



Full wwPDB EM Validation Report ⓘ

Jul 14, 2026 – 09:13 PM JST

PDB ID : 9XQS / pdb_00009xqs
EMDB ID : EMD-67121
Title : Structure of the inner peripheral region in the phage phiKZ baseplate complex
Authors : Xiao, H.; Peng, Z.; Zhou, J.; Liu, H.
Deposited on : 2025-11-18
Resolution : 3.65 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.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

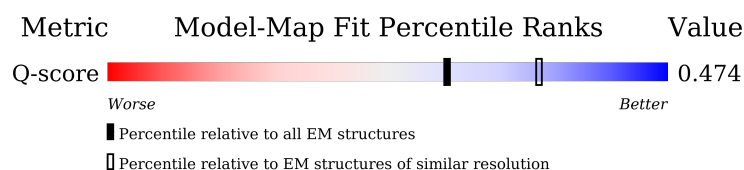
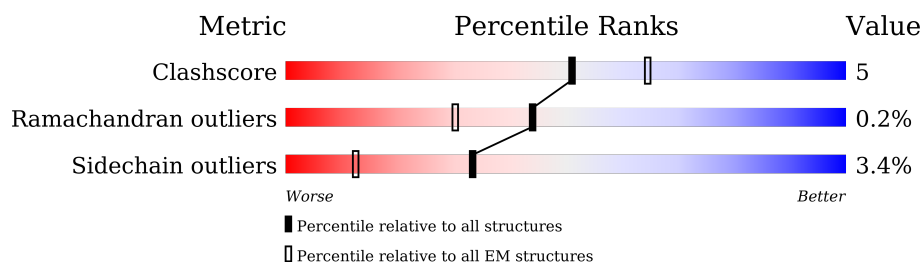
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 Å.

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



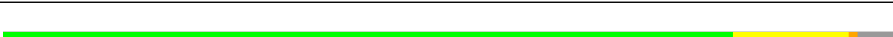
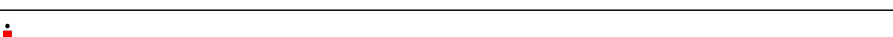
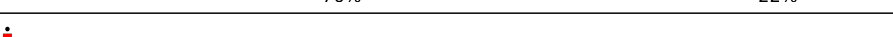
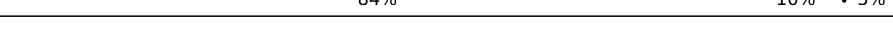
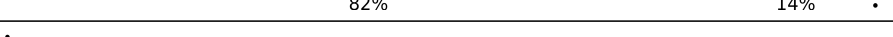
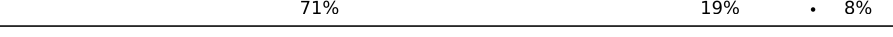
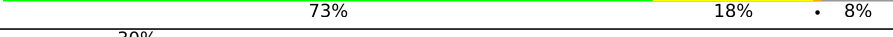
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11564 (3.15 - 4.15)

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	971	
1	B	971	
1	U	971	
1	V	971	

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Mol	Chain	Length	Quality of chain
2	C	724	
2	D	724	
3	E	203	
3	F	203	
3	G	203	
3	H	203	
4	I	349	
4	J	349	
5	K	664	
5	L	664	
6	M	138	
6	N	138	
6	O	138	
6	P	138	
6	Q	138	
6	R	138	
6	S	138	
6	T	138	
7	W	695	
7	X	695	
7	Y	695	
7	Z	695	
8	a	136	
8	b	136	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 91692 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 PHIKZ087.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	963	Total	C	N	O	S	0	0
			7705	4888	1288	1499	30		
1	B	963	Total	C	N	O	S	0	0
			7705	4888	1288	1499	30		
1	U	951	Total	C	N	O	S	0	0
			7627	4845	1274	1478	30		
1	V	951	Total	C	N	O	S	0	0
			7627	4845	1274	1478	30		

- Molecule 2 is a protein called PHIKZ128.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	610	Total	C	N	O	S	0	0
			5019	3217	836	949	17		
2	D	610	Total	C	N	O	S	0	0
			5019	3217	836	949	17		

- Molecule 3 is a protein called PHIKZ161.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	202	Total	C	N	O	S	0	0
			1583	1003	263	314	3		
3	F	199	Total	C	N	O	S	0	0
			1559	986	260	311	2		
3	G	202	Total	C	N	O	S	0	0
			1583	1003	263	314	3		
3	H	199	Total	C	N	O	S	0	0
			1559	986	260	311	2		

- Molecule 4 is a protein called PHIKZ088.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	314	Total	C	N	O	S	0	0
			2594	1655	434	490	15		
4	J	314	Total	C	N	O	S	0	0
			2594	1655	434	490	15		

- Molecule 5 is a protein called PHIKZ182.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	580	Total	C	N	O	S	0	0
			4604	2927	812	851	14		
5	L	570	Total	C	N	O	S	0	0
			4530	2884	796	836	14		

- Molecule 6 is a protein called PHIKZ049.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	133	Total	C	N	O	S	0	0
			1038	661	177	196	4		
6	N	135	Total	C	N	O	S	0	0
			1047	666	179	198	4		
6	O	133	Total	C	N	O	S	0	0
			1038	661	177	196	4		
6	P	135	Total	C	N	O	S	0	0
			1047	666	179	198	4		
6	Q	131	Total	C	N	O	S	0	0
			1025	653	175	193	4		
6	R	131	Total	C	N	O	S	0	0
			1025	653	175	193	4		
6	S	133	Total	C	N	O	S	0	0
			1030	657	176	193	4		
6	T	133	Total	C	N	O	S	0	0
			1030	657	176	193	4		

- Molecule 7 is a protein called PHIKZ029.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	636	Total	C	N	O	S	0	0
			5010	3170	846	973	21		
7	X	636	Total	C	N	O	S	0	0
			5010	3170	846	973	21		
7	Y	634	Total	C	N	O	S	0	0
			4986	3152	844	969	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	Z	634	Total	C	N	O	S	0	0
			4986	3152	844	969	21		

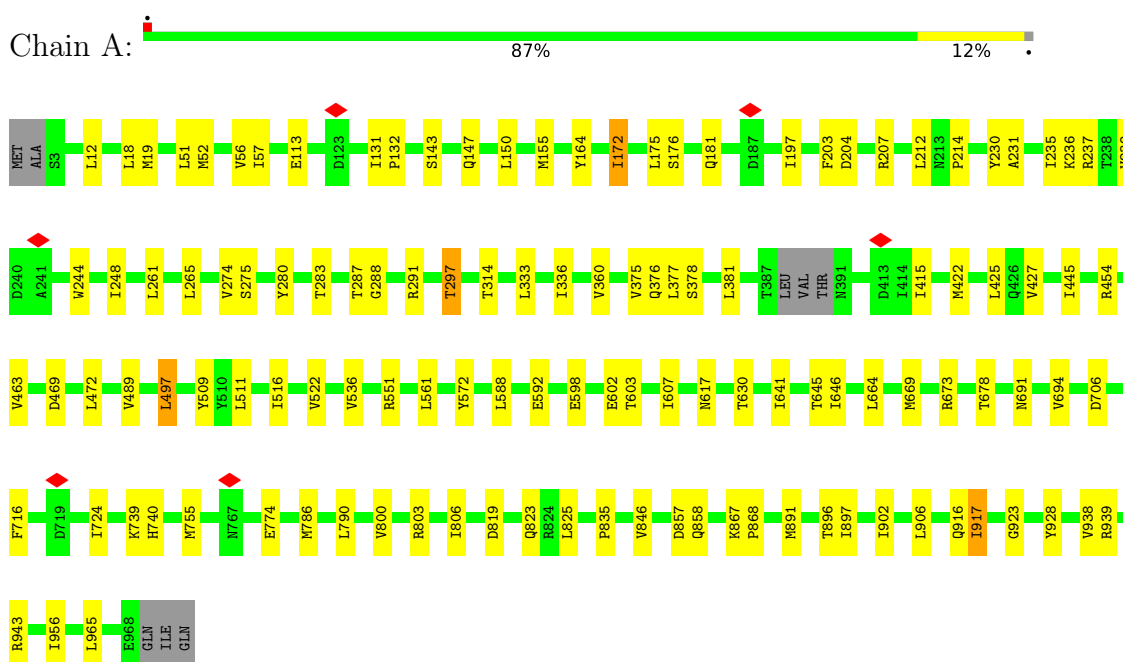
- Molecule 8 is a protein called PHIKZ062.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	133	Total	C	N	O	S	0	0
			1056	673	176	206	1		
8	b	133	Total	C	N	O	S	0	0
			1056	673	176	206	1		

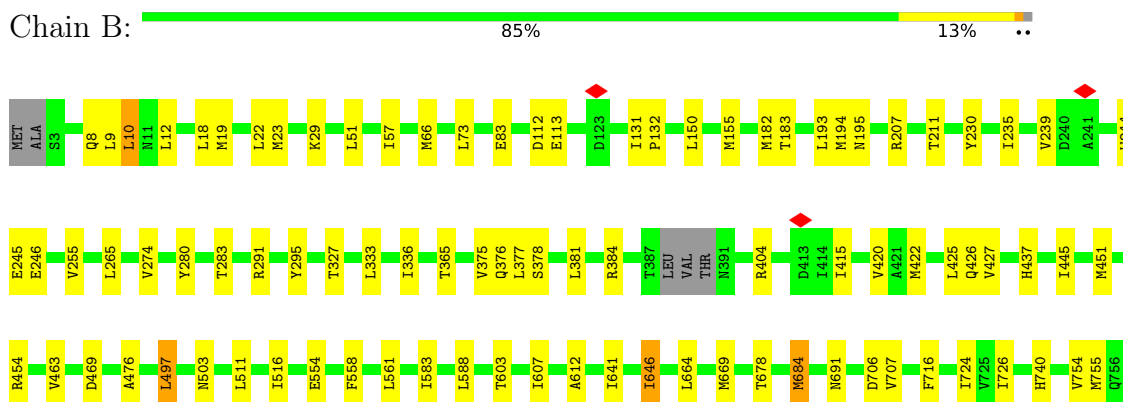
3 Residue-property plots

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: PHIKZ087



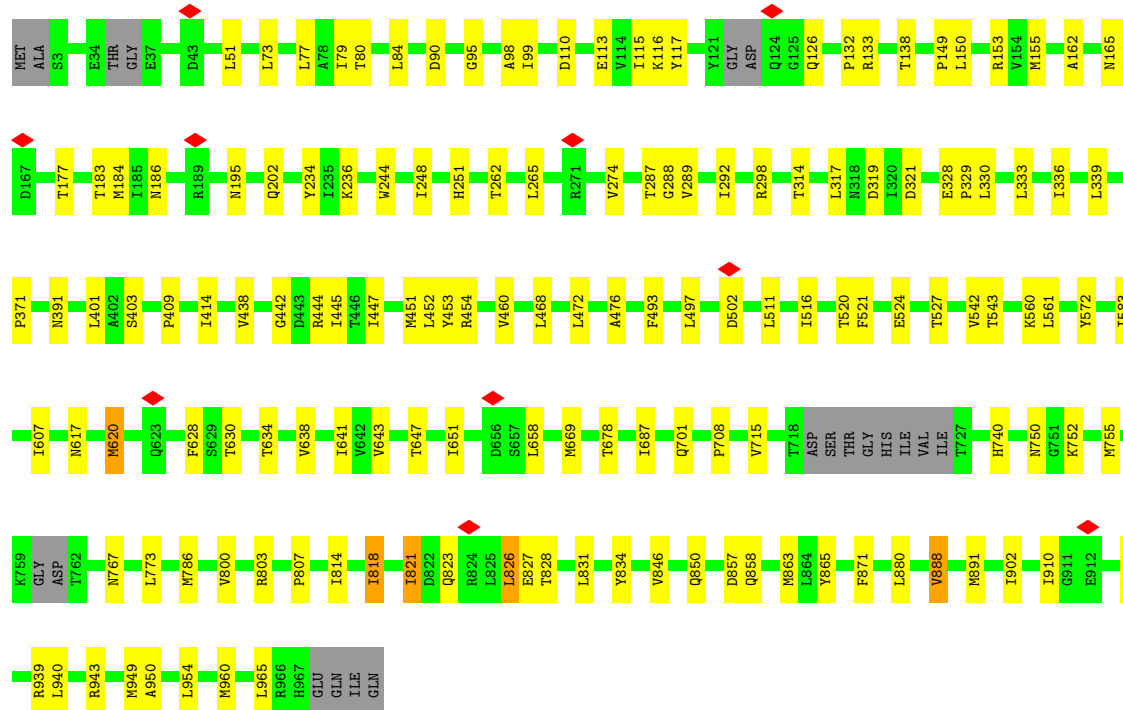
• Molecule 1: PHIKZ087





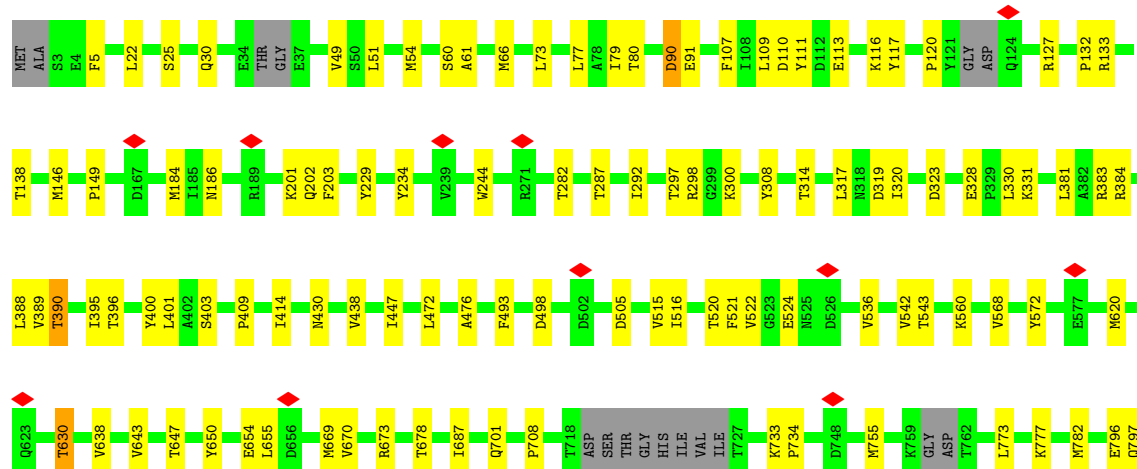
• Molecule 1: PHIKZ087

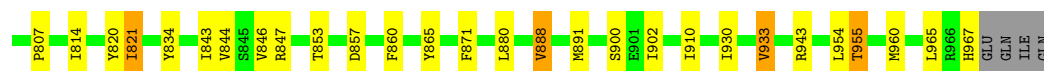
Chain U: 83% 15% ..



• Molecule 1: PHIKZ087

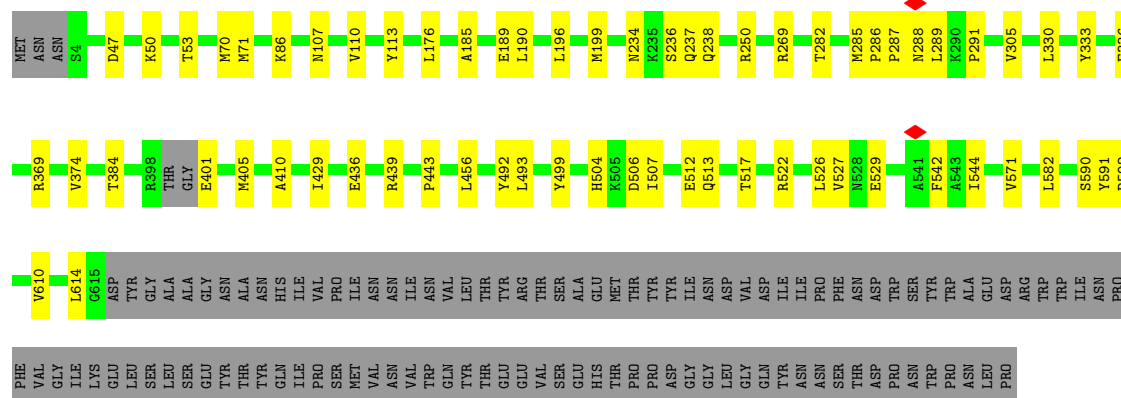
Chain V: 84% 13% ..





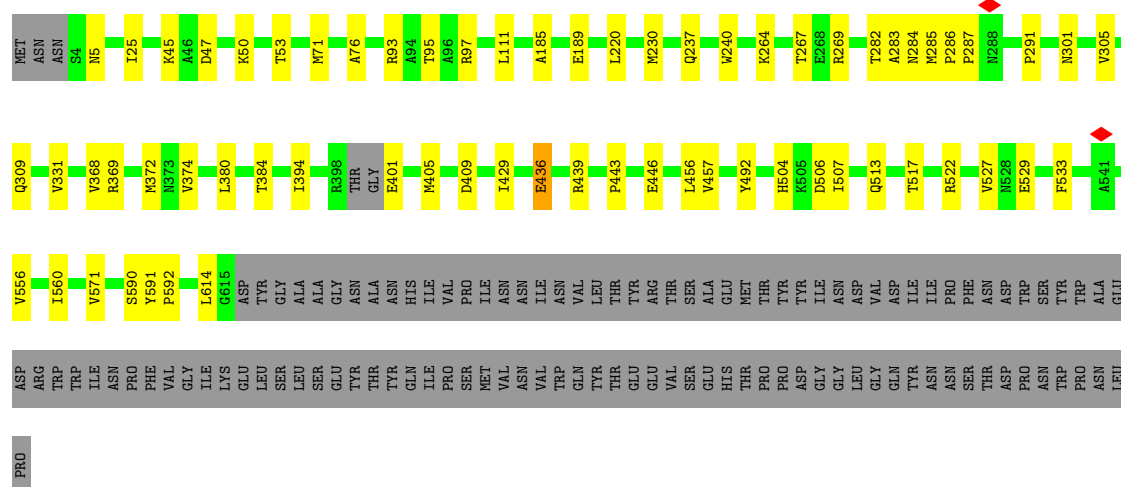
• Molecule 2: PHIKZ128

Chain C: 75% 9% 16%



• Molecule 2: PHIKZ128

Chain D: 75% 9% 16%



• Molecule 3: PHIKZ161

Chain E: 91% 8%



• Molecule 3: PHIKZ161

Chain F: 89% 9%



• Molecule 3: PHIKZ161

Chain G: 89% 11%



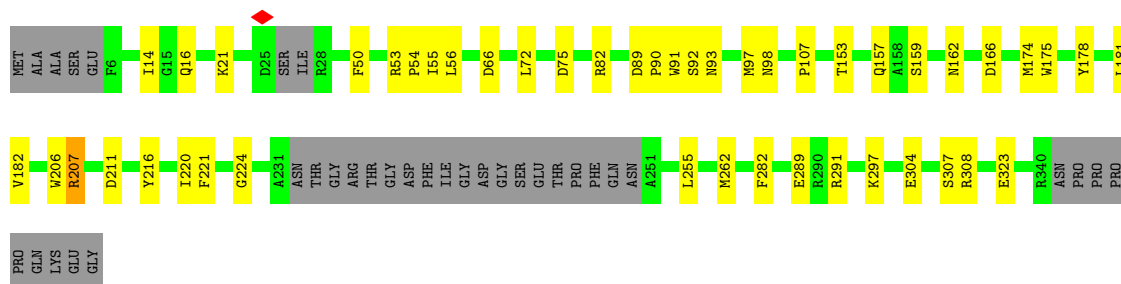
• Molecule 3: PHIKZ161

Chain H: 91% 7%



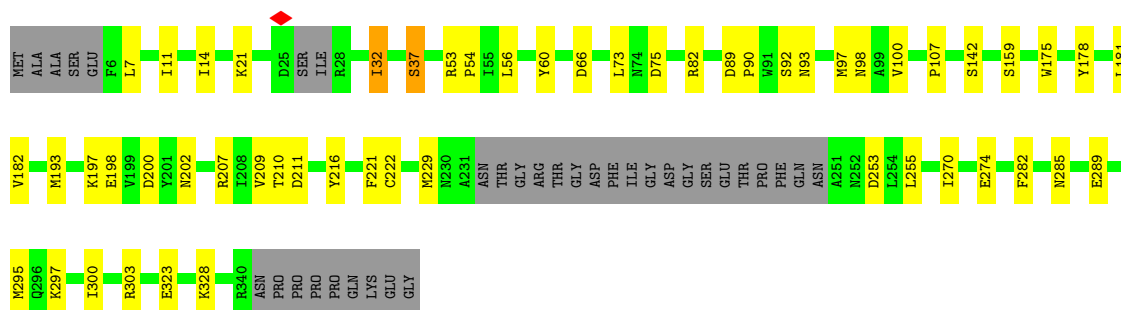
• Molecule 4: PHIKZ088

Chain I: 77% 13% 10%



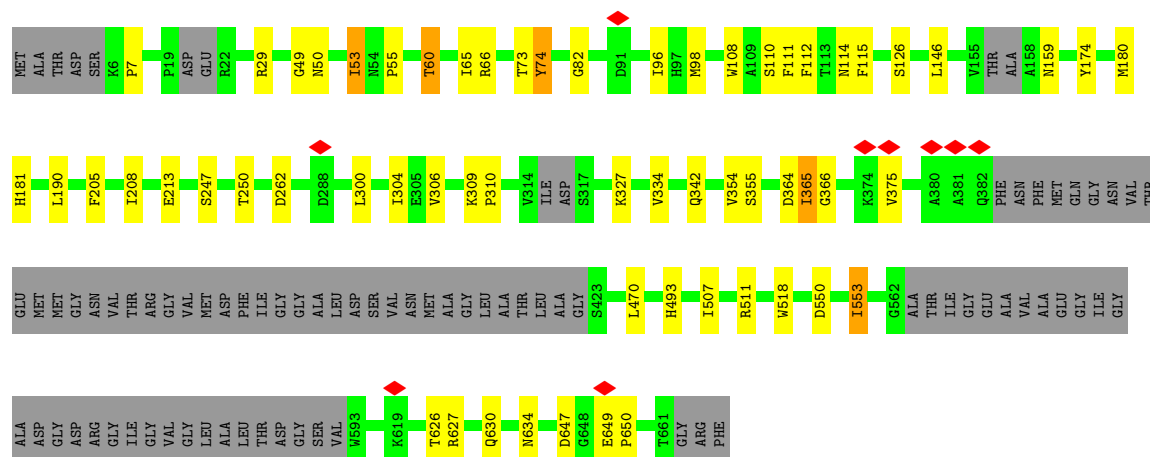
• Molecule 4: PHIKZ088

Chain J: 74% 15% 10%

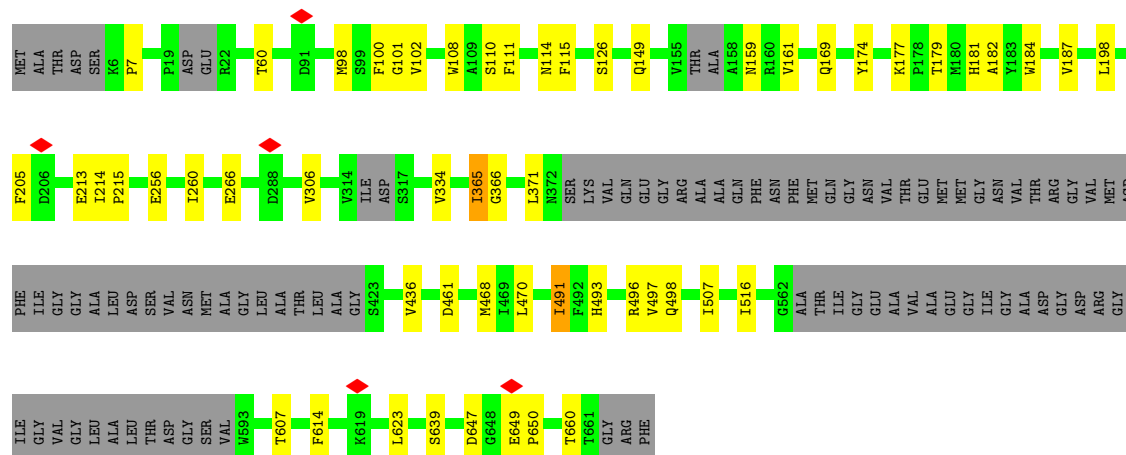
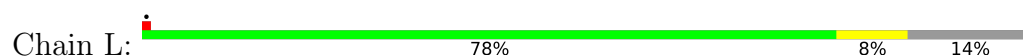


• Molecule 5: PHIKZ182

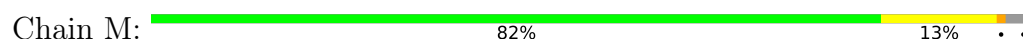
Chain K: 78% 8% 13%



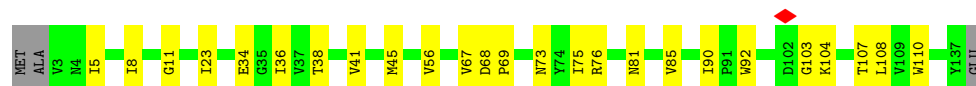
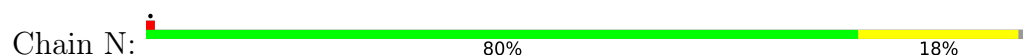
- Molecule 5: PHIKZ182



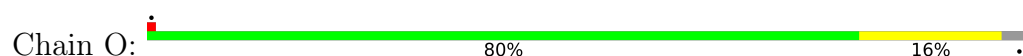
- Molecule 6: PHIKZ049



- Molecule 6: PHIKZ049

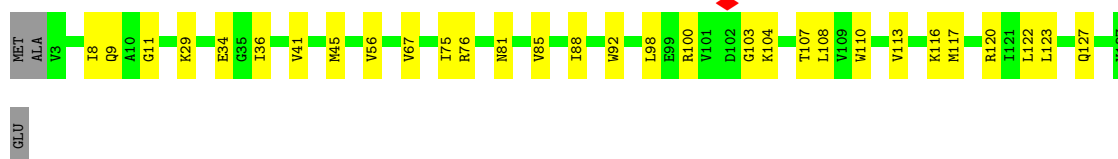
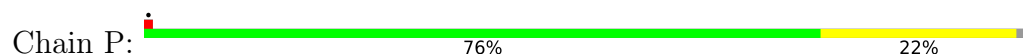


- Molecule 6: PHIKZ049

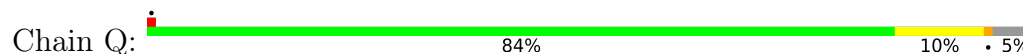




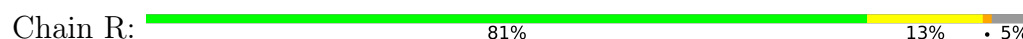
• Molecule 6: PHIKZ049



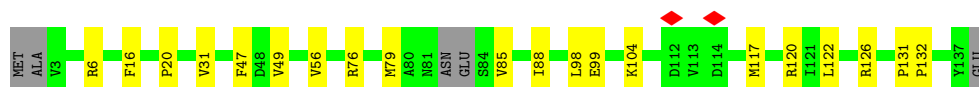
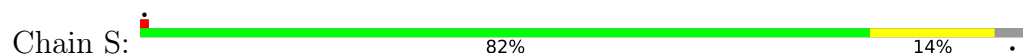
• Molecule 6: PHIKZ049



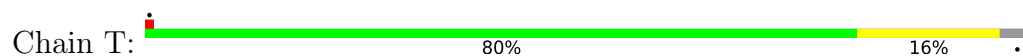
• Molecule 6: PHIKZ049



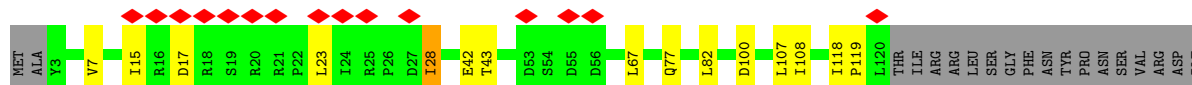
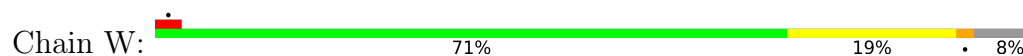
• Molecule 6: PHIKZ049

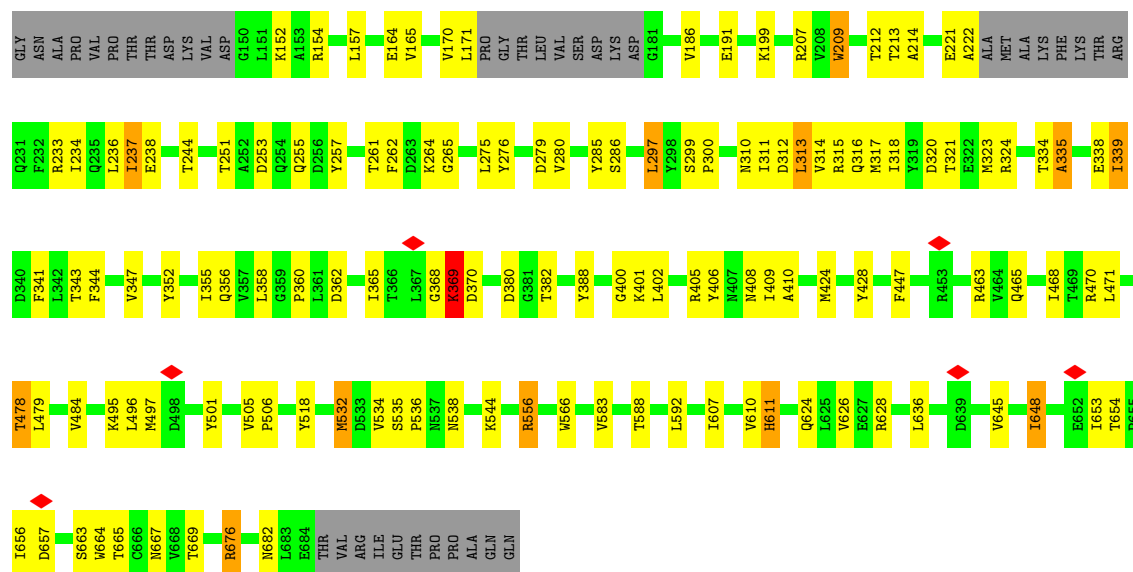


• Molecule 6: PHIKZ049



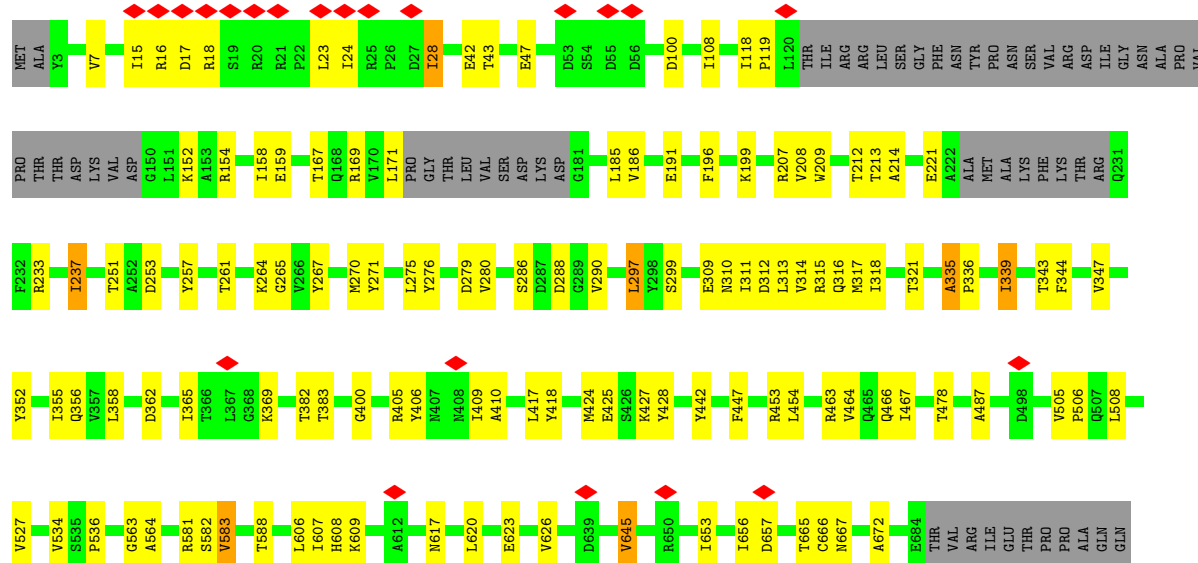
• Molecule 7: PHIKZ029





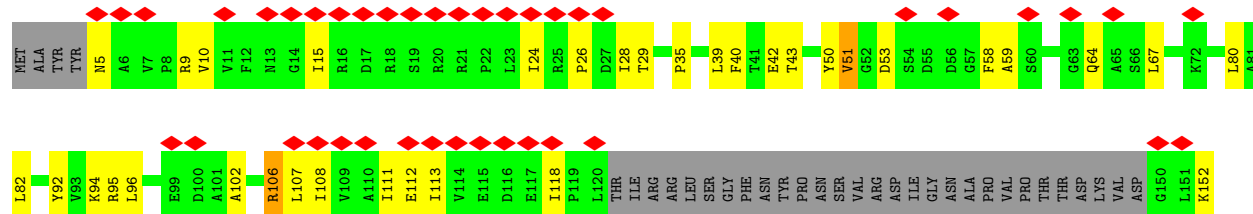
• Molecule 7: PHIKZ029

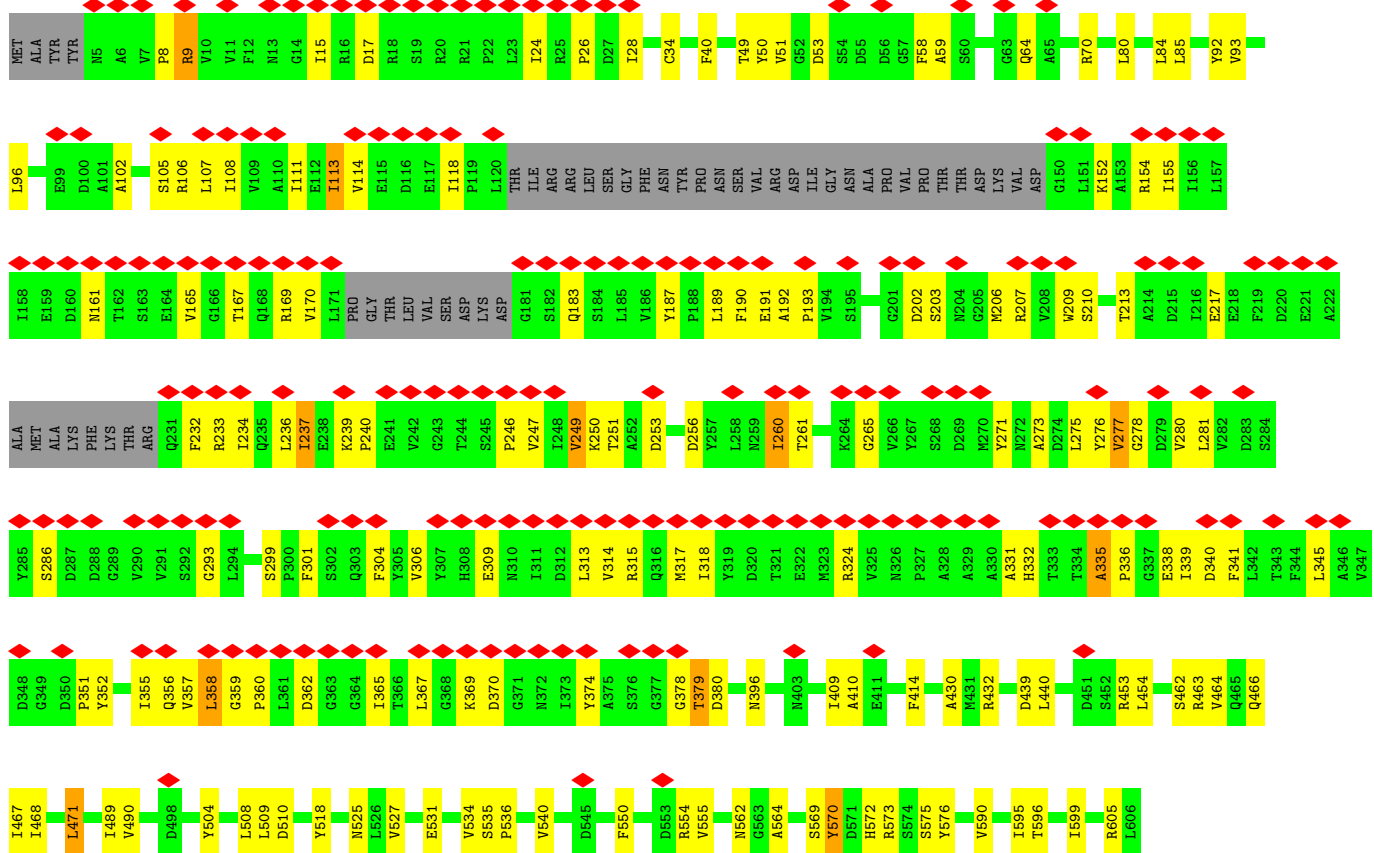
Chain X: 73% 18% 8%

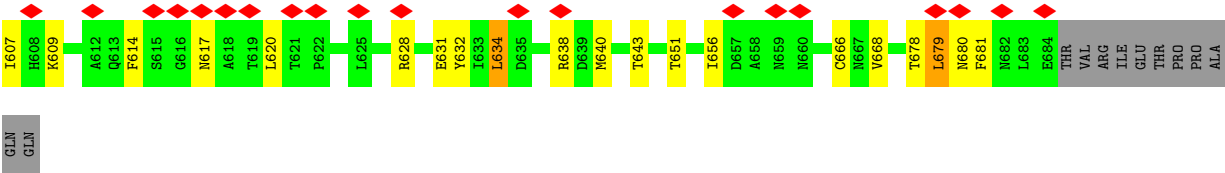


• Molecule 7: PHIKZ029

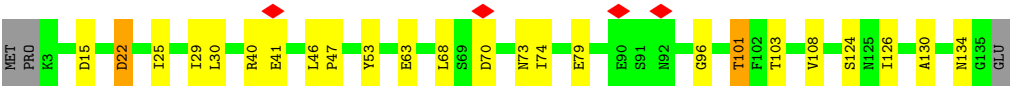
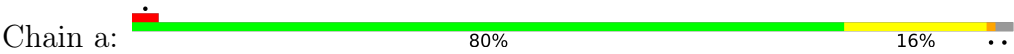
Chain Y: 30% 67% 23% 9%



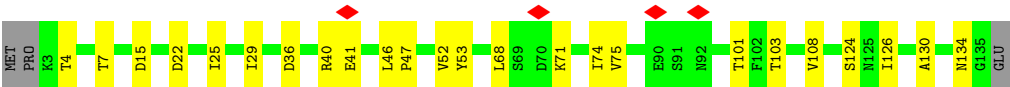
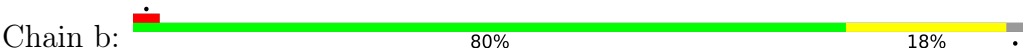




● Molecule 8: PHIKZ062



● Molecule 8: PHIKZ062



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22539	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.208	Depositor
Minimum map value	-0.651	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.23	Depositor
Map size ($\text{\AA}$)	544.0, 544.0, 544.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.36, 1.36, 1.36	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/7851	0.29	0/10649
1	B	0.14	0/7851	0.31	0/10649
1	U	0.18	0/7769	0.33	0/10534
1	V	0.15	0/7769	0.32	0/10534
2	C	0.15	0/5133	0.30	0/6968
2	D	0.13	0/5133	0.29	0/6968
3	E	0.13	0/1611	0.28	0/2198
3	F	0.12	0/1587	0.29	0/2166
3	G	0.13	0/1611	0.26	0/2198
3	H	0.12	0/1587	0.29	0/2166
4	I	0.17	0/2656	0.32	0/3608
4	J	0.18	0/2656	0.32	0/3608
5	K	0.17	0/4722	0.34	0/6404
5	L	0.17	0/4648	0.33	0/6306
6	M	0.15	0/1059	0.36	0/1447
6	N	0.14	0/1069	0.35	0/1462
6	O	0.16	0/1059	0.39	0/1447
6	P	0.13	0/1069	0.33	0/1462
6	Q	0.16	0/1044	0.38	0/1424
6	R	0.15	0/1044	0.36	0/1424
6	S	0.14	0/1051	0.34	0/1436
6	T	0.14	0/1051	0.35	0/1436
7	W	0.16	0/5113	0.40	0/6953
7	X	0.16	0/5113	0.40	0/6953
7	Y	0.19	0/5087	0.42	0/6917
7	Z	0.21	0/5087	0.43	0/6917
8	a	0.20	0/1073	0.45	0/1457
8	b	0.19	0/1073	0.44	0/1457
All	All	0.16	0/93576	0.34	0/127148

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7705	0	7652	65	0
1	B	7705	0	7652	80	0
1	U	7627	0	7594	75	0
1	V	7627	0	7594	75	0
2	C	5019	0	4947	37	0
2	D	5019	0	4947	40	0
3	E	1583	0	1591	16	0
3	F	1559	0	1557	15	0
3	G	1583	0	1591	11	0
3	H	1559	0	1557	15	0
4	I	2594	0	2511	26	0
4	J	2594	0	2511	32	0
5	K	4604	0	4465	37	0
5	L	4530	0	4390	33	0
6	M	1038	0	1029	11	0
6	N	1047	0	1038	14	0
6	O	1038	0	1029	18	0
6	P	1047	0	1038	18	0
6	Q	1025	0	1016	10	0
6	R	1025	0	1016	13	0
6	S	1030	0	1025	11	0
6	T	1030	0	1025	13	0
7	W	5010	0	4888	84	0
7	X	5010	0	4888	74	0
7	Y	4986	0	4870	109	0
7	Z	4986	0	4870	114	0
8	a	1056	0	1076	16	0
8	b	1056	0	1076	13	0
All	All	91692	0	90443	999	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:ASP:HB3	1:B:755:MET:HE1	1.41	0.99
7:Z:277:VAL:HG23	7:Z:278:GLY:H	1.35	0.92
7:Y:277:VAL:HG23	7:Y:278:GLY:H	1.34	0.88
8:a:130:ALA:O	8:a:134:ASN:HB2	1.74	0.86
8:b:40:ARG:HG2	8:b:41:GLU:H	1.40	0.82
8:a:40:ARG:HG2	8:a:41:GLU:H	1.46	0.80
1:B:949:MET:HE3	1:B:955:THR:HG21	1.66	0.77
4:I:55:ILE:HD13	4:I:91:TRP:HE1	1.49	0.76
7:X:318:ILE:HG21	7:X:339:ILE:HD12	1.67	0.76
1:V:891:MET:HG2	1:V:902:ILE:HG12	1.66	0.76
7:X:213:THR:HG22	7:X:214:ALA:H	1.50	0.76
1:B:9:LEU:HD11	1:B:19:MET:HE3	1.67	0.76
6:M:18:VAL:HG22	6:M:20:PRO:HD2	1.68	0.75
7:Y:315:ARG:HG3	7:Y:335:ALA:HB1	1.70	0.74
7:Y:213:THR:HG22	7:Y:214:ALA:H	1.53	0.74
7:Y:251:THR:HG23	7:Y:253:ASP:H	1.52	0.73
7:Y:40:PHE:HD2	7:Y:383:THR:HG23	1.53	0.73
5:K:365:ILE:HG22	5:K:366:GLY:H	1.54	0.73
7:X:534:VAL:HG13	7:X:536:PRO:HD2	1.69	0.73
3:E:33:ARG:HH11	3:E:38:ILE:HD13	1.53	0.72
7:Z:24:ILE:HG23	7:Z:26:PRO:HD3	1.71	0.72
6:O:18:VAL:HG22	6:O:20:PRO:HD2	1.71	0.72
6:M:76:ARG:HH21	6:N:41:VAL:HG22	1.54	0.72
7:Z:656:ILE:HD12	7:Z:656:ILE:H	1.55	0.71
7:Y:342:LEU:HD23	7:Y:343:THR:HG23	1.72	0.71
7:Y:656:ILE:HD12	7:Y:656:ILE:H	1.56	0.71
7:W:315:ARG:HG3	7:W:335:ALA:HB1	1.73	0.70
7:Y:51:VAL:HG21	7:Y:58:PHE:HD1	1.56	0.70
7:X:42:GLU:HG3	7:X:43:THR:HG22	1.72	0.70
7:W:213:THR:HG22	7:W:214:ALA:H	1.57	0.70
4:J:202:ASN:HB2	5:K:60:THR:HG23	1.74	0.70
7:W:154:ARG:HD2	7:W:362:ASP:HB3	1.72	0.70
7:X:409:ILE:HB	7:Y:5:ASN:HB3	1.73	0.70
5:K:53:ILE:HG13	5:L:468:MET:HE1	1.71	0.69
3:E:74:THR:HG22	3:E:80:PRO:HB3	1.75	0.68
7:X:358:LEU:HD21	7:X:365:ILE:HG22	1.75	0.68
7:Z:315:ARG:HG3	7:Z:335:ALA:HB1	1.76	0.68
1:A:516:ILE:HG13	1:A:678:THR:HG22	1.76	0.68
4:J:53:ARG:HH21	4:J:90:PRO:HA	1.58	0.68
1:V:202:GLN:HE22	1:V:298:ARG:HB2	1.59	0.67
7:Y:24:ILE:HG23	7:Y:26:PRO:HD3	1.75	0.67
1:B:437:HIS:HB2	1:B:451:MET:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:193:MET:HE2	4:J:200:ASP:HB3	1.75	0.67
1:V:132:PRO:HG2	1:V:317:LEU:HB3	1.75	0.67
7:Z:468:ILE:HA	7:Z:471:LEU:HB2	1.77	0.66
1:U:891:MET:HG2	1:U:902:ILE:HG12	1.76	0.66
7:X:563:GLY:HA2	7:X:581:ARG:HE	1.60	0.65
1:V:409:PRO:HG3	1:V:414:ILE:HG13	1.77	0.65
7:Z:106:ARG:HE	7:Z:161:ASN:HA	1.61	0.65
4:J:7:LEU:O	4:J:11:ILE:HD12	1.97	0.64
7:W:42:GLU:HG3	7:W:43:THR:HG22	1.78	0.64
7:Z:209:TRP:CG	7:Z:210:SER:H	2.16	0.64
7:Y:152:LYS:HA	7:Y:355:ILE:HB	1.79	0.64
1:A:230:TYR:HD1	1:A:231:ALA:H	1.44	0.64
1:A:716:PHE:HB2	1:A:724:ILE:HD12	1.79	0.63
1:U:516:ILE:HG12	1:U:678:THR:HG22	1.79	0.63
6:R:9:GLN:HG3	6:S:6:ARG:HD3	1.80	0.63
7:X:208:VAL:HG12	7:X:209:TRP:H	1.64	0.63
3:H:14:ILE:HG23	3:H:16:PRO:HD2	1.81	0.63
1:B:375:VAL:HG12	1:B:376:GLN:HG3	1.80	0.63
1:B:716:PHE:HB2	1:B:724:ILE:HD12	1.81	0.63
3:E:44:ASN:HB3	3:E:47:ASP:HB2	1.80	0.63
3:G:44:ASN:HB3	3:G:47:ASP:HB2	1.80	0.63
7:Z:367:LEU:HD21	7:Z:370:ASP:HB2	1.80	0.62
3:G:74:THR:HG22	3:G:80:PRO:HB3	1.81	0.62
1:A:131:ILE:HD12	1:A:150:LEU:HD23	1.81	0.62
7:Z:251:THR:HG23	7:Z:253:ASP:H	1.62	0.62
1:B:800:VAL:HG22	1:B:803:ARG:HH21	1.65	0.62
6:T:117:MET:O	6:T:121:ILE:HG13	2.00	0.62
1:B:255:VAL:HG21	2:C:236:SER:HB2	1.80	0.62
1:V:647:THR:HG23	1:V:669:MET:HE1	1.82	0.61
1:B:454:ARG:HH21	1:B:463:VAL:HG22	1.63	0.61
7:Z:464:VAL:HG21	7:Z:564:ALA:HB2	1.82	0.61
7:Y:108:ILE:HG13	7:Y:191:GLU:HG3	1.82	0.61
2:C:384:THR:HB	2:C:522:ARG:HH22	1.66	0.61
1:V:521:PHE:HZ	1:V:524:GLU:HB3	1.65	0.61
7:Z:51:VAL:HG21	7:Z:58:PHE:HD1	1.65	0.61
7:X:251:THR:HG23	7:X:253:ASP:H	1.66	0.60
1:B:790:LEU:HB3	1:B:956:ILE:HD11	1.83	0.60
7:X:315:ARG:HH21	7:X:316:GLN:HB3	1.65	0.60
8:a:53:TYR:HE2	8:a:63:GLU:HG3	1.66	0.60
1:A:790:LEU:HB3	1:A:956:ILE:HD11	1.82	0.60
2:C:405:MET:HE2	2:C:410:ALA:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:572:TYR:HE2	1:V:630:THR:HB	1.67	0.60
7:Z:277:VAL:HG23	7:Z:278:GLY:N	2.13	0.60
6:O:90:ILE:HD12	6:O:90:ILE:H	1.65	0.60
7:Y:96:LEU:HB3	7:Y:391:LEU:HD13	1.83	0.60
1:B:131:ILE:HD12	1:B:150:LEU:HD23	1.83	0.60
1:V:796:GLU:HG3	1:V:955:THR:HG23	1.84	0.60
7:Z:240:PRO:HD2	7:Z:246:PRO:HA	1.84	0.60
1:A:422:MET:HE1	1:A:835:PRO:HD2	1.83	0.59
7:Y:277:VAL:HG23	7:Y:278:GLY:N	2.13	0.59
7:X:344:PHE:HD2	7:X:356:GLN:HG3	1.67	0.59
4:J:300:ILE:HG23	4:J:303:ARG:HH21	1.67	0.59
6:R:48:ASP:HB3	6:R:51:ALA:HB3	1.85	0.59
7:Y:259:ASN:O	7:Y:260:ILE:HD13	2.03	0.59
1:B:51:LEU:HB3	1:V:51:LEU:HD21	1.84	0.59
1:B:422:MET:HE2	1:B:835:PRO:HD2	1.84	0.59
2:C:47:ASP:HB3	2:C:50:LYS:HB2	1.84	0.59
3:E:127:VAL:HG21	3:F:127:VAL:HG21	1.84	0.59
1:U:583:ILE:HD12	1:U:617:ASN:HD22	1.66	0.59
1:V:493:PHE:HE1	1:V:807:PRO:HB3	1.67	0.59
7:Z:152:LYS:HA	7:Z:355:ILE:HB	1.84	0.59
1:U:572:TYR:HE2	1:U:630:THR:HB	1.66	0.59
1:V:516:ILE:HG12	1:V:678:THR:HG22	1.84	0.59
1:B:365:THR:HA	2:C:250:ARG:HH21	1.68	0.59
6:T:18:VAL:HG22	6:T:20:PRO:HD2	1.85	0.59
5:L:498:GLN:HG2	5:L:614:PHE:HE2	1.67	0.58
3:G:127:VAL:HG21	3:H:127:VAL:HG21	1.84	0.58
1:U:186:ASN:H	1:U:520:THR:HG23	1.67	0.58
7:Y:106:ARG:HE	7:Y:161:ASN:HA	1.67	0.58
7:Z:232:PHE:HZ	7:Z:340:ASP:HA	1.68	0.58
7:Z:554:ARG:HH21	7:Z:555:VAL:HG23	1.68	0.58
5:L:101:GLY:HA2	5:L:179:THR:HG22	1.85	0.58
7:W:67:LEU:HD12	7:W:82:LEU:HB2	1.84	0.58
4:I:53:ARG:HH21	4:I:90:PRO:HA	1.68	0.58
6:N:107:THR:HG23	6:Q:109:VAL:HG22	1.85	0.58
1:A:454:ARG:HH21	1:A:463:VAL:HG22	1.68	0.58
1:A:641:ILE:HD13	1:A:664:LEU:HD11	1.86	0.58
7:Z:314:VAL:HA	7:Z:317:MET:HB2	1.83	0.58
5:K:7:PRO:HG2	7:Y:638:ARG:HH22	1.68	0.58
6:O:47:PHE:CD2	6:O:87:PHE:HB2	2.39	0.58
1:U:521:PHE:HZ	1:U:524:GLU:HB3	1.68	0.58
7:W:251:THR:HG23	7:W:253:ASP:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:VAL:HG12	1:A:376:GLN:HG3	1.84	0.58
5:K:29:ARG:HG2	5:K:74:TYR:HE2	1.69	0.58
7:Y:464:VAL:HG21	7:Y:564:ALA:HB2	1.86	0.57
5:L:365:ILE:HG13	5:L:366:GLY:H	1.69	0.57
5:L:493:HIS:HB3	5:L:497:VAL:HG12	1.86	0.57
6:M:23:ILE:HG22	6:M:24:LEU:HD12	1.84	0.57
1:V:395:ILE:HG23	1:V:396:THR:HG23	1.86	0.57
1:A:377:LEU:HD11	1:A:381:LEU:HG	1.86	0.57
7:Y:209:TRP:CD1	7:Y:210:SER:H	2.23	0.57
7:Y:344:PHE:HD2	7:Y:356:GLN:HG2	1.69	0.57
7:X:108:ILE:HG23	7:X:191:GLU:HB2	1.85	0.57
1:B:891:MET:HG2	1:B:902:ILE:HG12	1.87	0.57
7:Z:107:LEU:HD11	7:Z:206:MET:HE1	1.85	0.57
8:b:40:ARG:HG2	8:b:41:GLU:N	2.16	0.57
6:S:31:VAL:HG12	6:S:79:MET:HA	1.85	0.57
7:X:653:ILE:HG23	7:X:657:ASP:HB2	1.86	0.57
3:E:120:LEU:HD21	3:F:128:ILE:HD12	1.87	0.57
7:Y:207:ARG:HH21	7:Y:237:ILE:HG21	1.69	0.57
1:B:641:ILE:HD13	1:B:664:LEU:HD11	1.85	0.57
7:Z:80:LEU:HB2	7:Z:509:LEU:HD11	1.86	0.57
7:W:152:LYS:HG2	7:W:355:ILE:HD12	1.87	0.56
7:Y:107:LEU:HD11	7:Y:206:MET:HE1	1.87	0.56
7:Z:239:LYS:HG2	7:Z:246:PRO:HB3	1.87	0.56
1:B:858:GLN:NE2	1:B:923:GLY:H	2.03	0.56
1:A:800:VAL:HG22	1:A:803:ARG:HH21	1.70	0.56
1:V:708:PRO:HB3	1:V:755:MET:HE1	1.86	0.56
7:W:119:PRO:HG3	7:W:355:ILE:HD11	1.87	0.56
7:W:315:ARG:HH21	7:W:316:GLN:HB3	1.70	0.56
7:W:400:GLY:HA2	7:W:406:TYR:HD1	1.70	0.56
7:X:317:MET:O	7:X:321:THR:HG23	2.05	0.56
3:F:149:VAL:HG13	3:F:153:GLN:HB2	1.87	0.56
6:Q:117:MET:HE3	6:Q:117:MET:HA	1.87	0.56
1:U:202:GLN:HE22	1:U:298:ARG:HB2	1.71	0.56
7:W:648:ILE:HG23	7:W:669:THR:HB	1.88	0.56
7:Z:301:PHE:HZ	7:Z:304:PHE:HB2	1.70	0.56
7:X:169:ARG:HG2	7:X:169:ARG:HH11	1.71	0.56
7:W:164:GLU:HG2	7:W:165:VAL:H	1.70	0.56
7:Y:240:PRO:HD2	7:Y:246:PRO:HA	1.87	0.56
7:W:317:MET:O	7:W:321:THR:HG23	2.06	0.56
2:C:369:ARG:HH11	2:C:374:VAL:HG22	1.70	0.56
1:B:12:LEU:HD13	1:B:18:LEU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:35:PRO:HB3	7:Y:416:VAL:HG23	1.88	0.56
1:A:19:MET:HE2	1:A:56:VAL:HG13	1.88	0.56
1:U:800:VAL:HG22	1:U:803:ARG:HH21	1.71	0.56
1:V:116:LYS:HE3	1:V:117:TYR:CE1	2.40	0.56
5:K:550:ASP:HB3	5:K:553:ILE:HD11	1.87	0.55
1:V:186:ASN:H	1:V:520:THR:HG23	1.70	0.55
7:X:108:ILE:HB	7:X:158:ILE:HG22	1.87	0.55
7:Z:113:ILE:HG22	7:Z:114:VAL:H	1.71	0.55
7:Z:518:TYR:CE1	7:Z:531:GLU:HA	2.41	0.55
4:I:98:ASN:HD21	7:Y:643:THR:HG21	1.71	0.55
1:U:755:MET:HE2	1:U:755:MET:HA	1.88	0.55
7:W:313:LEU:O	7:W:316:GLN:HG3	2.06	0.55
7:Y:113:ILE:HG23	7:Y:153:ALA:HB2	1.88	0.55
6:P:110:TRP:HZ2	6:R:125:VAL:HG11	1.72	0.55
1:U:236:LYS:O	1:U:288:GLY:HA3	2.06	0.55
7:Y:343:THR:HG22	7:Y:367:LEU:HA	1.88	0.55
7:Z:190:PHE:HB3	7:Z:306:VAL:HG22	1.88	0.55
7:Z:209:TRP:HZ3	7:Z:369:LYS:HB2	1.71	0.55
1:V:438:VAL:HG12	1:V:447:ILE:HA	1.89	0.55
7:Y:365:ILE:HG22	7:Y:367:LEU:HB3	1.88	0.55
7:Z:265:GLY:HA2	7:Z:276:TYR:HB2	1.88	0.55
7:W:358:LEU:HD21	7:W:365:ILE:HG22	1.88	0.55
7:W:676:ARG:HD2	8:a:96:GLY:HA3	1.88	0.55
1:B:426:GLN:HG2	1:B:781:GLU:HG2	1.88	0.55
1:A:572:TYR:CE2	1:A:630:THR:HB	2.42	0.55
1:B:892:LEU:HD12	1:B:897:ILE:HG12	1.88	0.55
1:U:687:ILE:HD11	1:U:814:ILE:HD11	1.88	0.55
7:Z:234:ILE:HG13	7:Z:260:ILE:HD11	1.88	0.55
7:Z:236:LEU:HB3	7:Z:249:VAL:HG23	1.90	0.55
3:F:14:ILE:HG23	3:F:16:PRO:HD2	1.89	0.54
4:I:207:ARG:HB3	4:I:221:PHE:HB2	1.89	0.54
7:X:425:GLU:HA	7:X:428:TYR:HD2	1.73	0.54
5:K:66:ARG:HA	5:K:82:GLY:HA2	1.89	0.54
1:U:701:GLN:HG2	1:U:773:LEU:HD23	1.89	0.54
7:X:154:ARG:HD2	7:X:362:ASP:HB3	1.88	0.54
7:Y:462:SER:O	7:Y:466:GLN:HG2	2.07	0.54
2:D:556:VAL:O	2:D:560:ILE:HG22	2.08	0.54
1:V:234:TYR:HB3	1:V:244:TRP:HB3	1.88	0.54
3:G:8:LYS:HG2	3:G:28:VAL:HG22	1.89	0.54
5:K:7:PRO:HG2	7:Y:638:ARG:NH2	2.22	0.54
7:W:405:ARG:HD3	7:Y:550:PHE:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:213:THR:HG22	7:Y:214:ALA:N	2.20	0.54
5:L:214:ILE:HG13	5:L:215:PRO:HD3	1.90	0.54
1:A:891:MET:HG2	1:A:902:ILE:HG12	1.89	0.54
5:L:159:ASN:HB3	5:L:334:VAL:HG21	1.89	0.54
7:W:624:GLN:O	7:W:628:ARG:HG2	2.08	0.54
1:U:98:ALA:O	1:U:99:ILE:HD13	2.08	0.54
7:X:447:PHE:CD2	7:X:506:PRO:HG3	2.43	0.54
6:T:34:GLU:HB2	6:T:76:ARG:HB3	1.90	0.54
1:U:409:PRO:HG3	1:U:414:ILE:HG13	1.89	0.54
4:J:274:GLU:HG2	5:K:65:ILE:HB	1.90	0.53
1:U:330:LEU:HD12	1:U:333:LEU:HD13	1.91	0.53
7:Y:118:ILE:HD11	7:Y:324:ARG:HH12	1.73	0.53
1:V:888:VAL:HG21	1:V:960:MET:HE1	1.89	0.53
7:X:336:PRO:O	7:X:339:ILE:HG12	2.09	0.53
8:a:70:ASP:O	8:a:74:ILE:HG22	2.07	0.53
7:W:424:MET:HE2	7:W:463:ARG:HD2	1.90	0.53
1:V:843:ILE:HG12	1:V:853:THR:HG22	1.91	0.53
7:X:609:LYS:HA	7:Y:5:ASN:HD21	1.72	0.53
7:Y:236:LEU:HB3	7:Y:249:VAL:HG23	1.89	0.53
1:B:684:MET:HE1	1:B:811:VAL:HG22	1.89	0.53
7:Y:554:ARG:HH21	7:Y:555:VAL:HG23	1.73	0.53
7:Z:572:HIS:O	7:Z:573:ARG:HG2	2.08	0.53
2:D:237:GLN:HE22	2:D:269:ARG:HD3	1.74	0.53
7:X:313:LEU:O	7:X:316:GLN:HG3	2.09	0.53
7:Z:167:THR:HG23	7:Z:169:ARG:HH12	1.74	0.53
1:B:183:THR:OG1	1:B:195:ASN:HB3	2.09	0.53
5:K:354:VAL:HG23	5:K:511:ARG:HB2	1.90	0.53
5:K:518:TRP:HH2	5:L:496:ARG:HB2	1.73	0.53
7:W:471:LEU:HD13	7:W:583:VAL:HG11	1.91	0.53
6:T:31:VAL:HG12	6:T:79:MET:HA	1.91	0.52
7:Y:154:ARG:HE	7:Y:357:VAL:HB	1.74	0.52
7:Y:261:THR:HG23	7:Y:275:LEU:HB3	1.90	0.52
1:B:923:GLY:HA3	1:B:928:TYR:HD2	1.74	0.52
2:D:267:THR:HG22	2:D:301:ASN:HD21	1.73	0.52
2:D:429:ILE:HA	2:D:533:PHE:HE1	1.73	0.52
6:O:36:ILE:HG23	6:O:75:ILE:HG22	1.90	0.52
7:Z:617:ASN:HB3	7:Z:620:LEU:HG	1.90	0.52
3:G:14:ILE:HG22	3:G:16:PRO:HD2	1.90	0.52
4:I:162:ASN:HD21	4:I:166:ASP:HB2	1.75	0.52
4:J:54:PRO:HG3	4:J:175:TRP:CZ2	2.44	0.52
7:Y:107:LEU:HG	7:Y:192:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:154:ARG:HD3	7:Z:362:ASP:HB3	1.92	0.52
3:F:124:VAL:O	3:F:128:ILE:HG12	2.08	0.52
2:C:527:VAL:HG12	2:C:529:GLU:H	1.73	0.52
5:K:518:TRP:CH2	5:L:496:ARG:HB2	2.45	0.52
7:Z:261:THR:HG23	7:Z:275:LEU:HB3	1.91	0.52
6:T:78:ARG:HG3	6:T:78:ARG:HH11	1.75	0.52
2:D:369:ARG:HH11	2:D:374:VAL:HG22	1.74	0.52
7:Z:237:ILE:HD11	7:Z:374:TYR:CE1	2.45	0.52
6:P:113:VAL:HG13	6:P:117:MET:HB3	1.92	0.52
1:V:5:PHE:HB2	1:V:49:VAL:HG23	1.92	0.52
1:B:377:LEU:HD11	1:B:381:LEU:HG	1.92	0.52
2:D:47:ASP:HB2	2:D:50:LYS:HB2	1.92	0.52
6:O:73:ASN:HB2	6:O:90:ILE:HD11	1.92	0.52
1:B:858:GLN:HE22	1:B:923:GLY:H	1.57	0.51
5:L:7:PRO:HG2	7:Z:638:ARG:NH2	2.26	0.51
1:A:235:ILE:HD13	1:A:237:ARG:HH11	1.76	0.51
1:B:182:MET:SD	1:B:194:MET:HE1	2.50	0.51
5:K:159:ASN:HB3	5:K:334:VAL:HG21	1.92	0.51
1:U:865:TYR:HE1	1:U:965:LEU:HD12	1.74	0.51
2:C:285:MET:HE1	2:C:291:PRO:HB3	1.92	0.51
4:I:50:PHE:HB2	4:I:206:TRP:HB2	1.92	0.51
5:K:181:HIS:H	5:K:181:HIS:CD2	2.29	0.51
7:Y:190:PHE:HB3	7:Y:306:VAL:HG22	1.91	0.51
1:A:896:THR:C	1:A:897:ILE:HD13	2.34	0.51
6:T:41:VAL:O	6:T:45:MET:HG2	2.11	0.51
1:U:110:ASP:HB3	1:U:113:GLU:HB2	1.93	0.51
1:V:891:MET:HA	1:V:891:MET:HE2	1.92	0.51
7:Y:9:ARG:HH21	7:Z:679:LEU:HB3	1.75	0.51
6:N:103:GLY:O	6:N:104:LYS:HG3	2.10	0.51
6:R:34:GLU:OE2	6:R:34:GLU:HA	2.11	0.51
7:Z:108:ILE:HG13	7:Z:191:GLU:HG3	1.91	0.51
7:Z:345:LEU:HD23	7:Z:345:LEU:H	1.75	0.51
3:E:8:LYS:HG2	3:E:28:VAL:HG22	1.91	0.51
7:W:320:ASP:HB3	7:W:324:ARG:HH21	1.76	0.51
7:X:310:ASN:O	7:X:314:VAL:HG13	2.11	0.51
8:b:71:LYS:O	8:b:75:VAL:HG12	2.09	0.51
1:V:201:LYS:HB2	1:V:203:PHE:HE1	1.75	0.51
7:Y:67:LEU:HD22	7:Y:82:LEU:HB2	1.93	0.51
7:Y:572:HIS:O	7:Y:573:ARG:HG2	2.10	0.51
7:Z:207:ARG:HH21	7:Z:237:ILE:HG21	1.75	0.51
1:U:493:PHE:HE1	1:U:807:PRO:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:195:SER:HA	7:Y:302:SER:HB3	1.92	0.51
7:Z:409:ILE:HD11	7:Z:605:ARG:HA	1.93	0.51
1:B:333:LEU:HD23	1:B:336:ILE:HD11	1.93	0.51
1:U:708:PRO:HB3	1:U:755:MET:HE1	1.92	0.51
7:Y:50:TYR:HB2	7:Y:92:TYR:CE2	2.46	0.51
5:K:50:ASN:OD1	5:K:55:PRO:HB3	2.11	0.50
7:W:611:HIS:NE2	7:Y:678:THR:HG21	2.25	0.50
1:U:438:VAL:HG12	1:U:447:ILE:HA	1.93	0.50
1:B:807:PRO:O	1:B:811:VAL:HG23	2.11	0.50
4:J:297:LYS:NZ	4:J:323:GLU:HB3	2.27	0.50
1:U:452:LEU:HD12	1:U:468:LEU:HD13	1.92	0.50
1:U:858:GLN:HE22	1:U:940:LEU:HD13	1.76	0.50
7:X:315:ARG:HG3	7:X:335:ALA:HB1	1.92	0.50
7:Y:233:ARG:HH11	7:Y:259:ASN:HB2	1.76	0.50
1:A:175:LEU:HD12	1:A:176:SER:H	1.76	0.50
1:A:694:VAL:HG11	6:M:55:GLN:HG3	1.93	0.50
1:B:377:LEU:HD12	1:B:378:SER:N	2.25	0.50
7:W:607:ILE:HA	7:W:610:VAL:HG12	1.93	0.50
7:X:581:ARG:HG2	7:X:582:SER:O	2.12	0.50
1:A:858:GLN:HE22	1:A:923:GLY:H	1.59	0.50
1:B:858:GLN:HA	1:B:858:GLN:OE1	2.12	0.50
5:K:98:MET:HG2	5:L:491:ILE:HD13	1.93	0.50
7:Z:569:SER:HA	7:Z:575:SER:HA	1.94	0.50
4:J:297:LYS:HZ3	4:J:323:GLU:HB3	1.77	0.50
7:Z:118:ILE:HD11	7:Z:324:ARG:HH12	1.75	0.50
7:X:213:THR:HG22	7:X:214:ALA:N	2.25	0.50
7:X:487:ALA:HB3	7:X:583:VAL:HG21	1.94	0.50
7:Y:204:ASN:HD21	7:Y:300:PRO:HB2	1.77	0.50
2:C:333:TYR:O	2:C:336:GLU:HG3	2.11	0.50
4:I:211:ASP:OD2	4:I:216:TYR:HB2	2.11	0.50
7:Z:315:ARG:O	7:Z:318:ILE:HG13	2.11	0.50
1:B:910:ILE:HD12	1:B:914:VAL:HG11	1.94	0.49
2:D:527:VAL:HG12	2:D:529:GLU:H	1.77	0.49
7:W:276:TYR:O	7:W:280:VAL:HG22	2.11	0.49
2:C:429:ILE:HG21	2:C:527:VAL:HG23	1.93	0.49
4:I:72:LEU:HD21	4:I:174:MET:HG3	1.93	0.49
4:J:207:ARG:HB2	4:J:221:PHE:HB2	1.94	0.49
1:U:183:THR:HB	1:U:195:ASN:HB3	1.94	0.49
1:U:460:VAL:HG11	1:U:786:MET:HE2	1.94	0.49
7:W:653:ILE:HG23	7:W:657:ASP:HB2	1.94	0.49
1:B:503:ASN:H	2:C:282:THR:HG22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:201:LYS:HB2	1:V:203:PHE:CE1	2.46	0.49
7:Z:114:VAL:HB	7:Z:183:GLN:NE2	2.28	0.49
1:A:923:GLY:HA3	1:A:928:TYR:HD2	1.76	0.49
2:D:240:TRP:CE2	2:D:264:LYS:HD3	2.48	0.49
6:N:45:MET:HE2	6:N:45:MET:N	2.27	0.49
1:A:858:GLN:NE2	1:A:923:GLY:H	2.10	0.49
2:C:237:GLN:HE22	2:C:269:ARG:HD3	1.77	0.49
4:J:98:ASN:HD21	7:Z:643:THR:HG21	1.76	0.49
1:U:476:ALA:HB1	1:U:954:LEU:HD21	1.94	0.49
7:Y:315:ARG:O	7:Y:318:ILE:HG13	2.12	0.49
1:A:12:LEU:HD13	1:A:18:LEU:HB3	1.94	0.49
1:V:701:GLN:HG2	1:V:773:LEU:HD23	1.95	0.49
7:Z:628:ARG:HA	7:Z:631:GLU:CD	2.37	0.49
2:D:429:ILE:HG12	2:D:533:PHE:CE1	2.48	0.49
6:N:11:GLY:H	6:N:34:GLU:HA	1.76	0.49
3:G:176:VAL:O	3:G:179:GLU:HG3	2.13	0.49
4:J:93:ASN:HB2	4:J:97:MET:HE3	1.95	0.49
5:K:208:ILE:H	5:K:208:ILE:HD12	1.77	0.49
6:P:41:VAL:O	6:P:45:MET:HG2	2.13	0.49
7:Y:154:ARG:HH21	7:Y:357:VAL:HG11	1.78	0.49
6:M:122:LEU:O	6:M:126:ARG:HG3	2.13	0.48
1:V:687:ILE:HD11	1:V:814:ILE:HD11	1.95	0.48
7:W:233:ARG:HG2	7:W:257:TYR:CD2	2.48	0.48
7:Y:647:ILE:C	7:Y:648:ILE:HD12	2.38	0.48
7:Z:271:TYR:HD1	7:Z:273:ALA:HB3	1.77	0.48
4:I:308:ARG:NH2	4:J:37:SER:HB3	2.28	0.48
7:Y:238:GLU:HG3	7:Y:249:VAL:HG21	1.94	0.48
4:J:193:MET:HE3	4:J:198:GLU:HB2	1.95	0.48
7:Y:428:TYR:CD1	7:Y:470:ARG:HD2	2.49	0.48
1:B:384:ARG:HG2	1:B:404:ARG:HB2	1.94	0.48
1:V:542:VAL:HG12	1:V:543:THR:H	1.78	0.48
1:B:230:TYR:HB3	1:B:295:TYR:HD2	1.78	0.48
1:B:867:LYS:HG2	1:B:868:PRO:HD2	1.96	0.48
5:L:639:SER:HB2	5:L:660:THR:HG21	1.96	0.48
6:N:110:TRP:HZ2	6:Q:125:VAL:HG11	1.76	0.48
7:Z:111:ILE:HG13	7:Z:189:LEU:HG	1.95	0.48
2:D:372:MET:HA	2:D:372:MET:HE2	1.95	0.48
4:I:308:ARG:HH21	4:J:37:SER:HB3	1.78	0.48
5:K:630:GLN:HB3	5:K:634:ASN:HB2	1.95	0.48
6:O:47:PHE:CE2	6:O:87:PHE:HB2	2.48	0.48
7:Z:114:VAL:HB	7:Z:183:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:25:ILE:O	8:a:29:ILE:HG13	2.14	0.48
1:A:333:LEU:HD23	1:A:336:ILE:HD11	1.95	0.48
2:C:439:ARG:HD2	2:C:443:PRO:HD3	1.95	0.48
3:H:65:GLU:OE1	3:H:65:GLU:HA	2.13	0.48
3:H:193:GLU:OE2	1:V:734:PRO:HG2	2.14	0.48
6:P:120:ARG:HD2	6:R:129:ASN:HD21	1.78	0.48
1:U:826:LEU:H	1:U:826:LEU:HD23	1.79	0.48
1:V:755:MET:HA	1:V:755:MET:HE2	1.95	0.48
7:W:310:ASN:O	7:W:314:VAL:HG13	2.13	0.48
7:Y:113:ILE:HG21	7:Y:317:MET:SD	2.53	0.48
7:Y:640:MET:HE2	7:Y:640:MET:HB3	1.72	0.48
3:H:163:ALA:HB2	6:T:129:ASN:HB2	1.96	0.48
4:J:285:ASN:HB3	4:J:295:MET:HE3	1.94	0.48
7:W:209:TRP:HA	7:W:369:LYS:HZ1	1.79	0.48
7:W:607:ILE:HD13	7:Y:681:PHE:CZ	2.49	0.48
7:X:607:ILE:HD11	7:X:666:CYS:SG	2.54	0.48
7:Z:277:VAL:CG2	7:Z:278:GLY:H	2.18	0.48
1:B:73:LEU:HD12	1:V:73:LEU:HD21	1.96	0.48
6:R:29:LYS:HD3	6:R:29:LYS:C	2.39	0.48
6:R:76:ARG:HH12	6:R:85:VAL:HG11	1.79	0.48
1:V:22:LEU:O	1:V:25:SER:HB3	2.14	0.48
7:W:447:PHE:CD2	7:W:506:PRO:HG3	2.49	0.48
7:X:169:ARG:HG2	7:X:169:ARG:NH1	2.29	0.48
7:W:534:VAL:HG12	7:W:536:PRO:HD2	1.95	0.48
7:Y:237:ILE:HD11	7:Y:374:TYR:CE1	2.49	0.48
8:b:25:ILE:O	8:b:29:ILE:HG13	2.13	0.48
1:A:706:ASP:HB3	1:A:755:MET:SD	2.54	0.47
2:D:384:THR:HB	2:D:522:ARG:HH22	1.79	0.47
2:D:591:TYR:N	2:D:592:PRO:HD2	2.28	0.47
5:K:627:ARG:HG3	5:K:627:ARG:HH11	1.78	0.47
7:Z:9:ARG:H	7:Z:9:ARG:HE	1.62	0.47
1:B:377:LEU:HD12	1:B:378:SER:H	1.79	0.47
2:C:513:GLN:O	2:C:517:THR:HG23	2.14	0.47
2:C:590:SER:HB2	2:C:592:PRO:HD2	1.94	0.47
2:D:76:ALA:H	2:D:95:THR:HG22	1.78	0.47
6:T:60:LEU:H	6:T:60:LEU:HD12	1.78	0.47
1:V:77:LEU:HD23	1:V:77:LEU:H	1.78	0.47
1:V:844:VAL:HG12	1:V:933:VAL:HA	1.95	0.47
7:X:311:ILE:HA	7:X:314:VAL:HG22	1.96	0.47
7:Y:210:SER:HB2	7:Y:345:LEU:HD11	1.96	0.47
7:Z:250:LYS:HD2	7:Z:256:ASP:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:332:HIS:CE1	7:Z:339:ILE:H	2.31	0.47
4:I:93:ASN:HB2	4:I:97:MET:HE2	1.95	0.47
1:B:830:GLU:HA	1:B:830:GLU:OE1	2.15	0.47
2:C:591:TYR:N	2:C:592:PRO:HD2	2.28	0.47
2:D:93:ARG:HB3	2:D:97:ARG:HH12	1.79	0.47
1:V:390:THR:HG23	1:V:400:TYR:HE1	1.78	0.47
2:D:405:MET:HG3	2:D:409:ASP:HB2	1.96	0.47
3:E:33:ARG:HH21	3:H:33:ARG:CZ	2.27	0.47
1:V:300:LYS:HD2	1:V:300:LYS:HA	1.75	0.47
1:B:112:ASP:HB3	7:W:360:PRO:HD3	1.97	0.47
2:D:283:ALA:O	2:D:284:ASN:HB3	2.15	0.47
2:D:369:ARG:HD2	2:D:492:TYR:CE2	2.50	0.47
7:W:221:GLU:HG2	7:W:222:ALA:H	1.77	0.47
7:W:315:ARG:O	7:W:318:ILE:HG13	2.14	0.47
7:Z:154:ARG:HH21	7:Z:357:VAL:HG11	1.78	0.47
1:B:8:GLN:HG3	1:B:22:LEU:HD11	1.96	0.47
2:D:513:GLN:O	2:D:517:THR:HG23	2.15	0.47
3:G:189:LEU:HD21	3:H:188:ARG:HG2	1.96	0.47
7:X:208:VAL:HG12	7:X:209:TRP:N	2.29	0.47
7:X:400:GLY:HA2	7:X:406:TYR:HD2	1.80	0.47
7:X:623:GLU:HA	7:X:626:VAL:HG12	1.96	0.47
7:Z:570:TYR:HB3	7:Z:576:TYR:CD1	2.50	0.47
3:F:14:ILE:HG12	3:F:15:SER:H	1.79	0.47
4:J:56:LEU:HD22	4:J:178:TYR:CE2	2.50	0.47
4:J:107:PRO:HB3	4:J:282:PHE:CD2	2.50	0.47
7:Z:314:VAL:HG11	7:Z:341:PHE:HB3	1.96	0.47
1:A:857:ASP:HB3	1:A:943:ARG:HG2	1.97	0.47
1:B:131:ILE:HB	1:B:150:LEU:HB3	1.97	0.47
6:Q:48:ASP:HB3	6:Q:51:ALA:HB3	1.97	0.47
7:W:311:ILE:HA	7:W:314:VAL:HG22	1.97	0.47
7:Y:286:SER:HB3	7:Y:299:SER:N	2.30	0.47
7:Y:335:ALA:HB3	7:Y:336:PRO:HD3	1.97	0.47
7:Z:410:ALA:HA	7:Z:609:LYS:NZ	2.30	0.47
1:B:910:ILE:HD11	1:B:917:ILE:HD11	1.96	0.47
6:M:76:ARG:NH1	6:M:85:VAL:HG21	2.30	0.47
1:U:821:ILE:C	1:U:823:GLN:H	2.22	0.47
7:W:233:ARG:HG2	7:W:257:TYR:HD2	1.80	0.47
7:W:478:THR:HG23	7:W:479:LEU:HD12	1.96	0.47
7:Y:40:PHE:CD2	7:Y:383:THR:HG23	2.42	0.47
1:A:203:PHE:HB3	1:A:297:THR:HG22	1.97	0.46
1:A:916:GLN:HG2	1:V:900:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:286:PRO:HB2	2:C:287:PRO:HD3	1.97	0.46
6:P:103:GLY:O	6:P:104:LYS:HG3	2.15	0.46
7:X:207:ARG:HH21	7:X:237:ILE:HG21	1.80	0.46
8:b:130:ALA:O	8:b:134:ASN:HB2	2.15	0.46
1:B:476:ALA:HB1	1:B:954:LEU:HD21	1.96	0.46
2:D:282:THR:O	2:D:285:MET:HB2	2.15	0.46
4:I:89:ASP:CG	4:I:92:SER:HB2	2.40	0.46
1:U:234:TYR:HB3	1:U:244:TRP:HB3	1.97	0.46
7:W:323:MET:HE1	7:W:324:ARG:HG3	1.97	0.46
7:Y:260:ILE:HG22	7:Y:261:THR:N	2.31	0.46
7:Y:646:ASN:C	7:Y:647:ILE:HD13	2.40	0.46
7:Z:50:TYR:HB2	7:Z:92:TYR:CE1	2.50	0.46
1:A:551:ARG:HH12	1:A:592:GLU:HB2	1.81	0.46
1:B:497:LEU:HD22	1:B:782:MET:HE1	1.96	0.46
7:X:314:VAL:HB	7:X:339:ILE:HG21	1.97	0.46
1:A:377:LEU:HD12	1:A:378:SER:N	2.31	0.46
1:B:377:LEU:HD21	1:B:381:LEU:HD11	1.98	0.46
2:D:590:SER:HB2	2:D:592:PRO:HD2	1.97	0.46
4:I:159:SER:HA	4:I:255:LEU:O	2.16	0.46
6:S:122:LEU:O	6:S:126:ARG:HG3	2.15	0.46
1:U:560:LYS:HD2	1:U:560:LYS:HA	1.67	0.46
7:W:108:ILE:HG23	7:W:191:GLU:HB2	1.97	0.46
7:Z:111:ILE:HD11	7:Z:189:LEU:HD11	1.98	0.46
7:Z:351:PRO:HG3	7:Z:356:GLN:NE2	2.30	0.46
6:N:34:GLU:OE2	6:N:76:ARG:HG2	2.15	0.46
7:X:276:TYR:O	7:X:280:VAL:HG22	2.16	0.46
1:B:182:MET:HE2	1:B:182:MET:HA	1.97	0.46
6:O:60:LEU:H	6:O:60:LEU:HD12	1.80	0.46
1:V:498:ASP:HB3	1:V:505:ASP:OD1	2.15	0.46
7:Z:107:LEU:HG	7:Z:192:ALA:HB3	1.96	0.46
1:A:739:LYS:HB2	1:A:739:LYS:HE3	1.78	0.46
2:D:504:HIS:CE1	2:D:506:ASP:HB2	2.51	0.46
4:I:89:ASP:HB3	4:I:92:SER:O	2.16	0.46
5:L:111:PHE:O	5:L:115:PHE:HB3	2.16	0.46
6:O:75:ILE:O	6:O:75:ILE:HG13	2.16	0.46
6:O:87:PHE:C	6:O:88:ILE:HD13	2.40	0.46
7:W:532:MET:H	7:W:532:MET:HG2	1.53	0.46
7:Y:211:THR:HG23	7:Y:231:GLN:HB2	1.97	0.46
8:a:22:ASP:OD2	8:a:124:SER:HB2	2.15	0.46
1:B:113:GLU:HB3	1:B:333:LEU:HD11	1.98	0.46
2:C:504:HIS:CE1	2:C:506:ASP:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:33:ARG:HE	3:H:33:ARG:HD2	1.80	0.46
4:I:54:PRO:HG3	4:I:175:TRP:CZ2	2.51	0.46
6:P:11:GLY:H	6:P:34:GLU:HA	1.81	0.46
7:X:424:MET:HE2	7:X:427:LYS:HD2	1.98	0.46
7:X:617:ASN:HD21	7:Z:534:VAL:HG12	1.80	0.46
7:Y:106:ARG:HH21	7:Y:161:ASN:HA	1.80	0.46
7:Y:416:VAL:HG12	7:Y:441:GLN:HB2	1.98	0.46
1:A:52:MET:HB2	1:U:51:LEU:HD11	1.98	0.46
4:I:297:LYS:HZ3	4:I:323:GLU:HG2	1.81	0.46
5:L:98:MET:HE2	5:L:100:PHE:HE1	1.81	0.46
7:Z:210:SER:HB2	7:Z:345:LEU:HD21	1.98	0.46
2:C:86:LYS:HE3	2:C:86:LYS:HB2	1.76	0.46
2:C:369:ARG:HD2	2:C:492:TYR:CE2	2.51	0.46
5:K:364:ASP:C	5:K:365:ILE:HD12	2.41	0.46
6:M:10:ALA:HB1	6:N:38:THR:HG22	1.98	0.46
1:V:133:ARG:HG3	1:V:149:PRO:HD3	1.96	0.46
7:W:23:LEU:HD23	7:W:23:LEU:H	1.81	0.46
7:X:665:THR:HG22	7:Z:680:ASN:ND2	2.31	0.46
7:Y:534:VAL:HG23	7:Y:536:PRO:HD2	1.98	0.46
7:Z:554:ARG:HE	7:Z:555:VAL:HG23	1.81	0.46
1:A:522:VAL:HB	1:A:673:ARG:HG2	1.98	0.45
4:I:262:MET:HE1	4:J:142:SER:N	2.31	0.45
5:K:327:LYS:HE3	5:K:327:LYS:HB2	1.64	0.45
1:U:863:MET:HB2	1:U:918:ASP:OD1	2.15	0.45
1:V:389:VAL:HG12	1:V:401:LEU:HB2	1.98	0.45
7:Y:102:ALA:HB3	7:Y:379:THR:H	1.81	0.45
7:Y:106:ARG:HG3	7:Y:193:PRO:HA	1.97	0.45
7:Y:439:ASP:OD2	7:Y:605:ARG:HG3	2.15	0.45
7:Z:202:ASP:HB2	7:Z:378:GLY:HA3	1.98	0.45
7:Z:277:VAL:O	7:Z:281:LEU:HB2	2.15	0.45
7:Z:454:LEU:HD21	7:Z:504:TYR:CD2	2.51	0.45
2:C:50:LYS:O	2:C:53:THR:HG22	2.16	0.45
3:F:174:ARG:O	3:F:178:LEU:HG	2.16	0.45
1:U:150:LEU:HD11	1:U:162:ALA:HB1	1.97	0.45
1:V:116:LYS:HE3	1:V:117:TYR:CD1	2.51	0.45
7:W:402:LEU:HD23	7:W:402:LEU:HA	1.86	0.45
7:X:159:GLU:HG3	7:X:159:GLU:O	2.16	0.45
7:X:409:ILE:HG13	7:X:608:HIS:ND1	2.31	0.45
7:Y:632:TYR:O	7:Y:636:LEU:HG	2.16	0.45
7:Z:209:TRP:CG	7:Z:210:SER:N	2.84	0.45
7:Z:209:TRP:CD1	7:Z:210:SER:H	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:MET:HG2	1:B:963:THR:HB	1.99	0.45
4:J:75:ASP:HA	4:J:82:ARG:NH1	2.32	0.45
5:K:112:PHE:HZ	5:L:371:LEU:HD11	1.81	0.45
5:K:205:PHE:CE1	5:K:213:GLU:HG2	2.51	0.45
6:S:47:PHE:HD2	6:S:49:VAL:HG22	1.81	0.45
6:S:104:LYS:HD2	6:S:104:LYS:HA	1.69	0.45
7:Z:59:ALA:HB1	7:Z:64:GLN:HG2	1.98	0.45
2:D:331:VAL:O	2:D:331:VAL:HG13	2.17	0.45
1:U:818:ILE:HD12	1:U:818:ILE:HA	1.81	0.45
7:Y:80:LEU:HB2	7:Y:509:LEU:HD11	1.97	0.45
6:T:60:LEU:HD21	6:T:92:TRP:HD1	1.82	0.45
7:W:428:TYR:CD1	7:W:470:ARG:HD2	2.52	0.45
7:W:497:MET:HB3	7:W:544:LYS:HD2	1.98	0.45
7:Y:570:TYR:HB3	7:Y:576:TYR:CD1	2.50	0.45
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.78	0.45
1:A:906:LEU:HD13	1:A:917:ILE:HD11	1.99	0.45
1:B:280:TYR:HA	1:B:283:THR:HG22	1.98	0.45
2:D:285:MET:HE1	2:D:291:PRO:HB3	1.99	0.45
2:D:436:GLU:H	2:D:436:GLU:HG3	1.47	0.45
3:F:13:LEU:HD13	3:F:83:VAL:HG21	1.99	0.45
6:O:4:ASN:OD1	6:O:6:ARG:HG3	2.16	0.45
6:O:37:VAL:HB	6:O:41:VAL:HB	1.98	0.45
1:U:572:TYR:CE2	1:U:630:THR:HB	2.49	0.45
7:X:264:LYS:HG3	7:X:265:GLY:H	1.82	0.45
7:Z:286:SER:HB3	7:Z:299:SER:N	2.32	0.45
1:A:445:ILE:HB	1:A:497:LEU:HG	1.99	0.45
1:A:489:VAL:CG2	1:A:786:MET:HB3	2.45	0.45
2:C:70:MET:HE2	2:C:70:MET:HA	1.98	0.45
2:C:185:ALA:O	2:C:189:GLU:HG2	2.17	0.45
3:F:95:ASN:ND2	6:Q:27:ASN:HB3	2.32	0.45
3:H:174:ARG:O	3:H:178:LEU:HG	2.17	0.45
5:L:649:GLU:HB3	5:L:650:PRO:HD3	1.98	0.45
1:U:116:LYS:HE3	1:U:117:TYR:CD1	2.51	0.45
7:X:335:ALA:O	7:X:339:ILE:HD11	2.16	0.45
8:b:4:THR:HG22	8:b:15:ASP:HB3	1.99	0.45
1:B:912:GLU:HG3	2:D:5:ASN:HD21	1.80	0.45
6:R:94:VAL:HG12	6:R:96:ASN:H	1.82	0.45
6:S:99:GLU:OE1	6:S:99:GLU:N	2.49	0.45
1:U:454:ARG:O	1:U:460:VAL:HA	2.17	0.45
1:U:561:LEU:HD23	1:U:561:LEU:HA	1.76	0.45
1:V:846:VAL:HG22	1:V:847:ARG:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:857:ASP:HB3	1:V:943:ARG:HG2	1.99	0.45
7:X:16:ARG:HG3	7:X:18:ARG:HE	1.81	0.45
7:X:199:LYS:HD2	7:X:199:LYS:HA	1.77	0.45
1:A:236:LYS:O	1:A:288:GLY:HA3	2.17	0.45
2:D:439:ARG:HD2	2:D:443:PRO:HD3	1.98	0.45
5:L:198:LEU:HD23	5:L:198:LEU:HA	1.81	0.45
6:N:36:ILE:HG12	6:N:75:ILE:HG22	1.99	0.45
1:U:133:ARG:HG3	1:U:149:PRO:HD3	1.99	0.45
7:X:417:LEU:HB2	7:X:442:TYR:CE1	2.52	0.45
4:I:262:MET:HE1	4:J:142:SER:H	1.82	0.45
5:K:649:GLU:HB3	5:K:650:PRO:HD3	1.98	0.45
6:T:75:ILE:HG23	6:T:88:ILE:HB	1.98	0.45
7:W:496:LEU:HB2	7:W:505:VAL:HG21	1.98	0.45
7:Y:233:ARG:NH1	7:Y:259:ASN:HB2	2.32	0.45
7:Z:396:ASN:HD22	7:Z:430:ALA:HB1	1.81	0.45
1:B:819:ASP:O	1:B:823:GLN:HG2	2.16	0.44
1:B:857:ASP:HB3	1:B:943:ARG:HG2	1.98	0.44
2:D:286:PRO:HB2	2:D:287:PRO:HD3	1.99	0.44
4:J:211:ASP:OD2	4:J:216:TYR:HB2	2.17	0.44
6:M:37:VAL:HB	6:M:41:VAL:HB	1.98	0.44
6:O:6:ARG:HH22	6:P:9:GLN:HG3	1.82	0.44
6:P:88:ILE:HD13	6:P:88:ILE:HA	1.83	0.44
1:U:132:PRO:HG3	1:U:317:LEU:HB3	1.99	0.44
1:V:733:LYS:HD2	1:V:733:LYS:HA	1.88	0.44
7:W:207:ARG:HH21	7:W:237:ILE:HG21	1.82	0.44
7:X:410:ALA:HB3	7:Y:5:ASN:HB2	1.97	0.44
7:Z:462:SER:O	7:Z:466:GLN:HG2	2.17	0.44
3:E:33:ARG:HH21	3:H:33:ARG:NH1	2.15	0.44
6:O:6:ARG:NH2	6:P:9:GLN:HG3	2.32	0.44
7:Y:532:MET:HE2	7:Y:532:MET:HB3	1.82	0.44
8:b:15:ASP:OD1	8:b:15:ASP:C	2.61	0.44
8:b:52:VAL:HG12	8:b:53:TYR:CD1	2.51	0.44
1:B:554:GLU:HB2	1:B:558:PHE:HB3	2.00	0.44
2:D:456:LEU:HD13	2:D:507:ILE:HG12	1.99	0.44
3:E:132:ILE:HG13	3:E:134:VAL:H	1.82	0.44
1:V:90:ASP:OD1	1:V:91:GLU:HG2	2.17	0.44
7:W:338:GLU:HB2	7:W:347:VAL:HG13	2.00	0.44
7:W:495:LYS:HB2	7:W:544:LYS:HG3	1.98	0.44
7:X:119:PRO:HG3	7:X:355:ILE:HD11	1.99	0.44
7:Z:335:ALA:HB3	7:Z:336:PRO:HD3	1.99	0.44
4:J:89:ASP:HB3	4:J:92:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:149:PRO:HG2	1:U:165:ASN:HB3	1.99	0.44
7:X:405:ARG:HD3	7:Z:550:PHE:HE1	1.82	0.44
7:Y:277:VAL:O	7:Y:281:LEU:HB2	2.18	0.44
1:B:265:LEU:HD23	1:B:274:VAL:HG22	1.98	0.44
1:B:588:LEU:HD23	1:B:588:LEU:HA	1.84	0.44
4:J:193:MET:HE3	4:J:193:MET:HB3	1.89	0.44
5:L:214:ILE:HG13	5:L:215:PRO:CD	2.47	0.44
1:V:650:TYR:CE1	1:V:669:MET:HG2	2.52	0.44
7:X:209:TRP:CD1	7:X:369:LYS:HE3	2.52	0.44
7:X:264:LYS:HD3	7:X:264:LYS:HA	1.83	0.44
8:b:68:LEU:HD23	8:b:68:LEU:HA	1.80	0.44
1:A:846:VAL:HG21	1:A:928:TYR:CE1	2.52	0.44
4:I:56:LEU:HD22	4:I:178:TYR:CE2	2.53	0.44
4:J:89:ASP:CG	4:J:92:SER:HB2	2.42	0.44
5:K:53:ILE:HD11	5:K:247:SER:HB2	1.97	0.44
7:X:424:MET:HE1	7:X:467:ILE:HD11	2.00	0.44
6:Q:4:ASN:OD1	6:Q:4:ASN:C	2.60	0.44
1:V:110:ASP:HB3	1:V:113:GLU:HB2	1.99	0.44
1:V:229:TYR:HB2	1:V:297:THR:HG22	1.99	0.44
1:V:472:LEU:HD23	1:V:472:LEU:HA	1.79	0.44
7:W:314:VAL:HG11	7:W:341:PHE:CD2	2.53	0.44
7:W:344:PHE:HD2	7:W:356:GLN:HG3	1.83	0.44
7:W:368:GLY:HA3	7:W:369:LYS:HZ3	1.83	0.44
7:X:453:ARG:HG3	7:X:453:ARG:HH11	1.82	0.44
7:Y:314:VAL:HG11	7:Y:341:PHE:HB3	2.00	0.44
7:Y:438:ARG:O	7:Y:438:ARG:HG2	2.18	0.44
7:Z:105:SER:O	7:Z:193:PRO:HA	2.17	0.44
1:B:425:LEU:HG	1:B:427:VAL:HG23	2.00	0.44
3:H:14:ILE:HG12	3:H:15:SER:H	1.83	0.44
5:K:96:ILE:HG12	5:L:493:HIS:HD2	1.82	0.44
5:K:111:PHE:O	5:K:115:PHE:HB3	2.18	0.44
5:K:493:HIS:C	5:K:493:HIS:CD2	2.96	0.44
1:V:572:TYR:CE2	1:V:630:THR:HB	2.49	0.44
7:X:609:LYS:HA	7:Y:5:ASN:ND2	2.33	0.44
7:Z:113:ILE:HG21	7:Z:317:MET:HE3	1.98	0.44
1:B:244:TRP:CG	1:B:291:ARG:HH21	2.35	0.44
3:E:133:GLY:HA2	3:F:165:ILE:HG13	2.00	0.44
1:U:95:GLY:HA2	1:U:99:ILE:HD11	1.99	0.44
1:U:452:LEU:HD23	1:U:452:LEU:HA	1.82	0.44
1:U:880:LEU:HD22	1:U:910:ILE:HG21	2.00	0.44
1:V:320:ILE:HD12	1:V:320:ILE:HA	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:860:PHE:HB3	1:V:960:MET:HE3	1.99	0.44
7:W:369:LYS:HB2	7:W:370:ASP:H	1.67	0.44
7:X:464:VAL:HG21	7:X:564:ALA:HB2	2.00	0.44
7:Z:187:TYR:CG	7:Z:313:LEU:HD22	2.53	0.44
8:b:22:ASP:C	8:b:22:ASP:OD1	2.60	0.44
1:A:143:SER:HB2	1:A:204:ASP:OD1	2.18	0.43
3:H:124:VAL:O	3:H:128:ILE:HG22	2.18	0.43
1:U:527:THR:HG21	1:U:651:ILE:H	1.83	0.43
1:V:655:LEU:HB3	1:V:670:VAL:HG11	2.00	0.43
7:W:318:ILE:HG21	7:W:339:ILE:HD12	1.99	0.43
7:Z:169:ARG:NH2	7:Z:309:GLU:HG2	2.32	0.43
8:b:124:SER:OG	8:b:126:ILE:HG22	2.18	0.43
1:B:23:MET:HE2	1:V:54:MET:HB3	2.01	0.43
6:P:76:ARG:CZ	6:P:85:VAL:HG11	2.48	0.43
6:R:4:ASN:C	6:R:4:ASN:OD1	2.60	0.43
6:T:87:PHE:O	6:T:88:ILE:HD13	2.18	0.43
1:U:370:LEU:HD12	1:U:371:PRO:HD2	2.00	0.43
1:V:328:GLU:O	1:V:331:LYS:HG2	2.18	0.43
7:W:286:SER:HB3	7:W:299:SER:H	1.83	0.43
7:X:369:LYS:H	7:X:369:LYS:HZ3	1.65	0.43
1:A:147:GLN:CD	1:A:172:ILE:HD11	2.43	0.43
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.87	0.43
4:J:229:MET:HE2	4:J:229:MET:HB3	1.86	0.43
5:L:214:ILE:HG13	5:L:215:PRO:N	2.33	0.43
7:W:408:ASN:ND2	7:Y:550:PHE:HD2	2.15	0.43
7:X:152:LYS:HG2	7:X:355:ILE:HD12	2.00	0.43
1:A:155:MET:HE3	1:A:155:MET:HB3	1.83	0.43
1:A:280:TYR:HA	1:A:283:THR:HG22	1.99	0.43
3:E:187:GLN:NE2	3:E:188:ARG:HG2	2.34	0.43
4:I:66:ASP:OD2	4:I:181:LEU:HD11	2.19	0.43
4:I:107:PRO:HB3	4:I:282:PHE:CD2	2.54	0.43
5:L:470:LEU:HD12	5:L:470:LEU:HA	1.82	0.43
1:U:472:LEU:HD23	1:U:472:LEU:HA	1.78	0.43
1:U:511:LEU:HD11	1:U:607:ILE:HD11	2.00	0.43
7:Y:10:VAL:O	7:Y:10:VAL:HG22	2.17	0.43
7:Y:454:LEU:HD21	7:Y:504:TYR:CD1	2.53	0.43
7:Z:651:THR:HG22	7:Z:666:CYS:HB2	2.00	0.43
1:B:607:ILE:HA	1:B:612:ALA:O	2.19	0.43
2:D:380:LEU:HD23	2:D:380:LEU:HA	1.76	0.43
3:H:95:ASN:ND2	6:R:27:ASN:HB3	2.34	0.43
6:N:73:ASN:HB2	6:N:90:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:442:GLY:C	1:U:444:ARG:H	2.26	0.43
7:W:199:LYS:HA	7:W:199:LYS:HD2	1.79	0.43
7:W:535:SER:HA	7:W:538:ASN:HD21	1.84	0.43
7:W:656:ILE:HD13	7:W:656:ILE:HA	1.84	0.43
7:Y:621:THR:H	7:Y:624:GLN:HB2	1.83	0.43
7:Z:464:VAL:HG23	7:Z:489:ILE:HG21	2.00	0.43
3:E:115:LEU:HD22	3:E:115:LEU:HA	1.86	0.43
1:V:654:GLU:OE1	1:V:654:GLU:N	2.51	0.43
7:Y:207:ARG:HE	7:Y:237:ILE:HG21	1.83	0.43
7:Z:331:ALA:HB3	7:Z:352:TYR:OH	2.19	0.43
8:a:15:ASP:OD1	8:a:15:ASP:C	2.61	0.43
8:a:126:ILE:HD12	8:a:126:ILE:HA	1.94	0.43
1:B:707:VAL:HB	1:B:757:TYR:HB2	2.00	0.43
3:E:43:ARG:HD3	3:E:43:ARG:HA	1.77	0.43
4:I:308:ARG:HD2	4:I:308:ARG:HA	1.78	0.43
5:K:309:LYS:HD2	5:K:310:PRO:HD2	2.01	0.43
6:Q:118:TYR:CG	6:Q:137:TYR:HE2	2.36	0.43
7:X:212:THR:HG21	7:X:347:VAL:O	2.18	0.43
1:B:646:ILE:HA	1:B:669:MET:SD	2.58	0.43
5:K:205:PHE:CZ	5:K:213:GLU:HG2	2.53	0.43
1:U:630:THR:OG1	1:U:634:THR:HG21	2.19	0.43
7:X:267:TYR:CZ	7:Z:70:ARG:HD2	2.54	0.43
7:Z:53:ASP:OD1	7:Z:53:ASP:C	2.61	0.43
7:Z:358:LEU:HD21	7:Z:365:ILE:HA	1.99	0.43
1:A:819:ASP:O	1:A:823:GLN:HG2	2.18	0.43
2:C:542:PHE:HB3	2:C:544:ILE:HG12	2.00	0.43
6:Q:29:LYS:HD3	6:Q:30:ASN:HB2	2.00	0.43
6:S:117:MET:HG2	6:S:120:ARG:HH21	1.84	0.43
7:W:236:LEU:HD22	7:W:285:TYR:CE2	2.54	0.43
7:Y:277:VAL:CG2	7:Y:278:GLY:H	2.16	0.43
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.80	0.43
2:C:493:LEU:HD23	2:C:493:LEU:HA	1.84	0.43
3:E:38:ILE:HG21	3:E:45:VAL:HG22	2.01	0.43
3:G:132:ILE:HG13	3:G:134:VAL:H	1.83	0.43
6:R:118:TYR:CG	6:R:137:TYR:HE2	2.37	0.43
1:U:153:ARG:HE	1:U:153:ARG:HB3	1.68	0.43
7:W:171:LEU:HD12	7:W:171:LEU:H	1.84	0.43
7:W:663:SER:HB2	7:Y:680:ASN:HD21	1.84	0.43
7:X:167:THR:HG23	7:X:169:ARG:HH21	1.84	0.43
7:X:418:TYR:HD1	7:X:508:LEU:HD21	1.84	0.43
7:Z:510:ASP:OD2	7:Z:540:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:526:LEU:HD23	2:C:526:LEU:HA	1.82	0.42
2:D:50:LYS:O	2:D:53:THR:HG22	2.19	0.42
7:W:334:THR:OG1	7:W:335:ALA:N	2.51	0.42
7:Z:439:ASP:C	7:Z:440:LEU:HD23	2.44	0.42
8:b:46:LEU:HB3	8:b:47:PRO:HD3	2.01	0.42
1:B:783:MET:HE3	1:B:783:MET:HB3	1.81	0.42
3:F:22:LYS:HA	3:F:22:LYS:HD3	1.87	0.42
4:I:157:GLN:HA	4:I:157:GLN:OE1	2.18	0.42
4:I:291:ARG:HE	4:I:291:ARG:HB3	1.58	0.42
5:K:108:TRP:C	5:K:110:SER:H	2.27	0.42
5:L:108:TRP:C	5:L:110:SER:H	2.27	0.42
6:O:47:PHE:HD2	6:O:87:PHE:HB2	1.82	0.42
7:X:221:GLU:H	7:X:221:GLU:CD	2.27	0.42
7:Y:204:ASN:ND2	7:Y:300:PRO:HB2	2.34	0.42
7:Z:102:ALA:HB3	7:Z:379:THR:H	1.83	0.42
1:A:588:LEU:HD23	1:A:588:LEU:HA	1.85	0.42
2:C:71:MET:HG2	2:C:113:TYR:CE1	2.54	0.42
6:N:56:VAL:HG11	6:N:92:TRP:CZ2	2.53	0.42
6:P:108:LEU:HD13	6:R:110:TRP:HZ3	1.84	0.42
1:V:384:ARG:HG3	1:V:820:TYR:CE2	2.54	0.42
1:V:403:SER:HA	1:V:834:TYR:O	2.19	0.42
7:Z:187:TYR:CD2	7:Z:313:LEU:HD22	2.55	0.42
7:Z:453:ARG:HA	7:Z:453:ARG:HD3	1.83	0.42
8:b:22:ASP:OD2	8:b:124:SER:HB2	2.18	0.42
1:B:796:GLU:HB2	1:B:955:THR:HG22	2.02	0.42
5:K:49:GLY:HA2	5:K:250:THR:OG1	2.19	0.42
1:U:857:ASP:HB3	1:U:943:ARG:HG2	2.00	0.42
1:U:949:MET:HG2	1:U:950:ALA:H	1.85	0.42
7:Y:53:ASP:OD1	7:Y:53:ASP:C	2.63	0.42
7:Z:596:THR:O	7:Z:599:ILE:HG12	2.19	0.42
8:a:68:LEU:HA	8:a:68:LEU:HD23	1.74	0.42
1:A:561:LEU:HD23	1:A:561:LEU:HA	1.93	0.42
1:B:516:ILE:HG13	1:B:678:THR:HG22	2.00	0.42
5:L:181:HIS:CD2	5:L:182:ALA:H	2.38	0.42
6:N:108:LEU:HD13	6:Q:110:TRP:HZ3	1.85	0.42
6:S:76:ARG:NH1	6:S:85:VAL:HG11	2.34	0.42
1:V:111:TYR:CG	1:V:184:MET:HE1	2.54	0.42
1:V:120:PRO:HA	1:V:127:ARG:HG3	2.00	0.42
1:V:522:VAL:HB	1:V:673:ARG:HG2	2.01	0.42
7:Z:50:TYR:HB2	7:Z:92:TYR:HE1	1.84	0.42
7:Z:463:ARG:O	7:Z:467:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:825:LEU:HD23	1:B:825:LEU:HA	1.82	0.42
6:M:40:SER:HB3	1:U:767:ASN:ND2	2.34	0.42
6:O:23:ILE:HG22	6:O:24:LEU:HD23	2.00	0.42
6:O:93:ILE:H	6:O:93:ILE:HG13	1.67	0.42
1:U:184:MET:HE2	1:U:184:MET:HB2	1.93	0.42
7:X:233:ARG:HG2	7:X:257:TYR:CD2	2.54	0.42
7:Y:154:ARG:HD3	7:Y:362:ASP:HB3	2.02	0.42
1:A:265:LEU:HD23	1:A:274:VAL:HG22	2.00	0.42
1:A:867:LYS:HG2	1:A:868:PRO:HD2	2.00	0.42
2:D:45:LYS:HE2	2:D:45:LYS:HB2	1.80	0.42
5:L:371:LEU:HD23	5:L:371:LEU:HA	1.85	0.42
1:U:126:GLN:HG2	1:U:155:MET:HA	2.02	0.42
1:U:328:GLU:N	1:U:329:PRO:HD2	2.35	0.42
1:U:846:VAL:HG23	1:U:850:GLN:HB2	2.02	0.42
7:W:318:ILE:HG12	7:W:339:ILE:HD12	2.01	0.42
7:W:465:GLN:HA	7:W:468:ILE:HG22	2.02	0.42
7:W:636:LEU:HD12	7:W:636:LEU:HA	1.87	0.42
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.83	0.42
1:A:164:TYR:CD2	1:A:175:LEU:HD21	2.54	0.42
1:A:425:LEU:HG	1:A:427:VAL:HG23	2.02	0.42
1:A:938:VAL:O	1:A:939:ARG:HD2	2.20	0.42
2:C:199:MET:HE3	1:V:66:MET:HG2	2.02	0.42
2:D:220:LEU:HD23	2:D:220:LEU:HA	1.89	0.42
4:J:66:ASP:OD2	4:J:181:LEU:HD11	2.19	0.42
4:J:328:LYS:HE2	4:J:328:LYS:HB2	1.87	0.42
5:K:180:MET:HE2	5:K:342:GLN:C	2.44	0.42
5:L:365:ILE:HD12	5:L:365:ILE:HA	1.83	0.42
6:P:56:VAL:HG11	6:P:92:TRP:CZ2	2.55	0.42
7:W:401:LYS:HA	7:W:401:LYS:HD2	1.88	0.42
7:Z:24:ILE:HD12	7:Z:24:ILE:HA	1.96	0.42
7:Z:640:MET:HE2	7:Z:640:MET:HB3	1.77	0.42
8:a:73:ASN:C	8:a:73:ASN:OD1	2.63	0.42
1:A:131:ILE:HA	1:A:132:PRO:HD3	1.92	0.42
1:B:445:ILE:HB	1:B:497:LEU:HG	2.01	0.42
2:D:267:THR:HG22	2:D:301:ASN:ND2	2.34	0.42
5:K:470:LEU:HD23	5:K:470:LEU:HA	1.83	0.42
6:S:131:PRO:HA	6:S:132:PRO:HD3	1.96	0.42
1:U:403:SER:HA	1:U:834:TYR:O	2.20	0.42
1:U:620:MET:HG3	1:U:628:PHE:CZ	2.54	0.42
1:U:888:VAL:HG21	1:U:960:MET:HE1	2.02	0.42
1:V:30:GLN:HG2	1:V:60:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:308:TYR:HD1	1:V:308:TYR:HA	1.75	0.42
7:W:251:THR:HG23	7:W:253:ASP:N	2.34	0.42
7:W:264:LYS:HG2	7:W:265:GLY:H	1.84	0.42
7:X:286:SER:HB3	7:X:299:SER:H	1.85	0.42
7:Y:59:ALA:HB1	7:Y:64:GLN:HG2	2.02	0.42
7:Y:310:ASN:O	7:Y:314:VAL:HG22	2.20	0.42
7:Z:40:PHE:HE1	7:Z:96:LEU:HB2	1.85	0.42
6:N:68:ASP:HA	6:N:69:PRO:HD3	1.89	0.42
7:W:556:ARG:HG2	7:W:566:TRP:CZ2	2.55	0.42
7:Z:203:SER:HB2	7:Z:239:LYS:HE2	2.02	0.42
1:B:726:ILE:HD12	1:B:726:ILE:HA	1.89	0.41
1:B:843:ILE:HD11	6:O:21:TYR:CE1	2.55	0.41
1:B:923:GLY:HA3	1:B:928:TYR:CD2	2.55	0.41
5:K:300:LEU:O	5:K:304:ILE:HG23	2.19	0.41
5:L:102:VAL:O	5:L:177:LYS:HB3	2.20	0.41
7:W:409:ILE:N	7:W:409:ILE:HD12	2.35	0.41
7:Y:28:ILE:HG13	7:Y:29:THR:H	1.85	0.41
7:Y:209:TRP:HD1	7:Y:210:SER:H	1.65	0.41
7:Z:534:VAL:HG23	7:Z:536:PRO:HD2	2.02	0.41
8:a:46:LEU:HB3	8:a:47:PRO:HD3	2.03	0.41
2:D:429:ILE:HD12	2:D:527:VAL:HG21	2.02	0.41
2:D:439:ARG:NH1	2:D:443:PRO:HG3	2.35	0.41
3:F:175:ILE:H	3:F:175:ILE:HG13	1.65	0.41
1:U:236:LYS:HB2	1:U:289:VAL:HG22	2.03	0.41
1:U:391:ASN:ND2	1:U:401:LEU:HD11	2.36	0.41
7:X:288:ASP:OD1	7:X:290:VAL:HG22	2.21	0.41
7:Z:167:THR:HG23	7:Z:169:ARG:NH1	2.35	0.41
1:B:132:PRO:HG3	1:B:327:THR:HG21	2.02	0.41
1:B:561:LEU:HD23	1:B:561:LEU:HA	1.92	0.41
3:F:123:LYS:HB3	3:F:123:LYS:HE3	1.76	0.41
5:L:184:TRP:HA	5:L:187:VAL:HG12	2.02	0.41
6:P:116:LYS:HE3	6:P:116:LYS:HB2	1.69	0.41
1:U:73:LEU:HD12	1:U:73:LEU:HA	1.86	0.41
1:U:827:GLU:O	1:U:828:THR:C	2.63	0.41
1:U:939:ARG:HD3	1:U:939:ARG:HA	1.80	0.41
1:V:821:ILE:HD13	1:V:821:ILE:HA	1.85	0.41
1:V:865:TYR:HE1	1:V:965:LEU:HD12	1.84	0.41
1:V:880:LEU:HD22	1:V:910:ILE:HG21	2.02	0.41
7:W:212:THR:HG21	7:W:347:VAL:O	2.21	0.41
7:X:645:VAL:HG22	7:X:672:ALA:HB2	2.02	0.41
7:Y:256:ASP:OD1	7:Y:256:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:GLN:HG3	1:B:798:GLU:N	2.34	0.41
3:H:123:LYS:HE2	3:H:123:LYS:HB3	1.84	0.41
6:S:16:PHE:HB3	6:S:98:LEU:HD12	2.02	0.41
6:T:99:GLU:N	6:T:99:GLU:OE2	2.53	0.41
1:U:265:LEU:HD23	1:U:274:VAL:HG22	2.02	0.41
7:W:251:THR:HG22	7:W:255:GLN:H	1.85	0.41
7:X:24:ILE:HD12	7:X:24:ILE:HA	1.95	0.41
7:X:28:ILE:HD13	7:X:28:ILE:H	1.86	0.41
7:Y:351:PRO:HG3	7:Y:356:GLN:NE2	2.34	0.41
1:A:113:GLU:HB3	1:A:333:LEU:HD11	2.02	0.41
1:B:10:LEU:HD11	1:V:61:ALA:HB1	2.02	0.41
2:C:107:ASN:HA	2:C:110:VAL:HG12	2.02	0.41
2:C:439:ARG:NH1	2:C:443:PRO:HG3	2.36	0.41
2:D:111:LEU:HD12	2:D:111:LEU:HA	1.81	0.41
4:I:75:ASP:HA	4:I:82:ARG:NH1	2.35	0.41
4:I:224:GLY:O	4:I:262:MET:HB2	2.21	0.41
5:L:205:PHE:CE2	5:L:213:GLU:HB2	2.56	0.41
5:L:256:GLU:O	5:L:260:ILE:HG22	2.21	0.41
6:P:123:LEU:HD11	6:P:127:GLN:HE21	1.85	0.41
7:W:236:LEU:HD23	7:W:300:PRO:HG2	2.02	0.41
7:Y:42:GLU:OE2	7:Y:43:THR:HG22	2.20	0.41
7:Y:187:TYR:CG	7:Y:313:LEU:HD22	2.55	0.41
7:Z:92:TYR:CD2	7:Z:414:PHE:HD2	2.38	0.41
7:Z:631:GLU:H	7:Z:631:GLU:HG3	1.68	0.41
1:A:646:ILE:HA	1:A:669:MET:SD	2.60	0.41
1:A:858:GLN:OE1	1:A:858:GLN:HA	2.21	0.41
2:C:234:ASN:O	2:C:238:GLN:HG3	2.19	0.41
3:H:15:SER:HB2	3:H:16:PRO:HD3	2.02	0.41
1:U:647:THR:HG23	1:U:669:MET:HE1	2.03	0.41
7:W:335:ALA:O	7:W:339:ILE:HD11	2.20	0.41
7:Y:491:MET:HE3	7:Y:566:TRP:HB3	2.02	0.41
7:Z:490:VAL:HG21	7:Z:508:LEU:HD13	2.03	0.41
1:A:207:ARG:HD3	1:A:291:ARG:HD2	2.02	0.41
1:B:29:LYS:HB3	1:B:29:LYS:HE2	1.79	0.41
1:B:583:ILE:HD12	1:B:583:ILE:HA	1.83	0.41
1:B:846:VAL:HG21	1:B:928:TYR:CE1	2.56	0.41
2:C:196:LEU:HD23	2:C:196:LEU:HA	1.80	0.41
3:G:27:TYR:HD2	3:G:73:LEU:HB3	1.86	0.41
6:P:107:THR:HG23	6:R:109:VAL:HG22	2.01	0.41
6:T:131:PRO:HA	6:T:132:PRO:HD3	1.96	0.41
1:V:796:GLU:CD	1:V:797:GLN:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:592:LEU:HD23	7:W:592:LEU:HA	1.81	0.41
7:X:424:MET:HE2	7:X:424:MET:HA	2.02	0.41
7:Y:111:ILE:HD11	7:Y:189:LEU:HD11	2.01	0.41
7:Y:410:ALA:HA	7:Y:609:LYS:NZ	2.36	0.41
7:Z:525:ASN:HA	7:Z:640:MET:HA	2.02	0.41
8:a:79:GLU:OE2	8:a:79:GLU:N	2.53	0.41
1:A:536:VAL:HG22	1:A:551:ARG:HB3	2.02	0.41
1:B:826:LEU:HD23	1:B:826:LEU:HA	1.86	0.41
3:E:132:ILE:HG21	3:F:108:LEU:HD22	2.02	0.41
5:L:516:ILE:N	5:L:516:ILE:HD13	2.35	0.41
6:P:8:ILE:HG22	6:P:100:ARG:HH21	1.85	0.41
6:S:20:PRO:HG3	6:S:56:VAL:HG13	2.03	0.41
1:U:248:ILE:HG23	1:U:262:THR:HG23	2.02	0.41
1:U:445:ILE:HD11	1:U:497:LEU:HD12	2.03	0.41
1:V:107:PHE:CE2	1:V:109:LEU:HD21	2.55	0.41
1:V:330:LEU:HA	1:V:330:LEU:HD23	1.81	0.41
7:W:209:TRP:HB2	7:W:233:ARG:O	2.21	0.41
7:X:309:GLU:H	7:X:309:GLU:HG3	1.74	0.41
7:X:463:ARG:O	7:X:467:ILE:HG12	2.20	0.41
7:Y:236:LEU:HB2	7:Y:285:TYR:CZ	2.55	0.41
7:Y:406:TYR:HA	7:Y:412:TYR:CD2	2.56	0.41
1:A:214:PRO:HG3	1:A:287:THR:HG22	2.02	0.41
2:C:582:LEU:HD23	2:C:582:LEU:HA	1.91	0.41
2:D:93:ARG:HD3	2:D:93:ARG:HA	1.83	0.41
3:G:20:LEU:H	3:G:20:LEU:HD22	1.85	0.41
3:G:196:LEU:HD23	3:G:196:LEU:HA	1.93	0.41
4:J:159:SER:HA	4:J:255:LEU:O	2.20	0.41
5:K:190:LEU:HD12	5:K:190:LEU:HA	1.86	0.41
5:L:623:LEU:HA	5:L:623:LEU:HD23	1.89	0.41
6:N:5:ILE:HD12	6:N:8:ILE:HD11	2.03	0.41
6:Q:119:ASP:OD1	6:Q:119:ASP:C	2.64	0.41
1:U:542:VAL:HG12	1:U:543:THR:H	1.85	0.41
1:V:384:ARG:HG3	1:V:820:TYR:CZ	2.56	0.41
1:V:476:ALA:HB1	1:V:954:LEU:HD21	2.03	0.41
7:W:207:ARG:O	7:W:234:ILE:HA	2.21	0.41
7:W:682:ASN:O	8:a:101:THR:HA	2.21	0.41
7:X:261:THR:OG1	7:X:275:LEU:HB3	2.21	0.41
7:X:607:ILE:HD13	7:Z:681:PHE:CZ	2.56	0.41
7:Y:112:GLU:HB3	7:Y:186:VAL:HG22	2.03	0.41
7:Y:431:MET:SD	7:Y:471:LEU:HD22	2.61	0.41
7:Z:359:GLY:HA3	7:Z:360:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:595:ILE:HD12	7:Z:595:ILE:N	2.36	0.41
1:A:509:TYR:CZ	1:A:607:ILE:HG21	2.56	0.41
1:A:602:GLU:HB3	1:A:617:ASN:CG	2.46	0.41
1:U:453:TYR:CD1	1:U:786:MET:HE1	2.56	0.41
1:U:502:ASP:OD1	1:U:502:ASP:C	2.63	0.41
1:U:750:ASN:HD22	1:U:752:LYS:HD3	1.84	0.41
7:W:244:THR:HG22	7:W:244:THR:O	2.21	0.41
7:Y:598:ASN:O	7:Y:602:VAL:HG23	2.20	0.41
7:Z:338:GLU:HG2	7:Z:340:ASP:HB2	2.03	0.41
1:A:244:TRP:CG	1:A:291:ARG:HH21	2.39	0.40
2:C:456:LEU:HD13	2:C:507:ILE:HG12	2.02	0.40
2:C:504:HIS:ND1	2:C:507:ILE:HG13	2.36	0.40
4:J:32:ILE:H	4:J:32:ILE:HG12	1.70	0.40
5:L:7:PRO:HG2	7:Z:638:ARG:HH22	1.85	0.40
6:M:90:ILE:HA	6:M:90:ILE:HD13	1.82	0.40
6:P:36:ILE:HG23	6:P:75:ILE:HG22	2.03	0.40
1:U:84:LEU:HD23	1:U:84:LEU:HA	1.94	0.40
1:V:383:ARG:HE	1:V:383:ARG:HB2	1.74	0.40
7:Y:259:ASN:O	7:Y:275:LEU:HD23	2.21	0.40
7:Y:464:VAL:HG23	7:Y:489:ILE:HG21	2.03	0.40
7:Y:525:ASN:HA	7:Y:640:MET:HA	2.02	0.40
7:Z:271:TYR:CD1	7:Z:273:ALA:HB3	2.56	0.40
7:Z:634:LEU:HA	7:Z:634:LEU:HD22	1.82	0.40
8:a:40:ARG:HG2	8:a:41:GLU:N	2.25	0.40
3:F:15:SER:HB2	3:F:16:PRO:HD3	2.03	0.40
4:J:60:TYR:HD1	4:J:73:LEU:HD22	1.85	0.40
6:O:122:LEU:HD21	6:O:126:ARG:HE	1.86	0.40
1:V:560:LYS:HA	1:V:560:LYS:HD2	1.67	0.40
7:X:428:TYR:OH	7:X:466:GLN:HB3	2.21	0.40
7:Z:28:ILE:HD12	7:Z:28:ILE:HA	1.87	0.40
7:Z:379:THR:HG22	7:Z:380:ASP:H	1.85	0.40
8:a:22:ASP:OD1	8:a:22:ASP:C	2.64	0.40
1:A:825:LEU:HD12	1:A:825:LEU:HA	1.86	0.40
1:B:245:GLU:HG2	1:B:246:GLU:H	1.86	0.40
2:C:176:LEU:HD12	2:C:176:LEU:HA	1.88	0.40
2:C:499:TYR:CD1	2:C:512:GLU:HB2	2.57	0.40
2:D:285:MET:HB2	2:D:285:MET:HE2	1.84	0.40
4:J:197:LYS:HD3	5:L:461:ASP:OD1	2.21	0.40
6:P:122:LEU:HD12	6:P:122:LEU:HA	1.85	0.40
1:V:430:ASN:HD22	1:V:777:LYS:HE3	1.85	0.40
7:W:261:THR:OG1	7:W:275:LEU:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.87	0.40
2:D:185:ALA:O	2:D:189:GLU:HG2	2.22	0.40
5:K:50:ASN:O	5:K:50:ASN:CG	2.64	0.40
6:M:7:ASP:O	6:M:8:ILE:HD12	2.21	0.40
1:U:715:VAL:HB	1:U:740:HIS:HB2	2.02	0.40
7:W:77:GLN:HG3	7:W:388:TYR:OH	2.21	0.40
7:W:221:GLU:HG2	7:W:222:ALA:N	2.37	0.40
7:W:518:TYR:HD1	7:W:518:TYR:HA	1.79	0.40
1:A:181:GLN:HB2	1:A:197:ILE:HB	2.03	0.40
1:B:207:ARG:HD3	1:B:291:ARG:HD2	2.04	0.40
2:D:394:ILE:HD13	2:D:394:ILE:HA	1.97	0.40
1:V:66:MET:HE2	1:V:66:MET:HB2	1.92	0.40
7:W:28:ILE:H	7:W:28:ILE:HD13	1.86	0.40
7:Z:369:LYS:HD3	7:Z:369:LYS:HA	1.83	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	959/971 (99%)	926 (97%)	33 (3%)	0	100	100
1	B	959/971 (99%)	918 (96%)	41 (4%)	0	100	100
1	U	941/971 (97%)	891 (95%)	49 (5%)	1 (0%)	48	78
1	V	941/971 (97%)	893 (95%)	47 (5%)	1 (0%)	48	78
2	C	606/724 (84%)	584 (96%)	22 (4%)	0	100	100
2	D	606/724 (84%)	580 (96%)	26 (4%)	0	100	100
3	E	200/203 (98%)	195 (98%)	5 (2%)	0	100	100
3	F	197/203 (97%)	189 (96%)	8 (4%)	0	100	100
3	G	200/203 (98%)	196 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	197/203 (97%)	191 (97%)	6 (3%)	0	100	100
4	I	308/349 (88%)	301 (98%)	7 (2%)	0	100	100
4	J	308/349 (88%)	300 (97%)	8 (3%)	0	100	100
5	K	568/664 (86%)	532 (94%)	35 (6%)	1 (0%)	43	70
5	L	558/664 (84%)	535 (96%)	22 (4%)	1 (0%)	43	70
6	M	129/138 (94%)	119 (92%)	10 (8%)	0	100	100
6	N	133/138 (96%)	122 (92%)	11 (8%)	0	100	100
6	O	129/138 (94%)	118 (92%)	11 (8%)	0	100	100
6	P	133/138 (96%)	120 (90%)	13 (10%)	0	100	100
6	Q	125/138 (91%)	116 (93%)	9 (7%)	0	100	100
6	R	125/138 (91%)	119 (95%)	6 (5%)	0	100	100
6	S	129/138 (94%)	124 (96%)	5 (4%)	0	100	100
6	T	129/138 (94%)	122 (95%)	7 (5%)	0	100	100
7	W	628/695 (90%)	550 (88%)	71 (11%)	7 (1%)	11	39
7	X	628/695 (90%)	542 (86%)	82 (13%)	4 (1%)	21	51
7	Y	626/695 (90%)	550 (88%)	71 (11%)	5 (1%)	16	45
7	Z	626/695 (90%)	544 (87%)	77 (12%)	5 (1%)	16	45
8	a	131/136 (96%)	125 (95%)	6 (5%)	0	100	100
8	b	131/136 (96%)	128 (98%)	3 (2%)	0	100	100
All	All	11350/12326 (92%)	10630 (94%)	695 (6%)	25 (0%)	44	70

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	365	ILE
7	W	369	LYS
7	Y	277	VAL
7	Z	8	PRO
7	Z	277	VAL
5	K	365	ILE
7	W	410	ALA
7	Y	369	LYS
7	W	335	ALA
7	X	297	LEU
7	X	335	ALA

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Mol	Chain	Res	Type
7	Y	335	ALA
7	Z	335	ALA
1	U	90	ASP
1	V	90	ASP
7	W	297	LEU
7	W	501	TYR
7	Z	293	GLY
7	W	339	ILE
7	W	15	ILE
7	X	15	ILE
7	X	339	ILE
7	Y	15	ILE
7	Z	15	ILE
7	Y	339	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	858/866 (99%)	837 (98%)	21 (2%)	43	60
1	B	858/866 (99%)	837 (98%)	21 (2%)	43	60
1	U	851/866 (98%)	824 (97%)	27 (3%)	34	54
1	V	851/866 (98%)	823 (97%)	28 (3%)	33	54
2	C	562/664 (85%)	552 (98%)	10 (2%)	51	65
2	D	562/664 (85%)	550 (98%)	12 (2%)	47	62
3	E	177/178 (99%)	176 (99%)	1 (1%)	78	78
3	F	174/178 (98%)	173 (99%)	1 (1%)	78	78
3	G	177/178 (99%)	173 (98%)	4 (2%)	44	61
3	H	174/178 (98%)	174 (100%)	0	100	100
4	I	290/318 (91%)	280 (97%)	10 (3%)	32	53
4	J	290/318 (91%)	278 (96%)	12 (4%)	27	50
5	K	490/547 (90%)	474 (97%)	16 (3%)	33	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	L	483/547 (88%)	469 (97%)	14 (3%)	37	56
6	M	113/115 (98%)	107 (95%)	6 (5%)	20	45
6	N	113/115 (98%)	109 (96%)	4 (4%)	32	53
6	O	113/115 (98%)	111 (98%)	2 (2%)	51	65
6	P	113/115 (98%)	109 (96%)	4 (4%)	32	53
6	Q	111/115 (96%)	108 (97%)	3 (3%)	39	57
6	R	111/115 (96%)	108 (97%)	3 (3%)	39	57
6	S	111/115 (96%)	110 (99%)	1 (1%)	70	73
6	T	111/115 (96%)	109 (98%)	2 (2%)	51	65
7	W	550/602 (91%)	514 (94%)	36 (6%)	15	40
7	X	550/602 (91%)	518 (94%)	32 (6%)	18	43
7	Y	548/602 (91%)	524 (96%)	24 (4%)	25	49
7	Z	548/602 (91%)	513 (94%)	35 (6%)	16	41
8	a	122/125 (98%)	117 (96%)	5 (4%)	27	50
8	b	122/125 (98%)	116 (95%)	6 (5%)	22	47
All	All	10133/10812 (94%)	9793 (97%)	340 (3%)	33	53

All (340) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	172	ILE
1	A	239	VAL
1	A	248	ILE
1	A	275	SER
1	A	297	THR
1	A	314	THR
1	A	360	VAL
1	A	415	ILE
1	A	469	ASP
1	A	497	LEU
1	A	511	LEU
1	A	598	GLU
1	A	603	THR
1	A	645	THR
1	A	691	ASN
1	A	740	HIS

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Mol	Chain	Res	Type
1	A	774	GLU
1	A	806	ILE
1	A	917	ILE
1	A	965	LEU
1	B	10	LEU
1	B	57	ILE
1	B	66	MET
1	B	83	GLU
1	B	155	MET
1	B	211	THR
1	B	235	ILE
1	B	239	VAL
1	B	415	ILE
1	B	420	VAL
1	B	469	ASP
1	B	497	LEU
1	B	511	LEU
1	B	603	THR
1	B	646	ILE
1	B	684	MET
1	B	691	ASN
1	B	740	HIS
1	B	754	VAL
1	B	836	THR
1	B	963	THR
2	C	190	LEU
2	C	288	ASN
2	C	289	LEU
2	C	305	VAL
2	C	330	LEU
2	C	401	GLU
2	C	436	GLU
2	C	571	VAL
2	C	610	VAL
2	C	614	LEU
2	D	25	ILE
2	D	71	MET
2	D	230	MET
2	D	305	VAL
2	D	309	GLN
2	D	368	VAL
2	D	401	GLU

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Mol	Chain	Res	Type
2	D	436	GLU
2	D	446	GLU
2	D	457	VAL
2	D	571	VAL
2	D	614	LEU
3	E	115	LEU
3	F	5	ILE
3	G	5	ILE
3	G	53	LEU
3	G	97	VAL
3	G	124	VAL
4	I	14	ILE
4	I	16	GLN
4	I	21	LYS
4	I	153	THR
4	I	182	VAL
4	I	207	ARG
4	I	220	ILE
4	I	289	GLU
4	I	304	GLU
4	I	307	SER
4	J	14	ILE
4	J	21	LYS
4	J	32	ILE
4	J	37	SER
4	J	100	VAL
4	J	182	VAL
4	J	209	VAL
4	J	210	THR
4	J	222	CYS
4	J	253	ASP
4	J	270	ILE
4	J	289	GLU
5	K	53	ILE
5	K	60	THR
5	K	73	THR
5	K	74	TYR
5	K	114	ASN
5	K	126	SER
5	K	146	LEU
5	K	174	TYR
5	K	262	ASP

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Mol	Chain	Res	Type
5	K	306	VAL
5	K	355	SER
5	K	375	VAL
5	K	507	ILE
5	K	553	ILE
5	K	626	THR
5	K	647	ASP
5	L	60	THR
5	L	114	ASN
5	L	126	SER
5	L	149	GLN
5	L	161	VAL
5	L	169	GLN
5	L	174	TYR
5	L	266	GLU
5	L	306	VAL
5	L	436	VAL
5	L	491	ILE
5	L	507	ILE
5	L	607	THR
5	L	647	ASP
6	M	8	ILE
6	M	26	THR
6	M	45	MET
6	M	75	ILE
6	M	90	ILE
6	M	113	VAL
6	N	23	ILE
6	N	67	VAL
6	N	81	ASN
6	N	85	VAL
6	O	14	ILE
6	O	49	VAL
6	P	29	LYS
6	P	67	VAL
6	P	81	ASN
6	P	98	LEU
6	Q	43	SER
6	Q	60	LEU
6	Q	137	TYR
6	R	3	VAL
6	R	101	VAL

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Mol	Chain	Res	Type
6	R	137	TYR
6	S	88	ILE
6	T	27	ASN
6	T	59	SER
1	U	77	LEU
1	U	79	ILE
1	U	80	THR
1	U	115	ILE
1	U	138	THR
1	U	166	THR
1	U	177	THR
1	U	251	HIS
1	U	287	THR
1	U	292	ILE
1	U	314	THR
1	U	319	ASP
1	U	321	ASP
1	U	336	ILE
1	U	339	LEU
1	U	451	MET
1	U	620	MET
1	U	638	VAL
1	U	641	ILE
1	U	643	VAL
1	U	658	LEU
1	U	818	ILE
1	U	821	ILE
1	U	826	LEU
1	U	831	LEU
1	U	871	PHE
1	U	888	VAL
1	V	79	ILE
1	V	80	THR
1	V	138	THR
1	V	146	MET
1	V	282	THR
1	V	287	THR
1	V	292	ILE
1	V	314	THR
1	V	319	ASP
1	V	323	ASP
1	V	381	LEU

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Mol	Chain	Res	Type
1	V	388	LEU
1	V	390	THR
1	V	515	VAL
1	V	536	VAL
1	V	568	VAL
1	V	620	MET
1	V	630	THR
1	V	638	VAL
1	V	643	VAL
1	V	782	MET
1	V	821	ILE
1	V	871	PHE
1	V	888	VAL
1	V	930	ILE
1	V	933	VAL
1	V	955	THR
1	V	967	HIS
7	W	7	VAL
7	W	17	ASP
7	W	28	ILE
7	W	100	ASP
7	W	107	LEU
7	W	118	ILE
7	W	157	LEU
7	W	170	VAL
7	W	186	VAL
7	W	209	TRP
7	W	237	ILE
7	W	238	GLU
7	W	262	PHE
7	W	279	ASP
7	W	297	LEU
7	W	312	ASP
7	W	313	LEU
7	W	343	THR
7	W	352	TYR
7	W	369	LYS
7	W	380	ASP
7	W	382	THR
7	W	478	THR
7	W	484	VAL
7	W	532	MET

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Mol	Chain	Res	Type
7	W	556	ARG
7	W	588	THR
7	W	611	HIS
7	W	626	VAL
7	W	645	VAL
7	W	648	ILE
7	W	654	THR
7	W	664	TRP
7	W	665	THR
7	W	667	ASN
7	W	676	ARG
7	X	7	VAL
7	X	17	ASP
7	X	23	LEU
7	X	28	ILE
7	X	47	GLU
7	X	100	ASP
7	X	118	ILE
7	X	171	LEU
7	X	185	LEU
7	X	186	VAL
7	X	196	PHE
7	X	237	ILE
7	X	270	MET
7	X	271	TYR
7	X	279	ASP
7	X	297	LEU
7	X	312	ASP
7	X	343	THR
7	X	352	TYR
7	X	382	THR
7	X	383	THR
7	X	454	LEU
7	X	478	THR
7	X	505	VAL
7	X	527	VAL
7	X	583	VAL
7	X	588	THR
7	X	606	LEU
7	X	620	LEU
7	X	645	VAL
7	X	656	ILE

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Mol	Chain	Res	Type
7	X	667	ASN
7	Y	39	LEU
7	Y	51	VAL
7	Y	94	LYS
7	Y	95	ARG
7	Y	106	ARG
7	Y	158	ILE
7	Y	165	VAL
7	Y	216	ILE
7	Y	237	ILE
7	Y	247	VAL
7	Y	249	VAL
7	Y	301	PHE
7	Y	342	LEU
7	Y	348	ASP
7	Y	471	LEU
7	Y	485	CYS
7	Y	527	VAL
7	Y	532	MET
7	Y	535	SER
7	Y	546	LEU
7	Y	572	HIS
7	Y	590	VAL
7	Y	614	PHE
7	Y	668	VAL
7	Z	9	ARG
7	Z	17	ASP
7	Z	34	CYS
7	Z	49	THR
7	Z	84	LEU
7	Z	85	LEU
7	Z	93	VAL
7	Z	113	ILE
7	Z	155	ILE
7	Z	165	VAL
7	Z	170	VAL
7	Z	213	THR
7	Z	217	GLU
7	Z	233	ARG
7	Z	237	ILE
7	Z	247	VAL
7	Z	249	VAL

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Mol	Chain	Res	Type
7	Z	260	ILE
7	Z	280	VAL
7	Z	358	LEU
7	Z	379	THR
7	Z	432	ARG
7	Z	471	LEU
7	Z	527	VAL
7	Z	535	SER
7	Z	562	ASN
7	Z	570	TYR
7	Z	590	VAL
7	Z	607	ILE
7	Z	614	PHE
7	Z	632	TYR
7	Z	634	LEU
7	Z	668	VAL
7	Z	678	THR
7	Z	679	LEU
8	a	22	ASP
8	a	30	LEU
8	a	101	THR
8	a	103	THR
8	a	108	VAL
8	b	7	THR
8	b	36	ASP
8	b	74	ILE
8	b	101	THR
8	b	103	THR
8	b	108	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	191	HIS
1	A	391	ASN
1	A	723	HIS
1	B	723	HIS
1	B	797	GLN
2	C	237	GLN
2	D	237	GLN
2	D	309	GLN

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Mol	Chain	Res	Type
2	D	342	GLN
2	D	561	ASN
3	E	121	GLN
3	E	139	ASN
3	F	29	ASN
3	F	95	ASN
3	F	182	ASN
3	H	95	ASN
3	H	101	GLN
3	H	182	ASN
4	I	115	ASN
4	I	162	ASN
4	J	42	ASN
5	K	289	ASN
5	K	630	GLN
5	L	181	HIS
5	L	289	ASN
5	L	490	GLN
6	O	73	ASN
6	P	73	ASN
6	P	128	ASN
6	R	73	ASN
6	S	115	ASN
6	T	127	GLN
1	U	202	GLN
1	U	424	GLN
1	U	426	GLN
1	U	750	ASN
1	U	797	GLN
1	U	858	GLN
1	V	202	GLN
1	V	251	HIS
1	V	359	GLN
1	V	424	GLN
1	V	426	GLN
1	V	430	ASN
1	V	569	GLN
7	W	353	GLN
7	W	598	ASN
7	W	659	ASN
7	X	75	ASN
7	X	259	ASN

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Mol	Chain	Res	Type
7	X	353	GLN
7	X	562	ASN
7	X	617	ASN
7	X	659	ASN
7	X	674	ASN
7	Y	83	ASN
7	Y	353	GLN
7	Y	562	ASN
7	Y	660	ASN
7	Z	5	ASN
7	Z	183	GLN
7	Z	326	ASN
7	Z	356	GLN
7	Z	598	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

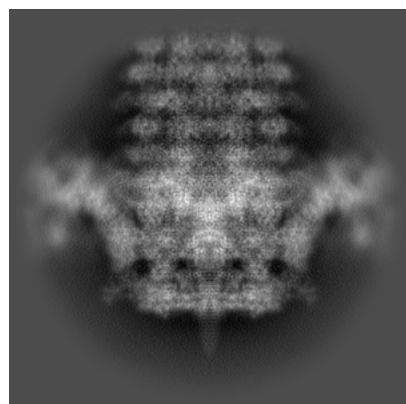
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67121. These allow visual inspection of the internal detail of the map and identification of artifacts.

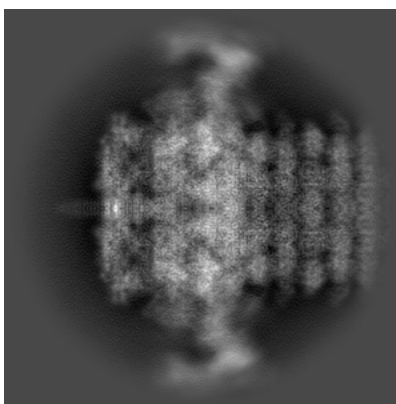
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

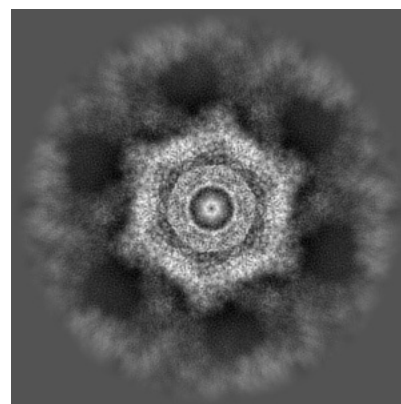
6.1.1 Primary map



X

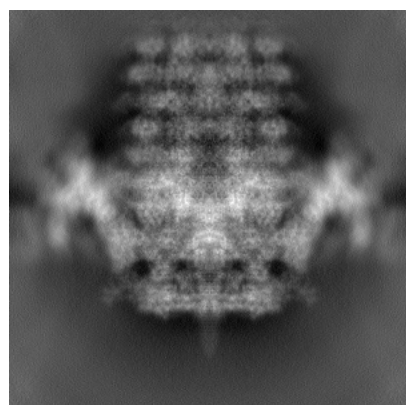


Y

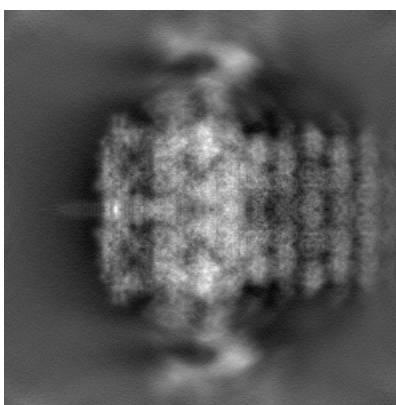


Z

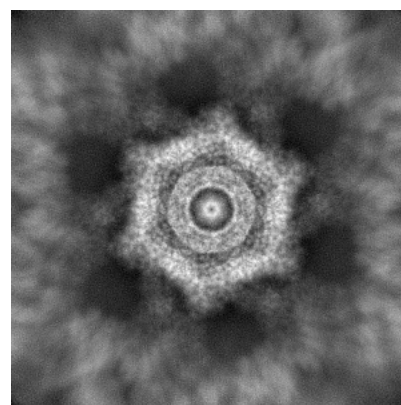
6.1.2 Raw map



X



Y

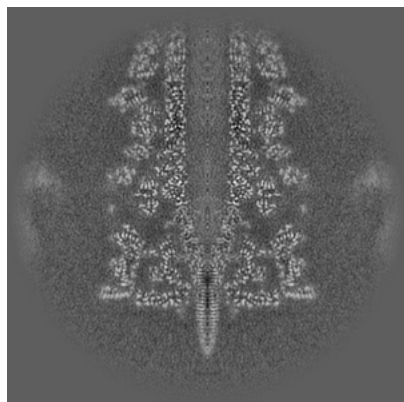


Z

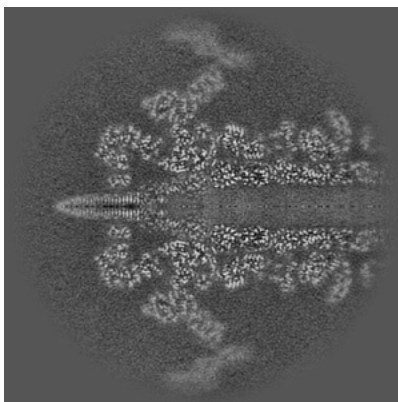
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

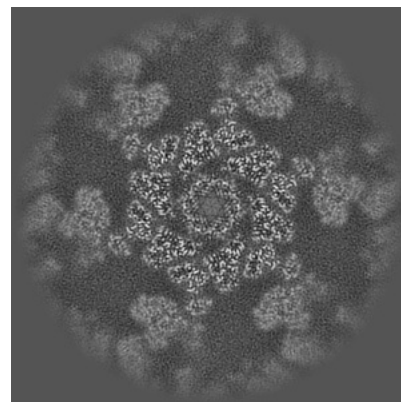
6.2.1 Primary map



X Index: 200

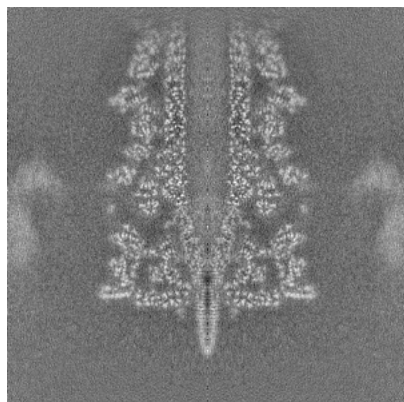


Y Index: 200

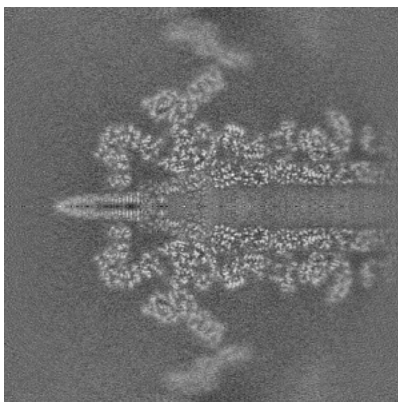


Z Index: 200

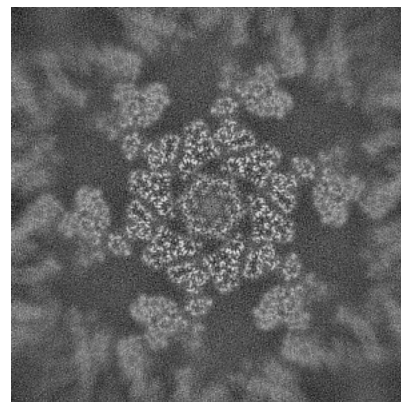
6.2.2 Raw map



X Index: 200



Y Index: 200

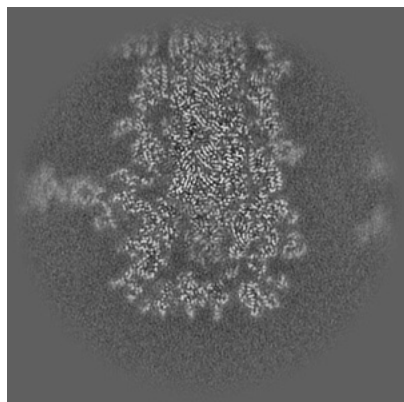


Z Index: 200

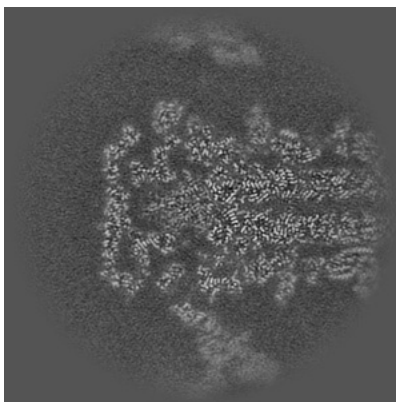
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

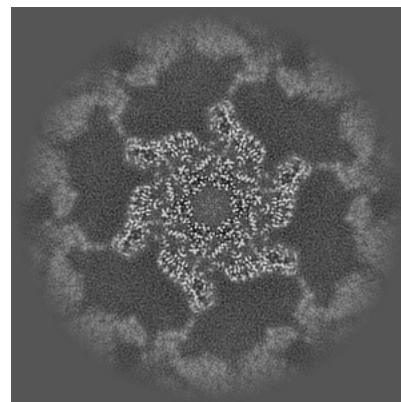
6.3.1 Primary map



X Index: 177

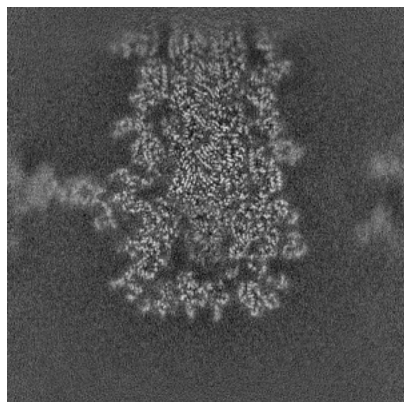


Y Index: 179

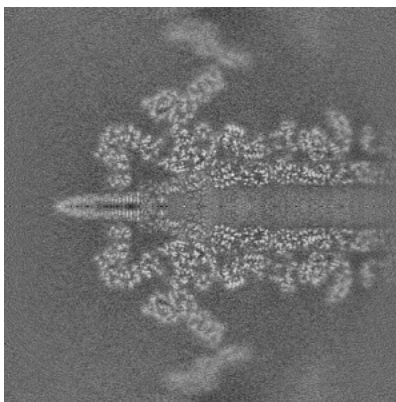


Z Index: 229

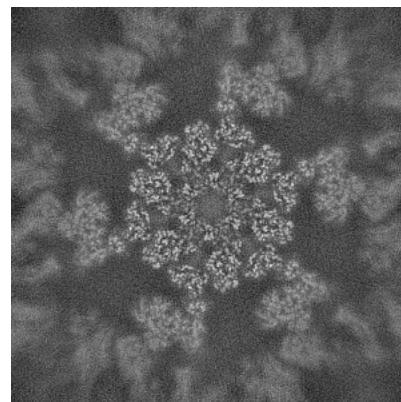
6.3.2 Raw map



X Index: 177



Y Index: 200

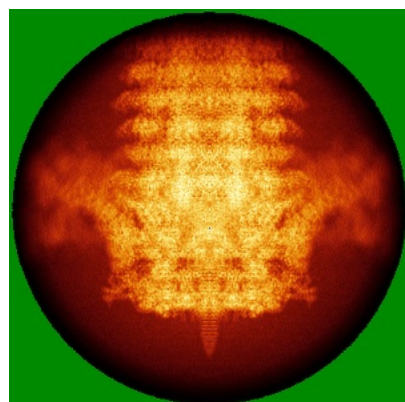


Z Index: 203

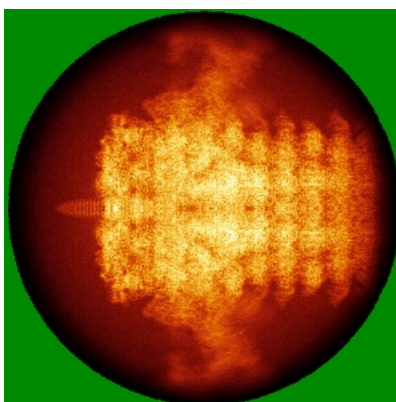
The images above show the largest variance slices of the map in three orthogonal directions.

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

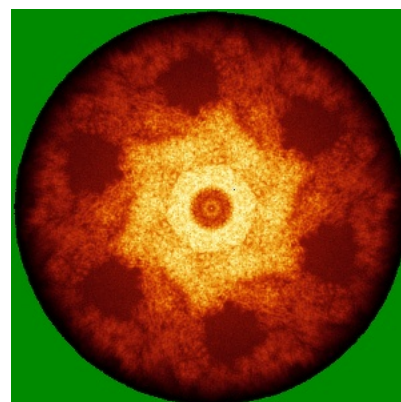
6.4.1 Primary map



X

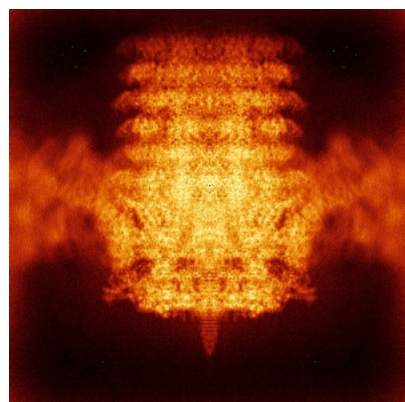


Y

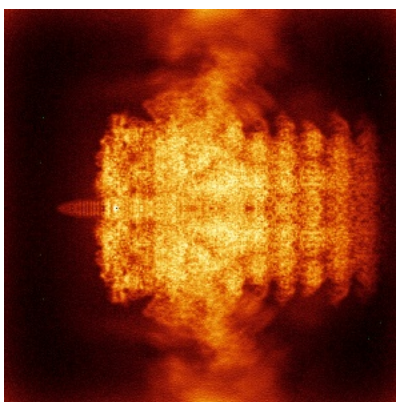


Z

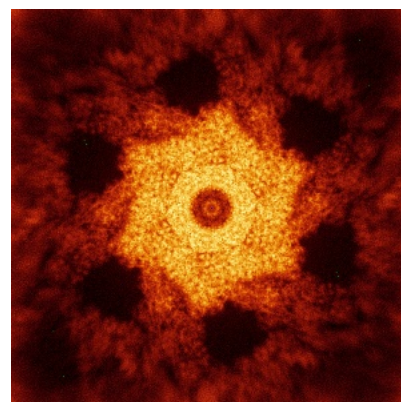
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

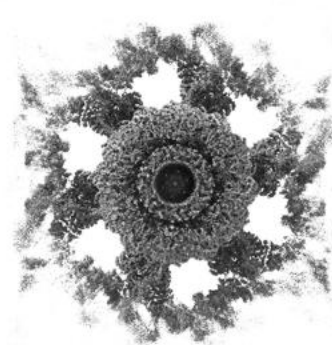
6.5.2 Raw map



X



Y



Z

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

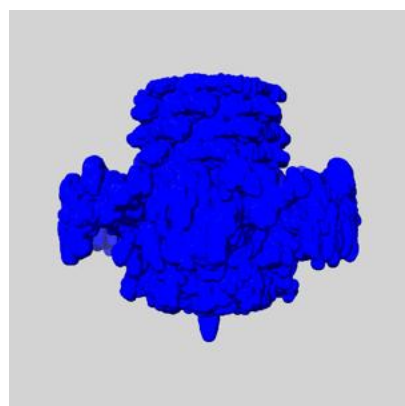
6.6 Mask visualisation [i](#)

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

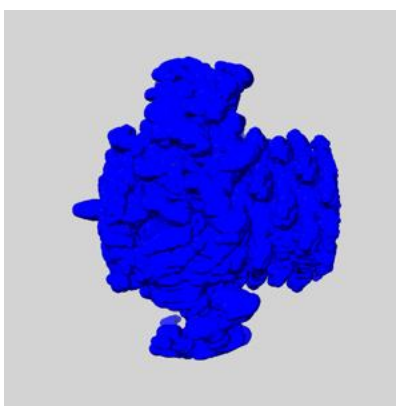
A mask typically either:

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

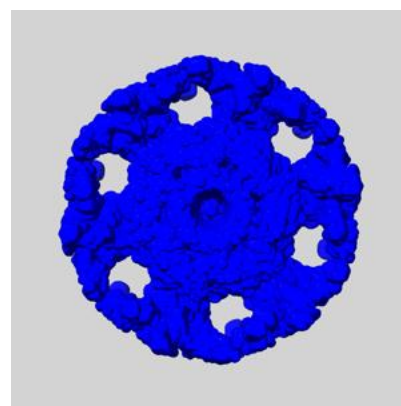
6.6.1 emd_67121_msk_1.map [i](#)



X



Y

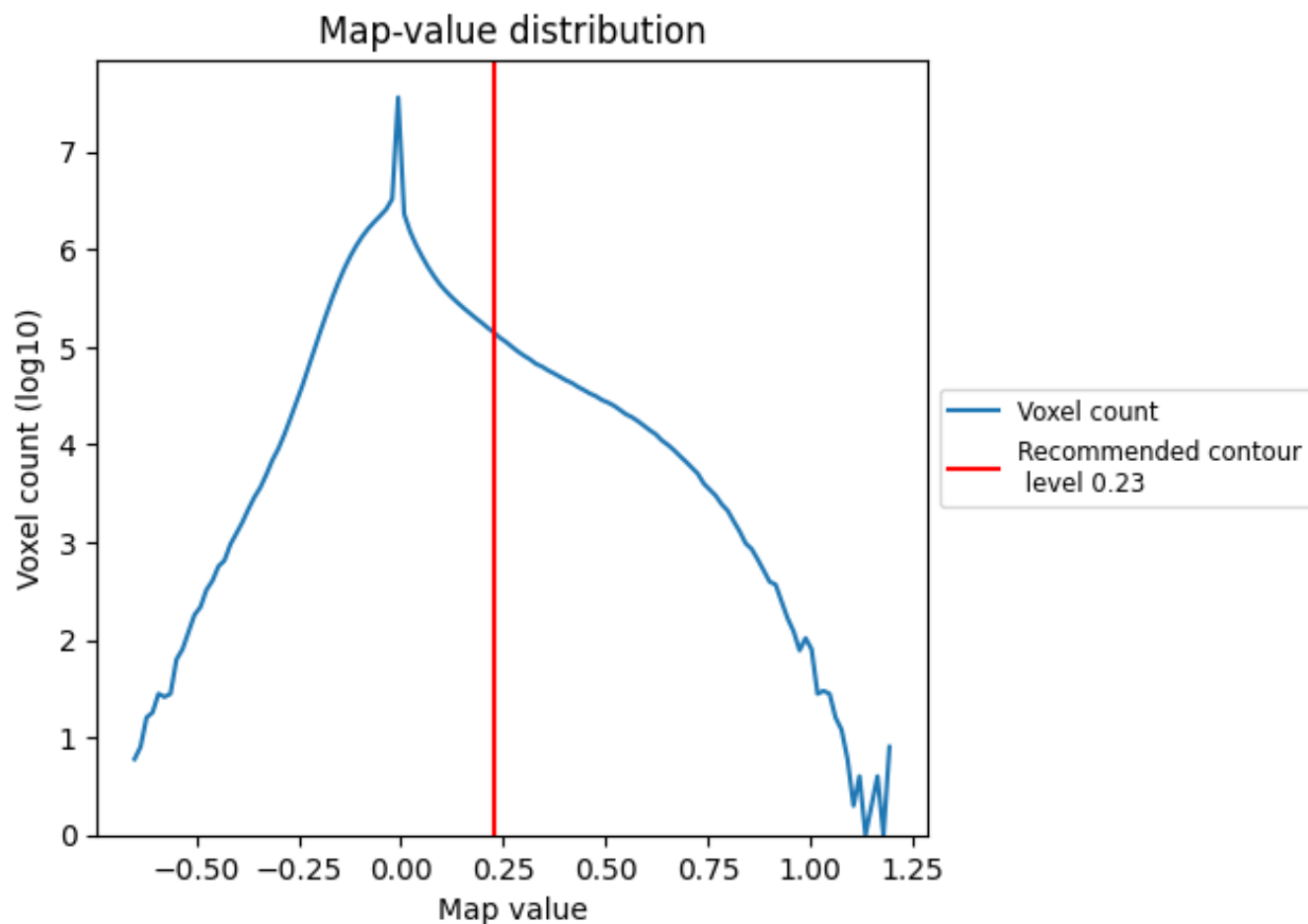


Z

7 Map analysis [i](#)

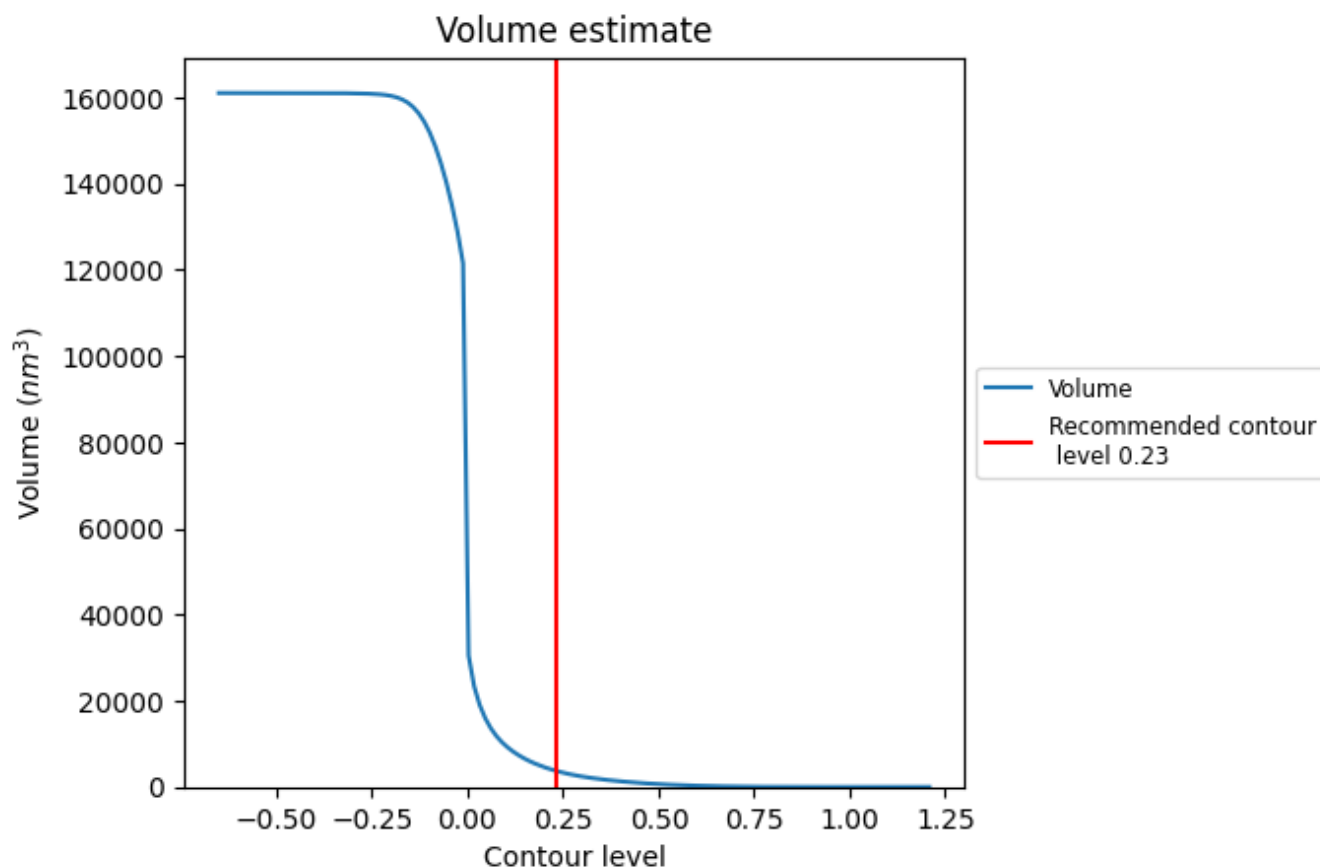
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

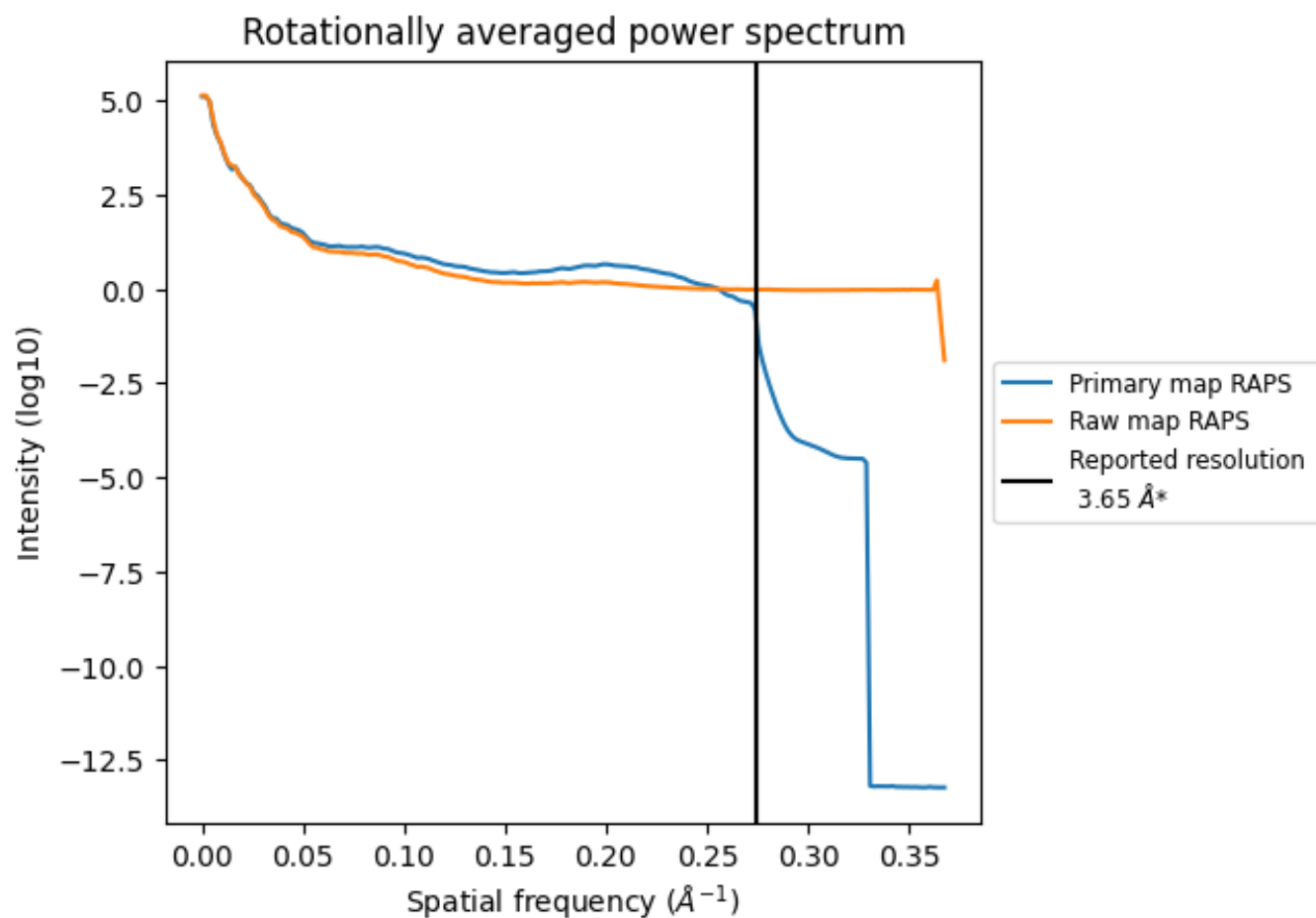
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3776 nm³; this corresponds to an approximate mass of 3411 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 ⓘ

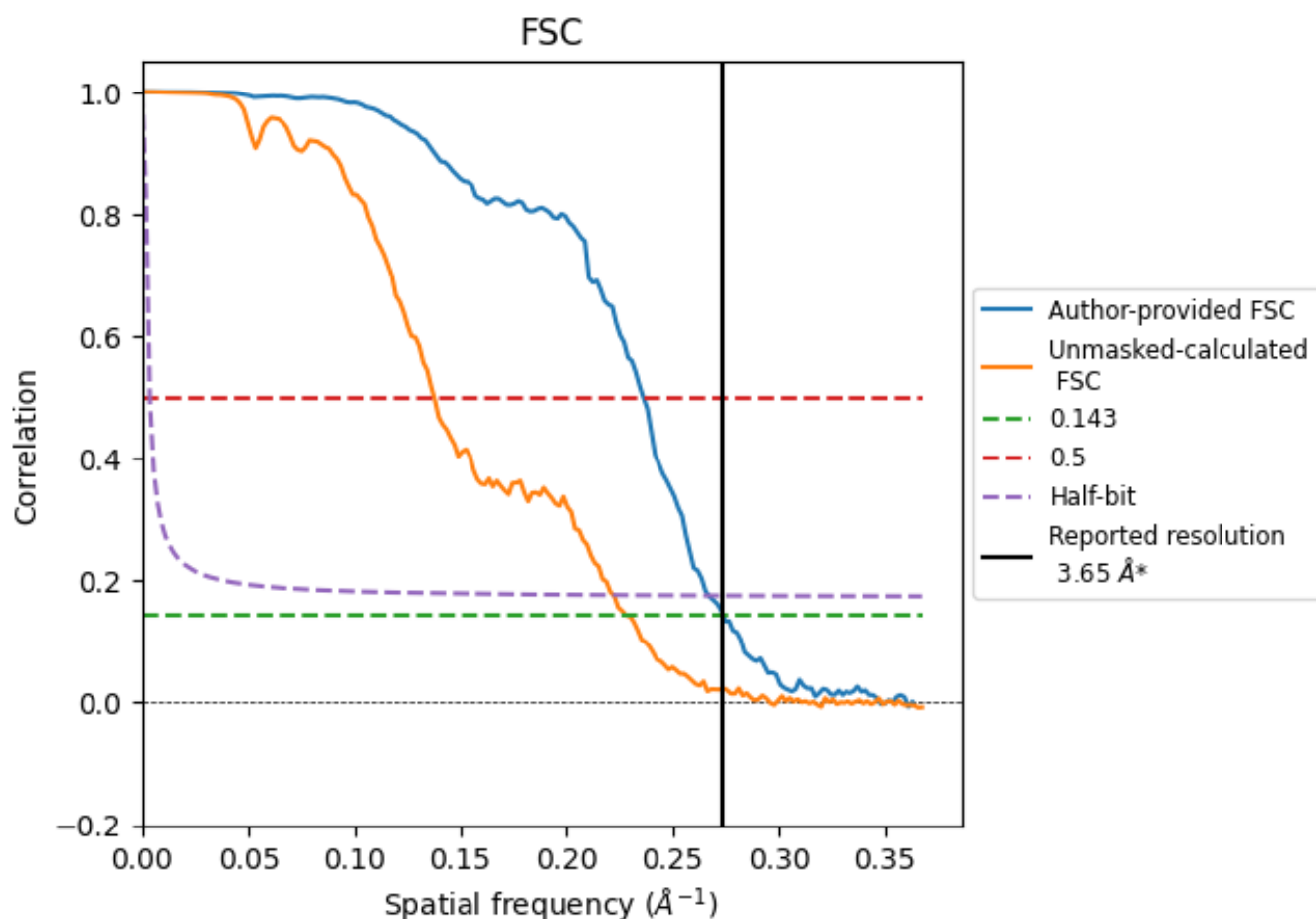


*Reported resolution corresponds to spatial frequency of 0.274 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.274 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.65	4.24	3.74
Unmasked-calculated*	4.38	7.28	4.50

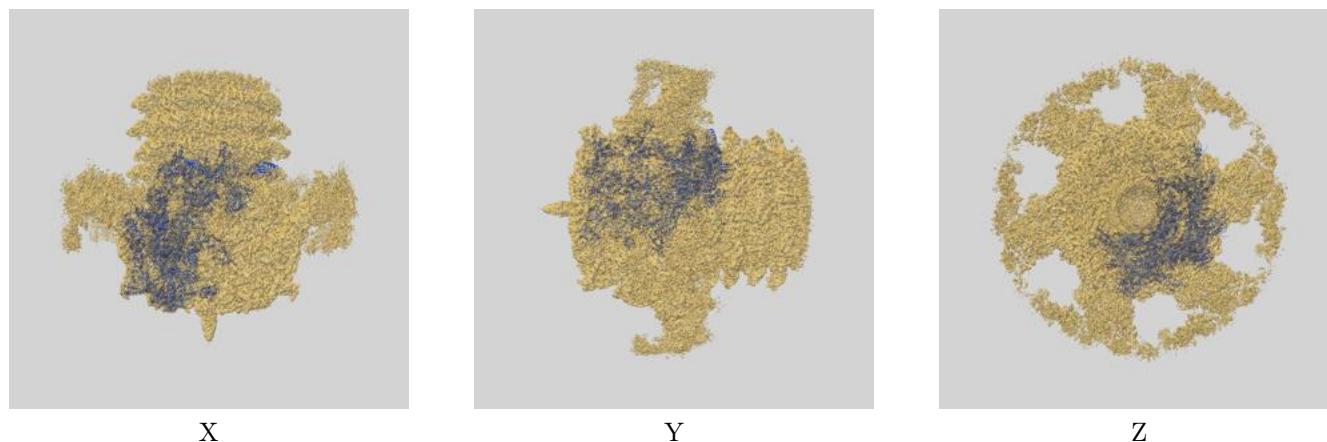
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.38 differs from the reported value 3.65 by more than 10 %

9 Map-model fit [i](#)

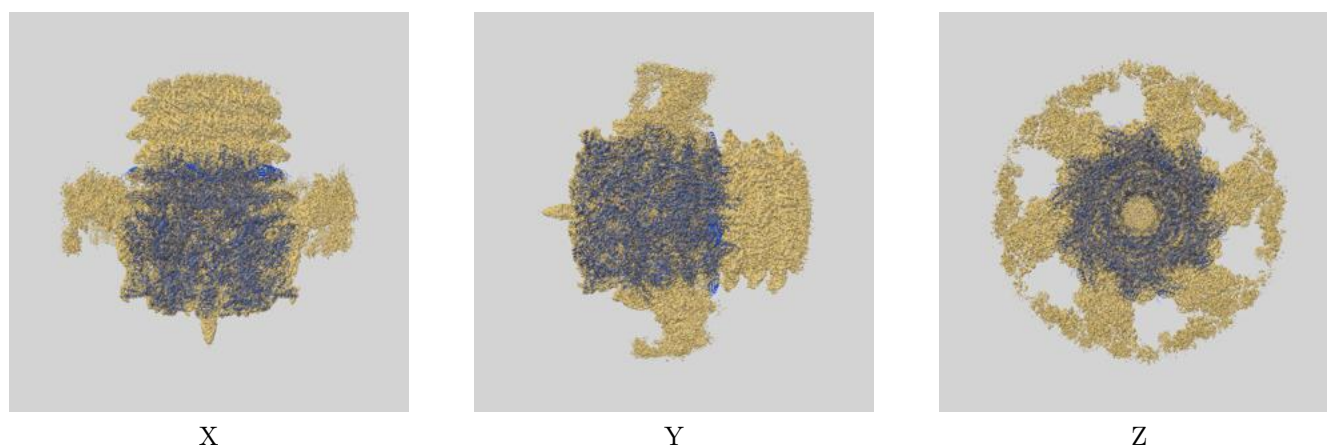
This section contains information regarding the fit between EMDB map EMD-67121 and PDB model 9XQS. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

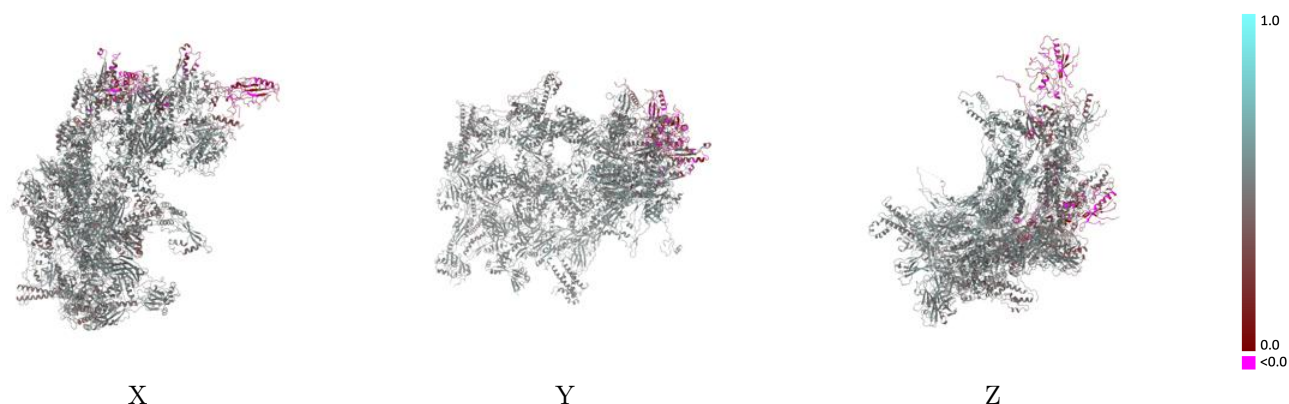


9.1.2 Map-model assembly overlay [i](#)



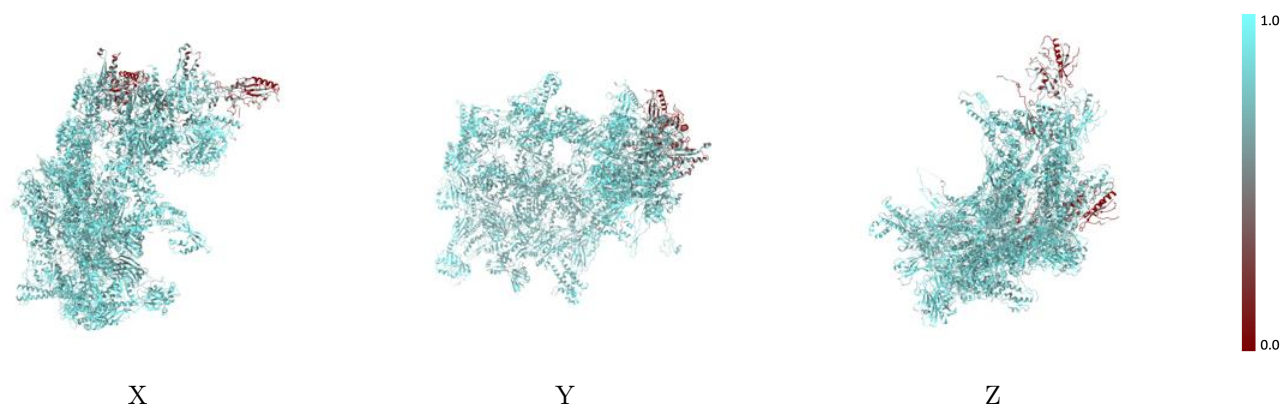
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



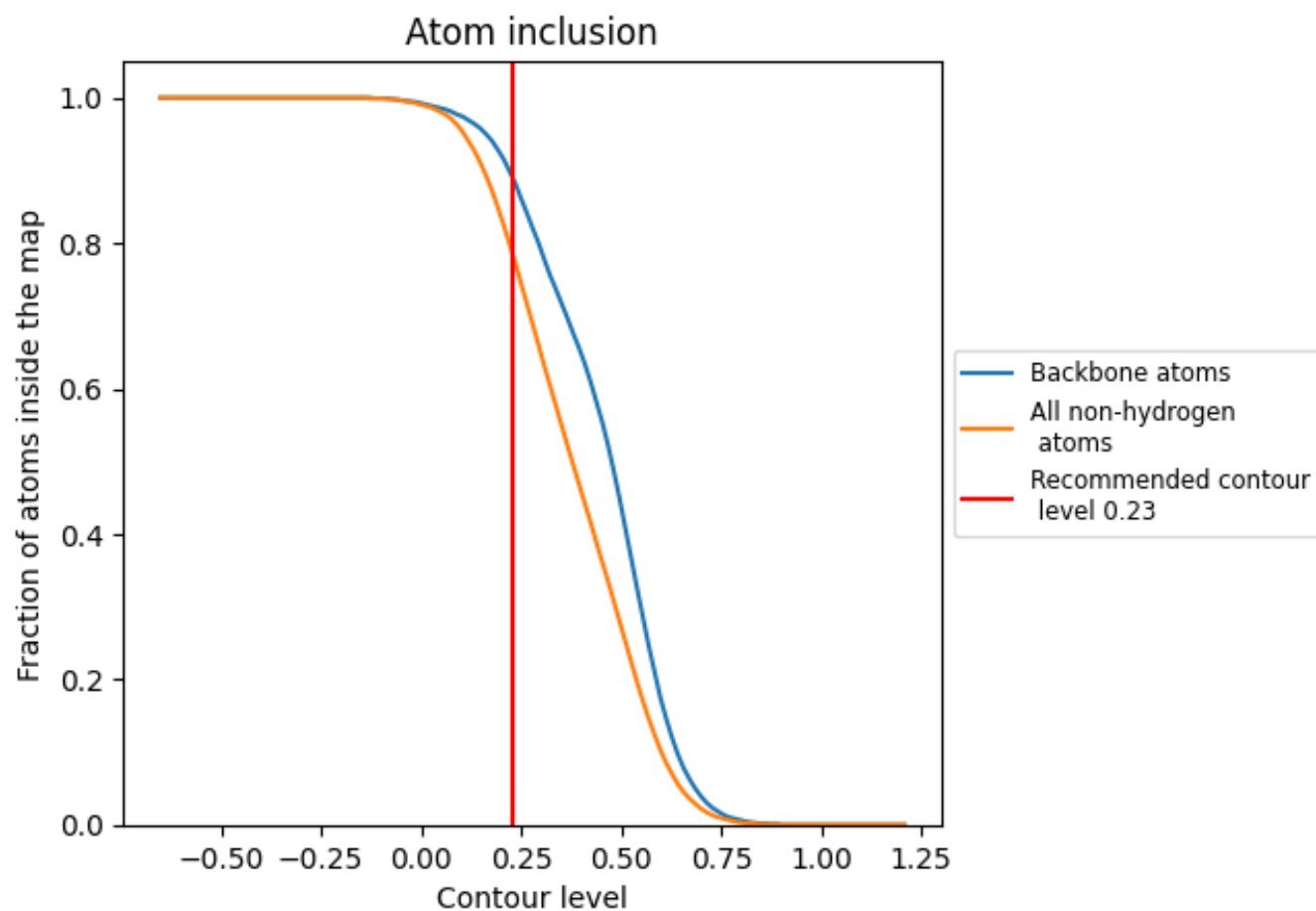
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 78% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7840	 0.4740
A	 0.8260	 0.4980
B	 0.8260	 0.4980
C	 0.8260	 0.4780
D	 0.8250	 0.4770
E	 0.8090	 0.4790
F	 0.8400	 0.4760
G	 0.8060	 0.4810
H	 0.8420	 0.4790
I	 0.8060	 0.5240
J	 0.8050	 0.5220
K	 0.8060	 0.5130
L	 0.8150	 0.5150
M	 0.8350	 0.4950
N	 0.8440	 0.4810
O	 0.8360	 0.4930
P	 0.8440	 0.4870
Q	 0.8580	 0.4810
R	 0.8480	 0.4840
S	 0.8270	 0.4960
T	 0.8340	 0.4910
U	 0.7850	 0.5030
V	 0.7840	 0.5030
W	 0.8000	 0.4730
X	 0.8000	 0.4710
Y	 0.5450	 0.3060
Z	 0.5460	 0.3040
a	 0.8030	 0.5040
b	 0.8020	 0.5040

