



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:06 AM UTC

PDB ID : 6YBA / pdb_00006yba
EMDB ID : EMD-10768
Title : HAdV-F41 Capsid
Authors : Perez Illana, M.; Martinez, M.; Mangroo, C.; Brown, M.; Marabini, R.; San Martin, C.
Deposited on : 2020-03-16
Resolution : 4.00 Å(reported)

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

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

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

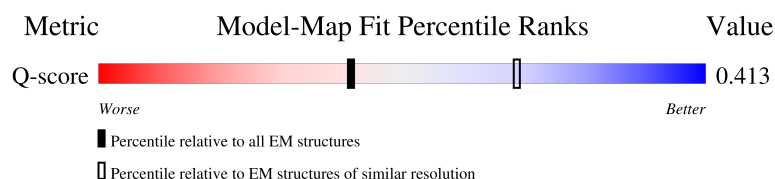
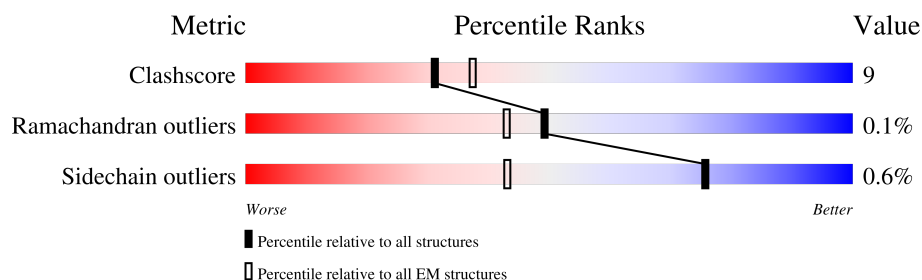
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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

Mol	Chain	Length	Quality of chain
1	A	925	24% 73% 25%
1	B	925	25% 75% 24%
1	C	925	23% 73% 25%
1	D	925	18% 75% 23%

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Mol	Chain	Length	Quality of chain
1	E	925	
1	F	925	
1	G	925	
1	H	925	
1	I	925	
1	J	925	
1	K	925	
1	L	925	
2	M	508	
3	N	579	
4	O	233	
4	P	233	
5	Q	133	
5	R	133	
5	S	133	
5	T	133	
6	U	266	
6	V	266	
6	Y	266	
6	u	266	
7	W	183	
7	w	183	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 98037 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	912	Total	C	N	O	S	0	0
			7244	4603	1226	1379	36		
1	B	913	Total	C	N	O	S	0	0
			7250	4607	1227	1380	36		
1	C	914	Total	C	N	O	S	0	0
			7254	4610	1227	1381	36		
1	D	908	Total	C	N	O	S	0	0
			7214	4585	1221	1372	36		
1	E	917	Total	C	N	O	S	0	0
			7273	4620	1231	1386	36		
1	F	910	Total	C	N	O	S	0	0
			7229	4595	1223	1375	36		
1	G	910	Total	C	N	O	S	0	0
			7229	4595	1223	1375	36		
1	H	915	Total	C	N	O	S	0	0
			7262	4615	1228	1382	37		
1	I	908	Total	C	N	O	S	0	0
			7214	4585	1221	1372	36		
1	J	914	Total	C	N	O	S	0	0
			7254	4610	1227	1381	36		
1	K	912	Total	C	N	O	S	0	0
			7242	4603	1225	1378	36		
1	L	911	Total	C	N	O	S	0	0
			7238	4601	1224	1377	36		

- Molecule 2 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	452	Total	C	N	O	S	0	0
			3609	2288	621	688	12		

- Molecule 3 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	298	Total	C	N	O	S	0	0
			2315	1447	413	451	4		

- Molecule 4 is a protein called Pre-hexon-linking protein VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	180	Total	C	N	O	S	0	0
			1379	865	236	273	5		
4	P	180	Total	C	N	O	S	0	0
			1379	865	236	273	5		

- Molecule 5 is a protein called Hexon-interlacing protein.

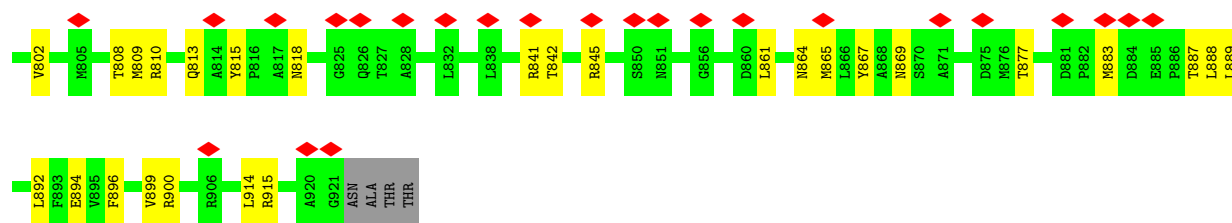
Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	50	Total	C	N	O	S	0	0
			365	232	65	67	1		
5	R	50	Total	C	N	O	S	0	0
			365	232	65	67	1		
5	S	50	Total	C	N	O	S	0	0
			365	232	65	67	1		
5	T	50	Total	C	N	O	S	0	0
			365	232	65	67	1		

- Molecule 6 is a protein called Pre-protein VI.

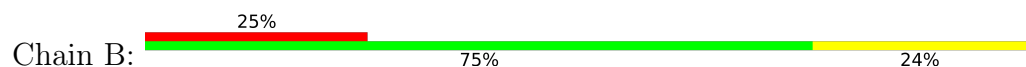
Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	29	Total	C	N	O	S	0	0
			218	135	42	40	1		
6	V	29	Total	C	N	O	S	0	0
			218	135	42	40	1		
6	Y	29	Total	C	N	O	S	0	0
			218	135	42	40	1		
6	u	29	Total	C	N	O	S	0	0
			218	135	42	40	1		

- Molecule 7 is a protein called Pre-histone-like nucleoprotein.

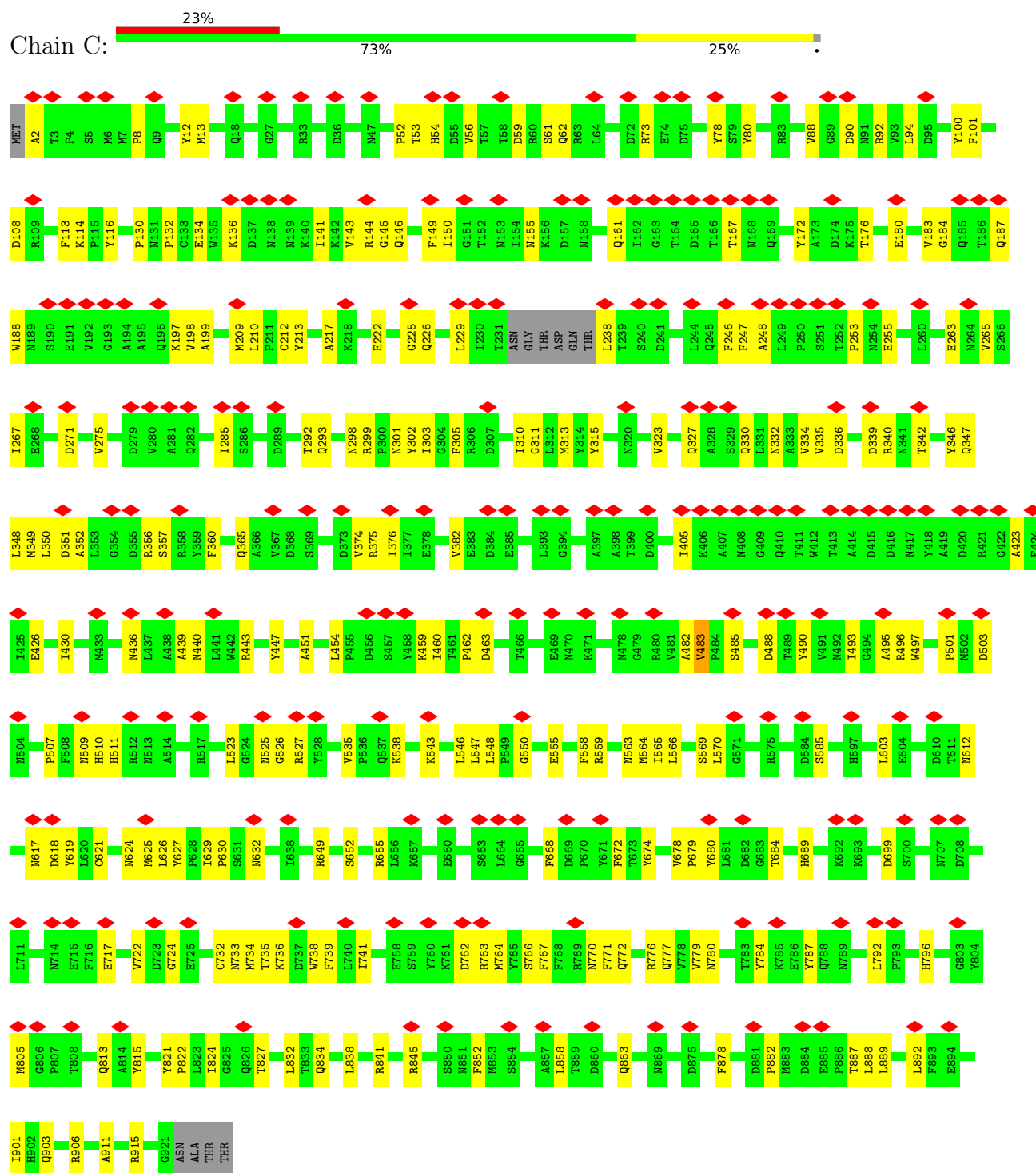
Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	6	Total	C	N	O	S	0	0
			37	23	6	7	1		
7	w	12	Total	C	N	O	S	0	0
			83	53	15	14	1		



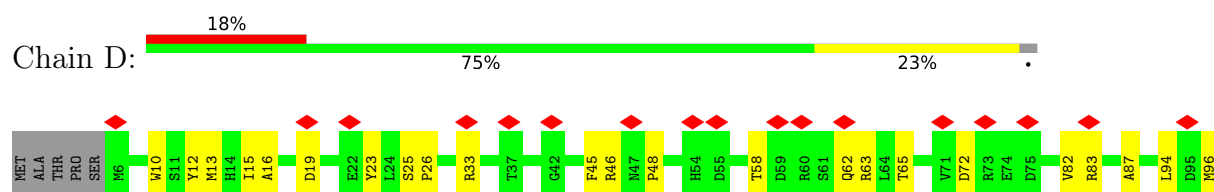
• Molecule 1: Hexon protein

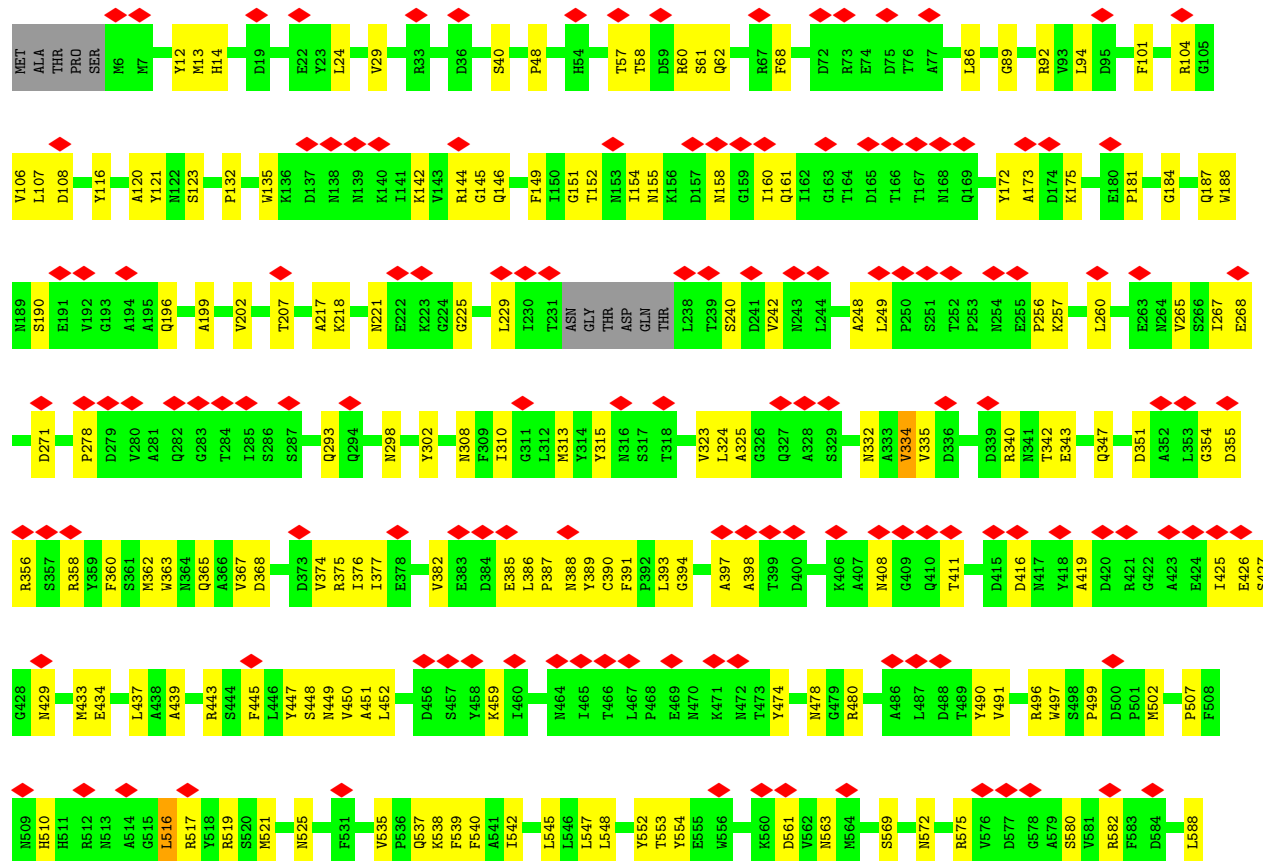


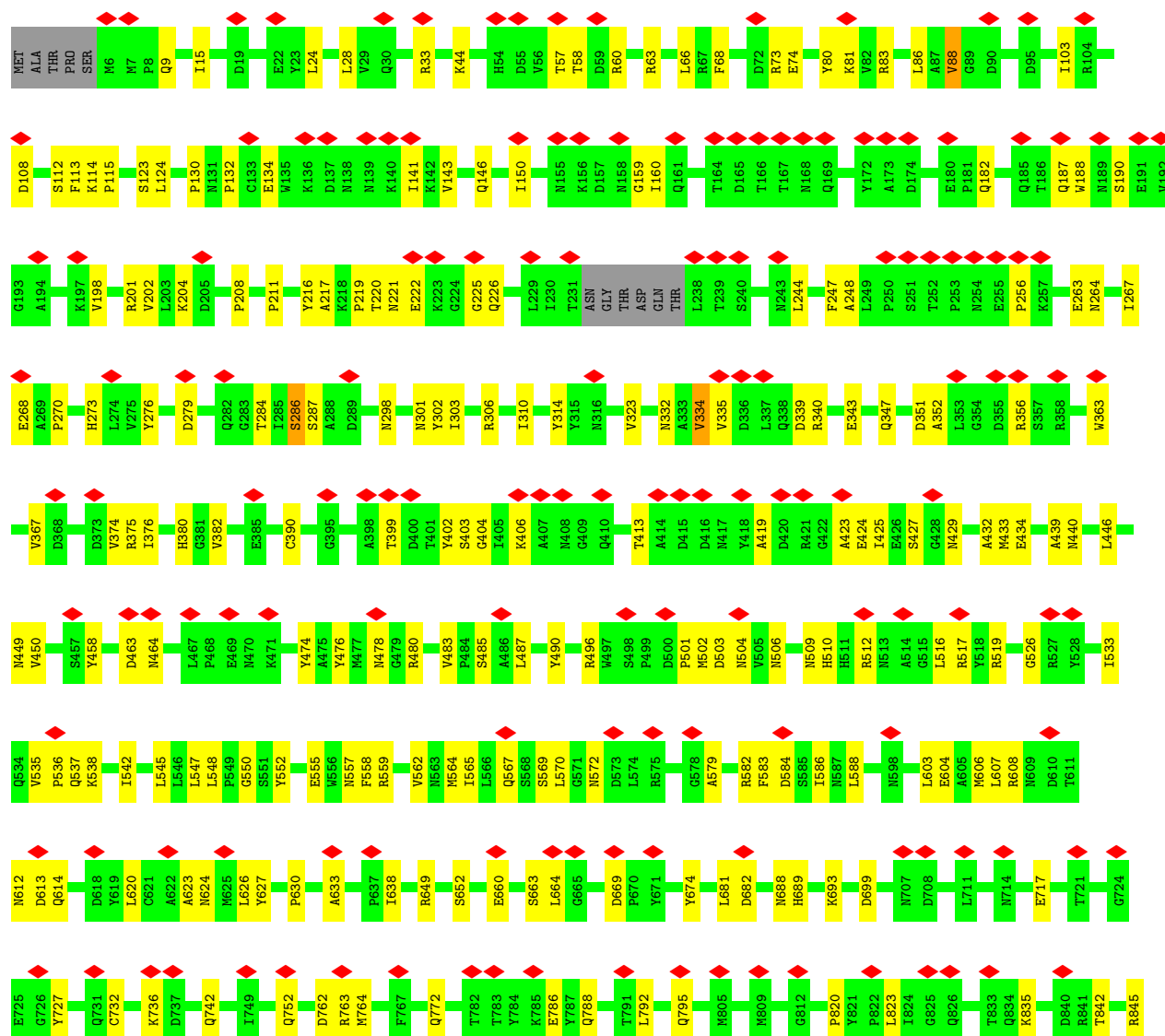
• Molecule 1: Hexon protein

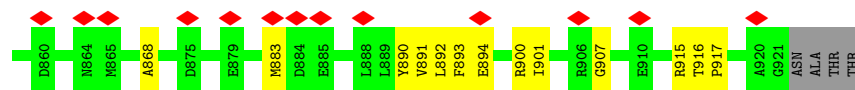


• Molecule 1: Hexon protein

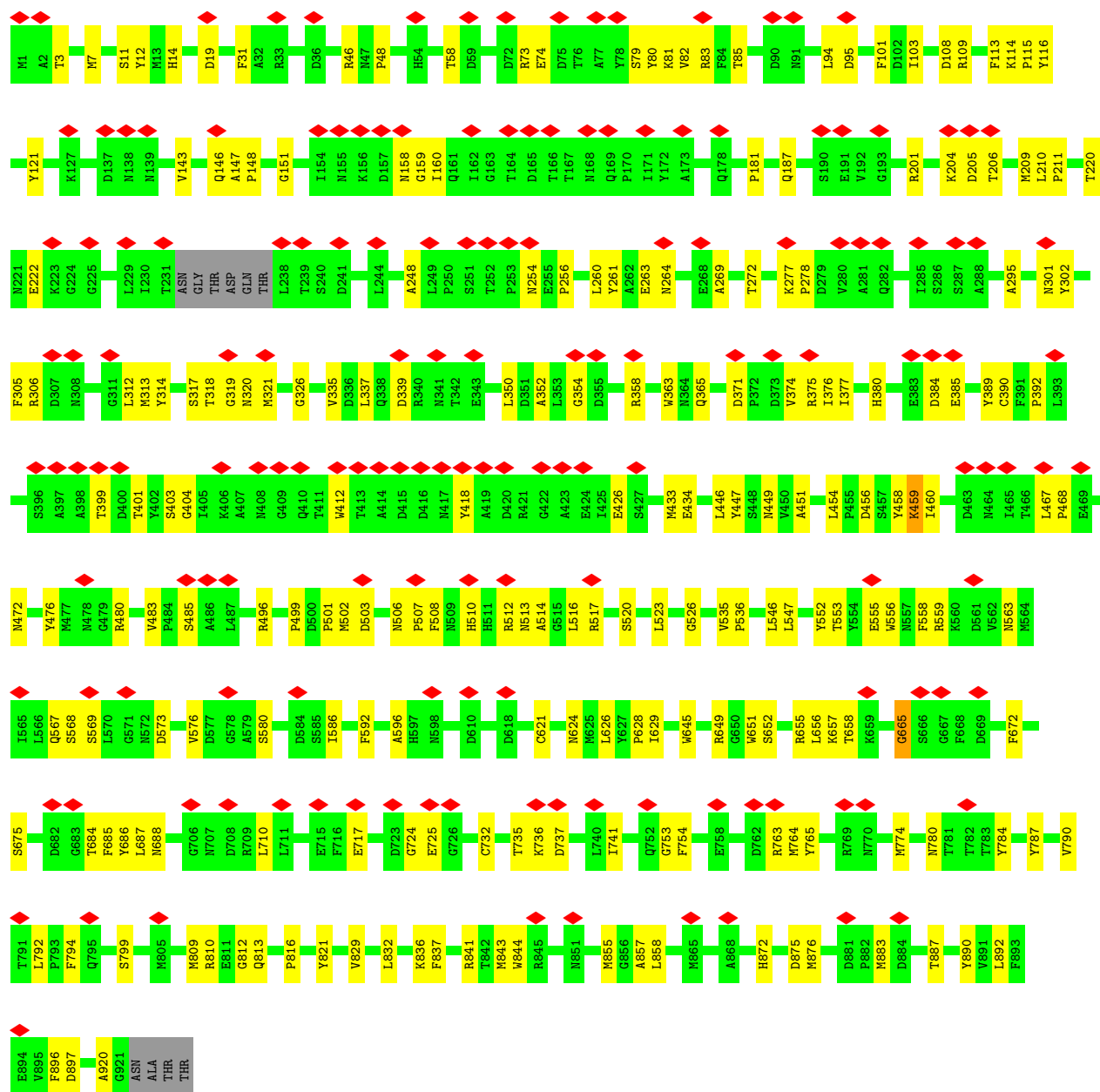
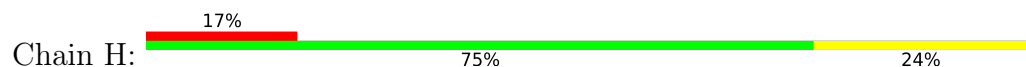




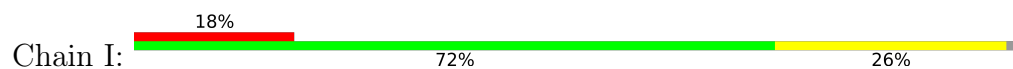


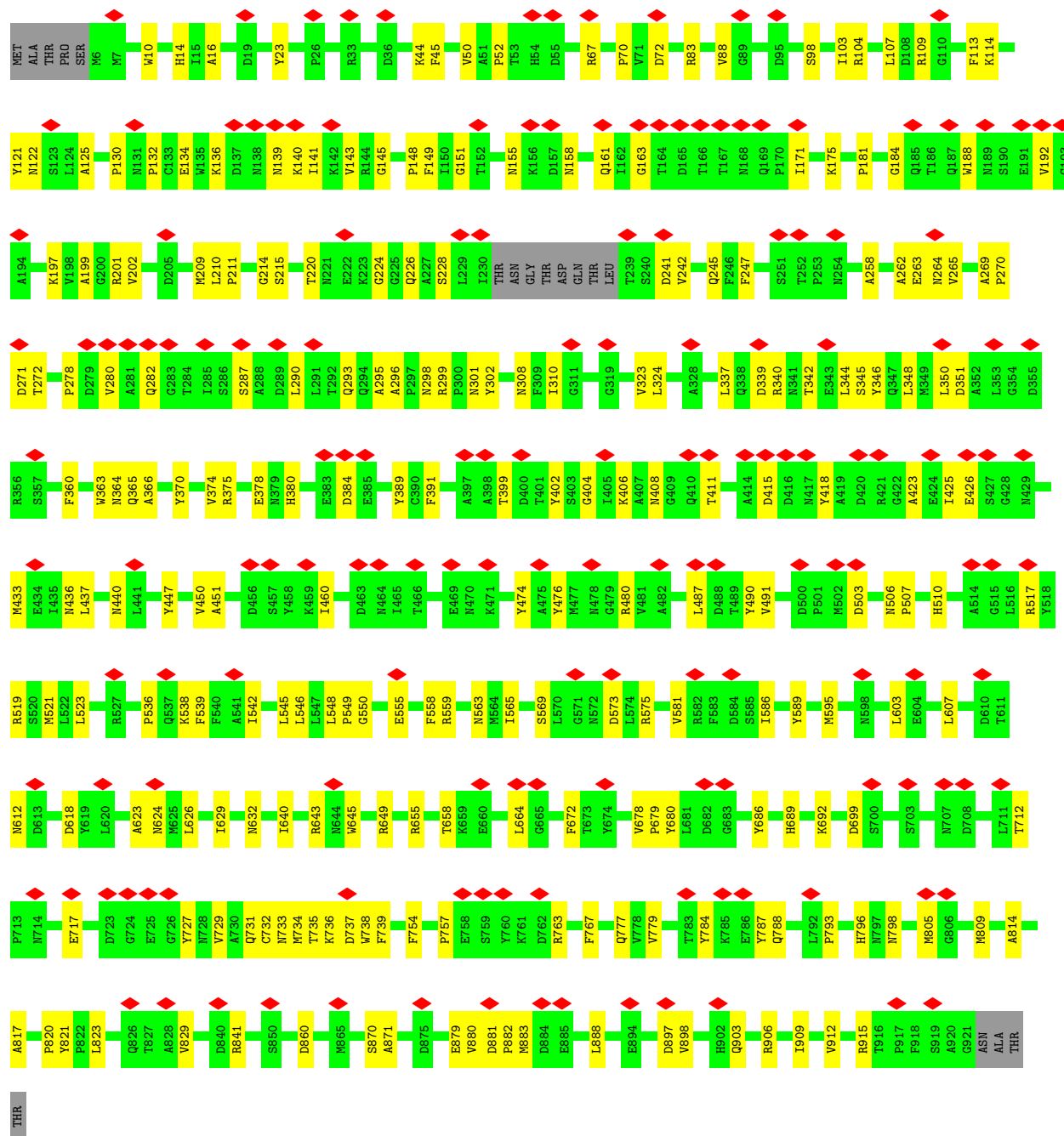


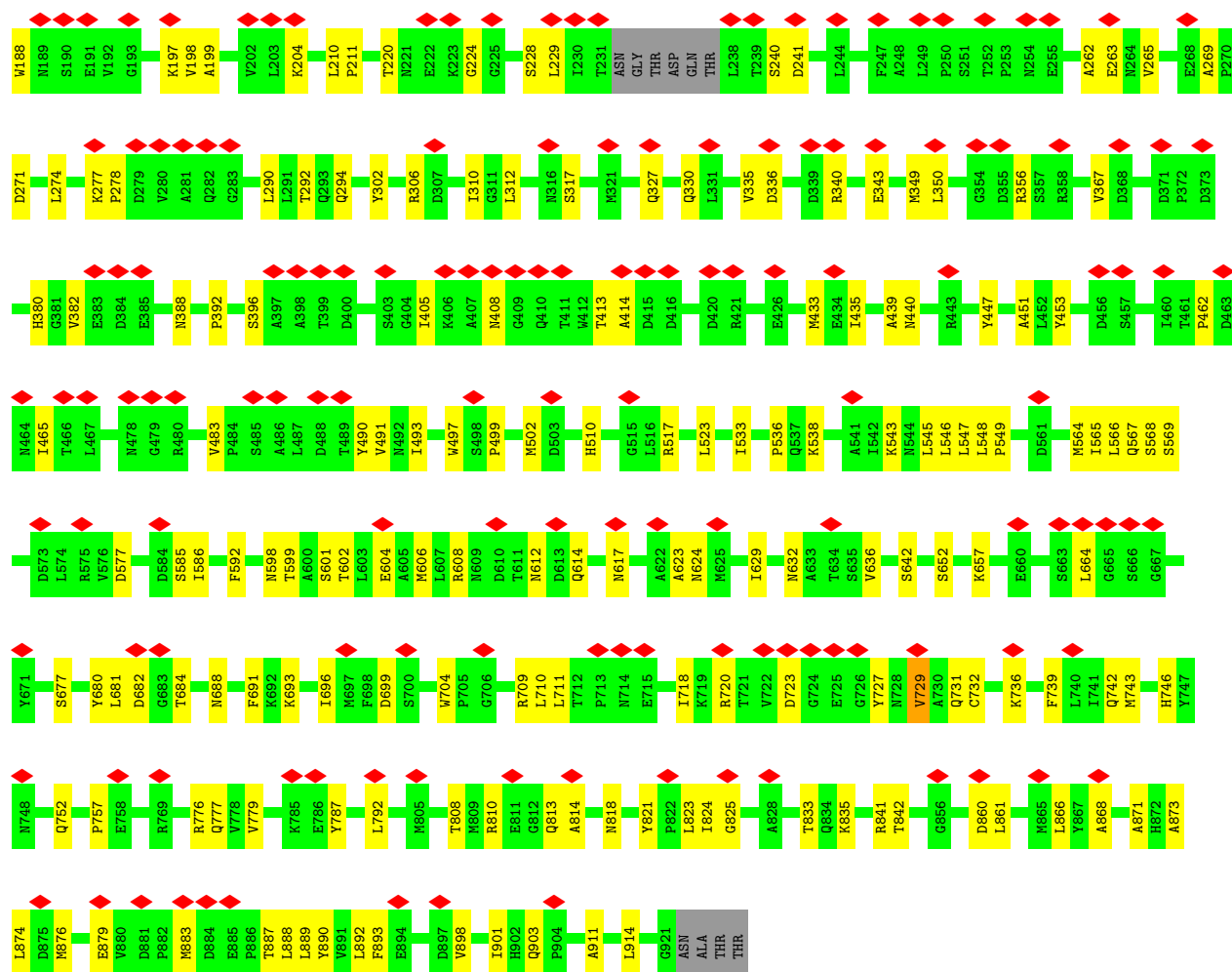
• Molecule 1: Hexon protein



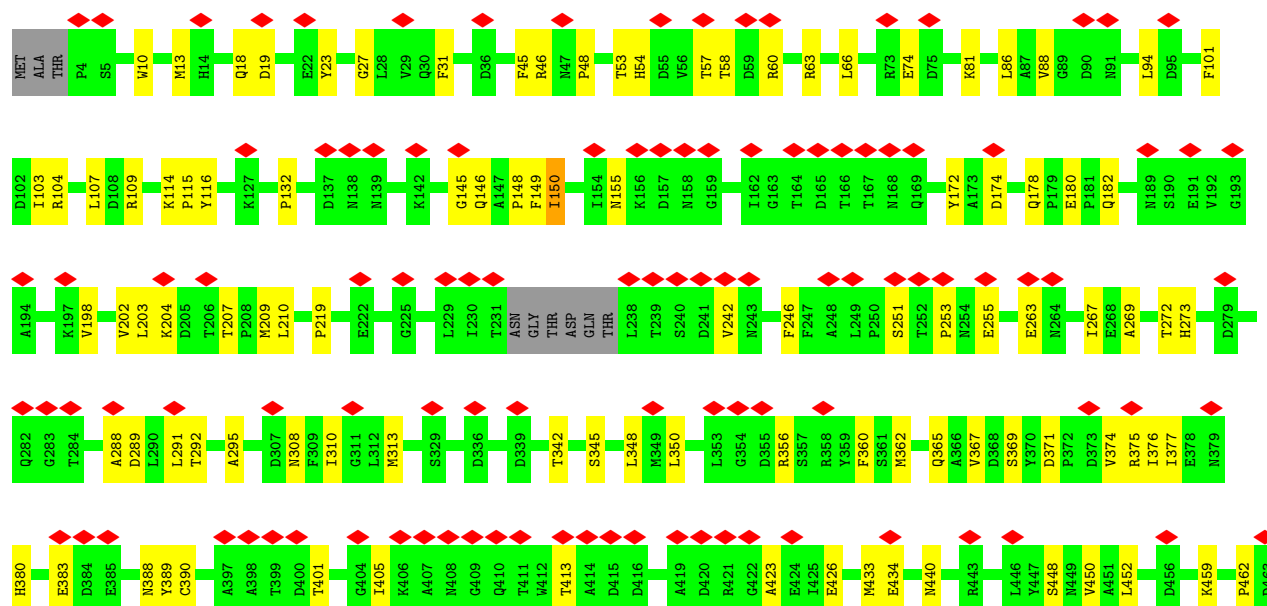
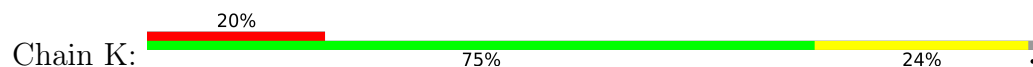
• Molecule 1: Hexon protein

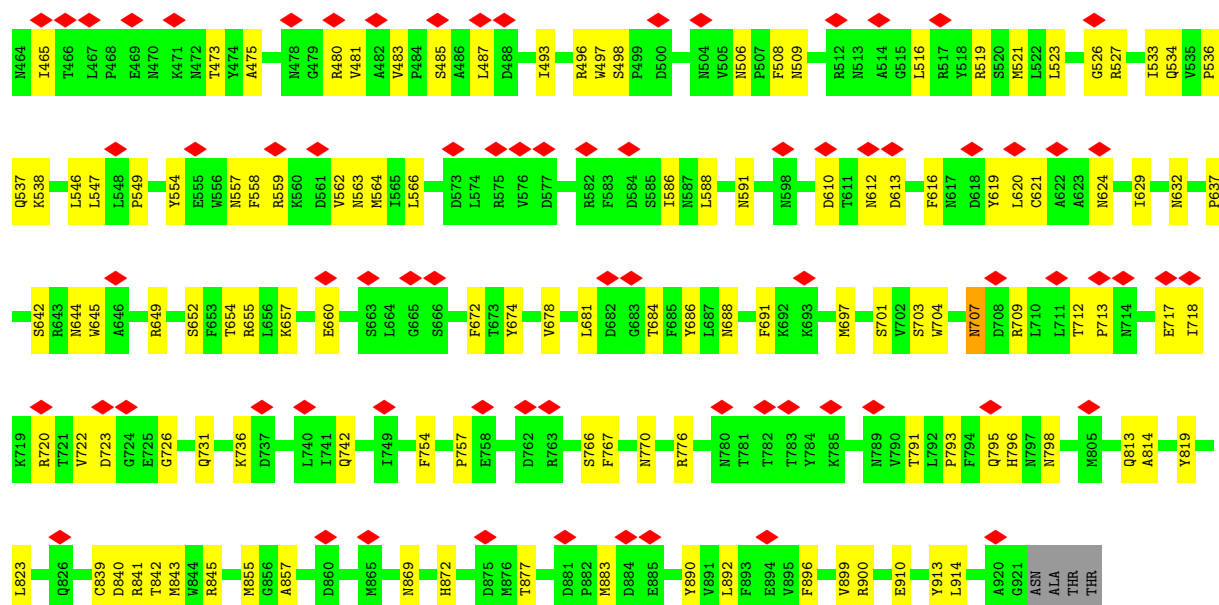




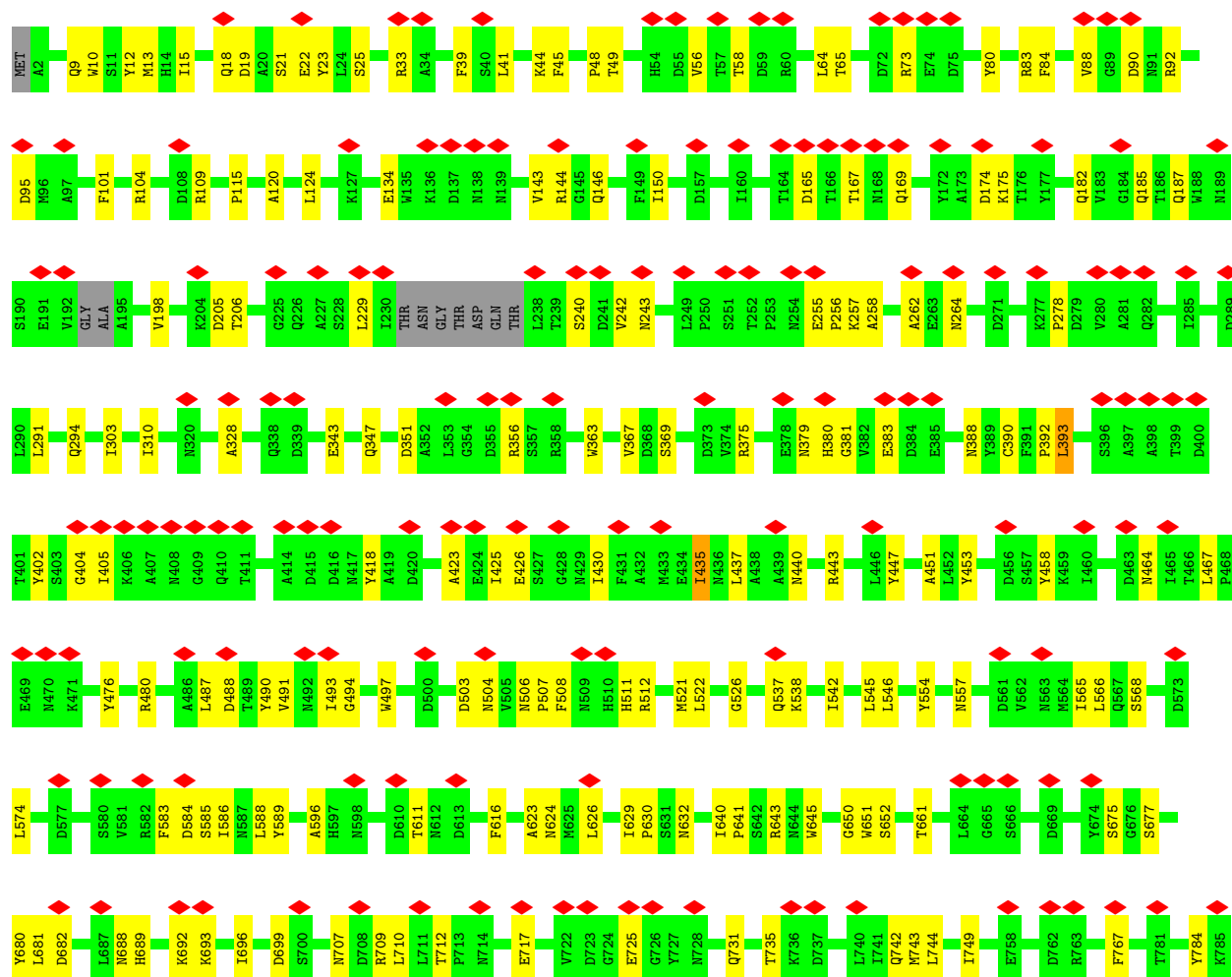
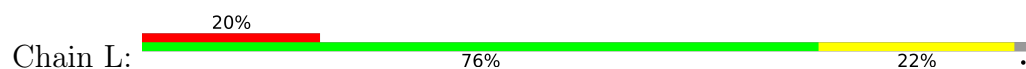


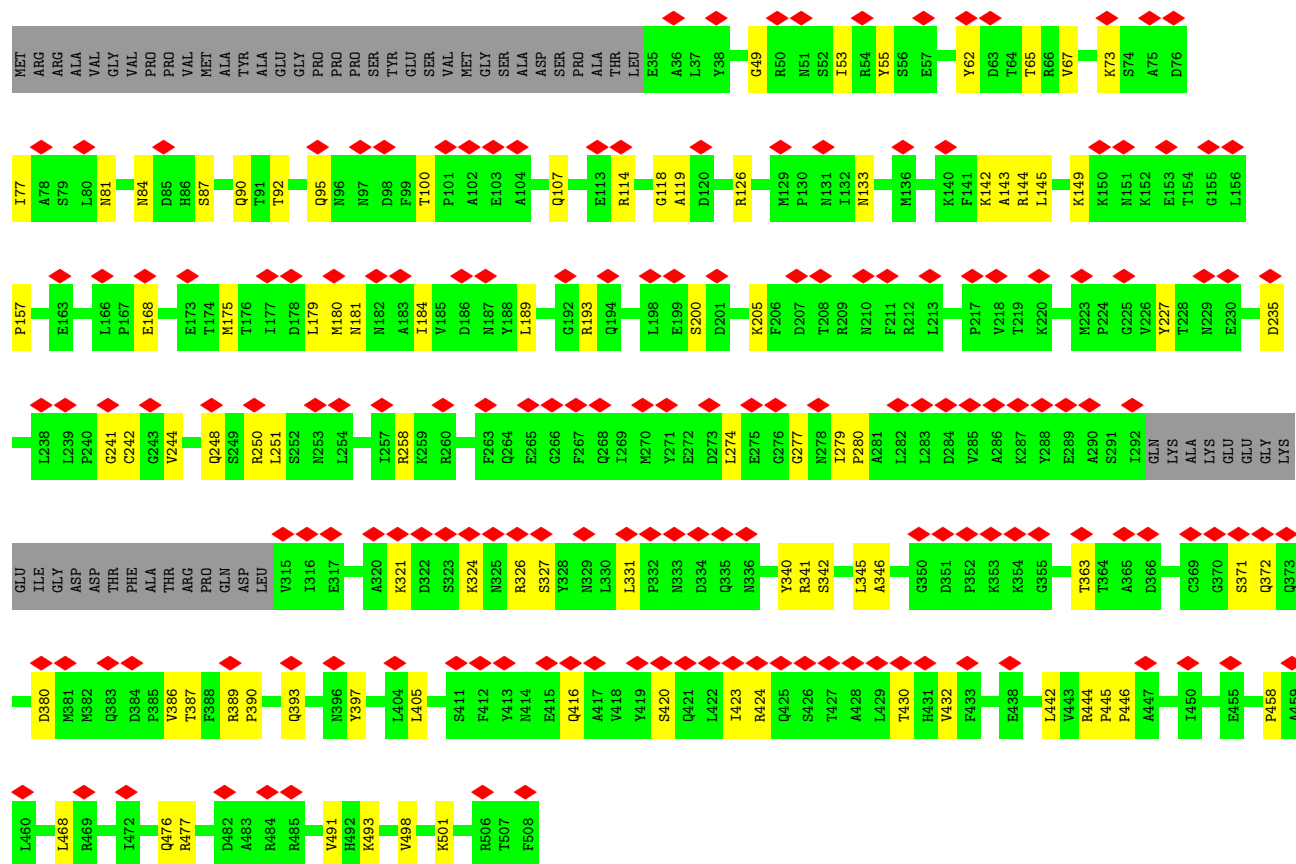
• Molecule 1: Hexon protein



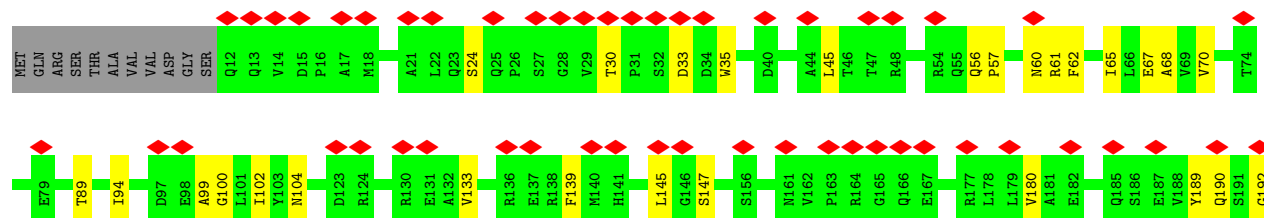
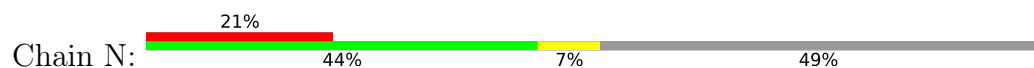


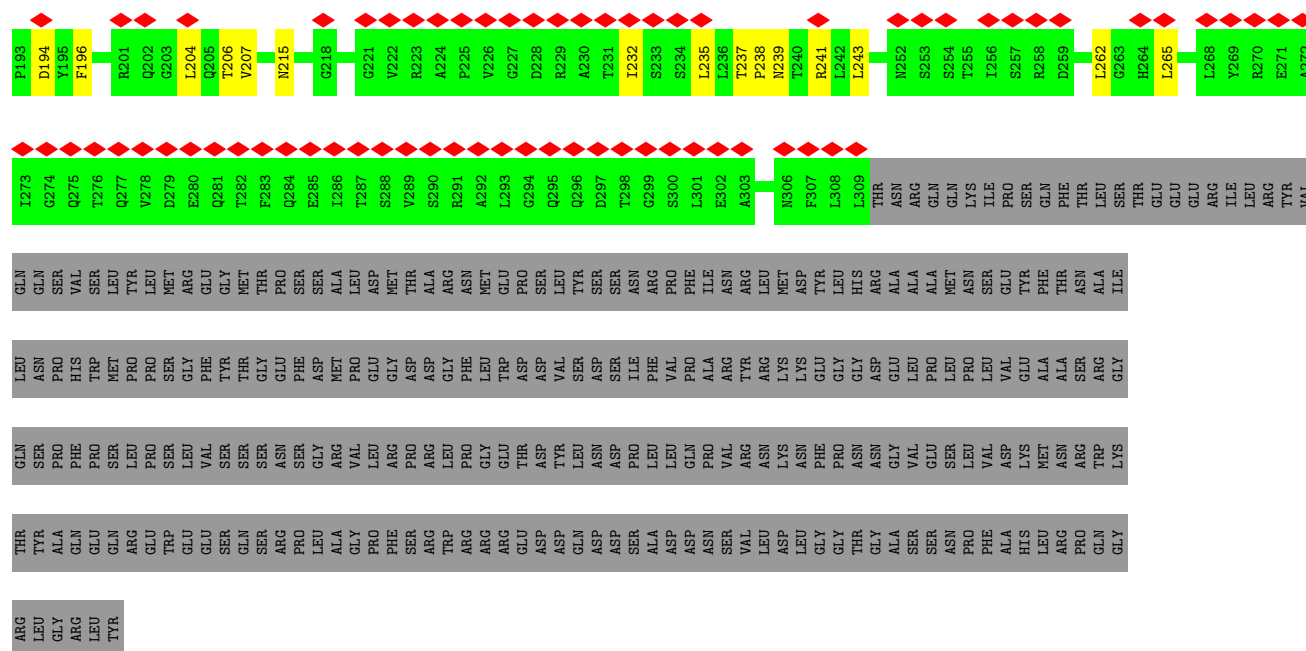
• Molecule 1: Hexon protein



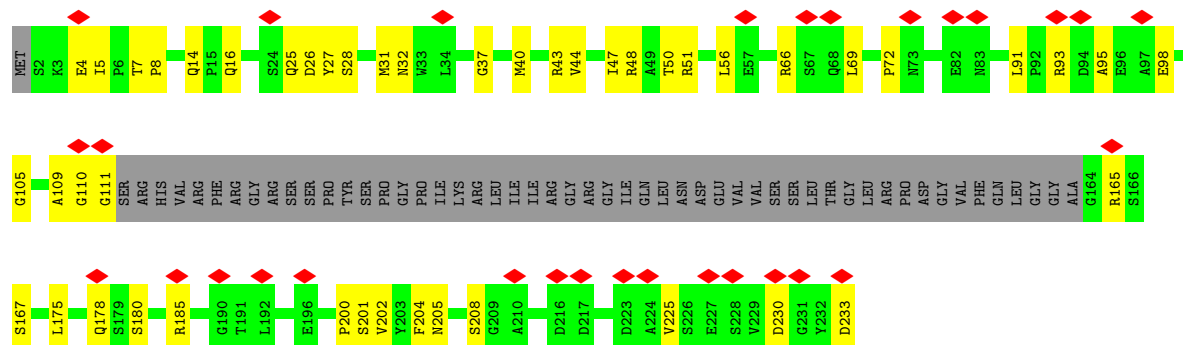


- Molecule 3: Pre-hexon-linking protein IIIa

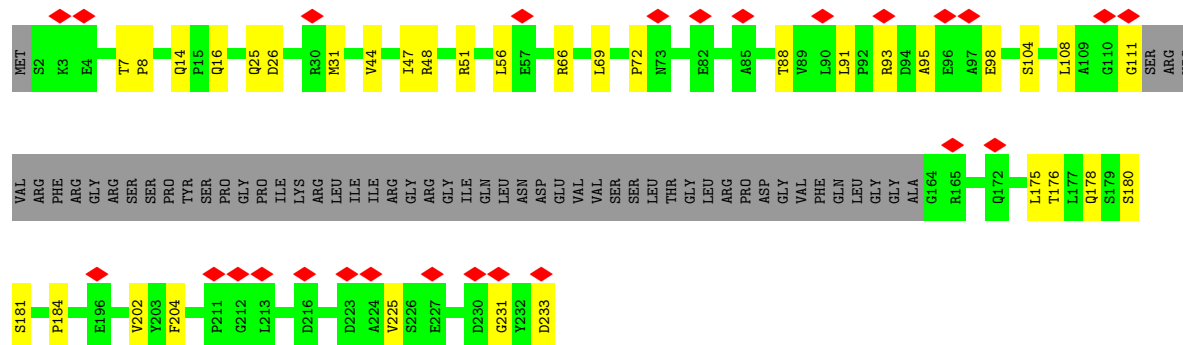




• Molecule 4: Pre-hexon-linking protein VIII



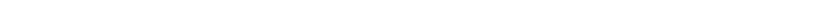
• Molecule 4: Pre-hexon-linking protein VIII



• Molecule 5: Hexon-interlacing protein

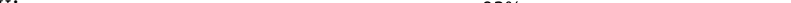
[illegible]

- Molecule 7: Pre-histone-like nucleoprotein

Chain W:  97%

[illegible]

- Molecule 7: Pre-histone-like nucleoprotein

Chain w:  5% 93%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	9926	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 ($e^-/\text{\AA}^2$)	42	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	0.364	Depositor
Minimum map value	-0.253	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	1060.8, 1060.8, 1060.8	wwPDB
Map dimensions	780, 780, 780	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.31	0/7444	0.67	2/10145 (0.0%)
1	B	0.32	0/7451	0.69	2/10154 (0.0%)
1	C	0.32	0/7455	0.70	6/10161 (0.1%)
1	D	0.33	0/7414	0.69	2/10103 (0.0%)
1	E	0.33	0/7474	0.68	1/10187 (0.0%)
1	F	0.34	0/7429	0.70	4/10124 (0.0%)
1	G	0.35	0/7429	0.73	4/10124 (0.0%)
1	H	0.35	0/7463	0.73	7/10171 (0.1%)
1	I	0.35	0/7414	0.69	3/10103 (0.0%)
1	J	0.33	0/7455	0.69	4/10161 (0.0%)
1	K	0.33	0/7443	0.71	4/10143 (0.0%)
1	L	0.34	0/7438	0.69	1/10136 (0.0%)
2	M	0.29	0/3695	0.53	0/5035
3	N	0.25	0/2353	0.56	1/3206 (0.0%)
4	O	0.30	0/1417	0.50	0/1935
4	P	0.30	0/1417	0.50	0/1935
5	Q	0.31	0/374	0.68	0/512
5	R	0.31	0/374	0.68	0/512
5	S	0.31	0/374	0.68	0/512
5	T	0.31	0/374	0.68	0/512
6	U	0.22	0/224	0.43	0/302
6	V	0.22	0/224	0.43	0/302
6	Y	0.22	0/224	0.43	0/302
6	u	0.22	0/224	0.43	0/302
7	W	0.19	0/37	0.41	0/47
7	w	0.29	0/86	0.54	0/114
All	All	0.33	0/100706	0.68	41/137240 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	6
1	C	0	8
1	D	0	2
1	E	0	7
1	F	0	3
1	G	0	4
1	H	0	4
1	I	0	5
1	J	0	6
1	K	0	8
1	L	0	3
2	M	0	3
All	All	0	63

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	139	ASN	N-CA-C	-8.39	105.05	114.62
3	N	133	VAL	N-CA-C	-7.36	105.37	112.29
1	H	576	VAL	N-CA-C	-6.85	106.81	113.53
1	L	95	ASP	N-CA-C	-6.14	106.77	114.56
1	C	771	PHE	CA-C-N	-5.92	117.07	122.28
1	C	771	PHE	C-N-CA	-5.92	117.07	122.28
1	E	433	MET	CB-CG-SD	5.91	130.44	112.70
1	D	574	LEU	CA-C-N	5.75	132.52	121.54
1	D	574	LEU	C-N-CA	5.75	132.52	121.54
1	H	181	PRO	CA-C-N	5.51	135.86	125.66
1	H	181	PRO	C-N-CA	5.51	135.86	125.66
1	F	398	ALA	CA-C-N	5.44	131.93	121.54
1	F	398	ALA	C-N-CA	5.44	131.93	121.54
1	K	707	ASN	CA-C-N	5.39	131.84	121.54
1	K	707	ASN	C-N-CA	5.39	131.84	121.54
1	C	253	PRO	CA-C-N	5.32	134.29	124.82
1	C	253	PRO	C-N-CA	5.32	134.29	124.82
1	H	459	LYS	CA-C-N	5.23	131.38	121.97
1	H	459	LYS	C-N-CA	5.23	131.38	121.97
1	J	408	ASN	CA-C-N	5.11	131.43	121.41
1	J	408	ASN	C-N-CA	5.11	131.43	121.41
1	G	463	ASP	CA-C-N	5.09	129.63	122.46
1	G	463	ASP	C-N-CA	5.09	129.63	122.46
1	K	619	TYR	CA-C-N	5.08	131.24	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	619	TYR	C-N-CA	5.08	131.24	121.54
1	I	491	VAL	CA-C-N	5.04	131.17	121.54
1	I	491	VAL	C-N-CA	5.04	131.17	121.54
1	G	699	ASP	CA-C-N	5.03	131.15	121.54
1	G	699	ASP	C-N-CA	5.03	131.15	121.54
1	C	463	ASP	CA-C-N	5.03	129.55	122.46
1	C	463	ASP	C-N-CA	5.03	129.55	122.46
1	A	707	ASN	CA-C-N	5.03	131.14	121.54
1	A	707	ASN	C-N-CA	5.03	131.14	121.54
1	B	619	TYR	CA-C-N	5.02	131.14	121.54
1	B	619	TYR	C-N-CA	5.02	131.14	121.54
1	F	491	VAL	CA-C-N	5.02	131.13	121.54
1	F	491	VAL	C-N-CA	5.02	131.13	121.54
1	J	491	VAL	CA-C-N	5.02	131.12	121.54
1	J	491	VAL	C-N-CA	5.02	131.12	121.54
1	H	384	ASP	CA-C-N	5.00	131.09	121.54
1	H	384	ASP	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	LEU	Peptide
1	A	612	ASN	Peptide
1	A	704	TRP	Peptide
1	A	756	VAL	Peptide
1	B	334	VAL	Peptide
1	B	409	GLY	Peptide
1	B	612	ASN	Peptide
1	B	704	TRP	Peptide
1	B	796	HIS	Peptide
1	B	916	THR	Peptide
1	C	167	THR	Peptide
1	C	285	ILE	Peptide
1	C	525	ASN	Peptide
1	C	59	ASP	Peptide
1	C	612	ASN	Peptide
1	C	630	PRO	Peptide
1	C	762	ASP	Peptide
1	C	796	HIS	Peptide
1	D	630	PRO	Peptide
1	D	641	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	E	149	PHE	Peptide
1	E	285	ILE	Peptide
1	E	314	TYR	Peptide
1	E	377	ILE	Peptide
1	E	70	PRO	Peptide
1	E	757	PRO	Peptide
1	E	916	THR	Peptide
1	F	397	ALA	Peptide
1	F	419	ALA	Peptide
1	F	617	ASN	Peptide
1	G	273	HIS	Peptide
1	G	286	SER	Peptide
1	G	536	PRO	Peptide
1	G	916	THR	Peptide
1	H	159	GLY	Peptide
1	H	319	GLY	Peptide
1	H	354	GLY	Peptide
1	H	401	THR	Peptide
1	I	384	ASP	Peptide
1	I	536	PRO	Peptide
1	I	618	ASP	Peptide
1	I	70	PRO	Peptide
1	I	796	HIS	Peptide
1	J	224	GLY	Peptide
1	J	292	THR	Peptide
1	J	536	PRO	Peptide
1	J	55	ASP	Peptide
1	J	704	TRP	Peptide
1	J	787	TYR	Peptide
1	K	149	PHE	Peptide
1	K	251	SER	Peptide
1	K	273	HIS	Peptide
1	K	288	ALA	Peptide
1	K	289	ASP	Peptide
1	K	536	PRO	Peptide
1	K	704	TRP	Peptide
1	K	796	HIS	Peptide
1	L	174	ASP	Peptide
1	L	630	PRO	Peptide
1	L	641	PRO	Peptide
2	M	100	THR	Peptide
2	M	331	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	M	62	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7244	0	6936	163	0
1	B	7250	0	6942	147	0
1	C	7254	0	6947	153	0
1	D	7214	0	6905	159	0
1	E	7273	0	6963	161	0
1	F	7229	0	6923	153	0
1	G	7229	0	6923	155	0
1	H	7262	0	6959	152	0
1	I	7214	0	6905	169	0
1	J	7254	0	6947	141	0
1	K	7242	0	6936	156	0
1	L	7238	0	6931	148	0
2	M	3609	0	3546	52	0
3	N	2315	0	2312	29	0
4	O	1379	0	1307	46	0
4	P	1379	0	1307	25	0
5	Q	365	0	363	4	0
5	R	365	0	363	0	0
5	S	365	0	363	2	0
5	T	365	0	363	2	0
6	U	218	0	202	1	0
6	V	218	0	202	1	0
6	Y	218	0	202	6	0
6	u	218	0	202	4	0
7	W	37	0	31	1	0
7	w	83	0	70	5	0
All	All	98037	0	94050	1685	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 9.

All (1685) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:754:PHE:HB2	1:F:363:TRP:HE1	1.43	0.84
1:A:201:ARG:H	1:C:813:GLN:HE22	1.35	0.75
1:D:754:PHE:HB2	1:E:363:TRP:HE1	1.51	0.74
1:G:74:GLU:HB3	1:G:81:LYS:HB2	1.71	0.73
1:D:360:PHE:HB3	1:D:365:GLN:HB3	1.72	0.72
1:J:731:GLN:HE21	1:K:533:ILE:HG22	1.55	0.72
1:G:310:ILE:HG22	1:G:538:LYS:HE3	1.72	0.71
1:K:356:ARG:HG3	1:K:367:VAL:HG12	1.73	0.71
1:B:734:MET:HE3	1:B:738:TRP:HD1	1.56	0.70
1:B:111:PRO:HA	1:B:527:ARG:HH12	1.56	0.70
1:D:643:ARG:NH2	1:I:699:ASP:O	2.24	0.70
1:J:777:GLN:HG2	1:K:526:GLY:HA3	1.72	0.70
1:A:512:ARG:HA	1:A:517:ARG:HH21	1.56	0.69
1:L:651:TRP:HZ3	1:L:696:ILE:HG12	1.58	0.69
1:G:449:ASN:HD21	1:G:512:ARG:HH21	1.38	0.69
2:M:250:ARG:HH21	2:M:372:GLN:HE21	1.40	0.69
1:E:248:ALA:HB2	1:E:256:PRO:HA	1.75	0.69
1:D:341:ASN:OD1	1:D:624:ASN:ND2	2.26	0.69
1:A:483:VAL:HG22	1:A:485:SER:H	1.58	0.69
1:E:906:ARG:NH2	1:L:328:ALA:O	2.26	0.69
1:A:68:PHE:HB2	1:A:588:LEU:HB3	1.73	0.69
1:G:81:LYS:HD2	1:G:557:ASN:HB3	1.73	0.68
1:I:114:LYS:NZ	1:I:270:PRO:O	2.26	0.68
1:D:322:GLY:HA3	1:D:556:TRP:HD1	1.59	0.68
1:H:725:GLU:HB3	1:I:67:ARG:HH12	1.58	0.68
1:C:734:MET:HE3	1:C:738:TRP:HD1	1.58	0.68
1:H:321:MET:HE1	1:H:335:VAL:HA	1.77	0.67
3:N:204:LEU:HD21	4:O:201:SER:HB3	1.76	0.67
1:F:101:PHE:HB2	1:F:535:VAL:HB	1.76	0.67
1:D:405:ILE:HG22	1:D:414:ALA:HA	1.77	0.66
1:I:643:ARG:NH2	1:L:699:ASP:O	2.29	0.66
1:J:310:ILE:HG22	1:J:538:LYS:HE3	1.76	0.66
1:B:306:ARG:HH12	1:B:678:VAL:H	1.44	0.66
1:K:701:SER:OG	4:O:16:GLN:NE2	2.29	0.66
1:C:217:ALA:O	1:C:226:GLN:NE2	2.29	0.65
1:D:374:VAL:HG23	1:D:450:VAL:HG22	1.79	0.65
1:G:44:LYS:HE2	1:I:546:LEU:HB2	1.78	0.65
1:H:652:SER:HB2	1:H:892:LEU:HB3	1.78	0.65
1:D:13:MET:HG3	1:F:914:LEU:HD21	1.76	0.65
1:D:201:ARG:HG2	1:D:261:TYR:HB2	1.78	0.65
1:J:67:ARG:HH12	1:L:725:GLU:HG3	1.62	0.65
1:A:402:TYR:HB3	1:C:247:PHE:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:749:ILE:HG22	1:E:752:GLN:HE21	1.61	0.65
1:H:19:ASP:HA	1:H:48:PRO:HD2	1.78	0.65
1:K:107:LEU:HD11	1:K:566:LEU:HD11	1.78	0.65
1:B:18:GLN:HE22	4:O:185:ARG:HA	1.62	0.65
1:K:174:ASP:H	1:K:178:GLN:HE21	1.43	0.65
1:E:629:ILE:HG12	1:E:636:VAL:HG11	1.79	0.65
1:K:94:LEU:HB3	1:K:547:LEU:HB3	1.79	0.65
1:K:624:ASN:ND2	1:K:890:TYR:OH	2.30	0.65
1:K:914:LEU:HD12	4:O:31:MET:HG2	1.79	0.65
1:A:734:MET:HE3	1:A:738:TRP:HD1	1.60	0.64
1:D:382:VAL:HG11	1:D:439:ALA:HA	1.79	0.64
1:I:563:ASN:ND2	1:I:672:PHE:O	2.30	0.64
1:I:360:PHE:HB3	1:I:365:GLN:HB3	1.79	0.64
1:A:423:ALA:HB1	1:C:143:VAL:H	1.63	0.64
1:B:509:ASN:ND2	1:B:674:TYR:OH	2.30	0.64
1:K:509:ASN:ND2	1:K:674:TYR:OH	2.31	0.64
1:F:774:MET:HE1	1:F:838:LEU:HB2	1.80	0.64
1:A:495:ALA:HB2	1:B:525:ASN:HB2	1.80	0.64
1:G:188:TRP:HB3	1:I:809:MET:HE1	1.79	0.64
1:J:388:ASN:HB3	1:K:440:ASN:HD21	1.63	0.64
1:K:132:PRO:HB2	1:K:202:VAL:HG12	1.79	0.64
1:D:12:TYR:O	1:F:900:ARG:NH2	2.31	0.64
1:H:732:CYS:HB2	1:H:837:PHE:HB3	1.80	0.64
1:E:495:ALA:HB2	1:F:525:ASN:HB2	1.79	0.64
1:E:786:GLU:HG2	1:F:218:LYS:HD3	1.80	0.63
1:J:134:GLU:HG2	1:J:143:VAL:HG12	1.80	0.63
1:K:360:PHE:HB3	1:K:365:GLN:HB3	1.80	0.63
1:G:124:LEU:H	1:I:798:ASN:HD21	1.44	0.63
1:G:217:ALA:HB3	1:G:226:GLN:HE21	1.61	0.63
1:G:374:VAL:HG11	1:G:510:HIS:HE1	1.63	0.63
1:J:447:TYR:HA	1:J:451:ALA:HB3	1.80	0.63
1:A:152:THR:OG1	1:A:161:GLN:NE2	2.31	0.63
1:F:135:TRP:HE1	1:F:142:LYS:HE3	1.64	0.63
1:G:545:LEU:HD13	1:G:901:ILE:HD12	1.80	0.63
1:A:341:ASN:H	1:A:624:ASN:HD22	1.45	0.63
1:D:612:ASN:HD21	1:E:25:SER:H	1.46	0.63
1:F:459:LYS:HB3	1:F:480:ARG:HB3	1.81	0.63
1:J:302:TYR:OH	1:J:517:ARG:NH1	2.32	0.63
1:K:563:ASN:ND2	1:K:672:PHE:O	2.31	0.63
1:A:307:ASP:HA	1:A:519:ARG:HH12	1.64	0.63
1:F:474:TYR:HB2	1:F:572:ASN:HD22	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:ASN:ND2	1:A:842:THR:O	2.32	0.63
1:G:134:GLU:HG2	1:G:143:VAL:HG22	1.81	0.62
1:E:380:HIS:HE2	1:F:521:MET:HE2	1.64	0.62
1:C:845:ARG:HH22	6:Y:32:GLY:HA3	1.64	0.62
1:D:649:ARG:NH2	7:W:21:TYR:O	2.33	0.62
1:H:74:GLU:HB3	1:H:81:LYS:HB3	1.80	0.62
1:I:643:ARG:HH22	1:L:699:ASP:HB3	1.65	0.62
1:J:306:ARG:HE	1:J:567:GLN:HB2	1.65	0.62
1:C:315:TYR:HE2	1:C:342:THR:HG23	1.64	0.62
1:E:340:ARG:HH21	1:E:915:ARG:HD3	1.64	0.62
1:F:218:LYS:NZ	1:F:268:GLU:OE2	2.33	0.62
1:F:408:ASN:HB3	1:F:411:THR:HB	1.81	0.62
1:G:506:ASN:ND2	1:G:509:ASN:OD1	2.33	0.62
1:J:752:GLN:NE2	1:L:39:PHE:O	2.33	0.62
1:E:356:ARG:HB3	1:E:367:VAL:HG11	1.81	0.62
1:C:699:ASP:O	1:E:643:ARG:NH2	2.32	0.62
1:J:274:LEU:HD21	1:J:277:LYS:HD3	1.81	0.62
1:C:459:LYS:HG2	1:C:482:ALA:HB2	1.81	0.61
1:D:558:PHE:HE2	1:D:586:ILE:HG21	1.62	0.61
1:E:911:ALA:HB3	4:O:109:ALA:HB3	1.82	0.61
1:A:559:ARG:NH1	1:A:564:MET:SD	2.73	0.61
1:L:104:ARG:HG3	1:L:584:ASP:HB3	1.81	0.61
1:E:146:GLN:NE2	1:F:429:ASN:OD1	2.33	0.61
1:G:483:VAL:HG22	1:G:485:SER:H	1.64	0.61
1:A:430:ILE:O	1:B:810:ARG:NH2	2.34	0.61
1:G:788:GLN:HB3	1:H:222:GLU:HA	1.81	0.61
1:J:111:PRO:HD2	1:J:577:ASP:HB3	1.83	0.61
1:C:546:LEU:HD21	1:C:603:LEU:HD21	1.82	0.61
1:D:433:MET:HE1	1:F:433:MET:HG3	1.82	0.61
1:G:376:ILE:HD13	1:G:496:ARG:HE	1.65	0.61
1:I:732:CYS:SG	1:I:733:ASN:N	2.73	0.61
1:L:375:ARG:HD3	1:L:507:PRO:HG3	1.81	0.61
1:D:146:GLN:HE22	1:E:430:ILE:HG13	1.66	0.61
1:F:313:MET:HE1	1:F:537:GLN:HA	1.83	0.61
1:J:657:LYS:HG2	1:J:887:THR:HG22	1.83	0.61
1:K:58:THR:HG22	1:K:60:ARG:H	1.65	0.61
1:A:818:ASN:OD1	1:B:226:GLN:NE2	2.34	0.61
1:B:388:ASN:HB3	1:C:440:ASN:HD21	1.65	0.61
1:K:203:LEU:HD12	1:K:207:THR:HG21	1.83	0.61
4:P:7:THR:O	4:P:25:GLN:NE2	2.34	0.61
1:D:813:GLN:HE22	1:E:201:ARG:H	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:TYR:HB3	1:B:558:PHE:HB2	1.83	0.60
1:C:483:VAL:HG11	1:C:792:LEU:HD21	1.82	0.60
1:E:563:ASN:ND2	1:E:672:PHE:O	2.34	0.60
1:H:459:LYS:HB3	1:H:480:ARG:HB3	1.83	0.60
1:L:623:ALA:HB2	1:L:915:ARG:HH22	1.64	0.60
1:C:509:ASN:ND2	1:C:674:TYR:OH	2.33	0.60
1:G:306:ARG:HE	1:G:567:GLN:HB2	1.66	0.60
1:L:565:ILE:HG23	1:L:566:LEU:HG	1.82	0.60
4:P:7:THR:HB	4:P:25:GLN:HE21	1.66	0.60
1:A:104:ARG:NH2	1:C:724:GLY:O	2.33	0.60
1:D:301:ASN:HA	1:D:569:SER:HB2	1.84	0.60
1:I:548:LEU:HD11	1:I:607:LEU:HB2	1.83	0.60
1:A:436:ASN:ND2	1:B:123:SER:O	2.35	0.60
1:G:247:PHE:HA	1:H:404:GLY:HA2	1.84	0.60
1:G:268:GLU:HG3	1:G:270:PRO:HD3	1.82	0.60
1:F:687:LEU:HD21	1:F:883:MET:HE1	1.84	0.60
4:O:7:THR:O	4:O:25:GLN:NE2	2.34	0.60
1:G:204:LYS:HD2	1:G:264:ASN:HB2	1.83	0.60
1:D:307:ASP:OD2	1:D:356:ARG:NH2	2.34	0.60
1:D:591:ASN:ND2	1:F:750:GLY:O	2.35	0.60
1:J:3:THR:HG22	1:J:5:SER:H	1.66	0.60
2:M:371:SER:HB3	2:M:405:LEU:HB3	1.82	0.60
3:N:239:ASN:N	4:O:4:GLU:OE2	2.35	0.60
1:C:132:PRO:HB3	1:C:145:GLY:HA2	1.82	0.60
1:L:643:ARG:HE	1:L:918:PHE:H	1.50	0.60
1:C:130:PRO:HA	1:C:212:CYS:H	1.67	0.59
1:D:762:ASP:HB3	1:D:769:ARG:HB2	1.84	0.59
1:G:559:ARG:NH1	1:G:564:MET:SD	2.75	0.59
1:I:209:MET:O	1:I:293:GLN:NE2	2.34	0.59
1:K:401:THR:HG23	1:K:423:ALA:H	1.66	0.59
1:L:583:PHE:HB3	1:L:586:ILE:HD11	1.83	0.59
1:D:210:LEU:HD12	1:D:267:ILE:HG22	1.83	0.59
1:D:363:TRP:HE1	1:F:754:PHE:HB2	1.66	0.59
1:E:459:LYS:O	1:E:480:ARG:NH2	2.35	0.59
1:I:52:PRO:HD3	6:u:11:PRO:HA	1.83	0.59
1:F:175:LYS:HB2	1:F:242:VAL:HG21	1.84	0.59
1:H:558:PHE:HE2	1:H:586:ILE:HG12	1.66	0.59
1:K:900:ARG:HH11	4:O:40:MET:HE3	1.66	0.59
1:E:226:GLN:HG3	1:E:265:VAL:HG11	1.85	0.59
1:G:380:HIS:HE1	1:H:517:ARG:HB2	1.67	0.59
1:A:900:ARG:NH1	1:B:12:TYR:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ARG:HH21	1:C:772:GLN:HE21	1.50	0.59
1:D:688:ASN:ND2	1:D:842:THR:O	2.36	0.59
1:I:161:GLN:NE2	1:I:163:GLY:O	2.35	0.59
1:J:335:VAL:O	1:J:340:ARG:NH2	2.35	0.59
1:K:613:ASP:OD2	1:K:900:ARG:NE	2.36	0.59
1:B:563:ASN:ND2	1:B:672:PHE:O	2.36	0.59
1:C:52:PRO:HD3	6:Y:11:PRO:HA	1.84	0.59
1:D:33:ARG:NH2	6:V:20:GLY:O	2.35	0.59
1:I:649:ARG:NH2	6:u:32:GLY:O	2.36	0.59
1:J:163:GLY:HA3	1:J:171:ILE:HB	1.85	0.59
1:B:508:PHE:O	1:B:513:ASN:ND2	2.35	0.59
1:E:73:ARG:HH12	1:E:585:SER:HA	1.68	0.59
1:D:575:ARG:HD3	5:S:40:VAL:HA	1.84	0.59
1:H:326:GLY:HA2	1:H:552:TYR:HA	1.85	0.59
1:C:114:LYS:HE3	1:C:298:ASN:HB2	1.85	0.59
1:F:368:ASP:O	1:F:841:ARG:NH2	2.36	0.59
1:J:174:ASP:HB3	1:J:177:TYR:HB3	1.85	0.59
1:K:114:LYS:NZ	1:K:116:TYR:O	2.34	0.59
4:O:7:THR:HB	4:O:25:GLN:HE21	1.66	0.59
1:C:624:ASN:HD21	1:C:892:LEU:HD12	1.68	0.58
1:H:621:CYS:O	1:H:649:ARG:NH2	2.36	0.58
1:A:725:GLU:O	1:B:104:ARG:NH2	2.36	0.58
1:D:436:ASN:ND2	1:E:123:SER:O	2.36	0.58
1:E:632:ASN:ND2	1:E:883:MET:O	2.36	0.58
2:M:142:LYS:NZ	2:M:248:GLN:OE1	2.35	0.58
1:F:496:ARG:NH1	1:F:773:PRO:O	2.36	0.58
1:H:146:GLN:HA	1:I:426:GLU:HB3	1.84	0.58
1:C:108:ASP:O	1:C:527:ARG:NH1	2.35	0.58
1:C:503:ASP:OD2	1:C:689:HIS:NE2	2.36	0.58
1:K:736:LYS:NZ	1:L:65:THR:OG1	2.36	0.58
1:A:629:ILE:HD11	1:A:889:LEU:HB2	1.86	0.58
1:I:565:ILE:HD11	1:I:581:VAL:HG11	1.85	0.58
1:G:86:LEU:HB2	1:G:552:TYR:HB2	1.84	0.58
1:H:337:LEU:HD21	1:H:920:ALA:HB2	1.86	0.58
1:J:546:LEU:HB3	1:J:614:GLN:HE22	1.69	0.58
1:L:458:TYR:O	1:L:480:ARG:NH2	2.36	0.58
1:B:101:PHE:HB2	1:B:535:VAL:HB	1.85	0.58
1:B:511:HIS:O	1:B:517:ARG:NH1	2.36	0.58
1:B:627:TYR:HB2	1:B:889:LEU:HB3	1.86	0.58
1:D:476:TYR:OH	1:D:480:ARG:NH1	2.36	0.58
1:H:305:PHE:HZ	1:H:312:LEU:HD22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:350:LEU:HD21	1:I:365:GLN:HG3	1.85	0.58
1:I:437:LEU:HA	1:I:440:ASN:HD22	1.69	0.58
1:I:912:VAL:HG12	4:P:108:LEU:HD22	1.86	0.58
1:G:823:LEU:HB3	1:H:526:GLY:HA2	1.85	0.58
1:J:107:LEU:HD23	1:J:109:ARG:HE	1.69	0.58
1:A:563:ASN:HB2	1:A:575:ARG:HB2	1.85	0.58
1:E:144:ARG:NH2	1:F:394:GLY:O	2.37	0.58
1:I:607:LEU:HD23	1:I:612:ASN:HB3	1.86	0.58
1:K:74:GLU:HB3	1:K:81:LYS:HB2	1.85	0.58
1:K:516:LEU:HA	1:K:519:ARG:HE	1.68	0.58
1:C:443:ARG:NH1	1:C:488:ASP:OD2	2.35	0.57
1:F:376:ILE:HD11	1:F:772:GLN:HE22	1.69	0.57
1:H:206:THR:OG1	1:H:264:ASN:ND2	2.37	0.57
1:H:318:THR:HA	1:H:321:MET:HB3	1.86	0.57
1:A:46:ARG:NH1	1:C:617:ASN:OD1	2.38	0.57
1:A:563:ASN:ND2	1:A:672:PHE:O	2.36	0.57
1:B:276:TYR:OH	1:C:187:GLN:NE2	2.38	0.57
1:B:900:ARG:NH1	1:C:12:TYR:O	2.37	0.57
1:C:655:ARG:HE	1:C:887:THR:HG21	1.69	0.57
1:D:437:LEU:HB2	1:F:437:LEU:HD11	1.84	0.57
1:G:363:TRP:NE1	1:I:754:PHE:O	2.36	0.57
1:H:101:PHE:HB2	1:H:535:VAL:HB	1.86	0.57
1:H:508:PHE:O	1:H:513:ASN:ND2	2.37	0.57
1:G:649:ARG:HH21	1:G:894:GLU:HG2	1.70	0.57
1:K:559:ARG:HD3	1:K:564:MET:HE3	1.87	0.57
2:M:342:SER:HB3	2:M:345:LEU:HB2	1.85	0.57
1:A:74:GLU:HG3	1:A:81:LYS:HE2	1.85	0.57
1:D:347:GLN:NE2	1:D:682:ASP:OD1	2.31	0.57
1:G:652:SER:HB2	1:G:892:LEU:HB3	1.86	0.57
1:I:269:ALA:HB1	1:I:272:THR:HB	1.85	0.57
1:J:709:ARG:NH2	4:P:233:ASP:OD2	2.38	0.57
2:M:144:ARG:HE	2:M:242:CYS:HA	1.70	0.57
2:M:397:TYR:OH	2:M:477:ARG:NH1	2.37	0.57
3:N:147:SER:HB3	3:N:180:VAL:HB	1.85	0.57
1:C:90:ASP:H	1:C:906:ARG:HH12	1.50	0.57
1:E:204:LYS:HD3	1:E:264:ASN:HB2	1.85	0.57
1:A:160:ILE:HB	1:A:259:VAL:HG11	1.86	0.57
1:A:509:ASN:ND2	1:A:674:TYR:OH	2.38	0.57
1:D:130:PRO:HA	1:D:212:CYS:H	1.69	0.57
1:D:278:PRO:O	1:D:464:ASN:ND2	2.38	0.57
1:D:340:ARG:NH2	1:D:622:ALA:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:306:ARG:NH2	1:J:564:MET:O	2.37	0.57
1:A:405:ILE:HG12	1:C:246:PHE:HB2	1.87	0.57
1:D:222:GLU:HG3	1:D:223:LYS:HG2	1.87	0.57
1:F:155:ASN:ND2	1:F:172:TYR:OH	2.38	0.57
1:F:202:VAL:HB	1:F:260:LEU:HD13	1.85	0.57
1:I:450:VAL:HG12	1:I:487:LEU:HD13	1.87	0.57
1:K:697:MET:HG2	1:K:703:SER:HA	1.86	0.57
1:L:73:ARG:NH1	1:L:80:TYR:OH	2.37	0.57
1:B:47:ASN:ND2	7:w:16:HIS:O	2.38	0.57
1:B:537:GLN:NE2	1:B:554:TYR:OH	2.37	0.57
1:C:629:ILE:HD11	1:C:889:LEU:HB2	1.87	0.57
1:J:413:THR:OG1	1:J:414:ALA:N	2.38	0.57
1:E:62:GLN:OE1	1:E:92:ARG:NH2	2.38	0.56
1:E:92:ARG:NH1	1:E:595:MET:O	2.38	0.56
1:H:449:ASN:OD1	1:H:510:HIS:NE2	2.38	0.56
1:H:685:PHE:HE2	1:H:843:MET:HE2	1.70	0.56
1:L:278:PRO:O	1:L:464:ASN:ND2	2.38	0.56
2:M:205:LYS:HE2	2:M:442:LEU:HA	1.86	0.56
1:A:382:VAL:HG11	1:A:439:ALA:HA	1.87	0.56
1:A:717:GLU:OE1	1:A:720:ARG:NH2	2.38	0.56
1:C:108:ASP:OD1	1:C:527:ARG:NH1	2.38	0.56
1:D:94:LEU:HD23	1:D:547:LEU:HD22	1.86	0.56
1:G:146:GLN:HE21	1:I:814:ALA:H	1.53	0.56
1:G:182:GLN:NE2	1:I:793:PRO:O	2.37	0.56
1:G:788:GLN:NE2	1:H:220:THR:O	2.37	0.56
1:H:201:ARG:NH2	1:H:263:GLU:OE1	2.38	0.56
1:A:521:MET:HB3	1:C:496:ARG:HB2	1.86	0.56
1:A:617:ASN:ND2	7:w:20:MET:SD	2.79	0.56
1:B:766:SER:O	1:B:770:ASN:ND2	2.37	0.56
1:C:313:MET:HE1	1:C:538:LYS:H	1.70	0.56
1:D:340:ARG:HH21	1:D:622:ALA:H	1.52	0.56
1:F:154:ILE:HD11	1:F:256:PRO:HB2	1.86	0.56
1:F:158:ASN:ND2	1:F:173:ALA:O	2.37	0.56
1:G:208:PRO:HB3	1:G:284:THR:HG22	1.87	0.56
1:G:219:PRO:O	1:I:788:GLN:NE2	2.38	0.56
1:G:474:TYR:HB2	1:G:572:ASN:HD22	1.70	0.56
1:G:607:LEU:HD21	1:G:614:GLN:HE22	1.70	0.56
1:H:301:ASN:HA	1:H:569:SER:HB2	1.88	0.56
1:J:94:LEU:HD12	1:J:592:PHE:HE1	1.70	0.56
1:L:650:GLY:H	1:L:848:PHE:H	1.54	0.56
1:L:717:GLU:HG2	1:L:735:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:TYR:OH	1:E:342:THR:O	2.22	0.56
1:E:899:VAL:HA	1:E:913:TYR:HB3	1.87	0.56
1:J:723:ASP:OD2	1:K:104:ARG:NH1	2.36	0.56
1:B:94:LEU:HD23	1:B:547:LEU:HD22	1.87	0.56
1:D:25:SER:H	1:F:612:ASN:HD21	1.54	0.56
1:G:132:PRO:HB2	1:G:202:VAL:HG22	1.88	0.56
1:K:709:ARG:HB3	1:L:64:LEU:HD13	1.88	0.56
1:L:503:ASP:OD1	1:L:689:HIS:NE2	2.38	0.56
2:M:49:GLY:O	2:M:114:ARG:NH1	2.38	0.56
1:B:705:PRO:HB3	1:B:710:LEU:HD22	1.86	0.56
1:C:161:GLN:HA	1:C:172:TYR:HA	1.88	0.56
1:C:360:PHE:HB3	1:C:365:GLN:HB3	1.88	0.56
1:I:136:LYS:HA	1:I:141:ILE:HG22	1.87	0.56
1:L:150:ILE:HD12	1:L:185:GLN:HE21	1.70	0.56
1:B:485:SER:O	1:B:490:TYR:OH	2.22	0.56
1:F:86:LEU:HB2	1:F:552:TYR:HB2	1.86	0.56
1:J:742:GLN:HE21	1:J:746:HIS:HE1	1.54	0.56
1:K:13:MET:O	1:K:46:ARG:NH2	2.38	0.56
2:M:180:MET:HE3	2:M:184:ILE:HB	1.87	0.56
4:P:14:GLN:NE2	4:P:16:GLN:OE1	2.39	0.56
1:C:94:LEU:HB3	1:C:547:LEU:HB3	1.88	0.56
1:C:447:TYR:HA	1:C:451:ALA:HB3	1.87	0.56
1:L:109:ARG:NH1	1:L:303:ILE:O	2.39	0.56
3:N:56:GLN:O	3:N:61:ARG:NH1	2.38	0.56
4:O:14:GLN:NE2	4:O:16:GLN:OE1	2.39	0.56
1:E:230:ILE:HG22	1:E:239:THR:H	1.71	0.56
1:G:517:ARG:HH11	1:I:380:HIS:CG	2.24	0.56
1:G:820:PRO:HG2	1:H:121:TYR:HE1	1.71	0.56
1:B:629:ILE:HD11	1:B:889:LEU:HB2	1.88	0.55
1:F:298:ASN:ND2	1:F:478:ASN:OD1	2.39	0.55
1:J:96:MET:HE2	1:J:547:LEU:HD21	1.88	0.55
1:A:279:ASP:O	1:A:464:ASN:ND2	2.39	0.55
1:B:632:ASN:ND2	1:B:883:MET:O	2.37	0.55
1:C:563:ASN:ND2	1:C:672:PHE:O	2.39	0.55
1:D:114:LYS:NZ	1:D:116:TYR:O	2.37	0.55
1:D:116:TYR:OH	1:D:271:ASP:OD2	2.23	0.55
1:D:306:ARG:NH2	1:D:563:ASN:O	2.40	0.55
1:G:201:ARG:NH2	1:G:263:GLU:OE1	2.39	0.55
1:G:483:VAL:HG21	1:G:792:LEU:HD21	1.88	0.55
1:K:388:ASN:HB3	1:L:440:ASN:HD21	1.71	0.55
1:B:210:LEU:HD12	1:B:267:ILE:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:ALA:H	1:C:146:GLN:HE21	1.53	0.55
1:K:180:GLU:HG2	1:K:182:GLN:H	1.71	0.55
1:K:462:PRO:HG2	1:K:465:ILE:HD12	1.89	0.55
1:K:814:ALA:H	1:L:146:GLN:HE21	1.54	0.55
2:M:389:ARG:HD3	2:M:390:PRO:HD2	1.89	0.55
1:A:123:SER:O	1:C:436:ASN:ND2	2.39	0.55
1:B:263:GLU:HB3	1:B:265:VAL:HG13	1.87	0.55
1:C:763:ARG:HE	1:C:764:MET:H	1.53	0.55
1:D:898:VAL:HG22	1:E:46:ARG:HH12	1.72	0.55
1:A:503:ASP:OD1	1:A:689:HIS:NE2	2.36	0.55
1:C:776:ARG:HD3	1:C:834:GLN:HE21	1.71	0.55
1:E:85:THR:OG1	1:L:83:ARG:NH2	2.40	0.55
1:E:519:ARG:NH2	1:E:567:GLN:OE1	2.40	0.55
1:G:626:LEU:HG	1:G:664:LEU:HD11	1.89	0.55
1:J:652:SER:HB2	1:J:892:LEU:HB3	1.88	0.55
2:M:73:LYS:NZ	2:M:92:THR:OG1	2.40	0.55
1:A:350:LEU:HD22	1:A:356:ARG:HH11	1.71	0.55
1:B:155:ASN:ND2	1:B:172:TYR:OH	2.40	0.55
1:C:349:MET:SD	1:C:543:LYS:NZ	2.76	0.55
1:F:447:TYR:HA	1:F:451:ALA:HB3	1.88	0.55
1:H:472:ASN:HB3	1:H:573:ASP:HB2	1.87	0.55
1:J:356:ARG:HB3	1:J:367:VAL:HG11	1.89	0.55
1:L:351:ASP:HB2	1:L:356:ARG:HE	1.72	0.55
1:A:72:ASP:HB3	1:A:83:ARG:HD3	1.89	0.55
1:C:176:THR:HG22	1:C:225:GLY:HA3	1.89	0.55
1:G:347:GLN:NE2	1:G:682:ASP:O	2.40	0.55
1:G:537:GLN:NE2	1:G:542:ILE:O	2.40	0.55
1:H:392:PRO:HA	1:I:433:MET:HG2	1.87	0.55
1:H:710:LEU:HD11	1:H:741:ILE:HD12	1.89	0.55
1:A:399:THR:HB	1:A:426:GLU:HA	1.89	0.55
1:D:613:ASP:HB2	1:D:900:ARG:HH11	1.72	0.55
1:G:548:LEU:HD11	1:G:607:LEU:HB3	1.88	0.55
1:G:786:GLU:HB2	1:G:788:GLN:HE22	1.72	0.55
1:K:620:LEU:HD21	1:K:892:LEU:HD21	1.89	0.55
1:A:15:ILE:HA	1:A:46:ARG:HH21	1.71	0.54
1:B:811:GLU:HB2	1:C:184:GLY:HA3	1.89	0.54
1:E:436:ASN:ND2	1:F:123:SER:O	2.37	0.54
1:G:490:TYR:OH	1:G:795:GLN:NE2	2.40	0.54
1:I:575:ARG:NH1	5:Q:38:SER:O	2.40	0.54
1:J:642:SER:HB3	1:J:871:ALA:HB1	1.89	0.54
3:N:238:PRO:HG2	4:O:5:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:ARG:HG2	1:B:561:ASP:H	1.72	0.54
1:D:65:THR:HG22	1:D:591:ASN:HB3	1.89	0.54
1:E:402:TYR:HB2	1:E:423:ALA:HB3	1.88	0.54
1:E:919:SER:OG	4:O:105:GLY:O	2.25	0.54
1:G:440:ASN:HD21	1:I:389:TYR:H	1.53	0.54
1:G:583:PHE:HB3	1:G:586:ILE:HD11	1.89	0.54
1:G:630:PRO:HB2	1:G:633:ALA:HB3	1.90	0.54
1:J:388:ASN:ND2	1:K:440:ASN:OD1	2.40	0.54
1:A:810:ARG:NH2	1:C:430:ILE:O	2.40	0.54
1:C:732:CYS:SG	1:C:733:ASN:N	2.79	0.54
1:H:563:ASN:ND2	1:H:672:PHE:O	2.40	0.54
1:J:107:LEU:HD11	1:J:566:LEU:HD21	1.88	0.54
1:E:24:LEU:HD22	1:E:28:LEU:HD23	1.89	0.54
1:E:472:ASN:HB3	1:E:573:ASP:HB2	1.88	0.54
1:F:548:LEU:HD11	1:F:607:LEU:HB2	1.89	0.54
1:C:548:LEU:HD12	1:C:903:GLN:HB2	1.89	0.54
1:H:657:LYS:HG2	1:H:887:THR:HG22	1.88	0.54
1:L:568:SER:OG	1:L:675:SER:O	2.26	0.54
1:E:76:THR:HB	1:E:79:SER:H	1.72	0.54
1:E:640:ILE:HD13	1:E:643:ARG:HH12	1.72	0.54
1:D:631:SER:OG	5:Q:11:SER:O	2.25	0.54
1:E:624:ASN:ND2	1:E:680:TYR:OH	2.41	0.54
1:E:762:ASP:OD2	1:F:358:ARG:NH1	2.41	0.54
1:G:83:ARG:HA	1:G:555:GLU:HA	1.90	0.54
1:J:382:VAL:HG11	1:J:439:ALA:HA	1.88	0.54
1:B:382:VAL:HG23	1:B:384:ASP:HB2	1.90	0.54
1:C:301:ASN:HA	1:C:569:SER:HB2	1.88	0.54
1:C:376:ILE:HD11	1:C:838:LEU:HG	1.89	0.54
1:D:378:GLU:HG2	1:D:496:ARG:HA	1.90	0.54
1:F:152:THR:OG1	1:F:161:GLN:NE2	2.37	0.54
1:F:688:ASN:ND2	1:F:842:THR:O	2.40	0.54
1:H:546:LEU:HB2	1:I:44:LYS:HE2	1.88	0.54
1:J:104:ARG:NH2	1:J:585:SER:OG	2.41	0.54
1:K:292:THR:HG21	1:L:187:GLN:HA	1.90	0.54
1:B:523:LEU:HB3	1:B:529:VAL:HG11	1.89	0.54
1:D:146:GLN:HG3	1:E:426:GLU:HB3	1.90	0.54
1:J:94:LEU:HB3	1:J:547:LEU:HB2	1.89	0.54
1:L:710:LEU:HD23	1:L:712:THR:H	1.72	0.54
1:A:229:LEU:HA	1:A:240:SER:HA	1.89	0.54
1:C:780:ASN:HD21	1:C:832:LEU:HB2	1.73	0.54
1:E:812:GLY:H	1:F:184:GLY:HA3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:744:LEU:HD21	1:L:853:MET:HG2	1.90	0.54
1:A:780:ASN:ND2	1:A:783:THR:OG1	2.41	0.53
1:H:313:MET:HG2	1:H:556:TRP:HE1	1.72	0.53
1:H:512:ARG:HG3	1:H:517:ARG:HH11	1.73	0.53
1:J:188:TRP:HB3	1:L:809:MET:HE1	1.91	0.53
1:L:632:ASN:HD22	1:L:882:PRO:HB2	1.73	0.53
1:A:226:GLN:HG3	1:A:265:VAL:HG11	1.90	0.53
1:C:780:ASN:HD21	1:C:832:LEU:H	1.56	0.53
1:D:798:ASN:HD21	1:E:124:LEU:HB2	1.73	0.53
1:E:910:GLU:OE2	4:O:93:ARG:NH1	2.40	0.53
1:G:390:CYS:HB2	1:G:433:MET:HB2	1.90	0.53
1:L:435:ILE:HD13	1:L:437:LEU:HB3	1.89	0.53
1:A:197:LYS:NZ	1:A:256:PRO:O	2.40	0.53
1:A:210:LEU:HD12	1:A:267:ILE:HG22	1.88	0.53
1:A:275:VAL:HA	1:A:465:ILE:HD11	1.89	0.53
1:C:73:ARG:HH12	1:C:585:SER:HA	1.71	0.53
1:C:150:ILE:HG13	1:C:198:VAL:HG23	1.91	0.53
1:C:327:GLN:O	1:C:330:GLN:NE2	2.41	0.53
1:C:565:ILE:HG23	1:C:566:LEU:HG	1.89	0.53
1:D:341:ASN:ND2	1:D:680:TYR:O	2.41	0.53
1:E:299:ARG:NH1	1:E:477:MET:O	2.40	0.53
1:F:374:VAL:HG13	1:F:449:ASN:HB3	1.90	0.53
1:H:688:ASN:OD1	1:H:844:TRP:NE1	2.42	0.53
1:J:396:SER:OG	1:L:144:ARG:NH2	2.42	0.53
1:J:688:ASN:ND2	1:J:842:THR:O	2.42	0.53
2:M:258:ARG:HH21	2:M:363:THR:HG21	1.73	0.53
1:A:360:PHE:HB3	1:A:365:GLN:HB2	1.91	0.53
1:A:485:SER:O	1:A:490:TYR:OH	2.25	0.53
1:C:352:ALA:HA	1:C:763:ARG:HD3	1.90	0.53
1:H:467:LEU:HD12	1:H:476:TYR:HA	1.89	0.53
1:I:23:TYR:OH	1:I:45:PHE:O	2.25	0.53
1:B:342:THR:HG21	1:B:539:PHE:HA	1.89	0.53
1:D:23:TYR:OH	1:D:45:PHE:O	2.27	0.53
1:G:620:LEU:HD12	1:G:892:LEU:HD21	1.90	0.53
1:H:456:ASP:O	1:H:480:ARG:NH2	2.42	0.53
2:M:81:ASN:HD22	2:M:90:GLN:H	1.56	0.53
1:C:770:ASN:OD1	1:C:841:ARG:NH2	2.41	0.53
1:D:764:MET:O	1:D:770:ASN:ND2	2.42	0.53
1:G:380:HIS:CE1	1:H:517:ARG:HB2	2.44	0.53
1:L:175:LYS:HB3	1:L:242:VAL:HG11	1.90	0.53
1:L:692:LYS:HB2	1:L:879:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:742:GLN:NE2	1:L:845:ARG:O	2.39	0.53
1:B:230:ILE:O	1:B:238:LEU:N	2.42	0.53
1:D:63:ARG:NH1	1:F:710:LEU:O	2.42	0.53
1:D:496:ARG:NH1	1:D:773:PRO:O	2.41	0.53
1:E:335:VAL:O	1:E:913:TYR:OH	2.24	0.53
1:E:654:THR:OG1	1:E:688:ASN:ND2	2.42	0.53
1:H:621:CYS:SG	1:H:649:ARG:NH2	2.81	0.53
1:A:134:GLU:HG2	1:A:143:VAL:HG12	1.89	0.53
1:A:220:THR:HG21	1:A:228:SER:HA	1.91	0.53
1:F:563:ASN:ND2	1:F:672:PHE:O	2.42	0.53
1:I:301:ASN:HA	1:I:569:SER:HB3	1.91	0.53
1:B:910:GLU:OE1	1:C:2:ALA:N	2.42	0.53
1:C:209:MET:O	1:C:293:GLN:NE2	2.42	0.53
1:G:279:ASP:HA	1:G:464:ASN:HD21	1.74	0.53
1:H:754:PHE:O	1:I:363:TRP:NE1	2.37	0.53
1:J:598:ASN:ND2	4:P:93:ARG:O	2.36	0.53
2:M:324:LYS:HD3	2:M:326:ARG:HH12	1.72	0.53
1:A:694:VAL:HB	1:A:716:PHE:HB2	1.89	0.52
1:B:565:ILE:HG23	1:B:566:LEU:HG	1.91	0.52
1:D:19:ASP:HA	1:D:48:PRO:HD2	1.91	0.52
1:F:58:THR:HG22	1:F:60:ARG:H	1.74	0.52
1:F:332:ASN:ND2	1:F:334:VAL:O	2.41	0.52
1:J:632:ASN:ND2	1:J:883:MET:O	2.42	0.52
1:K:310:ILE:HD12	1:K:681:LEU:HB3	1.90	0.52
1:A:865:MET:HE3	1:A:869:ASN:HD21	1.75	0.52
1:C:350:LEU:HB2	1:C:356:ARG:HH21	1.74	0.52
1:C:485:SER:O	1:C:490:TYR:OH	2.26	0.52
1:D:386:LEU:HD12	1:D:387:PRO:HD2	1.91	0.52
1:F:723:ASP:OD1	1:F:728:ASN:ND2	2.42	0.52
1:G:57:THR:OG1	1:I:860:ASP:OD2	2.27	0.52
1:G:68:PHE:HB2	1:G:588:LEU:HB3	1.90	0.52
1:I:308:ASN:HB3	1:I:310:ILE:HG23	1.91	0.52
1:J:604:GLU:O	1:J:608:ARG:NH1	2.42	0.52
1:K:448:SER:HA	1:K:452:LEU:HD23	1.91	0.52
2:M:144:ARG:NH1	2:M:241:GLY:O	2.41	0.52
1:A:446:LEU:HD11	1:A:487:LEU:HG	1.92	0.52
1:C:101:PHE:HB2	1:C:535:VAL:HB	1.92	0.52
1:C:621:CYS:SG	1:C:649:ARG:NH1	2.78	0.52
1:I:210:LEU:HD22	1:I:215:SER:HB3	1.90	0.52
1:K:766:SER:O	1:K:770:ASN:ND2	2.42	0.52
1:C:197:LYS:NZ	1:C:255:GLU:OE2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:ILE:HG12	1:F:248:ALA:HB2	1.92	0.52
1:D:807:PRO:HB3	1:F:386:LEU:HD23	1.92	0.52
1:H:375:ARG:HH11	1:H:507:PRO:HD2	1.74	0.52
1:H:460:ILE:HD11	1:H:483:VAL:HB	1.90	0.52
1:I:712:THR:OG1	1:I:737:ASP:OD2	2.26	0.52
1:J:103:ILE:HG12	1:J:586:ILE:HD12	1.91	0.52
1:B:327:GLN:O	2:M:389:ARG:NH1	2.39	0.52
1:D:402:TYR:HE1	1:F:249:LEU:HD23	1.75	0.52
1:H:371:ASP:HB3	1:H:374:VAL:HG22	1.92	0.52
1:I:550:GLY:HA2	1:I:906:ARG:HG2	1.92	0.52
1:A:504:ASN:ND2	1:A:883:MET:SD	2.78	0.52
1:E:276:TYR:OH	1:F:187:GLN:NE2	2.43	0.52
1:E:910:GLU:OE2	4:O:165:ARG:NH1	2.42	0.52
1:G:519:ARG:NH1	1:G:567:GLN:OE1	2.35	0.52
1:H:510:HIS:CD2	1:H:512:ARG:H	2.28	0.52
1:J:349:MET:HE2	1:J:543:LYS:HE3	1.92	0.52
1:C:454:LEU:HD22	1:C:501:PRO:HB2	1.92	0.52
1:D:531:PHE:HB2	1:D:533:ILE:HG23	1.91	0.52
1:F:196:GLN:O	1:F:257:LYS:NZ	2.42	0.52
1:G:688:ASN:ND2	1:G:842:THR:O	2.42	0.52
1:H:79:SER:OG	1:H:80:TYR:N	2.42	0.52
1:H:313:MET:O	1:H:559:ARG:NH2	2.42	0.52
1:H:765:TYR:HE1	1:H:841:ARG:HH11	1.58	0.52
1:I:247:PHE:HB2	1:I:258:ALA:HB3	1.92	0.52
1:E:640:ILE:HD11	1:E:874:LEU:HG	1.92	0.52
1:E:655:ARG:NH2	1:E:887:THR:OG1	2.42	0.52
1:F:94:LEU:HD23	1:F:547:LEU:HD23	1.91	0.52
1:K:210:LEU:HD12	1:K:267:ILE:HG22	1.92	0.52
1:L:402:TYR:HB2	1:L:423:ALA:HB3	1.92	0.52
2:M:227:TYR:OH	2:M:280:PRO:O	2.26	0.52
2:M:321:LYS:HA	2:M:327:SER:HA	1.91	0.52
1:B:708:ASP:HB3	1:C:61:SER:HB2	1.92	0.52
1:E:150:ILE:HG12	1:E:198:VAL:HG23	1.90	0.52
1:G:742:GLN:HE22	1:G:845:ARG:H	1.56	0.52
1:K:688:ASN:ND2	1:K:839:CYS:SG	2.83	0.52
1:L:423:ALA:HB1	1:L:425:ILE:HG23	1.91	0.52
1:A:302:TYR:HB3	1:A:520:SER:HB3	1.91	0.52
1:B:693:LYS:NZ	1:B:879:GLU:OE1	2.42	0.52
1:C:679:PRO:HA	1:C:684:THR:HB	1.91	0.52
1:D:102:ASP:OD2	1:F:736:LYS:NZ	2.43	0.52
1:E:910:GLU:HA	4:O:110:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:656:LEU:HD23	1:F:685:PHE:HE1	1.74	0.52
1:G:517:ARG:HB3	1:I:380:HIS:HE1	1.75	0.52
1:G:649:ARG:HE	1:G:894:GLU:HG2	1.74	0.52
1:L:537:GLN:NE2	1:L:554:TYR:OH	2.43	0.52
1:C:618:ASP:HB3	1:C:621:CYS:HB3	1.91	0.51
1:D:10:TRP:HB2	1:D:15:ILE:HB	1.91	0.51
1:D:660:GLU:HB2	1:D:678:VAL:HG12	1.92	0.51
1:E:107:LEU:HD11	1:E:566:LEU:HD21	1.92	0.51
1:H:385:GLU:HG3	1:I:296:ALA:HB1	1.93	0.51
1:I:346:TYR:HB3	1:I:538:LYS:HD3	1.92	0.51
1:L:388:ASN:OD1	1:L:388:ASN:N	2.42	0.51
1:C:382:VAL:HG11	1:C:439:ALA:HA	1.93	0.51
1:C:559:ARG:NH2	1:C:564:MET:O	2.44	0.51
1:C:621:CYS:O	1:C:649:ARG:NH2	2.42	0.51
1:F:217:ALA:HB2	1:F:267:ILE:HD13	1.92	0.51
1:G:276:TYR:OH	1:H:187:GLN:NE2	2.43	0.51
1:H:14:HIS:O	1:H:46:ARG:NH1	2.43	0.51
3:N:35:TRP:NE1	3:N:68:ALA:O	2.43	0.51
1:B:609:ASN:ND2	3:N:24:SER:OG	2.43	0.51
1:D:202:VAL:HB	1:D:260:LEU:HD13	1.91	0.51
1:G:458:TYR:HE2	1:G:501:PRO:HB3	1.75	0.51
1:I:366:ALA:O	1:I:519:ARG:NH1	2.43	0.51
1:J:165:ASP:HB2	1:J:169:GLN:HB2	1.91	0.51
1:K:562:VAL:HG23	1:K:566:LEU:HD12	1.92	0.51
1:L:443:ARG:HH12	1:L:802:VAL:HG12	1.75	0.51
1:L:767:PHE:HA	1:L:842:THR:HG21	1.91	0.51
1:A:766:SER:O	1:A:770:ASN:ND2	2.44	0.51
1:B:645:TRP:HD1	1:B:872:HIS:HB2	1.76	0.51
1:H:352:ALA:HA	1:H:763:ARG:HD3	1.92	0.51
1:I:476:TYR:OH	1:I:480:ARG:NH2	2.43	0.51
3:N:60:ASN:OD1	6:Y:12:ARG:NH2	2.43	0.51
1:D:46:ARG:HH12	1:F:898:VAL:HG22	1.74	0.51
1:E:728:ASN:H	1:E:736:LYS:HE2	1.76	0.51
1:E:756:VAL:HG23	1:F:365:GLN:HE21	1.76	0.51
1:G:503:ASP:OD2	1:G:689:HIS:NE2	2.41	0.51
1:J:392:PRO:HA	1:K:433:MET:HG2	1.91	0.51
1:K:342:THR:HA	1:K:345:SER:HB3	1.92	0.51
1:K:546:LEU:HB2	1:L:44:LYS:HD2	1.93	0.51
1:K:632:ASN:ND2	1:K:883:MET:O	2.43	0.51
1:G:425:ILE:HG22	1:I:145:GLY:HA3	1.92	0.51
1:I:542:ILE:HA	1:I:545:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:TYR:OH	1:J:45:PHE:O	2.28	0.51
1:K:86:LEU:HD12	1:K:94:LEU:HD11	1.92	0.51
1:A:626:LEU:HB3	1:A:888:LEU:HD12	1.91	0.51
1:A:780:ASN:OD1	1:A:781:THR:N	2.44	0.51
1:B:53:THR:OG1	1:B:54:HIS:N	2.43	0.51
1:C:180:GLU:HB2	1:C:183:VAL:HG23	1.92	0.51
1:D:322:GLY:HA3	1:D:556:TRP:CD1	2.43	0.51
1:D:742:GLN:HE22	1:D:767:PHE:HB2	1.76	0.51
1:E:726:GLY:HA2	1:F:104:ARG:HH22	1.76	0.51
1:F:151:GLY:HA3	1:F:160:ILE:HD11	1.92	0.51
1:G:112:SER:OG	1:G:572:ASN:ND2	2.44	0.51
1:H:657:LYS:HA	1:H:887:THR:HA	1.91	0.51
1:J:146:GLN:HA	1:K:426:GLU:H	1.75	0.51
1:K:637:PRO:HA	1:K:877:THR:HA	1.93	0.51
1:B:450:VAL:HG12	1:B:487:LEU:HD21	1.93	0.51
1:C:652:SER:HB2	1:C:892:LEU:HB3	1.92	0.51
1:D:243:ASN:O	1:D:262:ALA:N	2.42	0.51
1:D:780:ASN:HD22	1:D:832:LEU:HD23	1.76	0.51
1:E:292:THR:HG23	1:F:188:TRP:HD1	1.76	0.51
1:F:68:PHE:HB2	1:F:588:LEU:HB3	1.93	0.51
1:G:24:LEU:HD12	1:G:28:LEU:HD23	1.91	0.51
1:I:692:LYS:NZ	1:I:881:ASP:OD1	2.39	0.51
1:K:371:ASP:HB2	1:K:374:VAL:HG22	1.92	0.51
1:L:903:GLN:HE21	1:L:909:ILE:HD12	1.75	0.51
1:C:229:LEU:HB2	1:C:238:LEU:HD21	1.93	0.51
1:D:104:ARG:NH1	1:F:723:ASP:OD2	2.44	0.51
1:B:736:LYS:NZ	1:C:100:TYR:OH	2.36	0.51
1:D:622:ALA:HA	1:D:894:GLU:HA	1.93	0.51
1:I:404:GLY:HA3	1:I:418:TYR:HB2	1.92	0.51
1:J:606:MET:O	1:J:612:ASN:ND2	2.43	0.51
2:M:53:ILE:HD13	2:M:65:THR:HG22	1.92	0.51
1:A:83:ARG:HG3	1:A:555:GLU:HG2	1.93	0.50
1:E:622:ALA:HA	1:E:895:VAL:HG22	1.93	0.50
1:E:770:ASN:OD1	1:E:841:ARG:NH2	2.44	0.50
1:G:446:LEU:HD12	1:G:487:LEU:HD11	1.93	0.50
1:H:821:TYR:HB3	1:H:829:VAL:HG21	1.92	0.50
4:O:8:PRO:HB3	4:O:202:VAL:HG22	1.93	0.50
1:C:822:PRO:HG2	1:C:827:THR:HG21	1.93	0.50
1:G:220:THR:N	1:G:225:GLY:O	2.44	0.50
1:H:374:VAL:HG21	1:H:510:HIS:HE1	1.77	0.50
1:J:343:GLU:HB2	1:J:681:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:23:TYR:OH	1:K:45:PHE:O	2.29	0.50
1:A:81:LYS:HG2	1:A:557:ASN:HD22	1.76	0.50
1:A:187:GLN:HG3	1:C:292:THR:HG21	1.91	0.50
1:A:546:LEU:HB3	1:A:614:GLN:HE22	1.75	0.50
1:A:815:TYR:O	1:B:122:ASN:ND2	2.44	0.50
1:E:203:LEU:HB3	1:E:207:THR:HG21	1.92	0.50
1:G:302:TYR:HE2	1:G:517:ARG:HG2	1.76	0.50
1:J:128:THR:HG23	1:J:294:GLN:HB3	1.92	0.50
1:A:447:TYR:HA	1:A:451:ALA:HB3	1.93	0.50
1:E:909:ILE:O	4:O:111:GLY:N	2.41	0.50
1:G:332:ASN:ND2	1:G:334:VAL:O	2.45	0.50
1:K:707:ASN:OD1	1:K:707:ASN:N	2.45	0.50
1:K:791:THR:HG23	1:K:793:PRO:HD2	1.93	0.50
1:L:206:THR:OG1	1:L:264:ASN:OD1	2.28	0.50
1:D:103:ILE:HA	1:D:586:ILE:HG12	1.93	0.50
1:I:130:PRO:HA	1:I:211:PRO:HA	1.93	0.50
1:J:294:GLN:HE22	1:J:808:THR:HA	1.77	0.50
2:M:189:LEU:HG	2:M:193:ARG:HH12	1.77	0.50
1:G:382:VAL:HG11	1:G:439:ALA:HA	1.93	0.50
1:J:490:TYR:HA	1:J:493:ILE:HD11	1.93	0.50
1:A:217:ALA:HB2	1:A:267:ILE:HD13	1.94	0.50
1:A:813:GLN:HE21	1:B:147:ALA:HA	1.77	0.50
1:E:548:LEU:HD11	1:E:607:LEU:HB3	1.94	0.50
1:F:308:ASN:OD1	1:F:347:GLN:NE2	2.44	0.50
1:G:15:ILE:HG12	1:I:898:VAL:HG21	1.94	0.50
1:G:108:ASP:HB3	1:G:579:ALA:HA	1.94	0.50
1:G:433:MET:SD	1:I:433:MET:HE3	2.51	0.50
1:K:313:MET:HE1	1:K:537:GLN:HA	1.93	0.50
1:B:248:ALA:HB2	1:B:256:PRO:HA	1.94	0.50
1:B:705:PRO:HG2	1:B:708:ASP:H	1.76	0.50
1:D:378:GLU:OE1	1:E:517:ARG:NH1	2.45	0.50
1:F:542:ILE:HG22	1:F:545:LEU:HD13	1.92	0.50
1:H:143:VAL:H	1:I:423:ALA:HB3	1.76	0.50
1:K:380:HIS:NE2	1:L:521:MET:SD	2.85	0.50
3:N:215:ASN:ND2	3:N:237:THR:OG1	2.45	0.50
1:A:706:GLY:O	1:A:709:ARG:NH1	2.45	0.50
1:C:339:ASP:OD2	1:C:915:ARG:NH2	2.44	0.50
1:D:316:ASN:ND2	1:D:337:LEU:O	2.45	0.50
1:G:638:ILE:HD11	1:G:891:VAL:HG21	1.93	0.50
1:H:210:LEU:HD21	1:H:269:ALA:HB2	1.94	0.50
1:I:595:MET:HE1	1:I:603:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:88:VAL:HG13	1:J:549:PRO:HA	1.94	0.50
1:J:150:ILE:HG12	1:J:198:VAL:HG23	1.93	0.50
1:J:549:PRO:HD2	1:J:608:ARG:HH22	1.77	0.50
1:K:390:CYS:HB3	1:L:435:ILE:HG23	1.93	0.50
1:K:914:LEU:HD13	1:L:13:MET:HG3	1.93	0.50
3:N:99:ALA:HA	3:N:102:ILE:HG22	1.94	0.50
1:A:78:TYR:OH	1:K:723:ASP:OD2	2.29	0.49
1:E:208:PRO:HG2	1:E:267:ILE:HB	1.93	0.49
1:F:116:TYR:OH	1:F:271:ASP:OD2	2.27	0.49
1:F:278:PRO:HG3	1:F:293:GLN:H	1.77	0.49
1:F:354:GLY:O	1:F:763:ARG:NH2	2.45	0.49
1:G:476:TYR:OH	1:G:480:ARG:NH1	2.45	0.49
1:G:562:VAL:HG21	1:G:579:ALA:HB3	1.93	0.49
1:H:724:GLY:O	1:I:104:ARG:NH1	2.44	0.49
1:I:629:ILE:HD13	1:I:880:VAL:HG21	1.94	0.49
1:L:310:ILE:HG22	1:L:538:LYS:HE2	1.94	0.49
3:N:62:PHE:HA	3:N:65:ILE:HG22	1.93	0.49
1:A:390:CYS:HA	1:B:435:ILE:HB	1.94	0.49
1:C:302:TYR:HE2	1:C:511:HIS:HB2	1.76	0.49
1:D:710:LEU:HD21	1:D:741:ILE:HD13	1.93	0.49
1:D:797:ASN:HD21	1:E:121:TYR:HA	1.75	0.49
1:F:24:LEU:HB2	1:F:29:VAL:HG13	1.93	0.49
1:H:58:THR:HB	1:H:596:ALA:HA	1.94	0.49
1:H:645:TRP:HD1	1:H:872:HIS:HB2	1.77	0.49
1:I:344:LEU:HD11	1:I:348:LEU:HD12	1.93	0.49
1:J:12:TYR:O	1:L:900:ARG:NH1	2.37	0.49
1:K:798:ASN:HD21	1:L:124:LEU:H	1.58	0.49
1:L:388:ASN:HD22	1:L:437:LEU:HD23	1.77	0.49
2:M:73:LYS:HE3	2:M:95:GLN:HA	1.94	0.49
1:B:146:GLN:HE22	1:C:430:ILE:HD11	1.77	0.49
1:D:741:ILE:O	1:D:745:SER:OG	2.29	0.49
1:I:399:THR:HG21	1:I:426:GLU:HA	1.94	0.49
1:K:405:ILE:HD11	1:K:413:THR:HA	1.93	0.49
1:L:878:PHE:HD2	1:L:889:LEU:HD11	1.76	0.49
4:P:8:PRO:HB3	4:P:202:VAL:HG22	1.93	0.49
1:A:655:ARG:HH21	1:A:887:THR:HG21	1.77	0.49
1:C:323:VAL:HG22	1:C:555:GLU:HB2	1.92	0.49
1:I:132:PRO:HB2	1:I:202:VAL:HG22	1.95	0.49
1:K:652:SER:HB3	1:K:843:MET:HE2	1.94	0.49
1:L:134:GLU:HG2	1:L:205:ASP:HB3	1.95	0.49
1:E:201:ARG:HG2	1:E:261:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:ARG:NH1	6:u:20:GLY:O	2.42	0.49
1:G:517:ARG:HB3	1:I:380:HIS:CE1	2.48	0.49
1:G:557:ASN:OD1	1:G:557:ASN:N	2.44	0.49
1:H:147:ALA:HB2	1:H:260:LEU:HD21	1.93	0.49
1:K:272:THR:HB	1:K:295:ALA:HB1	1.95	0.49
1:A:188:TRP:HE1	1:C:292:THR:HA	1.77	0.49
1:B:652:SER:HB2	1:B:892:LEU:HB3	1.93	0.49
1:I:302:TYR:HE2	1:I:517:ARG:HG2	1.77	0.49
1:L:90:ASP:OD1	1:L:906:ARG:NH1	2.46	0.49
2:M:380:ASP:HB2	2:M:476:GLN:HE22	1.78	0.49
1:A:397:ALA:N	1:A:426:GLU:OE2	2.44	0.49
1:B:23:TYR:OH	1:B:45:PHE:O	2.25	0.49
1:B:474:TYR:O	1:B:478:ASN:N	2.46	0.49
1:C:310:ILE:HD13	1:C:347:GLN:HE21	1.78	0.49
1:C:901:ILE:HG22	1:C:911:ALA:HA	1.94	0.49
1:E:744:LEU:HD12	1:E:750:GLY:HA3	1.94	0.49
1:I:121:TYR:HE2	1:I:270:PRO:HG2	1.78	0.49
1:K:493:ILE:HD13	1:L:120:ALA:HB2	1.94	0.49
1:L:104:ARG:NH1	1:L:585:SER:OG	2.41	0.49
1:A:445:PHE:HE1	1:A:512:ARG:HH12	1.60	0.49
1:A:508:PHE:HD2	1:A:684:THR:HG23	1.78	0.49
1:D:657:LYS:HB2	1:D:660:GLU:HG2	1.95	0.49
1:K:900:ARG:NH1	1:L:12:TYR:OH	2.45	0.49
1:B:323:VAL:HG12	1:B:332:ASN:HD22	1.78	0.49
1:D:522:LEU:HD21	1:F:731:GLN:HE21	1.78	0.49
1:E:548:LEU:H	1:E:903:GLN:HE21	1.61	0.49
1:G:216:TYR:HD1	1:I:817:ALA:HB3	1.78	0.49
1:I:406:LYS:HB3	1:I:415:ASP:HB3	1.94	0.49
1:K:383:GLU:OE2	1:L:512:ARG:NH2	2.46	0.49
1:K:913:TYR:HB2	4:O:32:ASN:HB3	1.94	0.49
1:L:343:GLU:HG3	1:L:681:LEU:HD22	1.95	0.49
1:A:436:ASN:O	1:A:440:ASN:ND2	2.46	0.49
1:D:434:GLU:HG3	1:E:126:PRO:HB3	1.95	0.49
1:F:510:HIS:O	1:F:569:SER:OG	2.31	0.49
1:I:408:ASN:OD1	1:I:411:THR:OG1	2.30	0.49
1:J:173:ALA:HA	1:J:178:GLN:HE21	1.78	0.49
1:K:473:THR:HG22	1:K:475:ALA:H	1.76	0.49
1:K:629:ILE:HG13	1:K:655:ARG:HH12	1.77	0.49
3:N:207:VAL:HG21	3:N:243:LEU:HD13	1.94	0.49
1:A:602:THR:O	1:A:606:MET:N	2.46	0.48
1:B:456:ASP:OD1	1:B:476:TYR:OH	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:780:ASN:HD22	1:B:830:PRO:HB2	1.78	0.48
1:I:155:ASN:HD22	1:I:158:ASN:HB2	1.78	0.48
1:J:533:ILE:HG22	1:L:731:GLN:HE21	1.78	0.48
1:K:155:ASN:HD22	1:K:172:TYR:HE2	1.61	0.48
1:K:717:GLU:OE2	1:K:720:ARG:NH2	2.45	0.48
1:K:726:GLY:HA3	1:L:104:ARG:HH21	1.77	0.48
1:L:652:SER:OG	1:L:894:GLU:OE2	2.27	0.48
3:N:189:TYR:OH	4:O:208:SER:O	2.22	0.48
1:A:181:PRO:HB3	1:C:813:GLN:HE21	1.78	0.48
1:B:688:ASN:ND2	1:B:842:THR:O	2.46	0.48
1:C:52:PRO:HG2	1:C:56:VAL:HG21	1.95	0.48
1:C:134:GLU:HG2	1:C:143:VAL:HG12	1.95	0.48
1:D:434:GLU:HG2	1:F:393:LEU:HD23	1.95	0.48
1:D:493:ILE:O	1:E:525:ASN:ND2	2.36	0.48
1:G:612:ASN:OD1	1:G:612:ASN:N	2.44	0.48
1:G:613:ASP:OD2	1:G:900:ARG:NH2	2.32	0.48
1:H:73:ARG:NE	1:H:80:TYR:OH	2.41	0.48
1:B:107:LEU:HG	1:B:109:ARG:HG3	1.95	0.48
1:D:634:THR:OG1	1:D:879:GLU:OE2	2.32	0.48
1:E:217:ALA:HB2	1:E:267:ILE:HD13	1.94	0.48
1:F:691:PHE:HB2	1:F:718:ILE:HD13	1.95	0.48
1:G:399:THR:HG21	1:G:424:GLU:HG3	1.95	0.48
1:I:340:ARG:HH21	1:I:915:ARG:HD3	1.78	0.48
1:I:342:THR:HA	1:I:345:SER:HB3	1.96	0.48
1:I:375:ARG:HH22	1:I:503:ASP:HA	1.78	0.48
1:J:898:VAL:HG11	1:K:13:MET:HB3	1.94	0.48
1:K:369:SER:HA	1:K:841:ARG:HH22	1.78	0.48
2:M:235:ASP:OD2	2:M:342:SER:OG	2.32	0.48
3:N:190:GLN:NE2	3:N:192:GLY:O	2.45	0.48
1:A:202:VAL:HG21	1:A:260:LEU:HD12	1.95	0.48
1:D:224:GLY:O	1:D:226:GLN:NE2	2.46	0.48
1:G:351:ASP:O	1:G:763:ARG:NH1	2.47	0.48
1:H:499:PRO:HG2	1:H:502:MET:HB3	1.96	0.48
1:I:72:ASP:OD2	1:I:83:ARG:NH1	2.44	0.48
1:I:121:TYR:HB2	1:I:214:GLY:HA2	1.96	0.48
1:J:220:THR:HG21	1:J:228:SER:HA	1.95	0.48
1:K:132:PRO:HB3	1:K:145:GLY:HA2	1.94	0.48
1:L:453:TYR:OH	1:L:511:HIS:ND1	2.38	0.48
1:A:709:ARG:NH1	4:O:233:ASP:OD2	2.46	0.48
1:B:562:VAL:HA	1:B:565:ILE:HG22	1.96	0.48
1:B:564:MET:HB3	1:B:672:PHE:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:ARG:HD3	1:B:834:GLN:HE21	1.77	0.48
1:D:375:ARG:HH12	1:D:840:ASP:HB3	1.77	0.48
1:J:824:ILE:HG12	1:K:115:PRO:HD2	1.95	0.48
1:K:616:PHE:H	1:K:899:VAL:HG12	1.79	0.48
1:B:688:ASN:O	1:B:844:TRP:NE1	2.41	0.48
1:F:637:PRO:HA	1:F:877:THR:HA	1.94	0.48
1:G:187:GLN:O	1:G:190:SER:OG	2.30	0.48
1:H:248:ALA:HB2	1:H:256:PRO:HA	1.94	0.48
1:J:624:ASN:ND2	1:J:890:TYR:OH	2.47	0.48
1:L:379:ASN:HD21	1:L:493:ILE:HA	1.79	0.48
1:A:337:LEU:HD12	1:A:340:ARG:HH22	1.78	0.48
1:C:346:TYR:HB3	1:C:538:LYS:HD3	1.95	0.48
1:C:375:ARG:HD3	1:C:507:PRO:HB3	1.96	0.48
1:C:779:VAL:HG21	1:C:821:TYR:HD2	1.79	0.48
1:G:146:GLN:HA	1:H:426:GLU:H	1.79	0.48
1:H:94:LEU:HD12	1:H:547:LEU:HD13	1.96	0.48
1:H:855:MET:HE2	1:I:52:PRO:HD2	1.96	0.48
1:I:734:MET:HE3	1:I:738:TRP:HD1	1.79	0.48
1:K:94:LEU:HD22	1:K:547:LEU:HD13	1.96	0.48
1:B:697:MET:HA	1:B:703:SER:HA	1.96	0.48
1:C:88:VAL:O	1:C:550:GLY:N	2.47	0.48
1:C:351:ASP:HA	1:C:356:ARG:HB2	1.95	0.48
1:C:717:GLU:O	1:C:735:THR:OG1	2.28	0.48
1:G:339:ASP:OD1	1:G:915:ARG:NH1	2.42	0.48
1:H:350:LEU:HD21	1:H:365:GLN:HG3	1.94	0.48
1:J:684:THR:HG23	1:J:841:ARG:HG3	1.96	0.48
1:A:60:ARG:HH22	4:O:111:GLY:HA3	1.79	0.48
1:A:443:ARG:HH12	1:A:802:VAL:HG21	1.78	0.48
1:B:176:THR:HG22	1:B:225:GLY:HA3	1.95	0.48
1:D:434:GLU:N	1:F:391:PHE:O	2.46	0.48
1:E:210:LEU:HD13	1:E:269:ALA:HB2	1.96	0.48
1:G:73:ARG:NH2	1:G:80:TYR:OH	2.47	0.48
1:G:298:ASN:HA	1:G:478:ASN:HD21	1.78	0.48
1:I:717:GLU:O	1:I:735:THR:OG1	2.31	0.48
1:J:327:GLN:HA	1:J:330:GLN:HE21	1.79	0.48
1:K:678:VAL:HG23	1:K:681:LEU:HB2	1.95	0.48
1:L:294:GLN:NE2	1:L:807:PRO:O	2.47	0.48
1:B:613:ASP:OD2	1:B:900:ARG:NH2	2.46	0.48
1:C:632:ASN:HD22	1:C:882:PRO:HB2	1.79	0.48
1:G:323:VAL:HG22	1:G:555:GLU:HG2	1.94	0.48
1:G:406:LYS:N	1:G:413:THR:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:299:ARG:O	1:I:474:TYR:OH	2.32	0.48
1:J:109:ARG:HH22	1:J:523:LEU:HB3	1.78	0.48
1:K:506:ASN:HB2	1:K:508:PHE:H	1.79	0.48
2:M:77:ILE:HD13	2:M:92:THR:HG23	1.96	0.48
1:A:361:SER:OG	1:A:518:TYR:OH	2.26	0.47
1:A:717:GLU:O	1:A:735:THR:OG1	2.26	0.47
1:C:626:LEU:HD12	1:C:888:LEU:HD13	1.96	0.47
1:F:356:ARG:HB3	1:F:367:VAL:HG11	1.95	0.47
1:G:83:ARG:NH1	1:G:555:GLU:OE1	2.46	0.47
1:K:642:SER:O	4:O:27:TYR:OH	2.28	0.47
1:A:145:GLY:H	1:B:425:ILE:HG12	1.79	0.47
1:D:396:SER:OG	1:F:144:ARG:NH2	2.46	0.47
1:E:315:TYR:HE2	1:E:342:THR:HB	1.79	0.47
1:F:149:PHE:HB3	1:F:199:ALA:HB3	1.97	0.47
1:F:717:GLU:OE1	1:F:720:ARG:NH2	2.33	0.47
1:I:122:ASN:HB3	1:I:125:ALA:HB2	1.96	0.47
1:I:447:TYR:HA	1:I:451:ALA:HB3	1.96	0.47
1:L:467:LEU:HD12	1:L:476:TYR:HA	1.96	0.47
1:L:506:ASN:HB2	1:L:508:PHE:HD2	1.79	0.47
1:B:384:ASP:OD2	1:C:213:TYR:OH	2.28	0.47
1:B:539:PHE:O	1:B:543:LYS:N	2.48	0.47
1:B:698:PHE:N	1:B:702:VAL:O	2.46	0.47
1:D:99:THR:HB	1:D:588:LEU:HD12	1.96	0.47
1:D:144:ARG:NH2	1:E:396:SER:OG	2.47	0.47
1:D:360:PHE:HA	1:F:768:PHE:HZ	1.79	0.47
1:F:640:ILE:HD12	1:F:874:LEU:HD21	1.95	0.47
1:G:727:TYR:HA	1:G:736:LYS:HE2	1.96	0.47
1:K:652:SER:HB2	1:K:892:LEU:HB3	1.95	0.47
1:L:18:GLN:HB3	1:L:22:GLU:HB2	1.95	0.47
1:A:622:ALA:HB1	1:A:892:LEU:HB2	1.96	0.47
1:F:187:GLN:HB2	1:F:190:SER:HB3	1.97	0.47
1:F:772:GLN:HE21	1:F:838:LEU:HD22	1.79	0.47
1:G:88:VAL:HG13	1:G:550:GLY:H	1.80	0.47
1:H:496:ARG:H	1:I:521:MET:HB3	1.80	0.47
1:H:875:ASP:N	1:H:875:ASP:OD1	2.46	0.47
1:K:657:LYS:HB2	1:K:660:GLU:HG2	1.95	0.47
1:K:813:GLN:HB2	1:L:146:GLN:HG3	1.95	0.47
1:L:10:TRP:HA	1:L:15:ILE:HD12	1.96	0.47
1:L:347:GLN:NE2	1:L:682:ASP:O	2.47	0.47
1:L:404:GLY:HA2	1:L:418:TYR:HD2	1.78	0.47
1:D:692:LYS:HB3	1:D:879:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:613:ASP:HB2	1:E:900:ARG:HE	1.80	0.47
1:F:770:ASN:ND2	1:F:841:ARG:O	2.48	0.47
1:J:813:GLN:NE2	1:K:148:PRO:HD2	2.29	0.47
1:L:58:THR:HG22	1:L:596:ALA:HA	1.95	0.47
1:A:53:THR:OG1	1:A:54:HIS:N	2.47	0.47
1:B:143:VAL:HG22	1:C:423:ALA:HB1	1.95	0.47
1:B:443:ARG:O	1:B:447:TYR:N	2.48	0.47
1:D:72:ASP:OD1	1:D:83:ARG:N	2.47	0.47
1:D:303:ILE:HG23	1:D:566:LEU:HD13	1.96	0.47
1:D:376:ILE:HG22	1:D:378:GLU:HG3	1.97	0.47
1:E:905:HIS:HB2	1:E:908:VAL:HB	1.95	0.47
1:G:403:SER:H	1:G:423:ALA:HB3	1.78	0.47
1:G:582:ARG:NH1	1:G:584:ASP:OD1	2.47	0.47
1:I:575:ARG:NH1	5:Q:38:SER:OG	2.48	0.47
1:K:246:PHE:HB2	1:L:405:ILE:HG12	1.96	0.47
1:K:610:ASP:OD2	4:O:43:ARG:NH2	2.48	0.47
1:K:645:TRP:NE1	1:K:872:HIS:O	2.46	0.47
1:A:526:GLY:H	1:C:777:GLN:HG3	1.78	0.47
1:B:10:TRP:CE2	4:O:16:GLN:HB3	2.50	0.47
1:B:72:ASP:HB3	1:B:83:ARG:HG2	1.97	0.47
1:B:318:THR:OG1	1:B:336:ASP:O	2.32	0.47
1:E:652:SER:HB2	1:E:892:LEU:HB3	1.96	0.47
1:E:910:GLU:CD	4:O:93:ARG:HH11	2.22	0.47
1:G:402:TYR:N	1:G:423:ALA:O	2.48	0.47
1:I:624:ASN:ND2	1:I:680:TYR:OH	2.47	0.47
1:I:727:TYR:HA	1:I:736:LYS:NZ	2.30	0.47
1:J:72:ASP:HB2	1:J:83:ARG:HH11	1.78	0.47
1:K:209:MET:HE1	1:K:291:LEU:HD12	1.97	0.47
1:L:257:LYS:HG3	1:L:258:ALA:H	1.79	0.47
1:C:136:LYS:HA	1:C:141:ILE:HA	1.95	0.47
1:D:132:PRO:HB3	1:D:145:GLY:HA2	1.96	0.47
1:G:301:ASN:HA	1:G:569:SER:HB3	1.97	0.47
1:G:509:ASN:OD1	1:G:674:TYR:OH	2.32	0.47
1:J:146:GLN:HE21	1:L:813:GLN:HB2	1.79	0.47
4:P:95:ALA:HA	4:P:98:GLU:HB3	1.97	0.47
1:A:391:PHE:O	1:B:434:GLU:N	2.47	0.47
1:B:33:ARG:HG2	7:w:14:GLY:HA3	1.96	0.47
1:B:101:PHE:CE2	1:B:313:MET:HE2	2.50	0.47
1:D:254:ASN:ND2	1:E:412:TRP:O	2.48	0.47
1:G:221:ASN:HB2	1:G:225:GLY:HA3	1.96	0.47
1:G:547:LEU:HB2	1:G:552:TYR:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:860:ASP:OD2	1:K:57:THR:OG1	2.32	0.47
1:A:341:ASN:H	1:A:624:ASN:ND2	2.11	0.47
1:A:398:ALA:N	1:A:426:GLU:OE2	2.42	0.47
1:A:525:ASN:HB2	1:C:495:ALA:HB2	1.96	0.47
1:B:601:SER:OG	3:N:100:GLY:N	2.48	0.47
1:E:596:ALA:HB3	1:E:599:THR:HG22	1.97	0.47
1:F:207:THR:OG1	1:F:265:VAL:O	2.33	0.47
1:G:217:ALA:HB2	1:G:267:ILE:HD13	1.97	0.47
1:H:114:LYS:NZ	1:H:116:TYR:O	2.43	0.47
1:H:272:THR:HB	1:H:295:ALA:HB1	1.96	0.47
1:H:483:VAL:HG22	1:H:485:SER:H	1.79	0.47
1:J:776:ARG:O	1:J:833:THR:OG1	2.32	0.47
1:K:869:ASN:HB2	4:O:200:PRO:HD3	1.97	0.47
1:L:542:ILE:HG22	1:L:545:LEU:HD13	1.96	0.47
1:A:655:ARG:HE	1:A:887:THR:HG21	1.80	0.46
1:E:375:ARG:HD2	1:E:507:PRO:HG3	1.97	0.46
1:H:94:LEU:HD23	1:H:592:PHE:HD1	1.80	0.46
1:I:337:LEU:HD12	1:I:915:ARG:HE	1.80	0.46
1:I:490:TYR:HD2	1:I:820:PRO:HD3	1.80	0.46
1:J:312:LEU:HD13	1:J:565:ILE:HG12	1.96	0.46
3:N:57:PRO:HD2	6:Y:12:ARG:CZ	2.45	0.46
1:B:315:TYR:HE2	1:B:538:LYS:HB2	1.80	0.46
1:G:33:ARG:HG3	6:u:19:MET:HE3	1.97	0.46
1:H:858:LEU:HD11	1:I:16:ALA:HB2	1.96	0.46
1:I:163:GLY:HA3	1:I:171:ILE:HD11	1.96	0.46
1:I:506:ASN:HB3	1:I:686:TYR:CZ	2.50	0.46
1:K:390:CYS:N	1:K:433:MET:O	2.38	0.46
1:C:116:TYR:OH	1:C:271:ASP:OD2	2.34	0.46
1:C:210:LEU:HD12	1:C:267:ILE:HG22	1.97	0.46
1:I:151:GLY:N	1:I:197:LYS:O	2.47	0.46
1:J:736:LYS:NZ	1:K:591:ASN:OD1	2.49	0.46
1:K:798:ASN:ND2	1:L:124:LEU:H	2.13	0.46
1:L:504:ASN:ND2	1:L:883:MET:SD	2.88	0.46
3:N:89:THR:HG22	3:N:94:ILE:HB	1.97	0.46
1:B:74:GLU:OE1	2:M:393:GLN:NE2	2.49	0.46
1:B:699:ASP:N	1:B:873:ALA:O	2.49	0.46
1:C:217:ALA:HB2	1:C:267:ILE:HD13	1.96	0.46
1:G:496:ARG:HH22	1:G:772:GLN:HB2	1.81	0.46
1:H:103:ILE:HD12	1:H:312:LEU:HD21	1.97	0.46
1:H:306:ARG:HG2	1:H:567:GLN:HB2	1.98	0.46
1:J:693:LYS:HB3	1:J:879:GLU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:19:ASP:HA	1:K:48:PRO:HD2	1.97	0.46
2:M:386:VAL:HG22	2:M:387:THR:HG23	1.96	0.46
1:A:19:ASP:HA	1:A:48:PRO:HD2	1.97	0.46
1:A:79:SER:OG	1:A:80:TYR:N	2.48	0.46
1:A:627:TYR:O	1:A:889:LEU:N	2.49	0.46
1:A:864:ASN:ND2	4:O:230:ASP:O	2.48	0.46
1:B:116:TYR:OH	1:B:271:ASP:OD2	2.29	0.46
1:E:101:PHE:HB2	1:E:535:VAL:HB	1.98	0.46
1:F:221:ASN:OD1	1:F:225:GLY:N	2.47	0.46
1:I:241:ASP:OD2	1:I:264:ASN:ND2	2.47	0.46
1:I:370:TYR:HE1	1:I:841:ARG:HE	1.64	0.46
1:L:41:LEU:HB3	1:L:45:PHE:HE2	1.81	0.46
1:L:167:THR:HG23	1:L:169:GLN:HE22	1.81	0.46
1:B:906:ARG:HB2	3:N:104:ASN:HD21	1.80	0.46
1:C:626:LEU:HD21	1:C:680:TYR:HE1	1.80	0.46
1:D:101:PHE:HB2	1:D:535:VAL:HB	1.98	0.46
1:D:435:ILE:HD13	1:D:437:LEU:HB3	1.96	0.46
1:E:103:ILE:HG12	1:E:586:ILE:HG12	1.97	0.46
1:E:405:ILE:HG22	1:E:414:ALA:HA	1.98	0.46
1:E:690:THR:O	1:E:881:ASP:N	2.47	0.46
1:E:707:ASN:HB3	1:F:61:SER:HA	1.97	0.46
1:H:108:ASP:HB3	1:H:580:SER:H	1.81	0.46
1:I:640:ILE:HD11	1:I:645:TRP:HH2	1.81	0.46
1:J:699:ASP:N	1:J:873:ALA:O	2.46	0.46
1:A:18:GLN:HE21	1:A:22:GLU:HB3	1.80	0.46
1:B:137:ASP:HB2	1:B:140:LYS:HB2	1.97	0.46
1:K:375:ARG:NH1	1:K:840:ASP:OD2	2.49	0.46
1:B:323:VAL:HG22	1:B:555:GLU:HB2	1.97	0.46
1:E:912:VAL:HG12	1:F:13:MET:HE1	1.98	0.46
1:G:623:ALA:HB3	1:G:893:PHE:HB2	1.97	0.46
1:G:693:LYS:HA	1:G:717:GLU:HA	1.98	0.46
1:H:302:TYR:HB3	1:H:520:SER:HB3	1.98	0.46
1:I:460:ILE:HD11	1:I:805:MET:HE2	1.98	0.46
1:J:19:ASP:OD1	1:J:20:ALA:N	2.48	0.46
1:J:720:ARG:HH12	1:J:727:TYR:HD2	1.64	0.46
1:A:313:MET:HG2	1:A:556:TRP:HE1	1.80	0.46
1:C:766:SER:OG	1:C:767:PHE:N	2.47	0.46
1:D:325:ALA:HB2	1:D:332:ASN:HA	1.96	0.46
1:D:546:LEU:HB3	1:D:614:GLN:HE22	1.81	0.46
1:F:302:TYR:HE2	1:F:517:ARG:HD2	1.80	0.46
1:I:375:ARG:HD2	1:I:507:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:380:HIS:CD2	1:K:521:MET:HE1	2.51	0.46
1:K:795:GLN:HG3	1:K:819:TYR:HB2	1.97	0.46
2:M:430:THR:HB	2:M:432:VAL:HG23	1.98	0.46
1:B:376:ILE:HD12	1:B:774:MET:HE1	1.97	0.46
1:D:103:ILE:HG22	1:D:531:PHE:HE2	1.81	0.46
1:F:132:PRO:HB3	1:F:145:GLY:HA3	1.98	0.46
1:G:113:PHE:CD1	1:G:303:ILE:HG22	2.51	0.46
1:J:462:PRO:HD2	1:J:465:ILE:HD11	1.98	0.46
1:J:623:ALA:HB3	1:J:893:PHE:HB2	1.98	0.46
1:K:731:GLN:HG3	1:L:522:LEU:HD21	1.98	0.46
2:M:126:ARG:HB3	2:M:458:PRO:HB3	1.97	0.46
3:N:57:PRO:HD2	6:Y:12:ARG:NH2	2.30	0.46
1:A:120:ALA:HB2	1:C:493:ILE:HD13	1.98	0.45
1:B:709:ARG:HH22	1:B:850:SER:HB3	1.81	0.45
1:C:80:TYR:HD2	1:C:558:PHE:HB2	1.80	0.45
1:D:389:TYR:HE2	1:E:810:ARG:HB3	1.81	0.45
1:E:131:ASN:ND2	1:E:210:LEU:O	2.49	0.45
1:G:256:PRO:HG3	1:H:412:TRP:CG	2.51	0.45
1:G:606:MET:O	1:G:612:ASN:ND2	2.46	0.45
1:G:663:SER:N	1:G:669:ASP:OD2	2.43	0.45
1:G:868:ALA:HB3	1:H:3:THR:HG21	1.97	0.45
1:H:389:TYR:HB3	1:H:434:GLU:HB3	1.97	0.45
1:I:339:ASP:HB2	1:I:623:ALA:HB1	1.97	0.45
1:J:548:LEU:HB2	1:J:903:GLN:HE21	1.81	0.45
1:L:367:VAL:HG23	1:L:369:SER:H	1.81	0.45
1:L:381:GLY:HA2	1:L:493:ILE:HD11	1.98	0.45
1:A:100:TYR:HE2	1:C:736:LYS:HZ3	1.64	0.45
1:A:718:ILE:HD13	1:A:738:TRP:CD1	2.51	0.45
1:D:356:ARG:HG3	1:D:367:VAL:HG12	1.99	0.45
1:D:361:SER:HB2	1:D:522:LEU:HD11	1.98	0.45
1:E:314:TYR:HD1	1:E:559:ARG:HB2	1.81	0.45
1:E:649:ARG:NH2	1:E:895:VAL:O	2.44	0.45
1:F:62:GLN:HG3	1:F:594:PRO:HA	1.97	0.45
1:F:377:ILE:HD11	1:F:450:VAL:HG11	1.98	0.45
1:F:638:ILE:HD12	1:F:638:ILE:HA	1.83	0.45
1:G:123:SER:O	1:I:436:ASN:ND2	2.49	0.45
1:G:150:ILE:HG12	1:G:198:VAL:HG23	1.99	0.45
1:G:603:LEU:HD12	1:H:31:PHE:HE2	1.81	0.45
1:L:688:ASN:ND2	1:L:842:THR:O	2.49	0.45
1:A:405:ILE:HD13	1:A:412:TRP:CD1	2.52	0.45
1:B:292:THR:HG23	1:C:188:TRP:HD1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ASP:OD1	1:C:340:ARG:NH2	2.49	0.45
1:D:312:LEU:HD13	1:D:565:ILE:HD11	1.96	0.45
1:I:548:LEU:HB2	1:I:903:GLN:HE21	1.81	0.45
1:L:229:LEU:HA	1:L:240:SER:HA	1.97	0.45
1:A:558:PHE:HE2	1:A:586:ILE:HD13	1.81	0.45
1:B:399:THR:HG22	1:B:426:GLU:HG3	1.99	0.45
1:C:155:ASN:ND2	1:C:172:TYR:OH	2.49	0.45
1:C:878:PHE:HD2	1:C:889:LEU:HD11	1.81	0.45
1:D:433:MET:HE2	1:E:433:MET:SD	2.56	0.45
1:D:749:ILE:HD12	1:D:749:ILE:HA	1.85	0.45
1:J:263:GLU:HB3	1:J:265:VAL:HG13	1.97	0.45
1:K:10:TRP:CE2	4:P:16:GLN:HB3	2.51	0.45
1:K:150:ILE:HD13	1:K:198:VAL:HG12	1.98	0.45
1:K:709:ARG:NH2	1:L:58:THR:O	2.49	0.45
3:N:30:THR:OG1	3:N:33:ASP:OD1	2.32	0.45
1:F:315:TYR:HB2	1:F:343:GLU:HG2	1.97	0.45
1:I:201:ARG:NH2	1:I:263:GLU:OE2	2.36	0.45
1:K:506:ASN:HB3	1:K:686:TYR:CG	2.52	0.45
1:L:497:TRP:CH2	1:L:836:LYS:HG2	2.51	0.45
3:N:232:ILE:HA	3:N:235:LEU:HB3	1.99	0.45
1:A:10:TRP:O	1:A:14:HIS:N	2.49	0.45
1:A:598:ASN:ND2	4:O:93:ARG:O	2.44	0.45
1:D:87:ALA:HA	1:D:551:SER:HA	1.98	0.45
1:F:656:LEU:HD13	1:F:661:THR:HG21	1.99	0.45
1:I:374:VAL:HG11	1:I:510:HIS:CE1	2.52	0.45
1:I:573:ASP:OD1	1:I:573:ASP:N	2.49	0.45
1:I:626:LEU:HD21	1:I:680:TYR:HE1	1.82	0.45
1:I:655:ARG:NH1	1:I:883:MET:SD	2.87	0.45
1:J:350:LEU:HD22	1:J:356:ARG:HH11	1.81	0.45
1:J:732:CYS:HA	1:J:835:LYS:HB2	1.97	0.45
1:J:810:ARG:NH1	1:L:430:ILE:O	2.50	0.45
3:N:60:ASN:HB2	6:Y:12:ARG:HH22	1.80	0.45
3:N:262:LEU:HD23	3:N:265:LEU:HD12	1.98	0.45
1:A:375:ARG:HD3	1:A:507:PRO:HG2	1.99	0.45
1:A:483:VAL:HG11	1:A:792:LEU:HD21	1.98	0.45
1:A:593:PHE:HD2	1:A:595:MET:HG2	1.80	0.45
1:A:740:LEU:HD12	1:B:64:LEU:HD21	1.99	0.45
1:C:323:VAL:HG12	1:C:332:ASN:HD22	1.82	0.45
1:E:103:ILE:HD12	1:E:533:ILE:HD11	1.99	0.45
1:F:351:ASP:HB2	1:F:763:ARG:HE	1.81	0.45
1:G:58:THR:HG22	1:G:60:ARG:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:209:MET:HE2	1:H:209:MET:HB3	1.80	0.45
1:H:710:LEU:HD12	1:H:737:ASP:HB3	1.98	0.45
1:I:378:GLU:HB3	1:I:380:HIS:CD2	2.51	0.45
1:I:870:SER:OG	1:I:871:ALA:N	2.49	0.45
1:K:459:LYS:O	1:K:480:ARG:NH2	2.41	0.45
1:K:612:ASN:HD21	1:L:25:SER:H	1.65	0.45
1:K:896:PHE:HE2	1:L:15:ILE:HG12	1.82	0.45
2:M:81:ASN:HB2	2:M:84:ASN:HB2	1.98	0.45
4:O:56:LEU:HD11	4:O:204:PHE:HE2	1.82	0.45
1:D:697:MET:HA	1:D:703:SER:HA	1.98	0.45
1:D:752:GLN:NE2	1:F:40:SER:O	2.40	0.45
1:E:210:LEU:HD12	1:E:267:ILE:HG22	1.99	0.45
1:F:903:GLN:HE21	1:F:909:ILE:HD12	1.82	0.45
1:G:222:GLU:HA	1:I:788:GLN:HB3	1.99	0.45
1:G:762:ASP:OD2	1:H:358:ARG:NH2	2.50	0.45
1:H:858:LEU:HD12	1:I:50:VAL:HA	1.98	0.45
1:J:90:ASP:H	1:J:549:PRO:HB3	1.81	0.45
1:J:210:LEU:HD21	1:J:269:ALA:HB2	1.97	0.45
2:M:424:ARG:HH21	2:M:444:ARG:HH21	1.65	0.45
4:O:95:ALA:HA	4:O:98:GLU:HB3	1.97	0.45
1:B:388:ASN:ND2	1:C:440:ASN:OD1	2.50	0.45
1:F:561:ASP:OD1	1:F:575:ARG:NH2	2.50	0.45
1:G:141:ILE:N	1:H:418:TYR:O	2.49	0.45
1:G:552:TYR:HE1	1:G:907:GLY:HA2	1.81	0.45
1:G:624:ASN:ND2	1:G:890:TYR:OH	2.50	0.45
1:H:458:TYR:O	1:H:480:ARG:NH2	2.50	0.45
1:I:209:MET:HE1	1:I:287:SER:H	1.82	0.45
1:J:568:SER:OG	1:J:569:SER:N	2.50	0.45
1:J:779:VAL:HG21	1:J:821:TYR:HD2	1.81	0.45
4:P:66:ARG:HE	4:P:69:LEU:HA	1.81	0.45
1:A:292:THR:HG21	1:B:187:GLN:HG3	1.99	0.45
1:B:319:GLY:HA3	2:M:90:GLN:HE22	1.82	0.45
1:C:357:SER:OG	1:C:764:MET:SD	2.74	0.45
1:C:374:VAL:HG11	1:C:510:HIS:CE1	2.52	0.45
1:D:731:GLN:HE21	1:E:533:ILE:HG22	1.81	0.45
1:E:273:HIS:CE1	1:E:481:VAL:HG21	2.53	0.45
1:F:89:GLY:O	1:F:92:ARG:NH1	2.50	0.45
1:F:356:ARG:HD3	1:F:764:MET:HB3	1.98	0.45
1:G:286:SER:O	1:G:286:SER:OG	2.34	0.45
1:H:629:ILE:HD11	1:H:655:ARG:HH21	1.82	0.45
1:J:10:TRP:HE1	1:L:916:THR:HG21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:229:LEU:HA	1:J:240:SER:HA	1.99	0.45
2:M:133:ASN:HA	2:M:168:GLU:HG3	1.98	0.45
4:O:66:ARG:HE	4:O:69:LEU:HA	1.81	0.45
1:B:496:ARG:HH21	1:B:772:GLN:HE21	1.65	0.44
1:C:78:TYR:CG	1:C:668:PHE:HB2	2.52	0.44
1:D:301:ASN:HB2	1:D:569:SER:H	1.82	0.44
1:F:375:ARG:HH12	1:F:507:PRO:HG3	1.82	0.44
1:F:390:CYS:HB3	1:F:433:MET:HB2	2.00	0.44
1:G:558:PHE:HE2	1:G:586:ILE:HG12	1.81	0.44
1:K:483:VAL:HG22	1:K:485:SER:H	1.82	0.44
1:L:624:ASN:ND2	1:L:680:TYR:OH	2.50	0.44
1:B:301:ASN:HA	1:B:569:SER:HB2	1.99	0.44
1:G:352:ALA:HA	1:G:763:ARG:HH12	1.81	0.44
1:H:83:ARG:HG2	1:H:555:GLU:HB3	1.98	0.44
1:H:568:SER:N	1:H:675:SER:O	2.44	0.44
1:J:271:ASP:OD1	1:J:271:ASP:N	2.50	0.44
1:L:23:TYR:OH	1:L:45:PHE:O	2.35	0.44
1:L:693:LYS:HB2	1:L:879:GLU:HB3	1.99	0.44
1:A:845:ARG:HH22	7:w:22:GLY:HA3	1.82	0.44
1:B:220:THR:OG1	1:B:227:ALA:O	2.35	0.44
1:C:460:ILE:HD13	1:C:805:MET:HE3	1.98	0.44
1:E:151:GLY:N	1:E:197:LYS:O	2.49	0.44
1:E:515:GLY:O	1:E:519:ARG:NH1	2.50	0.44
1:E:804:TYR:N	1:E:811:GLU:OE2	2.50	0.44
1:H:447:TYR:HA	1:H:451:ALA:HB3	1.99	0.44
1:H:717:GLU:HB2	1:H:735:THR:HG21	2.00	0.44
1:A:107:LEU:HG	1:A:109:ARG:HG3	1.99	0.44
1:A:130:PRO:HA	1:A:211:PRO:HA	1.99	0.44
1:B:294:GLN:OE1	1:B:809:MET:N	2.50	0.44
1:B:451:ALA:HA	1:B:487:LEU:HD23	1.99	0.44
1:C:629:ILE:N	1:C:887:THR:O	2.47	0.44
1:E:292:THR:HA	1:F:188:TRP:HE1	1.82	0.44
1:E:860:ASP:OD2	1:F:57:THR:OG1	2.36	0.44
1:I:109:ARG:HH22	1:I:523:LEU:HB3	1.82	0.44
1:I:727:TYR:HA	1:I:736:LYS:HZ2	1.81	0.44
1:I:809:MET:HE2	1:I:809:MET:HB3	1.78	0.44
2:M:416:GLN:O	2:M:420:SER:N	2.44	0.44
4:P:7:THR:HG22	4:P:26:ASP:HB3	2.00	0.44
1:B:43:ASN:HB3	1:B:44:LYS:HG3	1.99	0.44
1:B:764:MET:HE3	1:B:841:ARG:HH11	1.82	0.44
1:D:748:ASN:HD21	1:D:854:SER:H	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:PRO:HB2	1:E:202:VAL:HG23	1.99	0.44
1:E:402:TYR:CE2	1:E:425:ILE:HG12	2.53	0.44
1:H:377:ILE:HG12	1:H:499:PRO:HD3	2.00	0.44
1:H:380:HIS:CE1	1:I:517:ARG:HD2	2.52	0.44
1:I:149:PHE:H	1:I:184:GLY:HA2	1.82	0.44
1:I:406:LYS:HD2	1:I:415:ASP:HA	1.99	0.44
1:J:179:PRO:HG3	1:J:199:ALA:HB1	2.00	0.44
1:J:629:ILE:HD11	1:J:889:LEU:HB2	2.00	0.44
1:K:462:PRO:HD3	1:K:481:VAL:HG12	2.00	0.44
1:L:497:TRP:HH2	1:L:836:LYS:HG2	1.82	0.44
2:M:67:VAL:HG23	2:M:498:VAL:HB	1.99	0.44
4:O:48:ARG:HA	4:O:51:ARG:HG2	2.00	0.44
1:B:824:ILE:HG23	1:C:114:LYS:H	1.83	0.44
1:D:506:ASN:HB3	1:D:509:ASN:H	1.82	0.44
1:E:52:PRO:HD3	6:U:11:PRO:HA	1.99	0.44
1:E:516:LEU:HD23	1:E:519:ARG:HH21	1.83	0.44
1:F:340:ARG:HD3	1:F:540:PHE:HE1	1.83	0.44
1:F:443:ARG:HH12	1:F:802:VAL:HG12	1.82	0.44
1:G:63:ARG:HD2	1:G:66:LEU:HB3	1.99	0.44
1:G:314:TYR:HE1	1:G:559:ARG:HE	1.66	0.44
1:H:363:TRP:HZ3	1:H:536:PRO:HA	1.82	0.44
1:I:228:SER:HB2	1:I:265:VAL:HA	1.99	0.44
1:J:278:PRO:HG3	1:J:290:LEU:HA	1.99	0.44
1:K:900:ARG:NH1	4:O:40:MET:HE3	2.32	0.44
1:B:445:PHE:HE1	1:B:512:ARG:HH12	1.66	0.44
1:C:130:PRO:O	1:C:144:ARG:NH2	2.50	0.44
1:E:174:ASP:H	1:E:178:GLN:HB2	1.82	0.44
1:E:776:ARG:HD2	1:E:834:GLN:HE21	1.83	0.44
1:F:374:VAL:HG11	1:F:510:HIS:CE1	2.52	0.44
1:G:434:GLU:N	1:I:391:PHE:O	2.48	0.44
1:H:512:ARG:HG3	1:H:517:ARG:NH1	2.32	0.44
1:I:779:VAL:HG21	1:I:821:TYR:HD2	1.83	0.44
1:J:901:ILE:HD12	1:J:911:ALA:HB2	2.00	0.44
1:K:109:ARG:HH22	1:K:523:LEU:HB2	1.83	0.44
1:L:506:ASN:ND2	1:L:677:SER:OG	2.51	0.44
4:O:7:THR:HG22	4:O:26:ASP:HB3	2.00	0.44
1:B:679:PRO:HA	1:B:684:THR:HB	1.99	0.44
1:E:326:GLY:HA2	1:E:552:TYR:HD1	1.82	0.44
1:E:617:ASN:ND2	1:E:897:ASP:O	2.50	0.44
1:F:360:PHE:HE2	1:F:363:TRP:H	1.65	0.44
1:H:390:CYS:N	1:H:433:MET:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:736:LYS:HE2	1:I:589:TYR:CD2	2.52	0.44
1:I:114:LYS:NZ	1:I:271:ASP:OD1	2.40	0.44
1:J:241:ASP:OD1	1:J:241:ASP:N	2.51	0.44
1:J:599:THR:HA	1:J:602:THR:HG22	1.99	0.44
1:J:629:ILE:H	1:J:888:LEU:HA	1.83	0.44
1:K:376:ILE:HD13	1:K:498:SER:HB2	2.00	0.44
2:M:90:GLN:HE21	2:M:477:ARG:HH21	1.65	0.44
1:D:509:ASN:ND2	1:D:674:TYR:OH	2.51	0.44
1:F:325:ALA:HB3	1:F:553:THR:HB	2.00	0.44
1:G:130:PRO:HA	1:G:211:PRO:HA	1.99	0.44
1:G:504:ASN:HB2	1:G:883:MET:HE1	2.00	0.44
1:H:7:MET:HE3	1:H:11:SER:HB2	2.00	0.44
1:H:483:VAL:HG11	1:H:792:LEU:HD21	2.00	0.44
1:I:280:VAL:HG22	1:I:282:GLN:H	1.83	0.44
1:J:61:SER:HA	1:L:707:ASN:HB3	1.98	0.44
1:K:27:GLY:O	1:K:31:PHE:N	2.51	0.44
1:K:101:PHE:HD1	1:K:588:LEU:HD23	1.83	0.44
1:K:146:GLN:HA	1:L:426:GLU:H	1.83	0.44
1:K:654:THR:OG1	1:K:655:ARG:N	2.51	0.44
1:L:626:LEU:HD12	1:L:888:LEU:HD11	2.00	0.44
4:P:178:GLN:NE2	4:P:180:SER:OG	2.48	0.44
1:B:28:LEU:O	1:B:32:ALA:N	2.49	0.43
1:D:109:ARG:HD3	1:D:113:PHE:CD1	2.53	0.43
1:D:587:ASN:OD1	1:D:587:ASN:N	2.50	0.43
1:E:474:TYR:HE1	1:E:570:LEU:HD21	1.82	0.43
1:E:901:ILE:HG22	1:E:911:ALA:HA	1.99	0.43
1:H:376:ILE:HG23	1:H:774:MET:HE2	1.98	0.43
1:J:94:LEU:O	1:J:547:LEU:N	2.46	0.43
1:L:88:VAL:HB	1:L:92:ARG:HB2	2.00	0.43
1:L:150:ILE:HA	1:L:198:VAL:HG23	2.00	0.43
4:P:56:LEU:HD11	4:P:204:PHE:HE2	1.82	0.43
1:C:311:GLY:O	1:C:559:ARG:NH1	2.51	0.43
1:D:374:VAL:HG11	1:D:510:HIS:CE1	2.53	0.43
1:E:730:ALA:HB2	1:F:362:MET:HB2	2.01	0.43
1:G:559:ARG:HB2	1:G:565:ILE:HD11	2.00	0.43
1:H:506:ASN:HB3	1:H:686:TYR:CG	2.53	0.43
1:J:818:ASN:HD22	1:K:219:PRO:HG3	1.83	0.43
1:L:134:GLU:HB3	1:L:143:VAL:HG12	2.00	0.43
1:A:276:TYR:OH	1:B:187:GLN:OE1	2.35	0.43
1:A:347:GLN:HE22	1:A:356:ARG:NH2	2.16	0.43
1:B:895:VAL:HB	1:B:917:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ARG:HH12	1:C:570:LEU:HB2	1.84	0.43
1:D:405:ILE:HD11	1:F:256:PRO:HB3	1.99	0.43
1:F:108:ASP:HB3	1:F:580:SER:H	1.83	0.43
1:H:339:ASP:O	1:H:624:ASN:N	2.47	0.43
1:H:813:GLN:HE22	1:I:201:ARG:H	1.64	0.43
1:I:107:LEU:HD23	1:I:109:ARG:HH21	1.83	0.43
1:I:658:THR:HA	1:I:888:LEU:HD22	1.99	0.43
1:J:499:PRO:HG2	1:J:502:MET:HB3	2.00	0.43
1:J:601:SER:HA	1:J:604:GLU:HG3	2.00	0.43
1:K:497:TRP:CD1	1:K:776:ARG:HD2	2.52	0.43
1:A:58:THR:HG22	1:A:596:ALA:HA	2.01	0.43
1:B:204:LYS:HB2	1:B:263:GLU:H	1.84	0.43
1:E:140:LYS:HZ1	1:F:416:ASP:HB3	1.83	0.43
1:E:459:LYS:HG2	1:E:482:ALA:HB2	2.00	0.43
1:H:624:ASN:ND2	1:H:890:TYR:OH	2.52	0.43
1:I:103:ILE:HG12	1:I:586:ILE:HG12	2.00	0.43
1:J:23:TYR:O	1:L:611:THR:OG1	2.37	0.43
1:J:382:VAL:HG21	1:J:439:ALA:HB2	2.00	0.43
1:J:433:MET:HG2	1:L:392:PRO:HA	2.00	0.43
1:K:742:GLN:HE22	1:K:845:ARG:H	1.66	0.43
1:L:443:ARG:NE	1:L:488:ASP:OD1	2.49	0.43
1:L:640:ILE:HD11	1:L:645:TRP:CZ2	2.54	0.43
1:A:637:PRO:HA	1:A:877:THR:HA	2.00	0.43
1:E:98:SER:OG	1:E:591:ASN:ND2	2.40	0.43
1:E:625:MET:HB2	1:E:891:VAL:HB	1.99	0.43
1:I:10:TRP:O	1:I:14:HIS:N	2.51	0.43
1:I:149:PHE:HD2	1:I:199:ALA:HB3	1.83	0.43
1:I:210:LEU:HD11	1:I:269:ALA:HB2	2.00	0.43
1:I:364:ASN:HD21	1:I:519:ARG:HD3	1.83	0.43
1:I:692:LYS:HE2	1:I:879:GLU:HG2	2.00	0.43
1:I:784:TYR:HD2	1:I:787:TYR:HB2	1.83	0.43
1:J:115:PRO:HG2	1:L:494:GLY:HA3	2.01	0.43
1:J:866:LEU:HD22	4:P:231:GLY:HA2	2.01	0.43
1:L:165:ASP:HB3	1:L:169:GLN:H	1.83	0.43
3:N:139:PHE:HE2	3:N:145:LEU:HD23	1.83	0.43
1:B:559:ARG:NH2	1:B:564:MET:O	2.52	0.43
1:D:16:ALA:HB2	1:F:858:LEU:HD21	2.01	0.43
1:D:341:ASN:H	1:D:624:ASN:HD22	1.67	0.43
1:D:509:ASN:ND2	1:D:676:GLY:O	2.40	0.43
1:F:490:TYR:HD1	1:F:820:PRO:HD3	1.84	0.43
1:G:404:GLY:HA2	1:I:247:PHE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:677:SER:OG	1:J:682:ASP:OD2	2.35	0.43
1:L:861:LEU:HA	1:L:864:ASN:HB2	2.01	0.43
2:M:87:SER:HB3	2:M:491:VAL:HB	2.01	0.43
2:M:145:LEU:HD21	2:M:184:ILE:HD11	2.00	0.43
4:P:44:VAL:HA	4:P:47:ILE:HD12	2.01	0.43
1:C:784:TYR:HD2	1:C:787:TYR:HB2	1.83	0.43
1:D:626:LEU:HD13	1:D:890:TYR:HD1	1.83	0.43
1:E:241:ASP:OD1	1:E:241:ASP:N	2.51	0.43
1:F:497:TRP:CD1	1:F:776:ARG:HD2	2.53	0.43
1:H:314:TYR:HD1	1:H:559:ARG:HG3	1.83	0.43
1:H:784:TYR:HD2	1:H:787:TYR:HB2	1.84	0.43
1:I:909:ILE:O	4:P:111:GLY:N	2.38	0.43
1:J:823:LEU:HB3	1:K:526:GLY:HA2	2.01	0.43
1:K:376:ILE:HG13	1:K:496:ARG:HH21	1.83	0.43
4:O:178:GLN:NE2	4:O:180:SER:OG	2.48	0.43
1:B:146:GLN:HA	1:C:426:GLU:H	1.83	0.43
1:C:53:THR:OG1	1:C:54:HIS:N	2.52	0.43
1:D:114:LYS:HE3	1:D:298:ASN:HB2	2.00	0.43
1:D:542:ILE:HG22	1:D:545:LEU:HD13	2.01	0.43
1:E:401:THR:HG21	1:E:421:ARG:HE	1.84	0.43
1:E:490:TYR:HD1	1:E:820:PRO:HD3	1.84	0.43
1:E:559:ARG:HD3	1:E:561:ASP:HB3	1.99	0.43
1:E:750:GLY:HA2	1:E:754:PHE:HE1	1.83	0.43
1:F:686:TYR:HA	1:F:840:ASP:HA	2.00	0.43
1:H:389:TYR:HA	1:H:434:GLU:HA	2.00	0.43
1:H:454:LEU:HD22	1:H:501:PRO:HB2	2.01	0.43
1:I:114:LYS:HD2	1:I:298:ASN:HB2	1.99	0.43
1:J:131:ASN:ND2	1:J:210:LEU:O	2.51	0.43
1:J:388:ASN:HB3	1:K:440:ASN:ND2	2.32	0.43
1:J:604:GLU:OE1	1:J:608:ARG:NH1	2.44	0.43
1:J:711:LEU:O	1:K:63:ARG:NH1	2.50	0.43
1:J:914:LEU:HB2	1:K:13:MET:HE3	2.00	0.43
1:A:402:TYR:O	1:C:248:ALA:N	2.52	0.43
1:A:815:TYR:HE2	1:A:818:ASN:HD21	1.67	0.43
1:D:126:PRO:HB3	1:F:434:GLU:HG2	2.01	0.43
1:D:900:ARG:HH22	1:E:14:HIS:CE1	2.36	0.43
1:E:91:ASN:ND2	1:E:597:HIS:HD2	2.16	0.43
1:E:813:GLN:HA	1:F:146:GLN:HE21	1.83	0.43
1:F:499:PRO:HD2	1:F:502:MET:HE3	2.00	0.43
1:G:9:GLN:NE2	4:P:104:SER:OG	2.52	0.43
1:H:467:LEU:HA	1:H:468:PRO:HD3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:LYS:HB3	1:I:242:VAL:HG21	2.01	0.43
1:I:823:LEU:HA	1:I:829:VAL:HG12	2.01	0.43
1:J:483:VAL:HG21	1:J:792:LEU:HD11	2.00	0.43
2:M:55:TYR:OH	2:M:107:GLN:OE1	2.30	0.43
1:A:649:ARG:HH21	1:A:894:GLU:HB2	1.83	0.43
1:B:626:LEU:HD21	1:B:680:TYR:HE1	1.83	0.43
1:B:780:ASN:HD21	1:B:783:THR:HG22	1.84	0.43
1:D:779:VAL:HG21	1:D:821:TYR:HD2	1.84	0.43
1:E:390:CYS:N	1:E:433:MET:O	2.51	0.43
1:F:845:ARG:NH2	1:F:894:GLU:OE2	2.52	0.43
1:G:429:ASN:ND2	1:H:812:GLY:H	2.17	0.43
1:G:474:TYR:HE1	1:G:570:LEU:HD21	1.84	0.43
1:G:660:GLU:HG2	1:G:674:TYR:CE2	2.54	0.43
1:H:375:ARG:HB2	1:H:507:PRO:HG3	2.00	0.43
1:L:115:PRO:HB2	1:L:521:MET:HE2	1.99	0.43
2:M:445:PRO:HA	2:M:446:PRO:HD3	1.85	0.43
1:A:316:ASN:N	1:A:336:ASP:OD2	2.51	0.42
1:A:792:LEU:HA	1:A:795:GLN:HB3	2.01	0.42
1:B:315:TYR:OH	1:B:538:LYS:N	2.42	0.42
1:B:552:TYR:HE1	1:B:907:GLY:HA2	1.83	0.42
1:C:655:ARG:HH21	1:C:887:THR:HG21	1.84	0.42
1:D:94:LEU:HD11	1:D:590:ALA:HB1	2.00	0.42
1:D:274:LEU:HD22	1:D:293:GLN:HE21	1.84	0.42
1:D:362:MET:HG2	1:D:534:GLN:HG2	2.01	0.42
1:G:533:ILE:HA	1:I:731:GLN:HE21	1.84	0.42
1:H:753:GLY:HA2	1:I:98:SER:HA	2.00	0.42
1:K:362:MET:HE3	1:K:534:GLN:HG2	2.01	0.42
1:K:823:LEU:HD23	1:L:526:GLY:HA3	2.00	0.42
1:D:521:MET:HB3	1:F:496:ARG:H	1.84	0.42
1:G:427:SER:HB3	1:I:192:VAL:HG21	2.00	0.42
1:H:85:THR:HA	1:H:553:THR:HG22	2.00	0.42
1:H:277:LYS:HA	1:H:278:PRO:HD3	1.89	0.42
1:H:321:MET:HB2	1:H:321:MET:HE3	1.80	0.42
1:H:513:ASN:HB3	1:H:516:LEU:HB2	2.00	0.42
1:I:402:TYR:HD2	1:I:425:ILE:HD11	1.84	0.42
1:I:558:PHE:HE2	1:I:586:ILE:HG21	1.84	0.42
1:J:59:ASP:OD1	1:L:709:ARG:NH2	2.48	0.42
1:L:243:ASN:O	1:L:262:ALA:N	2.51	0.42
1:L:380:HIS:CD2	1:L:383:GLU:HG2	2.54	0.42
4:O:91:LEU:HD11	4:O:175:LEU:HD23	2.01	0.42
1:A:324:LEU:HD23	1:A:554:TYR:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PHE:HE1	1:C:303:ILE:HB	1.84	0.42
1:C:722:VAL:HG11	1:E:668:PHE:HE2	1.84	0.42
1:D:58:THR:HG21	1:D:62:GLN:HE22	1.83	0.42
1:D:72:ASP:O	1:D:82:VAL:HG12	2.20	0.42
1:D:379:ASN:ND2	1:D:489:THR:O	2.49	0.42
1:E:324:LEU:HD13	1:E:554:TYR:HD1	1.84	0.42
1:E:498:SER:HB3	1:E:774:MET:HE1	2.02	0.42
1:E:607:LEU:HD21	1:E:614:GLN:HE22	1.83	0.42
1:H:621:CYS:HB2	1:H:897:ASP:H	1.84	0.42
1:J:453:TYR:CZ	1:J:510:HIS:HA	2.55	0.42
1:J:696:ILE:HG12	1:J:876:MET:HG2	2.00	0.42
1:K:53:THR:HG23	1:K:54:HIS:CD2	2.54	0.42
1:K:767:PHE:HA	1:K:842:THR:HG21	2.01	0.42
1:B:766:SER:OG	1:B:767:PHE:N	2.52	0.42
1:D:678:VAL:HA	1:D:679:PRO:HD3	1.91	0.42
1:E:310:ILE:HG22	1:E:538:LYS:HE3	2.01	0.42
1:E:657:LYS:HB2	1:E:660:GLU:HB2	2.01	0.42
1:E:815:TYR:CZ	1:F:181:PRO:HG2	2.54	0.42
1:F:784:TYR:HD2	1:F:787:TYR:HB2	1.84	0.42
1:I:245:GLN:HE22	1:I:262:ALA:HB2	1.83	0.42
1:I:729:VAL:HG11	1:I:739:PHE:CG	2.54	0.42
1:J:405:ILE:HB	1:J:413:THR:HG23	2.00	0.42
3:N:206:THR:HB	4:O:205:ASN:HB3	2.00	0.42
4:O:44:VAL:HA	4:O:47:ILE:HD12	2.01	0.42
1:A:141:ILE:HG13	1:B:418:TYR:HA	2.01	0.42
1:C:149:PHE:O	1:C:199:ALA:N	2.41	0.42
1:C:678:VAL:HA	1:C:679:PRO:HD3	1.90	0.42
1:D:96:MET:HA	1:D:99:THR:HG23	2.00	0.42
1:E:758:GLU:HB2	1:E:761:LYS:HE2	2.00	0.42
1:E:898:VAL:HG11	1:F:13:MET:HB3	2.00	0.42
1:F:342:THR:HG21	1:F:539:PHE:HA	2.01	0.42
1:G:340:ARG:HH11	1:G:915:ARG:HD3	1.85	0.42
1:G:526:GLY:HA3	1:I:777:GLN:HG3	2.00	0.42
1:H:204:LYS:HG2	1:H:205:ASP:H	1.84	0.42
1:H:799:SER:OG	1:I:181:PRO:O	2.37	0.42
1:K:204:LYS:HB2	1:K:263:GLU:H	1.84	0.42
1:L:661:THR:HG21	1:L:888:LEU:HD21	2.01	0.42
4:O:47:ILE:O	4:O:50:THR:OG1	2.34	0.42
4:P:48:ARG:HA	4:P:51:ARG:HG2	2.00	0.42
1:A:243:ASN:H	1:A:262:ALA:HB3	1.83	0.42
1:A:263:GLU:OE2	1:C:815:TYR:OH	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:GLN:OE1	1:D:553:THR:OG1	2.25	0.42
1:D:497:TRP:CG	1:D:776:ARG:HD3	2.54	0.42
1:D:509:ASN:OD1	1:D:567:GLN:NE2	2.52	0.42
1:D:510:HIS:CE1	1:D:512:ARG:HB2	2.53	0.42
1:F:445:PHE:O	1:F:449:ASN:ND2	2.50	0.42
1:F:791:THR:HG22	1:F:793:PRO:HD2	2.01	0.42
1:G:248:ALA:HB3	1:H:403:SER:HB2	2.01	0.42
1:H:210:LEU:HD12	1:H:211:PRO:HD2	2.00	0.42
1:I:134:GLU:HG2	1:I:143:VAL:HG12	1.99	0.42
1:A:24:LEU:HA	1:A:24:LEU:HD23	1.85	0.42
1:B:305:PHE:HE2	1:B:523:LEU:HD21	1.85	0.42
1:B:443:ARG:HH21	1:B:484:PRO:HB2	1.84	0.42
1:B:788:GLN:HG3	1:C:222:GLU:HA	2.02	0.42
1:F:315:TYR:HE2	1:F:538:LYS:HG3	1.84	0.42
1:H:151:GLY:HA3	1:H:160:ILE:HG22	2.02	0.42
1:H:503:ASP:OD2	1:H:836:LYS:NZ	2.39	0.42
1:H:658:THR:O	5:T:32:ARG:NH2	2.52	0.42
1:I:342:THR:HG21	1:I:539:PHE:HA	2.01	0.42
1:J:814:ALA:H	1:K:146:GLN:HE21	1.67	0.42
1:K:766:SER:OG	1:K:767:PHE:N	2.53	0.42
1:K:910:GLU:HG3	4:O:37:GLY:H	1.85	0.42
2:M:274:LEU:O	2:M:341:ARG:NH1	2.52	0.42
1:A:452:LEU:HD13	1:A:452:LEU:HA	1.88	0.42
1:A:511:HIS:O	1:A:517:ARG:NH2	2.53	0.42
1:A:808:THR:OG1	1:A:809:MET:N	2.53	0.42
1:C:263:GLU:HB3	1:C:265:VAL:HG13	2.02	0.42
1:D:242:VAL:HG22	1:D:263:GLU:HG2	2.02	0.42
1:E:147:ALA:HB2	1:F:425:ILE:HB	2.02	0.42
1:E:645:TRP:CD1	1:E:872:HIS:HB2	2.55	0.42
1:E:766:SER:OG	1:E:767:PHE:N	2.52	0.42
1:F:685:PHE:O	1:F:688:ASN:ND2	2.53	0.42
2:M:119:ALA:HB2	2:M:468:LEU:HD21	2.02	0.42
2:M:420:SER:HA	2:M:423:ILE:HB	2.02	0.42
1:A:340:ARG:HH21	1:A:915:ARG:HD3	1.84	0.42
1:B:248:ALA:HB3	1:C:405:ILE:HD13	2.02	0.42
1:B:624:ASN:HD21	1:B:892:LEU:HD13	1.84	0.42
1:E:498:SER:HA	1:E:499:PRO:HD3	1.93	0.42
1:F:516:LEU:HA	1:F:519:ARG:HB2	2.01	0.42
1:F:688:ASN:O	1:F:844:TRP:NE1	2.37	0.42
1:G:356:ARG:HG3	1:G:367:VAL:HG12	2.02	0.42
1:G:752:GLN:NE2	1:H:95:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:510:HIS:CE1	1:H:512:ARG:HB3	2.55	0.42
1:K:53:THR:OG1	1:K:54:HIS:N	2.51	0.42
1:L:9:GLN:HG2	4:O:31:MET:HE3	2.02	0.42
2:M:181:ASN:HA	2:M:184:ILE:HG22	2.01	0.42
2:M:321:LYS:HG2	2:M:327:SER:HB3	2.02	0.42
1:A:405:ILE:HD13	1:A:412:TRP:HD1	1.85	0.42
1:C:858:LEU:HD13	1:C:863:GLN:HB3	2.01	0.42
1:E:20:ALA:HA	1:E:23:TYR:HE1	1.84	0.42
1:E:617:ASN:HD22	1:E:618:ASP:N	2.18	0.42
1:E:712:THR:HA	1:E:713:PRO:HD3	1.91	0.42
1:F:310:ILE:HD12	1:F:681:LEU:HB3	2.01	0.42
1:G:419:ALA:HB2	1:I:140:LYS:HB3	2.01	0.42
1:H:73:ARG:HG2	1:H:82:VAL:HG12	2.01	0.42
1:H:790:VAL:HG12	1:I:224:GLY:HA2	2.01	0.42
1:H:794:PHE:HB3	1:I:224:GLY:HA3	2.02	0.42
1:H:857:ALA:HB1	1:H:896:PHE:HE1	1.84	0.42
1:J:545:LEU:HD22	1:J:547:LEU:HD22	2.02	0.42
1:J:691:PHE:HB2	1:J:718:ILE:HG21	2.01	0.42
1:L:144:ARG:HD3	1:L:291:LEU:HD11	2.02	0.42
1:A:249:LEU:HD12	1:A:250:PRO:HD2	2.01	0.41
1:A:914:LEU:HB2	1:B:13:MET:HE3	2.02	0.41
1:B:304:GLY:HA3	1:B:519:ARG:HG3	2.01	0.41
1:B:360:PHE:CE2	1:B:362:MET:HB3	2.55	0.41
1:B:515:GLY:O	1:B:519:ARG:NE	2.53	0.41
1:B:883:MET:HE2	1:B:883:MET:HB2	1.98	0.41
1:D:350:LEU:HD21	1:D:365:GLN:HE21	1.85	0.41
1:D:612:ASN:ND2	1:E:25:SER:H	2.15	0.41
1:E:454:LEU:HD11	1:E:487:LEU:HD23	2.02	0.41
1:F:387:PRO:HB2	1:F:389:TYR:CZ	2.54	0.41
1:G:159:GLY:HA2	1:G:244:LEU:HD21	2.01	0.41
1:G:517:ARG:HH11	1:I:380:HIS:CD2	2.38	0.41
1:H:101:PHE:O	1:H:535:VAL:N	2.52	0.41
1:L:784:TYR:HB2	1:L:830:PRO:HD2	2.02	0.41
2:M:277:GLY:HA3	2:M:346:ALA:HB2	2.01	0.41
3:N:196:PHE:CE2	4:O:208:SER:HB3	2.55	0.41
5:Q:21:LEU:HD13	5:S:21:LEU:HD22	2.02	0.41
1:A:427:SER:HB2	1:C:198:VAL:HG21	2.02	0.41
1:A:861:LEU:HD12	1:A:867:TYR:HE2	1.86	0.41
1:B:348:LEU:HD12	1:B:619:TYR:HE2	1.85	0.41
1:B:914:LEU:HD13	1:C:13:MET:HG3	2.02	0.41
1:F:106:VAL:H	1:F:582:ARG:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:764:MET:N	1:G:764:MET:SD	2.93	0.41
1:H:113:PHE:CE2	1:H:115:PRO:HG3	2.55	0.41
1:J:24:LEU:HD13	1:J:28:LEU:HD23	2.01	0.41
1:J:729:VAL:HG11	1:J:739:PHE:CG	2.55	0.41
1:K:253:PRO:HB2	1:K:255:GLU:HG2	2.02	0.41
1:K:342:THR:OG1	1:K:538:LYS:O	2.38	0.41
1:K:754:PHE:HB2	1:L:363:TRP:CZ3	2.55	0.41
1:B:777:GLN:HG3	1:C:526:GLY:H	1.85	0.41
1:C:305:PHE:HE2	1:C:523:LEU:HD21	1.85	0.41
1:C:736:LYS:HA	1:C:739:PHE:HB3	2.02	0.41
1:C:741:ILE:HG13	1:C:852:PHE:CD2	2.56	0.41
1:D:632:ASN:HB2	1:D:882:PRO:HB2	2.03	0.41
1:E:80:TYR:CE2	1:E:586:ILE:HD12	2.55	0.41
1:G:432:ALA:HB3	1:H:810:ARG:HE	1.86	0.41
1:H:780:ASN:ND2	1:H:832:LEU:HB2	2.36	0.41
1:I:729:VAL:N	1:I:734:MET:O	2.54	0.41
1:K:508:PHE:CE2	1:K:684:THR:HG22	2.55	0.41
2:M:200:SER:O	2:M:340:TYR:OH	2.38	0.41
4:P:91:LEU:HD11	4:P:175:LEU:HD23	2.01	0.41
1:B:648:PHE:HB2	1:B:895:VAL:HG12	2.02	0.41
1:D:690:THR:HB	1:D:881:ASP:HB3	2.02	0.41
1:E:562:VAL:HA	1:E:565:ILE:HG22	2.02	0.41
1:F:340:ARG:HH21	1:F:915:ARG:HD3	1.86	0.41
1:J:79:SER:OG	1:J:80:TYR:N	2.52	0.41
1:J:210:LEU:HD12	1:J:211:PRO:HD2	2.02	0.41
1:K:23:TYR:HA	4:P:181:SER:HB2	2.03	0.41
1:K:253:PRO:HB2	1:K:255:GLU:H	1.85	0.41
1:K:795:GLN:H	1:L:182:GLN:HE22	1.69	0.41
1:L:101:PHE:CD1	1:L:588:LEU:HD23	2.55	0.41
1:L:557:ASN:OD1	1:L:557:ASN:N	2.50	0.41
1:A:44:LYS:HE2	1:C:546:LEU:HB2	2.03	0.41
1:D:25:SER:HA	1:D:26:PRO:HD3	1.93	0.41
1:D:94:LEU:HB3	1:D:547:LEU:HB2	2.02	0.41
1:H:508:PHE:CE2	1:H:684:THR:HG22	2.56	0.41
1:H:651:TRP:HE1	1:H:876:MET:HE1	1.85	0.41
1:H:809:MET:HE1	1:I:188:TRP:HB3	2.02	0.41
1:K:377:ILE:HG22	1:K:450:VAL:HG21	2.02	0.41
4:P:72:PRO:HG3	4:P:225:VAL:HG13	2.03	0.41
1:A:53:THR:HG23	1:A:54:HIS:CD2	2.56	0.41
1:A:813:GLN:HE22	1:B:200:GLY:HA3	1.85	0.41
1:B:654:THR:OG1	1:B:655:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:VAL:HB	1:B:716:PHE:HB2	2.01	0.41
1:B:822:PRO:HG2	1:B:827:THR:HG21	2.03	0.41
1:D:574:LEU:HD23	1:D:574:LEU:HA	1.89	0.41
1:E:711:LEU:HD12	1:E:727:TYR:HE2	1.85	0.41
1:F:14:HIS:HB3	1:F:48:PRO:HD3	2.03	0.41
1:K:644:ASN:HB3	4:O:28:SER:HB2	2.02	0.41
1:K:726:GLY:O	1:L:589:TYR:OH	2.37	0.41
1:L:650:GLY:HA2	1:L:847:PRO:HA	2.02	0.41
1:A:618:ASP:OD1	1:A:619:TYR:N	2.54	0.41
1:A:736:LYS:HA	1:A:739:PHE:HB3	2.03	0.41
1:B:717:GLU:OE1	1:B:720:ARG:NH2	2.53	0.41
1:E:316:ASN:ND2	1:E:342:THR:H	2.18	0.41
1:H:254:ASN:ND2	1:I:411:THR:O	2.48	0.41
1:H:317:SER:OG	1:H:665:GLY:N	2.53	0.41
1:I:340:ARG:NE	1:I:897:ASP:OD2	2.54	0.41
1:J:44:LYS:HE3	1:L:546:LEU:HD22	2.03	0.41
1:J:46:ARG:HB2	1:L:616:PHE:HA	2.01	0.41
1:L:80:TYR:CE2	1:L:586:ILE:HD13	2.56	0.41
1:L:393:LEU:HD22	1:L:393:LEU:HA	1.97	0.41
1:A:379:ASN:HD21	1:A:493:ILE:HD13	1.85	0.41
1:A:474:TYR:O	1:A:478:ASN:N	2.54	0.41
1:C:497:TRP:CD2	1:C:776:ARG:HD2	2.55	0.41
1:D:134:GLU:HB3	1:D:143:VAL:HG12	2.02	0.41
1:E:493:ILE:HD13	1:F:120:ALA:HB2	2.03	0.41
1:F:229:LEU:HA	1:F:240:SER:HA	2.03	0.41
1:F:324:LEU:HD23	1:F:554:TYR:HD1	1.85	0.41
1:F:382:VAL:HG11	1:F:439:ALA:HA	2.03	0.41
1:G:900:ARG:NH1	1:H:12:TYR:O	2.51	0.41
1:H:514:ALA:HA	1:H:517:ARG:HG2	2.03	0.41
1:I:323:VAL:HG22	1:I:555:GLU:HB3	2.03	0.41
1:I:351:ASP:HB3	1:I:763:ARG:HB3	2.02	0.41
1:I:506:ASN:HB3	1:I:686:TYR:CE1	2.56	0.41
1:L:435:ILE:H	1:L:435:ILE:HG13	1.77	0.41
1:A:122:ASN:HB3	1:A:125:ALA:HB2	2.03	0.41
1:A:388:ASN:HD21	1:A:437:LEU:HB2	1.85	0.41
1:A:629:ILE:HG13	1:A:636:VAL:HG11	2.02	0.41
1:B:246:PHE:HA	1:B:259:VAL:HG12	2.02	0.41
1:B:378:GLU:HG2	1:B:380:HIS:CE1	2.55	0.41
1:B:490:TYR:HD1	1:B:820:PRO:HD3	1.86	0.41
1:B:779:VAL:HG21	1:B:821:TYR:HD2	1.86	0.41
1:C:275:VAL:HG23	1:C:462:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:SER:H	1:F:612:ASN:ND2	2.17	0.41
1:D:72:ASP:OD1	1:D:72:ASP:N	2.54	0.41
1:D:440:ASN:HD21	1:F:388:ASN:HA	1.85	0.41
1:D:705:PRO:HB3	1:D:852:PHE:HZ	1.86	0.41
1:E:406:LYS:N	1:E:414:ALA:O	2.54	0.41
1:E:650:GLY:HA3	1:E:847:PRO:HA	2.02	0.41
1:F:12:TYR:OH	4:O:167:SER:OG	2.28	0.41
1:G:374:VAL:HG11	1:G:510:HIS:CE1	2.50	0.41
1:G:424:GLU:O	1:I:145:GLY:N	2.48	0.41
1:H:109:ARG:HH22	1:H:523:LEU:HB2	1.86	0.41
1:H:628:PRO:HB3	5:T:25:LEU:HD22	2.02	0.41
1:I:211:PRO:HG2	1:I:295:ALA:HB2	2.03	0.41
1:I:220:THR:H	1:I:226:GLN:HA	1.86	0.41
1:J:204:LYS:HB2	1:J:262:ALA:HB1	2.02	0.41
1:J:435:ILE:HG13	1:L:390:CYS:HB3	2.03	0.41
1:J:497:TRP:CD2	1:J:776:ARG:HG3	2.56	0.41
1:J:825:GLY:O	1:K:527:ARG:NH1	2.53	0.41
1:J:868:ALA:O	4:P:14:GLN:NE2	2.44	0.41
1:J:874:LEU:HD13	1:J:876:MET:HG3	2.03	0.41
1:K:81:LYS:HE3	1:K:557:ASN:HD21	1.85	0.41
1:K:86:LEU:HD23	1:K:554:TYR:HB3	2.02	0.41
1:K:558:PHE:HE2	1:K:586:ILE:HG21	1.86	0.41
1:L:19:ASP:HA	1:L:48:PRO:HD2	2.03	0.41
1:L:490:TYR:HE2	1:L:819:TYR:HD2	1.68	0.41
1:L:629:ILE:HD13	1:L:889:LEU:HD12	2.02	0.41
2:M:126:ARG:HG3	2:M:493:LYS:HB3	2.01	0.41
2:M:143:ALA:HA	2:M:244:VAL:HA	2.03	0.41
3:N:238:PRO:HA	3:N:241:ARG:HB2	2.03	0.41
4:O:31:MET:HE1	4:O:47:ILE:HD13	2.02	0.41
4:P:31:MET:HE1	4:P:47:ILE:HD13	2.02	0.41
4:P:88:THR:HA	4:P:176:THR:HG22	2.03	0.41
1:A:301:ASN:HB2	1:A:569:SER:H	1.86	0.41
1:A:377:ILE:HD11	1:A:450:VAL:HG11	2.03	0.41
1:A:573:ASP:HB3	1:A:576:VAL:HG12	2.03	0.41
1:A:730:ALA:HB2	1:B:362:MET:HB2	2.03	0.41
1:A:865:MET:O	1:A:869:ASN:ND2	2.53	0.41
1:A:896:PHE:HE1	7:w:20:MET:HE1	1.86	0.41
1:C:332:ASN:ND2	1:C:334:VAL:O	2.54	0.41
1:G:343:GLU:HG3	1:G:681:LEU:HD22	2.02	0.41
1:H:687:LEU:HD21	1:H:883:MET:HE1	2.02	0.41
1:I:734:MET:HE1	1:I:767:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:617:ASN:ND2	1:K:46:ARG:HE	2.19	0.41
2:M:118:GLY:O	2:M:501:LYS:N	2.54	0.41
1:A:209:MET:HE3	1:A:209:MET:HB3	1.93	0.40
1:A:375:ARG:HB2	1:A:507:PRO:HG2	2.04	0.40
1:A:399:THR:H	1:A:426:GLU:HG2	1.86	0.40
1:A:764:MET:HE2	1:A:841:ARG:HD2	2.03	0.40
1:A:914:LEU:HD13	1:B:13:MET:HG3	2.03	0.40
1:B:32:ALA:HA	1:B:41:LEU:HD23	2.03	0.40
1:D:192:VAL:HG23	1:D:196:GLN:HB2	2.02	0.40
1:F:631:SER:HB2	1:F:886:PRO:HG3	2.03	0.40
1:F:795:GLN:HA	1:F:818:ASN:HD21	1.86	0.40
1:G:375:ARG:HD2	1:G:502:MET:HE1	2.02	0.40
1:G:604:GLU:OE2	1:G:608:ARG:NH2	2.54	0.40
1:I:559:ARG:HH22	1:I:664:LEU:HD21	1.86	0.40
1:K:210:LEU:HD13	1:K:269:ALA:HB2	2.02	0.40
1:L:84:PHE:N	1:L:554:TYR:O	2.45	0.40
1:L:255:GLU:HA	1:L:256:PRO:HD3	1.91	0.40
1:L:487:LEU:HB2	1:L:491:VAL:HG11	2.03	0.40
4:O:72:PRO:HG3	4:O:225:VAL:HG13	2.03	0.40
1:A:119:THR:OG1	1:A:120:ALA:N	2.55	0.40
1:A:287:SER:HB2	1:A:291:LEU:HG	2.04	0.40
1:A:302:TYR:HB2	1:A:516:LEU:HD13	2.02	0.40
1:A:322:GLY:HA3	1:A:556:TRP:CE3	2.57	0.40
1:E:271:ASP:HA	1:E:298:ASN:ND2	2.36	0.40
1:G:732:CYS:HA	1:G:835:LYS:HB3	2.03	0.40
1:H:94:LEU:HD23	1:H:592:PHE:CD1	2.56	0.40
1:H:380:HIS:HE1	1:I:517:ARG:HD2	1.85	0.40
1:I:88:VAL:HG23	1:I:549:PRO:HA	2.02	0.40
1:J:13:MET:HE3	1:L:914:LEU:HB2	2.03	0.40
1:K:88:VAL:HG13	1:K:549:PRO:HA	2.04	0.40
1:K:246:PHE:HB2	1:L:405:ILE:HG21	2.03	0.40
1:K:621:CYS:HB2	1:K:649:ARG:NH2	2.36	0.40
1:K:857:ALA:N	1:L:49:THR:OG1	2.51	0.40
1:L:21:SER:OG	1:L:33:ARG:NH2	2.54	0.40
1:L:652:SER:HB2	1:L:892:LEU:HB2	2.02	0.40
1:B:606:MET:HE2	1:B:606:MET:HB3	1.95	0.40
1:C:348:LEU:HD12	1:C:619:TYR:HE2	1.86	0.40
1:D:343:GLU:HG3	1:D:681:LEU:HD22	2.02	0.40
1:D:350:LEU:HD11	1:D:365:GLN:HG3	2.03	0.40
1:D:360:PHE:CE2	1:D:362:MET:HB3	2.57	0.40
1:E:258:ALA:HB1	1:F:425:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:HIS:CE1	1:F:521:MET:HG3	2.56	0.40
1:E:796:HIS:CD2	1:E:817:ALA:HA	2.57	0.40
1:E:820:PRO:O	1:F:121:TYR:OH	2.36	0.40
1:F:161:GLN:HA	1:F:172:TYR:HA	2.03	0.40
1:F:448:SER:HA	1:F:452:LEU:HD12	2.03	0.40
1:H:201:ARG:HD2	1:H:261:TYR:HB2	2.03	0.40
1:H:813:GLN:HB3	1:I:148:PRO:HD3	2.03	0.40
1:J:151:GLY:N	1:J:197:LYS:O	2.55	0.40
1:J:317:SER:N	1:J:336:ASP:OD2	2.46	0.40
1:J:743:MET:HE2	1:J:743:MET:HB3	1.87	0.40
1:K:389:TYR:HA	1:K:434:GLU:HA	2.03	0.40
2:M:149:LYS:HB3	2:M:157:PRO:HB3	2.02	0.40
2:M:279:ILE:HD11	2:M:342:SER:HB2	2.02	0.40
1:A:201:ARG:HD2	1:A:261:TYR:HB2	2.03	0.40
1:C:8:PRO:HD3	3:N:67:GLU:OE2	2.22	0.40
1:C:62:GLN:HB3	1:C:92:ARG:HH12	1.86	0.40
1:C:625:MET:HB3	1:C:627:TYR:CE2	2.56	0.40
1:D:145:GLY:N	1:E:424:GLU:O	2.36	0.40
1:D:474:TYR:HB2	1:D:572:ASN:HD22	1.86	0.40
1:E:202:VAL:HG11	1:E:260:LEU:HD13	2.02	0.40
1:G:627:TYR:CE2	1:G:638:ILE:HG13	2.56	0.40
1:I:678:VAL:HA	1:I:679:PRO:HD3	1.98	0.40
1:J:440:ASN:HD21	1:L:388:ASN:HB2	1.85	0.40
1:L:447:TYR:HA	1:L:451:ALA:HB3	2.03	0.40
1:L:743:MET:HG3	1:L:749:ILE:HB	2.03	0.40
3:N:194:ASP:OD1	3:N:194:ASP:N	2.54	0.40
1:A:115:PRO:HD2	1:C:824:ILE:HG12	2.04	0.40
1:B:134:GLU:HA	1:B:143:VAL:HG12	2.03	0.40
1:D:559:ARG:HD3	1:D:561:ASP:HB3	2.03	0.40
1:E:640:ILE:HD13	1:E:643:ARG:NH1	2.37	0.40
1:F:355:ASP:HA	1:F:763:ARG:HH22	1.86	0.40
1:F:426:GLU:HG2	1:F:427:SER:H	1.86	0.40
1:G:114:LYS:HA	1:G:115:PRO:HD3	1.82	0.40
1:H:741:ILE:HD13	1:H:741:ILE:HG21	1.86	0.40
1:I:109:ARG:HD3	1:I:113:PHE:CE1	2.57	0.40
1:I:503:ASP:OD1	1:I:689:HIS:NE2	2.45	0.40
1:I:632:ASN:HB2	1:I:882:PRO:HB2	2.04	0.40
1:J:664:LEU:HD12	1:J:680:TYR:HE2	1.86	0.40
1:K:18:GLN:NE2	4:P:184:PRO:O	2.54	0.40
1:K:103:ILE:HA	1:K:586:ILE:HG12	2.02	0.40
1:K:691:PHE:HB2	1:K:718:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:712:THR:HA	1:K:713:PRO:HD3	1.90	0.40
1:K:855:MET:HE1	1:L:56:VAL:HG11	2.04	0.40
2:M:175:MET:O	2:M:179:LEU:N	2.55	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	908/925 (98%)	776 (86%)	132 (14%)	0	100	100
1	B	909/925 (98%)	780 (86%)	129 (14%)	0	100	100
1	C	910/925 (98%)	792 (87%)	118 (13%)	0	100	100
1	D	904/925 (98%)	759 (84%)	145 (16%)	0	100	100
1	E	913/925 (99%)	779 (85%)	132 (14%)	2 (0%)	43	75
1	F	906/925 (98%)	764 (84%)	139 (15%)	3 (0%)	36	70
1	G	906/925 (98%)	760 (84%)	144 (16%)	2 (0%)	43	75
1	H	911/925 (98%)	761 (84%)	145 (16%)	5 (0%)	24	60
1	I	904/925 (98%)	751 (83%)	151 (17%)	2 (0%)	43	75
1	J	910/925 (98%)	761 (84%)	148 (16%)	1 (0%)	48	81
1	K	908/925 (98%)	760 (84%)	146 (16%)	2 (0%)	43	75
1	L	905/925 (98%)	769 (85%)	136 (15%)	0	100	100
2	M	448/508 (88%)	406 (91%)	42 (9%)	0	100	100
3	N	296/579 (51%)	272 (92%)	24 (8%)	0	100	100
4	O	176/233 (76%)	160 (91%)	16 (9%)	0	100	100
4	P	176/233 (76%)	160 (91%)	16 (9%)	0	100	100
5	Q	48/133 (36%)	39 (81%)	9 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	48/133 (36%)	39 (81%)	9 (19%)	0	100	100
5	S	48/133 (36%)	39 (81%)	9 (19%)	0	100	100
5	T	48/133 (36%)	39 (81%)	9 (19%)	0	100	100
6	U	27/266 (10%)	26 (96%)	1 (4%)	0	100	100
6	V	27/266 (10%)	26 (96%)	1 (4%)	0	100	100
6	Y	27/266 (10%)	26 (96%)	1 (4%)	0	100	100
6	u	27/266 (10%)	26 (96%)	1 (4%)	0	100	100
7	W	4/183 (2%)	2 (50%)	2 (50%)	0	100	100
7	w	10/183 (6%)	6 (60%)	4 (40%)	0	100	100
All	All	12304/14615 (84%)	10478 (85%)	1809 (15%)	17 (0%)	49	81

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	917	PRO
1	H	320	ASN
1	F	630	PRO
1	H	816	PRO
1	E	630	PRO
1	F	385	GLU
1	F	816	PRO
1	K	150	ILE
1	H	665	GLY
1	J	757	PRO
1	E	917	PRO
1	G	287	SER
1	H	148	PRO
1	H	764	MET
1	I	278	PRO
1	I	757	PRO
1	K	757	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	A	787/797 (99%)	782 (99%)	5 (1%)	78	81
1	B	788/797 (99%)	784 (100%)	4 (0%)	81	82
1	C	788/797 (99%)	786 (100%)	2 (0%)	86	85
1	D	783/797 (98%)	779 (100%)	4 (0%)	81	82
1	E	790/797 (99%)	786 (100%)	4 (0%)	81	82
1	F	785/797 (98%)	777 (99%)	8 (1%)	68	76
1	G	785/797 (98%)	777 (99%)	8 (1%)	68	76
1	H	789/797 (99%)	784 (99%)	5 (1%)	78	81
1	I	783/797 (98%)	781 (100%)	2 (0%)	86	85
1	J	788/797 (99%)	783 (99%)	5 (1%)	78	81
1	K	787/797 (99%)	780 (99%)	7 (1%)	70	76
1	L	787/797 (99%)	784 (100%)	3 (0%)	84	84
2	M	403/447 (90%)	402 (100%)	1 (0%)	87	87
3	N	253/501 (50%)	251 (99%)	2 (1%)	73	77
4	O	149/193 (77%)	149 (100%)	0	100	100
4	P	149/193 (77%)	149 (100%)	0	100	100
5	Q	38/97 (39%)	37 (97%)	1 (3%)	40	61
5	R	38/97 (39%)	37 (97%)	1 (3%)	40	61
5	S	38/97 (39%)	37 (97%)	1 (3%)	40	61
5	T	38/97 (39%)	37 (97%)	1 (3%)	40	61
6	U	22/227 (10%)	22 (100%)	0	100	100
6	V	22/227 (10%)	22 (100%)	0	100	100
6	Y	22/227 (10%)	22 (100%)	0	100	100
6	u	22/227 (10%)	22 (100%)	0	100	100
7	W	2/139 (1%)	2 (100%)	0	100	100
7	w	6/139 (4%)	6 (100%)	0	100	100
All	All	10642/12472 (85%)	10578 (99%)	64 (1%)	76	81

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ILE

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Mol	Chain	Res	Type
1	A	285	ILE
1	A	452	LEU
1	A	516	LEU
1	A	899	VAL
1	B	88	VAL
1	B	285	ILE
1	B	367	VAL
1	B	636	VAL
1	C	335	VAL
1	C	483	VAL
1	D	290	LEU
1	D	629	ILE
1	D	740	LEU
1	D	899	VAL
1	E	88	VAL
1	E	290	LEU
1	E	405	ILE
1	E	864	ASN
1	F	107	LEU
1	F	323	VAL
1	F	334	VAL
1	F	335	VAL
1	F	516	LEU
1	F	609	ASN
1	F	656	LEU
1	F	899	VAL
1	G	88	VAL
1	G	103	ILE
1	G	160	ILE
1	G	334	VAL
1	G	335	VAL
1	G	450	VAL
1	G	516	LEU
1	G	535	VAL
1	H	158	ASN
1	H	399	THR
1	H	446	LEU
1	H	626	LEU
1	H	656	LEU
1	I	290	LEU
1	I	324	LEU
1	J	155	ASN

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Mol	Chain	Res	Type
1	J	636	VAL
1	J	710	LEU
1	J	729	VAL
1	J	861	LEU
1	K	66	LEU
1	K	242	VAL
1	K	308	ASN
1	K	348	LEU
1	K	350	LEU
1	K	487	LEU
1	K	722	VAL
1	L	393	LEU
1	L	435	ILE
1	L	574	LEU
2	M	251	LEU
3	N	45	LEU
3	N	70	VAL
5	Q	39	ASN
5	R	39	ASN
5	S	39	ASN
5	T	39	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (342) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	18	GLN
1	A	47	ASN
1	A	54	HIS
1	A	62	GLN
1	A	91	ASN
1	A	138	ASN
1	A	155	ASN
1	A	161	GLN
1	A	178	GLN
1	A	185	GLN
1	A	226	GLN
1	A	308	ASN
1	A	330	GLN
1	A	347	GLN
1	A	379	ASN
1	A	408	ASN

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Mol	Chain	Res	Type
1	A	410	GLN
1	A	417	ASN
1	A	509	ASN
1	A	557	ASN
1	A	587	ASN
1	A	591	ASN
1	A	597	HIS
1	A	609	ASN
1	A	614	GLN
1	A	624	ASN
1	A	746	HIS
1	A	752	GLN
1	A	813	GLN
1	A	818	ASN
1	A	869	ASN
1	A	872	HIS
1	A	905	HIS
1	B	18	GLN
1	B	54	HIS
1	B	62	GLN
1	B	146	GLN
1	B	153	ASN
1	B	155	ASN
1	B	161	GLN
1	B	226	GLN
1	B	308	ASN
1	B	365	GLN
1	B	388	ASN
1	B	408	ASN
1	B	417	ASN
1	B	449	ASN
1	B	506	ASN
1	B	509	ASN
1	B	537	GLN
1	B	567	GLN
1	B	597	HIS
1	B	609	ASN
1	B	624	ASN
1	B	733	ASN
1	B	746	HIS
1	B	752	GLN
1	B	772	GLN

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Mol	Chain	Res	Type
1	B	834	GLN
1	C	155	ASN
1	C	158	ASN
1	C	185	GLN
1	C	187	GLN
1	C	282	GLN
1	C	294	GLN
1	C	308	ASN
1	C	332	ASN
1	C	347	GLN
1	C	440	ASN
1	C	509	ASN
1	C	510	HIS
1	C	532	HIS
1	C	557	ASN
1	C	563	ASN
1	C	624	ASN
1	C	632	ASN
1	C	728	ASN
1	C	733	ASN
1	C	746	HIS
1	C	772	GLN
1	C	780	ASN
1	C	813	GLN
1	C	834	GLN
1	C	872	HIS
1	D	30	GLN
1	D	54	HIS
1	D	122	ASN
1	D	131	ASN
1	D	138	ASN
1	D	153	ASN
1	D	196	GLN
1	D	243	ASN
1	D	273	HIS
1	D	282	GLN
1	D	293	GLN
1	D	308	ASN
1	D	365	GLN
1	D	612	ASN
1	D	614	GLN
1	D	624	ASN

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Mol	Chain	Res	Type
1	D	742	GLN
1	D	746	HIS
1	D	748	ASN
1	D	777	GLN
1	D	780	ASN
1	D	797	ASN
1	D	813	GLN
1	D	869	ASN
1	E	14	HIS
1	E	91	ASN
1	E	122	ASN
1	E	153	ASN
1	E	185	GLN
1	E	187	GLN
1	E	226	GLN
1	E	232	ASN
1	E	293	GLN
1	E	330	GLN
1	E	440	ASN
1	E	509	ASN
1	E	537	GLN
1	E	557	ASN
1	E	587	ASN
1	E	597	HIS
1	E	617	ASN
1	E	624	ASN
1	E	688	ASN
1	E	746	HIS
1	E	752	GLN
1	E	780	ASN
1	E	788	GLN
1	E	834	GLN
1	E	864	ASN
1	F	9	GLN
1	F	54	HIS
1	F	62	GLN
1	F	146	GLN
1	F	155	ASN
1	F	161	GLN
1	F	168	ASN
1	F	196	GLN
1	F	226	GLN

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Mol	Chain	Res	Type
1	F	243	ASN
1	F	293	GLN
1	F	298	ASN
1	F	308	ASN
1	F	330	GLN
1	F	341	ASN
1	F	347	GLN
1	F	417	ASN
1	F	478	ASN
1	F	557	ASN
1	F	597	HIS
1	F	609	ASN
1	F	612	ASN
1	F	632	ASN
1	F	772	GLN
1	F	777	GLN
1	F	834	GLN
1	F	869	ASN
1	G	9	GLN
1	G	91	ASN
1	G	178	GLN
1	G	226	GLN
1	G	298	ASN
1	G	308	ASN
1	G	341	ASN
1	G	388	ASN
1	G	408	ASN
1	G	449	ASN
1	G	464	ASN
1	G	470	ASN
1	G	472	ASN
1	G	537	GLN
1	G	563	ASN
1	G	572	ASN
1	G	598	ASN
1	G	614	GLN
1	G	742	GLN
1	G	746	HIS
1	G	752	GLN
1	G	788	GLN
1	G	795	GLN
1	G	796	HIS

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Mol	Chain	Res	Type
1	G	905	HIS
1	H	153	ASN
1	H	158	ASN
1	H	169	GLN
1	H	185	GLN
1	H	226	GLN
1	H	243	ASN
1	H	264	ASN
1	H	308	ASN
1	H	316	ASN
1	H	338	GLN
1	H	341	ASN
1	H	380	HIS
1	H	408	ASN
1	H	470	ASN
1	H	591	ASN
1	H	733	ASN
1	H	748	ASN
1	H	777	GLN
1	H	780	ASN
1	H	797	ASN
1	H	813	GLN
1	H	872	HIS
1	I	54	HIS
1	I	62	GLN
1	I	91	ASN
1	I	131	ASN
1	I	146	GLN
1	I	185	GLN
1	I	245	GLN
1	I	341	ASN
1	I	347	GLN
1	I	380	HIS
1	I	417	ASN
1	I	510	HIS
1	I	557	ASN
1	I	591	ASN
1	I	609	ASN
1	I	624	ASN
1	I	728	ASN
1	I	731	GLN
1	I	746	HIS

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Mol	Chain	Res	Type
1	I	752	GLN
1	I	796	HIS
1	I	798	ASN
1	I	864	ASN
1	I	872	HIS
1	I	905	HIS
1	J	18	GLN
1	J	54	HIS
1	J	122	ASN
1	J	153	ASN
1	J	155	ASN
1	J	158	ASN
1	J	161	GLN
1	J	168	ASN
1	J	169	GLN
1	J	178	GLN
1	J	245	GLN
1	J	273	HIS
1	J	294	GLN
1	J	298	ASN
1	J	308	ASN
1	J	330	GLN
1	J	341	ASN
1	J	379	ASN
1	J	388	ASN
1	J	470	ASN
1	J	478	ASN
1	J	510	HIS
1	J	557	ASN
1	J	563	ASN
1	J	587	ASN
1	J	609	ASN
1	J	614	GLN
1	J	624	ASN
1	J	632	ASN
1	J	728	ASN
1	J	731	GLN
1	J	742	GLN
1	J	777	GLN
1	K	9	GLN
1	K	54	HIS
1	K	91	ASN

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Mol	Chain	Res	Type
1	K	169	GLN
1	K	178	GLN
1	K	298	ASN
1	K	338	GLN
1	K	341	ASN
1	K	440	ASN
1	K	470	ASN
1	K	472	ASN
1	K	504	ASN
1	K	509	ASN
1	K	557	ASN
1	K	563	ASN
1	K	612	ASN
1	K	624	ASN
1	K	632	ASN
1	K	688	ASN
1	K	746	HIS
1	K	796	HIS
1	K	798	ASN
1	K	864	ASN
1	K	902	HIS
1	K	905	HIS
1	L	131	ASN
1	L	146	GLN
1	L	155	ASN
1	L	169	GLN
1	L	185	GLN
1	L	187	GLN
1	L	221	ASN
1	L	298	ASN
1	L	327	GLN
1	L	332	ASN
1	L	341	ASN
1	L	347	GLN
1	L	365	GLN
1	L	440	ASN
1	L	492	ASN
1	L	506	ASN
1	L	537	GLN
1	L	591	ASN
1	L	632	ASN
1	L	644	ASN

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Mol	Chain	Res	Type
1	L	707	ASN
1	L	780	ASN
1	L	798	ASN
1	L	813	GLN
1	L	902	HIS
1	L	905	HIS
2	M	86	HIS
2	M	90	GLN
2	M	181	ASN
2	M	195	ASN
2	M	253	ASN
2	M	335	GLN
2	M	372	GLN
2	M	393	GLN
2	M	425	GLN
2	M	439	ASN
2	M	463	HIS
2	M	476	GLN
3	N	49	ASN
3	N	215	ASN
3	N	296	GLN
4	O	25	GLN
4	O	32	ASN
4	O	53	GLN
4	P	25	GLN
4	P	32	ASN
5	Q	39	ASN
5	R	33	GLN
5	R	39	ASN
5	S	39	ASN
5	T	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

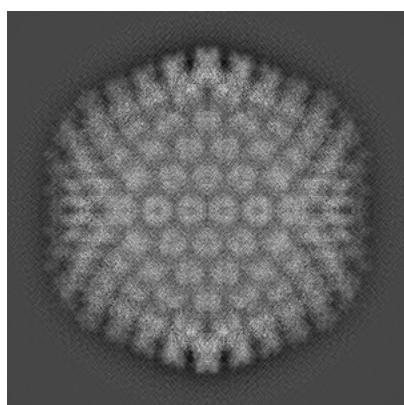
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10768. These allow visual inspection of the internal detail of the map and identification of artifacts.

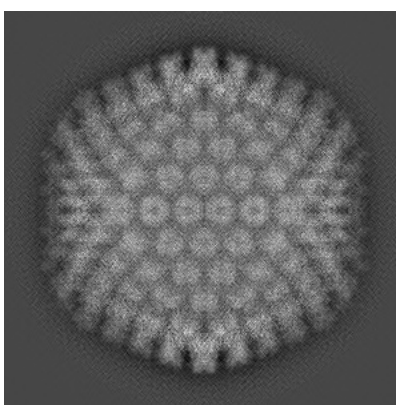
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

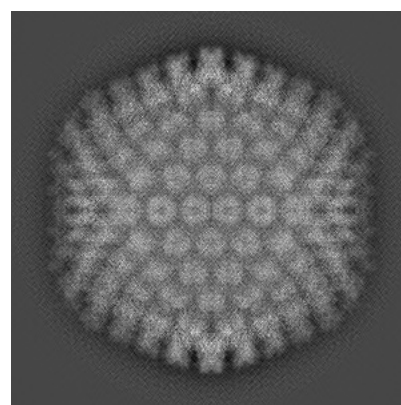
6.1.1 Primary map



X



Y

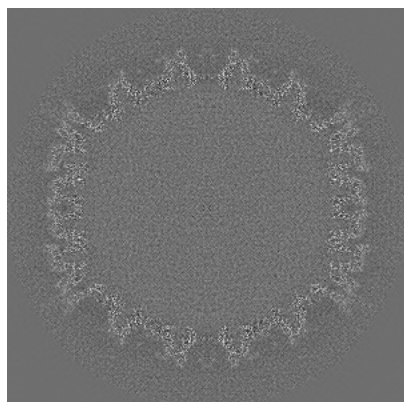


Z

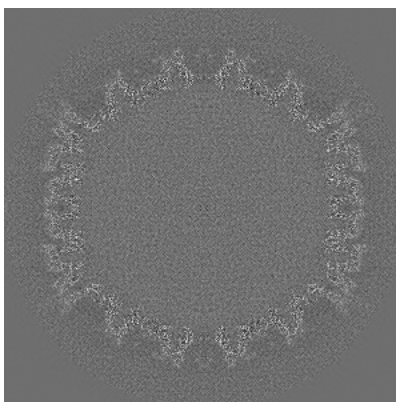
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

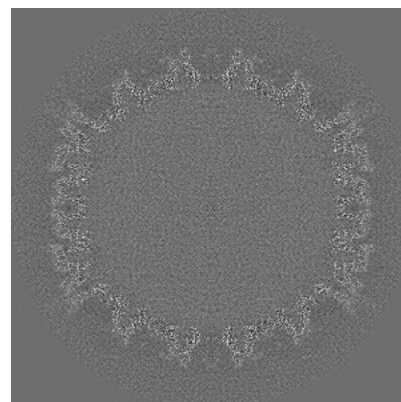
6.2.1 Primary map



X Index: 390



Y Index: 390

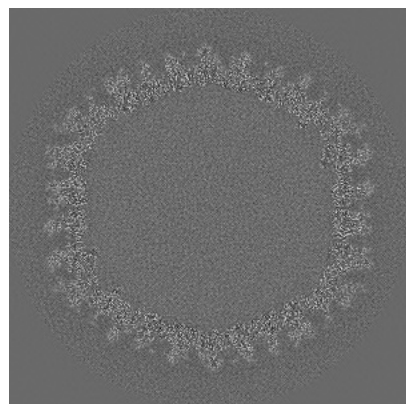


Z Index: 390

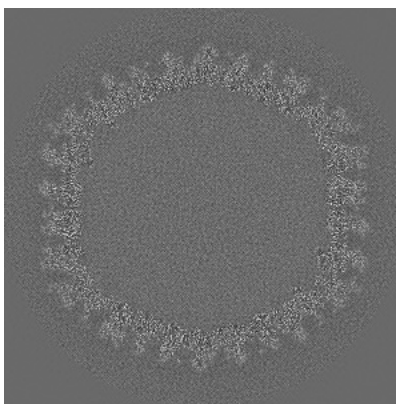
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

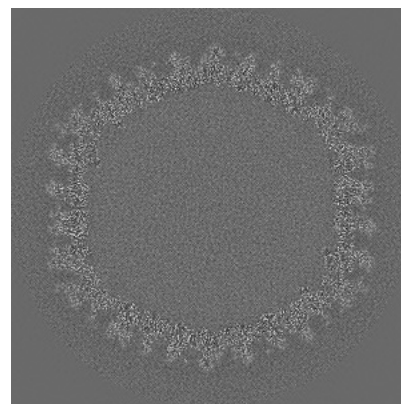
6.3.1 Primary map



X Index: 405



Y Index: 375

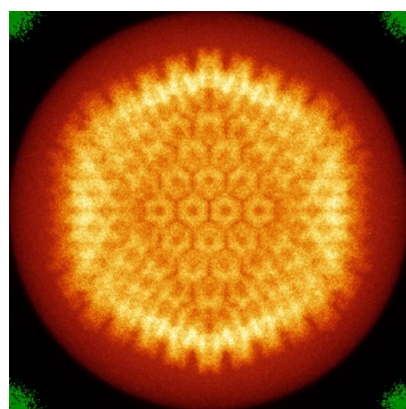


Z Index: 375

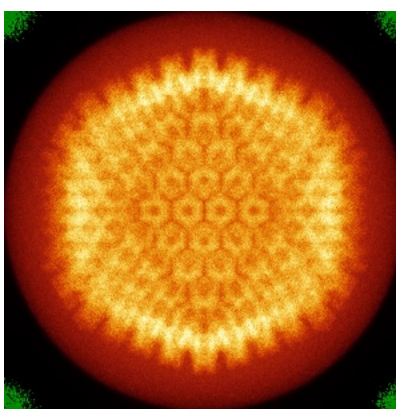
The images above show the largest variance slices of the map in three orthogonal directions.

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

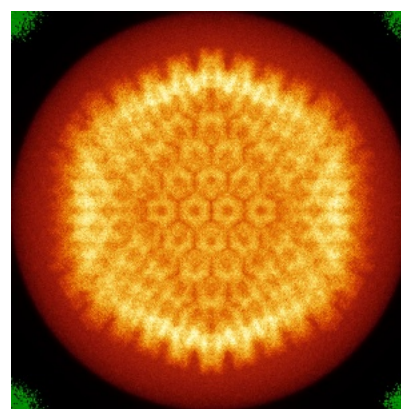
6.4.1 Primary map



X



Y

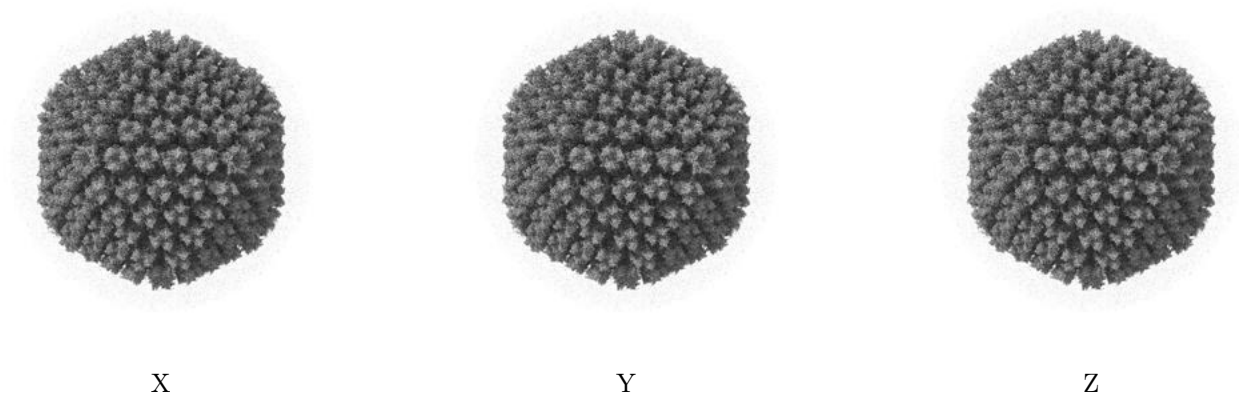


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

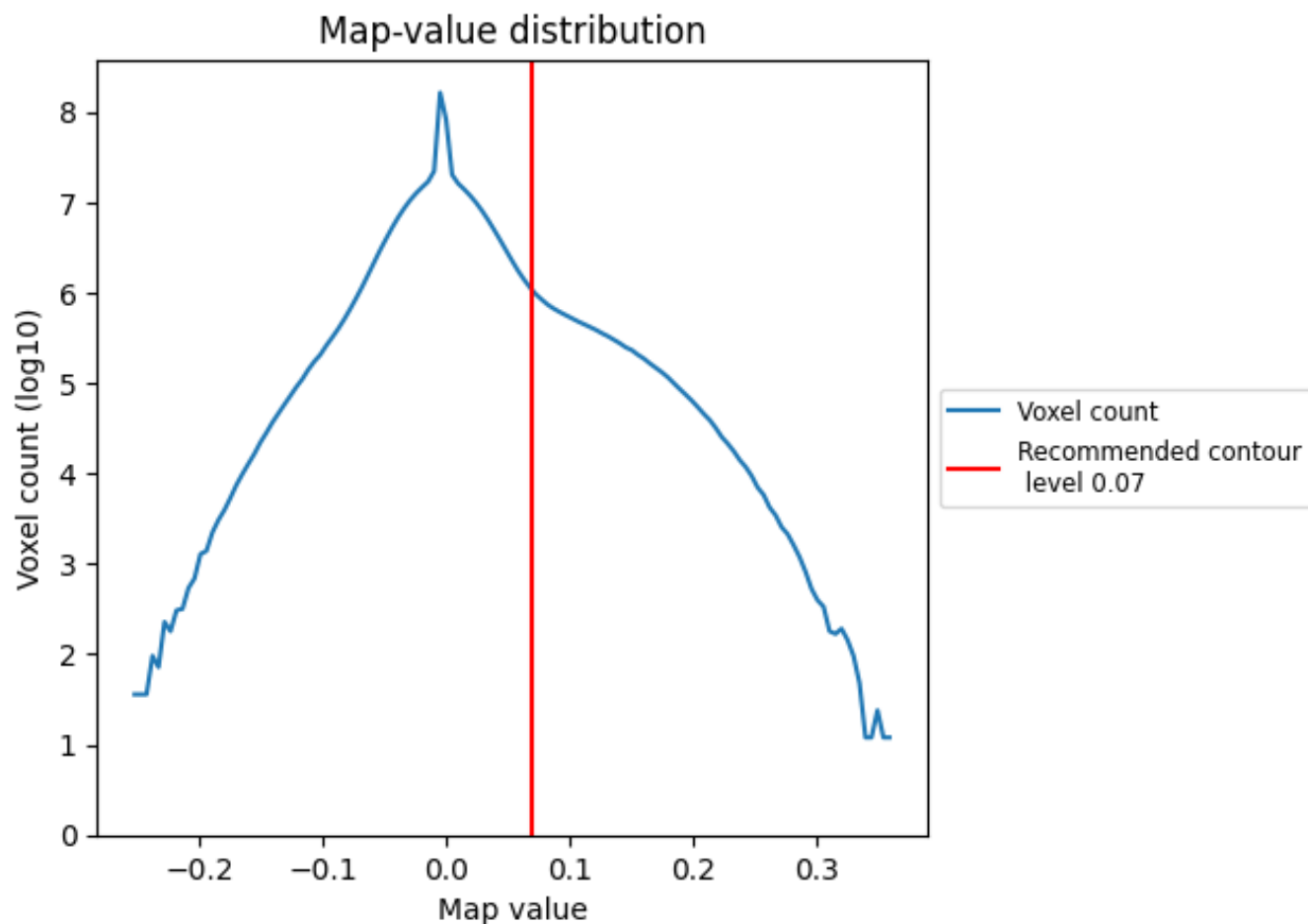
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

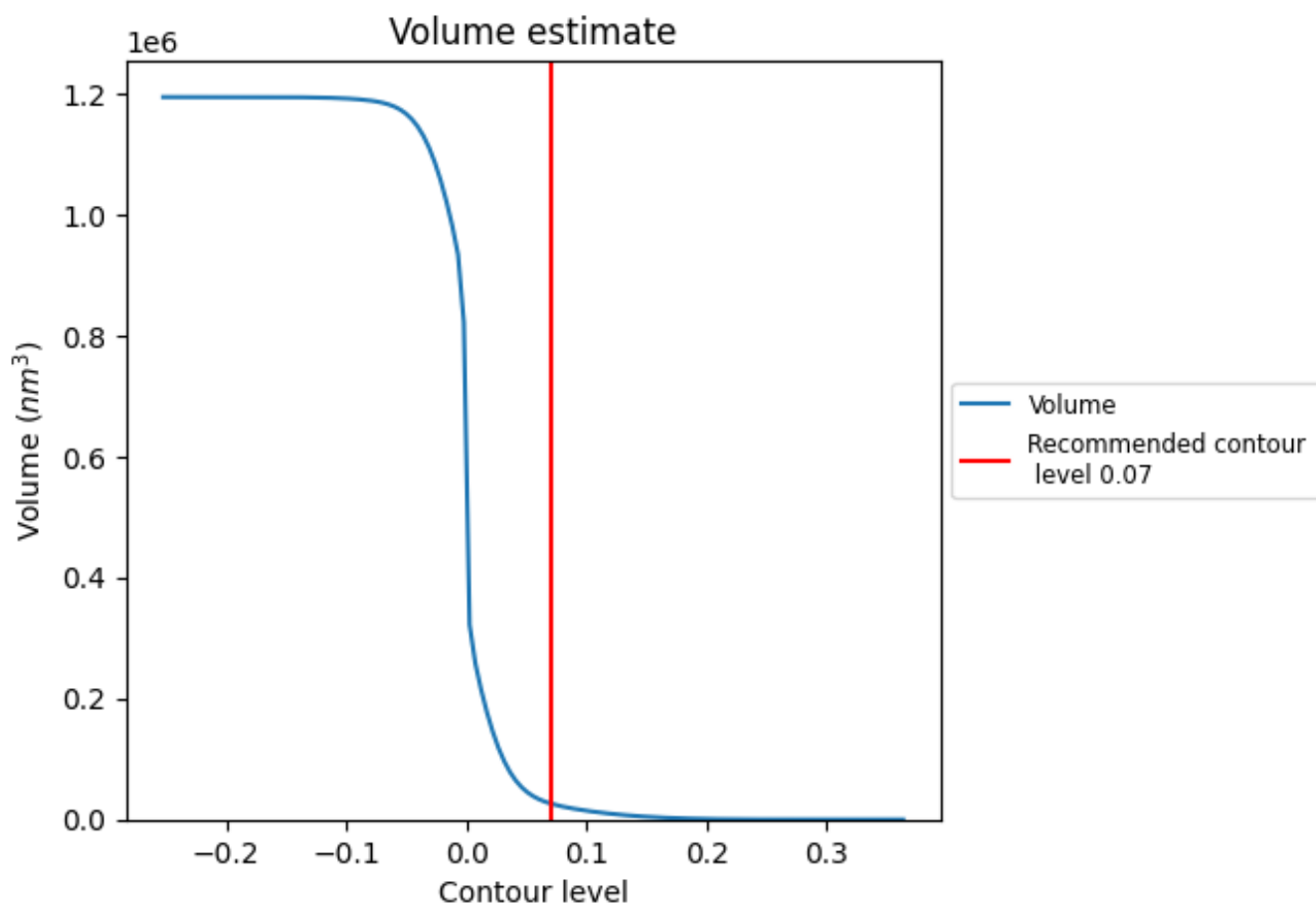
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

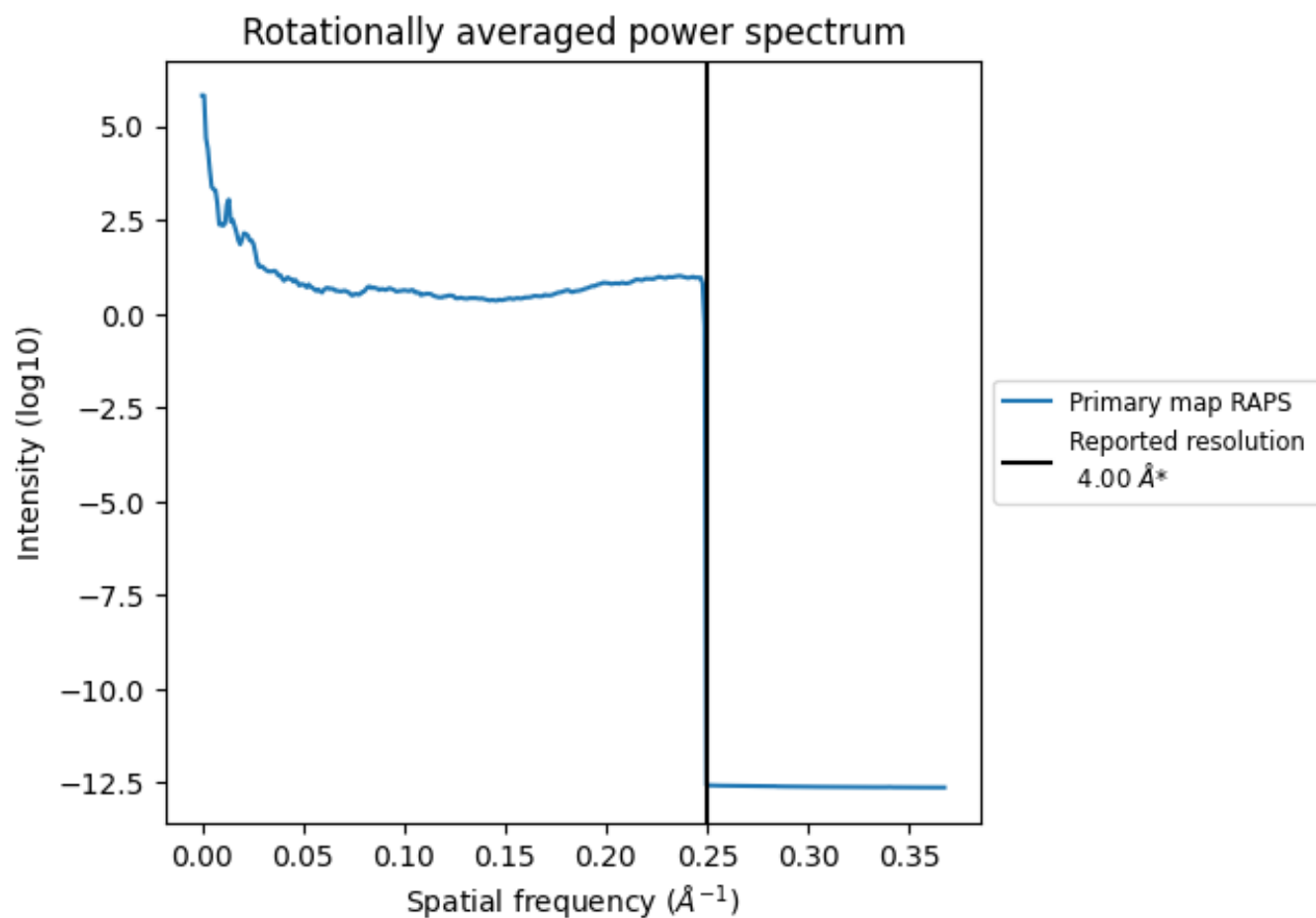
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 26562 nm³; this corresponds to an approximate mass of 23994 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation

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

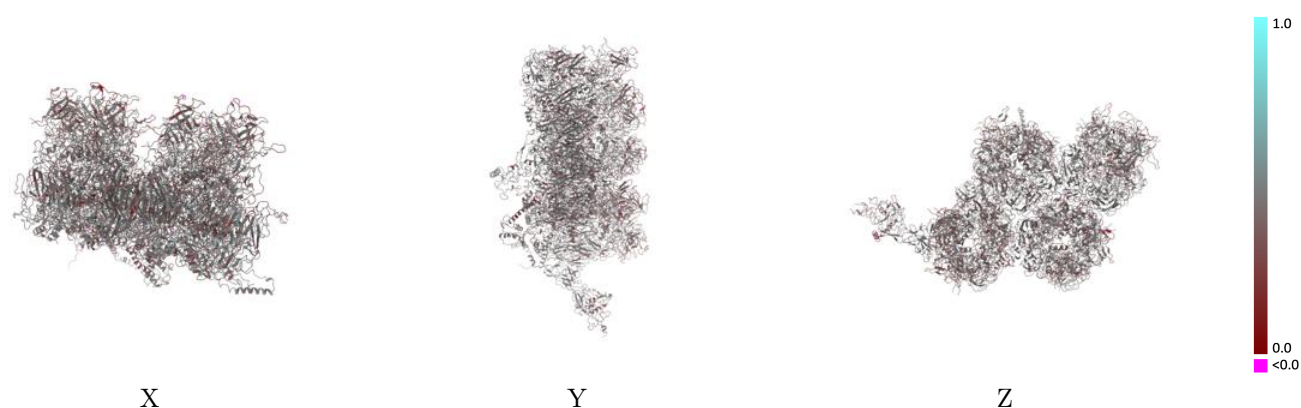
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10768 and PDB model 6YBA. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

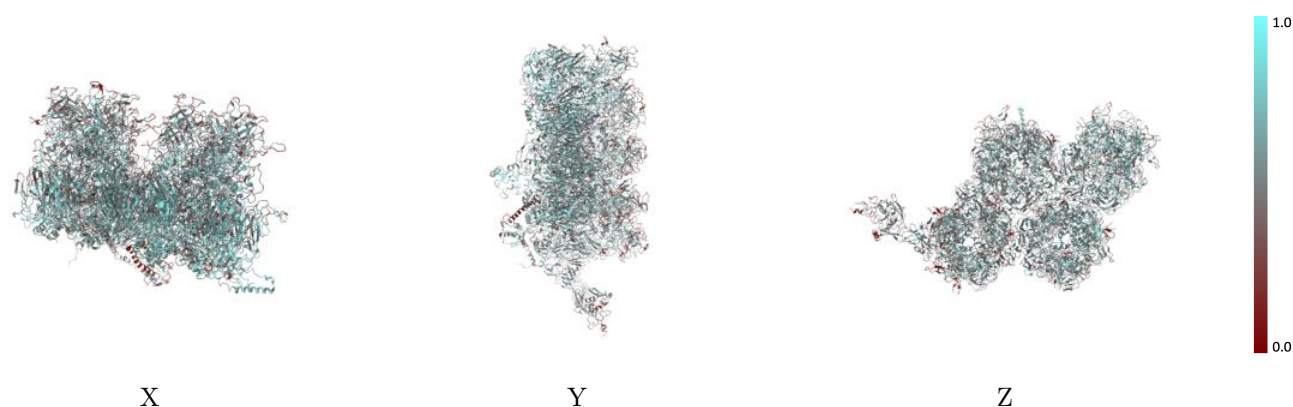
This section was not generated.

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



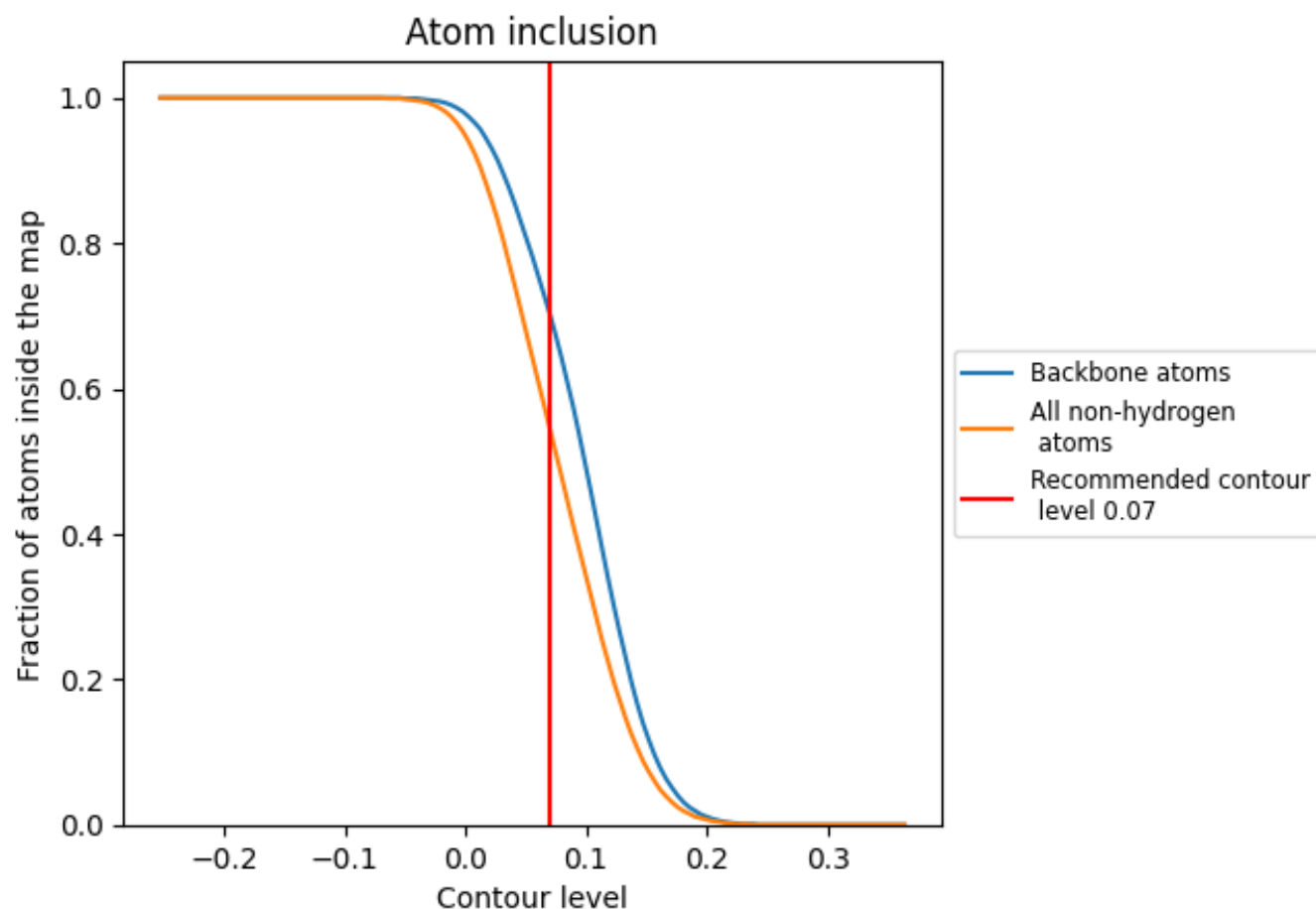
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5450	 0.4130
A	 0.5390	 0.4080
B	 0.5220	 0.4020
C	 0.5320	 0.4040
D	 0.5650	 0.4140
E	 0.5450	 0.4090
F	 0.5530	 0.4110
G	 0.5690	 0.4210
H	 0.5740	 0.4190
I	 0.5830	 0.4240
J	 0.5490	 0.4180
K	 0.5560	 0.4120
L	 0.5660	 0.4180
M	 0.4580	 0.4120
N	 0.4290	 0.4070
O	 0.5720	 0.4280
P	 0.5790	 0.4410
Q	 0.5080	 0.4170
R	 0.4640	 0.3940
S	 0.5000	 0.4060
T	 0.5360	 0.4130
U	 0.1830	 0.2820
V	 0.4270	 0.3870
W	 0.3330	 0.4110
Y	 0.4930	 0.3990
u	 0.1640	 0.2870
w	 0.3090	 0.3870

