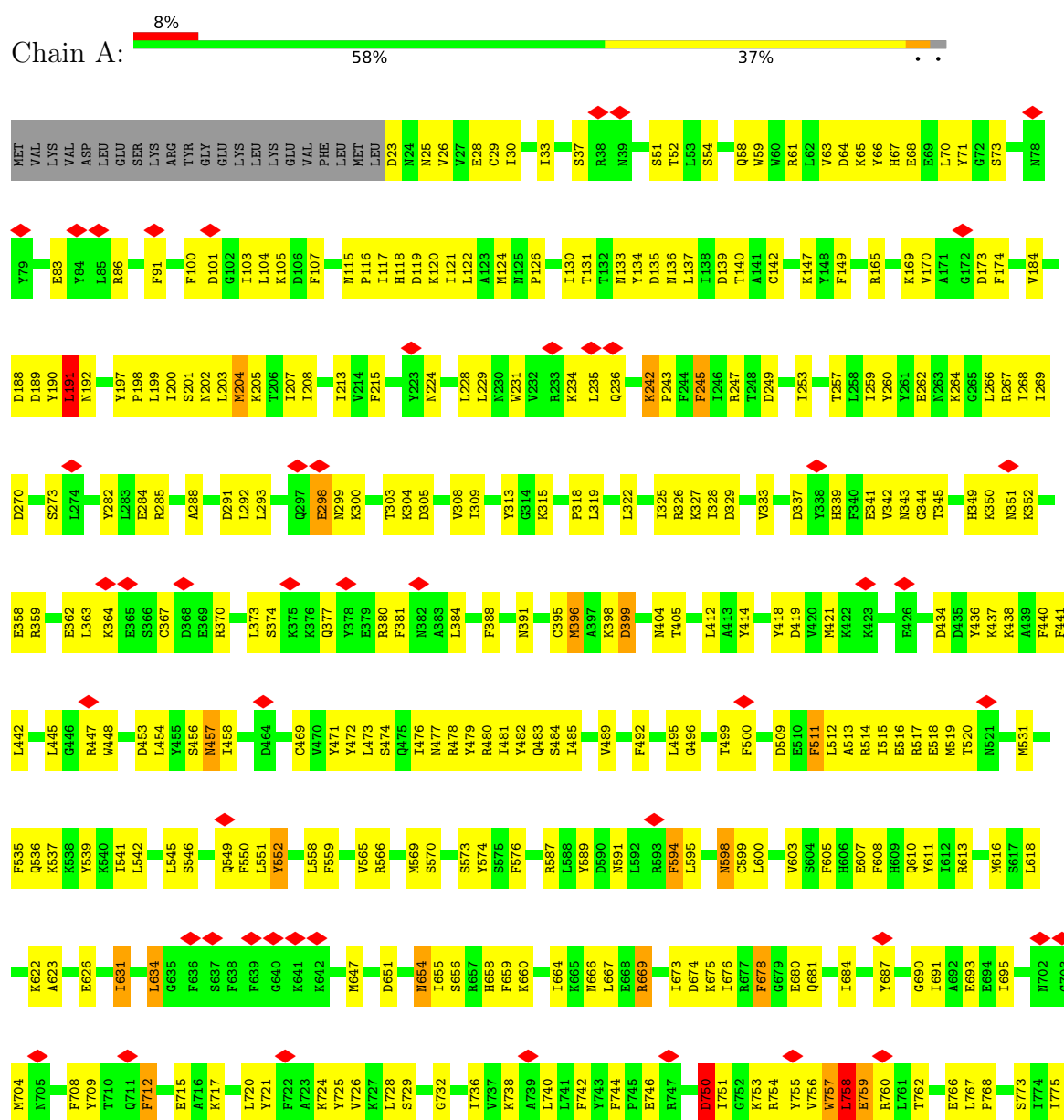
- Molecule 2 is a protein called SPR.

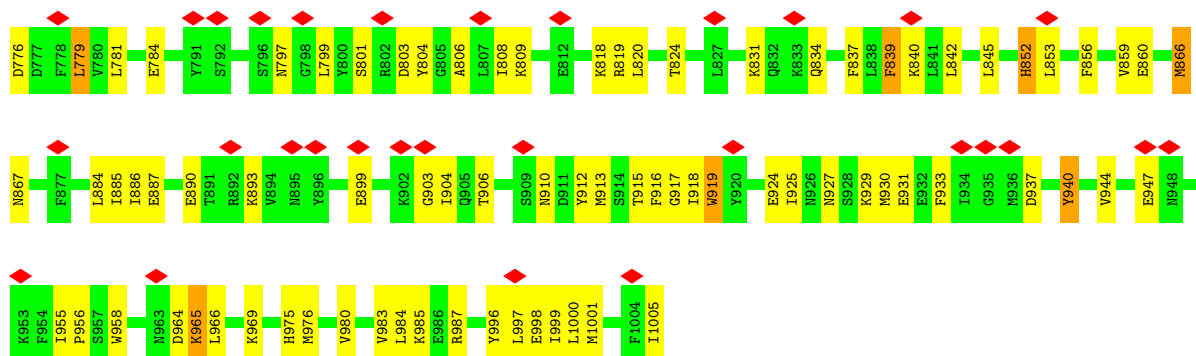
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	151	Total	C	N	O	S	0	0
			1198	758	189	247	4		
2	D	151	Total	C	N	O	S	0	0
			1198	758	189	247	4		
2	G	151	Total	C	N	O	S	0	0
			1198	758	189	247	4		
2	H	151	Total	C	N	O	S	0	0
			1198	758	189	247	4		

3 Residue-property plots

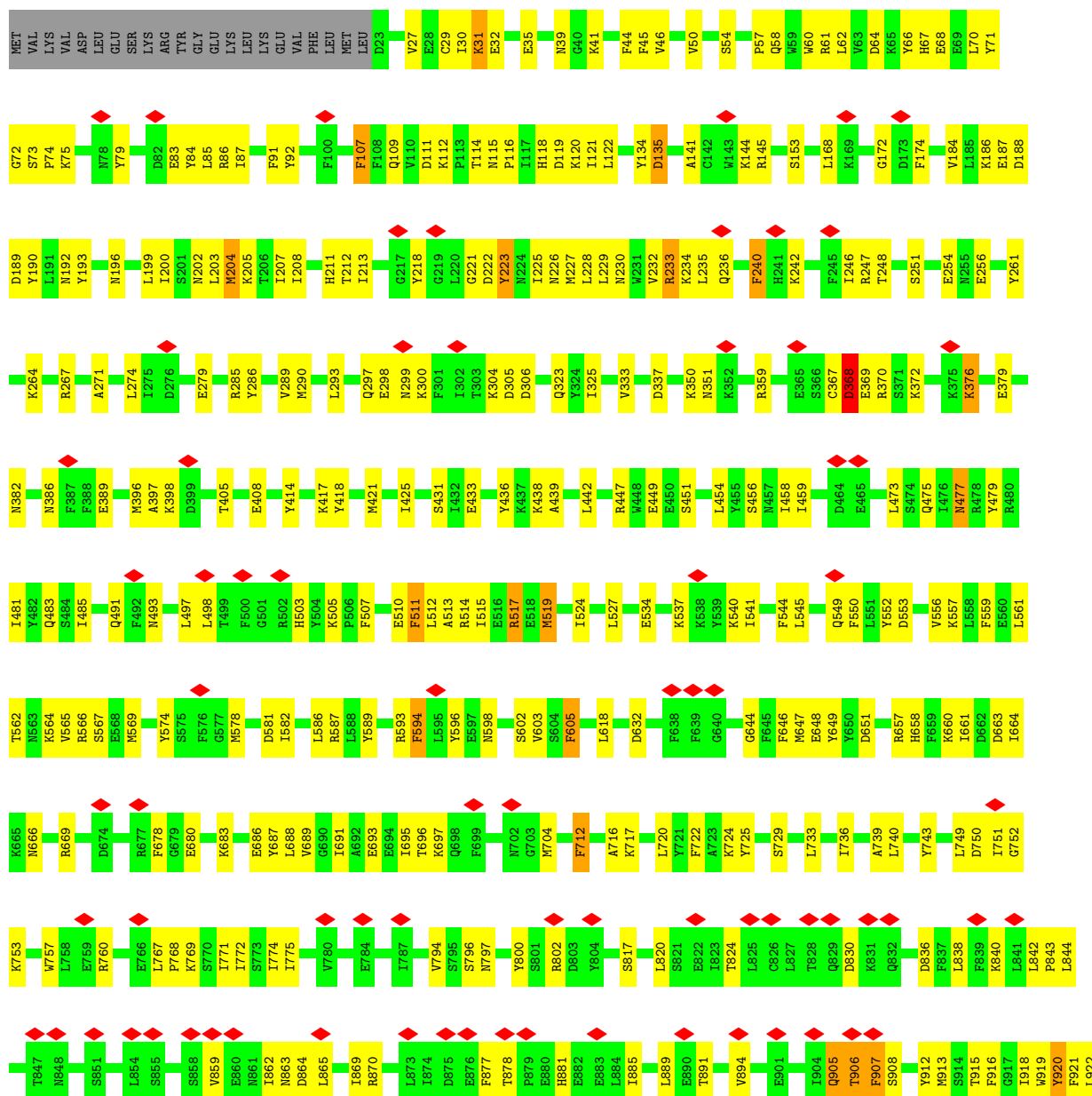
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: SIR2-like domain-containing protein



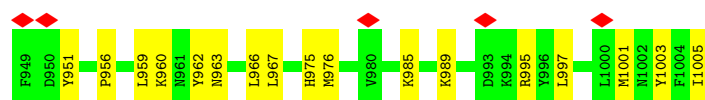


• Molecule 1: SIR2-like domain-containing protein

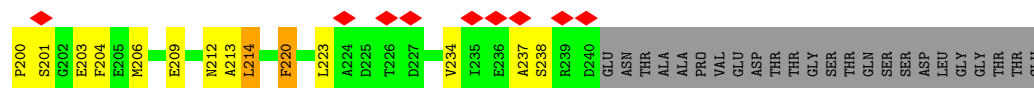
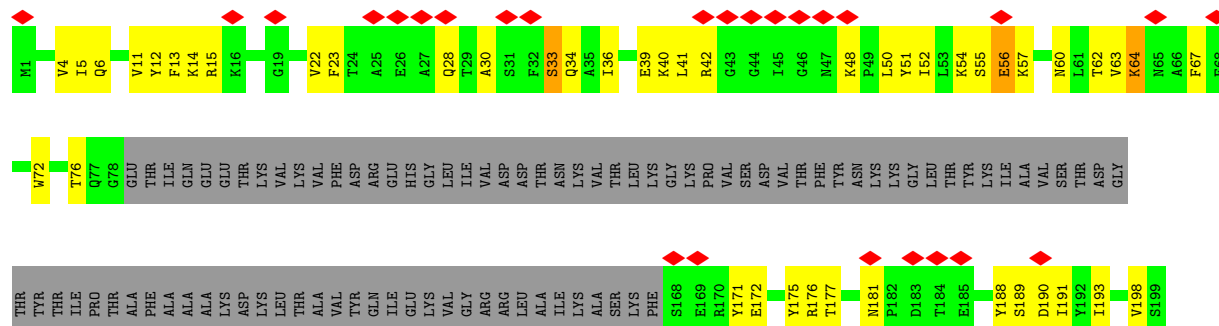
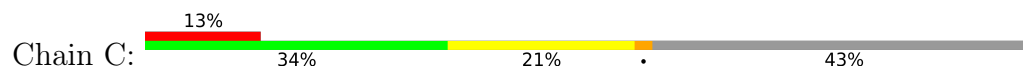




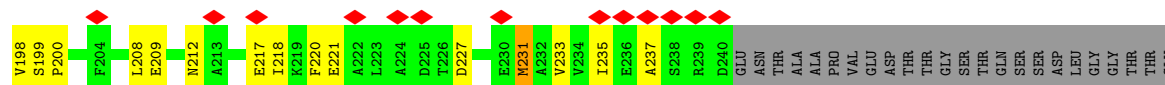
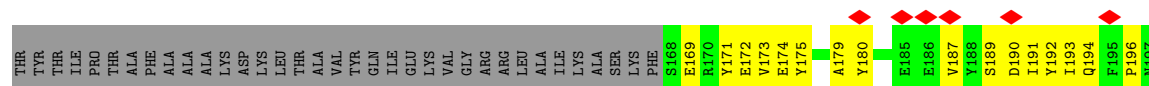
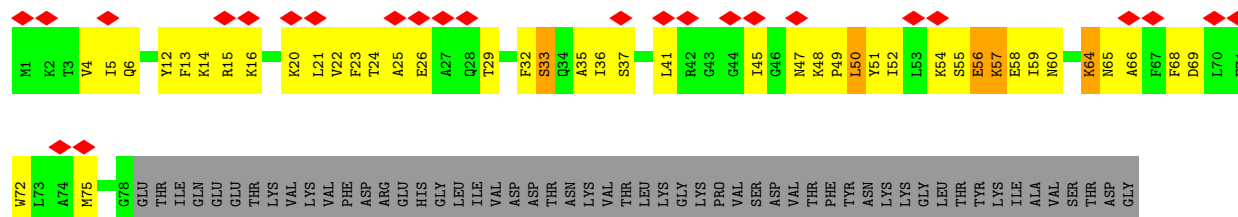
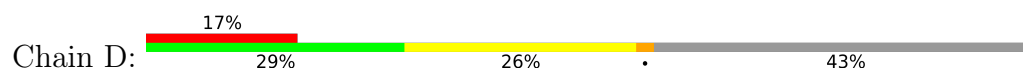




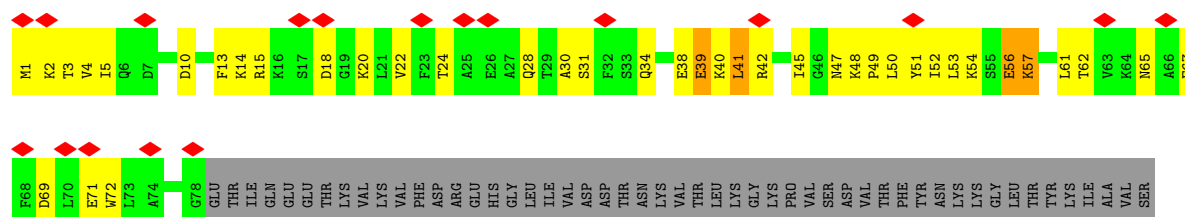
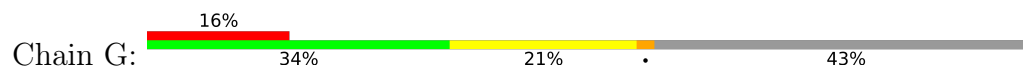
• Molecule 2: SPR



• Molecule 2: SPR

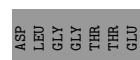
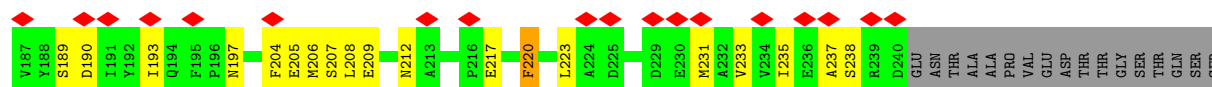
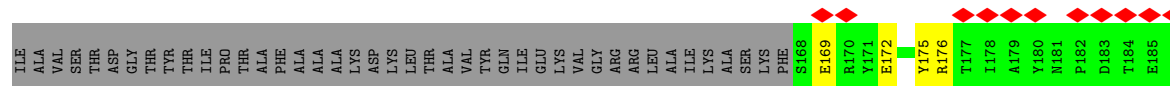
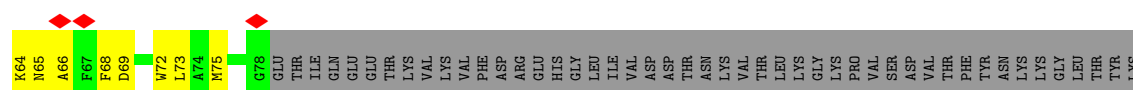
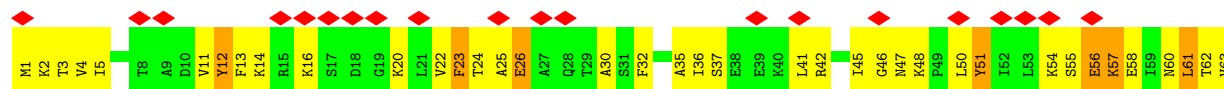
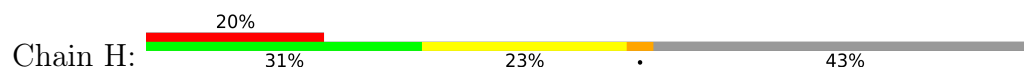


• Molecule 2: SPR





- Molecule 2: SPR



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37524	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.929	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	381.8, 381.8, 381.8	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/8374	0.56	6/11280 (0.1%)
1	B	0.27	0/8374	0.54	3/11280 (0.0%)
1	E	0.27	0/8374	0.53	1/11280 (0.0%)
1	F	0.28	0/8374	0.56	3/11280 (0.0%)
2	C	0.26	0/1218	0.54	0/1645
2	D	0.27	0/1218	0.59	1/1645 (0.1%)
2	G	0.27	0/1218	0.58	1/1645 (0.1%)
2	H	0.27	0/1218	0.58	1/1645 (0.1%)
All	All	0.27	0/38368	0.55	16/51700 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ASP	CB-CG-OD1	9.25	126.62	118.30
1	E	779	LEU	CA-CB-CG	7.50	132.56	115.30
1	A	758	LEU	CA-CB-CG	7.35	132.21	115.30
1	A	191	LEU	CA-CB-CG	6.93	131.24	115.30
1	F	843	PRO	CA-N-CD	-6.54	102.35	111.50
1	F	228	LEU	CA-CB-CG	6.46	130.16	115.30
1	A	204	MET	CA-CB-CG	6.13	123.72	113.30
1	F	688	LEU	CA-CB-CG	5.89	128.84	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	779	LEU	CA-CB-CG	5.87	128.81	115.30
2	D	50	LEU	CA-CB-CG	5.75	128.52	115.30
2	G	41	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	750	ASP	CB-CG-OD1	5.33	123.09	118.30
1	B	135	ASP	CB-CG-OD1	5.29	123.06	118.30
2	H	61	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	111	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	368	ASP	CB-CG-OD1	5.15	122.94	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	64	LYS	Peptide
1	E	297	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8183	0	8010	321	0
1	B	8183	0	8010	273	0
1	E	8183	0	8010	302	0
1	F	8183	0	8010	295	0
2	C	1198	0	1159	46	0
2	D	1198	0	1159	58	0
2	G	1198	0	1159	59	0
2	H	1198	0	1159	75	0
All	All	37524	0	36676	1339	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 18.

All (1339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ARG:HG3	1:E:90:ILE:HD11	1.48	0.93
1:F:724:LYS:HE2	1:F:760:ARG:HD2	1.53	0.90
1:F:235:LEU:HD12	1:F:236:GLN:HB2	1.54	0.89
1:B:208:ILE:HD12	1:B:213:ILE:HG13	1.55	0.88
2:D:25:ALA:O	2:D:65:ASN:ND2	2.07	0.88
2:C:190:ASP:H	2:C:237:ALA:HB3	1.42	0.81
1:B:594:PHE:O	1:B:598:ASN:ND2	2.13	0.81
2:G:15:ARG:HG2	2:G:20:LYS:HD2	1.59	0.81
1:F:910:ASN:HD21	2:G:229:ASP:H	1.26	0.80
1:E:919:TRP:HE1	2:H:50:LEU:HD13	1.47	0.79
1:A:852:HIS:HE1	1:A:856:PHE:HZ	1.31	0.79
2:D:50:LEU:HD12	2:D:51:TYR:H	1.47	0.78
2:H:14:LYS:N	2:H:172:GLU:O	2.15	0.78
2:G:190:ASP:H	2:G:237:ALA:HB3	1.49	0.78
1:A:917:GLY:HA2	1:A:944:VAL:HG23	1.65	0.78
1:E:657:ARG:HA	1:E:715:GLU:HG2	1.64	0.77
1:A:622:LYS:NZ	1:A:626:GLU:OE2	2.17	0.77
1:A:594:PHE:O	1:A:598:ASN:ND2	2.18	0.77
2:H:190:ASP:H	2:H:237:ALA:HB3	1.49	0.77
1:A:326:ARG:NH2	1:A:591:ASN:OD1	2.18	0.76
2:H:45:ILE:HG23	2:H:47:ASN:H	1.49	0.76
1:A:480:ARG:HD2	1:A:605:PHE:HE2	1.50	0.75
1:B:208:ILE:HG12	1:B:228:LEU:HD21	1.67	0.75
1:E:101:ASP:HA	1:E:104:LEU:HG	1.67	0.75
1:A:591:ASN:ND2	1:A:611:TYR:OH	2.19	0.75
2:H:50:LEU:HD12	2:H:51:TYR:H	1.50	0.75
2:D:64:LYS:HB3	2:D:217:GLU:HA	1.69	0.75
1:E:407:ILE:HG21	1:E:589:TYR:HB3	1.69	0.74
2:H:12:TYR:HA	2:H:23:PHE:CE2	2.23	0.74
1:E:478:ARG:NH2	1:E:518:GLU:OE2	2.21	0.74
1:F:126:PRO:O	1:F:165:ARG:NH2	2.20	0.73
1:F:871:ILE:HD12	1:F:872:GLY:N	2.03	0.73
1:E:278:ASN:O	1:E:285:ARG:NH2	2.19	0.73
1:E:684:ILE:HD11	1:E:726:VAL:HG21	1.70	0.73
1:B:974:LYS:O	1:B:976:MET:N	2.22	0.72
1:A:673:ILE:HG13	1:A:676:ILE:HD12	1.71	0.72
1:E:607:GLU:OE1	1:E:607:GLU:N	2.19	0.72
1:F:557:LYS:HD2	1:F:587:ARG:HH12	1.53	0.72
1:F:562:THR:HG22	1:F:618:LEU:HD22	1.71	0.71
2:H:16:LYS:HB3	2:H:169:GLU:HB3	1.73	0.71
1:B:248:THR:O	1:B:285:ARG:NH1	2.22	0.71
1:A:367:CYS:HA	1:A:370:ARG:HE	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:GLU:O	1:B:300:LYS:N	2.23	0.70
1:E:83:GLU:HB3	1:E:87:ILE:HD11	1.73	0.70
2:H:2:LYS:HG3	2:H:3:THR:HG22	1.72	0.70
1:F:802:ARG:H	1:F:840:LYS:HZ2	1.38	0.70
1:A:26:VAL:O	1:A:30:ILE:HD12	1.90	0.70
1:A:83:GLU:HA	1:A:86:ARG:HG2	1.73	0.70
2:C:189:SER:HB3	2:C:238:SER:HB3	1.72	0.70
1:F:951:TYR:OH	1:F:976:MET:SD	2.48	0.70
1:F:202:ASN:HA	1:F:205:LYS:HE2	1.73	0.69
1:A:231:TRP:HA	1:A:234:LYS:HE3	1.73	0.69
1:F:1001:MET:HA	1:F:1005:ILE:HD12	1.72	0.69
1:B:115:ASN:OD1	1:B:118:HIS:ND1	2.24	0.69
2:C:34:GLN:HE22	2:C:36:ILE:HG13	1.57	0.69
1:E:916:PHE:HA	1:E:919:TRP:CE3	2.28	0.69
1:E:105:LYS:HE2	1:E:105:LYS:HA	1.75	0.69
1:A:477:ASN:O	1:A:481:ILE:HG12	1.93	0.69
1:E:322:LEU:HD11	1:E:542:LEU:HD21	1.73	0.69
1:B:337:ASP:HA	1:B:350:LYS:HB3	1.73	0.69
1:E:771:ILE:O	1:E:775:ILE:HG13	1.93	0.68
1:B:271:ALA:HA	1:B:274:LEU:HD12	1.75	0.68
1:A:421:MET:HB3	1:A:445:LEU:HD11	1.76	0.68
2:H:11:VAL:HG13	2:H:175:TYR:HE1	1.59	0.68
1:E:867:ASN:HA	1:E:870:ARG:HG2	1.74	0.68
1:E:242:LYS:HG2	1:E:267:ARG:HH21	1.57	0.68
1:B:298:GLU:C	1:B:300:LYS:H	1.97	0.68
1:B:439:ALA:HB2	1:B:454:LEU:HD22	1.75	0.68
1:A:374:SER:OG	1:A:377:GLN:OE1	2.12	0.67
1:B:421:MET:O	1:B:425:ILE:HG13	1.94	0.67
1:F:683:LYS:HA	1:F:686:GLU:HG2	1.76	0.67
1:E:919:TRP:CD1	2:H:50:LEU:HB2	2.29	0.67
1:E:755:TYR:HE2	1:E:803:ASP:HB3	1.59	0.67
1:F:735:LYS:HA	1:F:738:LYS:HZ2	1.60	0.67
1:A:247:ARG:HE	1:A:249:ASP:HB2	1.59	0.67
1:B:29:CYS:SG	1:B:267:ARG:NH2	2.67	0.67
1:F:234:LYS:HD2	1:F:234:LYS:O	1.94	0.67
1:B:222:ASP:O	1:B:226:ASN:ND2	2.28	0.67
1:E:869:ILE:HG12	1:E:874:ILE:HG13	1.76	0.67
1:F:646:PHE:HB3	1:F:677:ARG:HH21	1.60	0.67
1:B:984:LEU:HD13	1:B:1000:LEU:HD13	1.75	0.67
1:F:905:GLN:O	1:F:906:THR:OG1	2.11	0.67
1:E:247:ARG:HD3	1:E:249:ASP:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:56:GLU:HG3	2:G:57:LYS:H	1.60	0.66
1:B:481:ILE:O	1:B:485:ILE:HG13	1.95	0.66
2:D:45:ILE:HG23	2:D:47:ASN:H	1.59	0.66
1:A:566:ARG:HH12	1:B:566:ARG:HH22	1.44	0.66
1:F:737:VAL:O	1:F:741:LEU:HG	1.95	0.66
1:E:984:LEU:HD22	1:E:1000:LEU:HB2	1.76	0.66
1:A:919:TRP:HB3	1:A:924:GLU:HB2	1.78	0.66
1:A:51:SER:HB3	1:A:133:ASN:HD22	1.61	0.66
1:A:54:SER:OG	1:A:115:ASN:ND2	2.29	0.66
1:A:474:SER:O	1:A:478:ARG:HG2	1.96	0.65
1:A:130:ILE:HD11	1:A:207:ILE:HG21	1.78	0.65
1:B:204:MET:HA	1:B:207:ILE:HD12	1.78	0.65
1:B:279:GLU:O	1:B:285:ARG:NH2	2.29	0.65
1:F:396:MET:SD	1:F:397:ALA:N	2.68	0.65
1:A:115:ASN:HD21	1:A:118:HIS:HD2	1.44	0.65
1:A:558:LEU:HD12	1:A:611:TYR:CD1	2.32	0.65
1:E:730:GLU:HA	1:E:733:LEU:HD12	1.78	0.65
1:F:657:ARG:NH1	1:F:715:GLU:OE2	2.30	0.65
1:F:683:LYS:N	1:F:683:LYS:HD3	2.11	0.65
1:A:744:PHE:HB2	1:A:754:ARG:HH22	1.61	0.65
1:E:89:GLN:OE1	1:E:188:ASP:N	2.29	0.65
1:B:688:LEU:HB3	1:B:736:ILE:HD11	1.78	0.65
1:E:613:ARG:HA	1:E:659:PHE:HE1	1.62	0.65
1:F:749:LEU:HD23	1:F:754:ARG:HD3	1.79	0.65
1:A:333:VAL:HB	1:A:541:ILE:HD12	1.78	0.65
1:B:168:LEU:HD22	1:B:203:LEU:HD22	1.78	0.65
1:B:802:ARG:HB3	1:B:840:LYS:HB3	1.77	0.65
1:F:689:VAL:HG22	1:F:735:LYS:HD2	1.79	0.65
1:A:724:LYS:HD2	1:A:725:TYR:CE1	2.32	0.64
1:B:57:PRO:HG2	1:B:107:PHE:HE1	1.62	0.64
1:F:298:GLU:C	1:F:300:LYS:H	2.00	0.64
1:F:619:LEU:HA	1:F:622:LYS:HE2	1.79	0.64
1:A:284:GLU:OE1	1:A:284:GLU:N	2.29	0.64
1:E:533:PHE:HB3	1:E:537:LYS:NZ	2.12	0.64
1:B:27:VAL:HG12	1:B:31:LYS:NZ	2.13	0.64
1:B:767:LEU:HG	1:B:772:ILE:HG12	1.80	0.64
1:A:480:ARG:HD2	1:A:605:PHE:CE2	2.32	0.64
1:E:459:ILE:HD11	1:E:475:GLN:HE22	1.62	0.64
1:E:757:TRP:HA	1:E:760:ARG:HE	1.62	0.64
1:A:651:ASP:O	1:A:655:ILE:HG12	1.97	0.64
1:B:939:GLN:NE2	1:B:962:TYR:OH	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:752:GLY:HA3	1:F:797:ASN:HB3	1.79	0.64
1:A:997:LEU:HD21	1:B:988:VAL:HB	1.80	0.64
1:B:493:ASN:HA	1:B:503:HIS:HE2	1.61	0.64
1:B:661:ILE:HD11	1:B:717:LYS:HD3	1.80	0.64
1:F:613:ARG:NH2	1:F:663:ASP:OD2	2.31	0.64
1:B:869:ILE:HG21	1:B:919:TRP:HH2	1.63	0.63
2:D:190:ASP:H	2:D:237:ALA:HB3	1.63	0.63
1:A:213:ILE:HB	1:A:243:PRO:HB3	1.79	0.63
1:A:518:GLU:OE1	1:B:145:ARG:NH2	2.30	0.63
1:E:404:ASN:HB3	2:G:1:MET:HA	1.80	0.63
1:A:492:PHE:HA	1:A:496:GLY:HA3	1.80	0.63
1:E:955:ILE:HB	1:E:958:TRP:CE2	2.34	0.63
1:A:820:LEU:O	1:A:824:THR:HG23	1.99	0.63
1:B:227:MET:SD	1:B:227:MET:N	2.71	0.63
1:B:184:VAL:HG23	1:B:189:ASP:HB3	1.80	0.63
1:B:794:VAL:HG22	2:C:223:LEU:HD12	1.81	0.63
1:E:770:SER:O	1:E:774:ILE:HD12	1.99	0.63
1:F:751:ILE:HA	1:F:754:ARG:HG2	1.80	0.63
1:F:754:ARG:O	1:F:758:LEU:HG	1.99	0.63
1:A:115:ASN:HD21	1:A:118:HIS:CD2	2.17	0.63
1:A:134:TYR:OH	1:A:184:VAL:O	2.17	0.63
1:E:500:PHE:HD1	1:E:747:ARG:HH22	1.45	0.63
1:F:801:SER:HA	1:F:804:TYR:CD2	2.33	0.63
1:A:147:LYS:HE3	1:A:147:LYS:HA	1.81	0.62
2:G:212:ASN:ND2	2:G:214:LEU:O	2.32	0.62
1:B:368:ASP:OD1	1:B:369:GLU:N	2.32	0.62
1:F:250:PRO:HG3	1:F:279:GLU:HG3	1.81	0.62
1:A:558:LEU:HD12	1:A:611:TYR:HD1	1.63	0.62
1:E:771:ILE:HD12	1:E:771:ILE:H	1.64	0.62
1:F:483:GLN:O	1:F:487:GLN:HG3	1.99	0.62
1:F:869:ILE:HA	1:F:874:ILE:H	1.63	0.62
1:A:469:CYS:HB2	1:A:539:TYR:HE2	1.64	0.62
1:A:613:ARG:HH22	1:A:659:PHE:HA	1.65	0.62
1:E:277:SER:OG	1:E:285:ARG:NH2	2.32	0.62
1:B:817:SER:HB2	1:B:820:LEU:HD23	1.81	0.62
1:E:956:PRO:HB3	1:E:987:ARG:HD3	1.80	0.62
1:B:286:TYR:O	1:B:290:MET:HG2	1.98	0.62
2:C:6:GLN:N	2:C:6:GLN:OE1	2.33	0.62
1:E:204:MET:O	1:E:208:ILE:HG12	2.00	0.62
1:F:83:GLU:O	1:F:87:ILE:HG12	2.00	0.62
1:B:549:GLN:HA	1:B:552:TYR:HB2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:613:ARG:NE	1:E:663:ASP:OD2	2.32	0.62
1:F:802:ARG:HB3	1:F:840:LYS:HG3	1.81	0.62
1:A:122:LEU:HD11	1:A:142:CYS:HA	1.82	0.62
1:A:976:MET:SD	1:A:976:MET:N	2.73	0.62
1:F:531:MET:SD	1:F:532:PRO:HD2	2.40	0.62
2:C:175:TYR:N	2:C:193:ILE:O	2.33	0.62
1:E:661:ILE:HA	1:E:664:ILE:HD12	1.82	0.62
1:A:687:TYR:O	1:A:691:ILE:HG13	1.99	0.61
2:C:55:SER:O	2:C:57:LYS:N	2.32	0.61
2:D:36:ILE:HG12	2:D:57:LYS:HG2	1.82	0.61
2:D:175:TYR:HB2	2:D:193:ILE:HB	1.81	0.61
1:E:120:LYS:HG3	1:E:290:MET:SD	2.39	0.61
1:B:720:LEU:HD13	1:B:740:LEU:HD12	1.82	0.61
1:E:499:THR:O	1:E:747:ARG:NH2	2.33	0.61
1:B:153:SER:HB2	1:B:172:GLY:HA2	1.82	0.61
1:B:751:ILE:HG21	1:B:800:TYR:HA	1.81	0.61
1:B:717:LYS:HG2	1:B:757:TRP:HH2	1.64	0.61
2:D:16:LYS:HB3	2:D:169:GLU:HB3	1.82	0.61
1:A:204:MET:HE2	1:A:208:ILE:HD11	1.81	0.61
2:C:212:ASN:ND2	2:C:214:LEU:O	2.34	0.61
1:B:565:VAL:HG11	1:B:618:LEU:HD11	1.82	0.61
1:B:680:GLU:HG2	1:B:683:LYS:HD2	1.81	0.61
2:D:199:SER:N	2:D:221:GLU:O	2.34	0.61
1:A:236:GLN:HG2	1:B:199:LEU:HD11	1.83	0.61
1:B:229:LEU:HA	1:B:232:VAL:HG22	1.82	0.61
1:F:199:LEU:HA	1:F:202:ASN:HD21	1.64	0.61
1:F:336:TYR:O	1:F:349:HIS:ND1	2.34	0.61
1:F:817:SER:OG	1:F:821:SER:OG	2.08	0.61
1:B:39:ASN:O	1:B:41:LYS:NZ	2.31	0.61
1:B:438:LYS:O	1:B:442:LEU:HG	2.00	0.61
2:C:175:TYR:HB2	2:C:193:ILE:HB	1.82	0.61
1:A:454:LEU:HA	1:A:457:ASN:ND2	2.15	0.61
1:E:418:TYR:HA	1:E:421:MET:HG3	1.83	0.61
1:E:762:THR:HB	1:E:767:LEU:HD21	1.82	0.60
1:F:865:LEU:HA	1:F:869:ILE:HD13	1.83	0.60
1:E:960:LYS:HE3	1:E:996:TYR:HE1	1.66	0.60
1:F:189:ASP:OD1	1:F:189:ASP:N	2.30	0.60
1:F:780:VAL:HG21	1:F:820:LEU:HD22	1.82	0.60
1:E:26:VAL:O	1:E:30:ILE:HG12	2.00	0.60
1:E:528:PHE:O	1:E:536:GLN:NE2	2.33	0.60
1:E:914:SER:O	1:E:918:ILE:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASP:O	1:A:456:SER:OG	2.18	0.60
1:F:549:GLN:HA	1:F:552:TYR:HB2	1.82	0.60
1:E:690:GLY:O	1:E:694:GLU:HG3	2.02	0.60
1:E:755:TYR:OH	1:E:807:LEU:HB2	2.01	0.60
1:A:247:ARG:N	1:A:269:ILE:O	2.33	0.60
1:E:724:LYS:HE2	1:E:725:TYR:CE1	2.37	0.60
1:E:919:TRP:HD1	2:H:50:LEU:HB2	1.65	0.60
2:H:11:VAL:HG13	2:H:175:TYR:CE1	2.37	0.60
1:A:396:MET:SD	1:A:396:MET:N	2.73	0.60
1:B:54:SER:O	1:B:112:LYS:NZ	2.31	0.60
1:B:913:MET:SD	1:B:913:MET:N	2.72	0.60
1:F:821:SER:O	1:F:825:LEU:HB3	2.02	0.60
1:A:753:LYS:HB3	1:A:757:TRP:CZ2	2.37	0.60
1:B:85:LEU:HD13	1:B:187:GLU:HG3	1.84	0.60
1:F:99:ALA:O	1:F:103:ILE:HG12	2.02	0.60
1:F:755:TYR:HA	1:F:804:TYR:HE1	1.67	0.60
1:F:337:ASP:HA	1:F:350:LYS:HB3	1.84	0.60
1:F:693:GLU:O	1:F:697:LYS:HD3	2.01	0.60
1:A:29:CYS:SG	1:A:267:ARG:NH2	2.75	0.59
1:A:326:ARG:HD2	1:A:329:ASP:HB2	1.82	0.59
1:E:676:ILE:HD12	1:E:676:ILE:H	1.67	0.59
1:F:230:ASN:OD1	1:F:231:TRP:N	2.35	0.59
2:G:10:ASP:HB2	2:G:176:ARG:HB3	1.84	0.59
1:B:920:TYR:CE2	1:B:944:VAL:HA	2.37	0.59
2:D:29:THR:HG23	2:D:64:LYS:HE2	1.83	0.59
1:F:475:GLN:HB3	1:F:527:LEU:HD21	1.84	0.59
2:C:33:SER:HB3	2:C:60:ASN:HB2	1.84	0.59
1:E:348:ARG:HE	1:E:351:ASN:HB3	1.66	0.59
1:F:767:LEU:HB2	1:F:811:PHE:HD2	1.67	0.59
2:G:71:GLU:HG2	2:G:72:TRP:HE3	1.66	0.59
2:H:11:VAL:HG12	2:H:23:PHE:CZ	2.37	0.59
1:A:298:GLU:O	1:A:300:LYS:N	2.36	0.59
1:E:406:SER:HB2	2:G:2:LYS:H	1.68	0.59
1:E:199:LEU:HD21	1:F:235:LEU:HD13	1.82	0.59
1:A:29:CYS:O	1:A:33:ILE:HG13	2.01	0.59
1:B:578:MET:HA	1:B:582:ILE:HD11	1.84	0.59
1:B:916:PHE:HA	1:B:919:TRP:HD1	1.68	0.59
1:A:188:ASP:O	1:A:192:ASN:ND2	2.36	0.59
1:A:728:LEU:HD11	1:A:732:GLY:HA3	1.84	0.59
1:F:956:PRO:HA	1:F:959:LEU:HG	1.83	0.59
1:F:959:LEU:HA	1:F:962:TYR:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:52:ILE:HD11	2:G:54:LYS:HD3	1.85	0.59
1:A:549:GLN:HA	1:A:552:TYR:HD2	1.68	0.58
1:A:904:ILE:HG12	2:D:235:ILE:HG23	1.85	0.58
1:B:41:LYS:O	1:B:212:THR:OG1	2.19	0.58
1:F:229:LEU:O	1:F:233:ARG:HG3	2.02	0.58
1:B:596:TYR:HE1	1:B:603:VAL:HB	1.68	0.58
1:B:649:TYR:HE1	1:B:687:TYR:HB2	1.68	0.58
1:B:687:TYR:O	1:B:691:ILE:HG12	2.03	0.58
2:C:42:ARG:NH1	2:C:51:TYR:OH	2.35	0.58
1:E:911:ASP:N	1:E:911:ASP:OD1	2.35	0.58
1:E:988:VAL:HG13	1:F:997:LEU:HD21	1.85	0.58
1:F:612:ILE:H	1:F:612:ILE:HD12	1.68	0.58
1:B:58:GLN:HB3	1:B:60:TRP:CD1	2.39	0.58
1:B:802:ARG:HD3	1:B:840:LYS:HD2	1.83	0.58
1:F:995:ARG:NH1	2:G:38:GLU:OE2	2.36	0.58
1:B:118:HIS:O	1:B:122:LEU:HG	2.02	0.58
1:E:83:GLU:O	1:E:87:ILE:HG12	2.03	0.58
1:E:348:ARG:NH2	1:E:351:ASN:O	2.34	0.58
1:B:44:PHE:CG	1:B:121:ILE:HD11	2.39	0.58
1:B:247:ARG:NH2	1:B:251:SER:O	2.36	0.58
2:G:24:THR:HB	2:G:65:ASN:HB3	1.85	0.58
1:A:319:LEU:HD21	1:A:541:ILE:HD13	1.86	0.58
1:A:472:TYR:OH	1:A:546:SER:HB3	2.03	0.58
1:A:516:GLU:O	1:A:520:THR:HG23	2.04	0.58
1:E:724:LYS:HD2	1:E:760:ARG:HB3	1.85	0.58
1:F:310:ASP:OD1	1:F:380:ARG:NH1	2.36	0.58
1:A:30:ILE:HG23	1:A:293:LEU:HD13	1.85	0.58
1:B:724:LYS:HD2	1:B:760:ARG:HD3	1.84	0.58
1:A:595:LEU:HA	1:A:600:LEU:HD12	1.84	0.58
1:E:531:MET:HG3	1:E:532:PRO:HD2	1.83	0.58
1:F:660:LYS:HB2	1:F:663:ASP:OD1	2.04	0.58
2:H:197:ASN:HB3	2:H:223:LEU:HB2	1.86	0.58
1:A:116:PRO:HD2	1:A:117:ILE:HD12	1.86	0.58
1:A:852:HIS:CE1	1:A:856:PHE:HZ	2.16	0.58
1:B:289:VAL:O	1:B:293:LEU:HG	2.04	0.58
1:F:804:TYR:O	1:F:807:LEU:HG	2.04	0.58
1:B:817:SER:OG	1:B:844:LEU:O	2.22	0.57
1:A:116:PRO:HB2	1:A:120:LYS:HZ3	1.69	0.57
1:A:377:GLN:OE1	1:A:377:GLN:N	2.34	0.57
1:A:842:LEU:HA	1:A:845:LEU:HD23	1.86	0.57
1:E:117:ILE:HD13	1:E:120:LYS:HZ2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:PHE:HE2	2:D:198:VAL:HG11	1.69	0.57
1:E:236:GLN:NE2	1:E:239:SER:O	2.38	0.57
1:E:589:TYR:OH	1:E:651:ASP:OD1	2.21	0.57
1:F:199:LEU:HA	1:F:202:ASN:ND2	2.19	0.57
1:A:448:TRP:CD1	1:A:448:TRP:N	2.72	0.57
2:D:172:GLU:HG2	2:D:196:PRO:HA	1.87	0.57
1:A:70:LEU:HD21	1:A:91:PHE:HA	1.86	0.57
1:B:367:CYS:SG	1:B:370:ARG:NH2	2.77	0.57
1:B:749:LEU:HA	1:B:753:LYS:HE3	1.85	0.57
1:E:116:PRO:C	1:E:120:LYS:HZ1	2.08	0.57
1:E:581:ASP:OD1	1:E:582:ILE:N	2.38	0.57
1:F:198:PRO:O	1:F:201:SER:OG	2.18	0.57
1:F:616:MET:O	1:F:620:ILE:HG13	2.04	0.57
1:F:652:PHE:HA	1:F:655:ILE:HD12	1.86	0.57
1:A:852:HIS:HE1	1:A:856:PHE:CZ	2.16	0.57
2:D:14:LYS:N	2:D:172:GLU:O	2.37	0.57
1:A:454:LEU:HA	1:A:457:ASN:HD22	1.70	0.57
1:B:602:SER:HA	1:B:605:PHE:HE1	1.70	0.57
1:B:771:ILE:HA	1:B:774:ILE:HD12	1.87	0.57
1:F:448:TRP:CH2	1:F:707:VAL:HG23	2.40	0.57
1:A:116:PRO:HB3	1:B:517:ARG:HH12	1.69	0.57
1:A:480:ARG:HD3	1:A:483:GLN:HE21	1.70	0.57
2:D:26:GLU:O	2:D:65:ASN:ND2	2.38	0.57
2:H:63:VAL:HG22	2:H:220:PHE:HZ	1.70	0.57
1:A:131:THR:O	1:A:170:VAL:N	2.30	0.56
1:B:304:LYS:NZ	1:B:306:ASP:H	2.03	0.56
2:G:52:ILE:HG12	2:G:54:LYS:H	1.68	0.56
1:A:595:LEU:HB3	1:A:603:VAL:HG12	1.87	0.56
1:A:721:TYR:OH	1:A:760:ARG:NH1	2.39	0.56
1:E:481:ILE:O	1:E:485:ILE:HG12	2.05	0.56
1:A:570:SER:O	1:B:669:ARG:NH1	2.39	0.56
1:E:919:TRP:NE1	2:H:50:LEU:HD13	2.18	0.56
1:F:962:TYR:HB3	1:F:967:LEU:HD12	1.86	0.56
2:H:13:PHE:HB2	2:H:23:PHE:CG	2.39	0.56
1:A:282:TYR:HD1	1:A:285:ARG:HH22	1.53	0.56
1:A:326:ARG:HD3	1:A:328:ILE:HG23	1.87	0.56
1:A:514:ARG:HA	1:A:517:ARG:HE	1.70	0.56
2:C:41:LEU:HB2	2:C:54:LYS:HE3	1.86	0.56
1:E:208:ILE:HD12	1:E:232:VAL:HG21	1.88	0.56
1:E:455:TYR:HE2	1:E:481:ILE:HG13	1.70	0.56
1:A:399:ASP:OD1	1:A:399:ASP:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ILE:HD11	1:B:541:ILE:HD13	1.88	0.56
1:F:910:ASN:ND2	2:G:229:ASP:H	2.00	0.56
2:G:20:LYS:HE2	2:G:22:VAL:HG23	1.86	0.56
1:A:469:CYS:O	1:A:473:LEU:HG	2.06	0.56
1:A:549:GLN:HA	1:A:552:TYR:CD2	2.40	0.56
1:B:752:GLY:HA3	1:B:797:ASN:HB3	1.88	0.56
1:A:100:PHE:O	1:A:104:LEU:HG	2.05	0.56
1:E:472:TYR:CE1	1:E:476:ILE:HD11	2.41	0.56
2:G:189:SER:HB3	2:G:238:SER:HB3	1.86	0.56
1:A:117:ILE:HD12	1:A:117:ILE:H	1.71	0.56
1:E:304:LYS:NZ	1:E:307:GLU:OE1	2.36	0.56
1:F:298:GLU:O	1:F:300:LYS:N	2.39	0.56
1:A:404:ASN:HA	2:C:4:VAL:HG12	1.87	0.55
1:B:256:GLU:OE1	1:B:256:GLU:N	2.40	0.55
2:G:38:GLU:HA	2:G:54:LYS:HG2	1.87	0.55
1:A:610:GLN:HA	1:A:613:ARG:HB3	1.87	0.55
1:B:379:GLU:HA	1:B:382:ASN:ND2	2.21	0.55
1:B:912:TYR:HB3	1:B:916:PHE:CZ	2.42	0.55
1:A:117:ILE:HA	1:A:120:LYS:HG2	1.86	0.55
1:B:75:LYS:HB3	1:B:79:TYR:CE2	2.41	0.55
1:B:122:LEU:HD11	1:B:141:ALA:HB1	1.89	0.55
1:F:592:LEU:O	1:F:596:TYR:HB2	2.06	0.55
1:F:871:ILE:HD12	1:F:872:GLY:H	1.72	0.55
1:A:337:ASP:HA	1:A:350:LYS:HB2	1.88	0.55
1:B:205:LYS:O	1:B:208:ILE:HG22	2.06	0.55
1:B:408:GLU:H	1:B:593:ARG:HH21	1.55	0.55
1:B:864:ASP:OD1	1:B:865:LEU:N	2.39	0.55
1:B:985:LYS:HA	1:B:988:VAL:HG22	1.86	0.55
1:E:253:ILE:HD13	1:E:268:ILE:HG12	1.88	0.55
1:A:198:PRO:HG2	1:B:235:LEU:HB3	1.89	0.55
1:A:405:THR:H	2:C:4:VAL:HG12	1.71	0.55
1:B:85:LEU:HD21	1:B:190:TYR:CE2	2.42	0.55
1:E:770:SER:O	1:E:773:SER:OG	2.15	0.55
1:F:69:GLU:HG2	1:F:91:PHE:HE1	1.72	0.55
1:F:821:SER:O	1:F:825:LEU:CB	2.54	0.55
1:A:666:ASN:OD1	1:A:669:ARG:NH2	2.38	0.55
1:B:230:ASN:O	1:B:234:LYS:NZ	2.39	0.55
1:B:483:GLN:NE2	2:C:209:GLU:O	2.35	0.55
1:B:589:TYR:OH	1:B:651:ASP:OD1	2.22	0.55
1:B:836:ASP:O	1:B:840:LYS:HG2	2.06	0.55
1:E:915:THR:HA	1:E:918:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:VAL:HG11	1:F:583:VAL:HG23	1.89	0.55
1:B:62:LEU:HD21	1:B:107:PHE:CG	2.41	0.55
1:B:870:ARG:HA	2:C:51:TYR:CZ	2.42	0.55
1:E:687:TYR:CE1	1:E:691:ILE:HD11	2.42	0.55
1:E:925:ILE:HG22	1:E:927:ASN:H	1.72	0.55
1:E:955:ILE:HG22	1:E:957:SER:H	1.72	0.55
2:H:189:SER:HB3	2:H:238:SER:HB3	1.89	0.55
1:E:147:LYS:NZ	1:F:526:ASP:OD2	2.40	0.55
1:F:895:ASN:O	1:F:899:GLU:HG2	2.06	0.55
1:B:768:PRO:O	1:B:772:ILE:HG13	2.07	0.54
1:E:469:CYS:SG	1:E:470:VAL:N	2.81	0.54
1:F:319:LEU:HD12	1:F:319:LEU:H	1.72	0.54
1:F:471:TYR:O	1:F:475:GLN:NE2	2.40	0.54
1:F:856:PHE:O	1:F:857:LYS:HG3	2.07	0.54
2:H:26:GLU:O	2:H:65:ASN:ND2	2.39	0.54
1:A:985:LYS:NZ	1:B:1001:MET:HB3	2.23	0.54
1:E:30:ILE:HG23	1:E:293:LEU:HD13	1.89	0.54
1:A:674:ASP:OD1	1:A:675:LYS:N	2.40	0.54
1:E:638:PHE:HZ	2:G:177:THR:HG21	1.71	0.54
1:E:664:ILE:O	1:E:668:GLU:HG3	2.08	0.54
1:F:661:ILE:HD11	1:F:717:LYS:HD3	1.90	0.54
1:E:99:ALA:O	1:E:103:ILE:HG12	2.07	0.54
2:H:72:TRP:HA	2:H:75:MET:HG2	1.89	0.54
1:A:980:VAL:HA	1:A:983:VAL:HG12	1.90	0.54
1:B:498:LEU:HG	2:C:200:PRO:HG3	1.89	0.54
1:E:374:SER:OG	1:E:377:GLN:OE1	2.16	0.54
1:E:474:SER:O	1:E:478:ARG:HG2	2.08	0.54
1:F:377:GLN:CD	1:F:377:GLN:H	2.10	0.54
2:H:25:ALA:O	2:H:26:GLU:HB2	2.07	0.54
1:B:534:GLU:OE1	1:B:534:GLU:N	2.34	0.54
1:E:661:ILE:HG22	1:E:665:LYS:NZ	2.22	0.54
1:E:984:LEU:HG	1:E:987:ARG:HH21	1.72	0.54
1:A:899:GLU:O	1:A:903:GLY:N	2.41	0.54
1:F:578:MET:HA	1:F:582:ILE:HD12	1.88	0.54
1:F:616:MET:HE1	1:F:655:ILE:HA	1.89	0.54
2:D:173:VAL:HG22	2:D:175:TYR:HE1	1.72	0.54
1:E:737:VAL:HG11	1:E:771:ILE:HG23	1.90	0.54
1:F:147:LYS:HD3	1:F:147:LYS:N	2.23	0.54
1:F:751:ILE:HD11	1:F:782:GLN:NE2	2.23	0.54
2:H:208:LEU:HD11	2:H:212:ASN:HB3	1.90	0.54
1:E:204:MET:SD	1:E:228:LEU:HD21	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:ILE:HD12	1:B:722:PHE:CE2	2.43	0.53
1:B:739:ALA:HA	1:B:743:TYR:HD2	1.73	0.53
1:E:243:PRO:HD2	1:E:266:LEU:HD23	1.90	0.53
1:E:303:THR:OG1	1:E:304:LYS:N	2.41	0.53
1:E:558:LEU:O	1:E:562:THR:HG23	2.08	0.53
1:F:298:GLU:C	1:F:300:LYS:N	2.61	0.53
1:A:479:TYR:O	1:A:483:GLN:HG2	2.08	0.53
1:A:801:SER:HA	1:A:804:TYR:CD1	2.44	0.53
1:E:756:VAL:O	1:E:760:ARG:HG3	2.07	0.53
1:F:482:TYR:O	1:F:486:THR:HG22	2.08	0.53
1:F:770:SER:O	1:F:774:ILE:HG13	2.08	0.53
2:H:42:ARG:HE	2:H:45:ILE:HD13	1.73	0.53
2:H:175:TYR:HB2	2:H:193:ILE:HB	1.89	0.53
1:A:116:PRO:HB2	1:A:120:LYS:NZ	2.22	0.53
1:B:58:GLN:HB3	1:B:60:TRP:HD1	1.73	0.53
1:E:904:ILE:HG12	2:H:235:ILE:HG23	1.90	0.53
1:F:138:ILE:HG22	1:F:167:LEU:HD11	1.90	0.53
1:E:456:SER:O	1:E:459:ILE:HG22	2.08	0.53
1:F:46:VAL:HG11	1:F:138:ILE:HD11	1.91	0.53
1:A:414:TYR:OH	1:A:654:ASN:OD1	2.13	0.53
1:A:573:SER:OG	1:A:574:TYR:N	2.42	0.53
1:F:959:LEU:HA	1:F:962:TYR:CZ	2.43	0.53
2:G:31:SER:HG	2:G:62:THR:HG1	1.57	0.53
1:F:245:PHE:HD1	1:F:246:ILE:N	2.06	0.53
1:A:373:LEU:HB3	1:A:377:GLN:HB2	1.91	0.53
1:A:773:SER:HA	1:A:776:ASP:OD2	2.09	0.53
1:B:46:VAL:HG13	1:B:50:VAL:HG11	1.91	0.53
1:B:246:ILE:HG12	1:B:289:VAL:HG11	1.89	0.53
1:E:247:ARG:HB2	1:E:268:ILE:HD11	1.91	0.53
1:E:491:GLN:HE22	2:H:205:GLU:HA	1.73	0.53
1:B:298:GLU:C	1:B:300:LYS:N	2.59	0.53
1:E:983:VAL:O	1:E:987:ARG:HG3	2.08	0.53
1:A:955:ILE:HB	1:A:958:TRP:HE1	1.74	0.53
1:B:114:THR:OG1	1:B:144:LYS:NZ	2.39	0.53
1:E:43:VAL:HG22	1:E:128:HIS:HB2	1.91	0.53
1:F:603:VAL:HA	1:F:608:PHE:HD2	1.74	0.53
1:A:61:ARG:HA	1:A:64:ASP:OD2	2.09	0.53
1:A:480:ARG:HH11	1:A:483:GLN:HE22	1.56	0.53
1:B:405:THR:HG22	2:D:4:VAL:HB	1.90	0.53
1:E:214:VAL:HA	1:E:244:PHE:HB2	1.91	0.53
1:E:484:SER:HA	1:E:487:GLN:HE21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:833:LYS:HA	1:F:836:ASP:OD2	2.09	0.53
1:B:232:VAL:HG23	1:B:233:ARG:HD2	1.90	0.52
2:G:22:VAL:HG22	2:G:72:TRP:HH2	1.74	0.52
1:A:204:MET:CE	1:A:208:ILE:HD11	2.39	0.52
1:B:418:TYR:HA	1:B:421:MET:SD	2.49	0.52
1:E:831:LYS:HB3	1:E:834:GLN:HB3	1.90	0.52
1:F:706:VAL:O	1:F:710:THR:HG23	2.09	0.52
1:F:873:LEU:O	1:F:875:ASP:N	2.40	0.52
1:E:899:GLU:O	1:E:903:GLY:N	2.43	0.52
1:F:425:ILE:HD13	1:F:438:LYS:HB2	1.92	0.52
1:F:663:ASP:O	1:F:667:LEU:HG	2.08	0.52
2:H:12:TYR:HA	2:H:23:PHE:HE2	1.72	0.52
1:A:775:ILE:HG21	1:A:808:ILE:HD11	1.92	0.52
2:G:13:PHE:HB2	2:G:22:VAL:HB	1.91	0.52
1:A:66:TYR:HE1	1:A:103:ILE:HG21	1.74	0.52
1:A:184:VAL:HG13	1:A:189:ASP:HB3	1.91	0.52
1:A:298:GLU:C	1:A:300:LYS:H	2.12	0.52
1:B:369:GLU:HA	1:B:372:LYS:HD3	1.90	0.52
1:F:776:ASP:O	1:F:780:VAL:HG23	2.09	0.52
1:F:918:ILE:HG21	2:G:51:TYR:HB2	1.92	0.52
1:A:298:GLU:C	1:A:300:LYS:N	2.63	0.52
1:B:323:GLN:NE2	1:B:598:ASN:OD1	2.43	0.52
1:B:885:ILE:O	1:B:889:LEU:HG	2.09	0.52
2:D:22:VAL:HG23	2:D:69:ASP:HB3	1.90	0.52
1:F:174:PHE:HD2	1:F:178:PHE:HA	1.74	0.52
1:F:229:LEU:HD22	1:F:266:LEU:HD21	1.90	0.52
1:F:709:TYR:CZ	1:F:713:ILE:HD11	2.44	0.52
2:D:15:ARG:HB2	2:D:20:LYS:HE2	1.91	0.52
1:A:116:PRO:CB	1:B:517:ARG:HH12	2.22	0.52
1:B:62:LEU:HD21	1:B:107:PHE:CD2	2.45	0.52
1:E:150:SER:HB3	1:E:161:ALA:HB1	1.92	0.52
1:E:612:ILE:HG21	1:E:658:HIS:CD2	2.44	0.52
1:E:776:ASP:O	1:E:779:LEU:HD12	2.10	0.52
1:A:117:ILE:O	1:A:121:ILE:HG13	2.10	0.52
1:B:564:LYS:HB2	1:B:564:LYS:NZ	2.25	0.52
2:C:56:GLU:HG3	2:C:57:LYS:H	1.74	0.52
2:D:55:SER:O	2:D:57:LYS:N	2.43	0.52
1:E:802:ARG:CZ	1:E:840:LYS:HG3	2.40	0.52
2:G:13:PHE:HD2	2:G:22:VAL:HB	1.75	0.52
2:G:22:VAL:HG22	2:G:72:TRP:CH2	2.45	0.52
2:G:31:SER:OG	2:G:62:THR:OG1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:175:TYR:HB2	2:G:193:ILE:HB	1.92	0.52
1:B:749:LEU:HD12	1:B:753:LYS:HD2	1.92	0.52
2:D:173:VAL:HG22	2:D:175:TYR:CE1	2.45	0.52
1:E:472:TYR:O	1:E:476:ILE:HG12	2.10	0.52
1:F:382:ASN:OD1	1:F:383:ALA:N	2.43	0.52
1:A:690:GLY:O	1:A:693:GLU:HG3	2.10	0.51
1:A:955:ILE:HD13	1:B:632:ASP:HA	1.92	0.51
1:E:720:LEU:HB2	1:E:757:TRP:HZ3	1.76	0.51
1:A:566:ARG:CZ	1:B:566:ARG:HH12	2.23	0.51
1:A:906:THR:HG22	2:D:233:VAL:HG13	1.91	0.51
1:B:963:ASN:HB2	2:C:52:ILE:HG12	1.92	0.51
1:E:274:LEU:HD12	1:E:289:VAL:HG12	1.91	0.51
1:F:417:LYS:HA	1:F:417:LYS:HE2	1.92	0.51
1:A:103:ILE:HG23	1:A:107:PHE:CE2	2.45	0.51
1:A:267:ARG:HD2	1:A:268:ILE:H	1.75	0.51
1:A:395:CYS:SG	1:A:396:MET:N	2.83	0.51
1:B:602:SER:HA	1:B:605:PHE:CE1	2.46	0.51
1:E:522:PHE:HE1	1:E:527:LEU:HD21	1.75	0.51
1:F:610:GLN:HA	1:F:613:ARG:HD3	1.92	0.51
1:A:364:LYS:HA	1:A:381:PHE:HZ	1.76	0.51
1:A:695:ILE:HG21	1:A:744:PHE:CE1	2.45	0.51
1:B:333:VAL:HG22	1:B:541:ILE:HB	1.92	0.51
1:E:565:VAL:O	1:E:569:MET:HG2	2.10	0.51
1:F:225:ILE:O	1:F:229:LEU:HG	2.10	0.51
1:A:607:GLU:OE1	1:A:607:GLU:N	2.23	0.51
1:A:965:LYS:O	1:A:969:LYS:HG2	2.09	0.51
1:E:616:MET:O	1:E:620:ILE:HG22	2.09	0.51
1:F:47:GLY:O	1:F:133:ASN:ND2	2.33	0.51
1:F:61:ARG:HA	1:F:64:ASP:OD2	2.10	0.51
1:A:101:ASP:O	1:A:105:LYS:HG3	2.11	0.51
1:A:442:LEU:HD12	1:A:447:ARG:HB2	1.93	0.51
1:A:509:ASP:N	1:A:509:ASP:OD1	2.44	0.51
2:H:61:LEU:HD12	2:H:62:THR:H	1.74	0.51
1:B:396:MET:SD	1:B:397:ALA:N	2.84	0.51
1:E:210:THR:C	1:E:211:HIS:HD1	2.14	0.51
1:E:492:PHE:HA	2:H:204:PHE:HZ	1.76	0.51
1:F:663:ASP:HA	1:F:666:ASN:OD1	2.10	0.51
1:F:869:ILE:HG21	1:F:919:TRP:HZ2	1.75	0.51
2:G:177:THR:HG23	2:G:191:ILE:HB	1.93	0.51
1:E:808:ILE:HG21	1:E:815:PHE:CD2	2.46	0.51
1:F:627:ARG:HG2	1:F:628:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:882:GLU:HA	1:F:885:ILE:HG22	1.92	0.51
1:A:987:ARG:HD3	1:A:996:TYR:CG	2.46	0.51
1:B:242:LYS:HE3	1:B:242:LYS:HA	1.92	0.51
1:B:771:ILE:O	1:B:775:ILE:HG12	2.11	0.51
2:D:35:ALA:HB3	2:D:58:GLU:HG3	1.92	0.51
1:E:98:MET:H	1:E:98:MET:CE	2.24	0.51
2:H:24:THR:HA	2:H:68:PHE:HA	1.92	0.51
2:C:12:TYR:OH	2:C:176:ARG:NH2	2.44	0.51
1:E:319:LEU:HD23	1:E:325:ILE:HG12	1.91	0.51
1:F:659:PHE:CE2	1:F:667:LEU:HD11	2.46	0.51
1:A:607:GLU:OE2	2:D:209:GLU:N	2.34	0.50
1:A:947:GLU:HA	1:A:975:HIS:CE1	2.46	0.50
1:B:724:LYS:HD2	1:B:760:ARG:HH11	1.75	0.50
1:E:56:TYR:CZ	1:E:135:ASP:HB3	2.46	0.50
1:E:66:TYR:CD1	1:E:91:PHE:HD2	2.29	0.50
1:E:91:PHE:HE1	1:E:95:LYS:HD2	1.76	0.50
1:A:762:THR:HB	1:A:767:LEU:HD21	1.92	0.50
1:B:915:THR:HA	1:B:918:ILE:HD12	1.94	0.50
2:D:33:SER:OG	2:D:60:ASN:HB2	2.10	0.50
1:F:728:LEU:HD23	1:F:733:LEU:HB3	1.94	0.50
1:B:254:GLU:OE1	1:B:254:GLU:N	2.44	0.50
1:B:456:SER:O	1:B:459:ILE:HG22	2.11	0.50
1:F:454:LEU:O	1:F:458:ILE:HG22	2.11	0.50
2:H:20:LYS:HG2	2:H:22:VAL:HG23	1.92	0.50
1:B:226:ASN:O	1:B:229:LEU:HG	2.11	0.50
1:B:693:GLU:O	1:B:697:LYS:HG2	2.11	0.50
1:B:973:ASN:HD21	1:B:980:VAL:HG21	1.77	0.50
1:E:235:LEU:HD13	1:F:198:PRO:HB2	1.93	0.50
1:F:967:LEU:HD22	1:F:1003:TYR:HD2	1.76	0.50
1:A:270:ASP:OD2	1:A:273:SER:N	2.44	0.50
1:B:907:PHE:HE2	2:C:234:VAL:HG13	1.76	0.50
1:E:757:TRP:HA	1:E:760:ARG:HH21	1.76	0.50
1:E:979:HIS:O	1:E:983:VAL:HG23	2.12	0.50
1:F:101:ASP:HA	1:F:104:LEU:HG	1.92	0.50
1:F:894:VAL:HA	1:F:897:ILE:HG12	1.93	0.50
1:F:922:LEU:HD11	1:F:966:LEU:HD22	1.93	0.50
1:A:717:LYS:HE3	1:A:720:LEU:HD21	1.94	0.50
1:B:27:VAL:HA	1:B:30:ILE:HG22	1.93	0.50
1:B:304:LYS:HZ2	1:B:306:ASP:H	1.58	0.50
1:F:771:ILE:O	1:F:775:ILE:HG22	2.12	0.50
1:A:147:LYS:NZ	1:B:527:LEU:HA	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:ILE:HB	1:A:958:TRP:NE1	2.27	0.50
1:B:261:TYR:HD1	1:B:264:LYS:HD2	1.76	0.50
1:B:691:ILE:HD12	1:B:712:PHE:HZ	1.77	0.50
2:C:30:ALA:HA	2:C:62:THR:O	2.11	0.50
1:A:480:ARG:HB3	1:A:605:PHE:HZ	1.76	0.50
1:A:600:LEU:O	1:A:603:VAL:HG13	2.11	0.50
1:B:660:LYS:H	1:B:663:ASP:HB2	1.77	0.50
1:E:578:MET:HB2	1:E:582:ILE:HD11	1.92	0.50
1:F:170:VAL:O	1:F:193:TYR:OH	2.30	0.50
2:H:22:VAL:HG13	2:H:68:PHE:CE2	2.47	0.50
2:H:61:LEU:HD12	2:H:62:THR:N	2.27	0.50
1:B:978:HIS:O	1:B:981:ILE:HG13	2.11	0.50
1:E:383:ALA:HA	1:E:386:ASN:ND2	2.27	0.50
1:F:787:ILE:HA	1:F:833:LYS:HZ2	1.77	0.50
1:A:208:ILE:HA	1:A:213:ILE:HD11	1.94	0.49
1:F:261:TYR:HD1	1:F:264:LYS:HE2	1.77	0.49
2:H:23:PHE:CD1	2:H:24:THR:N	2.80	0.49
1:A:454:LEU:O	1:A:458:ILE:HD12	2.13	0.49
2:C:12:TYR:HD1	2:C:23:PHE:HB2	1.77	0.49
2:C:13:PHE:HB2	2:C:22:VAL:HG23	1.94	0.49
1:E:203:LEU:O	1:E:207:ILE:HG12	2.12	0.49
1:F:351:ASN:ND2	1:F:355:GLY:HA2	2.27	0.49
1:F:783:ALA:HA	1:F:786:HIS:NE2	2.27	0.49
1:A:253:ILE:HG13	1:A:257:THR:HB	1.93	0.49
1:A:476:ILE:O	1:A:480:ARG:HG2	2.13	0.49
1:A:852:HIS:CE1	1:A:856:PHE:CZ	2.98	0.49
1:E:115:ASN:OD1	1:E:118:HIS:ND1	2.33	0.49
1:E:487:GLN:NE2	2:H:207:SER:HA	2.27	0.49
1:A:203:LEU:O	1:A:207:ILE:HG12	2.12	0.49
1:A:740:LEU:HA	1:A:744:PHE:CD2	2.47	0.49
2:D:179:ALA:HB2	2:D:191:ILE:HD11	1.94	0.49
1:E:683:LYS:HA	1:E:686:GLU:HG3	1.93	0.49
1:F:680:GLU:HG3	1:F:683:LYS:NZ	2.27	0.49
2:G:52:ILE:HG23	2:G:53:LEU:H	1.76	0.49
2:H:36:ILE:HG12	2:H:57:LYS:HG2	1.93	0.49
2:C:177:THR:HG23	2:C:191:ILE:HB	1.94	0.49
2:D:24:THR:HG22	2:D:66:ALA:O	2.12	0.49
1:E:749:LEU:HA	1:E:753:LYS:HD2	1.95	0.49
1:E:755:TYR:HB2	1:E:804:TYR:CZ	2.48	0.49
1:A:964:ASP:OD1	1:A:964:ASP:N	2.45	0.49
2:D:208:LEU:HD11	2:D:212:ASN:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:827:LEU:HD22	1:E:831:LYS:HD2	1.94	0.49
1:A:59:TRP:O	1:A:63:VAL:HG23	2.13	0.49
1:A:929:LYS:O	1:A:929:LYS:HG2	2.12	0.49
1:B:958:TRP:CD1	1:B:958:TRP:N	2.81	0.49
2:D:15:ARG:HA	2:D:171:TYR:HA	1.94	0.49
1:E:390:LYS:HD3	1:E:390:LYS:C	2.33	0.49
1:E:409:ILE:HG21	1:E:414:TYR:HD2	1.77	0.49
1:E:713:ILE:O	1:E:717:LYS:HG3	2.12	0.49
1:F:25:ASN:OD1	1:F:26:VAL:N	2.45	0.49
1:F:115:ASN:HB2	1:F:116:PRO:HD2	1.94	0.49
1:F:260:TYR:CE1	1:F:264:LYS:HD3	2.47	0.49
1:F:291:ASP:HA	1:F:294:ILE:HG22	1.95	0.49
1:F:893:LYS:HB2	1:F:933:PHE:HE1	1.77	0.49
1:B:141:ALA:HA	1:B:144:LYS:HE2	1.94	0.49
1:B:905:GLN:O	1:B:906:THR:OG1	2.21	0.49
1:E:159:ALA:HB1	1:F:241:HIS:CE1	2.47	0.49
1:E:706:VAL:HA	1:E:709:TYR:HB3	1.94	0.49
1:F:696:THR:O	1:F:700:SER:HB3	2.12	0.49
2:H:11:VAL:HG12	2:H:23:PHE:HZ	1.78	0.49
1:A:30:ILE:HA	1:A:33:ILE:HD12	1.94	0.49
1:A:576:PHE:HB2	2:C:30:ALA:HB3	1.94	0.49
1:B:454:LEU:O	1:B:458:ILE:HG22	2.13	0.49
1:B:497:LEU:HD21	1:B:503:HIS:HB2	1.95	0.49
1:B:767:LEU:HD12	1:B:771:ILE:CD1	2.43	0.49
1:B:842:LEU:N	1:B:843:PRO:HD2	2.27	0.49
1:E:562:THR:HG22	1:E:618:LEU:HD22	1.94	0.49
1:F:31:LYS:HD2	1:F:31:LYS:O	2.12	0.49
1:A:224:ASN:O	1:A:228:LEU:HB2	2.12	0.49
1:A:398:LYS:HE3	1:A:398:LYS:HA	1.94	0.49
1:A:831:LYS:HB3	1:A:834:GLN:HB3	1.95	0.49
1:B:767:LEU:HD12	1:B:771:ILE:HD12	1.95	0.49
1:E:126:PRO:O	1:E:165:ARG:NH2	2.32	0.49
1:E:418:TYR:O	1:E:422:LYS:HG2	2.13	0.49
1:A:623:ALA:HA	1:A:626:GLU:OE2	2.13	0.48
1:A:930:MET:O	1:A:940:TYR:OH	2.26	0.48
1:E:606:HIS:O	1:E:610:GLN:HG2	2.13	0.48
1:E:708:PHE:HA	1:E:711:GLN:HE22	1.76	0.48
1:F:57:PRO:HB3	1:F:61:ARG:NH1	2.28	0.48
1:F:212:THR:C	1:F:213:ILE:HD13	2.33	0.48
1:A:169:LYS:HD3	1:A:173:ASP:HB3	1.94	0.48
1:A:545:LEU:HD11	1:A:594:PHE:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:14:LYS:O	2:G:172:GLU:N	2.46	0.48
1:A:359:ARG:O	1:A:363:LEU:HG	2.13	0.48
1:E:624:GLU:HB2	1:E:671:CYS:SG	2.54	0.48
1:E:962:TYR:HB3	1:E:966:LEU:HD23	1.94	0.48
1:F:255:ASN:O	1:F:258:LEU:HG	2.14	0.48
1:F:278:ASN:ND2	1:F:281:ASP:OD2	2.46	0.48
1:F:407:ILE:H	2:H:2:LYS:HB3	1.77	0.48
1:F:769:LYS:HA	1:F:772:ILE:HD12	1.96	0.48
1:A:242:LYS:NZ	1:A:267:ARG:HH11	2.12	0.48
1:A:840:LYS:HD2	1:A:867:ASN:HB3	1.96	0.48
1:B:376:LYS:HA	1:B:379:GLU:HG3	1.95	0.48
1:E:228:LEU:O	1:E:232:VAL:HG23	2.12	0.48
1:E:732:GLY:O	1:E:736:ILE:HG12	2.13	0.48
1:E:906:THR:HG22	2:H:233:VAL:HG13	1.94	0.48
1:E:987:ARG:HD2	1:E:996:TYR:CE2	2.48	0.48
1:F:376:LYS:HG2	1:F:380:ARG:HH21	1.77	0.48
1:F:564:LYS:O	1:F:564:LYS:NZ	2.31	0.48
1:F:594:PHE:O	1:F:598:ASN:ND2	2.46	0.48
1:F:707:VAL:O	1:F:710:THR:OG1	2.20	0.48
2:H:22:VAL:HG13	2:H:68:PHE:HE2	1.77	0.48
1:A:205:LYS:HZ2	1:A:231:TRP:HE3	1.58	0.48
1:A:480:ARG:HD3	1:A:483:GLN:NE2	2.29	0.48
1:A:803:ASP:HA	1:A:806:ALA:HB3	1.94	0.48
1:A:937:ASP:HB3	1:A:940:TYR:HB3	1.93	0.48
1:E:98:MET:H	1:E:98:MET:HE2	1.78	0.48
1:F:188:ASP:OD1	1:F:189:ASP:N	2.46	0.48
1:A:674:ASP:HA	1:A:725:TYR:CD2	2.48	0.48
1:A:708:PHE:O	1:A:712:PHE:HB2	2.14	0.48
1:B:203:LEU:O	1:B:207:ILE:HG13	2.14	0.48
1:B:425:ILE:HG21	1:B:447:ARG:NH2	2.29	0.48
2:D:13:PHE:HA	2:D:173:VAL:HA	1.95	0.48
1:F:316:ILE:HD12	1:F:384:LEU:HD13	1.94	0.48
1:F:875:ASP:OD2	2:G:49:PRO:HD2	2.12	0.48
1:F:933:PHE:HB3	1:F:940:TYR:CE2	2.48	0.48
2:G:34:GLN:NE2	2:G:57:LYS:HE3	2.28	0.48
1:A:405:THR:H	2:C:4:VAL:CG1	2.25	0.48
1:A:495:LEU:HD13	2:D:218:ILE:HD12	1.95	0.48
1:E:612:ILE:HG21	1:E:658:HIS:CG	2.48	0.48
1:F:118:HIS:HA	1:F:121:ILE:HG22	1.95	0.48
1:F:388:PHE:O	1:F:392:GLY:N	2.46	0.48
2:D:13:PHE:HB2	2:D:23:PHE:CG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:ASN:O	1:E:259:ILE:HG12	2.14	0.48
1:F:308:VAL:HG13	1:F:356:TYR:HB2	1.96	0.48
1:F:722:PHE:C	1:F:724:LYS:H	2.17	0.48
1:A:107:PHE:CD1	1:A:107:PHE:N	2.81	0.48
1:A:607:GLU:HA	1:A:610:GLN:OE1	2.12	0.48
1:B:83:GLU:O	1:B:87:ILE:HG13	2.13	0.48
1:F:825:LEU:HD11	1:F:852:HIS:HB3	1.94	0.48
2:H:14:LYS:HB2	2:H:172:GLU:HG3	1.94	0.48
1:A:893:LYS:HD2	1:A:933:PHE:CE2	2.49	0.48
1:A:925:ILE:HG22	1:A:927:ASN:H	1.78	0.48
1:B:50:VAL:HG23	1:B:115:ASN:HD21	1.79	0.48
1:B:379:GLU:HA	1:B:382:ASN:HD21	1.78	0.48
1:A:71:TYR:OH	1:E:257:THR:OG1	2.32	0.47
1:A:587:ARG:O	1:A:591:ASN:ND2	2.47	0.47
1:A:664:ILE:O	1:A:667:LEU:HG	2.14	0.47
1:E:433:GLU:OE1	1:E:433:GLU:N	2.41	0.47
2:H:64:LYS:HB3	2:H:217:GLU:HA	1.95	0.47
1:A:37:SER:OG	1:A:124:MET:SD	2.63	0.47
1:A:437:LYS:HD3	1:A:437:LYS:N	2.30	0.47
1:E:32:GLU:OE1	1:E:267:ARG:NH1	2.47	0.47
1:E:916:PHE:HA	1:E:919:TRP:CZ3	2.49	0.47
1:F:649:TYR:HE1	1:F:687:TYR:HB2	1.79	0.47
2:G:52:ILE:C	2:G:54:LYS:H	2.17	0.47
2:H:60:ASN:OD1	2:H:60:ASN:N	2.46	0.47
1:A:199:LEU:HD23	1:A:202:ASN:HD21	1.79	0.47
1:A:341:GLU:HB2	1:A:345:THR:HG22	1.97	0.47
1:A:860:GLU:HB3	1:A:884:LEU:HD11	1.96	0.47
1:E:595:LEU:HD13	1:E:600:LEU:HD11	1.97	0.47
1:E:607:GLU:OE2	2:H:209:GLU:N	2.46	0.47
1:F:91:PHE:HE2	1:F:100:PHE:HA	1.79	0.47
1:F:546:SER:OG	1:F:547:ASP:N	2.48	0.47
1:A:229:LEU:HD22	1:A:266:LEU:HD21	1.97	0.47
1:A:476:ILE:HD11	1:A:480:ARG:NE	2.30	0.47
1:B:79:TYR:HB2	1:B:84:TYR:CE2	2.49	0.47
1:B:118:HIS:O	1:B:121:ILE:HG22	2.14	0.47
1:B:557:LYS:O	1:B:561:LEU:HD23	2.15	0.47
1:B:717:LYS:HG2	1:B:757:TRP:CH2	2.47	0.47
1:B:878:THR:H	1:B:881:HIS:CE1	2.32	0.47
1:F:89:GLN:HG2	1:F:186:LYS:HB2	1.96	0.47
1:A:288:ALA:O	1:A:292:LEU:HG	2.15	0.47
1:A:412:LEU:HD12	1:A:441:PHE:HZ	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:TYR:HA	1:A:421:MET:HG3	1.96	0.47
1:A:797:ASN:HD21	1:A:799:LEU:HD13	1.79	0.47
1:B:218:TYR:HE1	1:B:221:GLY:H	1.63	0.47
1:E:680:GLU:HG2	1:E:683:LYS:NZ	2.30	0.47
1:E:720:LEU:HD13	1:E:740:LEU:HD12	1.97	0.47
1:F:755:TYR:HE1	1:F:807:LEU:HD23	1.79	0.47
1:B:442:LEU:HD11	1:B:454:LEU:HD13	1.96	0.47
1:B:919:TRP:HZ3	2:C:50:LEU:HG	1.79	0.47
1:E:111:ASP:N	1:E:111:ASP:OD1	2.48	0.47
1:A:197:TYR:HB3	1:A:200:ILE:HG12	1.95	0.47
1:A:448:TRP:N	1:A:448:TRP:HD1	2.12	0.47
1:A:469:CYS:HB2	1:A:539:TYR:CE2	2.49	0.47
1:A:931:GLU:OE1	1:A:931:GLU:N	2.46	0.47
1:A:966:LEU:HB2	2:D:51:TYR:OH	2.14	0.47
1:B:564:LYS:O	1:B:567:SER:OG	2.27	0.47
1:B:796:SER:O	1:B:796:SER:OG	2.29	0.47
2:C:72:TRP:O	2:C:76:THR:HG22	2.14	0.47
1:E:121:ILE:HA	1:E:290:MET:CE	2.45	0.47
1:E:456:SER:O	1:E:460:LEU:HG	2.15	0.47
1:E:469:CYS:HB3	1:E:539:TYR:HE2	1.79	0.47
1:E:763:LYS:HD3	1:E:763:LYS:C	2.35	0.47
1:E:808:ILE:HG21	1:E:815:PHE:HD2	1.80	0.47
1:F:225:ILE:HA	1:F:228:LEU:HG	1.96	0.47
1:F:533:PHE:HA	1:F:536:GLN:HG3	1.96	0.47
1:F:574:TYR:N	2:H:32:PHE:O	2.37	0.47
1:F:802:ARG:HB3	1:F:840:LYS:CG	2.44	0.47
1:F:960:LYS:HE3	1:F:995:ARG:HG2	1.96	0.47
1:A:118:HIS:HA	1:A:121:ILE:CD1	2.45	0.47
1:A:728:LEU:HD12	1:A:729:SER:N	2.29	0.47
1:B:67:HIS:ND1	1:B:73:SER:O	2.48	0.47
1:B:212:THR:C	1:B:213:ILE:HD13	2.36	0.47
1:A:434:ASP:O	1:A:438:LYS:HG3	2.15	0.47
1:A:589:TYR:OH	1:A:651:ASP:OD1	2.32	0.47
1:B:233:ARG:HH12	1:B:240:PHE:HE2	1.62	0.47
1:B:510:GLU:O	1:B:514:ARG:HG2	2.15	0.47
2:D:4:VAL:HG21	2:D:6:GLN:HE21	1.79	0.47
1:E:704:MET:HE2	1:E:704:MET:HA	1.97	0.47
1:E:966:LEU:HB2	2:H:51:TYR:OH	2.14	0.47
1:F:406:SER:HA	2:H:2:LYS:H	1.78	0.47
1:A:419:ASP:N	1:A:419:ASP:OD1	2.47	0.47
1:A:531:MET:HB3	1:A:535:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:THR:HG23	1:E:261:TYR:CE1	2.49	0.47
1:E:609:HIS:O	1:E:612:ILE:HG22	2.14	0.47
1:F:456:SER:O	1:F:459:ILE:HG22	2.14	0.47
1:A:358:GLU:O	1:A:362:GLU:HG2	2.15	0.46
1:A:559:PHE:CD1	1:B:559:PHE:HD1	2.32	0.46
1:B:666:ASN:OD1	1:B:666:ASN:N	2.47	0.46
1:E:56:TYR:CE1	1:E:135:ASP:HB3	2.50	0.46
1:E:205:LYS:HE3	1:F:202:ASN:ND2	2.30	0.46
1:F:245:PHE:HD1	1:F:246:ILE:H	1.63	0.46
1:F:587:ARG:HA	1:F:590:ASP:OD2	2.15	0.46
1:A:267:ARG:HD2	1:A:268:ILE:N	2.31	0.46
1:A:282:TYR:HA	1:A:285:ARG:NH1	2.31	0.46
1:A:678:PHE:CE1	1:A:726:VAL:HG23	2.51	0.46
1:A:746:GLU:N	1:A:746:GLU:OE1	2.49	0.46
1:E:75:LYS:NZ	1:E:78:ASN:O	2.40	0.46
1:E:724:LYS:HD2	1:E:760:ARG:CB	2.46	0.46
1:F:31:LYS:HD2	1:F:31:LYS:C	2.36	0.46
1:F:153:SER:HB2	1:F:169:LYS:HE3	1.96	0.46
1:F:828:THR:N	1:F:830:ASP:OD2	2.47	0.46
2:H:12:TYR:CE2	2:H:176:ARG:HB2	2.50	0.46
1:A:489:VAL:HA	1:A:492:PHE:HD2	1.80	0.46
1:B:27:VAL:HG12	1:B:31:LYS:HZ2	1.80	0.46
1:B:449:GLU:HB2	1:B:511:PHE:CE2	2.51	0.46
1:B:544:PHE:O	1:B:550:PHE:HB3	2.15	0.46
1:B:891:THR:HA	1:B:894:VAL:HG22	1.98	0.46
1:E:86:ARG:O	1:E:90:ILE:HG13	2.15	0.46
1:E:711:GLN:OE1	1:E:711:GLN:N	2.38	0.46
1:F:705:ASN:HB2	1:F:707:VAL:HG12	1.97	0.46
2:G:56:GLU:O	2:G:57:LYS:HB2	2.15	0.46
1:A:199:LEU:HA	1:A:202:ASN:HD21	1.80	0.46
1:A:673:ILE:HG23	1:A:725:TYR:CE2	2.50	0.46
1:A:984:LEU:HD13	1:A:1000:LEU:HD13	1.97	0.46
1:B:109:GLN:OE1	1:B:109:GLN:N	2.39	0.46
1:B:405:THR:HG21	1:B:586:LEU:HD11	1.96	0.46
1:B:924:GLU:HG2	2:C:50:LEU:HD12	1.98	0.46
1:E:376:LYS:O	1:E:379:GLU:HG3	2.15	0.46
1:E:459:ILE:HD11	1:E:475:GLN:NE2	2.28	0.46
1:E:879:PRO:O	1:E:883:GLU:HG2	2.16	0.46
1:F:558:LEU:HD11	1:F:615:SER:HB3	1.96	0.46
1:F:576:PHE:CD2	2:H:30:ALA:HB1	2.50	0.46
1:A:448:TRP:HZ3	1:A:484:SER:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:TYR:OH	1:B:648:GLU:OE2	2.33	0.46
2:D:200:PRO:HB3	2:D:220:PHE:CE1	2.51	0.46
1:F:433:GLU:CD	1:F:433:GLU:H	2.19	0.46
1:F:531:MET:CE	1:F:535:PHE:HB2	2.45	0.46
1:F:541:ILE:HD12	1:F:541:ILE:H	1.80	0.46
1:F:603:VAL:HA	1:F:608:PHE:CD2	2.51	0.46
1:A:131:THR:HB	1:A:169:LYS:HA	1.97	0.46
1:B:942:PHE:HE1	1:B:949:PHE:CE2	2.34	0.46
1:B:980:VAL:HG11	1:B:1004:PHE:CZ	2.50	0.46
1:F:109:GLN:OE1	1:F:109:GLN:N	2.32	0.46
1:F:324:TYR:HE1	1:F:391:ASN:HA	1.81	0.46
1:A:65:LYS:HG2	1:A:107:PHE:CZ	2.51	0.46
1:A:482:TYR:CE2	1:A:519:MET:HG3	2.51	0.46
1:A:886:ILE:HB	1:A:929:LYS:NZ	2.31	0.46
1:B:68:GLU:HA	1:B:73:SER:N	2.31	0.46
1:B:398:LYS:HE2	1:B:398:LYS:HA	1.98	0.46
1:B:513:ALA:O	1:B:517:ARG:HG2	2.16	0.46
1:F:225:ILE:O	1:F:228:LEU:HD12	2.15	0.46
2:H:55:SER:O	2:H:57:LYS:N	2.48	0.46
1:A:126:PRO:O	1:A:165:ARG:NH2	2.45	0.46
1:A:436:TYR:CZ	1:A:599:CYS:HB2	2.51	0.46
2:D:58:GLU:C	2:D:59:ILE:HD13	2.36	0.46
1:A:188:ASP:O	1:A:191:LEU:HD12	2.16	0.46
1:A:678:PHE:HE1	1:A:681:GLN:HG3	1.80	0.46
1:B:683:LYS:HA	1:B:686:GLU:OE1	2.16	0.46
2:D:58:GLU:OE1	2:D:60:ASN:ND2	2.49	0.46
1:E:455:TYR:HA	1:E:458:ILE:HG12	1.98	0.46
1:F:869:ILE:HG23	1:F:874:ILE:HA	1.98	0.46
2:G:14:LYS:NZ	2:G:174:GLU:HB2	2.31	0.46
1:A:201:SER:O	1:A:205:LYS:HG2	2.16	0.46
1:B:61:ARG:HA	1:B:64:ASP:OD2	2.15	0.46
1:B:919:TRP:HB3	1:B:925:ILE:HD12	1.97	0.46
1:E:728:LEU:HG	1:E:733:LEU:HG	1.98	0.46
1:F:442:LEU:HB2	1:F:451:SER:HB3	1.98	0.46
1:F:757:TRP:O	1:F:760:ARG:HB3	2.15	0.46
1:A:23:ASP:HB3	1:A:26:VAL:HG23	1.96	0.45
1:B:188:ASP:O	1:B:192:ASN:ND2	2.48	0.45
1:B:553:ASP:HB3	1:B:557:LYS:NZ	2.31	0.45
1:B:927:ASN:HB3	1:B:930:MET:HE2	1.98	0.45
2:D:60:ASN:ND2	2:D:221:GLU:OE2	2.49	0.45
1:E:627:ARG:HD3	1:E:675:LYS:NZ	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:847:THR:HA	1:E:850:LYS:HG2	1.98	0.45
1:F:246:ILE:HD13	1:F:269:ILE:HB	1.98	0.45
1:F:967:LEU:HD22	1:F:1003:TYR:CD2	2.51	0.45
1:A:259:ILE:O	1:A:262:GLU:HG3	2.15	0.45
2:C:48:LYS:HD3	2:C:50:LEU:HD13	1.98	0.45
1:F:657:ARG:HA	1:F:715:GLU:HG2	1.98	0.45
2:H:231:MET:SD	2:H:231:MET:N	2.89	0.45
1:A:754:ARG:HD3	1:A:757:TRP:HZ3	1.81	0.45
1:E:144:LYS:HB2	1:E:144:LYS:HE2	1.71	0.45
1:E:323:GLN:O	1:E:390:LYS:NZ	2.28	0.45
1:F:56:TYR:CD1	1:F:57:PRO:HD2	2.51	0.45
1:F:446:GLY:O	1:F:448:TRP:N	2.48	0.45
1:F:788:ASP:H	1:F:833:LYS:HD3	1.81	0.45
1:A:199:LEU:HA	1:A:202:ASN:ND2	2.32	0.45
1:A:738:LYS:HD2	1:A:742:PHE:HD2	1.81	0.45
1:A:899:GLU:HG2	1:A:904:ILE:HB	1.99	0.45
1:B:45:PHE:CZ	1:B:208:ILE:HD13	2.52	0.45
1:F:308:VAL:O	1:F:312:ILE:HG12	2.17	0.45
1:F:558:LEU:O	1:F:562:THR:HG23	2.16	0.45
2:G:14:LYS:N	2:G:172:GLU:O	2.48	0.45
1:A:915:THR:HA	1:A:918:ILE:HD12	1.97	0.45
2:C:4:VAL:HG13	2:C:6:GLN:OE1	2.16	0.45
2:D:179:ALA:O	2:D:189:SER:OG	2.34	0.45
1:E:242:LYS:N	1:E:242:LYS:HD3	2.32	0.45
1:E:967:LEU:O	1:E:970:ILE:HG22	2.15	0.45
1:F:651:ASP:O	1:F:655:ILE:HG13	2.17	0.45
2:H:20:LYS:HG3	2:H:72:TRP:CD1	2.50	0.45
1:A:260:TYR:HB2	1:E:90:ILE:HG23	1.99	0.45
1:E:753:LYS:O	1:E:757:TRP:HD1	1.99	0.45
1:F:140:THR:O	1:F:144:LYS:HG3	2.17	0.45
1:F:522:PHE:HZ	1:F:527:LEU:HD22	1.80	0.45
2:G:13:PHE:HD1	2:G:173:VAL:HG22	1.80	0.45
1:A:309:ILE:O	1:A:313:TYR:HB2	2.15	0.45
1:A:437:LYS:O	1:A:441:PHE:HD1	2.00	0.45
1:A:440:PHE:CG	1:A:599:CYS:HB3	2.51	0.45
1:B:955:ILE:HD12	1:B:958:TRP:HZ2	1.82	0.45
2:C:198:VAL:HG12	2:C:220:PHE:CD1	2.52	0.45
1:A:303:THR:OG1	1:A:304:LYS:N	2.43	0.45
1:A:751:ILE:O	1:A:754:ARG:HB2	2.17	0.45
1:E:30:ILE:HA	1:E:33:ILE:HD12	1.98	0.45
1:E:33:ILE:HD13	1:E:293:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ASN:HB3	1:F:205:LYS:HE3	1.99	0.45
1:E:662:ASP:HA	1:E:665:LYS:NZ	2.32	0.45
1:E:779:LEU:HA	1:E:782:GLN:HG3	1.97	0.45
1:E:863:ASN:HA	1:E:866:MET:HG2	1.99	0.45
1:F:731:GLU:H	1:F:731:GLU:CD	2.20	0.45
1:F:869:ILE:O	1:F:874:ILE:HG12	2.16	0.45
1:F:904:ILE:HG23	2:G:235:ILE:HA	1.99	0.45
2:G:39:GLU:OE2	2:G:41:LEU:HG	2.16	0.45
1:E:103:ILE:HA	1:E:106:ASP:OD2	2.17	0.45
1:E:366:SER:O	1:E:370:ARG:NH1	2.49	0.45
1:F:386:ASN:O	1:F:389:GLU:HG3	2.16	0.45
1:F:625:TYR:CZ	1:F:629:ARG:HD3	2.52	0.45
1:A:325:ILE:N	1:A:325:ILE:HD12	2.32	0.45
1:A:565:VAL:O	1:A:569:MET:HG2	2.16	0.45
1:B:566:ARG:HA	1:B:569:MET:HG2	1.99	0.45
2:C:39:GLU:HG2	2:C:40:LYS:H	1.81	0.45
2:D:174:GLU:HG2	2:D:194:GLN:HB3	1.98	0.45
1:E:90:ILE:O	1:E:94:VAL:HG12	2.16	0.45
1:E:485:ILE:HG21	1:E:511:PHE:CZ	2.52	0.45
2:H:206:MET:HG3	2:H:208:LEU:HD22	1.99	0.45
1:A:512:LEU:HG	1:A:516:GLU:OE2	2.17	0.44
1:A:658:HIS:C	1:A:659:PHE:HD1	2.20	0.44
1:B:386:ASN:HA	1:B:389:GLU:OE1	2.17	0.44
1:B:405:THR:H	2:D:4:VAL:HG11	1.82	0.44
1:B:769:LYS:HD3	1:B:772:ILE:HD12	2.00	0.44
1:B:974:LYS:HD3	1:B:974:LYS:N	2.32	0.44
2:C:203:GLU:OE1	2:C:203:GLU:N	2.49	0.44
1:E:531:MET:HG2	1:E:535:PHE:HD2	1.82	0.44
1:E:687:TYR:O	1:E:691:ILE:HG12	2.16	0.44
1:F:79:TYR:HB2	1:F:84:TYR:CZ	2.52	0.44
1:A:605:PHE:CD1	1:A:605:PHE:N	2.84	0.44
1:A:622:LYS:HD2	1:A:622:LYS:O	2.17	0.44
1:A:913:MET:HA	1:A:916:PHE:HD2	1.81	0.44
1:E:326:ARG:HD2	1:E:329:ASP:HB2	1.98	0.44
1:E:963:ASN:HD22	2:H:51:TYR:HE1	1.64	0.44
2:H:68:PHE:CZ	2:H:73:LEU:HB2	2.52	0.44
1:A:755:TYR:O	1:A:758:LEU:HD12	2.17	0.44
1:A:818:LYS:HE3	1:A:819:ARG:HH12	1.81	0.44
1:B:1001:MET:SD	1:B:1001:MET:N	2.91	0.44
2:D:231:MET:HE2	2:D:231:MET:HB2	1.83	0.44
1:E:313:TYR:CE2	1:E:380:ARG:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:809:LYS:NZ	1:E:813:LYS:O	2.49	0.44
2:G:54:LYS:HD2	2:G:54:LYS:HA	1.82	0.44
1:A:30:ILE:HD12	1:A:30:ILE:H	1.83	0.44
1:A:1001:MET:HA	1:A:1005:ILE:HD12	2.00	0.44
1:B:545:LEU:HD21	1:B:594:PHE:HZ	1.81	0.44
1:B:830:ASP:N	1:B:830:ASP:OD1	2.51	0.44
1:E:560:GLU:HB3	1:E:564:LYS:HZ1	1.82	0.44
1:F:962:TYR:CB	1:F:967:LEU:HD12	2.48	0.44
2:H:24:THR:HG22	2:H:66:ALA:O	2.17	0.44
1:A:511:PHE:O	1:A:515:ILE:HG12	2.17	0.44
1:B:27:VAL:HG12	1:B:31:LYS:HZ1	1.81	0.44
1:B:729:SER:O	1:B:733:LEU:HG	2.18	0.44
2:D:52:ILE:HD11	2:D:54:LYS:HB2	2.00	0.44
1:F:728:LEU:HB3	1:F:733:LEU:HB3	1.99	0.44
1:F:946:PRO:HB2	1:F:976:MET:HE1	1.98	0.44
2:G:203:GLU:N	2:G:203:GLU:OE1	2.51	0.44
1:A:358:GLU:HG2	1:A:359:ARG:N	2.33	0.44
1:A:436:TYR:OH	1:A:599:CYS:O	2.35	0.44
1:A:603:VAL:HA	1:A:608:PHE:CD2	2.53	0.44
1:B:769:LYS:HA	1:B:772:ILE:HD12	2.00	0.44
1:E:383:ALA:HA	1:E:386:ASN:HD21	1.83	0.44
1:E:535:PHE:CD1	1:E:539:TYR:HB2	2.52	0.44
1:E:549:GLN:HA	1:E:552:TYR:HB2	1.98	0.44
1:E:578:MET:SD	2:G:28:GLN:HG3	2.57	0.44
1:F:818:LYS:HG3	1:F:820:LEU:HG	1.99	0.44
2:H:23:PHE:CG	2:H:24:THR:N	2.85	0.44
1:A:322:LEU:HD22	1:A:542:LEU:HD21	1.99	0.44
1:A:958:TRP:N	1:A:958:TRP:CD1	2.85	0.44
1:B:116:PRO:O	1:B:120:LYS:HG2	2.17	0.44
1:B:254:GLU:HB3	1:B:256:GLU:OE1	2.18	0.44
2:C:14:LYS:HB3	2:C:172:GLU:HG3	1.99	0.44
1:E:433:GLU:H	1:E:433:GLU:CD	2.17	0.44
1:A:327:LYS:HD2	1:A:342:VAL:HA	1.99	0.44
1:B:92:TYR:CG	1:B:186:LYS:HE2	2.53	0.44
1:B:824:THR:HG22	1:B:838:LEU:HD13	2.00	0.44
2:C:11:VAL:HG13	2:C:175:TYR:HE1	1.82	0.44
2:D:23:PHE:HA	2:D:68:PHE:HD2	1.83	0.44
1:E:210:THR:O	1:E:211:HIS:ND1	2.47	0.44
1:E:512:LEU:HA	1:E:515:ILE:HG22	2.00	0.44
1:E:866:MET:SD	1:E:866:MET:N	2.91	0.44
1:F:727:LYS:HA	1:F:727:LYS:HD3	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:794:VAL:HG22	2:G:223:LEU:HD12	1.99	0.44
2:G:54:LYS:O	2:G:56:GLU:HG2	2.17	0.44
1:A:215:PHE:HB2	1:A:245:PHE:HB2	1.99	0.44
1:A:766:GLU:O	1:A:768:PRO:HD3	2.17	0.44
1:A:910:ASN:ND2	2:D:227:ASP:O	2.50	0.44
1:E:576:PHE:HB2	2:G:30:ALA:HB3	2.00	0.44
1:E:690:GLY:O	1:E:693:GLU:HG3	2.17	0.44
1:E:755:TYR:CE2	1:E:803:ASP:HB3	2.48	0.44
1:E:847:THR:HA	1:E:850:LYS:HE3	2.00	0.44
1:F:131:THR:HG23	1:F:169:LYS:HG2	2.00	0.44
1:F:281:ASP:N	1:F:285:ARG:HH21	2.15	0.44
1:F:632:ASP:OD1	1:F:632:ASP:N	2.47	0.44
1:F:732:GLY:O	1:F:736:ILE:HG12	2.18	0.44
1:A:574:TYR:CE1	1:A:634:LEU:HD21	2.53	0.43
1:B:519:MET:SD	1:B:519:MET:N	2.91	0.43
1:B:965:LYS:HZ3	1:B:966:LEU:HD21	1.83	0.43
1:B:997:LEU:O	1:B:1001:MET:HG2	2.18	0.43
2:C:11:VAL:HG11	2:C:63:VAL:HG11	1.99	0.43
1:E:412:LEU:HD23	1:E:420:VAL:HG23	2.00	0.43
1:E:592:LEU:HD12	1:E:592:LEU:HA	1.87	0.43
1:F:119:ASP:HB3	1:F:145:ARG:HH21	1.83	0.43
1:F:448:TRP:HA	1:F:451:SER:OG	2.18	0.43
1:F:910:ASN:HD21	2:G:229:ASP:N	2.04	0.43
2:G:48:LYS:HA	2:G:48:LYS:HD3	1.88	0.43
1:A:122:LEU:CD1	1:A:142:CYS:HA	2.48	0.43
1:A:691:ILE:HG22	1:A:695:ILE:HD11	1.99	0.43
1:A:839:PHE:HA	1:A:853:LEU:HD21	1.99	0.43
1:B:534:GLU:HA	1:B:537:LYS:HG2	2.00	0.43
2:D:41:LEU:HD11	2:D:54:LYS:HE2	1.99	0.43
1:E:27:VAL:O	1:E:31:LYS:HG3	2.18	0.43
1:E:66:TYR:OH	1:E:104:LEU:HD23	2.18	0.43
1:E:913:MET:HA	1:E:916:PHE:CE2	2.53	0.43
1:F:459:ILE:HD12	1:F:459:ILE:HA	1.91	0.43
1:F:669:ARG:HB2	1:F:669:ARG:CZ	2.48	0.43
1:F:758:LEU:O	1:F:762:THR:HG23	2.18	0.43
1:A:134:TYR:HB3	1:A:174:PHE:HE1	1.82	0.43
1:A:352:LYS:HA	1:A:352:LYS:HD3	1.80	0.43
1:A:388:PHE:HA	1:A:391:ASN:ND2	2.34	0.43
1:A:680:GLU:O	1:A:684:ILE:HG13	2.17	0.43
1:A:890:GLU:O	1:A:893:LYS:HG2	2.18	0.43
1:B:70:LEU:HD22	1:B:71:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:SER:O	2:C:201:SER:OG	2.32	0.43
2:D:35:ALA:O	2:D:57:LYS:HA	2.18	0.43
2:D:217:GLU:C	2:D:218:ILE:HD13	2.39	0.43
1:E:148:TYR:CG	1:F:532:PRO:HD3	2.53	0.43
1:F:51:SER:HA	1:F:137:LEU:HD11	2.00	0.43
1:A:565:VAL:HB	1:A:618:LEU:HD11	1.99	0.43
1:A:656:SER:O	1:A:715:GLU:HB2	2.19	0.43
1:B:414:TYR:HD1	1:B:596:TYR:HE2	1.66	0.43
1:B:906:THR:HB	1:B:907:PHE:H	1.61	0.43
2:D:180:TYR:HE1	2:D:187:VAL:HG22	1.82	0.43
1:E:189:ASP:O	1:E:193:TYR:N	2.52	0.43
1:E:395:CYS:SG	1:E:396:MET:N	2.91	0.43
1:E:573:SER:O	1:E:629:ARG:NH2	2.38	0.43
1:E:655:ILE:HG23	1:E:659:PHE:CD2	2.53	0.43
1:F:419:ASP:OD1	1:F:419:ASP:N	2.51	0.43
2:G:65:ASN:ND2	2:G:67:PHE:O	2.52	0.43
1:A:919:TRP:HB3	1:A:924:GLU:CB	2.47	0.43
1:B:66:TYR:HB3	1:B:91:PHE:CD2	2.54	0.43
1:B:417:LYS:O	1:B:421:MET:HG3	2.18	0.43
2:D:15:ARG:HB3	2:D:20:LYS:HB3	1.99	0.43
1:E:516:GLU:O	1:E:520:THR:OG1	2.32	0.43
1:E:771:ILE:HA	1:E:774:ILE:HD13	2.00	0.43
1:E:983:VAL:HG12	1:E:987:ARG:CZ	2.48	0.43
1:F:780:VAL:CG2	1:F:820:LEU:HD22	2.47	0.43
1:F:922:LEU:HD21	1:F:966:LEU:HB2	2.00	0.43
1:F:963:ASN:ND2	2:G:52:ILE:H	2.16	0.43
2:H:48:LYS:H	2:H:48:LYS:HD2	1.84	0.43
1:A:339:HIS:CE1	2:C:213:ALA:HB2	2.54	0.43
1:A:616:MET:HG3	1:A:659:PHE:HZ	1.83	0.43
1:A:956:PRO:HB2	1:A:987:ARG:CZ	2.49	0.43
1:B:45:PHE:HZ	1:B:208:ILE:HD13	1.84	0.43
1:B:442:LEU:HD12	1:B:451:SER:HA	2.01	0.43
1:E:43:VAL:O	1:E:213:ILE:HA	2.19	0.43
1:E:83:GLU:HA	1:E:86:ARG:HB3	2.01	0.43
1:E:117:ILE:HD11	1:E:283:LEU:HD12	2.00	0.43
1:F:421:MET:O	1:F:425:ILE:HG22	2.19	0.43
2:H:48:LYS:HD2	2:H:48:LYS:N	2.33	0.43
1:B:203:LEU:HD23	1:B:207:ILE:HD11	2.01	0.43
1:B:724:LYS:HG3	1:B:725:TYR:N	2.33	0.43
1:E:220:LEU:HD11	1:E:247:ARG:NH2	2.34	0.43
1:E:595:LEU:CD1	1:E:600:LEU:HD11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:987:ARG:HD2	1:E:996:TYR:HE2	1.84	0.43
1:F:218:TYR:OH	1:F:226:ASN:OD1	2.36	0.43
1:F:705:ASN:OD1	1:F:705:ASN:N	2.50	0.43
1:F:899:GLU:O	1:F:903:GLY:N	2.44	0.43
1:A:67:HIS:ND1	1:A:73:SER:O	2.52	0.43
1:A:732:GLY:O	1:A:736:ILE:HG12	2.18	0.43
1:B:657:ARG:HB3	1:B:658:HIS:HD2	1.83	0.43
1:E:533:PHE:HB3	1:E:537:LYS:HZ1	1.84	0.43
1:E:585:LEU:HD12	1:E:588:LEU:HD23	2.00	0.43
1:F:544:PHE:O	1:F:550:PHE:HB3	2.19	0.43
1:F:627:ARG:NH2	1:F:672:SER:OG	2.49	0.43
2:H:61:LEU:O	2:H:220:PHE:N	2.47	0.43
1:A:480:ARG:HH11	1:A:483:GLN:NE2	2.16	0.43
1:B:168:LEU:HD11	1:B:200:ILE:HD12	2.00	0.43
1:E:75:LYS:HZ2	1:E:79:TYR:HA	1.84	0.43
1:E:808:ILE:O	1:E:812:GLU:N	2.51	0.43
1:F:377:GLN:O	1:F:380:ARG:HG2	2.19	0.43
1:F:404:ASN:O	2:H:1:MET:N	2.45	0.43
1:F:755:TYR:CZ	1:F:803:ASP:HB3	2.53	0.43
1:A:695:ILE:HD13	1:A:744:PHE:CZ	2.54	0.43
1:B:79:TYR:HB2	1:B:84:TYR:CZ	2.54	0.43
1:F:225:ILE:HG23	1:F:228:LEU:HD11	2.00	0.43
1:F:837:PHE:HB3	1:F:840:LYS:HD2	2.01	0.43
2:H:175:TYR:N	2:H:193:ILE:O	2.49	0.43
1:A:388:PHE:HA	1:A:391:ASN:HD21	1.84	0.42
1:E:75:LYS:HD2	1:E:79:TYR:CD1	2.54	0.42
1:E:407:ILE:HD13	1:E:589:TYR:CG	2.54	0.42
1:E:933:PHE:O	1:E:936:MET:HG2	2.19	0.42
1:F:38:ARG:HH22	1:F:298:GLU:HB2	1.84	0.42
2:G:2:LYS:HD2	2:G:3:THR:OG1	2.19	0.42
2:H:35:ALA:O	2:H:58:GLU:N	2.52	0.42
2:H:51:TYR:HD1	2:H:51:TYR:HA	1.69	0.42
1:A:198:PRO:HG3	1:B:235:LEU:HD22	2.01	0.42
1:A:724:LYS:HG2	1:A:760:ARG:O	2.19	0.42
1:B:32:GLU:O	1:B:35:GLU:HG2	2.19	0.42
1:B:966:LEU:O	1:B:970:ILE:HG22	2.20	0.42
1:E:168:LEU:HD21	1:E:203:LEU:HD23	1.99	0.42
1:E:386:ASN:OD1	1:E:387:PHE:N	2.52	0.42
1:E:491:GLN:NE2	2:H:204:PHE:O	2.52	0.42
1:E:553:ASP:HA	1:E:556:VAL:HG12	2.01	0.42
1:F:348:ARG:NH1	1:F:349:HIS:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:678:PHE:CZ	1:F:725:TYR:HB2	2.54	0.42
1:F:688:LEU:HD22	1:F:736:ILE:HG21	2.00	0.42
1:F:801:SER:HB2	1:F:840:LYS:HE3	2.00	0.42
2:H:68:PHE:CG	2:H:69:ASP:N	2.87	0.42
1:A:343:ASN:OD1	1:A:344:GLY:N	2.51	0.42
1:A:998:GLU:OE1	1:A:999:ILE:HG23	2.19	0.42
1:B:225:ILE:O	1:B:228:LEU:HB3	2.19	0.42
1:B:817:SER:OG	1:B:820:LEU:HB2	2.19	0.42
1:B:978:HIS:O	1:B:982:GLU:HG3	2.20	0.42
1:F:46:VAL:HB	1:F:131:THR:HB	2.01	0.42
1:F:749:LEU:HG	1:F:753:LYS:HB2	2.00	0.42
1:F:857:LYS:HD2	1:F:858:SER:O	2.20	0.42
1:A:200:ILE:HG13	1:A:201:SER:N	2.35	0.42
2:C:181:ASN:HB2	2:C:188:TYR:CE1	2.53	0.42
2:D:37:SER:OG	2:D:56:GLU:OE2	2.36	0.42
1:E:67:HIS:ND1	1:E:73:SER:O	2.45	0.42
1:E:260:TYR:O	1:E:264:LYS:HG2	2.20	0.42
1:E:664:ILE:O	1:E:667:LEU:HG	2.19	0.42
1:F:865:LEU:HD13	1:F:869:ILE:HD13	2.00	0.42
1:A:781:LEU:O	1:A:784:GLU:HG3	2.19	0.42
1:A:866:MET:HG2	1:A:912:TYR:HE2	1.84	0.42
1:B:68:GLU:OE2	1:B:74:PRO:HD3	2.19	0.42
1:B:236:GLN:HB3	1:B:240:PHE:HB2	2.00	0.42
1:B:696:THR:HG23	1:B:743:TYR:CZ	2.54	0.42
2:C:28:GLN:H	2:C:64:LYS:HG2	1.84	0.42
1:E:297:GLN:O	1:E:299:ASN:N	2.52	0.42
1:E:409:ILE:HD13	1:E:414:TYR:CD2	2.54	0.42
1:E:541:ILE:HG23	1:E:542:LEU:HD22	2.02	0.42
1:F:32:GLU:O	1:F:35:GLU:HG3	2.20	0.42
1:F:156:GLU:OE1	1:F:156:GLU:N	2.53	0.42
1:F:588:LEU:HD12	1:F:592:LEU:HD23	2.02	0.42
1:B:977:LYS:O	1:B:981:ILE:HG12	2.20	0.42
1:F:33:ILE:HG23	1:F:42:LEU:HD11	2.02	0.42
1:F:233:ARG:HE	1:F:264:LYS:HB2	1.84	0.42
1:F:508:THR:HG22	1:F:510:GLU:H	1.84	0.42
1:A:26:VAL:HG12	1:A:30:ILE:HD11	2.02	0.42
1:A:64:ASP:O	1:A:68:GLU:HG2	2.19	0.42
1:B:193:TYR:HA	1:B:196:ASN:OD1	2.19	0.42
1:B:459:ILE:HD11	1:B:475:GLN:HG2	2.01	0.42
1:B:479:TYR:CG	1:B:524:ILE:HD13	2.55	0.42
1:B:553:ASP:O	1:B:556:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:LYS:HZ3	1:E:78:ASN:C	2.20	0.42
1:E:751:ILE:O	1:E:804:TYR:OH	2.29	0.42
1:F:134:TYR:CE2	1:F:183:VAL:HB	2.55	0.42
1:F:559:PHE:O	1:F:562:THR:OG1	2.31	0.42
1:F:929:LYS:HB2	1:F:930:MET:HE1	2.02	0.42
2:H:23:PHE:C	2:H:68:PHE:HB2	2.40	0.42
1:A:740:LEU:O	1:A:754:ARG:NH1	2.53	0.42
1:E:100:PHE:CE1	1:E:104:LEU:HD21	2.53	0.42
1:E:345:THR:OG1	1:E:397:ALA:N	2.52	0.42
1:E:861:ASN:HB3	1:E:864:ASP:HB2	2.02	0.42
1:E:869:ILE:HB	2:H:50:LEU:HD21	2.01	0.42
1:F:242:LYS:HB2	1:F:242:LYS:HE2	1.90	0.42
1:F:673:ILE:O	1:F:676:ILE:HG22	2.19	0.42
2:G:40:LYS:NZ	2:G:42:ARG:HG2	2.35	0.42
2:G:71:GLU:HG2	2:G:72:TRP:H	1.85	0.42
1:A:100:PHE:CE2	1:A:104:LEU:HD21	2.55	0.42
1:B:62:LEU:HD11	1:B:107:PHE:CD2	2.54	0.42
1:B:116:PRO:HA	1:B:119:ASP:OD2	2.19	0.42
1:B:228:LEU:O	1:B:232:VAL:HG13	2.19	0.42
1:B:425:ILE:HG21	1:B:447:ARG:HH21	1.83	0.42
1:E:369:GLU:O	1:E:372:LYS:HG2	2.19	0.42
1:E:919:TRP:HB3	1:E:924:GLU:HB2	2.01	0.42
1:A:135:ASP:OD2	1:A:137:LEU:HB2	2.20	0.42
1:A:139:ASP:HA	1:A:142:CYS:SG	2.59	0.42
1:A:380:ARG:O	1:A:384:LEU:HG	2.20	0.42
1:B:204:MET:SD	1:B:205:LYS:N	2.93	0.42
1:B:229:LEU:HD22	1:B:264:LYS:HD3	2.01	0.42
1:B:557:LYS:HD3	1:B:587:ARG:CZ	2.50	0.42
1:B:660:LYS:O	1:B:664:ILE:HG22	2.19	0.42
1:B:689:VAL:O	1:B:693:GLU:HG2	2.20	0.42
1:B:862:ILE:HG13	1:B:863:ASN:OD1	2.20	0.42
1:E:695:ILE:O	1:E:699:PHE:HD2	2.03	0.42
1:F:495:LEU:O	1:F:495:LEU:HD12	2.19	0.42
1:F:963:ASN:HD21	2:G:50:LEU:HB2	1.84	0.42
2:H:45:ILE:HG13	2:H:46:GLY:H	1.85	0.42
1:A:326:ARG:O	1:A:329:ASP:HB3	2.20	0.41
1:A:448:TRP:CZ3	1:A:484:SER:HB2	2.55	0.41
1:A:919:TRP:HE1	2:D:50:LEU:HD13	1.84	0.41
1:B:491:GLN:HG2	2:C:204:PHE:CZ	2.55	0.41
2:C:15:ARG:HD3	2:C:171:TYR:HD1	1.84	0.41
1:E:214:VAL:HG22	1:E:244:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:ASP:HB3	1:E:285:ARG:NH2	2.35	0.41
1:E:728:LEU:HD11	1:E:732:GLY:HA3	2.02	0.41
1:E:755:TYR:HB2	1:E:804:TYR:CE1	2.55	0.41
1:F:564:LYS:HZ1	1:F:568:GLU:HB3	1.85	0.41
1:F:606:HIS:C	1:F:606:HIS:HD1	2.23	0.41
1:F:688:LEU:HD22	1:F:736:ILE:HD13	2.02	0.41
1:F:753:LYS:O	1:F:757:TRP:CD1	2.72	0.41
2:G:20:LYS:HD3	2:G:20:LYS:C	2.41	0.41
1:B:261:TYR:CD1	1:B:264:LYS:HD2	2.55	0.41
1:B:574:TYR:N	2:D:32:PHE:O	2.42	0.41
2:C:28:GLN:HB3	2:C:64:LYS:NZ	2.35	0.41
1:E:405:THR:H	2:G:4:VAL:HG11	1.85	0.41
1:E:755:TYR:O	1:E:758:LEU:HG	2.20	0.41
1:F:963:ASN:ND2	2:G:52:ILE:HG22	2.34	0.41
2:H:41:LEU:HD21	2:H:54:LYS:HE2	2.01	0.41
2:H:64:LYS:HD3	2:H:217:GLU:HB3	2.03	0.41
1:A:231:TRP:CZ2	1:A:235:LEU:HD11	2.55	0.41
1:A:305:ASP:O	1:A:308:VAL:HB	2.20	0.41
1:A:756:VAL:O	1:A:759:GLU:HG3	2.20	0.41
1:B:485:ILE:HG23	1:B:507:PHE:CE2	2.55	0.41
1:B:512:LEU:HA	1:B:515:ILE:HG12	2.01	0.41
1:B:922:LEU:HD21	1:B:966:LEU:HD22	2.02	0.41
1:E:417:LYS:O	1:E:420:VAL:HG22	2.20	0.41
1:F:324:TYR:CE1	1:F:391:ASN:HA	2.55	0.41
1:F:338:TYR:HA	1:F:349:HIS:HB3	2.03	0.41
1:F:708:PHE:CE1	1:F:712:PHE:HB2	2.56	0.41
1:F:775:ILE:O	1:F:779:LEU:HG	2.20	0.41
1:A:52:THR:HG22	1:A:58:GLN:HG2	2.03	0.41
1:A:481:ILE:O	1:A:485:ILE:HG12	2.21	0.41
1:B:304:LYS:NZ	1:B:305:ASP:HB2	2.35	0.41
1:B:431:SER:OG	1:B:433:GLU:OE2	2.28	0.41
1:B:940:TYR:O	1:B:944:VAL:HG22	2.20	0.41
1:E:259:ILE:O	1:E:263:ASN:OD1	2.39	0.41
1:E:556:VAL:HG21	1:F:552:TYR:CE1	2.55	0.41
1:F:649:TYR:CE1	1:F:687:TYR:HB2	2.55	0.41
2:G:61:LEU:HD23	2:G:175:TYR:CZ	2.56	0.41
1:A:291:ASP:OD1	1:A:292:LEU:HD23	2.21	0.41
1:A:660:LYS:HB2	1:A:660:LYS:HE2	1.92	0.41
1:B:877:PHE:HZ	1:B:919:TRP:CZ3	2.38	0.41
1:E:152:ILE:HA	1:E:157:ASP:CG	2.40	0.41
1:E:254:GLU:HG2	1:E:255:ASN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:749:LEU:HB3	1:E:754:ARG:HG3	2.03	0.41
1:E:981:ILE:HD11	1:E:985:LYS:HZ3	1.86	0.41
1:F:318:PRO:O	1:F:539:TYR:OH	2.24	0.41
1:F:549:GLN:HA	1:F:552:TYR:HD2	1.85	0.41
1:F:620:ILE:HG13	1:F:620:ILE:H	1.65	0.41
1:F:631:ILE:HD13	1:F:636:PHE:HB3	2.01	0.41
1:F:842:LEU:HD23	1:F:871:ILE:HD11	2.03	0.41
1:A:655:ILE:HG23	1:A:659:PHE:CE2	2.55	0.41
1:A:809:LYS:HD3	1:A:809:LYS:HA	1.85	0.41
1:B:503:HIS:ND1	1:B:505:LYS:HE3	2.36	0.41
2:D:21:LEU:HA	2:D:23:PHE:HE1	1.85	0.41
1:E:562:THR:HA	1:E:618:LEU:HD21	2.01	0.41
1:E:737:VAL:HG21	1:E:771:ILE:HG23	2.02	0.41
2:G:226:THR:HG22	2:G:226:THR:O	2.20	0.41
1:A:327:LYS:HG3	1:A:328:ILE:N	2.35	0.41
1:A:709:TYR:CD1	1:A:709:TYR:N	2.87	0.41
2:D:192:TYR:HB2	2:D:235:ILE:HB	2.01	0.41
1:E:657:ARG:HB3	1:E:658:HIS:ND1	2.35	0.41
1:F:205:LYS:O	1:F:208:ILE:HG22	2.20	0.41
1:F:840:LYS:HG2	1:F:841:LEU:HG	2.03	0.41
1:F:985:LYS:O	1:F:989:LYS:HG2	2.20	0.41
2:H:61:LEU:HD21	2:H:175:TYR:CE2	2.56	0.41
1:A:396:MET:SD	1:A:399:ASP:HB3	2.61	0.41
1:A:499:THR:HG23	1:A:500:PHE:CD1	2.56	0.41
1:A:550:PHE:CG	1:A:551:LEU:N	2.89	0.41
1:A:1005:ILE:HD13	1:B:1005:ILE:HD13	2.03	0.41
1:E:509:ASP:O	1:E:512:LEU:HG	2.21	0.41
1:E:559:PHE:HE1	1:F:614:ASN:ND2	2.19	0.41
1:E:706:VAL:O	1:E:710:THR:HG23	2.21	0.41
1:F:557:LYS:O	1:F:561:LEU:HG	2.21	0.41
2:G:47:ASN:O	2:G:48:LYS:HE2	2.21	0.41
1:A:119:ASP:HB2	1:B:517:ARG:NH2	2.36	0.41
1:A:859:VAL:HG12	1:A:860:GLU:HG3	2.03	0.41
1:B:109:GLN:O	1:B:109:GLN:HG2	2.20	0.41
1:B:359:ARG:HD2	1:B:359:ARG:HA	1.92	0.41
1:B:372:LYS:HB2	1:B:372:LYS:HE2	1.82	0.41
1:B:473:LEU:O	1:B:477:ASN:ND2	2.54	0.41
1:B:537:LYS:HA	1:B:540:LYS:NZ	2.36	0.41
1:B:632:ASP:OD1	1:B:632:ASP:N	2.48	0.41
1:B:647:MET:SD	1:B:678:PHE:HA	2.60	0.41
1:B:689:VAL:HG12	1:B:693:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:LYS:N	2:D:49:PRO:HD3	2.35	0.41
1:E:46:VAL:N	1:E:130:ILE:O	2.46	0.41
1:E:484:SER:HA	1:E:487:GLN:NE2	2.34	0.41
1:E:612:ILE:HD12	1:E:612:ILE:HA	1.90	0.41
1:E:741:LEU:HD12	1:E:778:PHE:CG	2.56	0.41
1:E:781:LEU:O	1:E:784:GLU:HG3	2.21	0.41
1:E:817:SER:O	1:E:821:SER:OG	2.23	0.41
1:F:140:THR:O	1:F:144:LYS:HE3	2.20	0.41
1:F:343:ASN:ND2	1:F:345:THR:OG1	2.49	0.41
1:F:547:ASP:N	1:F:547:ASP:OD1	2.53	0.41
1:F:682:GLU:HA	1:F:685:GLU:OE2	2.21	0.41
1:F:778:PHE:O	1:F:782:GLN:HB3	2.21	0.41
2:G:18:ASP:N	2:G:18:ASP:OD1	2.52	0.41
1:A:136:ASN:O	1:A:140:THR:HG23	2.21	0.41
1:A:315:LYS:O	1:A:318:PRO:HD2	2.21	0.41
1:A:537:LYS:HA	1:A:537:LYS:HD2	1.90	0.41
1:E:53:LEU:HD23	1:E:53:LEU:HA	1.92	0.41
1:E:338:TYR:CZ	1:E:357:MET:HB3	2.56	0.41
1:E:913:MET:HA	1:E:916:PHE:HE2	1.85	0.41
1:E:939:GLN:HG2	1:E:958:TRP:CE2	2.56	0.41
1:F:189:ASP:O	1:F:193:TYR:N	2.53	0.41
2:H:37:SER:OG	2:H:56:GLU:OE2	2.38	0.41
1:B:223:TYR:O	1:B:227:MET:HG2	2.21	0.40
1:B:304:LYS:HZ2	1:B:305:ASP:N	2.18	0.40
1:B:562:THR:OG1	1:B:618:LEU:HD22	2.20	0.40
2:C:15:ARG:HD3	2:C:171:TYR:CD1	2.56	0.40
1:E:471:TYR:OH	1:F:146:GLY:O	2.39	0.40
1:E:730:GLU:HG2	1:E:731:GLU:N	2.36	0.40
1:F:377:GLN:HA	1:F:380:ARG:HE	1.86	0.40
1:F:557:LYS:HE3	1:F:587:ARG:HH22	1.85	0.40
1:F:669:ARG:HB2	1:F:669:ARG:NH1	2.36	0.40
2:H:24:THR:HB	2:H:65:ASN:OD1	2.20	0.40
1:A:885:ILE:HG23	1:A:916:PHE:CE1	2.56	0.40
1:B:644:GLY:HA3	1:B:646:PHE:CE1	2.56	0.40
2:D:50:LEU:HD12	2:D:51:TYR:N	2.26	0.40
2:D:54:LYS:HD2	2:D:56:GLU:H	1.86	0.40
1:E:479:TYR:HB2	1:E:522:PHE:CE2	2.57	0.40
1:E:610:GLN:HA	1:E:613:ARG:HH11	1.86	0.40
1:F:137:LEU:H	1:F:137:LEU:HD23	1.86	0.40
1:A:65:LYS:HG2	1:A:107:PHE:CE2	2.56	0.40
1:A:339:HIS:ND1	1:A:349:HIS:HB2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:ILE:HD11	1:B:716:ALA:HB1	2.04	0.40
1:B:750:ASP:H	1:B:753:LYS:HE3	1.86	0.40
1:E:327:LYS:HE2	1:E:341:GLU:O	2.21	0.40
1:E:475:GLN:OE1	1:E:475:GLN:HA	2.21	0.40
1:F:261:TYR:HA	1:F:264:LYS:HE2	2.04	0.40
1:A:631:ILE:O	1:A:631:ILE:HG13	2.22	0.40
1:A:704:MET:SD	1:A:704:MET:N	2.95	0.40
1:A:717:LYS:HD2	1:A:717:LYS:N	2.36	0.40
1:B:859:VAL:HG23	1:B:859:VAL:O	2.22	0.40
1:E:595:LEU:HB3	1:E:603:VAL:HG12	2.02	0.40
1:E:735:LYS:O	1:E:738:LYS:HG2	2.21	0.40
1:E:984:LEU:HG	1:E:987:ARG:NH2	2.36	0.40
1:F:218:TYR:CZ	1:F:225:ILE:HB	2.57	0.40
1:A:264:LYS:HD3	1:A:264:LYS:HA	1.72	0.40
1:A:418:TYR:O	1:A:421:MET:HB2	2.21	0.40
1:A:513:ALA:O	1:A:517:ARG:HG3	2.21	0.40
1:A:750:ASP:OD1	1:A:750:ASP:C	2.60	0.40
1:A:887:GLU:HA	1:A:890:GLU:OE1	2.21	0.40
1:B:64:ASP:O	1:B:68:GLU:HG3	2.21	0.40
1:B:200:ILE:O	1:B:204:MET:HG3	2.21	0.40
1:B:507:PHE:HB2	1:B:512:LEU:HD21	2.03	0.40
1:E:215:PHE:N	1:E:244:PHE:O	2.38	0.40
1:E:441:PHE:O	1:E:445:LEU:HD12	2.20	0.40
1:F:89:GLN:CG	1:F:187:GLU:H	2.34	0.40
1:F:405:THR:H	2:H:4:VAL:HG11	1.86	0.40
1:F:759:GLU:O	1:F:763:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	981/1005 (98%)	937 (96%)	41 (4%)	3 (0%)	37	72
1	B	981/1005 (98%)	914 (93%)	60 (6%)	7 (1%)	19	56
1	E	981/1005 (98%)	935 (95%)	43 (4%)	3 (0%)	37	72
1	F	981/1005 (98%)	904 (92%)	72 (7%)	5 (0%)	25	64
2	C	147/264 (56%)	111 (76%)	33 (22%)	3 (2%)	6	32
2	D	147/264 (56%)	106 (72%)	38 (26%)	3 (2%)	6	32
2	G	147/264 (56%)	120 (82%)	22 (15%)	5 (3%)	3	21
2	H	147/264 (56%)	103 (70%)	40 (27%)	4 (3%)	4	25
All	All	4512/5076 (89%)	4130 (92%)	349 (8%)	33 (1%)	21	56

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	B	299	ASN
1	B	906	THR
1	B	975	HIS
2	C	56	GLU
1	E	298	GLU
1	F	299	ASN
1	F	906	THR
1	A	631	ILE
1	B	905	GLN
1	B	907	PHE
2	D	56	GLU
1	F	907	PHE
2	G	56	GLU
2	H	56	GLU
1	E	299	ASN
1	F	818	LYS
1	F	905	GLN
2	G	57	LYS
1	B	908	SER
2	D	5	ILE
1	E	631	ILE
1	A	298	GLU
2	C	5	ILE
2	G	5	ILE
2	G	45	ILE
2	H	5	ILE

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Mol	Chain	Res	Type
2	H	26	GLU
2	C	214	LEU
2	D	57	LYS
2	G	69	ASP
2	H	57	LYS
1	B	72	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	901/922 (98%)	867 (96%)	34 (4%)	28	49
1	B	901/922 (98%)	871 (97%)	30 (3%)	33	53
1	E	901/922 (98%)	859 (95%)	42 (5%)	22	44
1	F	901/922 (98%)	870 (97%)	31 (3%)	32	52
2	C	130/225 (58%)	125 (96%)	5 (4%)	28	49
2	D	130/225 (58%)	125 (96%)	5 (4%)	28	49
2	G	130/225 (58%)	128 (98%)	2 (2%)	60	75
2	H	130/225 (58%)	126 (97%)	4 (3%)	35	55
All	All	4124/4588 (90%)	3971 (96%)	153 (4%)	31	50

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	28	GLU
1	A	149	PHE
1	A	190	TYR
1	A	191	LEU
1	A	242	LYS
1	A	245	PHE
1	A	351	ASN
1	A	396	MET

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Mol	Chain	Res	Type
1	A	457	ASN
1	A	471	TYR
1	A	511	PHE
1	A	536	GLN
1	A	552	TYR
1	A	594	PHE
1	A	598	ASN
1	A	634	LEU
1	A	647	MET
1	A	654	ASN
1	A	669	ARG
1	A	678	PHE
1	A	712	PHE
1	A	750	ASP
1	A	757	TRP
1	A	758	LEU
1	A	759	GLU
1	A	779	LEU
1	A	837	PHE
1	A	839	PHE
1	A	852	HIS
1	A	866	MET
1	A	919	TRP
1	A	940	TYR
1	A	965	LYS
1	B	31	LYS
1	B	86	ARG
1	B	107	PHE
1	B	134	TYR
1	B	135	ASP
1	B	174	PHE
1	B	202	ASN
1	B	204	MET
1	B	211	HIS
1	B	223	TYR
1	B	233	ARG
1	B	240	PHE
1	B	297	GLN
1	B	351	ASN
1	B	368	ASP
1	B	376	LYS
1	B	436	TYR

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Mol	Chain	Res	Type
1	B	477	ASN
1	B	511	PHE
1	B	517	ARG
1	B	519	MET
1	B	581	ASP
1	B	594	PHE
1	B	605	PHE
1	B	704	MET
1	B	712	PHE
1	B	920	TYR
1	B	921	PHE
1	B	985	LYS
1	B	990	ASN
2	C	33	SER
2	C	64	LYS
2	C	67	PHE
2	C	206	MET
2	C	220	PHE
2	D	12	TYR
2	D	33	SER
2	D	72	TRP
2	D	75	MET
2	D	231	MET
1	E	45	PHE
1	E	60	TRP
1	E	84	TYR
1	E	89	GLN
1	E	98	MET
1	E	105	LYS
1	E	108	PHE
1	E	162	THR
1	E	204	MET
1	E	211	HIS
1	E	231	TRP
1	E	260	TYR
1	E	290	MET
1	E	330	LEU
1	E	339	HIS
1	E	343	ASN
1	E	357	MET
1	E	395	CYS
1	E	418	TYR

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Mol	Chain	Res	Type
1	E	445	LEU
1	E	452	TYR
1	E	469	CYS
1	E	511	PHE
1	E	516	GLU
1	E	522	PHE
1	E	537	LYS
1	E	569	MET
1	E	578	MET
1	E	596	TYR
1	E	645	PHE
1	E	658	HIS
1	E	709	TYR
1	E	721	TYR
1	E	779	LEU
1	E	810	HIS
1	E	815	PHE
1	E	911	ASP
1	E	912	TYR
1	E	916	PHE
1	E	919	TRP
1	E	965	LYS
1	E	989	LYS
1	F	45	PHE
1	F	147	LYS
1	F	189	ASP
1	F	196	ASN
1	F	223	TYR
1	F	228	LEU
1	F	233	ARG
1	F	234	LYS
1	F	245	PHE
1	F	260	TYR
1	F	286	TYR
1	F	290	MET
1	F	360	PHE
1	F	391	ASN
1	F	448	TRP
1	F	477	ASN
1	F	596	TYR
1	F	606	HIS
1	F	663	ASP

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Mol	Chain	Res	Type
1	F	688	LEU
1	F	704	MET
1	F	738	LYS
1	F	754	ARG
1	F	782	GLN
1	F	810	HIS
1	F	811	PHE
1	F	837	PHE
1	F	857	LYS
1	F	864	ASP
1	F	866	MET
1	F	975	HIS
2	G	39	GLU
2	G	231	MET
2	H	12	TYR
2	H	23	PHE
2	H	51	TYR
2	H	220	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	125	ASN
1	A	457	ASN
1	A	483	GLN
1	A	563	ASN
1	A	591	ASN
1	A	797	ASN
1	A	852	HIS
1	B	606	HIS
2	C	34	GLN
2	D	60	ASN
1	E	128	HIS
1	E	782	GLN
1	F	202	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

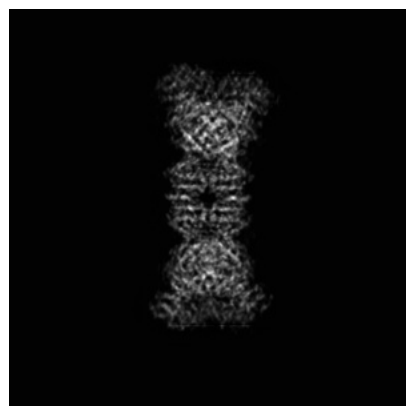
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39246. 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](#)

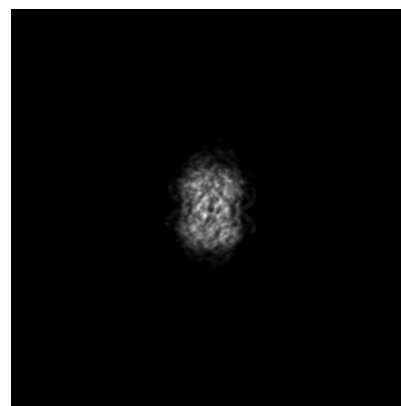
6.1.1 Primary map



X

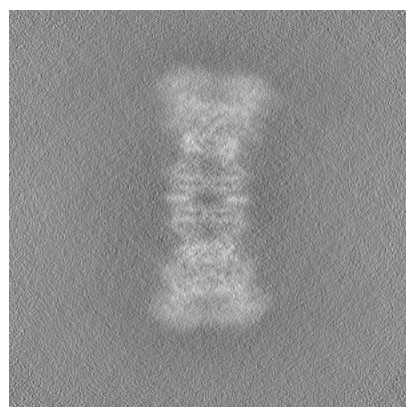


Y

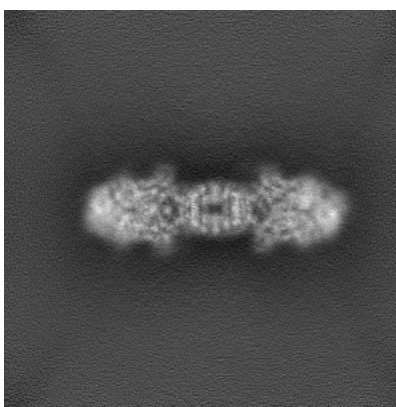


Z

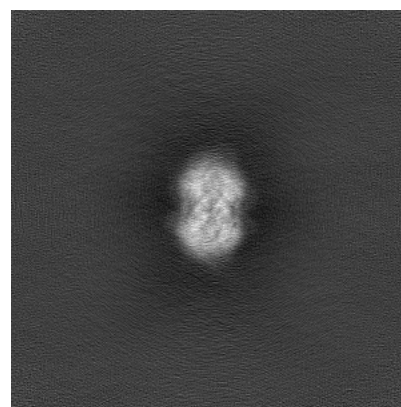
6.1.2 Raw map



X



Y



Z

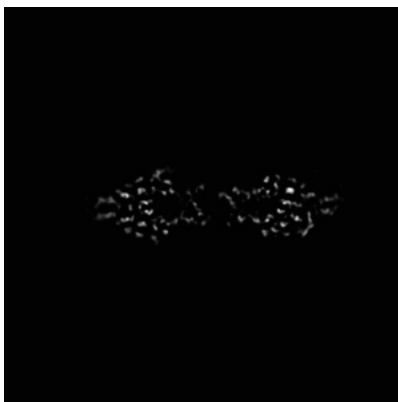
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

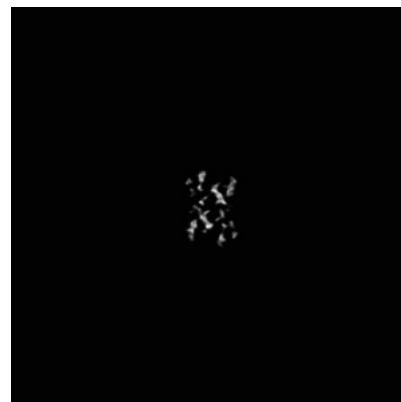
6.2.1 Primary map



X Index: 230

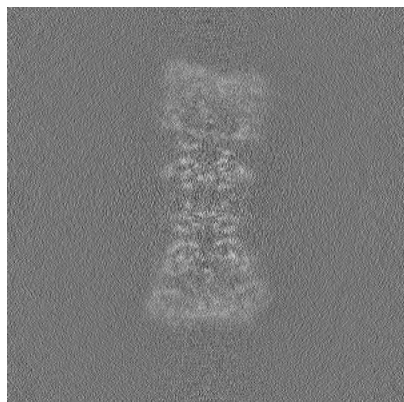


Y Index: 230

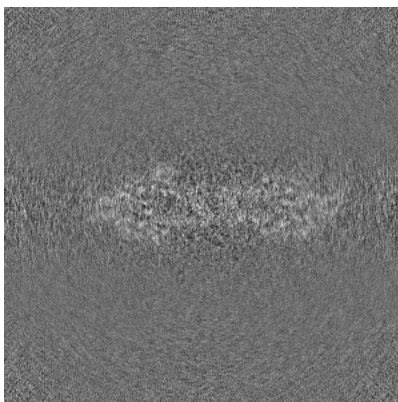


Z Index: 230

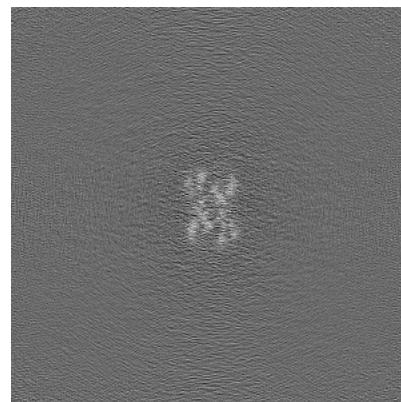
6.2.2 Raw map



X Index: 230



Y Index: 230



Z Index: 230

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: 224

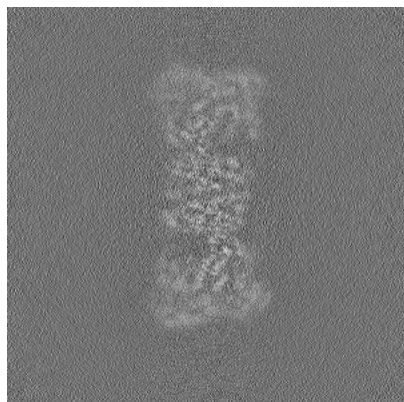


Y Index: 235

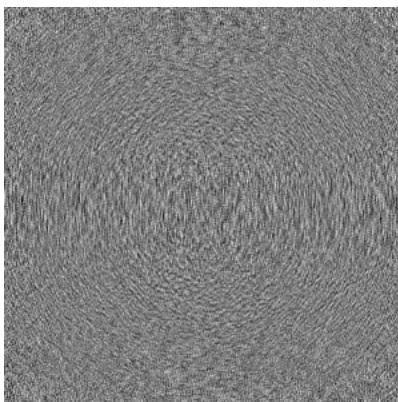


Z Index: 311

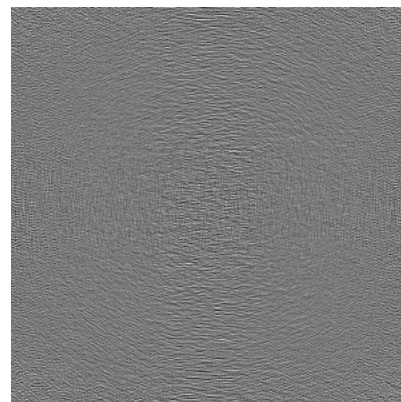
6.3.2 Raw map



X Index: 222



Y Index: 0

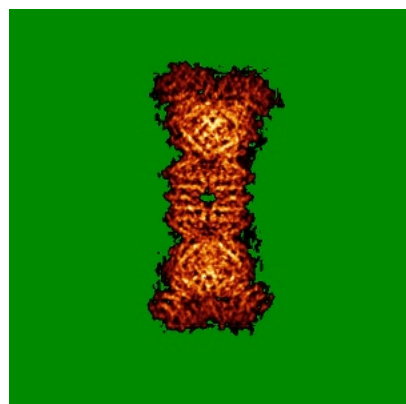


Z Index: 0

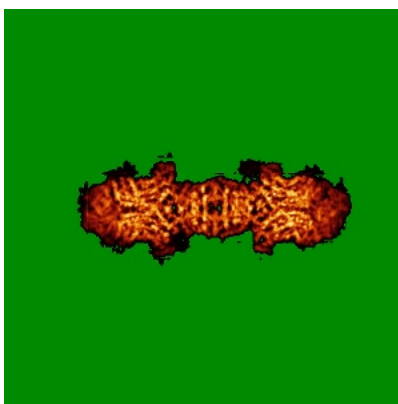
The images above show the largest variance slices of the map in three orthogonal directions.

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

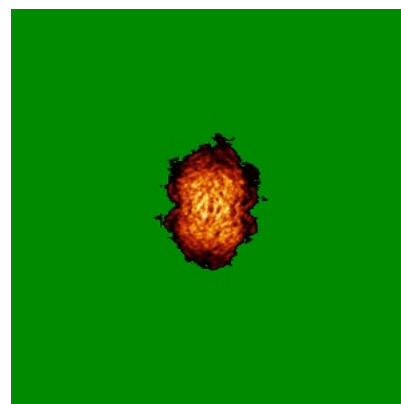
6.4.1 Primary map



X

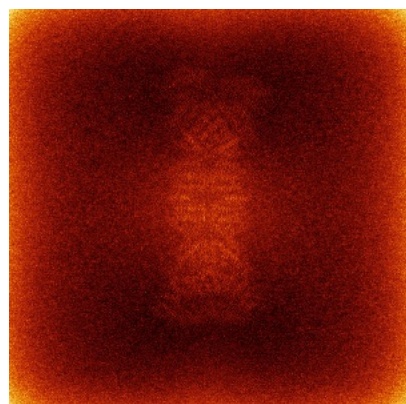


Y

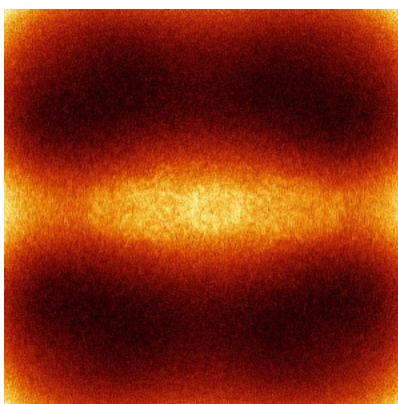


Z

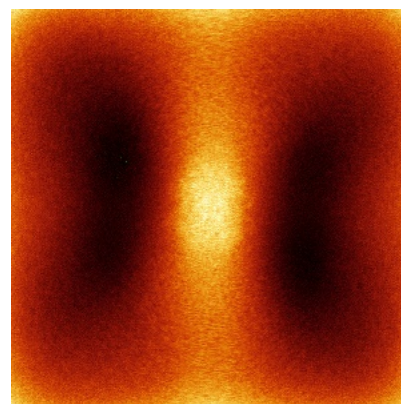
6.4.2 Raw map



X



Y

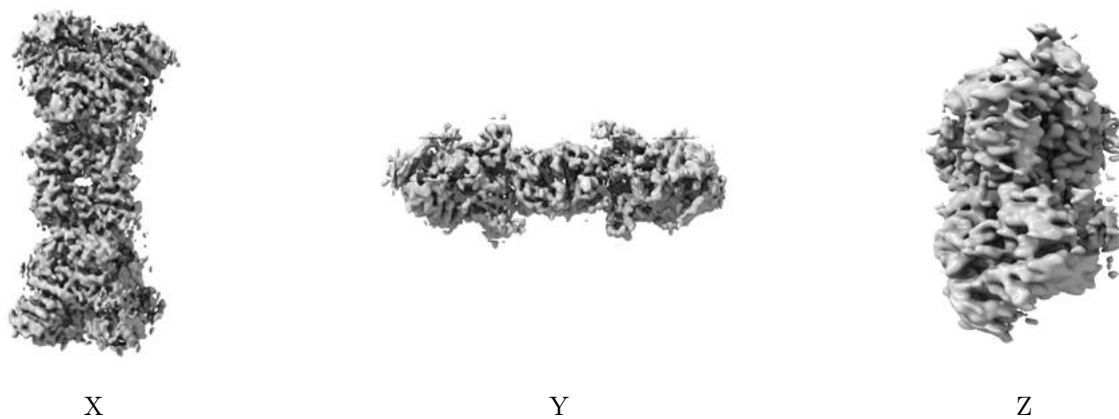


Z

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.

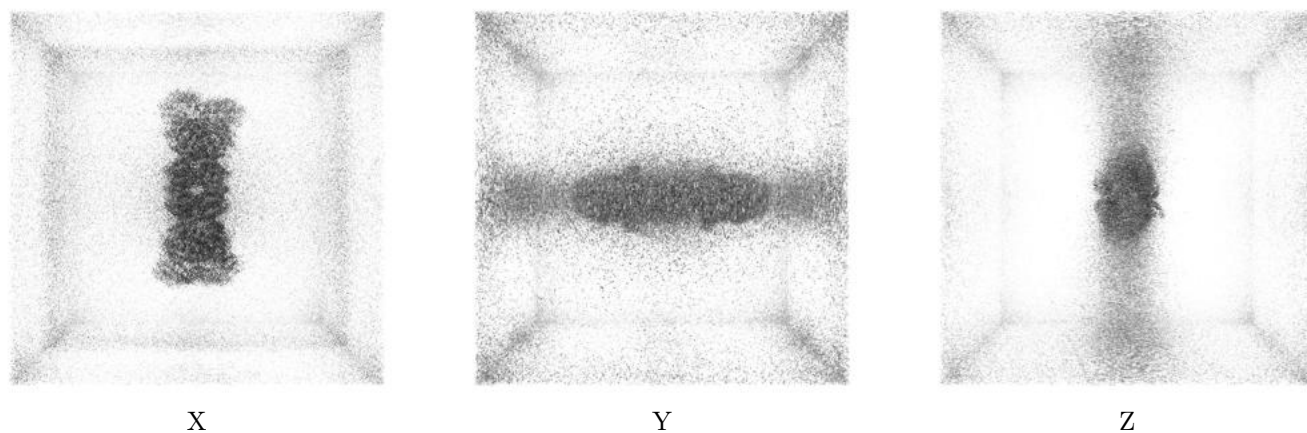
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

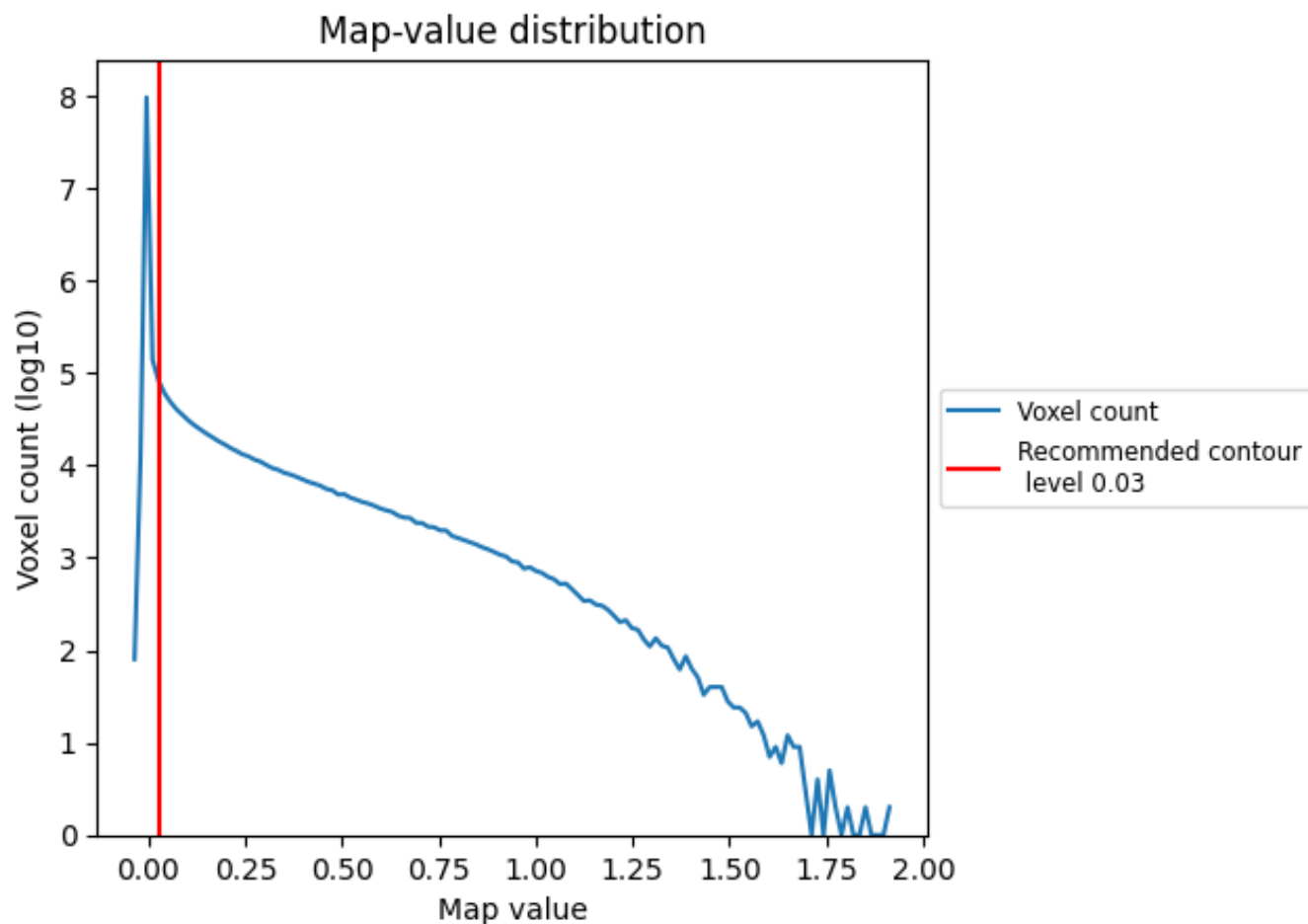
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

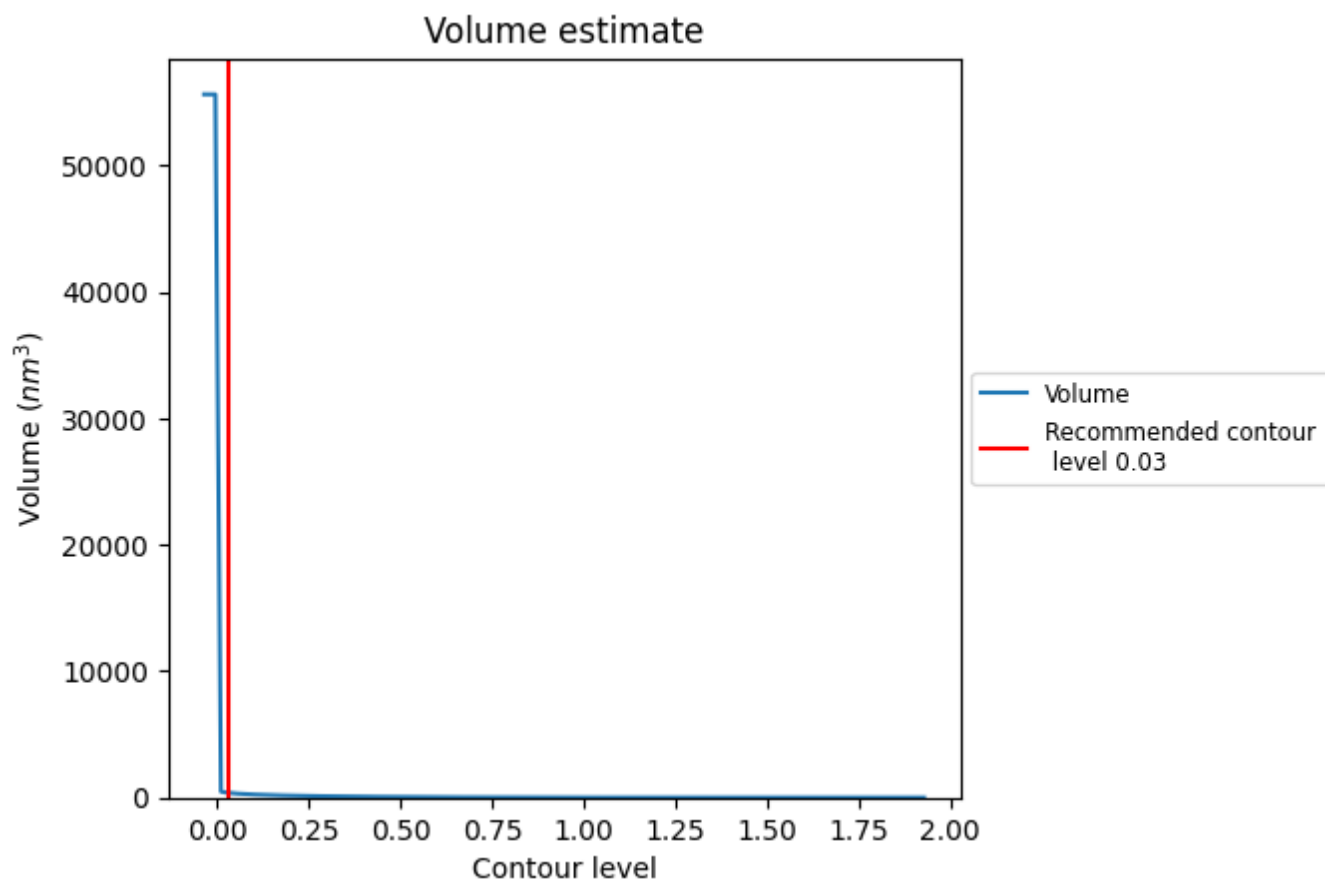
This section contains the results of statistical analysis of the map.

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.

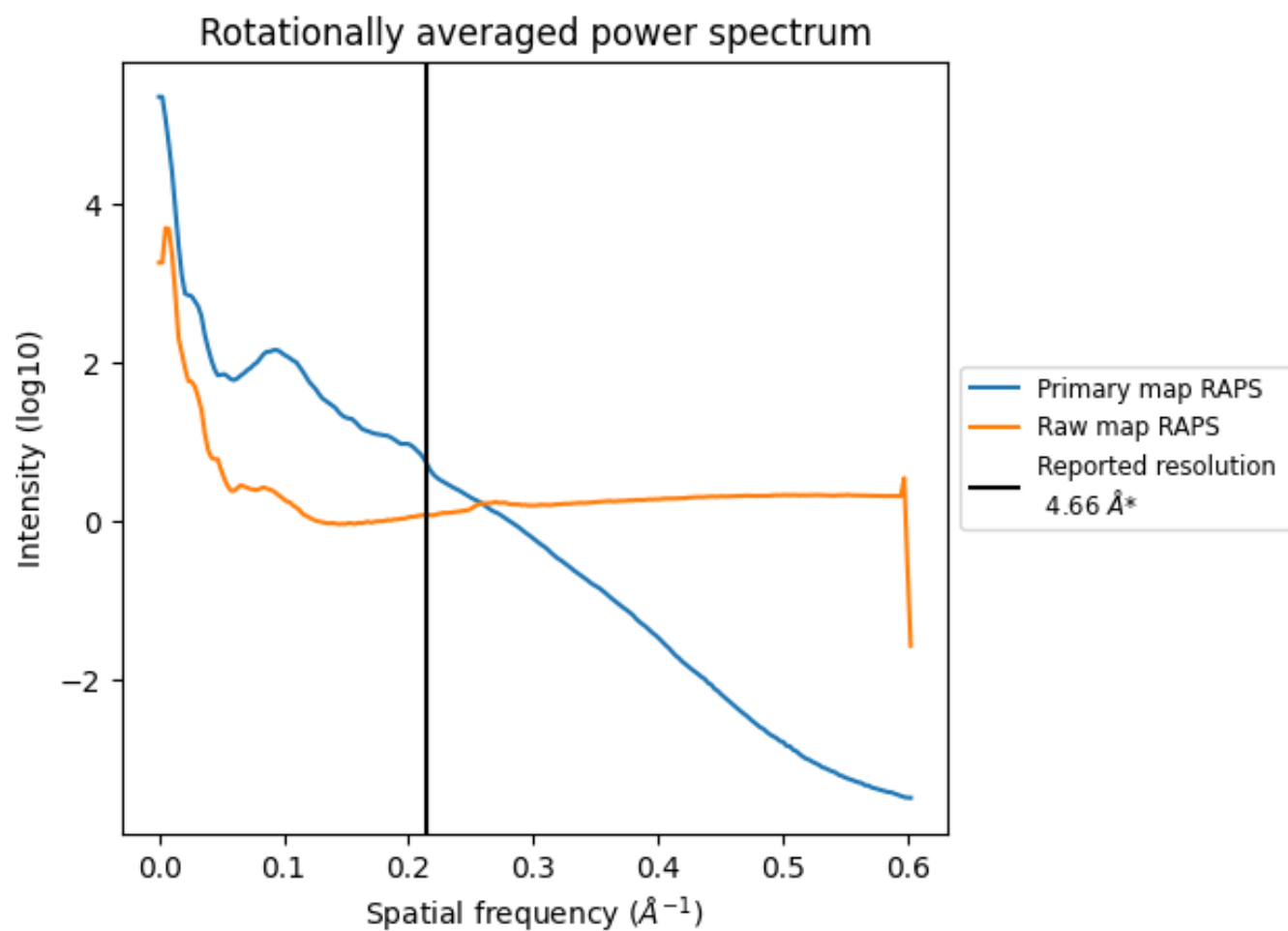
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 376 nm^3 ; this corresponds to an approximate mass of 339 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 ⓘ

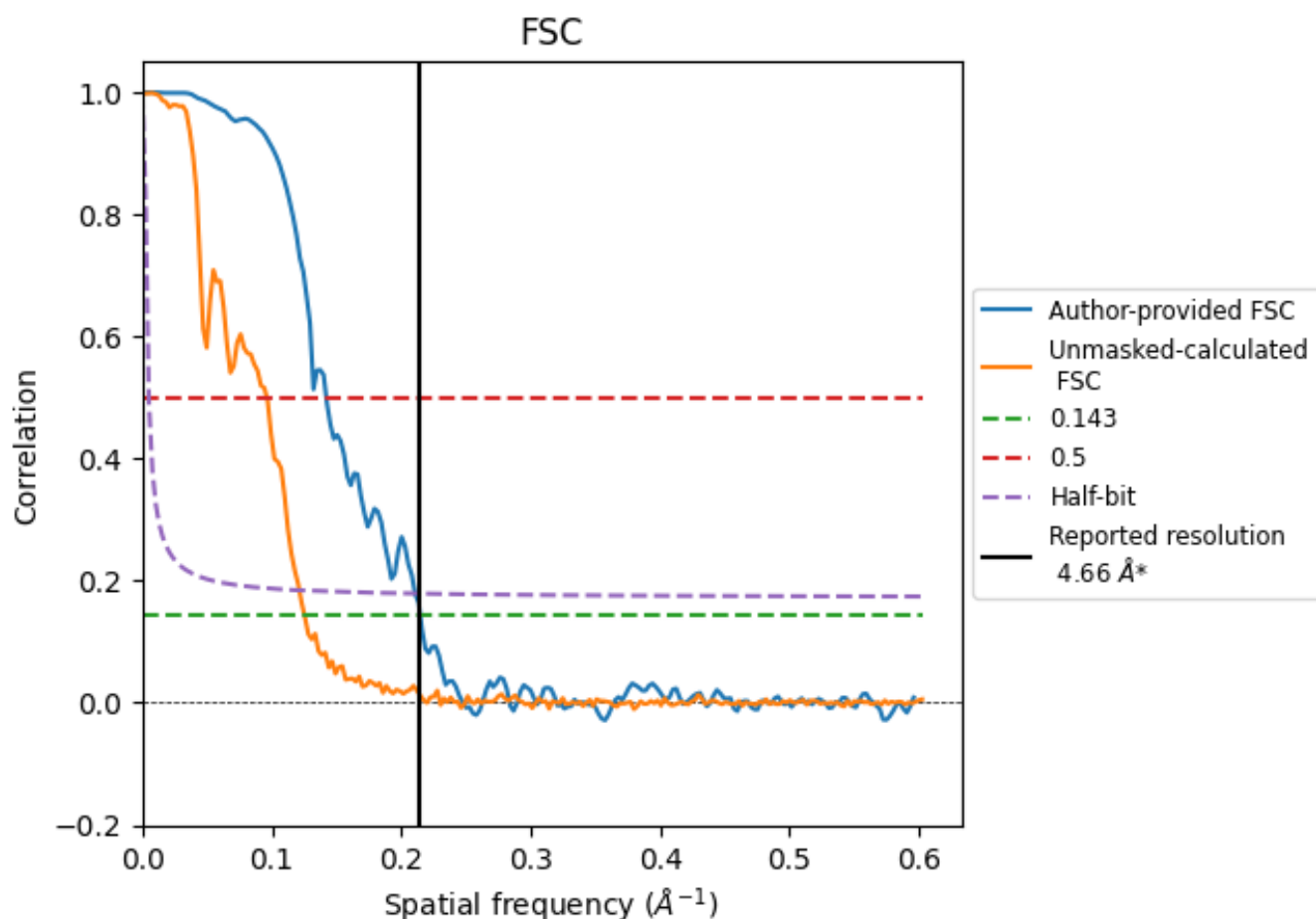


*Reported resolution corresponds to spatial frequency of 0.215 \AA^{-1}

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 0.215 Å⁻¹

8.2 Resolution estimates [i](#)

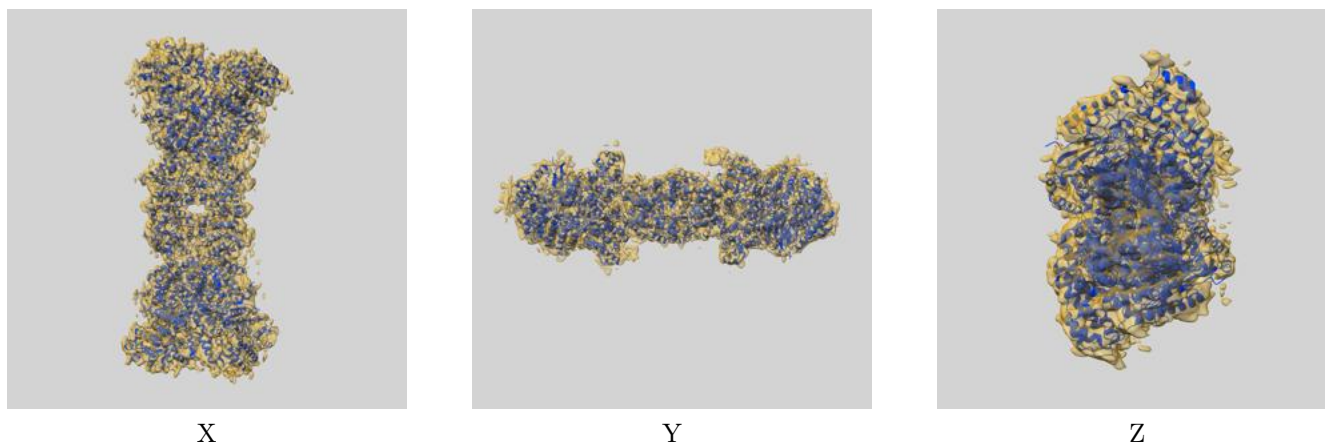
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.66	-	-
Author-provided FSC curve	4.66	7.03	4.74
Unmasked-calculated*	7.97	10.40	8.24

*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 7.97 differs from the reported value 4.66 by more than 10 %

9 Map-model fit [i](#)

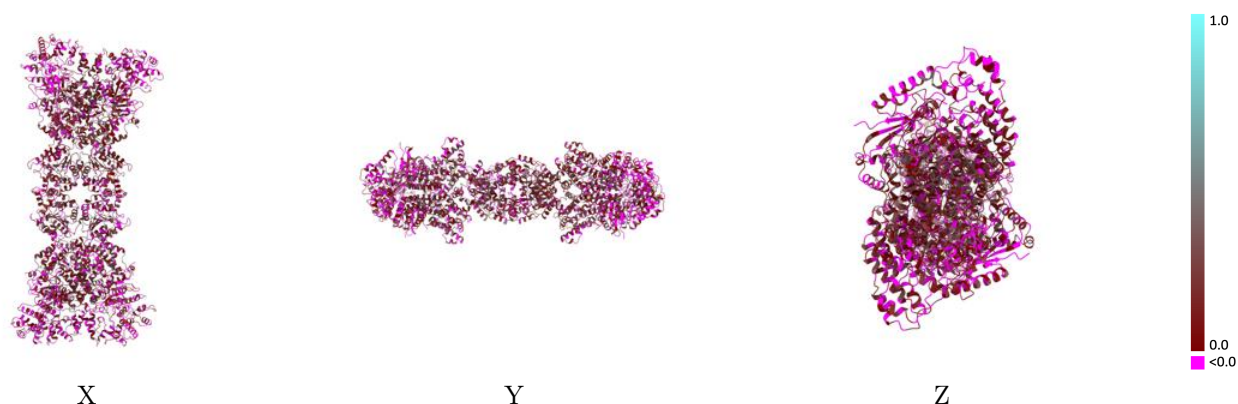
This section contains information regarding the fit between EMDB map EMD-39246 and PDB model 8YGF. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



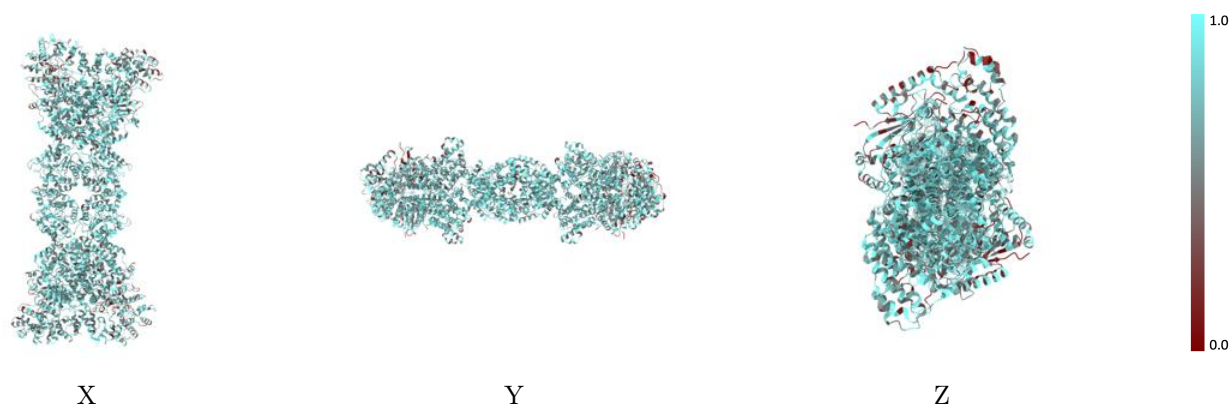
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



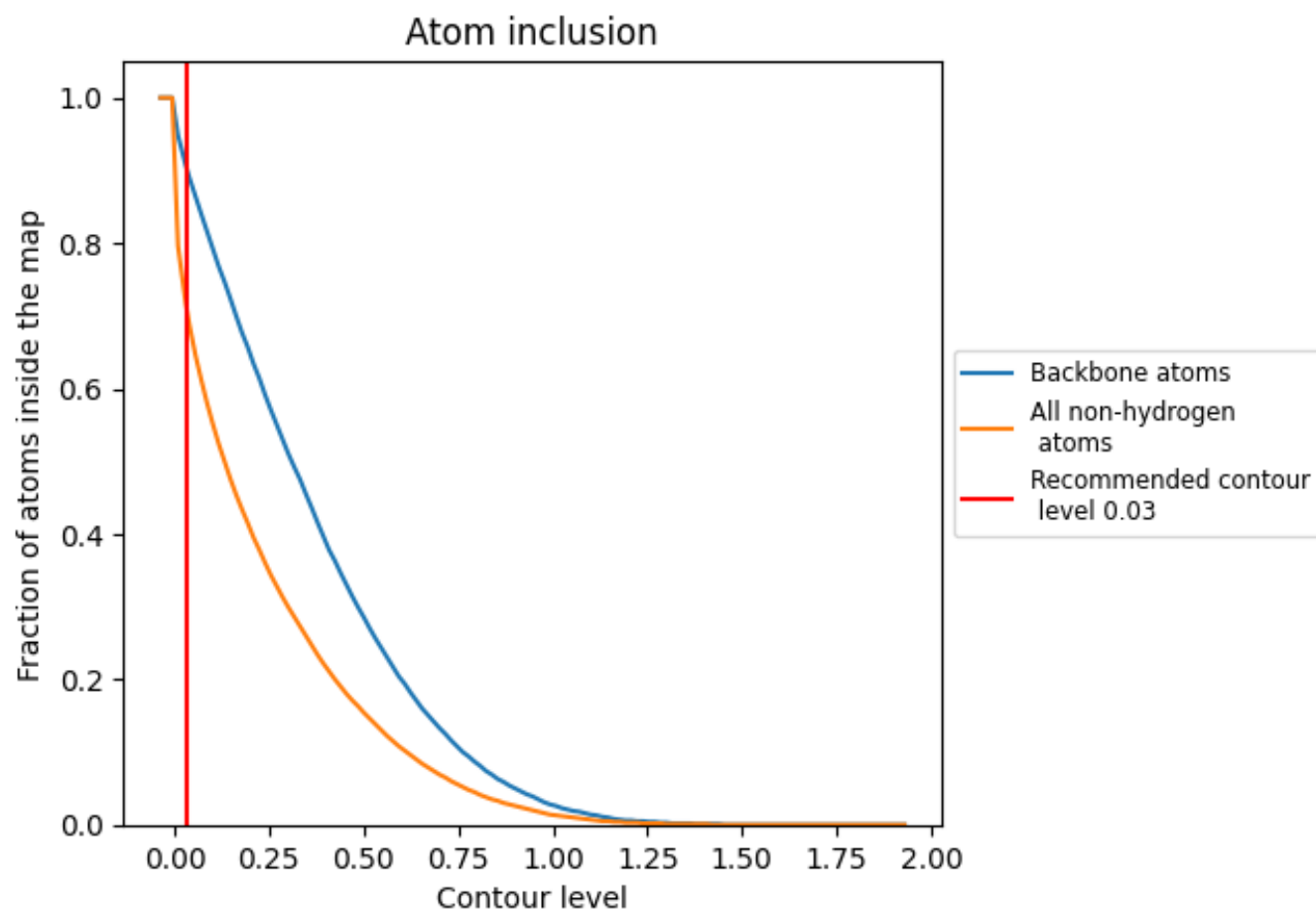
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 72% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7170	<div></div> 0.1240
A	<div></div> 0.7380	<div></div> 0.1310
B	<div></div> 0.7330	<div></div> 0.1290
C	<div></div> 0.5820	<div></div> 0.0570
D	<div></div> 0.5880	<div></div> 0.0400
E	<div></div> 0.7470	<div></div> 0.1390
F	<div></div> 0.7390	<div></div> 0.1420
G	<div></div> 0.5670	<div></div> 0.0530
H	<div></div> 0.5380	<div></div> 0.0410

1.0

0.0

<0.0