



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 08:57 AM UTC

PDB ID : 6XTY / pdb_00006xty
EMDB ID : EMD-10621
Title : CryoEM structure of human CMG bound to AND-1 (CMGA)
Authors : Rzechorzek, N.J.; Pellegrini, L.; Chirgadze, D.Y.; Hardwick, S.W.
Deposited on : 2020-01-16
Resolution : 6.77 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:

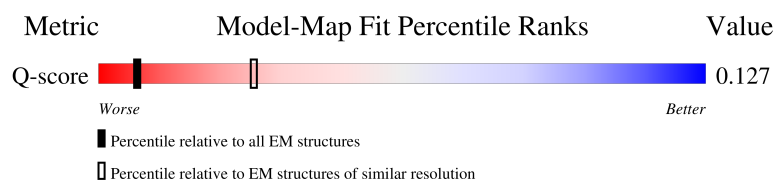
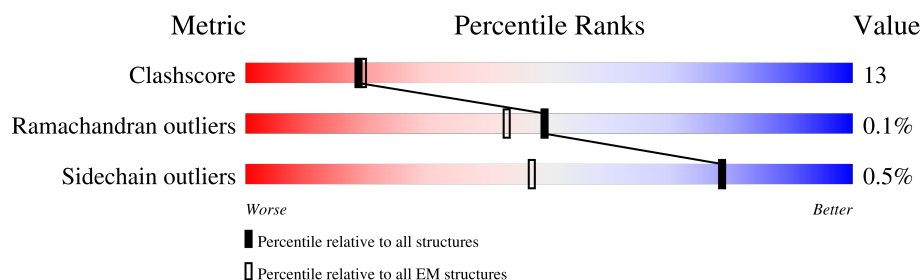
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 6.77 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	476 (6.29 - 7.25)

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	2	904	
2	3	853	
3	4	863	
4	5	734	

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Mol	Chain	Length	Quality of chain
5	6	821	
6	7	719	
7	A	196	
8	B	185	
9	C	216	
10	D	223	
11	E	566	
12	F	1171	
12	G	1171	
12	H	1171	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 48821 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	611	Total	C	N	O	S	0	0
			4832	3040	863	899	30		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	608	Total	C	N	O	S	0	0
			4782	2997	844	916	25		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	598	Total	C	N	O	S	0	0
			4784	3016	850	892	26		

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	577	Total	C	N	O	S	0	0
			4524	2841	805	843	35		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	609	Total	C	N	O	S	0	0
			4873	3068	862	917	26		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	598	Total	C	N	O	S	0	0
			4727	2960	837	901	29		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	196	Total	C	N	O	S	0	0
			1613	1016	290	295	12		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	176	Total	C	N	O	S	0	0
			1431	916	242	264	9		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	194	Total	C	N	O	S	0	0
			1552	985	268	293	6		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	203	Total	C	N	O	S	0	0
			1679	1065	290	314	10		

- Molecule 11 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	538	Total	C	N	O	S	0	0
			4380	2785	751	813	31		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	346	GLN	GLU	variant	UNP O75419

- Molecule 12 is a protein called WD repeat and HMG-box DNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	403	Total	C	N	O	S	3	0
			3213	2038	559	595	21		
12	G	403	Total	C	N	O	S	3	0
			3213	2038	559	595	21		
12	H	403	Total	C	N	O	S	3	0
			3213	2038	559	595	21		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-41	MET	-	initiating methionine	UNP O75717
F	-40	SER	-	expression tag	UNP O75717
F	-39	ALA	-	expression tag	UNP O75717
F	-38	TRP	-	expression tag	UNP O75717
F	-37	SER	-	expression tag	UNP O75717
F	-36	HIS	-	expression tag	UNP O75717
F	-35	PRO	-	expression tag	UNP O75717
F	-34	GLN	-	expression tag	UNP O75717
F	-33	PHE	-	expression tag	UNP O75717
F	-32	GLU	-	expression tag	UNP O75717
F	-31	LYS	-	expression tag	UNP O75717
F	-30	GLY	-	expression tag	UNP O75717
F	-29	GLY	-	expression tag	UNP O75717
F	-28	GLY	-	expression tag	UNP O75717
F	-27	SER	-	expression tag	UNP O75717
F	-26	GLY	-	expression tag	UNP O75717
F	-25	GLY	-	expression tag	UNP O75717
F	-24	GLY	-	expression tag	UNP O75717
F	-23	SER	-	expression tag	UNP O75717
F	-22	GLY	-	expression tag	UNP O75717
F	-21	GLY	-	expression tag	UNP O75717
F	-20	SER	-	expression tag	UNP O75717
F	-19	ALA	-	expression tag	UNP O75717
F	-18	TRP	-	expression tag	UNP O75717
F	-17	SER	-	expression tag	UNP O75717
F	-16	HIS	-	expression tag	UNP O75717
F	-15	PRO	-	expression tag	UNP O75717
F	-14	GLN	-	expression tag	UNP O75717
F	-13	PHE	-	expression tag	UNP O75717
F	-12	GLU	-	expression tag	UNP O75717
F	-11	LYS	-	expression tag	UNP O75717
F	-10	GLU	-	expression tag	UNP O75717
F	-9	ASN	-	expression tag	UNP O75717
F	-8	LEU	-	expression tag	UNP O75717
F	-7	TYR	-	expression tag	UNP O75717
F	-6	PHE	-	expression tag	UNP O75717
F	-5	GLN	-	expression tag	UNP O75717
F	-4	GLY	-	expression tag	UNP O75717
F	-3	SER	-	expression tag	UNP O75717
F	-2	SER	-	expression tag	UNP O75717
F	-1	ALA	-	expression tag	UNP O75717
F	0	THR	-	expression tag	UNP O75717

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-41	MET	-	initiating methionine	UNP O75717
G	-40	SER	-	expression tag	UNP O75717
G	-39	ALA	-	expression tag	UNP O75717
G	-38	TRP	-	expression tag	UNP O75717
G	-37	SER	-	expression tag	UNP O75717
G	-36	HIS	-	expression tag	UNP O75717
G	-35	PRO	-	expression tag	UNP O75717
G	-34	GLN	-	expression tag	UNP O75717
G	-33	PHE	-	expression tag	UNP O75717
G	-32	GLU	-	expression tag	UNP O75717
G	-31	LYS	-	expression tag	UNP O75717
G	-30	GLY	-	expression tag	UNP O75717
G	-29	GLY	-	expression tag	UNP O75717
G	-28	GLY	-	expression tag	UNP O75717
G	-27	SER	-	expression tag	UNP O75717
G	-26	GLY	-	expression tag	UNP O75717
G	-25	GLY	-	expression tag	UNP O75717
G	-24	GLY	-	expression tag	UNP O75717
G	-23	SER	-	expression tag	UNP O75717
G	-22	GLY	-	expression tag	UNP O75717
G	-21	GLY	-	expression tag	UNP O75717
G	-20	SER	-	expression tag	UNP O75717
G	-19	ALA	-	expression tag	UNP O75717
G	-18	TRP	-	expression tag	UNP O75717
G	-17	SER	-	expression tag	UNP O75717
G	-16	HIS	-	expression tag	UNP O75717
G	-15	PRO	-	expression tag	UNP O75717
G	-14	GLN	-	expression tag	UNP O75717
G	-13	PHE	-	expression tag	UNP O75717
G	-12	GLU	-	expression tag	UNP O75717
G	-11	LYS	-	expression tag	UNP O75717
G	-10	GLU	-	expression tag	UNP O75717
G	-9	ASN	-	expression tag	UNP O75717
G	-8	LEU	-	expression tag	UNP O75717
G	-7	TYR	-	expression tag	UNP O75717
G	-6	PHE	-	expression tag	UNP O75717
G	-5	GLN	-	expression tag	UNP O75717
G	-4	GLY	-	expression tag	UNP O75717
G	-3	SER	-	expression tag	UNP O75717
G	-2	SER	-	expression tag	UNP O75717
G	-1	ALA	-	expression tag	UNP O75717
G	0	THR	-	expression tag	UNP O75717

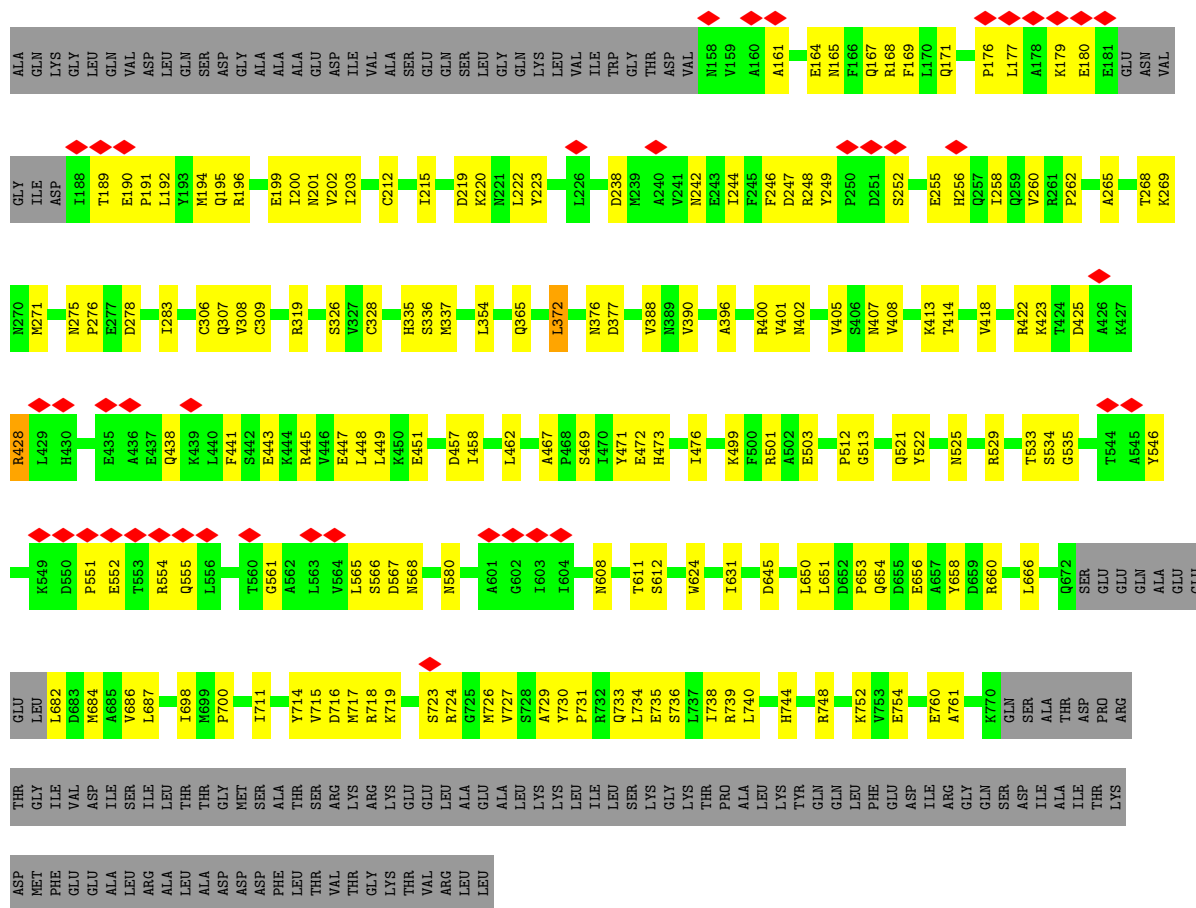
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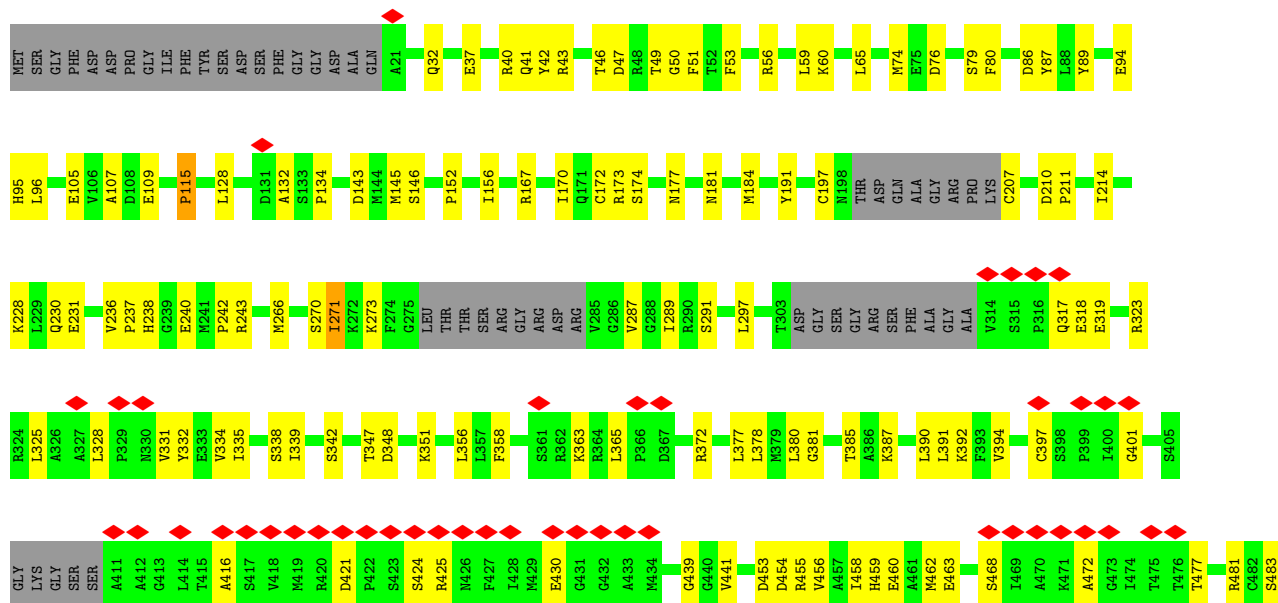
Chain	Residue	Modelled	Actual	Comment	Reference
H	-41	MET	-	initiating methionine	UNP O75717
H	-40	SER	-	expression tag	UNP O75717
H	-39	ALA	-	expression tag	UNP O75717
H	-38	TRP	-	expression tag	UNP O75717
H	-37	SER	-	expression tag	UNP O75717
H	-36	HIS	-	expression tag	UNP O75717
H	-35	PRO	-	expression tag	UNP O75717
H	-34	GLN	-	expression tag	UNP O75717
H	-33	PHE	-	expression tag	UNP O75717
H	-32	GLU	-	expression tag	UNP O75717
H	-31	LYS	-	expression tag	UNP O75717
H	-30	GLY	-	expression tag	UNP O75717
H	-29	GLY	-	expression tag	UNP O75717
H	-28	GLY	-	expression tag	UNP O75717
H	-27	SER	-	expression tag	UNP O75717
H	-26	GLY	-	expression tag	UNP O75717
H	-25	GLY	-	expression tag	UNP O75717
H	-24	GLY	-	expression tag	UNP O75717
H	-23	SER	-	expression tag	UNP O75717
H	-22	GLY	-	expression tag	UNP O75717
H	-21	GLY	-	expression tag	UNP O75717
H	-20	SER	-	expression tag	UNP O75717
H	-19	ALA	-	expression tag	UNP O75717
H	-18	TRP	-	expression tag	UNP O75717
H	-17	SER	-	expression tag	UNP O75717
H	-16	HIS	-	expression tag	UNP O75717
H	-15	PRO	-	expression tag	UNP O75717
H	-14	GLN	-	expression tag	UNP O75717
H	-13	PHE	-	expression tag	UNP O75717
H	-12	GLU	-	expression tag	UNP O75717
H	-11	LYS	-	expression tag	UNP O75717
H	-10	GLU	-	expression tag	UNP O75717
H	-9	ASN	-	expression tag	UNP O75717
H	-8	LEU	-	expression tag	UNP O75717
H	-7	TYR	-	expression tag	UNP O75717
H	-6	PHE	-	expression tag	UNP O75717
H	-5	GLN	-	expression tag	UNP O75717
H	-4	GLY	-	expression tag	UNP O75717
H	-3	SER	-	expression tag	UNP O75717
H	-2	SER	-	expression tag	UNP O75717
H	-1	ALA	-	expression tag	UNP O75717
H	0	THR	-	expression tag	UNP O75717

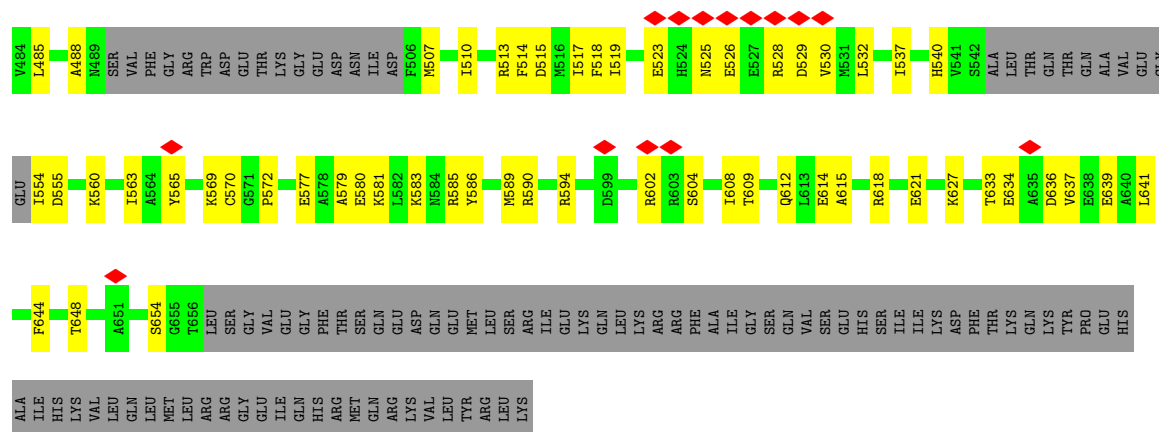
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	2	1	Total 1	Zn 1	0
13	4	1	Total 1	Zn 1	0
13	5	1	Total 1	Zn 1	0
13	6	1	Total 1	Zn 1	0
13	7	1	Total 1	Zn 1	0

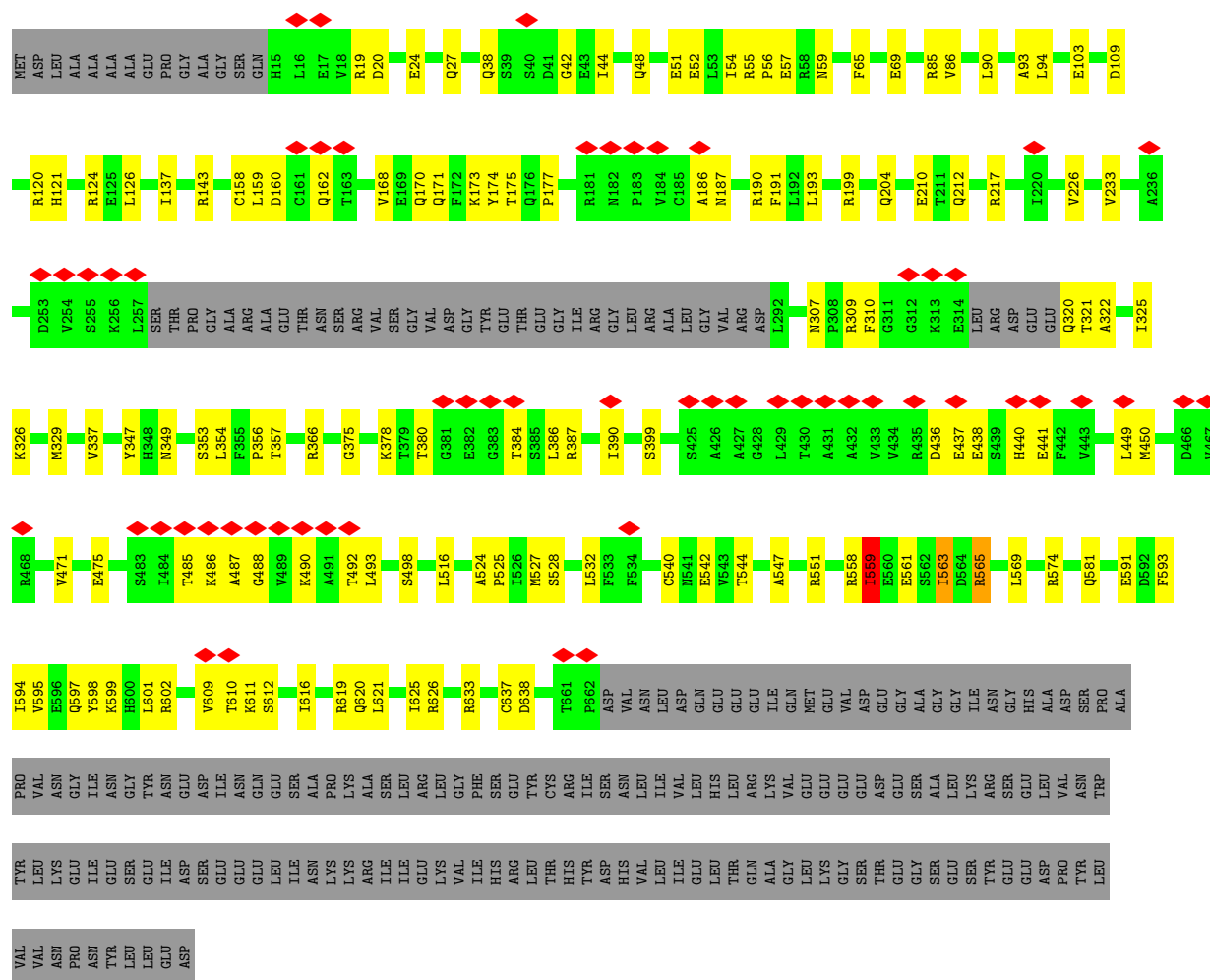


• Molecule 4: DNA replication licensing factor MCM5





• Molecule 5: DNA replication licensing factor MCM6



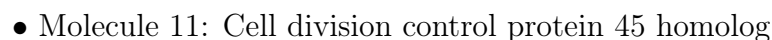
• Molecule 6: DNA replication licensing factor MCM7



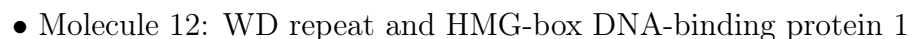
Frequency	Percentage
Daily	66%
Weekly	24%
Monthly	10%



Frequency	Percentage
Daily	73%
Weekly	18%
Monthly	9%

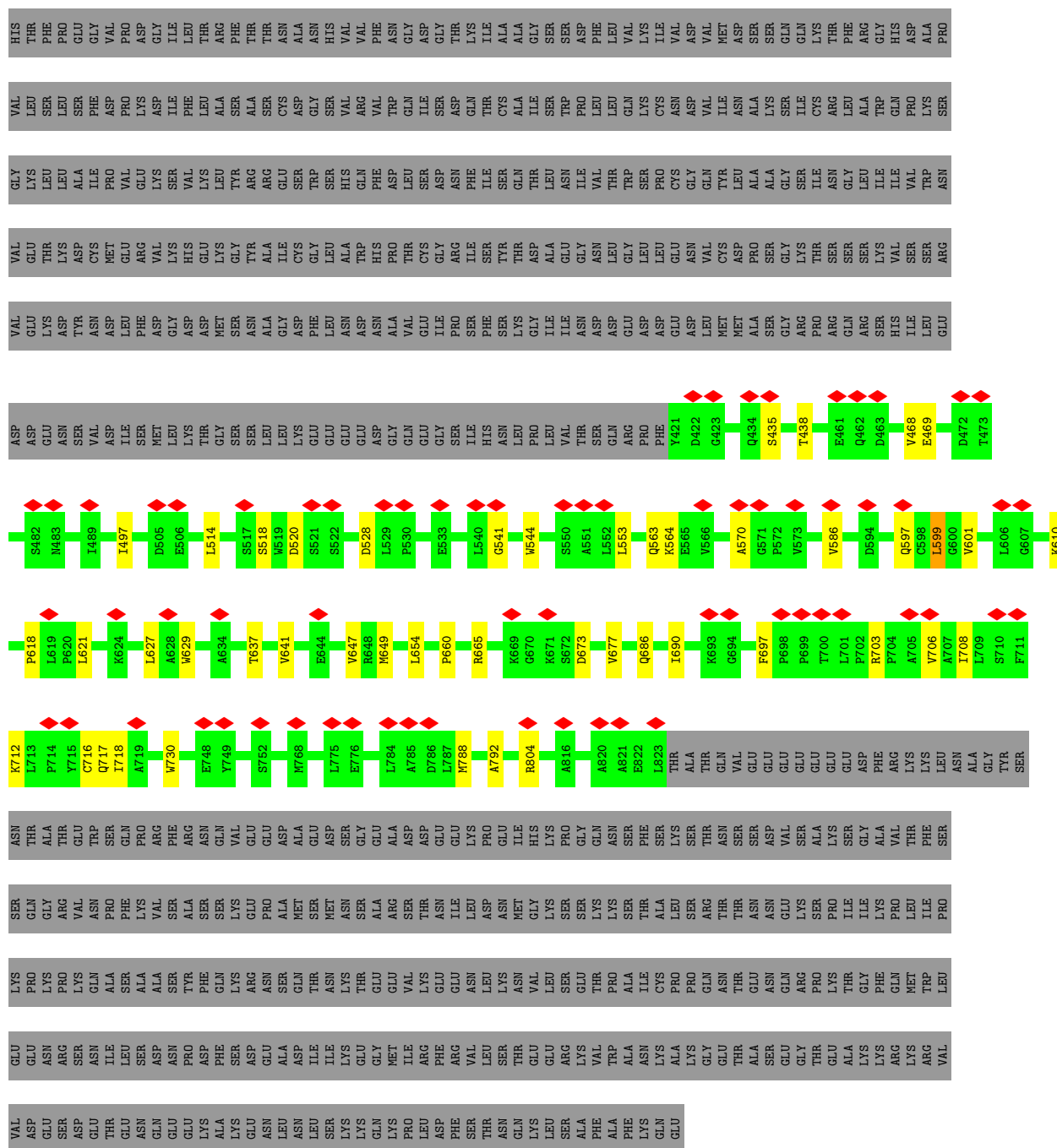


Response	Percentage
Yes	71%
No	23%
Don't know	5%

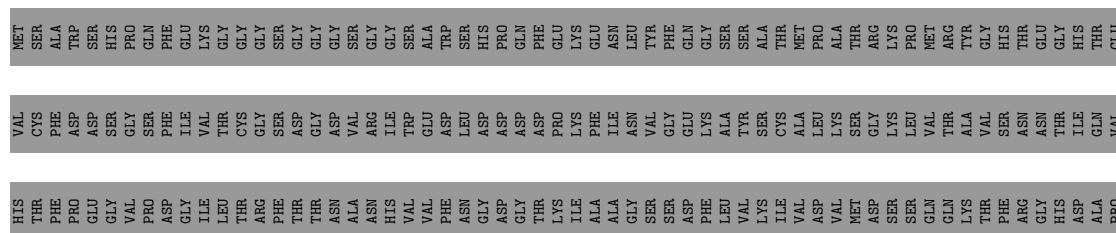


Response	Percentage
Yes	30%
No	66%





- Molecule 12: WD repeat and HMG-box DNA-binding protein 1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15393	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 ($e^-/\text{\AA}^2$)	54.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.639	Depositor
Minimum map value	-0.543	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	455.8, 455.8, 455.8	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	2	0.34	0/4923	0.44	0/6648
2	3	0.39	0/4859	0.47	0/6563
3	4	0.45	0/4870	0.50	1/6579 (0.0%)
4	5	0.40	0/4590	0.47	0/6171
5	6	0.43	0/4955	0.49	0/6685
6	7	0.43	0/4801	0.49	0/6482
7	A	0.37	0/1645	0.46	0/2210
8	B	0.44	0/1462	0.45	0/1981
9	C	0.41	0/1587	0.43	0/2143
10	D	0.41	0/1711	0.45	0/2305
11	E	0.39	0/4472	0.42	0/6037
12	F	0.09	0/3293	0.26	0/4462
12	G	0.09	0/3293	0.26	0/4462
12	H	0.09	0/3293	0.26	0/4462
All	All	0.37	0/49754	0.43	1/67190 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	458	ILE	N-CA-C	-5.10	105.89	113.39

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	4832	0	4839	252	0
2	3	4782	0	4826	155	0
3	4	4784	0	4825	141	0
4	5	4524	0	4608	219	0
5	6	4873	0	4901	156	0
6	7	4727	0	4758	122	0
7	A	1613	0	1606	84	0
8	B	1431	0	1456	101	0
9	C	1552	0	1504	45	0
10	D	1679	0	1700	33	0
11	E	4380	0	4331	239	0
12	F	3213	0	3168	30	0
12	G	3213	0	3168	94	0
12	H	3213	0	3168	31	0
13	2	1	0	0	0	0
13	4	1	0	0	0	0
13	5	1	0	0	0	0
13	6	1	0	0	0	0
13	7	1	0	0	0	0
All	All	48821	0	48858	1271	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 13.

All (1271) 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)
1:2:562:ARG:HH21	5:6:440:HIS:CD2	1.19	1.58
1:2:377:ARG:CG	1:2:565:VAL:HG22	1.33	1.57
8:B:59:ARG:CZ	12:G:703:ARG:HD2	1.20	1.57
1:2:377:ARG:CD	1:2:565:VAL:HG22	1.33	1.56
2:3:416:ARG:CG	4:5:456:VAL:HG11	1.31	1.55
1:2:511:HIS:CE1	4:5:342:SER:HB2	1.41	1.54
11:E:210:SER:HB2	12:G:473:THR:CG2	1.37	1.52
1:2:377:ARG:HG3	1:2:565:VAL:CG2	1.31	1.51
1:2:549:GLN:HG2	5:6:471:VAL:CG1	1.41	1.49
1:2:549:GLN:CG	5:6:471:VAL:HG11	1.43	1.46
3:4:521:GLN:NE2	6:7:464:GLN:HG2	1.29	1.45
11:E:254:HIS:CE1	12:G:458:TYR:CZ	1.79	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:549:GLN:CD	5:6:471:VAL:CG1	1.90	1.44
1:2:549:GLN:CG	5:6:471:VAL:CG1	1.93	1.42
8:B:59:ARG:CZ	12:G:703:ARG:CD	1.98	1.40
3:4:568:ASN:ND2	5:6:217:ARG:NH2	1.69	1.40
1:2:314:SER:HB3	1:2:563:HIS:NE2	1.33	1.38
11:E:254:HIS:HE1	12:G:458:TYR:CZ	1.03	1.37
5:6:357:THR:HA	5:6:551:ARG:NH1	1.05	1.36
11:E:255:ARG:O	12:G:701:LEU:CD1	1.72	1.35
1:2:549:GLN:CD	5:6:471:VAL:HG11	0.93	1.35
4:5:86:ASP:OD2	11:E:334:ILE:CG2	1.76	1.33
1:2:549:GLN:OE1	5:6:471:VAL:CG1	1.76	1.32
11:E:210:SER:CB	12:G:473:THR:CG2	2.06	1.31
1:2:580:ASP:HB3	4:5:238:HIS:NE2	1.43	1.31
11:E:255:ARG:O	12:G:701:LEU:HD11	1.16	1.31
8:B:111:ASP:OD1	11:E:265:VAL:N	1.61	1.30
1:2:276:ARG:NH2	11:E:318:MET:O	1.66	1.29
1:2:549:GLN:OE1	5:6:471:VAL:HG11	1.20	1.29
1:2:562:ARG:NH2	5:6:440:HIS:CD2	2.00	1.28
1:2:377:ARG:CG	1:2:565:VAL:CG2	1.94	1.28
5:6:357:THR:CA	5:6:551:ARG:NH1	1.99	1.26
8:B:59:ARG:NE	12:G:703:ARG:HD2	1.52	1.24
5:6:357:THR:CA	5:6:551:ARG:HH11	1.49	1.24
11:E:210:SER:CB	12:G:473:THR:HG23	1.67	1.23
2:3:416:ARG:HG2	4:5:456:VAL:CG1	1.68	1.22
2:3:487:LEU:CD2	6:7:241:SER:OG	1.88	1.20
1:2:765:ARG:NH2	4:5:385:THR:HG21	1.55	1.20
11:E:257:GLU:OE1	12:G:701:LEU:HD12	1.33	1.20
1:2:561:GLN:HE21	5:6:488:GLY:CA	1.54	1.20
8:B:59:ARG:NH1	12:G:703:ARG:CD	2.04	1.19
8:B:59:ARG:NH2	12:G:703:ARG:HB3	1.54	1.19
2:3:444:VAL:HG12	6:7:246:VAL:O	1.40	1.18
1:2:511:HIS:CE1	4:5:342:SER:CB	2.25	1.18
3:4:568:ASN:ND2	5:6:217:ARG:HH21	1.28	1.17
1:2:606:GLN:HE22	4:5:392:LYS:CE	1.57	1.17
1:2:561:GLN:CG	5:6:487:ALA:O	1.92	1.17
4:5:80:PHE:HD1	11:E:367:PHE:CE1	1.62	1.17
4:5:80:PHE:CD1	11:E:367:PHE:CE1	2.31	1.17
1:2:526:GLY:HA2	5:6:619:ARG:CZ	1.74	1.16
11:E:254:HIS:HE1	12:G:458:TYR:CE1	1.54	1.16
3:4:555:GLN:OE1	5:6:143:ARG:NH1	1.74	1.16
1:2:314:SER:CB	1:2:563:HIS:NE2	2.09	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:568:ASN:HD22	5:6:217:ARG:NH2	1.26	1.16
11:E:251:ARG:HD3	12:G:480:HIS:HB2	1.28	1.14
2:3:487:LEU:HD21	6:7:241:SER:OG	1.41	1.13
1:2:606:GLN:HE22	4:5:392:LYS:HE3	1.10	1.11
1:2:561:GLN:HG3	5:6:487:ALA:O	1.47	1.11
4:5:42:TYR:HA	11:E:367:PHE:CE2	1.84	1.11
1:2:377:ARG:HD3	1:2:565:VAL:HG22	1.29	1.11
1:2:561:GLN:HE21	5:6:488:GLY:HA2	1.10	1.10
4:5:86:ASP:OD2	11:E:334:ILE:HG22	1.36	1.09
4:5:56:ARG:NH2	8:B:119:ASP:OD1	1.85	1.09
8:B:40:LEU:HD21	12:G:688:ARG:CD	1.83	1.09
2:3:416:ARG:CB	4:5:456:VAL:HG11	1.82	1.08
8:B:59:ARG:NH1	12:G:703:ARG:HD3	1.61	1.08
2:3:416:ARG:CG	4:5:456:VAL:CG1	2.28	1.07
1:2:562:ARG:NH2	5:6:440:HIS:NE2	2.02	1.07
11:E:210:SER:HB2	12:G:473:THR:HG21	1.10	1.07
3:4:521:GLN:NE2	6:7:464:GLN:CG	2.18	1.06
4:5:43:ARG:HH21	11:E:266:ASP:CG	1.63	1.06
4:5:86:ASP:OD2	11:E:334:ILE:HG21	1.56	1.05
4:5:86:ASP:CG	11:E:334:ILE:HG22	1.80	1.05
8:B:40:LEU:HD11	12:G:688:ARG:CZ	1.87	1.05
11:E:259:GLU:OE2	12:G:701:LEU:C	1.98	1.05
1:2:377:ARG:HG3	1:2:565:VAL:HG21	1.06	1.04
1:2:271:TYR:OH	11:E:313:GLU:OE1	1.75	1.03
4:5:86:ASP:CG	11:E:334:ILE:CG2	2.32	1.03
1:2:564:PRO:HA	5:6:441:GLU:CD	1.80	1.02
1:2:377:ARG:CD	1:2:565:VAL:CG2	2.27	1.01
2:3:462:MET:O	6:7:407:ARG:NH1	1.94	1.00
1:2:271:TYR:CE1	11:E:313:GLU:OE1	2.14	1.00
8:B:111:ASP:OD2	11:E:264:SER:OG	1.80	0.99
3:4:521:GLN:HE21	6:7:464:GLN:HG2	1.23	0.99
1:2:562:ARG:HH21	5:6:440:HIS:HD2	1.07	0.99
1:2:549:GLN:HG2	5:6:471:VAL:HG12	1.01	0.98
2:3:439:GLU:OE1	4:5:472:ALA:O	1.82	0.98
8:B:59:ARG:NH2	12:G:703:ARG:CB	2.28	0.97
2:3:465:THR:CG2	6:7:407:ARG:HG2	1.94	0.96
11:E:254:HIS:CE1	12:G:458:TYR:CE1	2.14	0.96
1:2:511:HIS:HE1	4:5:342:SER:HB2	1.29	0.96
8:B:40:LEU:HD11	12:G:688:ARG:NH2	1.81	0.95
4:5:43:ARG:NE	11:E:266:ASP:OD1	1.98	0.95
1:2:549:GLN:OE1	5:6:471:VAL:CG2	2.15	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:42:TYR:HE1	11:E:367:PHE:HB3	1.29	0.94
1:2:561:GLN:HG2	5:6:487:ALA:O	1.68	0.94
11:E:259:GLU:OE2	12:G:701:LEU:CB	2.17	0.93
2:3:416:ARG:HG2	4:5:456:VAL:HG11	0.93	0.93
8:B:56:GLN:OE1	11:E:211:LYS:O	1.87	0.93
11:E:257:GLU:OE1	12:G:701:LEU:CD1	2.17	0.92
4:5:46:THR:HG21	11:E:406:ARG:O	1.69	0.92
1:2:765:ARG:HH21	4:5:385:THR:HG21	1.26	0.91
4:5:40:ARG:NH2	8:B:119:ASP:OD2	2.03	0.91
1:2:561:GLN:NE2	5:6:488:GLY:HA2	1.85	0.91
1:2:606:GLN:NE2	4:5:392:LYS:CE	2.34	0.91
1:2:511:HIS:NE2	4:5:342:SER:HB2	1.86	0.90
8:B:111:ASP:OD1	11:E:264:SER:HA	1.70	0.90
1:2:561:GLN:NE2	5:6:488:GLY:CA	2.34	0.90
1:2:271:TYR:CZ	11:E:313:GLU:OE1	2.24	0.90
8:B:59:ARG:HH21	12:G:703:ARG:HB3	1.31	0.90
8:B:111:ASP:OD1	11:E:264:SER:CA	2.19	0.90
1:2:549:GLN:HB3	5:6:475:GLU:OE2	1.73	0.89
3:4:568:ASN:HD22	5:6:217:ARG:CZ	1.85	0.89
7:A:166:SER:O	11:E:68:GLN:HG2	1.72	0.89
11:E:207:TRP:CZ2	12:G:478:ALA:O	2.25	0.88
11:E:259:GLU:OE2	12:G:701:LEU:HB3	1.72	0.88
1:2:549:GLN:OE1	5:6:471:VAL:HG21	1.71	0.88
8:B:111:ASP:OD1	11:E:264:SER:C	2.16	0.88
1:2:606:GLN:NE2	4:5:392:LYS:HE3	1.88	0.87
2:3:487:LEU:HD23	6:7:241:SER:OG	1.72	0.87
1:2:526:GLY:CA	5:6:619:ARG:CZ	2.51	0.87
3:4:555:GLN:HE22	5:6:143:ARG:HH22	1.23	0.87
4:5:42:TYR:CE1	11:E:367:PHE:CB	2.58	0.87
5:6:356:PRO:O	5:6:551:ARG:NH1	2.07	0.86
11:E:255:ARG:O	12:G:701:LEU:HD13	1.73	0.86
3:4:521:GLN:HE21	6:7:464:GLN:CG	1.81	0.85
2:3:534:MET:HE3	4:5:594:ARG:HG2	1.58	0.85
2:3:444:VAL:CG1	6:7:246:VAL:O	2.24	0.85
8:B:110:ALA:HB3	11:E:264:SER:HB2	1.59	0.85
3:4:568:ASN:ND2	5:6:217:ARG:CZ	2.40	0.85
1:2:606:GLN:HE22	4:5:392:LYS:NZ	1.74	0.85
4:5:80:PHE:CE1	11:E:367:PHE:CE1	2.65	0.85
3:4:521:GLN:HE22	6:7:464:GLN:HG2	1.32	0.84
1:2:314:SER:HB3	1:2:563:HIS:CD2	2.14	0.83
1:2:606:GLN:NE2	4:5:392:LYS:NZ	2.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:42:TYR:CE1	11:E:367:PHE:HB3	2.13	0.83
4:5:42:TYR:CD1	11:E:367:PHE:CD2	2.65	0.83
8:B:56:GLN:OE1	11:E:211:LYS:C	2.21	0.82
1:2:656:ARG:NH2	4:5:385:THR:OG1	2.13	0.81
1:2:765:ARG:HH22	4:5:385:THR:HG21	1.43	0.81
3:4:555:GLN:NE2	5:6:143:ARG:HH22	1.78	0.81
4:5:42:TYR:HE1	11:E:367:PHE:CB	1.92	0.81
1:2:377:ARG:CG	1:2:565:VAL:HG21	1.88	0.81
4:5:43:ARG:NH2	11:E:266:ASP:CG	2.39	0.81
1:2:564:PRO:HA	5:6:441:GLU:OE2	1.80	0.80
8:B:59:ARG:NH1	12:G:703:ARG:HD2	1.80	0.80
4:5:42:TYR:HA	11:E:367:PHE:HE2	1.46	0.80
3:4:512:PRO:HB2	6:7:600:TYR:CE2	2.17	0.80
11:E:207:TRP:HZ2	12:G:478:ALA:O	1.63	0.79
2:3:416:ARG:HG3	4:5:456:VAL:HG11	1.59	0.79
2:3:416:ARG:CB	4:5:456:VAL:CG1	2.56	0.79
5:6:159:LEU:HB3	5:6:187:ASN:HD21	1.48	0.79
8:B:129:ARG:NH2	9:C:151:ASP:OD2	2.16	0.79
9:C:34:VAL:HG12	9:C:86:VAL:HG12	1.65	0.79
5:6:356:PRO:C	5:6:551:ARG:HH12	1.91	0.79
8:B:109:LYS:HG3	11:E:262:THR:HB	1.63	0.78
7:A:98:LEU:H	7:A:103:ARG:HH21	1.31	0.78
1:2:561:GLN:HE21	5:6:488:GLY:HA3	1.45	0.78
1:2:765:ARG:HH21	4:5:385:THR:CG2	1.96	0.78
8:B:40:LEU:HD21	12:G:688:ARG:HD3	1.65	0.78
1:2:271:TYR:HE1	11:E:313:GLU:OE1	1.63	0.78
3:4:731:PRO:HD2	5:6:399:SER:OG	1.84	0.77
12:F:716:CYS:H	12:G:563:GLN:HE22	1.31	0.77
1:2:562:ARG:CZ	5:6:440:HIS:NE2	2.48	0.77
11:E:210:SER:HB2	12:G:473:THR:HG22	1.59	0.77
1:2:549:GLN:OE1	5:6:471:VAL:CB	2.31	0.77
3:4:521:GLN:HE21	6:7:464:GLN:CD	1.92	0.77
1:2:224:LYS:O	11:E:312:GLN:HB3	1.84	0.77
11:E:389:LYS:HZ1	11:E:462:ARG:HD2	1.50	0.77
12:F:563:GLN:HE22	12:H:716:CYS:H	1.31	0.77
12:G:716:CYS:H	12:H:563:GLN:HE22	1.31	0.77
2:3:4:ARG:NH1	9:C:107:VAL:HA	2.00	0.77
11:E:210:SER:OG	12:G:473:THR:HG23	1.85	0.76
11:E:257:GLU:HB2	12:G:458:TYR:HE1	1.49	0.76
1:2:561:GLN:HE22	1:2:564:PRO:HD3	1.49	0.76
3:4:161:ALA:O	3:4:165:ASN:ND2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:59:ARG:NH2	12:G:703:ARG:CG	2.49	0.76
8:B:111:ASP:CG	11:E:264:SER:HG	1.93	0.76
3:4:469:SER:HB3	6:7:369:MET:SD	2.25	0.75
1:2:377:ARG:HD2	1:2:565:VAL:HG22	1.65	0.75
3:4:555:GLN:CD	5:6:143:ARG:HH12	1.94	0.75
4:5:43:ARG:NH2	11:E:266:ASP:OD1	2.20	0.75
4:5:80:PHE:CE1	11:E:367:PHE:CZ	2.75	0.75
1:2:377:ARG:CB	1:2:565:VAL:CG2	2.65	0.74
2:3:100:ARG:NH2	2:3:150:SER:O	2.20	0.74
1:2:667:VAL:HG12	5:6:602:ARG:HH21	1.51	0.74
8:B:59:ARG:CZ	12:G:703:ARG:CG	2.65	0.74
7:A:170:LYS:NZ	11:E:64:GLU:OE2	2.16	0.74
8:B:40:LEU:HD11	12:G:688:ARG:NE	2.02	0.74
4:5:80:PHE:HD1	11:E:367:PHE:CD1	2.05	0.74
3:4:191:PRO:HB2	3:4:194:MET:HB2	1.70	0.73
8:B:7:GLU:OE1	9:C:189:TRP:NE1	2.21	0.73
11:E:257:GLU:CD	12:G:701:LEU:HD12	2.14	0.73
2:3:658:VAL:HG23	2:3:662:THR:HG21	1.71	0.73
2:3:416:ARG:HB3	4:5:456:VAL:CG1	2.18	0.73
11:E:99:ASP:OD1	11:E:100:THR:N	2.22	0.73
1:2:580:ASP:CB	4:5:238:HIS:NE2	2.39	0.72
8:B:109:LYS:CG	11:E:262:THR:HB	2.18	0.72
1:2:377:ARG:HG3	1:2:565:VAL:CB	2.16	0.72
1:2:561:GLN:NE2	5:6:488:GLY:HA3	2.02	0.72
7:A:179:ARG:NH2	7:A:183:GLU:OE2	2.23	0.72
5:6:187:ASN:ND2	5:6:190:ARG:O	2.23	0.72
8:B:40:LEU:HD21	12:G:688:ARG:NE	2.04	0.72
7:A:195:LEU:HD22	11:E:41:GLN:HE22	1.55	0.72
1:2:526:GLY:HA2	5:6:619:ARG:NH2	2.05	0.71
8:B:59:ARG:NH2	12:G:703:ARG:HD2	2.01	0.71
4:5:537:ILE:HA	4:5:540:HIS:HB3	1.71	0.71
5:6:27:GLN:HG3	5:6:93:ALA:HB2	1.73	0.71
5:6:307:ASN:O	5:6:309:ARG:NH1	2.23	0.71
5:6:54:ILE:HD11	5:6:103:GLU:HB2	1.71	0.71
2:3:347:SER:HG	2:3:608:VAL:N	1.88	0.71
11:E:210:SER:CB	12:G:473:THR:HG21	1.97	0.71
11:E:257:GLU:HB2	12:G:458:TYR:CE1	2.25	0.70
7:A:176:PHE:CE1	11:E:41:GLN:HG2	2.25	0.70
8:B:111:ASP:CG	11:E:264:SER:OG	2.34	0.70
4:5:43:ARG:CZ	11:E:266:ASP:OD1	2.40	0.70
5:6:310:PHE:CZ	5:6:574:ARG:HG2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:230:GLU:OE1	6:7:72:ARG:NH2	2.25	0.70
8:B:136:VAL:HG13	8:B:167:MET:HE1	1.74	0.70
4:5:79:SER:OG	11:E:368:LYS:HB3	1.91	0.69
11:E:287:HIS:HB2	11:E:325:VAL:HG12	1.73	0.69
3:4:568:ASN:HD22	5:6:217:ARG:HH21	0.75	0.69
7:A:147:TYR:HE2	11:E:46:GLN:HG2	1.56	0.69
1:2:818:PHE:HA	1:2:821:TYR:HB3	1.75	0.69
7:A:151:ARG:CZ	11:E:398:ILE:HG23	2.23	0.69
11:E:210:SER:HB3	12:G:473:THR:HG23	1.70	0.69
1:2:377:ARG:CB	1:2:565:VAL:HG22	2.19	0.69
2:3:4:ARG:NH1	9:C:106:VAL:O	2.26	0.69
8:B:40:LEU:CD2	12:G:688:ARG:HD3	2.22	0.69
1:2:325:VAL:HA	1:2:368:THR:HG23	1.74	0.68
1:2:754:SER:HB2	1:2:761:PRO:HB3	1.75	0.68
11:E:263:LEU:HD23	11:E:269:ARG:HH21	1.57	0.68
1:2:580:ASP:HB3	4:5:238:HIS:CD2	2.28	0.68
2:3:534:MET:CE	4:5:594:ARG:HG2	2.24	0.68
1:2:224:LYS:HB3	11:E:312:GLN:HB2	1.75	0.68
11:E:257:GLU:CB	12:G:458:TYR:HE1	2.06	0.68
3:4:219:ASP:OD1	3:4:220:LYS:N	2.26	0.68
1:2:593:ASN:ND2	1:2:596:ASP:OD2	2.27	0.68
5:6:390:ILE:O	5:6:498:SER:OG	2.12	0.68
3:4:335:HIS:O	3:4:335:HIS:ND1	2.27	0.68
2:3:416:ARG:HG2	4:5:456:VAL:CB	2.24	0.68
3:4:546:TYR:CE2	6:7:472:ALA:HB1	2.29	0.68
1:2:526:GLY:HA2	5:6:619:ARG:NE	2.09	0.67
4:5:47:ASP:HB2	11:E:406:ARG:HH22	1.58	0.67
11:E:251:ARG:HD3	12:G:480:HIS:CB	2.18	0.67
7:A:176:PHE:HB2	11:E:47:TYR:CE1	2.30	0.67
8:B:40:LEU:CD2	12:G:688:ARG:CD	2.68	0.67
2:3:444:VAL:O	6:7:246:VAL:HB	1.95	0.67
4:5:42:TYR:OH	11:E:368:LYS:NZ	2.25	0.67
1:2:507:PRO:HD3	1:2:513:VAL:HG12	1.77	0.67
4:5:80:PHE:CD1	11:E:367:PHE:CZ	2.83	0.67
1:2:549:GLN:CG	5:6:471:VAL:HG12	1.84	0.67
3:4:388:VAL:HG12	3:4:423:LYS:HG2	1.76	0.67
5:6:20:ASP:OD1	5:6:85:ARG:NH2	2.28	0.67
2:3:70:ASP:OD2	2:3:77:TYR:N	2.26	0.67
4:5:79:SER:CB	11:E:368:LYS:HB3	2.24	0.67
1:2:757:THR:HG22	1:2:758:GLY:H	1.60	0.66
2:3:645:GLN:OE1	2:3:654:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:447:TYR:OH	11:E:554:ARG:NH2	2.28	0.66
7:A:144:LYS:NZ	8:B:11:GLU:OE2	2.28	0.66
1:2:204:ARG:O	1:2:213:ASN:ND2	2.28	0.66
3:4:726:MET:HG3	3:4:727:VAL:H	1.59	0.66
7:A:149:GLU:OE2	7:A:174:GLN:NE2	2.28	0.66
8:B:56:GLN:OE1	11:E:211:LYS:HB3	1.96	0.66
1:2:328:ASN:HD22	1:2:364:ASN:HB2	1.60	0.66
10:D:202:SER:HG	10:D:204:HIS:HE2	1.43	0.66
2:3:91:ARG:NH2	2:3:268:ASP:OD1	2.28	0.66
1:2:198:ARG:NH2	1:2:241:GLU:OE2	2.29	0.66
2:3:465:THR:HG22	6:7:407:ARG:HG2	1.76	0.66
1:2:301:HIS:HB3	1:2:306:ILE:HD11	1.77	0.66
4:5:132:ALA:HA	11:E:328:LYS:HD2	1.78	0.66
8:B:23:LEU:HB3	8:B:36:PHE:HD2	1.61	0.66
7:A:74:ARG:NH2	9:C:18:ASN:O	2.29	0.66
1:2:365:MET:HB2	4:5:273:LYS:HZ1	1.59	0.65
2:3:465:THR:HG21	6:7:407:ARG:HG2	1.76	0.65
3:4:400:ARG:HG2	3:4:408:VAL:HG12	1.76	0.65
4:5:86:ASP:CG	11:E:334:ILE:HG21	2.13	0.65
10:D:71:GLU:OE1	10:D:73:LEU:N	2.25	0.65
2:3:151:PHE:H	2:3:155:HIS:HE1	1.43	0.65
4:5:441:VAL:HG22	4:5:483:SER:HB2	1.78	0.65
10:D:22:THR:HG22	10:D:24:ALA:H	1.60	0.65
11:E:257:GLU:CB	12:G:458:TYR:CE1	2.80	0.65
3:4:246:PHE:HA	3:4:249:TYR:CD2	2.32	0.65
5:6:310:PHE:HZ	5:6:574:ARG:HG2	1.61	0.65
1:2:564:PRO:CA	5:6:441:GLU:CD	2.62	0.65
11:E:323:LYS:HG3	11:E:324:GLN:HE21	1.61	0.65
11:E:448:CYS:SG	11:E:449:SER:N	2.70	0.65
1:2:514:ARG:O	1:2:772:ARG:NH1	2.30	0.65
1:2:733:PRO:HA	1:2:784:ASP:HB3	1.79	0.65
3:4:568:ASN:HD21	5:6:217:ARG:NH2	1.89	0.65
5:6:558:ARG:HB3	5:6:561:GLU:HB2	1.79	0.65
2:3:544:ASP:OD2	2:3:548:ARG:NH2	2.31	0.64
4:5:416:ALA:HA	4:5:430:GLU:O	1.97	0.64
2:3:152:GLY:HA3	9:C:103:ASP:HB2	1.77	0.64
8:B:51:ASN:ND2	10:D:80:MET:SD	2.70	0.64
2:3:381:ARG:NH2	2:3:385:ASN:OD1	2.28	0.64
7:A:175:HIS:HA	11:E:48:THR:HA	1.78	0.64
4:5:115:PRO:HA	8:B:130:VAL:HG22	1.79	0.64
4:5:167:ARG:HH11	4:5:181:ASN:HA	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:436:ASP:O	5:6:440:HIS:N	2.31	0.64
11:E:28:ASP:OD1	11:E:197:SER:OG	2.15	0.64
2:3:61:GLN:HG3	2:3:124:ALA:HB2	1.79	0.64
4:5:47:ASP:CB	11:E:406:ARG:HH22	2.11	0.64
4:5:42:TYR:OH	11:E:368:LYS:HG2	1.97	0.64
4:5:53:PHE:HZ	8:B:114:ARG:HG2	1.62	0.64
6:7:416:ALA:HB3	6:7:469:ILE:HD11	1.80	0.64
4:5:421:ASP:HB3	4:5:424:SER:OG	1.98	0.64
9:C:35:ARG:NH1	9:C:37:GLU:OE2	2.30	0.64
3:4:471:TYR:HD2	3:4:658:TYR:HE1	1.46	0.63
3:4:555:GLN:OE1	5:6:143:ARG:CZ	2.44	0.63
12:G:654:LEU:HD12	12:H:610:LYS:HG2	1.80	0.63
5:6:380:THR:HG1	5:6:384:THR:HG1	1.43	0.63
7:A:176:PHE:HB3	11:E:47:TYR:H	1.63	0.63
1:2:377:ARG:HG3	1:2:565:VAL:CG1	2.27	0.63
1:2:485:ILE:HD11	1:2:531:GLN:HB2	1.80	0.63
11:E:259:GLU:OE2	12:G:701:LEU:O	2.16	0.63
3:4:425:ASP:HB3	3:4:428:ARG:HG3	1.81	0.63
7:A:175:HIS:ND1	11:E:48:THR:HG23	2.14	0.63
8:B:55:ARG:HH21	11:E:43:ASP:HA	1.63	0.63
12:F:654:LEU:HD12	12:G:610:LYS:HG2	1.80	0.63
8:B:175:GLN:HB2	10:D:188:THR:HG21	1.80	0.63
4:5:80:PHE:HE1	11:E:367:PHE:CZ	2.16	0.63
4:5:42:TYR:CE1	11:E:367:PHE:HB2	2.33	0.62
5:6:187:ASN:HB2	5:6:190:ARG:HB2	1.80	0.62
7:A:111:MET:O	7:A:115:ASN:ND2	2.29	0.62
7:A:174:GLN:HG3	11:E:49:LEU:HB3	1.80	0.62
10:D:21:LEU:HD21	10:D:29:ARG:HH12	1.63	0.62
3:4:365:GLN:NE2	6:7:266:GLN:OE1	2.33	0.62
2:3:162:THR:OG1	2:3:164:CYS:SG	2.54	0.62
12:F:610:LYS:HG2	12:H:654:LEU:HD12	1.80	0.62
1:2:500:PHE:O	1:2:728:LYS:NZ	2.33	0.62
2:3:416:ARG:HG2	4:5:456:VAL:CG2	2.29	0.62
12:G:518:SER:OG	12:G:520:ASP:OD1	2.17	0.62
1:2:567:ARG:HD2	5:6:440:HIS:HD2	1.64	0.62
1:2:377:ARG:HD3	1:2:565:VAL:CG2	2.15	0.62
5:6:594:ILE:HD13	5:6:625:ILE:HG22	1.82	0.62
2:3:416:ARG:HG2	4:5:456:VAL:HG21	1.81	0.62
1:2:489:GLU:HA	1:2:492:LYS:HD2	1.81	0.62
9:C:7:ARG:NH2	9:C:23:ASP:OD2	2.33	0.62
1:2:667:VAL:HG12	5:6:602:ARG:NH2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:40:LEU:HD21	12:G:688:ARG:HD2	1.75	0.62
4:5:42:TYR:CD1	11:E:367:PHE:CG	2.87	0.61
4:5:65:LEU:HD11	9:C:155:ASN:O	1.99	0.61
4:5:347:THR:O	4:5:351:LYS:N	2.32	0.61
1:2:314:SER:HB2	1:2:565:VAL:CG2	2.30	0.61
2:3:115:PHE:CZ	2:3:287:ARG:HD3	2.35	0.61
12:F:518:SER:OG	12:F:520:ASP:OD1	2.17	0.61
3:4:402:ASN:HB2	3:4:405:VAL:HG22	1.83	0.61
1:2:683:HIS:CE1	5:6:386:LEU:HD13	2.35	0.61
1:2:742:LYS:HD2	1:2:788:GLU:HG3	1.82	0.61
1:2:314:SER:CB	1:2:563:HIS:CD2	2.79	0.61
3:4:719:LYS:HE2	5:6:542:GLU:OE2	2.01	0.61
6:7:56:ALA:HB2	6:7:63:VAL:HG21	1.82	0.61
6:7:520:LEU:HD23	6:7:644:LEU:HD11	1.82	0.61
3:4:469:SER:CB	6:7:369:MET:SD	2.88	0.60
6:7:222:LEU:HD12	6:7:223:GLN:H	1.66	0.60
12:H:518:SER:OG	12:H:520:ASP:OD1	2.17	0.60
7:A:174:GLN:O	11:E:49:LEU:N	2.32	0.60
5:6:124:ARG:NH2	5:6:210:GLU:OE2	2.34	0.60
6:7:171:SER:OG	6:7:172:GLU:N	2.35	0.60
2:3:440:ALA:CB	6:7:247:GLY:HA2	2.30	0.60
4:5:43:ARG:HD3	8:B:114:ARG:HD3	1.84	0.60
4:5:174:SER:OG	4:5:207:CYS:SG	2.60	0.60
4:5:231:GLU:OE2	4:5:243:ARG:N	2.28	0.60
5:6:109:ASP:OD1	5:6:109:ASP:N	2.34	0.60
6:7:52:LEU:HD12	6:7:141:PRO:HD3	1.84	0.60
1:2:355:CYS:SG	1:2:357:SER:OG	2.59	0.60
3:4:306:CYS:SG	3:4:308:VAL:N	2.67	0.60
5:6:159:LEU:HB3	5:6:187:ASN:ND2	2.16	0.60
2:3:465:THR:CB	6:7:407:ARG:HG2	2.30	0.60
3:4:718:ARG:NH1	3:4:729:ALA:O	2.31	0.60
11:E:210:SER:OG	12:G:473:THR:CG2	2.45	0.60
1:2:314:SER:HB2	1:2:565:VAL:HG23	1.84	0.59
1:2:329:CYS:HB3	1:2:332:CYS:SG	2.41	0.59
1:2:562:ARG:NH2	5:6:440:HIS:HD2	1.73	0.59
4:5:80:PHE:CD1	11:E:367:PHE:HE1	2.16	0.59
5:6:52:GLU:OE2	5:6:55:ARG:NH1	2.35	0.59
1:2:549:GLN:OE1	5:6:471:VAL:HG13	1.93	0.59
1:2:563:HIS:HD2	1:2:565:VAL:H	1.49	0.59
8:B:56:GLN:OE1	11:E:211:LYS:CA	2.50	0.59
2:3:212:ALA:HB2	2:3:287:ARG:HH22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:528:ARG:O	4:5:532:LEU:HG	2.02	0.59
6:7:374:ASN:HB3	6:7:483:SER:HB3	1.84	0.59
11:E:259:GLU:CD	12:G:701:LEU:HB3	2.26	0.59
1:2:343:GLN:HA	4:5:287:VAL:HG11	1.84	0.59
2:3:6:PRO:HD2	2:3:149:GLY:O	2.02	0.59
5:6:611:LYS:NZ	5:6:612:SER:O	2.35	0.59
7:A:43:ASN:O	7:A:47:VAL:HG23	2.02	0.59
12:G:641:VAL:HG21	12:G:677:VAL:HG21	1.84	0.59
2:3:663:LEU:HD23	6:7:537:ILE:HD12	1.83	0.59
7:A:135:ASP:OD2	7:A:138:GLN:NE2	2.32	0.59
12:H:641:VAL:HG21	12:H:677:VAL:HG21	1.84	0.59
2:3:173:GLU:HG3	2:3:281:GLN:HG2	1.83	0.59
4:5:42:TYR:HD1	11:E:367:PHE:CD2	2.20	0.59
1:2:477:ILE:O	1:2:480:SER:OG	2.19	0.59
1:2:514:ARG:NH2	1:2:516:ASP:O	2.36	0.59
2:3:173:GLU:N	2:3:173:GLU:OE1	2.36	0.59
2:3:447:ASP:HB3	6:7:246:VAL:CG1	2.33	0.59
3:4:476:ILE:CD1	3:4:650:LEU:HD11	2.32	0.59
2:3:344:LEU:HD11	2:3:616:TYR:HE2	1.67	0.59
3:4:247:ASP:HB2	3:4:248:ARG:HD2	1.85	0.59
2:3:141:GLU:OE1	2:3:237:VAL:HG11	2.03	0.59
4:5:51:PHE:CE1	11:E:266:ASP:HB3	2.38	0.59
4:5:507:MET:HB2	4:5:510:ILE:HG22	1.83	0.59
6:7:403:TYR:OH	6:7:445:ASP:OD2	2.19	0.59
1:2:384:LYS:HG2	1:2:385:VAL:HG23	1.85	0.58
4:5:42:TYR:HA	11:E:367:PHE:CD2	2.37	0.58
11:E:257:GLU:HG2	11:E:258:ASP:N	2.18	0.58
1:2:463:MET:O	1:2:467:LEU:HG	2.03	0.58
1:2:762:ILE:HG23	1:2:766:HIS:HB2	1.85	0.58
6:7:324:LEU:HA	6:7:327:ILE:HG22	1.84	0.58
9:C:106:VAL:O	9:C:167:ARG:NH2	2.36	0.58
2:3:447:ASP:CB	6:7:246:VAL:HG12	2.34	0.58
5:6:598:TYR:HB2	5:6:621:LEU:HD13	1.84	0.58
9:C:204:GLN:N	9:C:204:GLN:OE1	2.36	0.58
10:D:175:VAL:HG12	10:D:220:VAL:HG12	1.83	0.58
12:F:641:VAL:HG21	12:F:677:VAL:HG21	1.84	0.58
1:2:276:ARG:HH21	11:E:318:MET:C	2.03	0.58
1:2:377:ARG:HD2	1:2:565:VAL:HA	1.85	0.58
6:7:311:ASP:O	6:7:313:GLU:HG2	2.04	0.58
1:2:580:ASP:OD2	4:5:238:HIS:CD2	2.57	0.58
4:5:47:ASP:HB2	11:E:406:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:29:ARG:HE	10:D:50:ILE:HD11	1.68	0.58
1:2:314:SER:CB	1:2:565:VAL:HG23	2.34	0.58
2:3:440:ALA:CB	6:7:247:GLY:CA	2.82	0.58
3:4:566:SER:OG	3:4:567:ASP:N	2.35	0.58
1:2:377:ARG:NH2	1:2:393:SER:OG	2.37	0.57
3:4:278:ASP:HB3	3:4:283:ILE:HD11	1.85	0.57
11:E:536:ARG:HE	11:E:550:LYS:HE2	1.69	0.57
1:2:315:CYS:HB2	1:2:374:GLN:HE21	1.69	0.57
1:2:731:VAL:O	1:2:732:HIS:ND1	2.36	0.57
3:4:428:ARG:HH11	3:4:428:ARG:HB3	1.69	0.57
3:4:546:TYR:CE2	6:7:472:ALA:CB	2.87	0.57
6:7:567:ARG:O	6:7:618:ARG:NH1	2.37	0.57
8:B:57:LYS:NZ	11:E:211:LYS:NZ	2.53	0.57
1:2:763:THR:HG22	1:2:764:VAL:H	1.69	0.57
4:5:439:GLY:N	4:5:481:ARG:O	2.37	0.57
11:E:385:GLU:OE1	11:E:462:ARG:NE	2.37	0.57
4:5:60:LYS:NZ	8:B:122:ASP:OD2	2.23	0.57
1:2:517:ILE:O	1:2:625:THR:OG1	2.21	0.57
6:7:178:VAL:HG12	6:7:179:VAL:HG23	1.87	0.57
10:D:37:GLU:HG3	10:D:92:TYR:HE1	1.70	0.57
1:2:224:LYS:HB3	11:E:312:GLN:CB	2.35	0.57
2:3:447:ASP:HB3	6:7:246:VAL:HG12	1.87	0.57
3:4:555:GLN:HE22	5:6:143:ARG:NH2	1.98	0.57
8:B:78:GLU:OE1	8:B:85:THR:OG1	2.22	0.56
2:3:527:LEU:HD23	2:3:655:THR:HB	1.87	0.56
7:A:168:LEU:CD2	11:E:64:GLU:HB3	2.35	0.56
8:B:2:ASP:N	8:B:2:ASP:OD1	2.35	0.56
1:2:656:ARG:HH22	4:5:385:THR:HG1	1.50	0.56
2:3:385:ASN:HD22	2:3:493:VAL:H	1.54	0.56
2:3:509:THR:HG23	2:3:511:MET:H	1.71	0.56
2:3:616:TYR:OH	2:3:676:ALA:O	2.21	0.56
7:A:194:ILE:HG13	7:A:195:LEU:H	1.70	0.56
9:C:168:LEU:O	9:C:173:ARG:NH1	2.38	0.56
9:C:169:ASP:OD1	9:C:169:ASP:N	2.37	0.56
10:D:123:SER:HB3	10:D:126:GLU:HG3	1.88	0.56
12:F:637:THR:HG21	12:F:649:MET:HE3	1.87	0.56
4:5:325:LEU:HA	4:5:328:LEU:HD23	1.86	0.56
6:7:459:HIS:O	6:7:514:ARG:NH1	2.32	0.56
11:E:207:TRP:CE2	12:G:478:ALA:O	2.58	0.56
1:2:325:VAL:HG11	1:2:347:VAL:HG11	1.88	0.56
1:2:377:ARG:HD2	1:2:565:VAL:HG13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:562:ARG:NE	5:6:440:HIS:NE2	2.53	0.56
2:3:73:ASP:OD1	2:3:74:GLN:N	2.37	0.56
6:7:40:LEU:HD23	6:7:45:GLN:HB3	1.87	0.56
4:5:586:TYR:CZ	4:5:590:ARG:HD2	2.40	0.56
2:3:393:SER:CB	4:5:609:THR:HB	2.36	0.56
2:3:465:THR:HB	6:7:407:ARG:HG2	1.88	0.56
3:4:199:GLU:HA	3:4:202:VAL:HG12	1.88	0.56
4:5:172:CYS:HB3	4:5:177:ASN:H	1.70	0.56
4:5:377:LEU:HB2	4:5:485:LEU:HD12	1.87	0.56
5:6:329:MET:HE1	5:6:337:VAL:HG21	1.88	0.56
7:A:162:ASP:OD2	7:A:181:LYS:NZ	2.39	0.56
8:B:55:ARG:O	11:E:42:CYS:SG	2.63	0.56
2:3:409:ARG:NH2	2:3:447:ASP:O	2.24	0.56
6:7:169:ARG:HH11	6:7:236:LYS:HD3	1.71	0.56
11:E:282:GLN:O	11:E:330:GLN:NE2	2.39	0.56
1:2:765:ARG:HG3	1:2:765:ARG:O	2.06	0.55
6:7:363:ASP:OD1	6:7:363:ASP:N	2.37	0.55
8:B:110:ALA:HB3	11:E:264:SER:CB	2.34	0.55
3:4:533:THR:HG22	3:4:534:SER:H	1.70	0.55
4:5:170:ILE:HG22	4:5:214:ILE:HD13	1.87	0.55
11:E:259:GLU:OE2	12:G:701:LEU:CA	2.53	0.55
2:3:662:THR:O	2:3:665:THR:HG22	2.06	0.55
3:4:390:VAL:HG23	3:4:418:VAL:HG23	1.87	0.55
3:4:654:GLN:HG3	6:7:589:ARG:HH21	1.70	0.55
3:4:476:ILE:HD11	3:4:650:LEU:HD11	1.89	0.55
5:6:601:LEU:HG	5:6:616:ILE:HD13	1.88	0.55
3:4:328:CYS:SG	3:4:336:SER:OG	2.65	0.55
3:4:405:VAL:HG23	3:4:407:ASN:H	1.72	0.55
4:5:372:ARG:HB2	4:5:618:ARG:NH2	2.22	0.55
4:5:633:THR:OG1	4:5:634:GLU:N	2.38	0.55
9:C:90:LYS:HA	9:C:93:GLN:HB2	1.89	0.55
11:E:230:GLN:NE2	11:E:381:MET:SD	2.79	0.55
12:H:637:THR:HG21	12:H:649:MET:HE3	1.87	0.55
2:3:460:SER:OG	2:3:463:ASP:OD2	2.25	0.55
3:4:189:THR:HB	3:4:195:GLN:HE22	1.71	0.55
4:5:565:TYR:CE1	4:5:569:LYS:HG3	2.41	0.55
5:6:174:TYR:OH	5:6:193:LEU:HD22	2.06	0.55
8:B:59:ARG:CD	12:G:703:ARG:HD2	2.36	0.55
12:G:665:ARG:NH1	12:G:673:ASP:O	2.40	0.55
7:A:62:ILE:O	7:A:66:HIS:N	2.34	0.55
11:E:515:SER:O	11:E:515:SER:OG	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:637:THR:HG21	12:G:649:MET:HE3	1.87	0.55
2:3:267:ASP:OD2	2:3:268:ASP:N	2.40	0.55
3:4:200:ILE:HG21	3:4:258:ILE:HD11	1.87	0.55
4:5:589:MET:HE1	4:5:644:PHE:HE2	1.72	0.55
6:7:269:ASP:OD1	6:7:270:HIS:N	2.40	0.55
2:3:244:ILE:HD13	2:3:266:LEU:HD11	1.89	0.54
3:4:716:ASP:OD1	3:4:717:MET:N	2.39	0.54
11:E:443:GLY:O	11:E:485:ARG:NH2	2.39	0.54
1:2:377:ARG:HB2	1:2:565:VAL:CG2	2.37	0.54
1:2:580:ASP:OD2	4:5:238:HIS:HD2	1.88	0.54
3:4:354:LEU:HD13	3:4:372:LEU:HD11	1.88	0.54
5:6:170:GLN:OE1	5:6:170:GLN:N	2.40	0.54
1:2:680:VAL:HG11	5:6:591:GLU:HG3	1.88	0.54
8:B:24:ASP:OD1	8:B:24:ASP:N	2.36	0.54
1:2:402:LEU:O	1:2:405:SER:OG	2.12	0.54
1:2:592:MET:HE3	1:2:597:ARG:HG2	1.89	0.54
12:H:665:ARG:NH1	12:H:673:ASP:O	2.40	0.54
1:2:765:ARG:HH21	4:5:385:THR:CB	2.20	0.54
9:C:78:ASP:CG	9:C:82:ARG:H	2.13	0.54
10:D:106:HIS:NE2	10:D:162:VAL:O	2.39	0.54
12:F:665:ARG:NH1	12:F:673:ASP:O	2.40	0.54
4:5:380:LEU:HA	4:5:488:ALA:HB3	1.88	0.54
4:5:37:GLU:OE1	4:5:41:GLN:NE2	2.40	0.54
6:7:5:ASP:OD1	6:7:6:TYR:N	2.36	0.54
6:7:500:SER:O	6:7:504:ASN:ND2	2.41	0.54
6:7:135:GLU:HG3	6:7:137:TYR:CZ	2.43	0.54
3:4:457:ASP:N	3:4:457:ASP:OD1	2.38	0.53
3:4:748:ARG:HH22	3:4:754:GLU:HG2	1.74	0.53
4:5:634:GLU:HA	4:5:637:VAL:HG12	1.91	0.53
5:6:320:GLN:O	5:6:581:GLN:NE2	2.41	0.53
7:A:129:GLY:H	7:A:133:GLY:HA2	1.73	0.53
1:2:570:THR:OG1	1:2:571:LEU:N	2.41	0.53
5:6:109:ASP:OD2	5:6:199:ARG:NH2	2.42	0.53
6:7:445:ASP:OD1	6:7:445:ASP:N	2.33	0.53
6:7:521:ILE:HG13	6:7:522:GLN:H	1.73	0.53
5:6:171:GLN:H	5:6:175:THR:HG21	1.74	0.53
6:7:186:GLN:HE21	6:7:215:ARG:HH11	1.55	0.53
12:F:599:LEU:HD22	12:F:621:LEU:HD11	1.90	0.53
1:2:765:ARG:NH2	4:5:385:THR:CG2	2.46	0.53
2:3:469:GLU:HA	2:3:473:GLN:OE1	2.08	0.53
6:7:51:ASP:OD1	6:7:52:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:178:ARG:NE	10:D:180:GLU:OE2	2.39	0.53
12:H:468:VAL:HG21	12:H:497:ILE:HD13	1.90	0.53
1:2:366:GLU:N	1:2:366:GLU:OE2	2.42	0.53
2:3:191:HIS:HB3	2:3:229:LEU:HD22	1.89	0.53
11:E:496:PRO:HA	11:E:504:VAL:HG12	1.90	0.53
4:5:156:ILE:HD12	4:5:230:GLN:HB2	1.90	0.53
6:7:528:ASP:N	6:7:528:ASP:OD1	2.42	0.53
8:B:57:LYS:HZ3	11:E:211:LYS:NZ	2.07	0.53
12:G:599:LEU:HD22	12:G:621:LEU:HD11	1.90	0.53
12:H:712:LYS:HE3	12:H:718:ILE:HD13	1.91	0.53
3:4:501:ARG:O	3:4:739:ARG:NH2	2.41	0.53
12:F:597:GLN:HB3	12:F:599:LEU:HD13	1.91	0.53
1:2:792:ASN:O	1:2:796:ARG:HB2	2.09	0.53
2:3:390:GLY:O	2:3:396:LYS:NZ	2.41	0.53
4:5:380:LEU:HD23	4:5:381:GLY:N	2.23	0.53
12:H:597:GLN:HB3	12:H:599:LEU:HD13	1.91	0.53
12:H:599:LEU:HD22	12:H:621:LEU:HD11	1.90	0.53
1:2:687:HIS:O	1:2:689:SER:N	2.41	0.53
3:4:179:LYS:HG3	3:4:180:GLU:HG2	1.91	0.53
12:G:468:VAL:HG21	12:G:497:ILE:HD13	1.90	0.53
1:2:225:GLU:OE2	11:E:312:GLN:NE2	2.42	0.53
11:E:386:SER:O	11:E:389:LYS:NZ	2.32	0.53
12:G:597:GLN:HB3	12:G:599:LEU:HD13	1.91	0.53
4:5:43:ARG:CD	8:B:114:ARG:HD3	2.39	0.52
2:3:437:ARG:HH11	6:7:249:ILE:HD12	1.72	0.52
4:5:79:SER:HB2	11:E:367:PHE:O	2.10	0.52
4:5:172:CYS:SG	4:5:173:ARG:N	2.82	0.52
5:6:559:ILE:H	5:6:559:ILE:HD12	1.74	0.52
8:B:144:LYS:HE2	10:D:204:HIS:CE1	2.44	0.52
12:G:712:LYS:HE3	12:G:718:ILE:HD13	1.91	0.52
1:2:804:ASP:N	1:2:804:ASP:OD1	2.35	0.52
4:5:526:GLU:HA	4:5:529:ASP:HB2	1.91	0.52
1:2:606:GLN:NE2	4:5:392:LYS:HZ1	2.06	0.52
2:3:440:ALA:HB2	6:7:247:GLY:HA2	1.92	0.52
6:7:223:GLN:HE21	6:7:225:ARG:HB2	1.74	0.52
11:E:25:SER:OG	11:E:384:MET:SD	2.66	0.52
2:3:627:LEU:HA	2:3:682:VAL:HG22	1.91	0.52
3:4:199:GLU:O	3:4:203:ILE:HG12	2.10	0.52
7:A:161:VAL:HG13	7:A:181:LYS:HZ2	1.74	0.52
10:D:187:ASP:OD1	10:D:188:THR:N	2.38	0.52
12:F:468:VAL:HG21	12:F:497:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:525:PRO:O	5:6:528:SER:OG	2.22	0.52
7:A:83:ARG:HH21	7:A:110:GLU:CD	2.18	0.52
2:3:133:ASP:OD1	2:3:136:TYR:N	2.34	0.52
3:4:448:LEU:O	3:4:451:GLU:HG3	2.09	0.52
4:5:96:LEU:HD22	4:5:297:LEU:HD22	1.91	0.52
8:B:144:LYS:HE2	10:D:204:HIS:HE1	1.75	0.52
7:A:161:VAL:HG13	7:A:181:LYS:NZ	2.25	0.52
12:F:712:LYS:HE3	12:F:718:ILE:HD13	1.91	0.52
2:3:634:TYR:OH	2:3:688:GLU:OE1	2.14	0.52
2:3:638:GLU:OE1	2:3:641:ARG:NH2	2.35	0.52
4:5:363:LYS:NZ	4:5:621:GLU:OE2	2.42	0.52
7:A:149:GLU:CD	11:E:47:TYR:OH	2.53	0.51
4:5:332:TYR:HE2	4:5:351:LYS:HE2	1.75	0.51
4:5:585:ARG:HG2	4:5:641:LEU:HD22	1.93	0.51
8:B:59:ARG:NE	12:G:703:ARG:CD	2.46	0.51
1:2:644:SER:OG	1:2:651:GLU:OE1	2.25	0.51
3:4:167:GLN:HG2	3:4:244:ILE:HD11	1.92	0.51
10:D:199:GLU:HG3	10:D:200:LYS:H	1.75	0.51
1:2:777:HIS:HA	1:2:780:ILE:HG22	1.92	0.51
4:5:53:PHE:CZ	8:B:114:ARG:HG2	2.44	0.51
6:7:257:VAL:HG13	6:7:261:ASN:HB2	1.93	0.51
11:E:28:ASP:OD2	11:E:76:ASN:ND2	2.36	0.51
11:E:368:LYS:O	11:E:369:HIS:ND1	2.44	0.51
1:2:558:ALA:HB3	1:2:611:ILE:HD13	1.93	0.51
1:2:592:MET:HE1	1:2:600:ILE:HG21	1.92	0.51
2:3:673:HIS:HD2	2:3:686:ASP:HA	1.74	0.51
4:5:319:GLU:O	4:5:323:ARG:HG2	2.10	0.51
5:6:609:VAL:HG22	5:6:610:THR:HG23	1.93	0.51
7:A:39:LEU:HD22	7:A:65:ARG:HG2	1.93	0.51
4:5:87:TYR:HB3	4:5:95:HIS:CE1	2.45	0.51
5:6:349:ASN:O	5:6:353:SER:OG	2.23	0.51
7:A:158:GLU:HG3	7:A:166:SER:HB3	1.92	0.51
8:B:100:LEU:O	8:B:104:SER:HB2	2.10	0.51
4:5:236:VAL:HG21	4:5:242:PRO:HG3	1.93	0.51
6:7:280:ILE:HD12	6:7:295:GLU:HG3	1.92	0.51
8:B:103:ALA:O	8:B:107:ILE:HG12	2.11	0.51
2:3:88:ASN:HA	2:3:136:TYR:OH	2.10	0.51
3:4:171:GLN:HE21	3:4:244:ILE:HD12	1.76	0.51
11:E:98:CYS:HB2	11:E:118:LEU:HD12	1.93	0.51
5:6:321:THR:OG1	5:6:322:ALA:N	2.42	0.51
6:7:642:ASP:C	6:7:644:LEU:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:451:MET:HG2	11:E:453:GLY:H	1.76	0.50
2:3:623:ILE:HG22	2:3:625:PRO:HD3	1.92	0.50
4:5:590:ARG:HG2	4:5:608:ILE:HG21	1.94	0.50
8:B:56:GLN:OE1	11:E:211:LYS:CB	2.59	0.50
1:2:377:ARG:CB	1:2:565:VAL:HG21	2.38	0.50
4:5:590:ARG:HG2	4:5:608:ILE:CG2	2.42	0.50
5:6:19:ARG:NH1	5:6:24:GLU:OE2	2.45	0.50
7:A:109:GLU:OE2	7:A:109:GLU:N	2.40	0.50
9:C:100:PHE:CE1	9:C:107:VAL:HG11	2.47	0.50
11:E:527:GLU:O	11:E:531:GLU:HG3	2.11	0.50
1:2:276:ARG:HE	11:E:319:GLY:HA3	1.76	0.50
2:3:655:THR:OG1	2:3:698:TYR:O	2.24	0.50
4:5:387:LYS:O	4:5:391:LEU:HG	2.12	0.50
6:7:317:GLY:HA2	6:7:561:ARG:HE	1.76	0.50
1:2:315:CYS:SG	1:2:408:PRO:HD3	2.51	0.50
2:3:122:GLN:HG2	2:3:145:VAL:HG12	1.94	0.50
2:3:151:PHE:H	2:3:155:HIS:CE1	2.27	0.50
3:4:568:ASN:HD22	5:6:217:ARG:NE	2.08	0.50
4:5:338:SER:O	4:5:338:SER:OG	2.27	0.50
5:6:485:THR:HG23	5:6:490:LYS:HE2	1.94	0.50
8:B:49:ALA:HB1	8:B:60:LEU:HD21	1.93	0.50
11:E:5:ASP:OD1	11:E:5:ASP:N	2.45	0.50
4:5:390:LEU:O	4:5:394:VAL:HG23	2.11	0.50
6:7:36:GLN:HE22	6:7:39:ARG:CZ	2.25	0.50
9:C:128:SER:OG	9:C:129:PRO:HD2	2.12	0.50
1:2:462:LYS:HG3	1:2:463:MET:SD	2.51	0.50
3:4:656:GLU:O	3:4:660:ARG:HG3	2.10	0.50
1:2:548:GLY:N	1:2:587:ASP:O	2.44	0.49
1:2:676:ALA:HB3	5:6:595:VAL:HG23	1.94	0.49
3:4:698:ILE:HG22	3:4:700:PRO:HD3	1.92	0.49
4:5:47:ASP:H	11:E:406:ARG:NH2	2.10	0.49
6:7:153:ARG:HH12	6:7:251:ARG:NH1	2.10	0.49
1:2:560:VAL:H	1:2:613:LYS:HE2	1.77	0.49
1:2:802:PHE:HE2	1:2:814:MET:HE1	1.78	0.49
2:3:85:ILE:HD11	2:3:129:VAL:HG23	1.93	0.49
4:5:453:ASP:OD2	4:5:454:ASP:N	2.45	0.49
7:A:58:LEU:HD23	9:C:41:PRO:HG2	1.94	0.49
2:3:81:VAL:HG21	2:3:128:PHE:HE2	1.77	0.49
3:4:396:ALA:HB2	3:4:414:THR:HG22	1.93	0.49
4:5:380:LEU:HD22	4:5:519:ILE:HD12	1.94	0.49
6:7:575:GLU:CD	6:7:575:GLU:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:179:CYS:HB3	2:3:242:GLN:NE2	2.28	0.49
2:3:462:MET:HB3	6:7:407:ARG:HH11	1.78	0.49
3:4:580:ASN:N	3:4:580:ASN:OD1	2.45	0.49
7:A:88:ARG:NH2	10:D:101:GLU:OE1	2.45	0.49
7:A:149:GLU:OE2	11:E:37:GLN:NE2	2.45	0.49
1:2:642:THR:HG23	1:2:645:GLU:HG2	1.94	0.49
3:4:376:ASN:OD1	3:4:377:ASP:N	2.45	0.49
3:4:401:VAL:HG12	3:4:407:ASN:O	2.11	0.49
3:4:512:PRO:HB2	6:7:600:TYR:HE2	1.73	0.49
4:5:42:TYR:HD1	11:E:367:PHE:CG	2.30	0.49
4:5:143:ASP:OD1	4:5:143:ASP:N	2.45	0.49
6:7:153:ARG:HH12	6:7:251:ARG:HH12	1.60	0.49
8:B:26:ILE:HG13	8:B:33:LEU:HB2	1.93	0.49
1:2:248:LEU:HD21	1:2:285:ILE:HD13	1.95	0.49
1:2:314:SER:OG	1:2:563:HIS:CD2	2.66	0.49
1:2:462:LYS:O	1:2:465:THR:OG1	2.31	0.49
1:2:526:GLY:N	5:6:619:ARG:NH1	2.61	0.49
3:4:319:ARG:HG2	6:7:221:TYR:CE2	2.48	0.49
4:5:614:GLU:HG2	4:5:618:ARG:NH1	2.28	0.49
5:6:357:THR:HA	5:6:551:ARG:HH11	0.67	0.49
7:A:194:ILE:HG13	7:A:195:LEU:N	2.27	0.49
8:B:56:GLN:HE22	11:E:216:MET:HE1	1.77	0.49
8:B:109:LYS:HG2	11:E:262:THR:HB	1.94	0.49
1:2:373:TYR:CE1	4:5:289:ILE:HD11	2.47	0.49
3:4:740:LEU:HB3	3:4:761:ALA:HB1	1.94	0.49
4:5:134:PRO:HB2	4:5:152:PRO:HD3	1.93	0.49
5:6:159:LEU:O	5:6:162:GLN:NE2	2.45	0.49
11:E:477:PHE:O	11:E:480:SER:N	2.43	0.49
1:2:314:SER:CA	1:2:563:HIS:NE2	2.75	0.49
1:2:547:THR:OG1	1:2:588:GLU:OE1	2.30	0.49
7:A:10:ILE:HD12	9:C:22:LEU:HD22	1.95	0.49
7:A:195:LEU:HD22	11:E:41:GLN:NE2	2.26	0.49
1:2:633:ILE:HB	1:2:648:ASP:OD2	2.12	0.49
4:5:515:ASP:OD1	4:5:515:ASP:N	2.42	0.49
5:6:378:LYS:HB2	5:6:386:LEU:HD12	1.95	0.49
6:7:501:LEU:C	6:7:503:GLN:H	2.21	0.49
6:7:521:ILE:HG13	6:7:522:GLN:N	2.27	0.49
11:E:172:ARG:O	11:E:176:GLU:HG3	2.13	0.49
1:2:750:LEU:HD21	1:2:762:ILE:HG12	1.94	0.49
2:3:226:ASN:OD1	2:3:227:ASN:N	2.45	0.49
2:3:467:ILE:HG22	2:3:471:MET:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:190:GLU:O	3:4:192:LEU:N	2.45	0.49
3:4:723:SER:OG	3:4:724:ARG:NH1	2.46	0.49
4:5:356:LEU:HD13	4:5:377:LEU:HD12	1.95	0.49
8:B:57:LYS:NZ	11:E:211:LYS:HZ3	2.11	0.49
1:2:381:SER:HB3	1:2:384:LYS:HE2	1.94	0.48
6:7:500:SER:H	6:7:503:GLN:NE2	2.11	0.48
11:E:257:GLU:HG2	11:E:258:ASP:H	1.77	0.48
1:2:178:LYS:HD3	1:2:179:GLY:N	2.28	0.48
2:3:436:ARG:NH1	2:3:481:ALA:HB3	2.28	0.48
2:3:646:ASP:N	2:3:646:ASP:OD1	2.44	0.48
3:4:242:ASN:O	3:4:249:TYR:OH	2.16	0.48
5:6:86:VAL:O	5:6:90:LEU:HG	2.13	0.48
1:2:500:PHE:CZ	1:2:724:ILE:HG22	2.48	0.48
3:4:682:LEU:HG	3:4:686:VAL:HG11	1.94	0.48
4:5:156:ILE:HG22	4:5:228:LYS:HB3	1.94	0.48
1:2:207:VAL:O	1:2:240:ARG:NH2	2.46	0.48
4:5:51:PHE:CZ	11:E:266:ASP:HB3	2.47	0.48
5:6:160:ASP:OD2	5:6:186:ALA:N	2.29	0.48
10:D:197:ASP:OD1	10:D:197:ASP:N	2.46	0.48
2:3:458:LYS:NZ	4:5:459:HIS:HD2	2.12	0.48
4:5:47:ASP:CB	11:E:406:ARG:NH2	2.76	0.48
11:E:265:VAL:HG13	11:E:266:ASP:OD2	2.14	0.48
11:E:490:PRO:HD3	11:E:511:PRO:HG3	1.94	0.48
1:2:377:ARG:CG	1:2:565:VAL:CG1	2.90	0.48
1:2:594:ASP:O	1:2:598:THR:HG23	2.13	0.48
2:3:462:MET:CB	6:7:407:ARG:HH11	2.27	0.48
2:3:501:TYR:OH	2:3:508:LYS:NZ	2.47	0.48
5:6:565:ARG:C	5:6:565:ARG:HD2	2.38	0.48
7:A:83:ARG:NH2	7:A:110:GLU:OE1	2.46	0.48
7:A:124:TYR:O	7:A:127:SER:OG	2.26	0.48
11:E:126:GLU:N	11:E:126:GLU:OE1	2.47	0.48
4:5:115:PRO:HA	8:B:130:VAL:CG2	2.44	0.48
6:7:336:LEU:HD22	6:7:559:MET:HE3	1.96	0.48
8:B:66:MET:HE2	8:B:96:THR:HG22	1.96	0.48
11:E:257:GLU:HB3	12:G:458:TYR:CE1	2.49	0.48
2:3:95:ASN:HA	2:3:148:GLU:O	2.14	0.48
12:F:528:ASP:H	12:H:717:GLN:HE21	1.62	0.48
1:2:207:VAL:HA	1:2:212:HIS:O	2.14	0.48
2:3:10:ARG:NH1	9:C:90:LYS:HB2	2.29	0.48
7:A:168:LEU:HD22	11:E:64:GLU:HB3	1.94	0.48
12:G:686:GLN:HB2	12:G:708:ILE:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:385:VAL:O	1:2:387:ALA:N	2.46	0.48
11:E:74:LEU:HD11	11:E:95:PHE:HD1	1.79	0.48
1:2:720:LEU:O	1:2:724:ILE:HG23	2.14	0.47
2:3:400:LEU:HD12	2:3:454:ASP:HB3	1.95	0.47
11:E:389:LYS:NZ	11:E:462:ARG:HD2	2.23	0.47
12:F:686:GLN:HB2	12:F:708:ILE:HG23	1.96	0.47
3:4:624:TRP:CE2	3:4:651:LEU:HD21	2.49	0.47
5:6:44:ILE:H	5:6:44:ILE:HD12	1.79	0.47
5:6:637:CYS:SG	5:6:638:ASP:N	2.86	0.47
7:A:149:GLU:OE1	11:E:41:GLN:NE2	2.47	0.47
11:E:133:ILE:O	11:E:181:ARG:HD2	2.13	0.47
10:D:104:PHE:CD2	10:D:105:PRO:HD3	2.49	0.47
11:E:343:MET:SD	11:E:343:MET:N	2.87	0.47
1:2:549:GLN:CD	5:6:471:VAL:CB	2.77	0.47
1:2:586:ILE:HB	1:2:628:ALA:HB2	1.96	0.47
2:3:447:ASP:CB	6:7:246:VAL:CG1	2.93	0.47
3:4:714:TYR:HB2	3:4:734:LEU:HD13	1.96	0.47
4:5:76:ASP:OD1	11:E:368:LYS:HD3	2.14	0.47
6:7:420:ARG:HG2	6:7:427:LEU:HG	1.96	0.47
10:D:175:VAL:HG11	10:D:198:LEU:HD13	1.95	0.47
12:F:717:GLN:HE21	12:G:528:ASP:H	1.62	0.47
12:G:788:MET:HB3	12:G:792:ALA:HB3	1.96	0.47
1:2:343:GLN:NE2	1:2:399:LEU:HD11	2.30	0.47
3:4:521:GLN:O	3:4:525:ASN:ND2	2.48	0.47
4:5:80:PHE:CE1	11:E:367:PHE:HE1	2.30	0.47
12:G:717:GLN:HE21	12:H:528:ASP:H	1.62	0.47
3:4:306:CYS:HB2	3:4:337:MET:SD	2.55	0.47
4:5:40:ARG:NH2	8:B:75:ARG:NH1	2.63	0.47
4:5:43:ARG:HH22	8:B:111:ASP:CG	2.23	0.47
4:5:237:PRO:HG2	4:5:240:GLU:OE1	2.15	0.47
5:6:375:GLY:O	5:6:633:ARG:NH2	2.48	0.47
7:A:73:ARG:HG3	10:D:149:MET:HE1	1.97	0.47
8:B:55:ARG:NE	11:E:42:CYS:O	2.27	0.47
8:B:55:ARG:HA	11:E:42:CYS:SG	2.54	0.47
12:F:788:MET:HB3	12:F:792:ALA:HB3	1.96	0.47
2:3:391:ASP:HB2	2:3:532:ASP:HB2	1.97	0.47
4:5:380:LEU:N	4:5:518:PHE:O	2.48	0.47
7:A:165:THR:HB	11:E:18:ARG:HH22	1.79	0.47
8:B:17:ILE:HG22	8:B:60:LEU:HD23	1.96	0.47
11:E:133:ILE:HG13	11:E:181:ARG:HG3	1.97	0.47
12:H:788:MET:HB3	12:H:792:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:249:MET:HE2	2:3:279:ARG:HH21	1.79	0.47
4:5:577:GLU:HA	4:5:580:GLU:OE2	2.14	0.47
5:6:527:MET:HE2	5:6:527:MET:HB3	1.77	0.47
1:2:526:GLY:CA	5:6:619:ARG:NH1	2.77	0.47
3:4:265:ALA:O	3:4:422:ARG:NH1	2.48	0.47
3:4:726:MET:HG3	3:4:727:VAL:N	2.28	0.47
4:5:519:ILE:HD12	4:5:654:SER:OG	2.15	0.47
5:6:38:GLN:CD	5:6:42:GLY:HA2	2.40	0.47
5:6:120:ARG:O	5:6:121:HIS:ND1	2.48	0.47
1:2:276:ARG:NE	11:E:319:GLY:O	2.48	0.47
2:3:436:ARG:HH12	2:3:481:ALA:HB3	1.80	0.47
3:4:513:GLY:HA3	6:7:602:SER:HB2	1.97	0.47
6:7:554:LEU:H	6:7:554:LEU:HD12	1.80	0.47
11:E:491:LEU:HD23	11:E:492:VAL:N	2.30	0.47
1:2:481:ILE:HD11	1:2:496:ALA:HB2	1.97	0.46
4:5:49:THR:CG2	11:E:407:SER:CB	2.92	0.46
4:5:94:GLU:HG3	4:5:95:HIS:HD2	1.79	0.46
11:E:250:SER:O	11:E:254:HIS:HB3	2.15	0.46
12:H:686:GLN:HB2	12:H:708:ILE:HG23	1.96	0.46
1:2:186:VAL:HG13	1:2:195:ILE:HD12	1.97	0.46
2:3:184:PRO:HA	2:3:239:LYS:O	2.15	0.46
2:3:326:ILE:HG12	2:3:330:LYS:HE3	1.98	0.46
4:5:525:ASN:O	4:5:529:ASP:N	2.43	0.46
4:5:608:ILE:HD12	4:5:612:GLN:OE1	2.15	0.46
5:6:56:PRO:O	5:6:57:GLU:HG2	2.16	0.46
5:6:173:LYS:HG2	5:6:174:TYR:H	1.80	0.46
9:C:201:ASN:HA	9:C:204:GLN:CD	2.40	0.46
1:2:526:GLY:N	5:6:619:ARG:CZ	2.78	0.46
4:5:50:GLY:HA2	8:B:101:ASN:HD21	1.80	0.46
7:A:147:TYR:CE2	11:E:46:GLN:HG2	2.44	0.46
7:A:94:TYR:CE2	9:C:202:LEU:HD11	2.50	0.46
9:C:88:LEU:HD22	9:C:123:LEU:HD23	1.97	0.46
1:2:566:SER:OG	1:2:568:GLU:HG2	2.16	0.46
11:E:181:ARG:HA	11:E:184:ILE:HG22	1.97	0.46
12:H:586:VAL:HG11	12:H:627:LEU:HD22	1.98	0.46
1:2:587:ASP:OD1	1:2:588:GLU:N	2.49	0.46
1:2:751:ARG:HD3	4:5:532:LEU:HD13	1.97	0.46
2:3:151:PHE:N	2:3:155:HIS:HE1	2.13	0.46
3:4:730:TYR:HB3	5:6:399:SER:CB	2.45	0.46
4:5:115:PRO:CA	8:B:130:VAL:HG22	2.44	0.46
8:B:81:GLU:HG3	8:B:83:THR:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:71:GLU:OE1	10:D:74:LYS:N	2.44	0.46
1:2:284:ARG:HD2	1:2:442:ASN:O	2.15	0.46
1:2:288:LEU:HD21	1:2:305:LEU:HD23	1.96	0.46
2:3:431:GLN:HA	4:5:425:ARG:NH2	2.31	0.46
4:5:32:GLN:NE2	4:5:105:GLU:OE2	2.48	0.46
4:5:49:THR:OG1	4:5:50:GLY:N	2.49	0.46
8:B:111:ASP:CG	11:E:264:SER:HA	2.39	0.46
1:2:463:MET:SD	1:2:463:MET:N	2.88	0.46
7:A:176:PHE:CB	11:E:47:TYR:CE1	2.99	0.46
10:D:104:PHE:CG	10:D:105:PRO:HD3	2.51	0.46
2:3:202:ARG:NH2	2:3:220:PRO:HG3	2.31	0.46
2:3:324:GLU:HG2	2:3:328:LYS:HE3	1.98	0.46
2:3:547:LEU:O	2:3:551:ARG:HG3	2.15	0.46
4:5:109:GLU:HB3	8:B:79:ARG:CZ	2.45	0.46
4:5:401:GLY:HA2	4:5:441:VAL:O	2.16	0.46
4:5:468:SER:HB3	4:5:477:THR:HG22	1.98	0.46
4:5:570:CYS:SG	4:5:572:PRO:HD3	2.56	0.46
5:6:187:ASN:OD1	5:6:187:ASN:N	2.49	0.46
10:D:37:GLU:HG3	10:D:92:TYR:CE1	2.50	0.46
12:F:586:VAL:HG11	12:F:627:LEU:HD22	1.98	0.46
1:2:750:LEU:HB2	1:2:818:PHE:CE2	2.51	0.45
2:3:673:HIS:CD2	2:3:686:ASP:HA	2.50	0.45
3:4:164:GLU:O	3:4:168:ARG:HG3	2.16	0.45
3:4:258:ILE:HD12	3:4:258:ILE:HA	1.77	0.45
3:4:438:GLN:HG2	3:4:441:PHE:CE2	2.51	0.45
4:5:378:LEU:HD23	4:5:517:ILE:HD12	1.98	0.45
12:G:618:PRO:HB2	12:H:570:ALA:HB1	1.98	0.45
2:3:148:GLU:HG2	2:3:149:GLY:N	2.32	0.45
2:3:471:MET:HE2	2:3:471:MET:HB3	1.87	0.45
3:4:171:GLN:NE2	3:4:244:ILE:HD12	2.32	0.45
7:A:175:HIS:ND1	11:E:48:THR:CG2	2.77	0.45
8:B:96:THR:HG21	8:B:117:VAL:HG21	1.97	0.45
1:2:726:TYR:CE2	1:2:730:ARG:HD2	2.50	0.45
2:3:206:ASP:HB2	6:7:292:LEU:HD12	1.99	0.45
2:3:535:ASP:HB3	2:3:538:GLN:HE22	1.82	0.45
4:5:210:ASP:OD1	4:5:210:ASP:N	2.43	0.45
4:5:615:ALA:HA	4:5:618:ARG:HG2	1.98	0.45
8:B:27:TYR:HA	8:B:32:ASP:OD1	2.16	0.45
1:2:223:CYS:O	11:E:316:ALA:HB2	2.17	0.45
1:2:585:LEU:HD23	1:2:627:ILE:HB	1.98	0.45
3:4:191:PRO:O	3:4:195:GLN:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:145:MET:O	4:5:146:SER:OG	2.24	0.45
6:7:223:GLN:HG2	6:7:225:ARG:H	1.81	0.45
7:A:9:LEU:HB3	7:A:79:TYR:CD2	2.51	0.45
11:E:208:MET:O	12:G:477:HIS:HB3	2.16	0.45
12:F:570:ALA:HB1	12:H:618:PRO:HB2	1.98	0.45
1:2:377:ARG:HD2	1:2:565:VAL:CB	2.46	0.45
2:3:152:GLY:HA3	9:C:103:ASP:CB	2.45	0.45
3:4:222:LEU:HD12	3:4:223:TYR:N	2.32	0.45
4:5:335:ILE:O	4:5:339:ILE:HG23	2.16	0.45
4:5:463:GLU:HG3	4:5:513:ARG:CZ	2.46	0.45
6:7:534:ALA:O	6:7:538:THR:HG23	2.16	0.45
11:E:451:MET:HE2	11:E:453:GLY:HA3	1.99	0.45
1:2:276:ARG:CZ	11:E:318:MET:O	2.53	0.45
6:7:148:VAL:HG12	6:7:149:ILE:H	1.81	0.45
6:7:539:TYR:CG	6:7:547:PRO:HG3	2.51	0.45
11:E:39:LEU:HD23	11:E:39:LEU:HA	1.80	0.45
1:2:203:LEU:HD23	1:2:215:PHE:CD2	2.52	0.45
3:4:201:ASN:OD1	3:4:252:SER:OG	2.18	0.45
7:A:20:GLN:NE2	9:C:205:ASN:OD1	2.49	0.45
8:B:59:ARG:HH11	12:G:703:ARG:HD3	1.68	0.45
11:E:130:TYR:HE1	11:E:134:PHE:HD2	1.64	0.45
12:F:618:PRO:HB2	12:G:570:ALA:HB1	1.98	0.45
1:2:319:LEU:HD13	4:5:289:ILE:HG21	1.99	0.45
3:4:533:THR:HG22	3:4:534:SER:N	2.31	0.45
3:4:555:GLN:NE2	5:6:438:GLU:OE2	2.50	0.45
3:4:730:TYR:H	3:4:733:GLN:NE2	2.15	0.45
4:5:358:PHE:CE1	4:5:563:ILE:HG12	2.52	0.45
4:5:526:GLU:O	4:5:530:VAL:HG23	2.17	0.45
6:7:395:ASP:OD1	6:7:401:SER:OG	2.24	0.45
7:A:46:ASP:HA	7:A:49:GLU:HB3	1.98	0.45
10:D:29:ARG:NE	10:D:50:ILE:HD11	2.31	0.45
1:2:377:ARG:CD	1:2:565:VAL:CB	2.93	0.45
1:2:562:ARG:NH1	1:2:567:ARG:O	2.50	0.45
1:2:651:GLU:HB3	1:2:652:PRO:HD3	1.99	0.45
4:5:581:LYS:HG3	4:5:634:GLU:HG2	1.99	0.45
6:7:236:LYS:HE3	6:7:236:LYS:HB3	1.80	0.45
1:2:276:ARG:HE	11:E:319:GLY:C	2.25	0.45
1:2:530:SER:O	1:2:534:LYS:HG2	2.17	0.45
2:3:91:ARG:HB3	2:3:144:TYR:HB2	1.99	0.45
4:5:65:LEU:CD2	9:C:152:SER:HA	2.46	0.45
6:7:182:TYR:HE2	6:7:193:GLN:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:203:PHE:HE2	11:E:248:HIS:CD2	2.35	0.45
4:5:266:MET:HE2	4:5:266:MET:HB3	1.78	0.44
5:6:569:LEU:HD23	5:6:569:LEU:HA	1.78	0.44
6:7:48:LEU:HD23	6:7:136:LEU:HD12	2.00	0.44
8:B:55:ARG:CA	11:E:42:CYS:SG	3.05	0.44
2:3:126:LYS:HA	2:3:129:VAL:HG12	1.98	0.44
2:3:158:PRO:HD3	2:3:172:VAL:HG13	2.00	0.44
10:D:82:MET:HE2	10:D:82:MET:HB3	1.75	0.44
11:E:474:LEU:HD12	11:E:474:LEU:HA	1.81	0.44
12:G:690:ILE:HD13	12:G:706:VAL:HA	1.99	0.44
1:2:365:MET:SD	4:5:270:SER:HB2	2.58	0.44
1:2:493:ARG:O	1:2:497:LEU:HG	2.16	0.44
1:2:532:PHE:O	1:2:536:ILE:HG12	2.17	0.44
1:2:795:ILE:O	1:2:798:MET:HG3	2.17	0.44
3:4:306:CYS:SG	3:4:307:GLN:N	2.89	0.44
4:5:40:ARG:NH2	8:B:75:ARG:HH12	2.15	0.44
4:5:636:ASP:O	4:5:639:GLU:HG3	2.17	0.44
5:6:616:ILE:HG23	5:6:620:GLN:HG3	1.98	0.44
6:7:153:ARG:HB2	6:7:155:ASP:OD2	2.17	0.44
7:A:174:GLN:NE2	11:E:37:GLN:HE22	2.16	0.44
12:G:586:VAL:HG11	12:G:627:LEU:HD22	1.98	0.44
12:H:438:THR:HG22	12:H:697:PHE:HB2	2.00	0.44
3:4:238:ASP:OD2	3:4:260:VAL:HG12	2.17	0.44
3:4:271:MET:HE1	3:4:354:LEU:HB3	1.99	0.44
8:B:66:MET:HG2	8:B:113:ILE:HD13	1.99	0.44
12:G:438:THR:HG22	12:G:697:PHE:HB2	1.99	0.44
2:3:627:LEU:HD23	2:3:682:VAL:HG21	2.00	0.44
4:5:86:ASP:CB	11:E:334:ILE:HG21	2.48	0.44
4:5:579:ALA:O	4:5:583:LYS:HG3	2.17	0.44
7:A:98:LEU:N	7:A:103:ARG:HH21	2.08	0.44
8:B:67:ASP:OD1	8:B:68:VAL:N	2.51	0.44
11:E:62:PHE:O	11:E:66:LYS:HB3	2.17	0.44
2:3:59:GLU:OE1	2:3:62:ARG:NH2	2.51	0.44
2:3:378:SER:OG	6:7:343:GLU:OE2	2.30	0.44
3:4:220:LYS:HE2	3:4:220:LYS:HB3	1.81	0.44
5:6:347:TYR:OH	5:6:366:ARG:HB3	2.18	0.44
6:7:43:ARG:HH22	6:7:133:ARG:HH11	1.66	0.44
6:7:566:CYS:SG	6:7:619:LEU:HA	2.57	0.44
6:7:582:THR:O	6:7:586:VAL:HG23	2.17	0.44
9:C:40:MET:HB3	9:C:60:VAL:HB	1.99	0.44
10:D:173:LEU:HD13	10:D:211:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:299:ARG:HG2	11:E:353:MET:HG2	1.99	0.44
4:5:197:CYS:HB2	4:5:211:PRO:HG3	2.00	0.44
12:H:690:ILE:HD13	12:H:706:VAL:HA	1.99	0.44
1:2:720:LEU:HA	1:2:723:TYR:HB3	1.99	0.44
5:6:126:LEU:HD21	5:6:137:ILE:HD11	2.00	0.44
10:D:152:ASN:N	10:D:152:ASN:OD1	2.49	0.44
12:F:438:THR:HG22	12:F:697:PHE:HB2	2.00	0.44
1:2:306:ILE:HD12	1:2:418:TYR:HB2	2.00	0.44
1:2:377:ARG:HD2	1:2:565:VAL:CA	2.48	0.44
2:3:166:LEU:HD11	2:3:288:CYS:HB3	2.00	0.44
3:4:476:ILE:HD11	3:4:650:LEU:CD1	2.48	0.44
4:5:317:GLN:NE2	4:5:318:GLU:HG2	2.33	0.44
4:5:614:GLU:HG2	4:5:618:ARG:HH12	1.83	0.44
5:6:354:LEU:HD12	5:6:354:LEU:HA	1.81	0.44
12:F:690:ILE:HD13	12:F:706:VAL:HA	1.99	0.44
1:2:500:PHE:HE1	1:2:727:ALA:HB3	1.83	0.43
3:4:413:LYS:HB3	3:4:413:LYS:HE2	1.76	0.43
4:5:43:ARG:NH2	8:B:111:ASP:OD2	2.51	0.43
6:7:233:GLN:HG2	6:7:262:THR:HG22	2.00	0.43
6:7:248:ASN:OD1	6:7:249:ILE:N	2.49	0.43
7:A:176:PHE:HB2	11:E:47:TYR:CD1	2.53	0.43
1:2:567:ARG:HD2	5:6:440:HIS:CD2	2.49	0.43
2:3:118:LEU:HA	2:3:118:LEU:HD23	1.69	0.43
2:3:207:LEU:HD23	2:3:207:LEU:HA	1.82	0.43
3:4:268:THR:HG22	3:4:269:LYS:HG3	2.00	0.43
3:4:534:SER:OG	3:4:535:GLY:N	2.52	0.43
4:5:331:VAL:HG11	4:5:627:LYS:HG2	1.99	0.43
5:6:357:THR:C	5:6:551:ARG:HH11	2.18	0.43
6:7:148:VAL:HG12	6:7:149:ILE:N	2.33	0.43
7:A:30:ARG:HH21	7:A:31:GLN:HG3	1.83	0.43
7:A:144:LYS:HD2	7:A:144:LYS:HA	1.75	0.43
1:2:332:CYS:HB3	1:2:355:CYS:SG	2.58	0.43
1:2:399:LEU:HA	1:2:399:LEU:HD23	1.69	0.43
1:2:536:ILE:HA	1:2:539:VAL:HG12	1.99	0.43
2:3:487:LEU:HD21	6:7:241:SER:HG	1.69	0.43
2:3:525:ASP:OD2	2:3:665:THR:OG1	2.36	0.43
3:4:255:GLU:HG2	3:4:256:HIS:N	2.32	0.43
3:4:711:ILE:O	3:4:715:VAL:HG23	2.19	0.43
5:6:168:VAL:HB	5:6:177:PRO:HG3	1.99	0.43
7:A:28:GLY:O	7:A:32:VAL:HG13	2.18	0.43
7:A:102:LEU:C	7:A:104:PHE:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:541:GLY:HA3	12:G:544:TRP:CE2	2.53	0.43
1:2:271:TYR:HH	11:E:313:GLU:CD	2.17	0.43
1:2:382:PRO:HB3	5:6:492:THR:O	2.19	0.43
1:2:384:LYS:HE2	1:2:384:LYS:HB3	1.80	0.43
2:3:447:ASP:HB3	6:7:246:VAL:HG11	2.01	0.43
3:4:551:PRO:HG2	3:4:552:GLU:CD	2.42	0.43
4:5:507:MET:HE2	4:5:510:ILE:HG21	2.00	0.43
5:6:387:ARG:O	5:6:626:ARG:NH1	2.50	0.43
11:E:210:SER:CB	12:G:473:THR:HG22	2.28	0.43
3:4:169:PHE:CZ	3:4:215:ILE:HG22	2.54	0.43
9:C:35:ARG:HA	9:C:64:SER:O	2.18	0.43
9:C:93:GLN:O	9:C:97:ARG:NH1	2.51	0.43
9:C:161:THR:HG21	9:C:180:GLN:NE2	2.34	0.43
11:E:445:PHE:HD1	11:E:446:LEU:O	2.01	0.43
12:G:641:VAL:HG22	12:G:647:VAL:HG22	2.01	0.43
1:2:248:LEU:HB3	1:2:249:PRO:HD3	2.00	0.43
3:4:611:THR:OG1	3:4:612:SER:N	2.52	0.43
5:6:390:ILE:HG22	5:6:626:ARG:HD2	2.00	0.43
6:7:24:ASP:C	6:7:26:LEU:H	2.25	0.43
6:7:155:ASP:OD2	6:7:155:ASP:N	2.44	0.43
6:7:182:TYR:OH	6:7:193:GLN:NE2	2.51	0.43
7:A:188:GLN:O	9:C:202:LEU:HG	2.19	0.43
9:C:32:LEU:HA	9:C:33:PRO:HD3	1.90	0.43
9:C:78:ASP:OD1	9:C:82:ARG:N	2.38	0.43
11:E:106:VAL:HG11	11:E:133:ILE:HG21	2.00	0.43
11:E:125:LEU:HD23	11:E:125:LEU:HA	1.86	0.43
12:H:641:VAL:HG22	12:H:647:VAL:HG22	2.01	0.43
1:2:749:ASP:O	1:2:753:GLU:HG2	2.19	0.43
3:4:238:ASP:O	3:4:242:ASN:ND2	2.52	0.43
3:4:551:PRO:HG2	3:4:552:GLU:OE1	2.19	0.43
4:5:74:MET:HE2	4:5:89:TYR:CE1	2.54	0.43
6:7:185:ASP:OD1	6:7:185:ASP:N	2.49	0.43
7:A:176:PHE:CB	11:E:47:TYR:CD1	3.02	0.43
9:C:167:ARG:C	9:C:168:LEU:HD12	2.43	0.43
1:2:757:THR:HG22	1:2:758:GLY:N	2.30	0.43
2:3:486:ARG:O	6:7:242:ASP:OD1	2.36	0.43
3:4:276:PRO:HB3	6:7:175:PRO:HB3	2.00	0.43
3:4:566:SER:C	3:4:568:ASN:H	2.26	0.43
4:5:51:PHE:CD2	8:B:114:ARG:NH2	2.86	0.43
10:D:33:ALA:O	10:D:37:GLU:HG2	2.18	0.43
11:E:305:VAL:HG12	11:E:309:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:521:LEU:HD12	2:3:521:LEU:HA	1.77	0.43
11:E:305:VAL:HG12	11:E:309:LYS:HZ2	1.83	0.43
2:3:437:ARG:NH1	6:7:249:ILE:HD12	2.22	0.43
3:4:561:GLY:O	3:4:565:LEU:HG	2.19	0.43
4:5:50:GLY:HA2	8:B:101:ASN:ND2	2.34	0.43
4:5:462:MET:HE1	4:5:514:PHE:CE2	2.53	0.43
5:6:532:LEU:HD12	5:6:532:LEU:HA	1.91	0.43
6:7:559:MET:HB3	6:7:559:MET:HE2	1.67	0.43
7:A:41:GLU:HG3	7:A:42:GLN:N	2.34	0.43
8:B:40:LEU:CD2	12:G:688:ARG:NE	2.79	0.43
10:D:187:ASP:CG	10:D:188:THR:H	2.27	0.43
11:E:259:GLU:OE2	12:G:701:LEU:HB2	2.12	0.43
1:2:723:TYR:OH	1:2:780:ILE:O	2.37	0.42
3:4:326:SER:O	3:4:326:SER:OG	2.36	0.42
4:5:523:GLU:HB2	4:5:528:ARG:HD2	2.01	0.42
8:B:148:LEU:HD23	8:B:148:LEU:HA	1.79	0.42
11:E:36:LEU:HD12	11:E:36:LEU:HA	1.63	0.42
11:E:499:MET:SD	11:E:500:GLU:N	2.92	0.42
11:E:508:GLY:O	11:E:520:ASN:ND2	2.45	0.42
12:F:541:GLY:HA3	12:F:544:TRP:CE2	2.53	0.42
1:2:746:MET:HE2	1:2:795:ILE:HG23	2.02	0.42
4:5:238:HIS:O	4:5:238:HIS:CG	2.72	0.42
4:5:348:ASP:HA	4:5:351:LYS:HB2	2.00	0.42
7:A:33:LEU:HD13	10:D:148:HIS:HB2	2.01	0.42
9:C:27:MET:HE1	9:C:122:GLN:HG3	2.01	0.42
11:E:200:MET:O	11:E:204:GLU:HG2	2.19	0.42
2:3:671:THR:HG22	2:3:682:VAL:HG11	1.99	0.42
3:4:212:CYS:HB3	3:4:262:PRO:HB3	2.01	0.42
5:6:326:LYS:HA	5:6:329:MET:HG3	2.00	0.42
5:6:544:THR:O	5:6:547:ALA:N	2.52	0.42
11:E:132:ASP:OD2	11:E:132:ASP:N	2.50	0.42
1:2:315:CYS:H	1:2:563:HIS:CE1	2.38	0.42
1:2:526:GLY:CA	5:6:619:ARG:NH2	2.77	0.42
2:3:74:GLN:HG3	2:3:76:ILE:HG12	2.02	0.42
2:3:356:ASP:OD1	2:3:357:TYR:N	2.53	0.42
2:3:383:ASP:HB3	2:3:492:SER:HB3	2.02	0.42
3:4:568:ASN:CG	5:6:217:ARG:HH21	2.13	0.42
4:5:644:PHE:O	4:5:648:THR:HG22	2.19	0.42
7:A:31:GLN:O	7:A:35:GLU:HG2	2.19	0.42
8:B:19:PRO:HD2	8:B:40:LEU:O	2.19	0.42
1:2:534:LYS:O	1:2:537:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:394:VAL:HG12	2:3:394:VAL:O	2.19	0.42
2:3:415:GLY:HA3	2:3:455:GLU:O	2.19	0.42
3:4:255:GLU:OE1	3:4:255:GLU:N	2.50	0.42
3:4:443:GLU:O	3:4:447:GLU:HG3	2.19	0.42
3:4:529:ARG:HA	3:4:529:ARG:HD2	1.83	0.42
7:A:190:VAL:HG12	7:A:191:LEU:HD12	2.01	0.42
12:H:541:GLY:HA3	12:H:544:TRP:CE2	2.53	0.42
2:3:465:THR:HG22	6:7:407:ARG:CG	2.47	0.42
3:4:654:GLN:N	3:4:654:GLN:OE1	2.53	0.42
4:5:46:THR:HG21	11:E:406:ARG:HB3	2.02	0.42
7:A:3:CYS:SG	7:A:72:ASN:ND2	2.92	0.42
12:F:641:VAL:HG22	12:F:647:VAL:HG22	2.01	0.42
1:2:315:CYS:HB2	1:2:374:GLN:NE2	2.35	0.42
1:2:561:GLN:HB3	1:2:572:GLU:HG2	2.01	0.42
3:4:196:ARG:O	3:4:200:ILE:HG12	2.20	0.42
3:4:306:CYS:HB3	3:4:309:CYS:SG	2.59	0.42
3:4:684:MET:O	3:4:687:LEU:N	2.53	0.42
5:6:449:LEU:HD23	5:6:449:LEU:HA	1.74	0.42
7:A:151:ARG:NH2	11:E:398:ILE:HG23	2.35	0.42
9:C:40:MET:HE2	9:C:43:LEU:HD12	2.02	0.42
11:E:122:ASP:OD1	11:E:122:ASP:N	2.53	0.42
11:E:207:TRP:NE1	12:G:478:ALA:O	2.52	0.42
1:2:668:ASP:HA	1:2:669:PRO:HD3	1.95	0.42
1:2:723:TYR:CE1	1:2:727:ALA:HB2	2.55	0.42
2:3:353:HIS:HB3	2:3:542:ILE:HG12	2.02	0.42
2:3:399:LEU:O	2:3:403:VAL:HG23	2.20	0.42
3:4:467:ALA:HB2	3:4:522:TYR:CD2	2.55	0.42
3:4:735:GLU:O	3:4:738:ILE:HB	2.19	0.42
4:5:348:ASP:OD1	4:5:351:LYS:HD2	2.19	0.42
7:A:151:ARG:CZ	11:E:398:ILE:CG2	2.97	0.42
8:B:81:GLU:HG2	8:B:85:THR:HG22	2.01	0.42
9:C:113:GLY:HA3	9:C:114:PRO:HA	1.81	0.42
11:E:494:ALA:HB2	11:E:506:VAL:HG22	2.02	0.42
11:E:536:ARG:HH21	11:E:550:LYS:HE2	1.84	0.42
12:G:660:PRO:HG2	12:H:553:LEU:HD21	2.02	0.42
1:2:197:HIS:CE1	1:2:201:ASN:HD21	2.37	0.42
1:2:685:ARG:HG3	1:2:686:HIS:CE1	2.55	0.42
1:2:762:ILE:HA	1:2:766:HIS:ND1	2.34	0.42
2:3:81:VAL:HG21	2:3:128:PHE:CE2	2.53	0.42
2:3:462:MET:HB3	6:7:407:ARG:NH1	2.35	0.42
5:6:48:GLN:HA	5:6:51:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:94:LEU:HD12	5:6:94:LEU:HA	1.84	0.42
5:6:593:PHE:O	5:6:597:GLN:HG2	2.20	0.42
7:A:174:GLN:CG	11:E:49:LEU:HB3	2.50	0.42
12:F:660:PRO:HG2	12:G:553:LEU:HD21	2.02	0.42
12:H:469:GLU:OE2	12:H:703:ARG:NH2	2.53	0.42
1:2:314:SER:HB2	1:2:565:VAL:HG21	2.00	0.42
1:2:331:LYS:HD2	1:2:357:SER:HB3	2.01	0.42
4:5:397:CYS:C	4:5:560:LYS:HE3	2.45	0.42
6:7:269:ASP:OD2	6:7:305:LYS:HE3	2.19	0.42
9:C:130:GLU:OE1	9:C:130:GLU:N	2.33	0.42
11:E:482:LYS:HD3	11:E:482:LYS:HA	1.88	0.42
1:2:524:ASP:HA	1:2:632:PRO:HG3	2.01	0.41
3:4:608:ASN:ND2	5:6:212:GLN:NE2	2.68	0.41
4:5:184:MET:HE1	4:5:191:TYR:CG	2.54	0.41
6:7:77:PHE:O	6:7:81:VAL:HG23	2.20	0.41
10:D:206:ILE:HG22	10:D:207:ARG:N	2.34	0.41
12:F:730:TRP:HZ2	12:G:564:LYS:HD2	1.85	0.41
1:2:673:GLU:OE2	5:6:599:LYS:NZ	2.33	0.41
2:3:206:ASP:CG	2:3:207:LEU:H	2.28	0.41
4:5:455:ARG:O	4:5:458:ILE:HG22	2.20	0.41
12:F:469:GLU:OE2	12:F:703:ARG:NH2	2.52	0.41
12:F:553:LEU:HD21	12:H:660:PRO:HG2	2.02	0.41
2:3:416:ARG:HB3	4:5:456:VAL:HG11	1.74	0.41
2:3:509:THR:OG1	2:3:510:PRO:HD2	2.20	0.41
3:4:445:ARG:O	3:4:449:LEU:HG	2.20	0.41
4:5:59:LEU:HD22	4:5:107:ALA:HB2	2.02	0.41
5:6:120:ARG:HG2	5:6:121:HIS:H	1.86	0.41
11:E:83:LEU:HA	11:E:83:LEU:HD12	1.86	0.41
12:G:469:GLU:OE2	12:G:703:ARG:NH2	2.53	0.41
1:2:588:GLU:HB3	1:2:591:LYS:HD2	2.02	0.41
2:3:511:MET:HE3	2:3:511:MET:HB2	1.91	0.41
3:4:551:PRO:O	3:4:554:ARG:HD3	2.21	0.41
5:6:486:LYS:HD3	5:6:486:LYS:HA	1.74	0.41
7:A:21:LEU:HD12	7:A:22:PRO:HD2	2.01	0.41
7:A:98:LEU:HB3	7:A:102:LEU:HD12	2.02	0.41
7:A:151:ARG:NH1	11:E:398:ILE:HG23	2.35	0.41
1:2:203:LEU:HD23	1:2:203:LEU:HA	1.90	0.41
1:2:342:SER:OG	1:2:344:ASN:OD1	2.29	0.41
1:2:464:ILE:HD13	1:2:467:LEU:HD12	2.01	0.41
2:3:281:GLN:HG3	2:3:313:MET:HG3	2.02	0.41
3:4:275:ASN:OD1	6:7:263:ARG:NH2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:503:GLU:HB3	3:4:612:SER:HB3	2.02	0.41
3:4:744:HIS:CE1	3:4:760:GLU:HG2	2.55	0.41
4:5:334:VAL:HG22	4:5:554:ILE:HG13	2.02	0.41
6:7:533:LEU:O	6:7:537:ILE:HG13	2.20	0.41
6:7:645:LEU:HD23	6:7:645:LEU:HA	1.91	0.41
7:A:195:LEU:CD2	11:E:41:GLN:OE1	2.69	0.41
9:C:88:LEU:HD13	9:C:134:ILE:HD11	2.02	0.41
11:E:67:GLU:OE2	11:E:67:GLU:N	2.53	0.41
12:H:435:SER:HB3	12:H:629:TRP:CD1	2.56	0.41
5:6:65:PHE:O	5:6:69:GLU:HG3	2.19	0.41
5:6:322:ALA:O	5:6:326:LYS:HB2	2.21	0.41
5:6:450:MET:HE3	5:6:450:MET:HB2	1.87	0.41
6:7:166:ILE:HA	6:7:269:ASP:O	2.20	0.41
7:A:24:PHE:CG	7:A:107:ALA:HB2	2.55	0.41
9:C:165:VAL:HA	9:C:168:LEU:HD13	2.02	0.41
11:E:254:HIS:O	11:E:254:HIS:ND1	2.54	0.41
11:E:416:LEU:HD23	11:E:416:LEU:HA	1.88	0.41
12:F:435:SER:HB3	12:F:629:TRP:CD1	2.56	0.41
12:G:730:TRP:HZ2	12:H:564:LYS:HD2	1.85	0.41
4:5:167:ARG:NH1	4:5:181:ASN:HD22	2.18	0.41
4:5:555:ASP:OD1	4:5:555:ASP:N	2.52	0.41
5:6:450:MET:HE1	5:6:493:LEU:HD13	2.03	0.41
6:7:182:TYR:HB2	6:7:191:THR:HG23	2.03	0.41
7:A:151:ARG:NH2	11:E:398:ILE:CG2	2.84	0.41
7:A:165:THR:HB	11:E:18:ARG:NH2	2.35	0.41
1:2:377:ARG:NH1	1:2:377:ARG:HB3	2.36	0.41
1:2:606:GLN:NE2	4:5:392:LYS:HZ2	2.15	0.41
1:2:718:GLU:HG3	1:2:722:LYS:NZ	2.36	0.41
2:3:468:HIS:O	2:3:523:ARG:NH2	2.50	0.41
3:4:176:PRO:O	3:4:177:LEU:HD23	2.21	0.41
5:6:158:CYS:HA	5:6:191:PHE:HD1	1.86	0.41
5:6:357:THR:CA	5:6:551:ARG:HH12	2.00	0.41
6:7:135:GLU:HG3	6:7:137:TYR:OH	2.21	0.41
7:A:7:MET:HE3	7:A:7:MET:HB3	1.89	0.41
7:A:116:ASN:OD1	7:A:119:ARG:NH2	2.53	0.41
7:A:194:ILE:O	7:A:196:SER:N	2.53	0.41
1:2:311:VAL:HG22	1:2:411:GLU:HG3	2.03	0.41
1:2:616:ILE:HD12	1:2:616:ILE:HA	1.77	0.41
1:2:765:ARG:HD3	1:2:768:GLU:OE1	2.20	0.41
2:3:156:VAL:HG21	2:3:161:LEU:HD13	2.03	0.41
3:4:472:GLU:HG3	3:4:473:HIS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:46:THR:CG2	11:E:406:ARG:O	2.56	0.41
4:5:529:ASP:HA	4:5:532:LEU:HD12	2.03	0.41
4:5:602:ARG:C	4:5:604:SER:H	2.27	0.41
5:6:325:ILE:O	5:6:329:MET:HG2	2.20	0.41
5:6:437:GLU:C	5:6:440:HIS:H	2.29	0.41
6:7:348:GLU:OE2	6:7:348:GLU:N	2.36	0.41
7:A:152:CYS:SG	7:A:169:LEU:HG	2.61	0.41
7:A:176:PHE:CG	11:E:47:TYR:CE1	3.09	0.41
8:B:84:PHE:O	8:B:147:ASN:ND2	2.48	0.41
8:B:173:ASN:OD1	9:C:135:SER:OG	2.28	0.41
11:E:364:HIS:CD2	11:E:370:LYS:HD2	2.56	0.41
1:2:233:ASN:HB3	1:2:236:ASP:OD1	2.21	0.41
1:2:715:LEU:HA	1:2:716:PRO:HD3	1.91	0.41
1:2:726:TYR:CZ	1:2:730:ARG:HD2	2.56	0.41
1:2:793:MET:HB3	1:2:793:MET:HE3	1.80	0.41
2:3:414:THR:OG1	4:5:460:GLU:OE2	2.38	0.41
2:3:480:LYS:HD3	2:3:480:LYS:HA	1.80	0.41
3:4:631:ILE:HG13	3:4:631:ILE:O	2.20	0.41
5:6:59:ASN:OD1	5:6:59:ASN:N	2.53	0.41
5:6:187:ASN:HD22	5:6:190:ARG:HB2	1.86	0.41
5:6:516:LEU:HD12	5:6:516:LEU:HA	1.90	0.41
8:B:40:LEU:CD1	12:G:688:ARG:NE	2.77	0.41
11:E:23:VAL:HG12	11:E:24:ALA:O	2.21	0.41
12:G:435:SER:HB3	12:G:629:TRP:CD1	2.56	0.41
1:2:328:ASN:HA	1:2:335:VAL:HA	2.03	0.40
2:3:526:LEU:HD23	2:3:526:LEU:HA	1.85	0.40
3:4:499:LYS:HB3	3:4:499:LYS:HE3	1.83	0.40
4:5:507:MET:SD	4:5:507:MET:N	2.94	0.40
6:7:427:LEU:HD12	6:7:427:LEU:H	1.85	0.40
7:A:43:ASN:HB2	7:A:65:ARG:HD3	2.02	0.40
8:B:57:LYS:NZ	11:E:211:LYS:HZ1	2.18	0.40
11:E:284:TRP:HE1	11:E:424:ARG:NH2	2.20	0.40
2:3:114:ALA:HB2	2:3:169:VAL:HG23	2.03	0.40
2:3:509:THR:HG23	2:3:511:MET:N	2.35	0.40
3:4:462:LEU:HD23	3:4:462:LEU:HA	1.90	0.40
4:5:42:TYR:CD1	11:E:367:PHE:CB	3.04	0.40
4:5:128:LEU:O	4:5:128:LEU:HD12	2.21	0.40
4:5:271:ILE:HG12	4:5:291:SER:O	2.21	0.40
5:6:204:GLN:HB2	5:6:233:VAL:HG22	2.04	0.40
8:B:60:LEU:HD23	8:B:60:LEU:HA	1.93	0.40
9:C:40:MET:O	9:C:59:ALA:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:414:THR:HA	2:3:454:ASP:OD1	2.22	0.40
2:3:549:MET:HE2	4:5:365:LEU:HD13	2.03	0.40
2:3:659:THR:O	2:3:662:THR:HG22	2.22	0.40
3:4:471:TYR:HD2	3:4:658:TYR:CE1	2.32	0.40
5:6:524:ALA:HB3	5:6:525:PRO:HD3	2.02	0.40
6:7:400:ARG:O	6:7:440:GLY:HA3	2.21	0.40
7:A:166:SER:C	11:E:68:GLN:HG2	2.40	0.40
9:C:21:SER:O	9:C:21:SER:OG	2.39	0.40
12:H:554:LEU:HD22	12:H:567:PHE:CE1	2.57	0.40
1:2:271:TYR:OH	11:E:313:GLU:CD	2.59	0.40
1:2:814:MET:HE2	1:2:814:MET:HB3	1.88	0.40
2:3:65:LEU:HD12	2:3:65:LEU:HA	1.94	0.40
2:3:180:SER:OG	2:3:181:LEU:N	2.54	0.40
2:3:242:GLN:HG2	2:3:243:THR:H	1.86	0.40
3:4:752:LYS:HE2	3:4:752:LYS:HB3	1.86	0.40
4:5:49:THR:CG2	11:E:407:SER:HB2	2.51	0.40
7:A:124:TYR:CE2	10:D:97:LEU:HD11	2.56	0.40
12:F:497:ILE:HB	12:F:514:LEU:HB2	2.03	0.40
1:2:236:ASP:OD2	1:2:237:LEU:N	2.54	0.40
1:2:461:VAL:O	1:2:464:ILE:N	2.54	0.40
3:4:645:ASP:HB2	3:4:736:SER:OG	2.22	0.40
3:4:666:LEU:HD23	3:4:666:LEU:HA	1.93	0.40
6:7:51:ASP:OD1	6:7:53:ASP:N	2.45	0.40
6:7:339:SER:HB3	6:7:553:PRO:HA	2.03	0.40
7:A:94:TYR:HE2	9:C:202:LEU:HD11	1.87	0.40
11:E:165:VAL:HG22	11:E:169:MET:HG3	2.03	0.40
11:E:549:LEU:HD12	11:E:549:LEU:HA	1.88	0.40
12:F:564:LYS:HD2	12:H:730:TRP:HZ2	1.85	0.40
12:H:497:ILE:HB	12:H:514:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	603/904 (67%)	523 (87%)	80 (13%)	0	100	100
2	3	602/853 (71%)	532 (88%)	70 (12%)	0	100	100
3	4	592/863 (69%)	507 (86%)	84 (14%)	1 (0%)	43	78
4	5	563/734 (77%)	503 (89%)	59 (10%)	1 (0%)	43	78
5	6	603/821 (73%)	538 (89%)	62 (10%)	3 (0%)	24	63
6	7	592/719 (82%)	528 (89%)	63 (11%)	1 (0%)	43	78
7	A	194/196 (99%)	170 (88%)	24 (12%)	0	100	100
8	B	174/185 (94%)	161 (92%)	13 (8%)	0	100	100
9	C	190/216 (88%)	173 (91%)	17 (9%)	0	100	100
10	D	201/223 (90%)	186 (92%)	15 (8%)	0	100	100
11	E	534/566 (94%)	480 (90%)	54 (10%)	0	100	100
12	F	404/1171 (34%)	396 (98%)	8 (2%)	0	100	100
12	G	404/1171 (34%)	396 (98%)	8 (2%)	0	100	100
12	H	404/1171 (34%)	396 (98%)	8 (2%)	0	100	100
All	All	6060/9793 (62%)	5489 (91%)	565 (9%)	6 (0%)	49	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	540	CYS
3	4	653	PRO
4	5	115	PRO
5	6	559	ILE
5	6	563	ILE
6	7	490	PRO

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	2	535/781 (68%)	535 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3	527/742 (71%)	527 (100%)	0	100	100
3	4	530/753 (70%)	528 (100%)	2 (0%)	84	84
4	5	494/625 (79%)	493 (100%)	1 (0%)	87	87
5	6	545/724 (75%)	541 (99%)	4 (1%)	76	81
6	7	514/619 (83%)	507 (99%)	7 (1%)	59	72
7	A	174/174 (100%)	173 (99%)	1 (1%)	78	83
8	B	160/169 (95%)	160 (100%)	0	100	100
9	C	167/186 (90%)	167 (100%)	0	100	100
10	D	188/205 (92%)	188 (100%)	0	100	100
11	E	491/517 (95%)	489 (100%)	2 (0%)	84	84
12	F	350/1017 (34%)	347 (99%)	3 (1%)	70	79
12	G	350/1017 (34%)	347 (99%)	3 (1%)	70	79
12	H	350/1017 (34%)	347 (99%)	3 (1%)	70	79
All	All	5375/8546 (63%)	5349 (100%)	26 (0%)	78	83

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	372	LEU
3	4	428	ARG
4	5	271	ILE
5	6	226	VAL
5	6	559	ILE
5	6	563	ILE
5	6	565	ARG
6	7	311	ASP
6	7	312	ASP
6	7	319	LEU
6	7	320	THR
6	7	527	ARG
6	7	528	ASP
6	7	529	ASN
7	A	80	LEU
11	E	132	ASP
11	E	284	TRP
12	F	599	LEU
12	F	601	VAL

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Mol	Chain	Res	Type
12	F	804	ARG
12	G	599	LEU
12	G	601	VAL
12	G	804	ARG
12	H	599	LEU
12	H	601	VAL
12	H	804	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	180	HIS
1	2	196	HIS
1	2	197	HIS
1	2	201	ASN
1	2	206	HIS
1	2	282	HIS
1	2	328	ASN
1	2	419	HIS
1	2	443	HIS
1	2	488	HIS
1	2	511	HIS
1	2	561	GLN
1	2	601	HIS
1	2	606	GLN
1	2	607	GLN
1	2	683	HIS
2	3	97	ASN
2	3	112	ASN
2	3	155	HIS
2	3	241	HIS
2	3	488	ASN
2	3	513	ASN
2	3	545	HIS
3	4	165	ASN
3	4	171	GLN
3	4	195	GLN
3	4	214	HIS
3	4	256	HIS
3	4	368	HIS
3	4	415	HIS
3	4	473	HIS

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Mol	Chain	Res	Type
3	4	521	GLN
3	4	525	ASN
3	4	568	ASN
3	4	588	HIS
3	4	633	ASN
3	4	695	HIS
3	4	733	GLN
3	4	744	HIS
4	5	95	HIS
4	5	181	ASN
4	5	244	HIS
4	5	376	ASN
4	5	426	ASN
4	5	459	HIS
5	6	27	GLN
5	6	70	GLN
5	6	212	GLN
5	6	342	GLN
5	6	349	ASN
6	7	36	GLN
6	7	186	GLN
6	7	223	GLN
6	7	243	GLN
6	7	503	GLN
6	7	543	HIS
7	A	20	GLN
7	A	72	ASN
7	A	174	GLN
7	A	188	GLN
8	B	51	ASN
8	B	101	ASN
8	B	102	HIS
8	B	166	HIS
9	C	136	GLN
9	C	155	ASN
9	C	177	GLN
9	C	180	GLN
10	D	60	HIS
10	D	78	HIS
11	E	15	GLN
11	E	37	GLN
11	E	248	HIS

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Mol	Chain	Res	Type
11	E	253	ASN
11	E	324	GLN
11	E	339	ASN
11	E	364	HIS
11	E	414	HIS
12	F	563	GLN
12	F	602	GLN
12	F	615	HIS
12	F	663	ASN
12	F	667	HIS
12	F	717	GLN
12	G	459	ASN
12	G	563	GLN
12	G	602	GLN
12	G	615	HIS
12	G	663	ASN
12	G	667	HIS
12	G	717	GLN
12	H	563	GLN
12	H	602	GLN
12	H	615	HIS
12	H	663	ASN
12	H	667	HIS
12	H	717	GLN
12	H	738	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

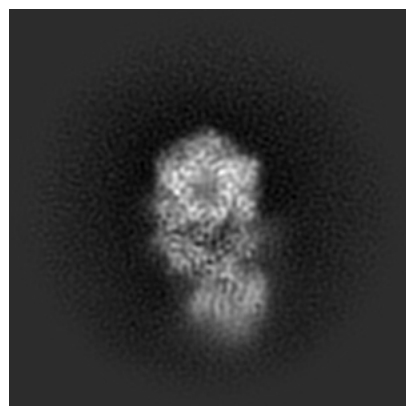
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10621. These allow visual inspection of the internal detail of the map and identification of artifacts.

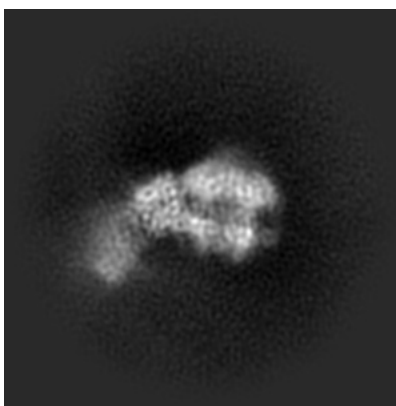
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

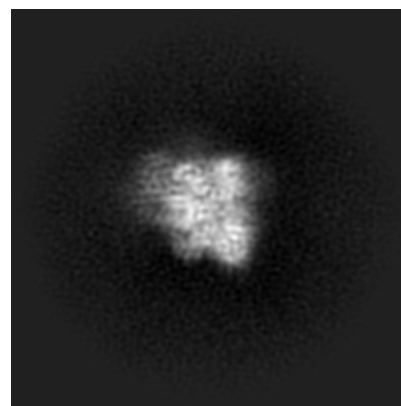
6.1.1 Primary map



X

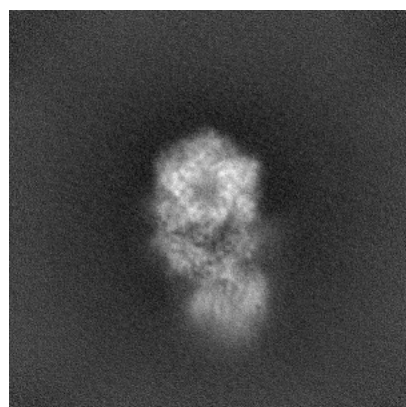


Y

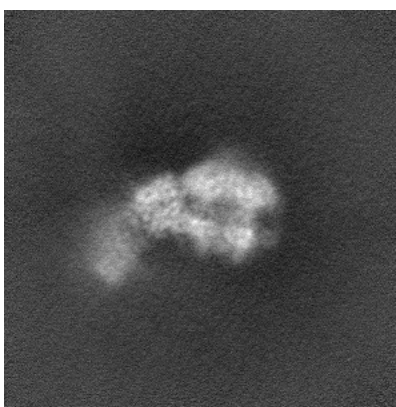


Z

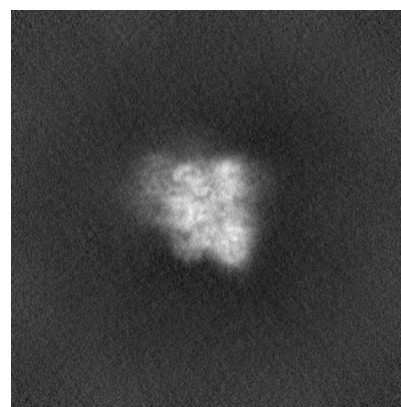
6.1.2 Raw map



X



Y

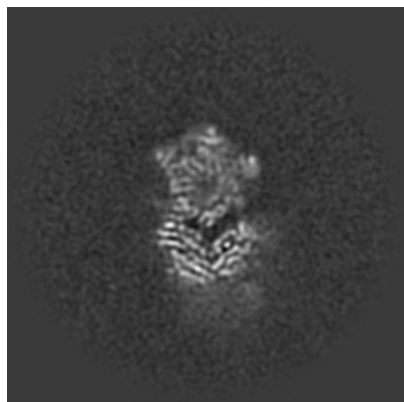


Z

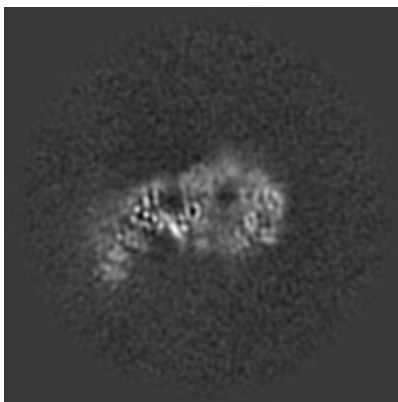
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

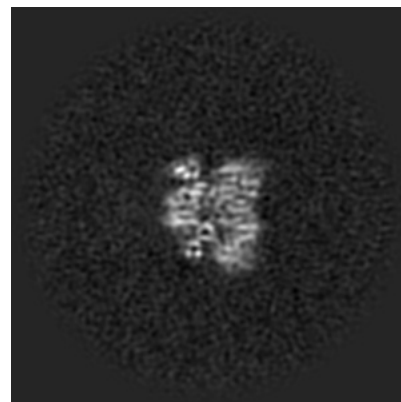
6.2.1 Primary map



X Index: 215

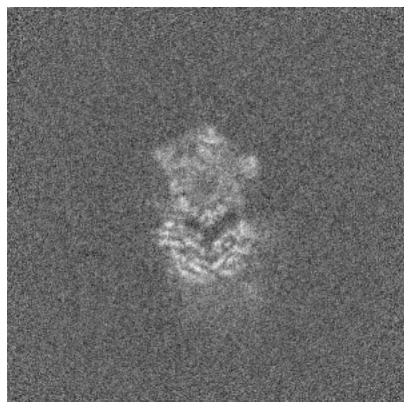


Y Index: 215

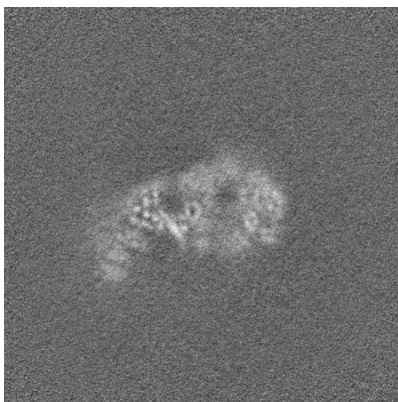


Z Index: 215

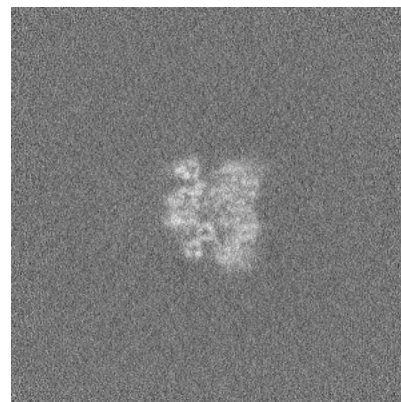
6.2.2 Raw map



X Index: 215



Y Index: 215

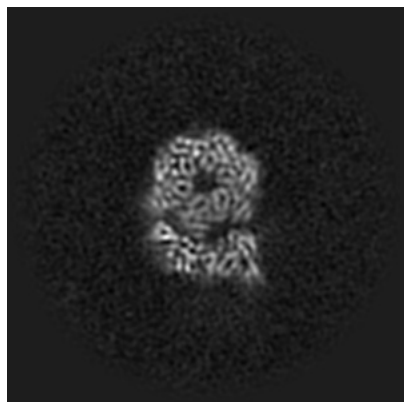


Z Index: 215

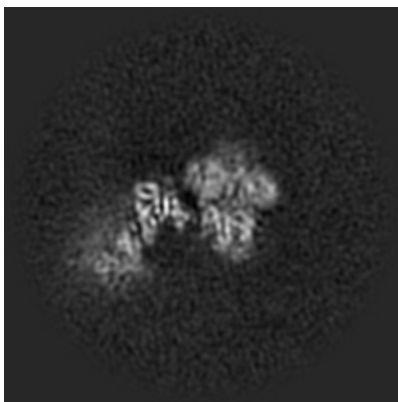
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

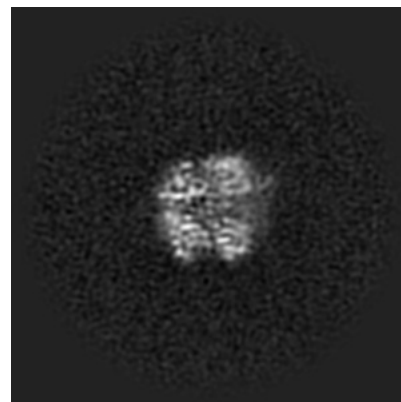
6.3.1 Primary map



X Index: 233

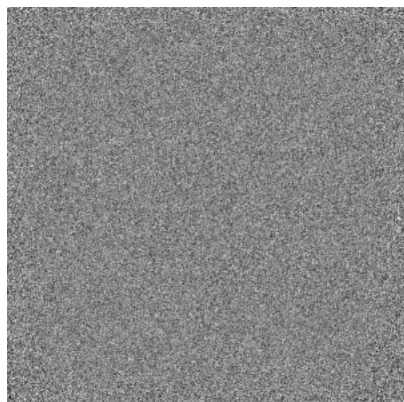


Y Index: 236

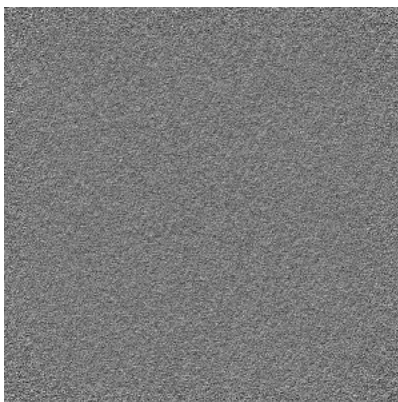


Z Index: 254

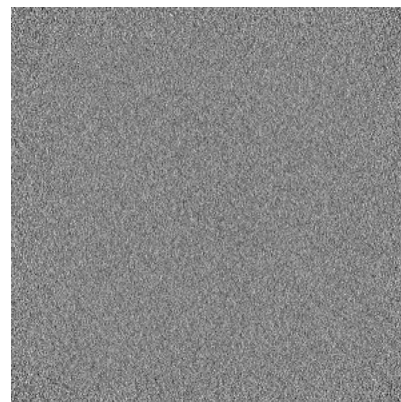
6.3.2 Raw map



X Index: 0



Y Index: 0

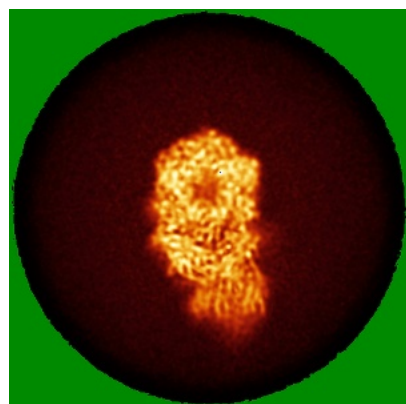


Z Index: 0

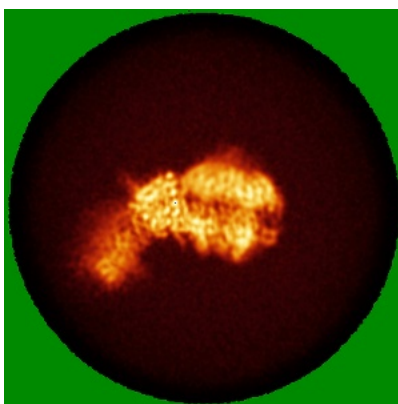
The images above show the largest variance slices of the map in three orthogonal directions.

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

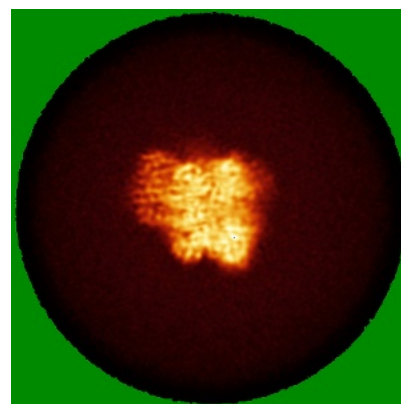
6.4.1 Primary map



X

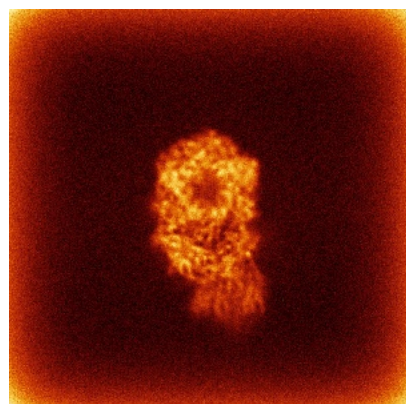


Y

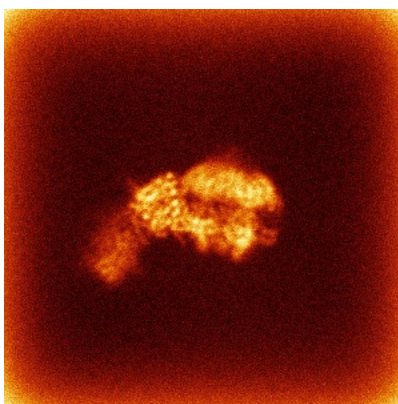


Z

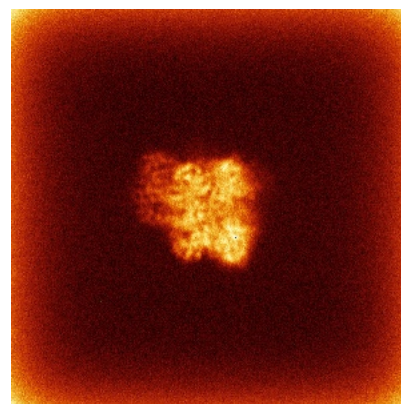
6.4.2 Raw map



X



Y

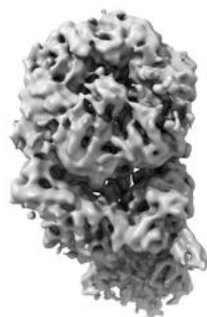


Z

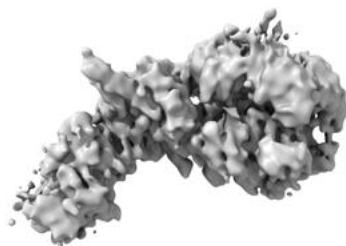
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

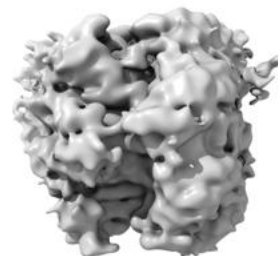
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

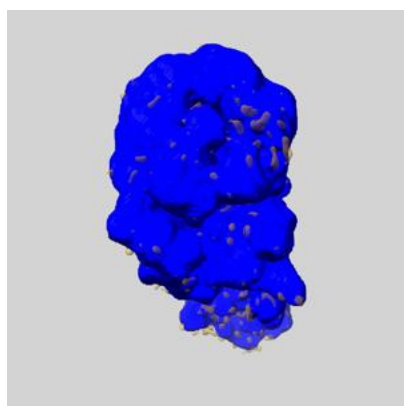
6.6 Mask visualisation [i](#)

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

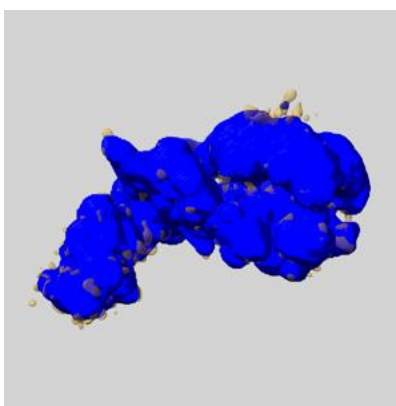
A mask typically either:

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

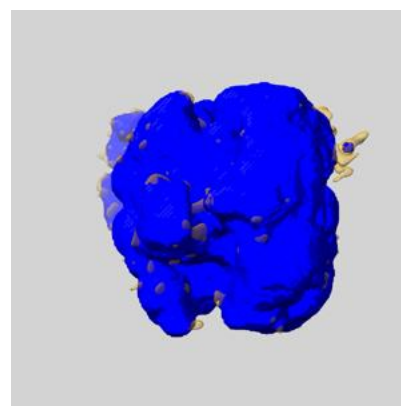
6.6.1 emd_10621_msk_1.map [i](#)



X



Y

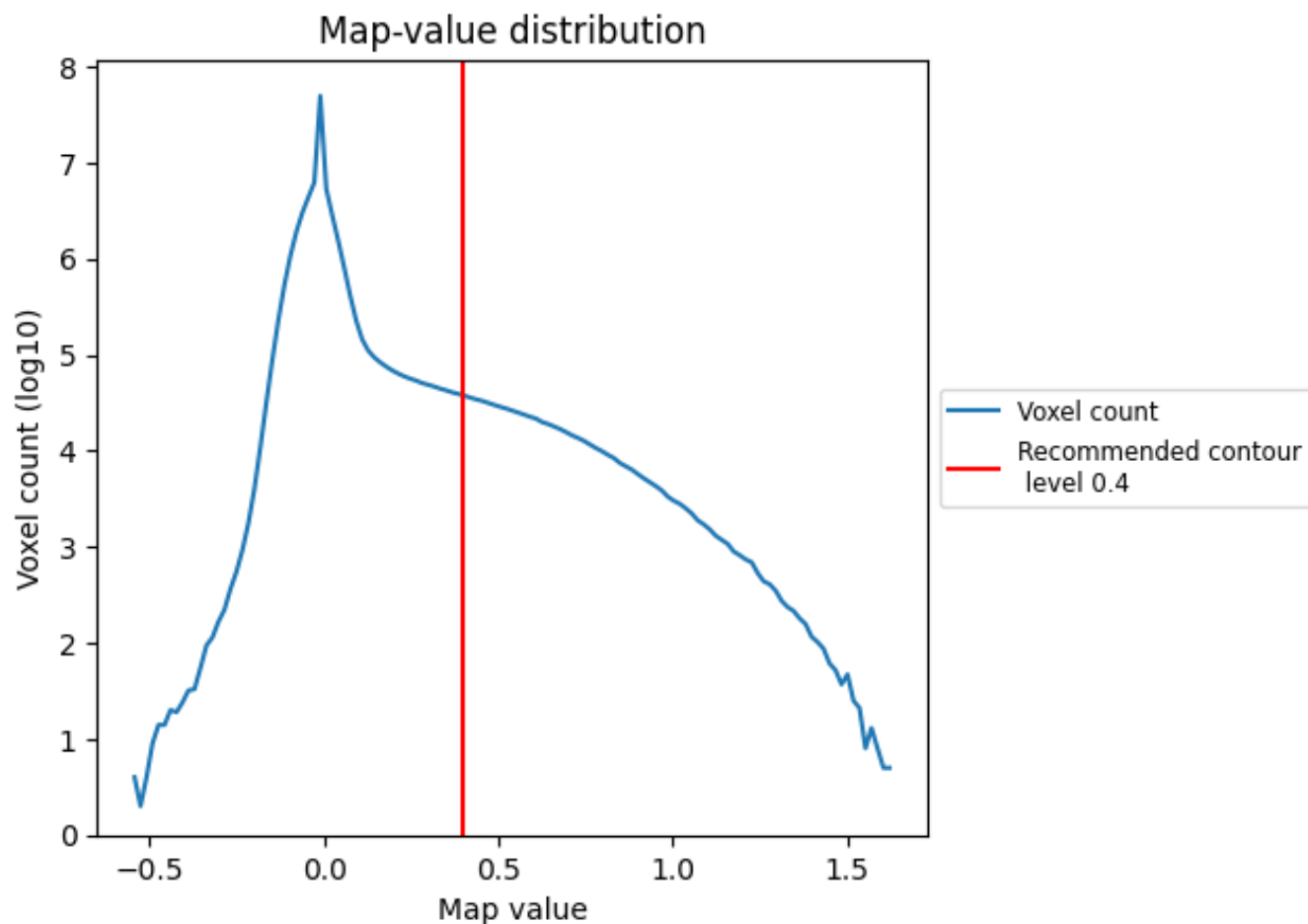


Z

7 Map analysis [i](#)

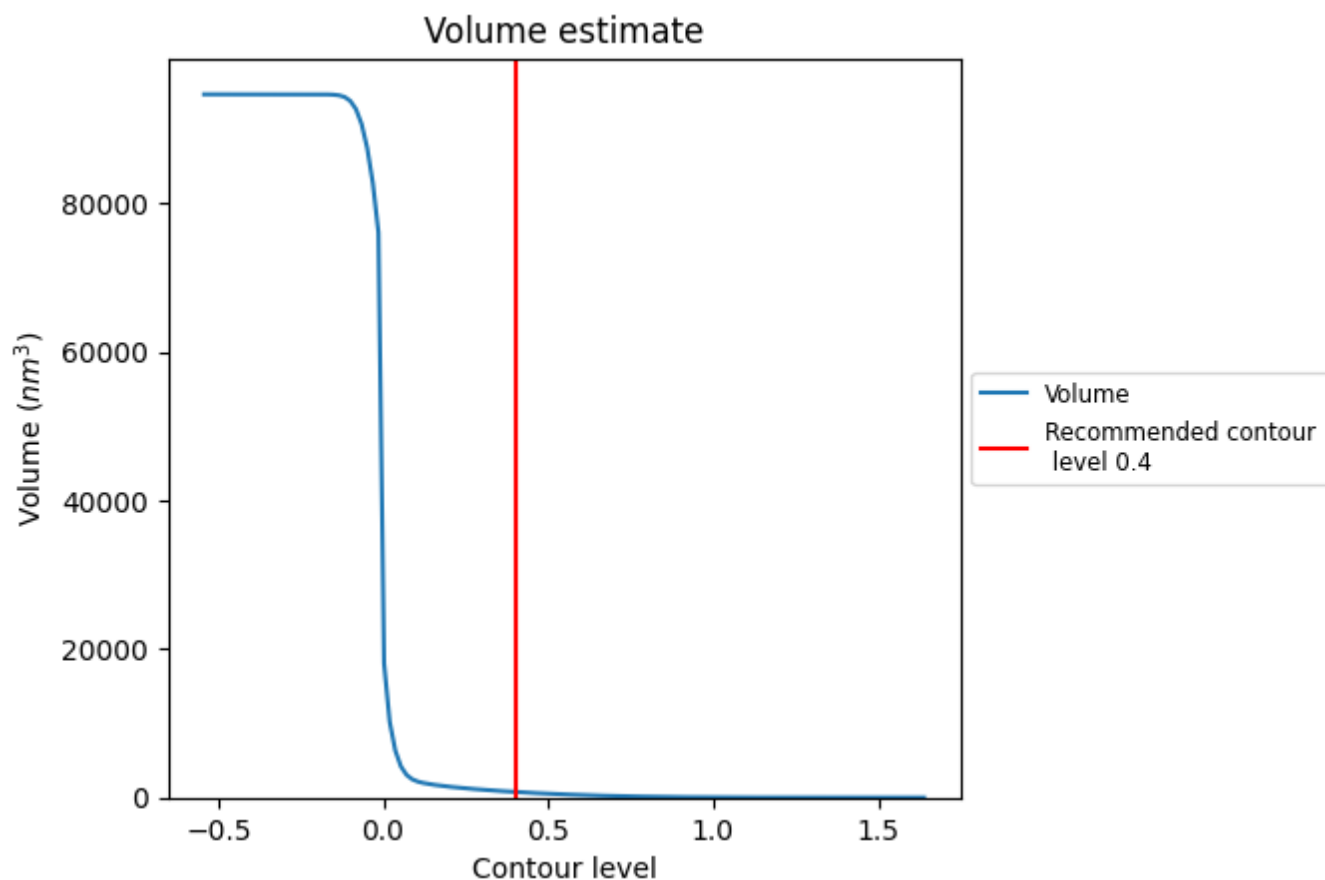
This section contains the results of statistical analysis of the map.

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.

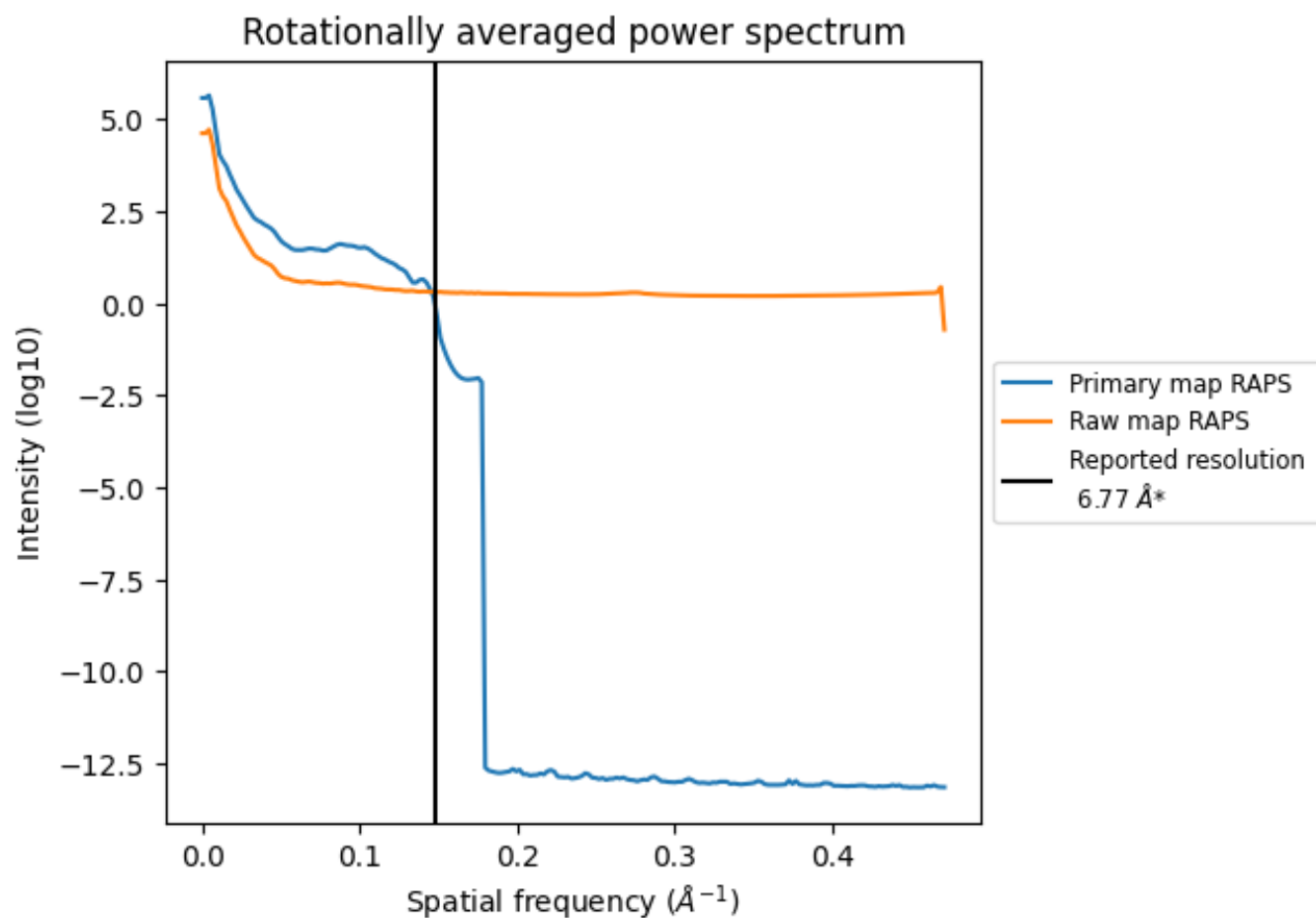
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 757 nm³; this corresponds to an approximate mass of 683 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 ⓘ

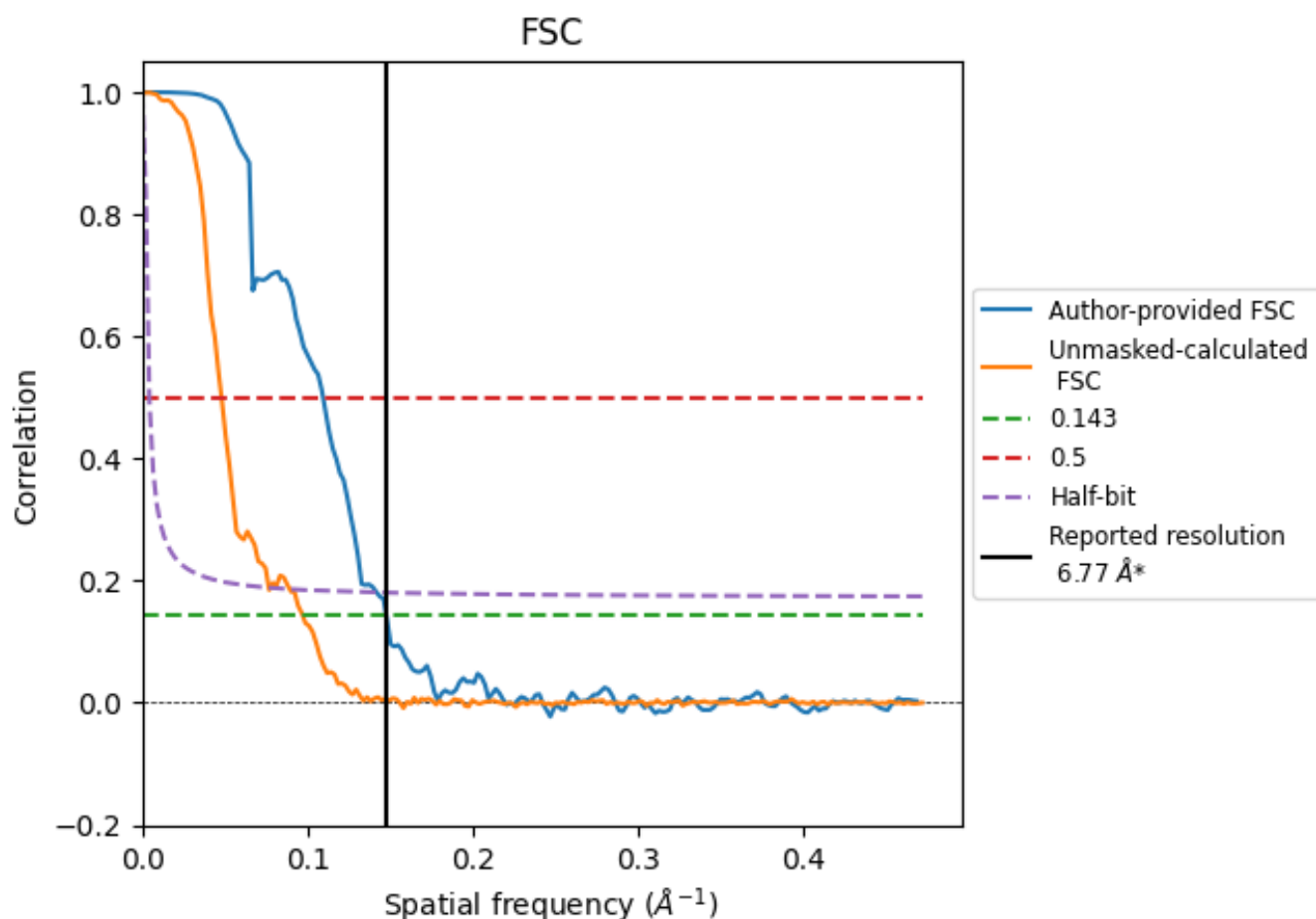


*Reported resolution corresponds to spatial frequency of 0.148 Å⁻¹

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 0.148 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

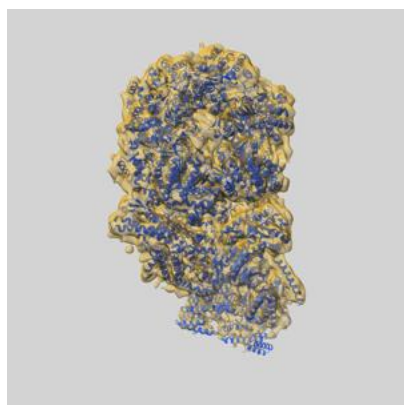
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.77	-	-
Author-provided FSC curve	6.78	9.14	7.05
Unmasked-calculated*	10.31	20.88	13.05

*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 10.31 differs from the reported value 6.77 by more than 10 %

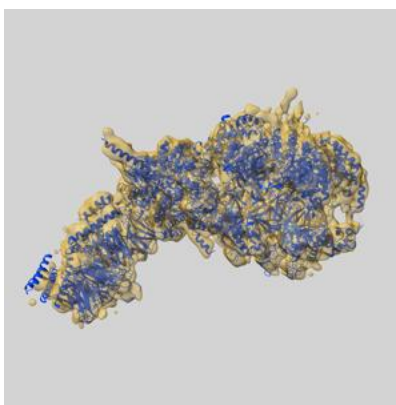
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10621 and PDB model 6XTY. Per-residue inclusion information can be found in section [3](#) on page [10](#).

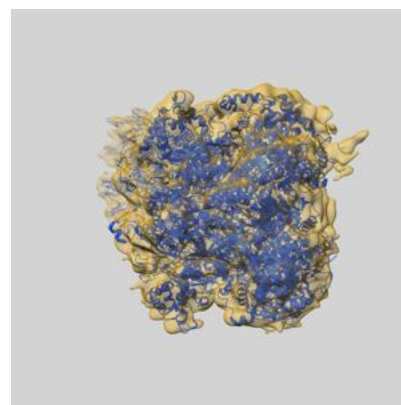
9.1 Map-model overlay [i](#)



X



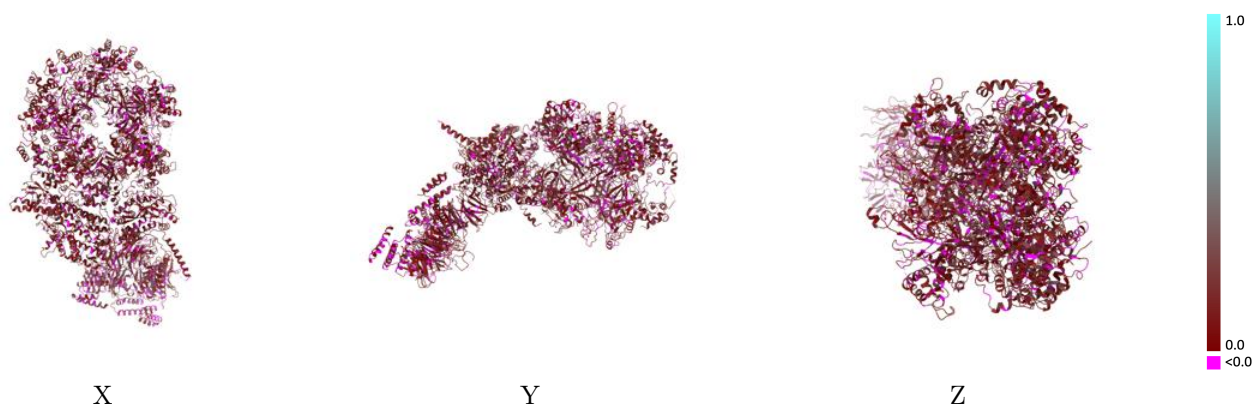
Y



Z

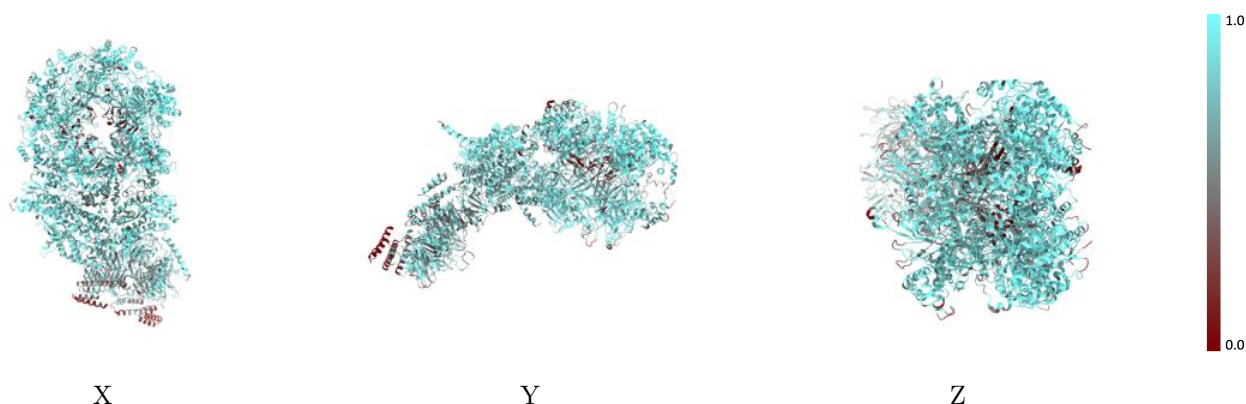
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



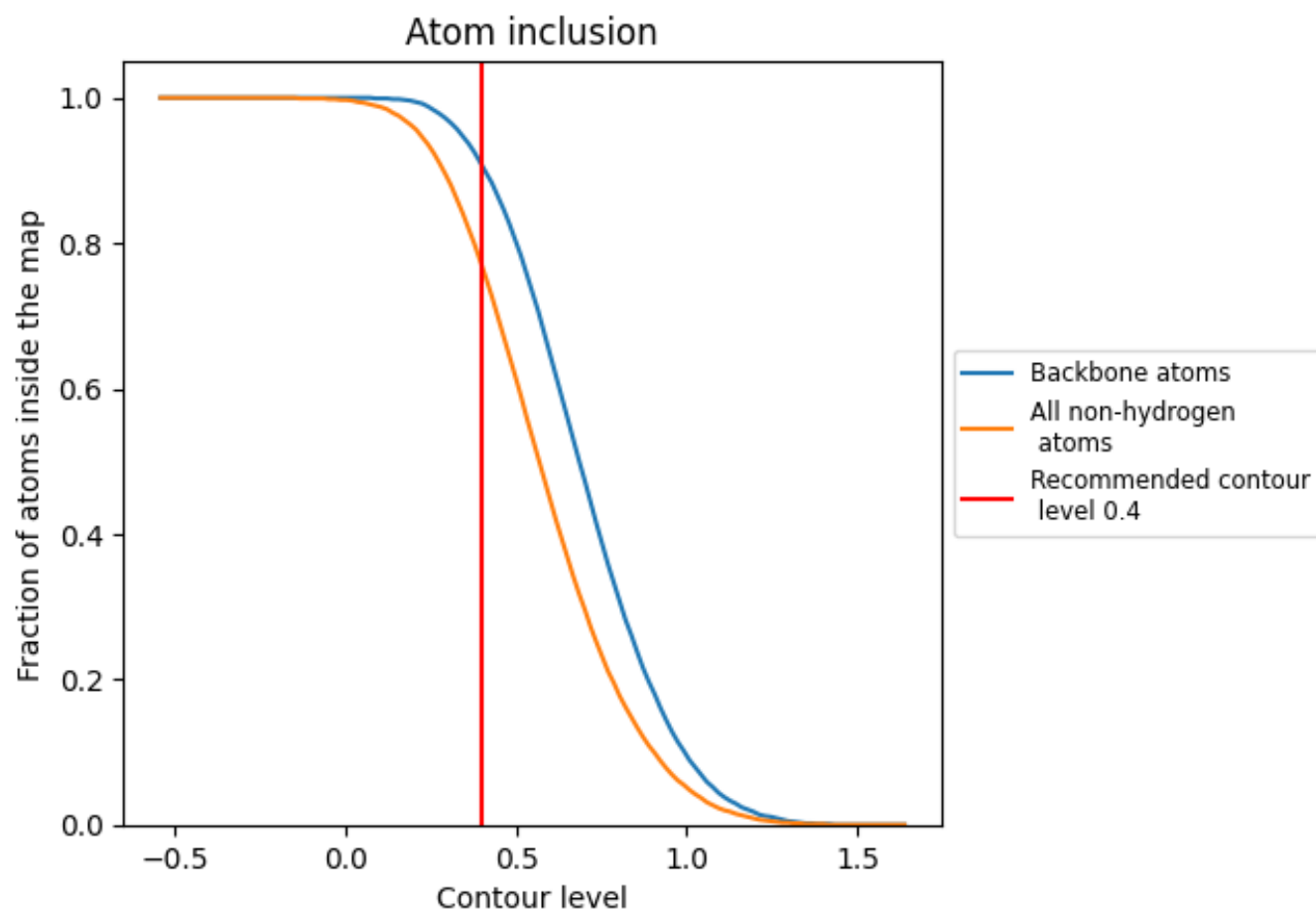
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 77% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7680	0.1270
2	0.8100	0.1330
3	0.8100	0.1200
4	0.8170	0.1280
5	0.7610	0.1260
6	0.8180	0.1210
7	0.8260	0.1250
A	0.8330	0.1430
B	0.8010	0.1520
C	0.8150	0.1420
D	0.8350	0.1380
E	0.7980	0.1410
F	0.6680	0.1200
G	0.5650	0.1270
H	0.5750	0.0990

1.0

0.0

<0.0