



Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 05:28 pm GMT

PDB ID : 6QI5
EMDB ID : EMD-4551
Title : Near Atomic Structure of an Atadenovirus Shows a possible gene duplication event and Intergenera Variations in Cementing Proteins
Authors : Condezo, G.N.; Marabini, R.; Gomez-Blanco, J.; SanMartin, C.
Deposited on : 2019-01-17
Resolution : 3.40 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

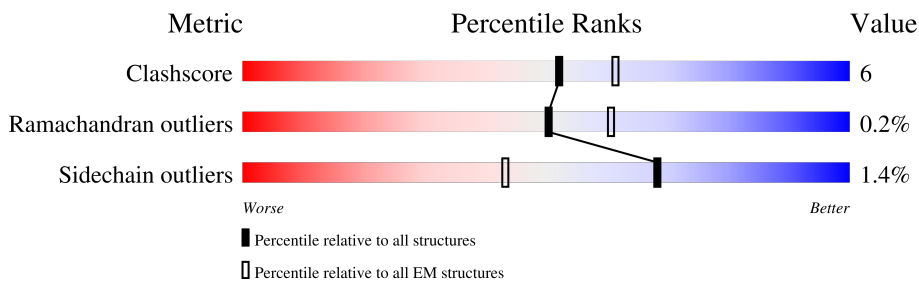
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	909	
1	B	909	
1	C	909	
1	D	909	
1	E	909	
1	F	909	
1	G	909	
1	H	909	

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Mol	Chain	Length	Quality of chain
1	I	909	 82% 17%
1	J	909	 84% 16%
1	K	909	 83% 16%
1	L	909	 82% 16%
2	Q	370	 84% 15%
2	R	370	 83% 16%
2	S	370	 83% 16%
2	T	370	 86% 13%
3	O	278	 60% 7% 33%
3	P	278	 60% 7% 33%
4	N	609	 37% 5% 58%
5	M	451	 15% 80% 20%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 106009 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
			Total	C	N	O	S		
1	A	905	Total 7168	C 4547	N 1226	O 1366	S 29	0	0
1	L	906	Total 7174	C 4550	N 1227	O 1368	S 29	0	0
1	K	908	Total 7184	C 4556	N 1229	O 1370	S 29	0	0
1	J	906	Total 7171	C 4548	N 1227	O 1368	S 28	0	0
1	H	905	Total 7166	C 4545	N 1226	O 1367	S 28	0	0
1	I	906	Total 7171	C 4548	N 1227	O 1368	S 28	0	0
1	G	906	Total 7171	C 4548	N 1227	O 1368	S 28	0	0
1	F	906	Total 7172	C 4548	N 1227	O 1368	S 29	0	0
1	E	906	Total 7171	C 4548	N 1227	O 1368	S 28	0	0
1	D	906	Total 7174	C 4550	N 1227	O 1368	S 29	0	0
1	C	907	Total 7179	C 4553	N 1228	O 1369	S 29	0	0
1	B	904	Total 7161	C 4542	N 1225	O 1365	S 29	0	0

- Molecule 2 is a protein called Protein LH3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S	367	Total 2874	C 1830	N 494	O 529	S 21	0	0
2	T	367	Total 2874	C 1830	N 494	O 529	S 21	0	0
2	R	367	Total 2874	C 1830	N 494	O 529	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	367	Total	C	N	O	S	0	0
			2874	1830	494	529	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	186	Total	C	N	O	S	0	0
			1452	922	248	280	2		
3	O	186	Total	C	N	O	S	0	0
			1452	922	248	280	2		

- Molecule 4 is a protein called PIIIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	255	Total	C	N	O	S	0	0
			1980	1250	346	378	6		

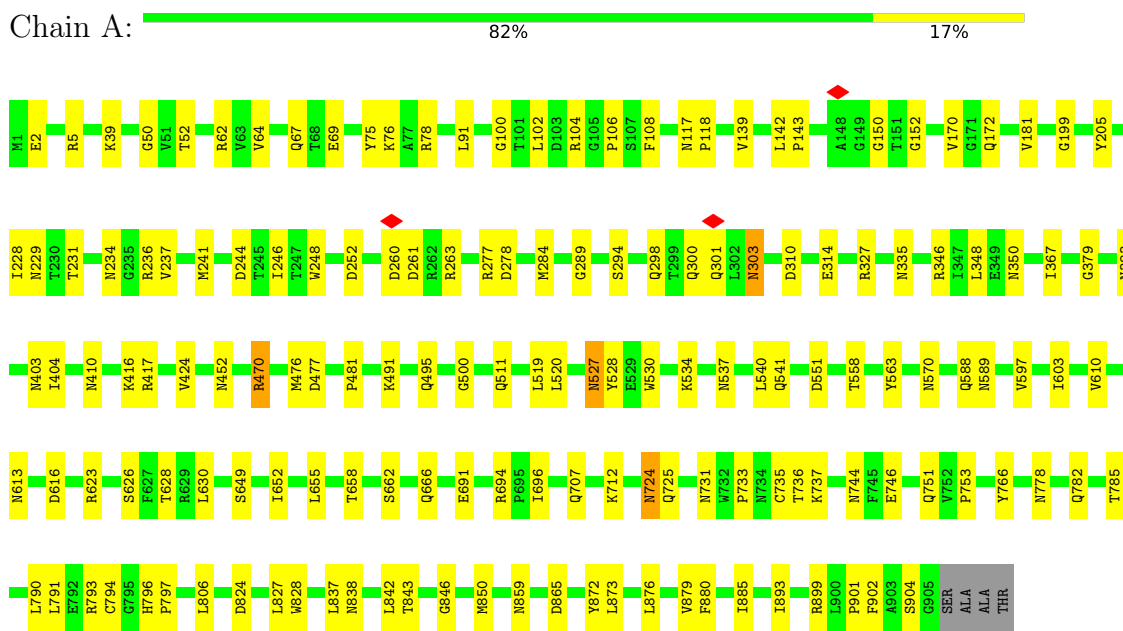
- Molecule 5 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	451	Total	C	N	O	S	0	0
			3567	2270	598	687	12		

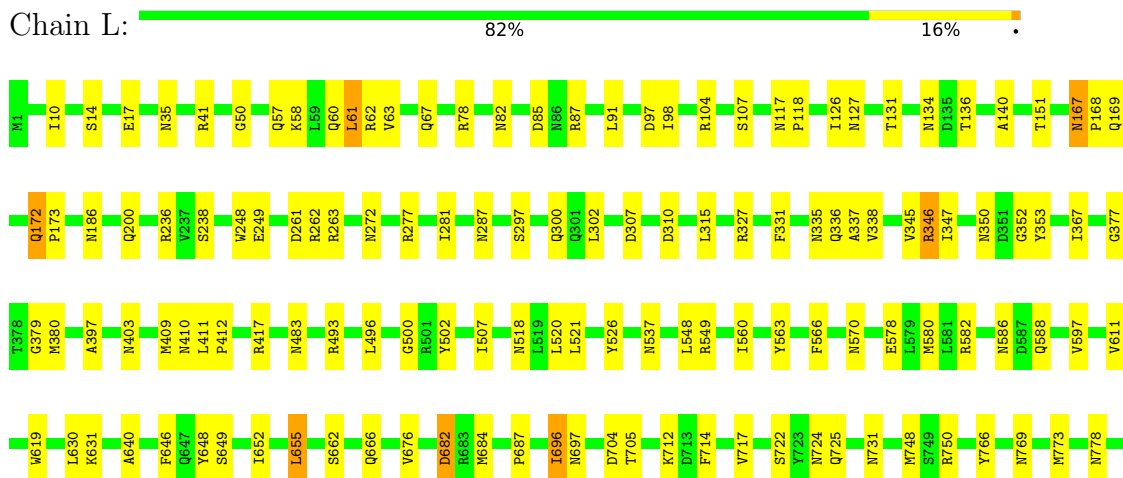
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Hexon protein

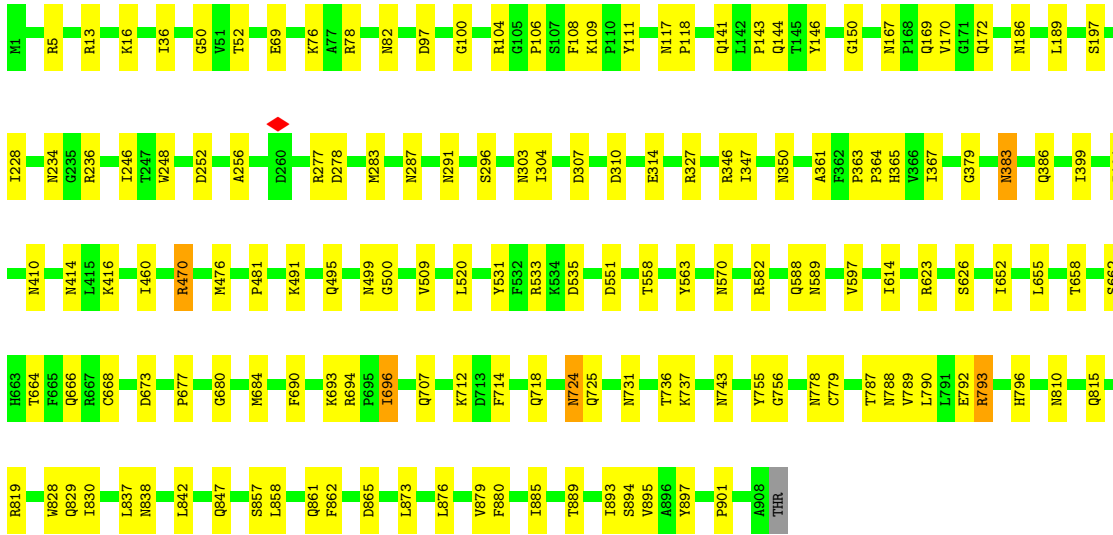
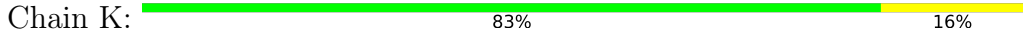


- Molecule 1: Hexon protein

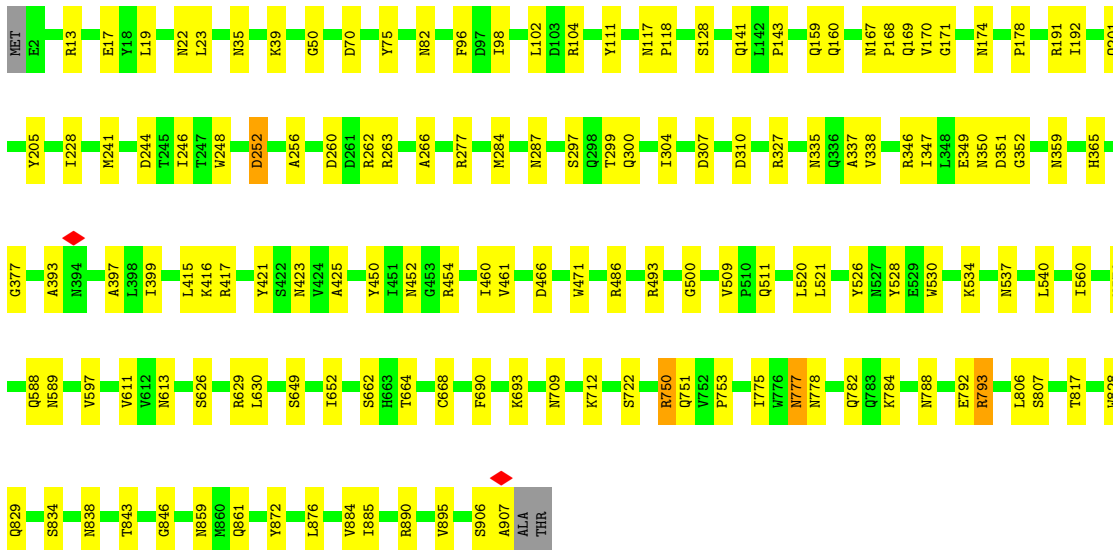
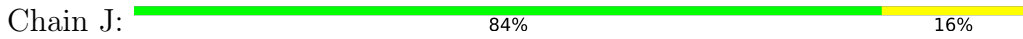




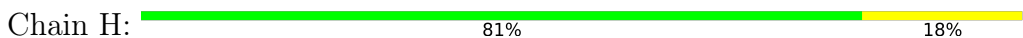
• Molecule 1: Hexon protein

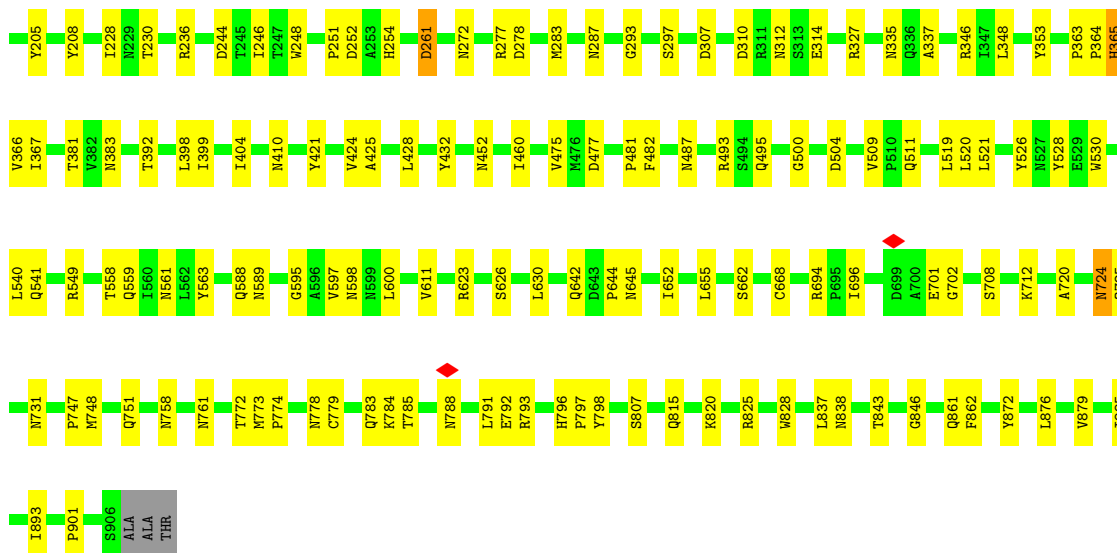


• Molecule 1: Hexon protein

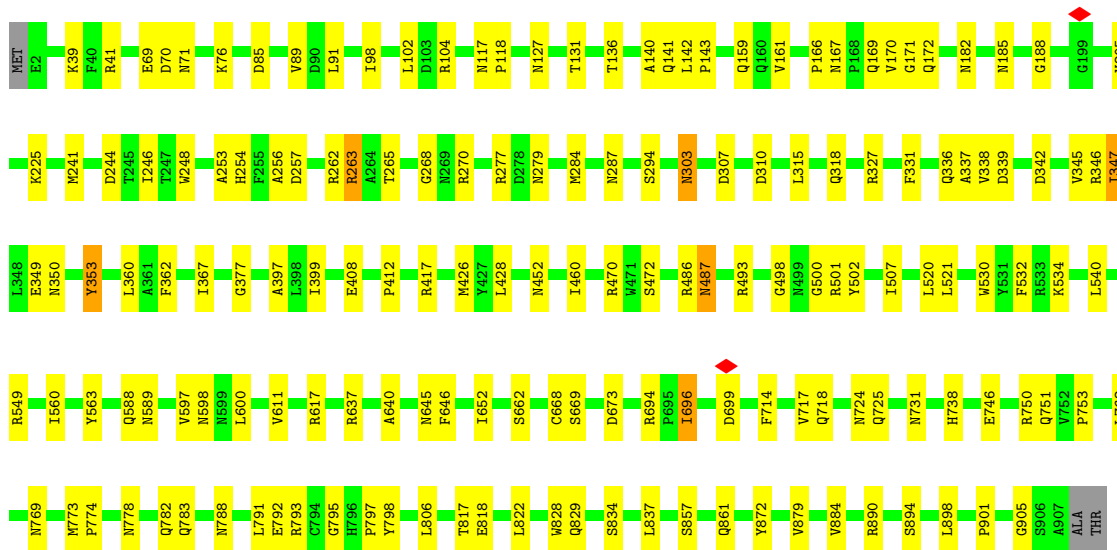
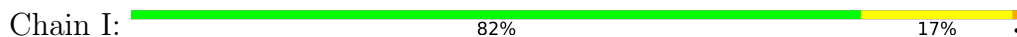


• Molecule 1: Hexon protein

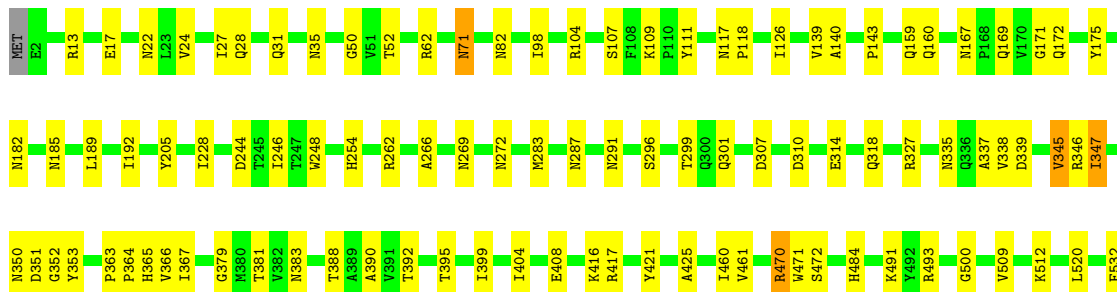
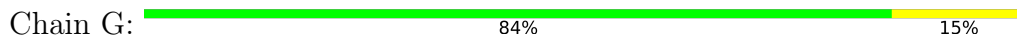


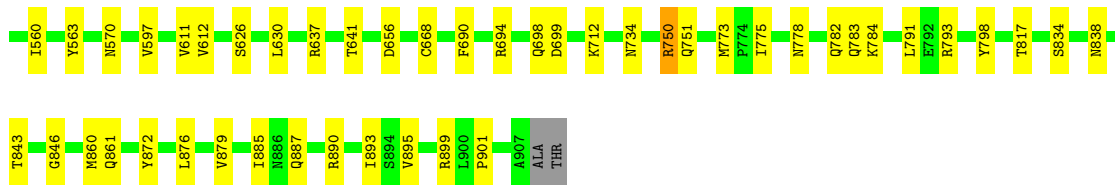


• Molecule 1: Hexon protein

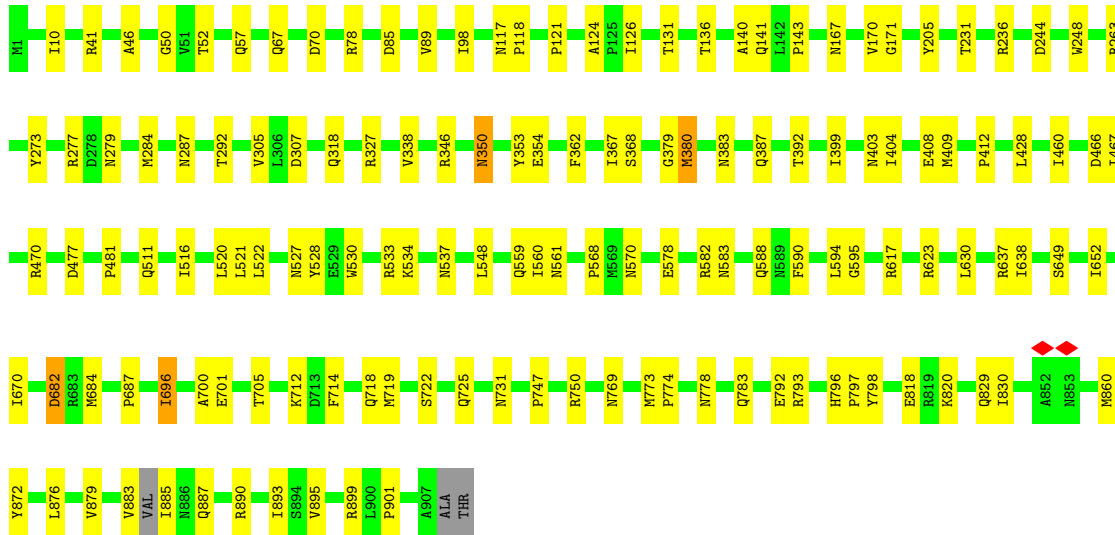
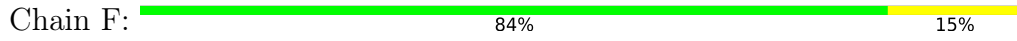


• Molecule 1: Hexon protein

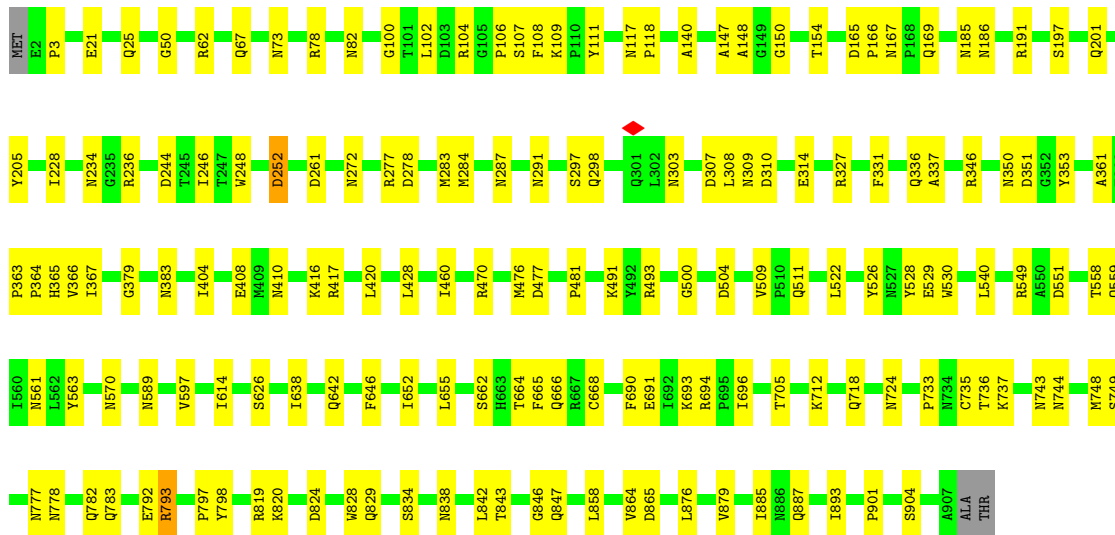
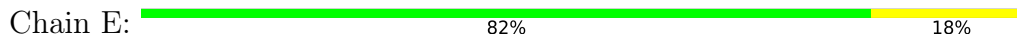




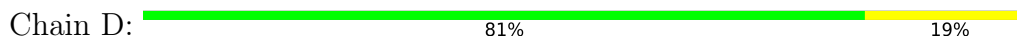
• Molecule 1: Hexon protein

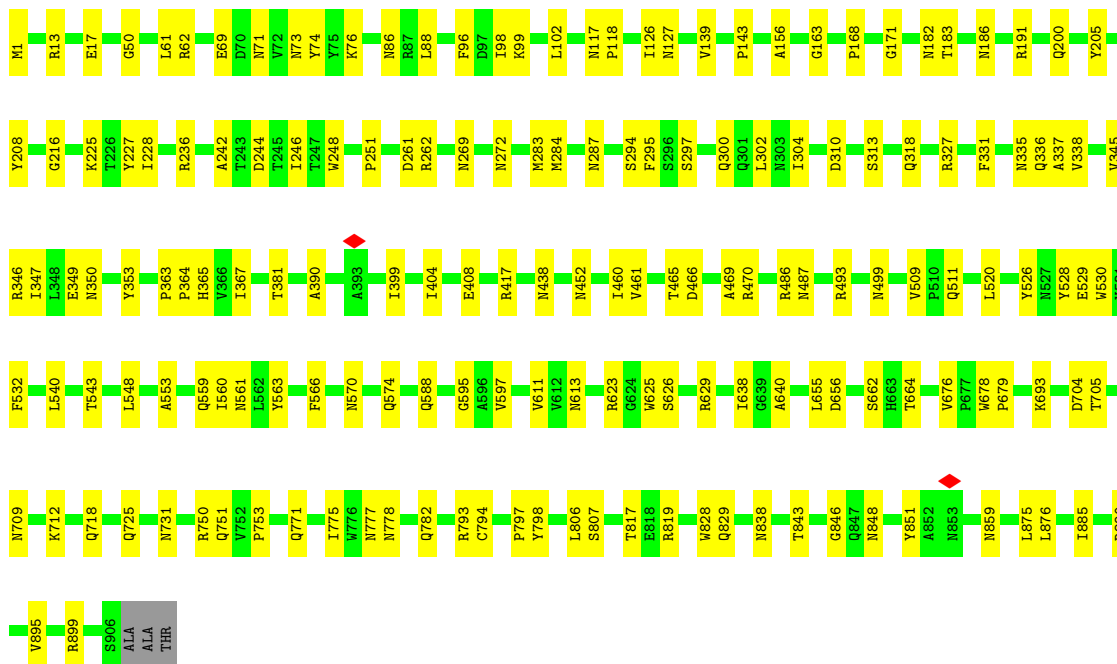


• Molecule 1: Hexon protein

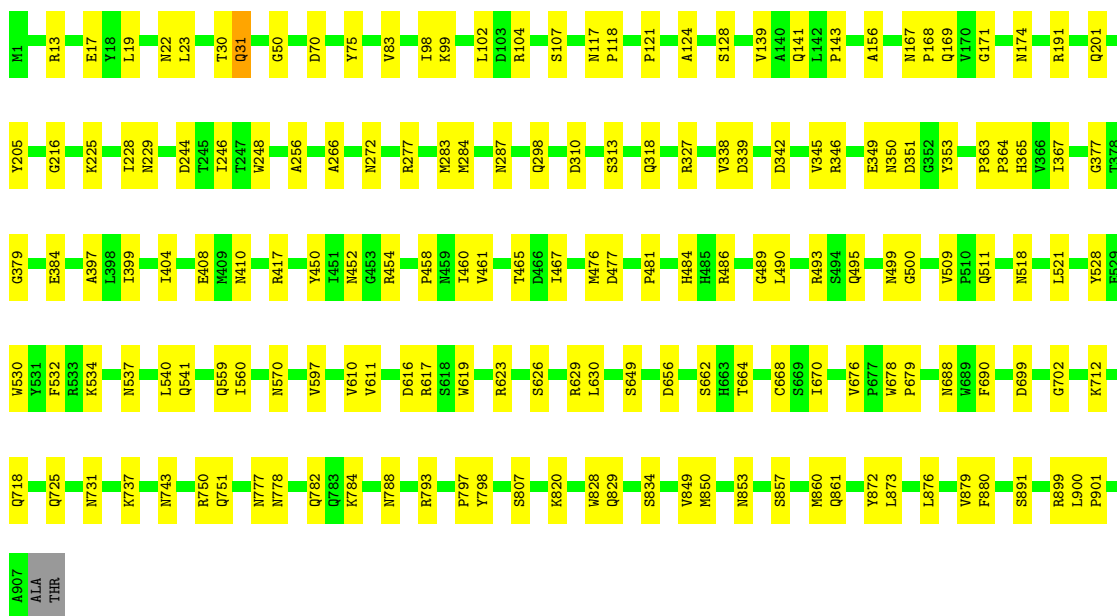
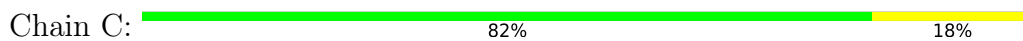


• Molecule 1: Hexon protein

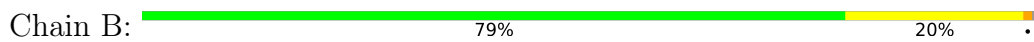


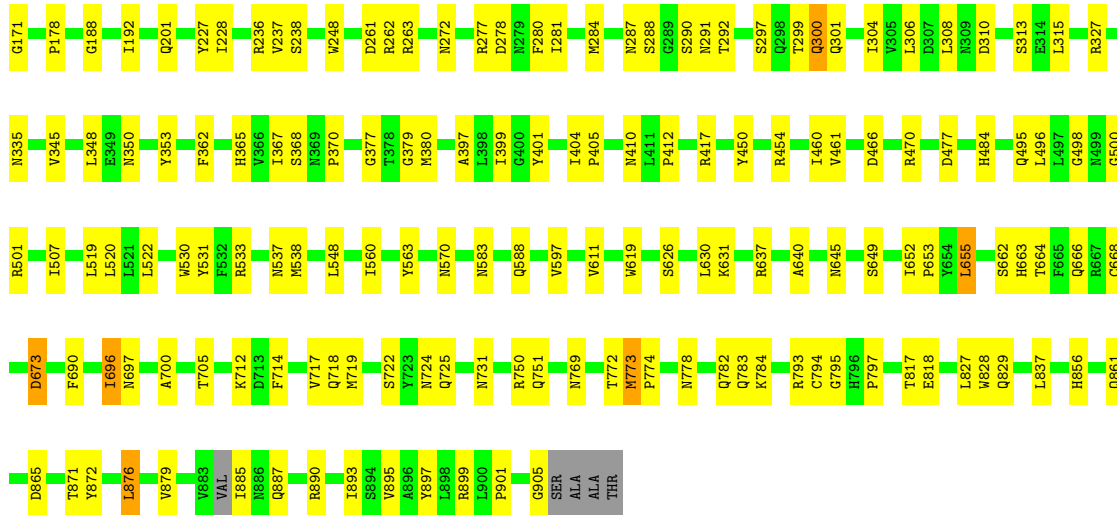


• Molecule 1: Hexon protein

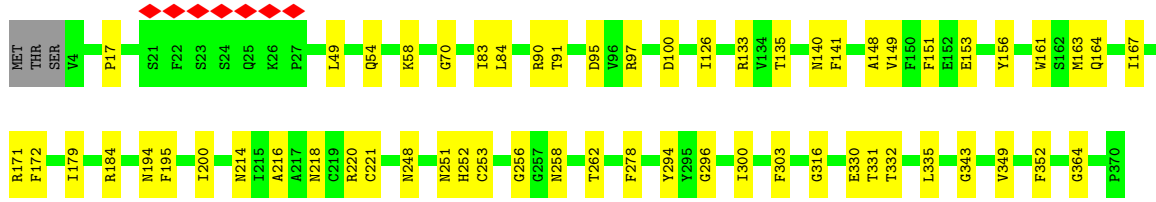
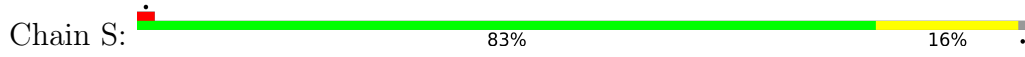


• Molecule 1: Hexon protein

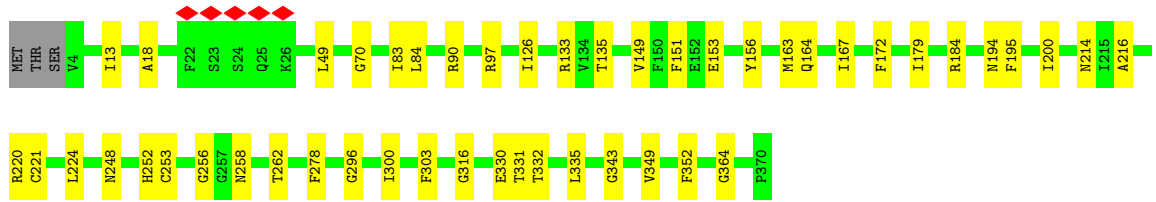
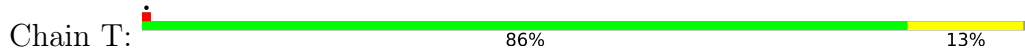




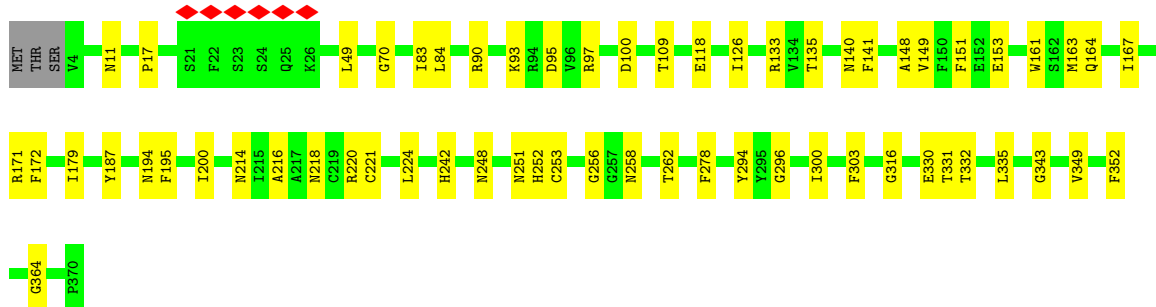
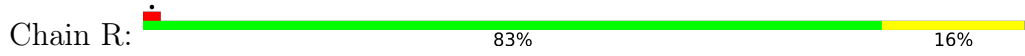
• Molecule 2: Protein LH3



• Molecule 2: Protein LH3



• Molecule 2: Protein LH3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	16071	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.536	Depositor
Minimum map value	-0.296	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	1053.0, 1053.0, 1053.0	wwPDB
Map dimensions	780, 780, 780	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.35, 1.35, 1.35	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	0.35	0/7373	0.59	4/10074 (0.0%)
1	B	0.34	0/7365	0.60	6/10061 (0.1%)
1	C	0.35	0/7384	0.59	1/10089 (0.0%)
1	D	0.38	0/7379	0.59	0/10082
1	E	0.37	0/7376	0.60	2/10079 (0.0%)
1	F	0.37	0/7376	0.60	4/10076 (0.0%)
1	G	0.38	0/7376	0.59	0/10079
1	H	0.38	0/7371	0.61	3/10072 (0.0%)
1	I	0.38	0/7376	0.61	6/10079 (0.1%)
1	J	0.36	0/7376	0.58	2/10079 (0.0%)
1	K	0.36	0/7389	0.59	2/10096 (0.0%)
1	L	0.37	0/7379	0.61	5/10082 (0.0%)
2	Q	0.34	0/2954	0.54	0/4016
2	R	0.34	0/2954	0.55	0/4016
2	S	0.34	0/2954	0.55	0/4016
2	T	0.34	0/2954	0.55	0/4016
3	O	0.34	0/1494	0.55	0/2048
3	P	0.34	0/1494	0.55	0/2048
4	N	0.30	0/2014	0.59	0/2741
5	M	0.30	0/3660	0.61	1/5005 (0.0%)
All	All	0.36	0/108998	0.59	36/148854 (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	4
1	C	0	1
1	D	0	3
1	E	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	4
1	H	0	3
1	I	0	2
1	J	0	3
1	K	0	2
1	L	0	5
5	M	0	3
All	All	0	37

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	LEU	CA-CB-CG	8.97	135.93	115.30
1	L	61	LEU	CA-CB-CG	7.24	131.96	115.30
1	I	315	LEU	CA-CB-CG	7.12	131.67	115.30
1	E	252	ASP	CB-CG-OD1	6.78	124.40	118.30
1	H	791	LEU	CA-CB-CG	6.67	130.63	115.30
1	L	315	LEU	CA-CB-CG	6.34	129.89	115.30
1	J	252	ASP	CB-CG-OD1	6.18	123.87	118.30
1	K	252	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	252	ASP	CB-CG-OD1	6.09	123.79	118.30
1	A	790	LEU	CA-CB-CG	5.94	128.96	115.30
1	H	252	ASP	CB-CG-OD1	5.92	123.63	118.30
1	C	900	LEU	CA-CB-CG	5.86	128.77	115.30
1	B	773	MET	C-N-CD	-5.74	107.98	120.60
1	E	696	ILE	C-N-CA	5.59	135.69	121.70
1	B	315	LEU	CA-CB-CG	5.58	128.13	115.30
1	I	696	ILE	C-N-CA	5.58	135.64	121.70
1	L	876	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	696	ILE	C-N-CA	5.48	135.40	121.70
1	B	876	LEU	CA-CB-CG	5.46	127.87	115.30
1	F	876	LEU	CA-CB-CG	5.46	127.85	115.30
1	H	696	ILE	C-N-CA	5.40	135.20	121.70
1	I	898	LEU	CA-CB-CG	5.39	127.69	115.30
5	M	239	LEU	CA-CB-CG	5.38	127.68	115.30
1	L	696	ILE	C-N-CA	5.37	135.12	121.70
1	I	91	LEU	CA-CB-CG	5.35	127.60	115.30
1	K	696	ILE	C-N-CA	5.33	135.03	121.70
1	F	696	ILE	C-N-CA	5.32	134.99	121.70
1	A	873	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	696	ILE	C-N-CA	5.17	134.63	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	521	LEU	CA-CB-CG	5.16	127.17	115.30
1	F	682	ASP	CB-CG-OD1	5.16	122.94	118.30
1	I	241	MET	CA-CB-CG	5.15	122.06	113.30
1	I	353	TYR	CA-CB-CG	5.11	123.10	113.40
1	F	368	SER	C-N-CA	5.10	134.46	121.70
1	B	673	ASP	CB-CG-OD1	5.05	122.84	118.30
1	L	682	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	ASP	Peptide
1	A	261	ASP	Peptide
1	A	298	GLN	Peptide
1	A	791	LEU	Peptide
1	B	178	PRO	Peptide
1	B	299	THR	Peptide
1	B	697	ASN	Peptide
1	B	772	THR	Peptide
1	C	365	HIS	Peptide
1	D	345	VAL	Peptide
1	D	346	ARG	Peptide
1	D	365	HIS	Peptide
1	E	298	GLN	Peptide
1	E	3	PRO	Peptide
1	E	365	HIS	Peptide
1	G	345	VAL	Peptide
1	G	346	ARG	Peptide
1	G	365	HIS	Peptide
1	G	791	LEU	Peptide
1	H	261	ASP	Peptide
1	H	365	HIS	Peptide
1	H	701	GLU	Peptide
1	I	345	VAL	Peptide
1	I	346	ARG	Peptide
1	J	299	THR	Peptide
1	J	346	ARG	Peptide
1	J	393	ALA	Peptide
1	K	146	TYR	Peptide
1	K	365	HIS	Peptide
1	L	172	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	L	345	VAL	Peptide
1	L	346	ARG	Peptide
1	L	697	ASN	Peptide
1	L	884	VAL	Peptide
5	M	118	ASP	Peptide
5	M	119	PRO	Peptide
5	M	40	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7168	0	6800	100	0
1	B	7161	0	6790	115	0
1	C	7179	0	6810	102	0
1	D	7174	0	6805	107	0
1	E	7171	0	6798	103	0
1	F	7172	0	6800	90	0
1	G	7171	0	6798	91	0
1	H	7166	0	6793	104	0
1	I	7171	0	6798	105	0
1	J	7171	0	6798	85	0
1	K	7184	0	6815	103	0
1	L	7174	0	6805	96	0
2	Q	2874	0	2742	38	0
2	R	2874	0	2742	44	0
2	S	2874	0	2742	38	0
2	T	2874	0	2742	26	0
3	O	1452	0	1400	11	0
3	P	1452	0	1400	12	0
4	N	1980	0	2014	15	0
5	M	3567	0	3505	53	0
All	All	106009	0	100897	1180	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 6.

All (1180) 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:H:312:ASN:HB2	1:H:598:ASN:HD21	1.48	0.78
1:B:50:GLY:HA2	1:B:570:ASN:HD22	1.56	0.71
4:N:186:ASN:HB3	4:N:218:ASN:HD21	1.56	0.70
1:F:50:GLY:HA2	1:F:570:ASN:HD22	1.55	0.70
1:K:246:ILE:HG22	1:K:248:TRP:H	1.57	0.70
1:K:662:SER:O	1:K:828:TRP:NE1	2.25	0.69
1:I:143:PRO:HB2	1:I:171:GLY:HA2	1.73	0.69
1:D:771:GLN:HG3	2:S:54:GLN:HG2	1.75	0.69
2:R:218:ASN:HD21	2:Q:161:TRP:HD1	1.41	0.69
1:G:327:ARG:HB3	1:G:338:VAL:HG11	1.75	0.69
1:F:705:THR:HG23	1:F:712:LYS:HG2	1.76	0.68
3:P:23:ARG:HH12	3:P:259:PRO:HD3	1.58	0.68
3:O:23:ARG:HH12	3:O:259:PRO:HD3	1.58	0.68
1:J:160:GLN:HB3	2:Q:91:THR:HG22	1.75	0.68
1:H:149:GLY:HA2	1:H:185:ASN:HA	1.76	0.68
1:L:352:GLY:H	1:J:111:TYR:HB2	1.60	0.67
1:D:50:GLY:HA2	1:D:570:ASN:HD22	1.58	0.67
1:H:662:SER:O	1:H:828:TRP:NE1	2.27	0.67
1:E:662:SER:O	1:E:828:TRP:NE1	2.26	0.67
1:E:246:ILE:HG22	1:E:248:TRP:H	1.60	0.67
1:B:5:ARG:HG3	1:B:10:ILE:HB	1.77	0.67
1:L:666:GLN:NE2	1:L:865:ASP:OD1	2.28	0.66
1:I:246:ILE:HG22	1:I:248:TRP:H	1.61	0.66
1:A:520:LEU:HB3	1:A:588:GLN:HE22	1.61	0.66
1:J:143:PRO:HB2	1:J:171:GLY:HA2	1.78	0.66
1:I:349:GLU:HG2	1:I:470:ARG:HG2	1.78	0.66
1:D:246:ILE:HG22	1:D:248:TRP:H	1.61	0.65
1:C:287:ASN:HD21	1:C:313:SER:H	1.45	0.65
1:L:327:ARG:HB3	1:L:338:VAL:HG21	1.79	0.65
1:C:143:PRO:HB2	1:C:171:GLY:HA2	1.77	0.65
1:A:150:GLY:H	1:A:236:ARG:HH12	1.45	0.65
1:F:797:PRO:HD3	1:E:404:ILE:HD11	1.79	0.65
1:L:50:GLY:HA2	1:L:570:ASN:HD22	1.61	0.64
1:E:50:GLY:HA2	1:E:570:ASN:HD22	1.61	0.64
1:I:520:LEU:HB3	1:I:588:GLN:HE22	1.62	0.64
1:D:294:SER:HB3	1:D:529:GLU:HB3	1.80	0.64
1:G:626:SER:HB3	1:G:876:LEU:HB2	1.79	0.64
1:I:140:ALA:HB3	1:G:399:ILE:HG22	1.80	0.64
1:B:104:ARG:NH2	1:B:500:GLY:O	2.31	0.63
1:B:705:THR:HG23	1:B:712:LYS:HG2	1.81	0.63
1:B:666:GLN:NE2	1:B:865:ASP:OD1	2.32	0.63
1:K:725:GLN:NE2	1:K:731:ASN:OD1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:140:ALA:HB3	1:J:399:ILE:HG22	1.81	0.62
1:L:520:LEU:HB3	1:L:588:GLN:HE22	1.64	0.62
1:K:626:SER:HB2	1:K:876:LEU:HB2	1.80	0.62
1:G:318:GLN:HG3	1:G:656:ASP:HA	1.81	0.62
4:N:139:VAL:HA	4:N:144:GLN:HE22	1.64	0.62
1:B:345:VAL:HG11	1:B:484:HIS:HE2	1.65	0.62
1:A:797:PRO:HD3	1:C:404:ILE:HD11	1.81	0.61
1:J:890:ARG:HD2	3:P:120:GLY:HA3	1.82	0.61
1:D:287:ASN:HD21	1:D:313:SER:H	1.48	0.61
1:A:5:ARG:NH2	1:C:850:MET:SD	2.67	0.61
1:B:696:ILE:HD11	1:B:818:GLU:HA	1.82	0.61
1:H:797:PRO:HD3	1:G:404:ILE:HD11	1.82	0.61
1:E:511:GLN:NE2	1:E:528:TYR:OH	2.33	0.61
1:L:104:ARG:NH2	1:L:500:GLY:O	2.34	0.61
1:H:589:ASN:HB2	1:I:41:ARG:H	1.64	0.61
1:I:104:ARG:NH2	1:I:500:GLY:O	2.33	0.61
1:F:10:ILE:HG22	1:E:842:LEU:HD12	1.81	0.61
1:B:724:ASN:HD22	1:B:837:LEU:HB2	1.66	0.61
1:I:725:GLN:NE2	1:I:731:ASN:OD1	2.33	0.61
1:B:287:ASN:HD21	1:B:313:SER:H	1.48	0.61
1:B:353:TYR:HB2	1:B:412:PRO:HB2	1.81	0.61
2:S:218:ASN:HD21	2:R:161:TRP:HD1	1.46	0.61
1:F:399:ILE:HG22	1:E:140:ALA:HB3	1.83	0.61
1:I:879:VAL:HG12	1:I:901:PRO:HD2	1.83	0.60
1:I:696:ILE:HD11	1:I:818:GLU:HA	1.83	0.60
1:E:197:SER:HG	1:E:248:TRP:HE1	1.50	0.60
1:K:143:PRO:O	1:K:172:GLN:NE2	2.35	0.60
1:H:398:LEU:HB2	1:G:139:VAL:HG22	1.84	0.60
1:F:404:ILE:HD11	1:D:797:PRO:HD3	1.82	0.60
1:J:626:SER:HB2	1:J:876:LEU:HB2	1.84	0.60
1:G:637:ARG:NH1	1:G:872:TYR:OH	2.34	0.60
1:A:662:SER:O	1:A:828:TRP:NE1	2.26	0.60
1:J:246:ILE:HG22	1:J:248:TRP:H	1.66	0.60
1:H:246:ILE:HG22	1:H:248:TRP:H	1.65	0.60
1:B:284:MET:HB3	1:B:530:TRP:HE1	1.67	0.60
1:H:205:TYR:HH	1:G:353:TYR:HH	1.49	0.60
1:L:127:ASN:OD1	1:K:796:HIS:ND1	2.34	0.60
5:M:200:ASP:HB2	5:M:286:TRP:HB3	1.83	0.60
1:A:278:ASP:OD2	1:A:327:ARG:NH2	2.32	0.60
1:L:676:VAL:HG22	1:I:905:GLY:H	1.67	0.60
1:L:682:ASP:HA	1:L:687:PRO:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:417:ARG:NH2	1:G:782:GLN:OE1	2.35	0.60
1:G:104:ARG:NH2	1:G:500:GLY:O	2.35	0.60
2:R:171:ARG:HH22	2:Q:135:THR:HG1	1.48	0.60
1:L:346:ARG:HH21	1:L:822:LEU:HB3	1.67	0.60
1:E:346:ARG:HD3	1:E:481:PRO:HB3	1.83	0.60
1:B:725:GLN:NE2	1:B:731:ASN:OD1	2.35	0.60
1:K:287:ASN:ND2	1:K:307:ASP:OD1	2.35	0.59
2:S:161:TRP:HD1	2:Q:218:ASN:HD21	1.47	0.59
1:G:337:ALA:O	1:G:493:ARG:NH1	2.35	0.59
1:E:350:ASN:OD1	1:E:416:LYS:NZ	2.34	0.59
1:E:904:SER:HA	1:C:676:VAL:HG22	1.84	0.59
1:C:246:ILE:HG22	1:C:248:TRP:H	1.66	0.59
1:K:563:TYR:HE2	1:J:712:LYS:HZ3	1.50	0.59
1:H:97:ASP:HB3	1:H:561:ASN:HB2	1.84	0.59
1:H:170:VAL:HG22	1:G:784:LYS:HE2	1.84	0.59
1:G:310:ASP:HB3	1:G:597:VAL:HG13	1.85	0.59
1:A:796:HIS:ND1	1:B:127:ASN:OD1	2.35	0.59
1:K:170:VAL:HG22	1:J:784:LYS:HE2	1.84	0.59
1:H:783:GLN:NE2	1:H:792:GLU:O	2.36	0.59
1:H:626:SER:HB2	1:H:876:LEU:HB2	1.83	0.59
1:F:140:ALA:HB3	1:D:399:ILE:HG22	1.83	0.59
1:C:310:ASP:HB3	1:C:597:VAL:HG13	1.85	0.59
1:L:797:PRO:HD3	1:K:404:ILE:HD11	1.82	0.59
1:K:792:GLU:OE1	1:K:793:ARG:NH2	2.36	0.59
1:J:104:ARG:NH2	1:J:500:GLY:O	2.36	0.59
1:F:118:PRO:O	1:E:410:ASN:ND2	2.36	0.59
1:L:724:ASN:HD22	1:L:837:LEU:HB2	1.67	0.59
1:L:337:ALA:O	1:L:493:ARG:NH1	2.36	0.59
1:F:403:ASN:ND2	1:D:794:CYS:O	2.34	0.59
1:C:99:LYS:HD3	1:C:559:GLN:HE21	1.68	0.59
1:A:842:LEU:HD12	1:B:10:ILE:HG22	1.84	0.59
1:L:631:LYS:NZ	1:L:869:GLU:OE2	2.36	0.59
1:K:106:PRO:HD2	1:K:551:ASP:HB2	1.84	0.59
1:G:139:VAL:HG11	1:G:262:ARG:HH12	1.68	0.59
1:F:696:ILE:HD11	1:F:818:GLU:HA	1.84	0.59
1:B:310:ASP:HB3	1:B:597:VAL:HG13	1.85	0.59
1:A:410:ASN:ND2	1:B:118:PRO:O	2.36	0.58
1:A:301:GLN:HB2	1:L:61:LEU:HD22	1.83	0.58
1:F:617:ARG:NH2	1:F:901:PRO:O	2.36	0.58
1:K:144:GLN:HB2	1:K:189:LEU:HB3	1.86	0.58
1:H:563:TYR:HE2	1:G:712:LYS:HZ3	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:778:ASN:HB3	1:D:118:PRO:HD2	1.84	0.58
1:C:70:ASP:OD1	1:C:534:LYS:NZ	2.35	0.58
1:A:626:SER:HB2	1:A:876:LEU:HB2	1.86	0.58
1:L:885:ILE:HG12	1:L:895:VAL:HG12	1.83	0.58
1:K:346:ARG:HD3	1:K:481:PRO:HB3	1.86	0.58
1:H:519:LEU:HD11	1:H:885:ILE:HD13	1.85	0.58
1:C:399:ILE:HG22	1:B:140:ALA:HB3	1.86	0.58
1:I:694:ARG:NH1	1:I:699:ASP:OD2	2.37	0.58
3:O:255:LYS:NZ	3:O:267:VAL:O	2.37	0.58
4:N:63:LEU:HD12	4:N:77:VAL:HG12	1.86	0.58
1:L:725:GLN:NE2	1:L:731:ASN:OD1	2.35	0.58
1:C:104:ARG:NH2	1:C:500:GLY:O	2.37	0.58
1:B:16:LYS:O	3:O:221:ARG:NH1	2.37	0.58
1:K:186:ASN:O	1:K:236:ARG:NH2	2.36	0.58
1:L:705:THR:HG23	1:L:712:LYS:HG2	1.85	0.58
1:J:284:MET:HB3	1:J:530:TRP:HE1	1.69	0.58
1:I:89:VAL:HB	1:I:521:LEU:HB3	1.84	0.58
1:F:284:MET:HB3	1:F:530:TRP:HE1	1.69	0.58
1:C:327:ARG:HB3	1:C:338:VAL:HG11	1.85	0.58
1:B:277:ARG:HH12	1:B:652:ILE:HD12	1.68	0.58
2:T:49:LEU:HD12	2:T:70:GLY:HA2	1.86	0.58
3:P:255:LYS:NZ	3:P:267:VAL:O	2.37	0.58
1:A:346:ARG:HD3	1:A:481:PRO:HB3	1.86	0.57
1:L:277:ARG:HH12	1:L:652:ILE:HD12	1.69	0.57
1:A:104:ARG:NH2	1:A:500:GLY:O	2.37	0.57
1:K:737:LYS:O	1:K:743:ASN:ND2	2.37	0.57
1:E:104:ARG:NH2	1:E:500:GLY:O	2.37	0.57
1:E:626:SER:HB2	1:E:876:LEU:HB2	1.84	0.57
5:M:183:LEU:O	5:M:278:LYS:NZ	2.37	0.57
1:E:109:LYS:HE2	1:E:252:ASP:HB2	1.86	0.57
1:B:121:PRO:HG2	1:B:124:ALA:HB2	1.85	0.57
2:Q:49:LEU:HD12	2:Q:70:GLY:HA2	1.86	0.57
1:A:117:ASN:HD22	1:C:778:ASN:HA	1.70	0.57
1:F:379:GLY:HA2	1:E:228:ILE:HA	1.86	0.57
5:M:390:ASP:OD1	5:M:393:GLN:NE2	2.37	0.57
1:A:778:ASN:HB3	1:B:118:PRO:HD2	1.86	0.57
1:L:778:ASN:HB3	1:J:118:PRO:HD2	1.86	0.57
2:S:49:LEU:HD12	2:S:70:GLY:HA2	1.86	0.57
3:O:96:THR:HG22	3:O:99:ARG:HD3	1.86	0.57
1:J:192:ILE:HG12	1:J:241:MET:HB3	1.87	0.57
1:J:277:ARG:HH12	1:J:652:ILE:HD12	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:254:HIS:NE2	1:H:452:ASN:O	2.34	0.57
1:H:694:ARG:NH2	1:H:702:GLY:O	2.38	0.57
1:K:50:GLY:HA2	1:K:570:ASN:HD22	1.69	0.57
3:P:96:THR:HG22	3:P:99:ARG:HD3	1.86	0.57
1:K:16:LYS:O	3:P:221:ARG:NH1	2.37	0.56
1:H:283:MET:HG2	1:H:509:VAL:HG11	1.86	0.56
1:G:611:VAL:HG22	1:G:861:GLN:HG2	1.87	0.56
1:G:694:ARG:NH2	1:G:698:GLN:O	2.38	0.56
1:E:417:ARG:NH2	1:E:782:GLN:OE1	2.38	0.56
1:C:559:GLN:NE2	1:B:700:ALA:O	2.34	0.56
5:M:243:ASN:HB2	5:M:280:GLN:HE21	1.69	0.56
1:A:100:GLY:HA2	1:A:558:THR:HG22	1.86	0.56
1:J:111:TYR:OH	1:J:252:ASP:OD2	2.21	0.56
1:E:283:MET:HG2	1:E:509:VAL:HG11	1.87	0.56
1:B:127:ASN:HB3	1:B:192:ILE:HD13	1.86	0.56
2:R:49:LEU:HD12	2:R:70:GLY:HA2	1.86	0.56
3:P:79:GLN:HE22	3:P:224:ARG:H	1.52	0.56
3:O:79:GLN:HE22	3:O:224:ARG:H	1.52	0.56
5:M:93:LYS:HB2	5:M:435:LYS:HB3	1.86	0.56
1:A:346:ARG:NH1	1:A:476:MET:O	2.39	0.56
1:H:353:TYR:HH	1:I:205:TYR:HH	1.53	0.56
1:I:256:ALA:HB3	1:I:265:THR:HG23	1.88	0.56
1:G:291:ASN:HD21	1:G:641:THR:HG22	1.71	0.56
1:F:700:ALA:O	1:D:559:GLN:NE2	2.38	0.56
1:L:85:ASP:OD1	1:L:890:ARG:NH1	2.38	0.56
1:J:843:THR:HG23	1:J:846:GLY:H	1.70	0.56
1:F:887:GLN:HG3	1:F:893:ILE:HG22	1.88	0.56
1:E:310:ASP:HB3	1:E:597:VAL:HG13	1.87	0.56
1:C:50:GLY:HA2	1:C:570:ASN:HD22	1.70	0.56
1:A:404:ILE:HD11	1:B:797:PRO:HD3	1.88	0.56
1:K:346:ARG:NH1	1:K:476:MET:O	2.39	0.56
1:H:549:ARG:HH12	1:H:644:PRO:HA	1.71	0.56
1:A:244:ASP:OD2	1:C:798:TYR:OH	2.24	0.56
1:I:277:ARG:HH12	1:I:652:ILE:HD12	1.71	0.56
1:I:337:ALA:O	1:I:493:ARG:NH1	2.39	0.56
1:A:470:ARG:NH2	1:A:746:GLU:OE1	2.39	0.56
1:A:904:SER:O	1:K:861:GLN:NE2	2.38	0.56
1:H:778:ASN:HA	1:I:117:ASN:HD22	1.71	0.56
1:I:70:ASP:OD1	1:I:534:LYS:NZ	2.38	0.56
1:D:626:SER:HB2	1:D:876:LEU:HB2	1.87	0.56
1:D:613:ASN:HD21	2:R:11:ASN:HD21	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:ILE:HG22	1:G:248:TRP:H	1.70	0.55
1:E:504:ASP:H	1:D:817:THR:HG21	1.71	0.55
1:A:879:VAL:HG12	1:A:901:PRO:HD2	1.88	0.55
1:K:533:ARG:HG2	1:K:535:ASP:H	1.71	0.55
1:E:749:SER:OG	1:E:819:ARG:NH1	2.39	0.55
1:C:718:GLN:NE2	1:C:829:GLN:O	2.39	0.55
1:H:879:VAL:HG12	1:H:901:PRO:HD2	1.87	0.55
1:F:350:ASN:HB3	1:F:467:ILE:HA	1.89	0.55
1:B:450:TYR:OH	1:B:454:ARG:NH1	2.39	0.55
1:J:310:ASP:HB3	1:J:597:VAL:HG13	1.87	0.55
1:I:284:MET:HB3	1:I:530:TRP:HE1	1.71	0.55
2:S:97:ARG:NH1	2:Q:100:ASP:OD1	2.33	0.55
1:E:150:GLY:O	1:E:236:ARG:NH1	2.39	0.55
1:E:244:ASP:OD2	1:D:798:TYR:OH	2.23	0.55
1:C:532:PHE:HE2	1:C:560:ILE:HG21	1.72	0.55
1:A:794:CYS:HB2	1:B:171:GLY:HA2	1.88	0.55
1:K:495:GLN:NE2	1:J:351:ASP:OD1	2.40	0.55
1:C:169:GLN:HE21	1:B:773:MET:HG3	1.71	0.55
4:N:194:LEU:O	4:N:198:TRP:NE1	2.39	0.55
5:M:168:GLY:HA2	5:M:204:LEU:HD12	1.87	0.55
1:L:411:LEU:HD21	1:J:415:LEU:HD12	1.89	0.55
1:K:117:ASN:HD22	1:J:778:ASN:HA	1.72	0.55
1:J:885:ILE:HG12	1:J:895:VAL:HG12	1.88	0.55
1:H:140:ALA:HB3	1:I:399:ILE:HG22	1.87	0.55
1:E:666:GLN:NE2	1:E:865:ASP:OD1	2.40	0.55
1:C:117:ASN:HD22	1:B:778:ASN:HA	1.72	0.55
4:N:85:MET:O	4:N:89:HIS:ND1	2.38	0.55
1:A:143:PRO:O	1:A:172:GLN:NE2	2.40	0.55
1:L:57:GLN:HB2	1:L:87:ARG:HH12	1.72	0.55
1:L:346:ARG:HE	1:L:822:LEU:HD13	1.71	0.55
1:K:278:ASP:OD2	1:K:327:ARG:NH2	2.39	0.55
1:H:798:TYR:OH	1:I:244:ASP:OD2	2.25	0.55
1:I:640:ALA:HB2	2:Q:17:PRO:HD3	1.89	0.55
1:F:98:ILE:HG22	1:F:560:ILE:HG23	1.88	0.55
2:R:100:ASP:OD1	2:Q:97:ARG:NH1	2.32	0.55
1:L:563:TYR:HE2	1:K:712:LYS:HZ2	1.55	0.55
1:L:97:ASP:OD1	1:K:712:LYS:NZ	2.40	0.55
1:K:5:ARG:HG3	3:P:15:GLN:HB2	1.89	0.55
1:K:100:GLY:HA2	1:K:558:THR:HG22	1.87	0.55
1:K:104:ARG:NH2	1:K:500:GLY:O	2.40	0.55
1:I:724:ASN:HD22	1:I:837:LEU:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:701:GLU:OE2	1:D:561:ASN:ND2	2.40	0.55
1:E:735:CYS:SG	1:E:737:LYS:NZ	2.76	0.55
1:C:256:ALA:O	1:C:788:ASN:ND2	2.40	0.55
1:H:52:THR:HG21	1:G:834:SER:HB3	1.89	0.54
1:H:104:ARG:NH2	1:H:500:GLY:O	2.41	0.54
1:H:150:GLY:O	1:H:236:ARG:NH1	2.41	0.54
1:H:346:ARG:HD3	1:H:481:PRO:HB3	1.89	0.54
1:H:520:LEU:HB3	1:H:588:GLN:HE22	1.71	0.54
1:H:118:PRO:HD2	1:G:778:ASN:HB3	1.89	0.54
1:G:460:ILE:HD12	1:G:461:VAL:HG23	1.89	0.54
1:E:169:GLN:NE2	1:D:775:ILE:O	2.40	0.54
1:D:337:ALA:O	1:D:493:ARG:NH1	2.40	0.54
1:L:118:PRO:O	1:K:410:ASN:ND2	2.40	0.54
1:J:50:GLY:HA2	1:J:570:ASN:HD22	1.72	0.54
1:H:101:THR:HA	1:H:504:ASP:HA	1.89	0.54
1:I:327:ARG:HH11	1:I:338:VAL:HG21	1.71	0.54
1:E:549:ARG:NH1	1:E:646:PHE:O	2.40	0.54
1:D:13:ARG:HB3	1:D:17:GLU:HG3	1.89	0.54
1:J:337:ALA:O	1:J:493:ARG:NH1	2.40	0.54
1:H:399:ILE:HG13	1:G:228:ILE:HD13	1.89	0.54
1:L:696:ILE:HD11	1:L:818:GLU:HA	1.87	0.54
1:D:460:ILE:HD12	1:D:461:VAL:HG23	1.89	0.54
1:C:75:TYR:HB2	1:C:534:LYS:HE3	1.89	0.54
1:C:98:ILE:HG12	1:C:560:ILE:HG12	1.88	0.54
1:C:121:PRO:HG2	1:C:124:ALA:HB2	1.89	0.54
1:L:131:THR:HA	1:L:136:THR:HA	1.88	0.54
1:L:798:TYR:OH	1:J:244:ASP:OD2	2.25	0.54
1:A:563:TYR:HE2	1:C:712:LYS:HZ3	1.54	0.54
1:K:666:GLN:NE2	1:K:865:ASP:OD1	2.41	0.54
1:I:645:ASN:ND2	2:Q:18:ALA:O	2.40	0.54
1:E:309:ASN:OD1	1:C:688:ASN:ND2	2.39	0.54
2:S:252:HIS:HD2	2:S:256:GLY:HA3	1.73	0.54
2:T:252:HIS:HD2	2:T:256:GLY:HA3	1.73	0.54
2:Q:253:CYS:HB2	2:Q:296:GLY:HA2	1.90	0.54
1:K:350:ASN:OD1	1:K:416:LYS:NZ	2.36	0.54
1:G:379:GLY:H	1:G:395:THR:HG21	1.73	0.54
1:D:417:ARG:NH2	1:D:782:GLN:OE1	2.38	0.54
1:L:200:GLN:NE2	1:L:261:ASP:OD1	2.41	0.54
1:D:327:ARG:HB3	1:D:338:VAL:HG11	1.90	0.54
1:C:460:ILE:HD12	1:C:461:VAL:HG23	1.90	0.54
1:F:277:ARG:HH12	1:F:652:ILE:HD12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:253:CYS:HB2	2:S:296:GLY:HA2	1.90	0.54
2:R:253:CYS:HB2	2:R:296:GLY:HA2	1.90	0.54
1:L:549:ARG:NH1	1:L:646:PHE:O	2.40	0.53
1:K:862:PHE:HD2	1:K:873:LEU:HD11	1.72	0.53
1:J:460:ILE:HD12	1:J:461:VAL:HG23	1.89	0.53
1:I:600:LEU:HD12	2:Q:13:ILE:HD11	1.90	0.53
1:I:894:SER:HA	3:P:112:GLY:HA3	1.90	0.53
1:F:354:GLU:OE2	1:D:486:ARG:NH2	2.40	0.53
1:G:352:GLY:O	1:G:416:LYS:NZ	2.41	0.53
1:E:793:ARG:NH1	1:D:404:ILE:O	2.41	0.53
1:B:370:PRO:HB3	1:B:405:PRO:HB3	1.90	0.53
1:B:887:GLN:HG3	1:B:893:ILE:HG12	1.89	0.53
5:M:98:ASN:ND2	5:M:136:TYR:O	2.41	0.53
1:G:143:PRO:HB2	1:G:171:GLY:HA2	1.90	0.53
1:E:109:LYS:NZ	1:E:111:TYR:O	2.40	0.53
1:C:298:GLN:HB2	1:C:891:SER:HB3	1.89	0.53
1:B:520:LEU:HB3	1:B:588:GLN:HE22	1.74	0.53
2:Q:252:HIS:HD2	2:Q:256:GLY:HA3	1.73	0.53
1:H:100:GLY:HA2	1:H:558:THR:HG22	1.90	0.53
1:F:885:ILE:HG12	1:F:895:VAL:HG12	1.89	0.53
1:E:102:LEU:HD11	1:E:540:LEU:HD11	1.89	0.53
4:N:164:VAL:HG22	4:N:177:VAL:HG12	1.90	0.53
5:M:47:LEU:HB3	5:M:57:TYR:HB2	1.90	0.53
1:A:367:ILE:HG22	1:C:141:GLN:HB2	1.90	0.53
1:J:304:ILE:HG23	1:J:895:VAL:HG11	1.91	0.53
1:G:62:ARG:HG3	1:G:563:TYR:HE1	1.74	0.53
1:C:128:SER:OG	1:C:201:GLN:NE2	2.41	0.53
1:K:491:LYS:NZ	1:J:349:GLU:OE1	2.41	0.53
1:G:299:THR:O	1:G:301:GLN:NE2	2.42	0.53
1:F:167:ASN:HB3	1:F:170:VAL:HG23	1.90	0.53
1:E:346:ARG:NH2	1:E:477:ASP:O	2.41	0.53
1:E:718:GLN:NE2	1:E:829:GLN:O	2.39	0.53
2:R:252:HIS:HD2	2:R:256:GLY:HA3	1.73	0.53
1:A:613:ASN:OD1	1:A:859:ASN:ND2	2.40	0.53
1:L:118:PRO:HD2	1:K:778:ASN:HB3	1.91	0.53
1:H:89:VAL:HG22	1:H:521:LEU:HB2	1.90	0.53
1:H:815:GLN:HE21	1:I:502:TYR:H	1.56	0.53
1:B:722:SER:OG	1:B:829:GLN:NE2	2.41	0.53
1:A:537:ASN:HD22	1:A:649:SER:HB3	1.74	0.53
1:A:603:ILE:HG12	1:A:610:VAL:HG21	1.91	0.53
1:L:640:ALA:HB2	2:R:17:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:417:ARG:NH2	1:J:782:GLN:OE1	2.41	0.53
1:F:121:PRO:HG2	1:F:124:ALA:HB2	1.90	0.53
1:B:637:ARG:HB3	5:M:46:ASN:HD21	1.74	0.53
1:B:879:VAL:HG12	1:B:901:PRO:HD2	1.90	0.53
1:I:549:ARG:NH1	1:I:646:PHE:O	2.41	0.53
1:B:85:ASP:OD1	1:B:890:ARG:NH1	2.42	0.53
2:T:253:CYS:HB2	2:T:296:GLY:HA2	1.90	0.53
1:A:205:TYR:OH	1:C:353:TYR:OH	2.26	0.53
1:A:350:ASN:OD1	1:A:416:LYS:NZ	2.42	0.53
1:A:495:GLN:NE2	1:C:351:ASP:OD1	2.42	0.53
1:K:677:PRO:HG2	1:K:680:GLY:HA3	1.91	0.53
1:G:887:GLN:HG2	1:G:893:ILE:HG22	1.90	0.53
1:F:718:GLN:NE2	1:F:829:GLN:O	2.42	0.53
1:C:617:ARG:NH2	1:C:901:PRO:O	2.41	0.53
1:K:310:ASP:HB3	1:K:597:VAL:HG13	1.92	0.52
1:H:611:VAL:HG22	1:H:861:GLN:HG2	1.90	0.52
1:F:205:TYR:HH	1:E:353:TYR:HH	1.57	0.52
1:F:353:TYR:HB2	1:F:412:PRO:HB2	1.91	0.52
2:S:332:THR:HB	2:S:335:LEU:HD13	1.92	0.52
2:T:330:GLU:HA	2:T:352:PHE:HB2	1.92	0.52
1:H:97:ASP:OD1	1:G:712:LYS:NZ	2.42	0.52
1:I:98:ILE:HG22	1:I:560:ILE:HG23	1.90	0.52
1:K:414:ASN:HB3	1:J:359:ASN:HD22	1.75	0.52
1:K:582:ARG:NH1	1:K:889:THR:O	2.41	0.52
1:J:70:ASP:OD1	1:J:534:LYS:NZ	2.40	0.52
1:A:199:GLY:HA3	1:A:248:TRP:HB2	1.91	0.52
1:K:144:GLN:NE2	1:K:170:VAL:O	2.42	0.52
1:H:174:ASN:HD21	1:G:783:GLN:HE22	1.55	0.52
1:H:511:GLN:NE2	1:H:528:TYR:OH	2.41	0.52
1:A:310:ASP:HB3	1:A:597:VAL:HG13	1.92	0.52
1:K:283:MET:HG2	1:K:509:VAL:HG11	1.91	0.52
1:E:797:PRO:HD3	1:D:404:ILE:HD11	1.91	0.52
1:K:718:GLN:NE2	1:K:829:GLN:O	2.42	0.52
1:H:102:LEU:HD11	1:H:540:LEU:HD11	1.91	0.52
1:E:331:PHE:HB3	1:E:336:GLN:HB3	1.92	0.52
1:C:277:ARG:HE	1:C:541:GLN:HB2	1.75	0.52
5:M:307:ASP:HA	5:M:351:GLN:HE22	1.75	0.52
1:A:205:TYR:HH	1:C:353:TYR:HH	1.51	0.52
1:H:144:GLN:HB2	1:H:189:LEU:HB3	1.92	0.52
1:G:24:VAL:HG12	1:G:28:GLN:HE22	1.74	0.52
1:G:381:THR:HB	1:G:390:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ARG:H	1:E:589:ASN:HB2	1.73	0.52
1:C:118:PRO:HD2	1:B:778:ASN:HB3	1.92	0.52
2:R:330:GLU:HA	2:R:352:PHE:HB2	1.92	0.52
1:A:102:LEU:HD11	1:A:540:LEU:HD11	1.92	0.52
1:L:186:ASN:O	1:L:236:ARG:NH2	2.42	0.52
1:L:722:SER:OG	1:L:829:GLN:NE2	2.43	0.52
1:J:520:LEU:HB3	1:J:588:GLN:HE22	1.75	0.52
1:C:168:PRO:HG3	1:C:191:ARG:HD3	1.92	0.52
1:A:277:ARG:HH12	1:A:652:ILE:HD12	1.75	0.52
1:A:301:GLN:NE2	1:L:60:GLN:O	2.43	0.52
1:L:98:ILE:HG22	1:L:560:ILE:HG23	1.92	0.52
1:F:67:GLN:HE21	1:F:78:ARG:HE	1.58	0.52
1:F:798:TYR:OH	1:D:244:ASP:OD2	2.24	0.52
1:E:106:PRO:HD2	1:E:551:ASP:HB2	1.92	0.52
1:I:778:ASN:HB3	1:G:118:PRO:HD2	1.92	0.51
1:I:798:TYR:OH	1:G:244:ASP:OD2	2.24	0.51
1:C:737:LYS:O	1:C:743:ASN:ND2	2.38	0.51
2:R:332:THR:HB	2:R:335:LEU:HD13	1.92	0.51
4:N:177:VAL:O	4:N:183:ASN:ND2	2.40	0.51
4:N:189:SER:OG	4:N:218:ASN:ND2	2.43	0.51
1:J:613:ASN:OD1	1:J:859:ASN:ND2	2.42	0.51
1:I:668:CYS:SG	1:I:669:SER:N	2.83	0.51
1:E:73:ASN:ND2	1:E:642:GLN:OE1	2.43	0.51
1:B:662:SER:O	1:B:828:TRP:NE1	2.34	0.51
2:S:330:GLU:HA	2:S:352:PHE:HB2	1.92	0.51
1:L:41:ARG:H	1:K:589:ASN:HB2	1.75	0.51
1:H:843:THR:HG23	1:H:846:GLY:H	1.74	0.51
1:F:346:ARG:HD3	1:F:481:PRO:HB3	1.91	0.51
1:D:163:GLY:O	1:D:191:ARG:NH1	2.43	0.51
1:L:502:TYR:H	1:K:815:GLN:HE21	1.59	0.51
1:G:160:GLN:HB3	2:S:91:THR:HG22	1.91	0.51
1:F:725:GLN:NE2	1:F:731:ASN:O	2.43	0.51
1:D:310:ASP:HB3	1:D:597:VAL:HG13	1.91	0.51
2:R:151:PHE:HE2	2:R:167:ILE:HD11	1.76	0.51
5:M:180:ARG:HD2	5:M:245:PRO:HG3	1.92	0.51
1:A:118:PRO:HD2	1:C:778:ASN:HB3	1.93	0.51
1:L:379:GLY:HA2	1:K:228:ILE:HA	1.91	0.51
1:H:337:ALA:O	1:H:493:ARG:NH1	2.44	0.51
1:G:347:ILE:HA	1:G:472:SER:HB3	1.92	0.51
1:D:725:GLN:NE2	1:D:731:ASN:OD1	2.43	0.51
2:S:151:PHE:HE2	2:S:167:ILE:HD11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:97:ASP:OD1	1:J:712:LYS:NZ	2.40	0.51
1:E:118:PRO:HD2	1:D:778:ASN:HB3	1.92	0.51
1:E:367:ILE:HD13	1:D:139:VAL:HG23	1.92	0.51
1:B:131:THR:HA	1:B:136:THR:HA	1.91	0.51
1:B:308:LEU:HD22	5:M:73:THR:HG23	1.92	0.51
1:A:231:THR:HG21	1:A:236:ARG:HD3	1.93	0.51
1:E:337:ALA:O	1:E:493:ARG:NH1	2.44	0.51
1:E:737:LYS:O	1:E:743:ASN:ND2	2.44	0.51
1:D:156:ALA:O	1:D:225:LYS:NZ	2.43	0.51
1:D:99:LYS:HD3	1:D:559:GLN:HE21	1.75	0.51
1:D:613:ASN:OD1	1:D:859:ASN:ND2	2.38	0.51
1:C:384:GLU:HG2	1:B:157:ILE:HD11	1.93	0.51
1:B:537:ASN:HD22	1:B:649:SER:HB3	1.75	0.51
2:R:83:ILE:HG22	2:R:84:LEU:HB2	1.93	0.51
2:Q:330:GLU:HA	2:Q:352:PHE:HB2	1.92	0.51
5:M:180:ARG:NH2	5:M:280:GLN:OE1	2.42	0.51
1:H:163:GLY:O	1:H:191:ARG:NH1	2.44	0.51
1:E:559:GLN:OE1	1:E:561:ASN:ND2	2.44	0.51
1:E:664:THR:HB	1:E:865:ASP:HB2	1.93	0.51
1:D:885:ILE:HG12	1:D:895:VAL:HG12	1.92	0.51
2:Q:83:ILE:HG22	2:Q:84:LEU:HB2	1.93	0.51
2:Q:332:THR:HB	2:Q:335:LEU:HD13	1.92	0.51
1:H:117:ASN:HD22	1:G:778:ASN:HA	1.75	0.51
1:F:141:GLN:HB2	1:D:367:ILE:HG22	1.92	0.51
1:F:273:TYR:OH	1:E:351:ASP:OD1	2.29	0.51
1:C:879:VAL:HG12	1:C:901:PRO:HD2	1.93	0.51
2:T:83:ILE:HG22	2:T:84:LEU:HB2	1.93	0.51
2:T:151:PHE:HE2	2:T:167:ILE:HD11	1.76	0.51
4:N:169:SER:OG	4:N:172:ASP:OD1	2.29	0.51
1:K:277:ARG:HH12	1:K:652:ILE:HD12	1.76	0.50
1:H:410:ASN:ND2	1:I:118:PRO:O	2.37	0.50
1:F:520:LEU:HB3	1:F:588:GLN:HE22	1.76	0.50
1:E:117:ASN:HD22	1:D:778:ASN:HA	1.75	0.50
1:D:705:THR:HG22	1:D:712:LYS:HD3	1.93	0.50
1:B:718:GLN:NE2	1:B:829:GLN:O	2.44	0.50
1:H:630:LEU:O	1:H:872:TYR:N	2.44	0.50
1:H:645:ASN:ND2	2:T:18:ALA:O	2.44	0.50
1:I:347:ILE:HD13	1:I:472:SER:HB3	1.92	0.50
1:F:327:ARG:HB3	1:F:338:VAL:HG21	1.94	0.50
2:Q:151:PHE:HE2	2:Q:167:ILE:HD11	1.76	0.50
1:G:310:ASP:HB2	1:G:899:ARG:HH22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ASP:OD1	1:C:493:ARG:NH2	2.45	0.50
1:C:611:VAL:HG22	1:C:861:GLN:HG2	1.92	0.50
1:A:52:THR:HG21	1:C:834:SER:HB3	1.92	0.50
1:J:168:PRO:HG3	1:J:191:ARG:HD3	1.93	0.50
1:D:704:ASP:O	1:D:712:LYS:NZ	2.44	0.50
1:B:145:THR:HA	1:B:188:GLY:HA2	1.92	0.50
1:A:885:ILE:HD11	1:A:893:ILE:HD11	1.94	0.50
1:J:13:ARG:HB3	1:J:17:GLU:HG3	1.94	0.50
1:G:109:LYS:NZ	1:G:111:TYR:O	2.35	0.50
1:F:725:GLN:HE21	1:F:731:ASN:H	1.59	0.50
1:E:100:GLY:HA2	1:E:558:THR:HG22	1.94	0.50
1:D:284:MET:HB3	1:D:530:TRP:HE1	1.77	0.50
1:L:236:ARG:NH1	1:L:238:SER:OG	2.44	0.50
1:L:704:ASP:H	1:L:712:LYS:HE3	1.75	0.50
1:J:352:GLY:O	1:J:416:LYS:NZ	2.43	0.50
1:G:314:GLU:OE2	1:G:512:LYS:NZ	2.43	0.50
1:D:318:GLN:HG3	1:D:656:ASP:HA	1.94	0.50
1:K:109:LYS:NZ	1:K:111:TYR:O	2.43	0.50
1:H:495:GLN:NE2	1:G:351:ASP:OD1	2.45	0.50
1:G:13:ARG:HB3	1:G:17:GLU:HG3	1.94	0.50
1:G:381:THR:HG1	1:G:392:THR:HG1	1.60	0.50
1:G:879:VAL:HG12	1:G:901:PRO:HD2	1.93	0.50
1:E:287:ASN:HA	1:E:307:ASP:HB3	1.93	0.50
1:E:308:LEU:HD11	3:O:109:GLN:HE22	1.77	0.50
1:D:438:ASN:HD21	2:S:58:LYS:HB3	1.75	0.50
1:B:201:GLN:NE2	1:B:261:ASP:O	2.45	0.50
1:J:260:ASP:HB3	1:J:263:ARG:HB2	1.93	0.50
1:I:143:PRO:O	1:I:172:GLN:NE2	2.44	0.50
1:D:62:ARG:HG3	1:D:563:TYR:HE1	1.77	0.50
1:C:477:ASP:OD2	1:C:820:LYS:NZ	2.37	0.50
1:C:346:ARG:HD3	1:C:481:PRO:HB3	1.94	0.50
1:B:91:LEU:HD12	1:B:519:LEU:HB3	1.94	0.50
1:B:377:GLY:N	1:B:397:ALA:O	2.42	0.50
5:M:275:SER:HB3	5:M:278:LYS:HB2	1.94	0.50
1:A:64:VAL:O	1:E:67:GLN:NE2	2.45	0.49
1:L:537:ASN:HD22	1:L:649:SER:HB3	1.77	0.49
1:I:673:ASP:HA	1:I:857:SER:HB2	1.94	0.49
1:D:843:THR:HG23	1:D:846:GLY:H	1.77	0.49
1:C:377:GLY:HA2	1:C:397:ALA:H	1.77	0.49
1:C:619:TRP:HB2	1:C:849:VAL:HG11	1.93	0.49
1:B:905:GLY:HA2	5:M:75:THR:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:83:ILE:HG22	2:S:84:LEU:HB2	1.93	0.49
2:T:332:THR:HB	2:T:335:LEU:HD13	1.92	0.49
1:I:783:GLN:NE2	1:I:792:GLU:O	2.45	0.49
1:F:353:TYR:HH	1:D:205:TYR:HH	1.58	0.49
1:E:107:SER:O	1:E:272:ASN:ND2	2.45	0.49
1:E:614:ILE:HB	1:E:858:LEU:HB3	1.94	0.49
2:S:100:ASP:OD1	2:R:97:ARG:NH1	2.39	0.49
1:A:379:GLY:HA2	1:C:228:ILE:HG22	1.94	0.49
1:L:91:LEU:HD13	1:L:521:LEU:HD13	1.94	0.49
1:I:182:ASN:ND2	1:I:185:ASN:OD1	2.45	0.49
1:C:490:LEU:HB2	1:C:493:ARG:HH21	1.78	0.49
1:K:520:LEU:HB3	1:K:588:GLN:HE22	1.78	0.49
1:I:339:ASP:HA	1:I:487:ASN:HD21	1.78	0.49
1:I:762:LEU:HD12	1:I:774:PRO:HB2	1.92	0.49
5:M:22:TYR:HD2	5:M:25:ILE:HG12	1.76	0.49
5:M:271:VAL:HG12	5:M:281:THR:HG22	1.94	0.49
1:H:297:SER:HA	1:H:526:TYR:HA	1.94	0.49
1:I:131:THR:HA	1:I:136:THR:HA	1.95	0.49
1:I:349:GLU:OE1	1:G:491:LYS:NZ	2.46	0.49
1:I:778:ASN:HA	1:G:117:ASN:HD22	1.75	0.49
1:E:346:ARG:NH1	1:E:476:MET:O	2.45	0.49
1:B:53:THR:HB	1:B:570:ASN:HA	1.93	0.49
1:B:885:ILE:HG12	1:B:895:VAL:HG12	1.93	0.49
1:A:108:PHE:O	1:C:807:SER:OG	2.31	0.49
1:L:249:GLU:OE1	1:K:810:ASN:ND2	2.45	0.49
1:J:792:GLU:HG3	1:J:793:ARG:HD3	1.93	0.49
1:H:208:TYR:HB3	1:H:251:PRO:HD2	1.94	0.49
1:F:362:PHE:O	1:D:408:GLU:N	2.40	0.49
1:C:128:SER:H	1:C:139:VAL:HG13	1.78	0.49
1:C:417:ARG:NH2	1:C:782:GLN:OE1	2.38	0.49
4:N:179:ILE:O	4:N:183:ASN:ND2	2.45	0.49
5:M:320:PRO:HG2	5:M:419:ARG:HD3	1.94	0.49
1:A:91:LEU:HD12	1:A:519:LEU:HB3	1.93	0.49
1:A:246:ILE:HG22	1:A:248:TRP:H	1.78	0.49
1:A:843:THR:HG23	1:A:846:GLY:H	1.77	0.49
1:H:885:ILE:HD11	1:H:893:ILE:HD11	1.95	0.49
1:L:367:ILE:HG22	1:K:141:GLN:HB2	1.95	0.49
1:K:696:ILE:HD13	1:K:819:ARG:HH11	1.76	0.49
1:K:885:ILE:HD11	1:K:893:ILE:HD11	1.95	0.49
1:J:611:VAL:HG22	1:J:861:GLN:HG2	1.95	0.49
1:E:522:LEU:HD12	1:E:887:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:666:GLN:HA	1:E:693:LYS:H	1.76	0.49
1:B:106:PRO:HD3	1:B:501:ARG:HH21	1.77	0.49
4:N:129:LEU:HG	4:N:158:VAL:HG21	1.95	0.49
1:E:879:VAL:HG12	1:E:901:PRO:HD2	1.94	0.49
1:B:783:GLN:HE21	1:B:784:LYS:HG2	1.78	0.49
2:S:195:PHE:HB2	2:S:216:ALA:HA	1.95	0.49
1:L:107:SER:O	1:L:272:ASN:ND2	2.46	0.49
1:L:126:ILE:HD11	1:L:248:TRP:HH2	1.77	0.49
1:D:304:ILE:HG23	1:D:895:VAL:HG11	1.94	0.49
1:D:548:LEU:HD12	1:D:553:ALA:HB2	1.94	0.49
1:L:10:ILE:HG22	1:K:842:LEU:HD12	1.94	0.48
1:J:722:SER:OG	1:J:829:GLN:NE2	2.46	0.48
1:D:96:PHE:HB2	1:D:509:VAL:HG22	1.94	0.48
2:S:171:ARG:NH2	2:R:135:THR:OG1	2.36	0.48
5:M:192:TYR:OH	5:M:245:PRO:O	2.30	0.48
5:M:216:ILE:HA	5:M:219:MET:HG3	1.94	0.48
1:A:228:ILE:HA	1:B:379:GLY:HA2	1.94	0.48
1:E:500:GLY:H	1:D:751:GLN:HE21	1.61	0.48
1:L:353:TYR:HB2	1:L:412:PRO:HB2	1.93	0.48
1:J:668:CYS:HB3	1:J:690:PHE:HB2	1.96	0.48
1:F:131:THR:HA	1:F:136:THR:HA	1.95	0.48
1:F:778:ASN:HA	1:D:117:ASN:HD22	1.77	0.48
1:D:168:PRO:HG3	1:D:191:ARG:HD3	1.95	0.48
1:C:19:LEU:HD13	1:C:23:LEU:HD12	1.95	0.48
2:R:195:PHE:HB2	2:R:216:ALA:HA	1.95	0.48
5:M:36:ILE:HD11	5:M:438:ALA:HB3	1.94	0.48
1:A:39:LYS:NZ	1:C:518:ASN:O	2.46	0.48
1:A:691:GLU:OE1	1:A:694:ARG:NH2	2.44	0.48
1:G:143:PRO:O	1:G:172:GLN:NE2	2.46	0.48
1:F:522:LEU:HB2	1:F:887:GLN:HG2	1.95	0.48
1:D:297:SER:HA	1:D:526:TYR:HA	1.94	0.48
1:D:350:ASN:ND2	1:D:465:THR:O	2.38	0.48
5:M:54:SER:OG	5:M:422:LEU:O	2.27	0.48
5:M:75:THR:HG22	5:M:415:THR:HA	1.94	0.48
1:L:630:LEU:O	1:L:872:TYR:N	2.46	0.48
1:H:778:ASN:HB3	1:I:118:PRO:HD2	1.96	0.48
1:F:682:ASP:HA	1:F:687:PRO:HB3	1.95	0.48
1:C:283:MET:HG2	1:C:509:VAL:HG11	1.95	0.48
1:C:662:SER:O	1:C:828:TRP:NE1	2.35	0.48
2:T:195:PHE:HB2	2:T:216:ALA:HA	1.95	0.48
1:L:281:ILE:HG21	1:L:655:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:GLN:NE2	1:H:170:VAL:O	2.46	0.48
1:I:141:GLN:HE21	1:G:367:ILE:HA	1.79	0.48
1:G:287:ASN:ND2	1:G:307:ASP:OD1	2.46	0.48
1:G:612:VAL:HG22	1:G:860:MET:HB2	1.95	0.48
1:F:287:ASN:HA	1:F:307:ASP:HB3	1.94	0.48
1:D:629:ARG:HD3	1:D:664:THR:HG23	1.94	0.48
1:C:537:ASN:HD22	1:C:649:SER:HB3	1.78	0.48
1:I:362:PHE:O	1:G:408:GLU:N	2.36	0.48
1:G:471:TRP:CE2	1:G:750:ARG:HG2	2.49	0.48
1:E:314:GLU:HG3	1:E:655:LEU:HD22	1.94	0.48
2:Q:195:PHE:HB2	2:Q:216:ALA:HA	1.95	0.48
1:A:181:VAL:HB	1:B:401:TYR:HB3	1.95	0.48
1:A:228:ILE:HD13	1:B:399:ILE:HD13	1.95	0.48
1:K:623:ARG:HD3	1:K:880:PHE:HE1	1.78	0.48
1:B:417:ARG:NH2	1:B:782:GLN:OE1	2.47	0.48
1:H:200:GLN:O	1:H:248:TRP:NE1	2.46	0.48
1:I:327:ARG:HD2	1:I:338:VAL:HG11	1.94	0.48
1:I:751:GLN:HG3	1:I:817:THR:HG22	1.96	0.48
1:L:778:ASN:HA	1:J:117:ASN:HD22	1.78	0.48
1:K:894:SER:HB3	3:O:35:ALA:HA	1.95	0.48
1:H:230:THR:HG22	1:I:377:GLY:HA3	1.96	0.48
1:H:748:MET:SD	1:H:820:LYS:NZ	2.83	0.48
1:G:182:ASN:ND2	1:G:185:ASN:OD1	2.46	0.48
1:A:150:GLY:O	1:A:236:ARG:NH1	2.46	0.47
1:A:623:ARG:HD3	1:A:880:PHE:HE1	1.79	0.47
1:L:518:ASN:HB3	1:J:39:LYS:HE2	1.95	0.47
1:L:619:TRP:HB2	1:L:849:VAL:HG11	1.96	0.47
1:K:256:ALA:O	1:K:788:ASN:ND2	2.47	0.47
1:K:383:ASN:OD1	1:K:386:GLN:NE2	2.47	0.47
1:G:345:VAL:HG11	1:G:484:HIS:HE2	1.79	0.47
1:G:347:ILE:HG21	1:G:470:ARG:HE	1.79	0.47
1:F:637:ARG:NH2	1:F:872:TYR:OH	2.47	0.47
1:B:640:ALA:H	5:M:46:ASN:HD22	1.62	0.47
1:L:417:ARG:NH2	1:L:782:GLN:OE1	2.47	0.47
1:I:611:VAL:HG22	1:I:861:GLN:HG3	1.96	0.47
1:F:533:ARG:HH22	1:F:638:ILE:HG23	1.78	0.47
1:E:205:TYR:HH	1:D:353:TYR:HH	1.53	0.47
1:C:346:ARG:NH1	1:C:476:MET:O	2.46	0.47
1:B:611:VAL:HG22	1:B:861:GLN:HG2	1.96	0.47
1:A:346:ARG:NH2	1:A:477:ASP:O	2.42	0.47
1:K:169:GLN:NE2	1:J:775:ILE:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:ASN:ND2	1:H:642:GLN:OE1	2.47	0.47
1:I:287:ASN:HA	1:I:307:ASP:HB3	1.96	0.47
1:F:387:GLN:HG2	1:E:154:THR:HB	1.96	0.47
2:R:253:CYS:O	2:R:258:ASN:ND2	2.48	0.47
1:K:118:PRO:HD2	1:J:778:ASN:HB3	1.96	0.47
1:H:520:LEU:HB2	1:I:39:LYS:HE2	1.96	0.47
1:I:470:ARG:NH2	1:I:746:GLU:OE2	2.47	0.47
1:D:331:PHE:HB3	1:D:336:GLN:HB3	1.97	0.47
5:M:370:ASN:O	5:M:372:THR:OG1	2.28	0.47
1:F:590:PHE:H	1:F:883:VAL:HG22	1.79	0.47
1:D:98:ILE:HG13	1:D:560:ILE:HG12	1.97	0.47
2:T:253:CYS:O	2:T:258:ASN:ND2	2.48	0.47
1:K:108:PHE:O	1:J:807:SER:OG	2.33	0.47
1:K:117:ASN:HA	1:J:778:ASN:HB3	1.97	0.47
1:H:109:LYS:NZ	1:H:111:TYR:O	2.44	0.47
1:H:421:TYR:HA	1:H:425:ALA:HB3	1.96	0.47
1:D:1:MET:SD	1:D:1:MET:N	2.73	0.47
1:D:183:THR:O	1:D:236:ARG:NH1	2.47	0.47
1:C:489:GLY:O	1:C:493:ARG:N	2.40	0.47
1:B:630:LEU:O	1:B:872:TYR:N	2.41	0.47
2:Q:97:ARG:HG2	2:Q:135:THR:HB	1.97	0.47
1:A:753:PRO:HD3	1:A:806:LEU:HD21	1.96	0.47
1:K:788:ASN:O	1:K:790:LEU:N	2.48	0.47
1:J:471:TRP:CE2	1:J:750:ARG:HG2	2.49	0.47
1:H:346:ARG:NH2	1:H:477:ASP:O	2.44	0.47
1:I:417:ARG:NH2	1:I:782:GLN:OE1	2.44	0.47
1:E:166:PRO:HG2	1:E:191:ARG:HH11	1.79	0.47
1:E:885:ILE:HD11	1:E:893:ILE:HD11	1.96	0.47
1:C:668:CYS:HB3	1:C:690:PHE:HB2	1.97	0.47
1:B:531:TYR:OH	5:M:334:THR:O	2.32	0.47
1:B:637:ARG:HH22	1:B:645:ASN:HB2	1.79	0.47
1:B:719:MET:HG3	1:B:725:GLN:HB2	1.96	0.47
2:Q:253:CYS:O	2:Q:258:ASN:ND2	2.48	0.47
1:A:712:LYS:HZ3	1:B:563:TYR:HE2	1.62	0.47
1:A:744:ASN:ND2	1:A:824:ASP:O	2.47	0.47
1:L:409:MET:HB3	1:K:361:ALA:HA	1.96	0.47
1:K:714:PHE:HE1	1:K:830:ILE:HD11	1.79	0.47
1:K:885:ILE:HB	1:K:895:VAL:HG12	1.97	0.47
1:J:589:ASN:HB3	1:J:884:VAL:HG12	1.97	0.47
1:H:600:LEU:HD12	2:T:13:ILE:HD11	1.97	0.47
1:F:783:GLN:NE2	1:F:792:GLU:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:HG	1:D:566:PHE:HE2	1.78	0.47
1:D:200:GLN:NE2	1:D:261:ASP:OD1	2.48	0.47
2:S:171:ARG:HH22	2:R:135:THR:HG1	1.57	0.47
2:S:253:CYS:O	2:S:258:ASN:ND2	2.48	0.47
5:M:17:ARG:HH12	5:M:449:THR:HG21	1.80	0.47
1:K:150:GLY:O	1:K:236:ARG:NH1	2.47	0.47
1:J:693:LYS:HB2	1:J:709:ASN:HB3	1.97	0.47
1:H:381:THR:HG23	1:H:392:THR:HB	1.96	0.47
1:H:772:THR:HG23	1:H:774:PRO:HD3	1.96	0.47
1:E:277:ARG:HH12	1:E:652:ILE:HD12	1.80	0.47
1:D:466:ASP:HB3	1:D:469:ALA:HB3	1.95	0.47
1:D:625:TRP:HD1	1:D:875:LEU:HD21	1.80	0.47
2:R:126:ILE:HB	2:R:149:VAL:HG12	1.97	0.47
1:K:379:GLY:HA2	1:J:228:ILE:HA	1.97	0.47
1:K:614:ILE:HB	1:K:858:LEU:HB3	1.97	0.47
1:H:310:ASP:HB3	1:H:597:VAL:HG13	1.97	0.47
1:H:725:GLN:NE2	1:H:731:ASN:OD1	2.48	0.47
1:I:532:PHE:HE2	1:I:560:ILE:HG21	1.79	0.47
1:F:409:MET:HB3	1:E:361:ALA:HA	1.95	0.47
1:E:62:ARG:NH1	1:E:563:TYR:OH	2.47	0.47
1:E:408:GLU:HB2	1:D:364:PRO:HG3	1.97	0.47
1:D:381:THR:HB	1:D:390:ALA:HB3	1.96	0.47
1:C:670:ILE:HG12	1:C:860:MET:HG2	1.95	0.47
2:S:97:ARG:HG2	2:S:135:THR:HB	1.97	0.47
1:A:67:GLN:O	1:A:76:LYS:NZ	2.49	0.46
1:D:693:LYS:HB2	1:D:709:ASN:HB3	1.96	0.46
1:C:284:MET:HB3	1:C:530:TRP:HE1	1.80	0.46
1:B:477:ASP:OD2	1:B:663:HIS:NE2	2.41	0.46
1:A:491:LYS:NZ	1:C:349:GLU:OE1	2.48	0.46
1:K:668:CYS:O	1:K:690:PHE:N	2.49	0.46
1:F:126:ILE:HD11	1:F:248:TRP:HH2	1.80	0.46
2:T:90:ARG:NH1	2:T:153:GLU:OE2	2.39	0.46
2:T:97:ARG:HG2	2:T:135:THR:HB	1.96	0.46
1:K:499:ASN:ND2	1:J:466:ASP:OD1	2.47	0.46
1:I:85:ASP:OD1	1:I:890:ARG:NH1	2.48	0.46
1:E:165:ASP:OD1	2:R:93:LYS:NZ	2.47	0.46
1:D:182:ASN:O	1:D:186:ASN:N	2.47	0.46
1:C:626:SER:HB2	1:C:876:LEU:HB2	1.96	0.46
1:B:236:ARG:NH1	1:B:238:SER:OG	2.48	0.46
1:B:301:GLN:NE2	5:M:332:ASN:OD1	2.49	0.46
2:S:126:ILE:HB	2:S:149:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:748:MET:HE3	1:L:820:LYS:HG3	1.98	0.46
1:J:256:ALA:O	1:J:788:ASN:ND2	2.48	0.46
1:I:342:ASP:OD2	1:I:486:ARG:NE	2.48	0.46
1:I:662:SER:O	1:I:828:TRP:NE1	2.41	0.46
1:G:751:GLN:HG2	1:G:817:THR:HG22	1.97	0.46
1:E:278:ASP:OD2	1:E:327:ARG:NH2	2.48	0.46
1:C:118:PRO:O	1:B:410:ASN:ND2	2.47	0.46
2:R:97:ARG:HG2	2:R:135:THR:HB	1.97	0.46
1:A:152:GLY:HA3	1:A:237:VAL:H	1.80	0.46
1:A:628:THR:HG23	1:A:827:LEU:HA	1.98	0.46
1:A:827:LEU:HD21	1:A:876:LEU:HD12	1.98	0.46
1:L:578:GLU:OE2	1:L:582:ARG:NE	2.38	0.46
1:H:244:ASP:OD2	1:G:798:TYR:OH	2.33	0.46
1:H:773:MET:HB2	1:I:167:ASN:HD21	1.81	0.46
1:I:253:ALA:HA	1:I:268:GLY:HA2	1.97	0.46
1:I:753:PRO:HD3	1:I:806:LEU:HD21	1.97	0.46
1:F:70:ASP:OD1	1:F:534:LYS:NZ	2.41	0.46
2:T:126:ILE:HB	2:T:149:VAL:HG12	1.97	0.46
1:A:229:ASN:HB2	1:B:380:MET:HE1	1.97	0.46
1:A:294:SER:HA	1:A:303:ASN:HD21	1.81	0.46
1:I:284:MET:SD	1:I:530:TRP:NE1	2.89	0.46
1:D:102:LEU:HD11	1:D:540:LEU:HD21	1.97	0.46
2:R:90:ARG:NH1	2:R:153:GLU:OE2	2.39	0.46
1:J:327:ARG:HB3	1:J:338:VAL:HG11	1.97	0.46
1:H:708:SER:HB3	1:H:747:PRO:HB3	1.98	0.46
2:R:171:ARG:NH2	2:Q:135:THR:OG1	2.37	0.46
1:A:78:ARG:NH2	1:A:527:ASN:OD1	2.47	0.46
1:A:289:GLY:O	1:K:694:ARG:NH2	2.49	0.46
1:K:367:ILE:HG22	1:J:141:GLN:HB2	1.97	0.46
1:I:353:TYR:HB2	1:I:412:PRO:HB2	1.97	0.46
1:I:673:ASP:HB3	1:I:857:SER:H	1.80	0.46
1:C:169:GLN:HA	1:B:795:GLY:HA3	1.97	0.46
5:M:150:VAL:HB	5:M:377:ARG:HH21	1.81	0.46
1:A:751:GLN:HE22	1:B:498:GLY:HA3	1.81	0.46
1:F:714:PHE:HE1	1:F:830:ILE:HD11	1.81	0.46
1:E:491:LYS:NZ	1:D:349:GLU:OE1	2.49	0.46
1:B:522:LEU:HD12	1:B:887:GLN:HB2	1.97	0.46
1:L:61:LEU:HB2	1:L:566:PHE:HE2	1.81	0.46
1:H:559:GLN:HE22	1:H:561:ASN:ND2	2.13	0.46
1:G:532:PHE:HE2	1:G:560:ILE:HG21	1.81	0.46
1:C:205:TYR:HB3	1:C:266:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:466:ASP:OD1	1:D:499:ASN:ND2	2.49	0.45
1:F:511:GLN:OE1	1:F:528:TYR:OH	2.33	0.45
1:F:719:MET:HG3	1:F:725:GLN:HB3	1.98	0.45
1:D:283:MET:HG2	1:D:509:VAL:HG11	1.99	0.45
1:C:318:GLN:HG3	1:C:656:ASP:HA	1.98	0.45
1:B:306:LEU:H	1:B:897:TYR:HE2	1.63	0.45
1:I:257:ASP:HB2	1:I:265:THR:HG22	1.98	0.45
1:G:50:GLY:HA2	1:G:570:ASN:HD22	1.82	0.45
1:E:783:GLN:NE2	1:E:792:GLU:O	2.48	0.45
1:D:595:GLY:O	1:D:623:ARG:NH2	2.49	0.45
1:C:350:ASN:ND2	1:C:465:THR:O	2.43	0.45
1:L:496:LEU:HD23	1:K:707:GLN:HE21	1.81	0.45
1:H:277:ARG:HH12	1:H:652:ILE:HD12	1.81	0.45
1:A:69:GLU:HB3	1:A:76:LYS:HB3	1.97	0.45
1:A:511:GLN:NE2	1:A:528:TYR:OH	2.41	0.45
1:A:666:GLN:NE2	1:A:865:ASP:OD1	2.49	0.45
1:J:159:GLN:HE22	2:R:109:THR:HG21	1.81	0.45
1:B:297:SER:OG	1:B:300:GLN:O	2.33	0.45
1:B:619:TRP:HA	1:B:901:PRO:HB3	1.98	0.45
5:M:57:TYR:OH	5:M:419:ARG:NH1	2.50	0.45
5:M:138:VAL:HB	5:M:308:ILE:HD11	1.99	0.45
1:A:106:PRO:HD2	1:A:551:ASP:HB2	1.99	0.45
1:A:470:ARG:N	1:B:495:GLN:OE1	2.49	0.45
1:L:580:MET:O	1:L:586:ASN:ND2	2.45	0.45
1:K:668:CYS:HB3	1:K:690:PHE:HB2	1.97	0.45
1:H:668:CYS:HG	1:H:862:PHE:HE1	1.64	0.45
1:E:148:ALA:O	1:E:236:ARG:NH2	2.41	0.45
1:E:416:LYS:HE2	1:E:420:LEU:HD11	1.97	0.45
1:A:724:ASN:HD22	1:A:837:LEU:HD22	1.82	0.45
1:I:142:LEU:HD13	1:I:188:GLY:HA3	1.98	0.45
1:E:147:ALA:HA	1:E:186:ASN:HD22	1.82	0.45
4:N:63:LEU:HD21	4:N:84:LEU:HD12	1.97	0.45
1:A:300:GLN:HG3	1:L:63:VAL:HG23	1.99	0.45
1:K:664:THR:HB	1:K:865:ASP:HB2	1.99	0.45
1:D:71:ASN:HB3	1:D:74:TYR:H	1.82	0.45
1:C:623:ARG:HD3	1:C:880:PHE:HE1	1.81	0.45
1:B:281:ILE:HG21	1:B:655:LEU:HD13	1.98	0.45
2:T:220:ARG:HE	2:T:262:THR:HG22	1.82	0.45
5:M:91:ILE:HG12	5:M:402:VAL:HG22	1.98	0.45
1:A:314:GLU:HG3	1:A:655:LEU:HD22	1.98	0.45
1:J:511:GLN:OE1	1:J:528:TYR:OH	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:314:GLU:HG3	1:H:655:LEU:HD22	1.98	0.45
1:E:297:SER:HA	1:E:526:TYR:HA	1.98	0.45
1:B:537:ASN:HD21	1:B:548:LEU:H	1.63	0.45
2:R:220:ARG:HE	2:R:262:THR:HG22	1.82	0.45
1:G:27:ILE:O	1:G:31:GLN:NE2	2.50	0.45
1:G:159:GLN:HE21	1:G:189:LEU:HD22	1.81	0.45
2:S:294:TYR:HE2	2:R:242:HIS:HB3	1.81	0.45
2:T:316:GLY:N	2:T:343:GLY:O	2.48	0.45
2:Q:126:ILE:HB	2:Q:149:VAL:HG12	1.97	0.45
1:F:594:LEU:O	1:F:623:ARG:NH2	2.50	0.45
1:C:83:VAL:HG21	1:C:521:LEU:HD11	1.99	0.45
2:S:316:GLY:N	2:S:343:GLY:O	2.48	0.45
1:A:725:GLN:NE2	1:A:731:ASN:OD1	2.49	0.44
1:K:197:SER:HG	1:K:248:TRP:HE1	1.65	0.44
1:K:314:GLU:HG3	1:K:655:LEU:HD22	1.99	0.44
1:K:755:TYR:HA	1:K:756:GLY:HA2	1.69	0.44
1:H:807:SER:HA	1:I:501:ARG:HG2	1.97	0.44
1:F:537:ASN:HD22	1:F:649:SER:HB3	1.83	0.44
1:D:662:SER:O	1:D:828:TRP:NE1	2.41	0.44
2:Q:316:GLY:N	2:Q:343:GLY:O	2.48	0.44
5:M:14:THR:HA	5:M:29:GLN:HE21	1.81	0.44
1:A:118:PRO:O	1:C:410:ASN:ND2	2.37	0.44
1:A:589:ASN:HB2	1:B:41:ARG:H	1.83	0.44
1:K:879:VAL:HG12	1:K:901:PRO:HD2	1.99	0.44
1:H:404:ILE:HD11	1:I:797:PRO:HD3	1.98	0.44
1:F:630:LEU:O	1:F:872:TYR:N	2.45	0.44
1:C:495:GLN:HE21	1:B:470:ARG:HG3	1.82	0.44
1:B:109:LYS:NZ	1:B:111:TYR:O	2.49	0.44
1:B:310:ASP:HB2	1:B:899:ARG:HH22	1.82	0.44
1:B:533:ARG:HH11	1:B:538:MET:HG2	1.82	0.44
2:R:133:ARG:HG2	2:R:164:GLN:HG2	1.99	0.44
1:L:904:SER:HA	1:D:676:VAL:HG22	1.98	0.44
1:G:694:ARG:NH1	1:G:699:ASP:OD1	2.51	0.44
1:E:748:MET:SD	1:E:820:LYS:NZ	2.86	0.44
1:D:225:LYS:HA	1:D:242:ALA:HA	2.00	0.44
2:T:133:ARG:HG2	2:T:164:GLN:HG2	1.99	0.44
3:P:89:PRO:HG3	3:P:212:VAL:HG22	2.00	0.44
1:A:277:ARG:HD3	1:A:541:GLN:HB2	2.00	0.44
1:L:287:ASN:HA	1:L:307:ASP:HB3	1.98	0.44
1:H:773:MET:SD	1:H:785:THR:OG1	2.72	0.44
1:F:85:ASP:OD1	1:F:890:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:477:ASP:OD2	1:F:820:LYS:NZ	2.40	0.44
1:E:21:GLU:OE2	1:E:25:GLN:NE2	2.50	0.44
1:E:78:ARG:HG3	1:E:529:GLU:HB3	1.99	0.44
1:C:156:ALA:O	1:C:225:LYS:NZ	2.41	0.44
1:K:291:ASN:HB2	1:K:531:TYR:CD2	2.53	0.44
1:K:363:PRO:HA	1:K:364:PRO:HD3	1.83	0.44
1:H:779:CYS:HB2	1:I:169:GLN:HB3	2.00	0.44
1:I:783:GLN:HE21	1:I:791:LEU:HG	1.81	0.44
1:G:283:MET:HG2	1:G:509:VAL:HG11	1.99	0.44
1:F:57:GLN:HE21	1:F:568:PRO:HA	1.81	0.44
1:F:559:GLN:OE1	1:F:561:ASN:ND2	2.50	0.44
1:E:504:ASP:O	1:D:819:ARG:NH2	2.51	0.44
1:D:640:ALA:HB2	2:S:17:PRO:HD3	2.00	0.44
1:C:379:GLY:HA2	1:B:228:ILE:HD12	1.98	0.44
1:B:227:TYR:HD1	1:B:237:VAL:HG11	1.83	0.44
2:Q:220:ARG:HE	2:Q:262:THR:HG22	1.82	0.44
1:L:377:GLY:O	1:L:397:ALA:N	2.51	0.44
1:K:673:ASP:HA	1:K:857:SER:HB3	1.99	0.44
1:E:638:ILE:HD11	1:E:655:LEU:HD21	2.00	0.44
1:B:109:LYS:NZ	1:B:113:GLY:O	2.47	0.44
2:R:300:ILE:HB	2:R:331:THR:HG22	2.00	0.44
1:L:331:PHE:HB3	1:L:336:GLN:HE21	1.83	0.44
1:J:75:TYR:HB2	1:J:534:LYS:HE3	2.00	0.44
1:J:753:PRO:HD3	1:J:806:LEU:HD21	2.00	0.44
1:H:720:ALA:HB1	1:H:837:LEU:HD23	2.00	0.44
1:E:108:PHE:O	1:D:807:SER:OG	2.31	0.44
1:E:379:GLY:HA2	1:D:228:ILE:HG22	2.00	0.44
2:S:300:ILE:HB	2:S:331:THR:HG22	2.00	0.44
1:A:50:GLY:HA2	1:A:570:ASN:HD22	1.83	0.44
1:A:630:LEU:O	1:A:872:TYR:N	2.51	0.44
1:H:751:GLN:HE22	1:I:498:GLY:HA3	1.82	0.44
1:I:347:ILE:HD11	1:I:822:LEU:HD12	2.00	0.44
1:I:834:SER:HB3	1:G:52:THR:HG21	2.00	0.44
1:F:98:ILE:HB	1:F:560:ILE:HG12	1.99	0.44
1:E:705:THR:HG23	1:E:712:LYS:HG2	2.00	0.44
1:C:616:ASP:HA	1:C:857:SER:HB3	2.00	0.44
2:S:220:ARG:HA	2:S:258:ASN:HD21	1.83	0.44
5:M:57:TYR:HE1	5:M:419:ARG:HG3	1.83	0.44
1:L:249:GLU:HB2	1:K:810:ASN:HD21	1.83	0.44
1:L:773:MET:HB3	1:J:169:GLN:HE21	1.82	0.44
1:H:348:LEU:HD13	1:H:424:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:712:LYS:HG3	1:I:563:TYR:HE2	1.83	0.44
1:H:773:MET:HB3	1:I:169:GLN:HE21	1.83	0.44
1:I:310:ASP:HB3	1:I:597:VAL:HG13	1.99	0.44
1:G:98:ILE:HG12	1:G:560:ILE:HG12	2.00	0.44
1:C:363:PRO:HA	1:C:364:PRO:HD3	1.81	0.44
1:B:630:LEU:HD22	1:B:653:PRO:HG2	2.00	0.44
3:O:89:PRO:HG3	3:O:212:VAL:HG22	2.00	0.44
4:N:176:GLN:HG2	4:N:183:ASN:HB3	2.00	0.44
1:A:766:TYR:OH	1:A:785:THR:O	2.34	0.43
1:I:360:LEU:HD23	1:I:408:GLU:HB2	2.00	0.43
1:G:140:ALA:HB2	1:G:192:ILE:HD13	2.00	0.43
1:G:339:ASP:OD1	1:G:339:ASP:N	2.51	0.43
1:F:118:PRO:HD2	1:E:778:ASN:HB3	2.00	0.43
1:E:363:PRO:HA	1:E:364:PRO:HD3	1.87	0.43
1:C:107:SER:O	1:C:272:ASN:ND2	2.50	0.43
1:B:278:ASP:OD2	1:B:327:ARG:NH2	2.51	0.43
1:B:631:LYS:HG2	1:B:871:THR:HG22	1.99	0.43
2:S:220:ARG:HE	2:S:262:THR:HG22	1.82	0.43
1:L:297:SER:HA	1:L:526:TYR:HA	2.01	0.43
1:H:595:GLY:O	1:H:623:ARG:NH2	2.52	0.43
1:F:231:THR:HG21	1:F:236:ARG:HD3	1.99	0.43
1:D:511:GLN:OE1	1:D:528:TYR:OH	2.35	0.43
1:D:848:ASN:HB3	1:D:851:TYR:HD2	1.83	0.43
1:B:107:SER:O	1:B:272:ASN:ND2	2.51	0.43
2:T:349:VAL:H	2:T:364:GLY:HA2	1.83	0.43
2:Q:90:ARG:NH1	2:Q:153:GLU:OE2	2.39	0.43
2:Q:300:ILE:HB	2:Q:331:THR:HG22	2.00	0.43
1:A:850:MET:HA	3:O:260:LEU:HD22	2.00	0.43
1:L:58:LYS:NZ	1:K:684:MET:O	2.49	0.43
1:I:69:GLU:HB3	1:I:76:LYS:HB3	2.00	0.43
1:F:470:ARG:NH2	1:F:747:PRO:O	2.49	0.43
1:B:619:TRP:NE1	1:B:856:HIS:O	2.45	0.43
2:Q:349:VAL:H	2:Q:364:GLY:HA2	1.84	0.43
1:J:19:LEU:HD13	1:J:23:LEU:HD12	2.00	0.43
1:H:363:PRO:HA	1:H:364:PRO:HD3	1.84	0.43
1:H:778:ASN:HB3	1:I:117:ASN:HA	1.99	0.43
1:I:98:ILE:HD11	1:I:507:ILE:HD11	2.00	0.43
1:E:691:GLU:OE2	1:E:694:ARG:NE	2.43	0.43
1:C:408:GLU:N	1:B:362:PHE:O	2.43	0.43
1:C:797:PRO:HD3	1:B:404:ILE:HD11	2.00	0.43
1:B:827:LEU:HD13	1:B:876:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:300:ILE:HB	2:T:331:THR:HG22	2.00	0.43
1:A:2:GLU:HB3	1:A:5:ARG:HD2	1.99	0.43
1:K:666:GLN:HA	1:K:693:LYS:H	1.83	0.43
1:J:287:ASN:HA	1:J:307:ASP:HB3	2.00	0.43
1:J:777:ASN:HD22	1:J:778:ASN:H	1.67	0.43
1:G:421:TYR:HA	1:G:425:ALA:HB3	2.01	0.43
1:D:225:LYS:HE2	1:D:227:TYR:HE1	1.84	0.43
1:D:718:GLN:NE2	1:D:829:GLN:O	2.50	0.43
1:B:98:ILE:HG22	1:B:560:ILE:HG23	1.99	0.43
1:A:707:GLN:HE21	1:B:496:LEU:HD23	1.84	0.43
1:K:724:ASN:HD22	1:K:837:LEU:HD22	1.83	0.43
1:J:128:SER:OG	1:J:201:GLN:NE2	2.52	0.43
1:J:537:ASN:HD22	1:J:649:SER:HB3	1.83	0.43
1:I:279:ASN:ND2	1:I:318:GLN:OE1	2.48	0.43
1:G:363:PRO:HA	1:G:364:PRO:HD3	1.86	0.43
1:F:879:VAL:HG12	1:F:901:PRO:HD2	2.00	0.43
1:E:733:PRO:HG2	1:E:736:THR:HG22	2.01	0.43
1:D:86:ASN:HD22	1:D:574:GLN:HE21	1.65	0.43
1:B:460:ILE:HD12	1:B:461:VAL:HG13	1.99	0.43
2:S:133:ARG:HG2	2:S:164:GLN:HG2	1.99	0.43
2:R:251:ASN:HD22	2:Q:187:TYR:HE1	1.66	0.43
5:M:112:LEU:HD12	5:M:127:PHE:HZ	1.83	0.43
1:L:14:SER:OG	1:L:17:GLU:OE1	2.30	0.43
1:L:766:TYR:OH	1:L:785:THR:O	2.28	0.43
1:H:428:LEU:HD13	1:H:460:ILE:HD11	2.00	0.43
1:G:383:ASN:OD1	1:G:388:THR:OG1	2.36	0.43
1:F:52:THR:HG21	1:E:834:SER:HB3	1.99	0.43
2:Q:133:ARG:HG2	2:Q:164:GLN:HG2	1.99	0.43
3:O:74:TYR:HB3	3:O:225:THR:HG22	2.01	0.43
5:M:271:VAL:HA	5:M:281:THR:HA	2.01	0.43
1:A:284:MET:HB3	1:A:530:TRP:HE1	1.84	0.43
1:J:98:ILE:HG13	1:J:560:ILE:HG12	2.01	0.43
1:F:305:VAL:HG22	1:F:516:ILE:HD11	2.00	0.43
1:F:367:ILE:H	1:F:367:ILE:HG13	1.67	0.43
1:D:143:PRO:HB2	1:D:171:GLY:HA2	2.00	0.43
5:M:341:VAL:HG12	5:M:343:GLY:H	1.83	0.43
1:L:537:ASN:HD21	1:L:548:LEU:H	1.66	0.43
1:K:842:LEU:HD21	1:K:847:GLN:HB3	2.00	0.43
1:I:331:PHE:HB3	1:I:336:GLN:HB3	1.99	0.43
1:F:773:MET:SD	1:F:773:MET:N	2.92	0.43
1:C:630:LEU:O	1:C:872:TYR:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:140:ASN:ND2	2:Q:95:ASP:OD2	2.43	0.43
2:R:220:ARG:HA	2:R:258:ASN:HD21	1.83	0.43
2:R:294:TYR:HE2	2:Q:242:HIS:HB3	1.82	0.43
2:R:349:VAL:H	2:R:364:GLY:HA2	1.83	0.43
1:L:62:ARG:HG3	1:L:563:TYR:HE1	1.83	0.43
1:L:67:GLN:HE21	1:L:78:ARG:CZ	2.32	0.43
1:H:62:ARG:HG3	1:H:563:TYR:HE1	1.84	0.43
1:C:13:ARG:HB3	1:C:17:GLU:HG3	2.00	0.43
1:C:450:TYR:CZ	1:C:454:ARG:HD2	2.53	0.43
2:S:172:PHE:HE2	2:S:179:ILE:HG13	1.84	0.43
5:M:37:ILE:HD12	5:M:39:ASN:HB2	2.00	0.43
1:K:36:ILE:HD12	1:J:520:LEU:HD22	2.00	0.42
1:E:843:THR:HG23	1:E:846:GLY:H	1.82	0.42
1:B:280:PHE:CZ	1:B:335:ASN:HB2	2.54	0.42
1:A:139:VAL:HG22	1:B:367:ILE:HG21	2.01	0.42
1:L:662:SER:O	1:L:828:TRP:NE1	2.33	0.42
1:K:296:SER:HB3	1:K:303:ASN:HA	2.02	0.42
1:K:304:ILE:O	1:K:897:TYR:OH	2.29	0.42
1:G:885:ILE:HG12	1:G:895:VAL:HG12	2.01	0.42
1:F:46:ALA:O	1:E:847:GLN:NE2	2.52	0.42
1:F:117:ASN:HA	1:E:778:ASN:HB3	1.99	0.42
1:C:678:TRP:CD1	1:C:679:PRO:HA	2.54	0.42
2:Q:220:ARG:HA	2:Q:258:ASN:HD21	1.83	0.42
5:M:185:SER:HB2	5:M:278:LYS:HD3	2.01	0.42
1:A:899:ARG:NE	1:A:902:PHE:O	2.52	0.42
1:L:502:TYR:H	1:K:815:GLN:NE2	2.17	0.42
1:L:717:VAL:HG23	1:L:836:PHE:HB3	2.01	0.42
1:K:399:ILE:HG13	1:J:228:ILE:HD13	2.02	0.42
1:I:102:LEU:HD11	1:I:540:LEU:HD21	2.01	0.42
1:I:795:GLY:HA3	1:G:169:GLN:HA	2.01	0.42
1:F:205:TYR:OH	1:E:353:TYR:OH	2.32	0.42
2:S:349:VAL:H	2:S:364:GLY:HA2	1.84	0.42
5:M:54:SER:HA	5:M:422:LEU:HB3	2.01	0.42
1:A:348:LEU:HD13	1:A:424:VAL:HG21	2.01	0.42
1:K:787:THR:HB	1:K:788:ASN:H	1.61	0.42
1:I:327:ARG:HG2	1:I:738:HIS:CE1	2.55	0.42
1:G:205:TYR:HB3	1:G:266:ALA:HB3	2.02	0.42
1:F:143:PRO:HB2	1:F:171:GLY:HA2	2.01	0.42
1:D:69:GLU:HB3	1:D:76:LYS:HB3	2.01	0.42
1:D:88:LEU:HD12	1:D:520:LEU:HD11	2.02	0.42
2:S:140:ASN:ND2	2:R:95:ASP:OD2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:172:PHE:HE2	2:R:179:ILE:HG13	1.84	0.42
2:R:316:GLY:N	2:R:343:GLY:O	2.48	0.42
1:I:637:ARG:NH2	1:I:872:TYR:OH	2.49	0.42
1:D:300:GLN:HE21	1:D:302:LEU:HD12	1.85	0.42
1:C:367:ILE:HG22	1:B:141:GLN:HB2	2.00	0.42
1:C:511:GLN:OE1	1:C:528:TYR:OH	2.37	0.42
2:Q:172:PHE:HE2	2:Q:179:ILE:HG13	1.85	0.42
5:M:320:PRO:HD2	5:M:419:ARG:HB3	2.01	0.42
1:J:423:ASN:HD21	1:J:486:ARG:HH21	1.67	0.42
1:H:39:LYS:HE2	1:G:520:LEU:HB2	2.02	0.42
1:I:263:ARG:HB2	1:G:175:TYR:CG	2.55	0.42
1:I:270:ARG:NH1	1:I:426:MET:O	2.41	0.42
1:E:665:PHE:HA	1:E:864:VAL:HG12	2.00	0.42
1:C:342:ASP:OD2	1:C:486:ARG:NH1	2.52	0.42
1:B:288:SER:O	1:B:292:THR:OG1	2.33	0.42
1:B:304:ILE:HG23	1:B:895:VAL:HG11	2.01	0.42
5:M:324:LYS:HD2	5:M:409:PRO:HB2	2.01	0.42
1:L:310:ASP:HB3	1:L:597:VAL:HG13	2.00	0.42
1:C:30:THR:OG1	1:C:31:GLN:N	2.50	0.42
1:C:629:ARG:HD3	1:C:664:THR:HG23	2.01	0.42
1:B:13:ARG:NH1	3:O:222:ILE:O	2.45	0.42
1:A:75:TYR:HB2	1:A:534:LYS:HE2	2.02	0.42
1:H:287:ASN:ND2	1:H:307:ASP:OD1	2.53	0.42
1:H:365:HIS:O	1:H:367:ILE:N	2.53	0.42
1:I:718:GLN:HE22	1:I:829:GLN:H	1.68	0.42
1:E:201:GLN:NE2	1:E:261:ASP:OD2	2.41	0.42
1:C:499:ASN:ND2	1:B:466:ASP:OD1	2.52	0.42
2:T:172:PHE:HE2	2:T:179:ILE:HG13	1.84	0.42
2:T:220:ARG:HA	2:T:258:ASN:HD21	1.83	0.42
2:T:278:PHE:HE2	2:T:303:PHE:HB3	1.85	0.42
1:A:142:LEU:HD21	1:A:241:MET:HG2	2.02	0.42
1:L:714:PHE:HA	1:L:717:VAL:HG12	2.02	0.42
1:H:167:ASN:HD21	1:G:773:MET:HB2	1.85	0.42
1:H:278:ASP:OD2	1:H:327:ARG:NH2	2.52	0.42
1:F:244:ASP:OD2	1:E:798:TYR:OH	2.36	0.42
1:C:17:GLU:HB2	4:N:9:SER:HB3	2.02	0.42
1:J:421:TYR:HA	1:J:425:ALA:HB3	2.02	0.42
1:I:367:ILE:H	1:I:367:ILE:HG13	1.42	0.42
1:C:467:ILE:H	1:C:467:ILE:HG13	1.65	0.42
3:P:74:TYR:HB3	3:P:225:THR:HG22	2.01	0.42
5:M:115:ASP:HA	5:M:160:LYS:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:169:GLN:HB3	1:K:779:CYS:HB2	2.01	0.41
1:K:52:THR:HG21	1:J:834:SER:HB3	2.02	0.41
1:K:736:THR:HB	1:K:743:ASN:HD21	1.85	0.41
1:H:228:ILE:HG21	1:I:399:ILE:HD13	2.02	0.41
1:H:482:PHE:HZ	1:H:825:ARG:HD2	1.85	0.41
1:I:773:MET:HB2	1:G:167:ASN:HD21	1.85	0.41
1:F:537:ASN:HD21	1:F:548:LEU:H	1.68	0.41
1:C:102:LEU:HD11	1:C:540:LEU:HD21	2.02	0.41
5:M:170:LYS:NZ	5:M:172:ASP:OD1	2.50	0.41
1:A:417:ARG:NH2	1:A:782:GLN:OE1	2.53	0.41
1:L:483:ASN:ND2	1:L:648:TYR:OH	2.40	0.41
1:J:96:PHE:HB2	1:J:509:VAL:HG22	2.02	0.41
1:J:178:PRO:HG3	1:J:365:HIS:CE1	2.56	0.41
1:J:377:GLY:HA2	1:J:397:ALA:H	1.85	0.41
1:H:724:ASN:HD22	1:H:837:LEU:HD22	1.84	0.41
1:E:744:ASN:ND2	1:E:824:ASP:O	2.52	0.41
1:D:139:VAL:HB	1:D:262:ARG:HH12	1.84	0.41
1:C:191:ARG:NH2	1:C:244:ASP:OD2	2.52	0.41
2:S:90:ARG:NH1	2:S:153:GLU:OE2	2.39	0.41
2:S:200:ILE:HG12	2:S:221:CYS:HB3	2.03	0.41
2:S:214:ASN:N	2:S:248:ASN:OD1	2.53	0.41
5:M:143:ASP:OD1	5:M:386:GLN:NE2	2.53	0.41
1:J:630:LEU:O	1:J:872:TYR:N	2.43	0.41
1:I:161:VAL:HG12	1:I:166:PRO:HD3	2.03	0.41
1:G:71:ASN:HD22	1:G:71:ASN:HA	1.65	0.41
1:G:107:SER:O	1:G:272:ASN:ND2	2.53	0.41
1:D:71:ASN:ND2	1:D:73:ASN:OD1	2.53	0.41
1:C:725:GLN:NE2	1:C:731:ASN:OD1	2.53	0.41
1:B:365:HIS:CD2	1:B:368:SER:HB3	2.55	0.41
1:B:668:CYS:HB3	1:B:690:PHE:HB2	2.01	0.41
1:B:751:GLN:HG3	1:B:817:THR:HB	2.02	0.41
1:A:735:CYS:SG	1:A:737:LYS:NZ	2.88	0.41
1:L:327:ARG:HH12	1:L:336:GLN:HB2	1.85	0.41
1:J:102:LEU:HD11	1:J:540:LEU:HD21	2.02	0.41
1:J:450:TYR:CZ	1:J:454:ARG:HD2	2.55	0.41
1:I:428:LEU:HD13	1:I:460:ILE:HD11	2.01	0.41
1:F:578:GLU:OE2	1:F:582:ARG:NE	2.45	0.41
1:F:722:SER:OG	1:F:829:GLN:NE2	2.53	0.41
1:D:678:TRP:CD1	1:D:679:PRO:HA	2.56	0.41
1:B:714:PHE:HA	1:B:717:VAL:HG12	2.01	0.41
2:S:251:ASN:HD22	2:R:187:TYR:HE1	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:214:ASN:N	2:R:248:ASN:OD1	2.53	0.41
2:Q:214:ASN:N	2:Q:248:ASN:OD1	2.54	0.41
1:A:500:GLY:H	1:C:751:GLN:HE21	1.68	0.41
1:J:167:ASN:HB3	1:J:170:VAL:HG22	2.03	0.41
1:H:796:HIS:HB2	1:I:127:ASN:HD21	1.85	0.41
1:G:630:LEU:O	1:G:872:TYR:N	2.49	0.41
1:F:89:VAL:HB	1:F:521:LEU:HB3	2.01	0.41
1:D:638:ILE:HD11	1:D:655:LEU:HD11	2.02	0.41
2:Q:278:PHE:HE2	2:Q:303:PHE:HB3	1.85	0.41
5:M:314:GLN:NE2	5:M:316:TYR:OH	2.42	0.41
1:L:611:VAL:HG11	2:Q:11:ASN:HD22	1.84	0.41
1:F:380:MET:HA	1:F:392:THR:HG22	2.03	0.41
1:E:668:CYS:HB3	1:E:690:PHE:HB2	2.01	0.41
1:D:295:PHE:HD2	1:D:304:ILE:HD12	1.86	0.41
1:D:520:LEU:HB3	1:D:588:GLN:HE22	1.84	0.41
5:M:337:SER:HB2	5:M:427:ARG:HG3	2.02	0.41
1:L:167:ASN:HD22	1:L:168:PRO:HD2	1.86	0.41
1:K:13:ARG:NH1	3:P:222:ILE:O	2.45	0.41
1:J:662:SER:O	1:J:828:TRP:NE1	2.48	0.41
1:G:296:SER:HA	1:G:893:ILE:HD11	2.02	0.41
1:G:843:THR:HG23	1:G:846:GLY:H	1.85	0.41
1:F:670:ILE:HG12	1:F:860:MET:HG2	2.03	0.41
1:E:563:TYR:HE2	1:D:712:LYS:HE2	1.85	0.41
1:B:126:ILE:HD11	1:B:248:TRP:HH2	1.86	0.41
2:S:278:PHE:HE2	2:S:303:PHE:HB3	1.85	0.41
2:R:200:ILE:HG12	2:R:221:CYS:HB3	2.03	0.41
1:I:377:GLY:N	1:I:397:ALA:O	2.52	0.41
1:G:126:ILE:HD11	1:G:248:TRP:CH2	2.55	0.41
1:G:656:ASP:OD1	1:G:656:ASP:N	2.50	0.41
1:F:408:GLU:HB2	1:E:364:PRO:HG3	2.01	0.41
2:S:95:ASP:OD2	2:Q:140:ASN:ND2	2.47	0.41
2:T:156:TYR:HE1	2:T:184:ARG:HB3	1.86	0.41
1:A:616:ASP:OD1	1:A:616:ASP:N	2.53	0.41
1:A:733:PRO:HG2	1:A:736:THR:HG22	2.03	0.41
1:L:151:THR:HA	1:L:236:ARG:HA	2.02	0.41
1:K:69:GLU:HG2	1:K:76:LYS:HB3	2.02	0.41
1:K:347:ILE:HG21	1:K:470:ARG:HE	1.85	0.41
1:J:297:SER:HA	1:J:526:TYR:HA	2.03	0.41
1:J:629:ARG:HD3	1:J:664:THR:HG23	2.02	0.41
1:J:751:GLN:HG2	1:J:817:THR:HG22	2.03	0.41
1:H:148:ALA:HB2	1:H:155:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:367:ILE:HD13	1:G:139:VAL:HG13	2.03	0.41
1:I:141:GLN:NE2	1:G:367:ILE:HA	2.36	0.41
1:I:294:SER:HA	1:I:303:ASN:HD21	1.85	0.41
1:F:292:THR:HG22	1:F:307:ASP:HB2	2.02	0.41
1:F:428:LEU:HD11	1:F:460:ILE:HD11	2.02	0.41
1:F:774:PRO:HB2	1:D:216:GLY:HA3	2.02	0.41
1:D:272:ASN:HA	1:D:543:THR:HB	2.03	0.41
1:C:216:GLY:HA3	1:B:774:PRO:HB2	2.02	0.41
1:B:290:SER:HA	5:M:57:TYR:HE2	1.86	0.41
1:B:626:SER:HB2	1:B:876:LEU:HG	2.03	0.41
1:B:668:CYS:O	1:B:690:PHE:N	2.53	0.41
2:T:200:ILE:HD13	2:T:224:LEU:HD22	2.03	0.41
2:T:200:ILE:HG12	2:T:221:CYS:HB3	2.03	0.41
5:M:244:ILE:HD11	5:M:285:SER:HB3	2.02	0.41
1:A:403:ASN:HD21	1:B:794:CYS:HA	1.86	0.41
1:L:134:ASN:HD22	2:R:118:GLU:HG2	1.85	0.41
1:K:460:ILE:H	1:K:460:ILE:HG13	1.75	0.41
1:D:269:ASN:ND2	1:D:452:ASN:HD21	2.19	0.41
1:D:753:PRO:HD3	1:D:806:LEU:HD21	2.03	0.41
1:B:291:ASN:HB3	1:B:531:TYR:HD2	1.86	0.41
3:P:79:GLN:NE2	3:P:224:ARG:H	2.19	0.41
1:L:403:ASN:HD21	1:K:172:GLN:HB2	1.85	0.40
1:H:169:GLN:NE2	1:G:775:ILE:O	2.54	0.40
1:H:293:GLY:HA3	1:H:530:TRP:CE3	2.56	0.40
1:H:783:GLN:HG2	1:H:788:ASN:O	2.21	0.40
1:I:589:ASN:HB3	1:I:884:VAL:HG12	2.03	0.40
1:I:773:MET:HB3	1:G:169:GLN:HE21	1.86	0.40
1:G:254:HIS:ND1	1:G:269:ASN:OD1	2.49	0.40
1:F:279:ASN:ND2	1:F:318:GLN:OE1	2.47	0.40
1:E:291:ASN:OD1	1:E:291:ASN:N	2.54	0.40
1:E:428:LEU:HD21	1:E:460:ILE:HD13	2.03	0.40
1:D:208:TYR:HB3	1:D:251:PRO:HD2	2.02	0.40
1:D:363:PRO:HA	1:D:364:PRO:HD3	1.81	0.40
2:S:141:PHE:HD2	2:S:148:ALA:HB1	1.86	0.40
2:R:278:PHE:HE2	2:R:303:PHE:HB3	1.85	0.40
5:M:286:TRP:CD1	5:M:297:LEU:HD21	2.56	0.40
1:G:668:CYS:HB3	1:G:690:PHE:HB2	2.02	0.40
1:E:284:MET:HB3	1:E:530:TRP:HE1	1.85	0.40
1:D:126:ILE:HD11	1:D:248:TRP:CH2	2.57	0.40
2:S:156:TYR:HE1	2:S:184:ARG:HB3	1.86	0.40
2:T:214:ASN:N	2:T:248:ASN:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:212:SER:HA	4:N:215:LEU:HD23	2.02	0.40
5:M:66:VAL:HG22	5:M:70:ASP:HB3	2.03	0.40
1:L:117:ASN:HA	1:K:778:ASN:HB3	2.04	0.40
1:L:773:MET:HG3	1:J:167:ASN:HD21	1.85	0.40
1:J:906:SER:OG	1:J:907:ALA:N	2.53	0.40
1:H:784:LYS:HD2	1:I:170:VAL:HA	2.02	0.40
1:D:611:VAL:HG11	2:R:11:ASN:HD22	1.87	0.40
1:C:699:ASP:OD1	1:C:702:GLY:N	2.51	0.40
2:R:200:ILE:HD13	2:R:224:LEU:HD22	2.03	0.40
5:M:215:ARG:HG3	5:M:218:ASN:HD22	1.86	0.40
1:L:300:GLN:O	1:L:302:LEU:N	2.54	0.40
1:H:432:TYR:HE2	1:H:475:VAL:HG11	1.86	0.40
1:F:595:GLY:O	1:F:623:ARG:NH2	2.47	0.40
1:D:532:PHE:HE2	1:D:560:ILE:HG21	1.85	0.40
1:C:345:VAL:HG11	1:C:484:HIS:NE2	2.37	0.40
1:C:610:VAL:HG11	1:C:873:LEU:HD22	2.04	0.40
5:M:111:LEU:HD13	5:M:126:TRP:CD2	2.56	0.40
1:A:170:VAL:HG22	1:C:784:LYS:HD3	2.03	0.40
1:L:98:ILE:HD11	1:L:507:ILE:HD11	2.03	0.40
1:L:724:ASN:HD21	1:L:838:ASN:H	1.69	0.40
1:J:205:TYR:HB3	1:J:266:ALA:HB3	2.03	0.40
1:H:277:ARG:HD3	1:H:541:GLN:HB2	2.03	0.40
1:I:159:GLN:HB2	1:I:225:LYS:HZ2	1.87	0.40
1:I:714:PHE:HA	1:I:717:VAL:HG12	2.04	0.40
1:F:796:HIS:HB2	1:D:127:ASN:HD21	1.87	0.40
1:E:379:GLY:HA2	1:D:228:ILE:HA	2.02	0.40
1:B:98:ILE:HD11	1:B:507:ILE:HD11	2.03	0.40
1:B:167:ASN:HD22	1:B:168:PRO:HD2	1.87	0.40
2:R:141:PHE:HD2	2:R:148:ALA:HB1	1.86	0.40
2:Q:156:TYR:HE1	2:Q:184:ARG:HB3	1.86	0.40
2:Q:229:MET:HA	2:Q:266:LEU:HD22	2.04	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	903/909 (99%)	825 (91%)	77 (8%)	1 (0%)	51	82
1	B	900/909 (99%)	816 (91%)	82 (9%)	2 (0%)	47	78
1	C	905/909 (100%)	816 (90%)	87 (10%)	2 (0%)	47	78
1	D	904/909 (99%)	838 (93%)	65 (7%)	1 (0%)	51	82
1	E	904/909 (99%)	835 (92%)	68 (8%)	1 (0%)	51	82
1	F	902/909 (99%)	829 (92%)	73 (8%)	0	100	100
1	G	904/909 (99%)	834 (92%)	68 (8%)	2 (0%)	47	78
1	H	903/909 (99%)	822 (91%)	79 (9%)	2 (0%)	47	78
1	I	904/909 (99%)	829 (92%)	73 (8%)	2 (0%)	47	78
1	J	904/909 (99%)	841 (93%)	61 (7%)	2 (0%)	47	78
1	K	906/909 (100%)	822 (91%)	82 (9%)	2 (0%)	47	78
1	L	904/909 (99%)	833 (92%)	67 (7%)	4 (0%)	34	67
2	Q	365/370 (99%)	325 (89%)	39 (11%)	1 (0%)	41	72
2	R	365/370 (99%)	325 (89%)	39 (11%)	1 (0%)	41	72
2	S	365/370 (99%)	325 (89%)	39 (11%)	1 (0%)	41	72
2	T	365/370 (99%)	326 (89%)	38 (10%)	1 (0%)	41	72
3	O	182/278 (66%)	161 (88%)	21 (12%)	0	100	100
3	P	182/278 (66%)	160 (88%)	22 (12%)	0	100	100
4	N	253/609 (42%)	230 (91%)	23 (9%)	0	100	100
5	M	449/451 (100%)	391 (87%)	55 (12%)	3 (1%)	22	55
All	All	13369/14004 (96%)	12183 (91%)	1158 (9%)	28 (0%)	50	78

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	789	VAL
1	L	173	PRO
1	I	347	ILE
1	G	347	ILE
1	L	347	ILE
1	J	347	ILE
1	H	261	ASP
1	C	31	GLN

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Mol	Chain	Res	Type
1	B	673	ASP
5	M	359	ALA
1	A	658	THR
1	L	172	GLN
1	K	658	THR
1	J	300	GLN
1	I	254	HIS
2	S	163	MET
2	R	163	MET
1	B	300	GLN
2	T	163	MET
2	Q	163	MET
5	M	360	VAL
1	L	885	ILE
1	C	458	PRO
1	H	366	VAL
1	D	347	ILE
1	G	366	VAL
5	M	119	PRO
1	E	366	VAL

5.3.2 Protein sidechains [i](#)

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	775/777 (100%)	763 (98%)	12 (2%)	65	82
1	B	774/777 (100%)	762 (98%)	12 (2%)	62	81
1	C	776/777 (100%)	766 (99%)	10 (1%)	69	84
1	D	776/777 (100%)	767 (99%)	9 (1%)	71	85
1	E	775/777 (100%)	764 (99%)	11 (1%)	67	83
1	F	775/777 (100%)	764 (99%)	11 (1%)	67	83
1	G	775/777 (100%)	763 (98%)	12 (2%)	65	82
1	H	775/777 (100%)	763 (98%)	12 (2%)	65	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	775/777 (100%)	762 (98%)	13 (2%)	60	80
1	J	775/777 (100%)	763 (98%)	12 (2%)	65	82
1	K	776/777 (100%)	767 (99%)	9 (1%)	71	85
1	L	776/777 (100%)	762 (98%)	14 (2%)	59	79
2	Q	301/304 (99%)	300 (100%)	1 (0%)	92	97
2	R	301/304 (99%)	300 (100%)	1 (0%)	92	97
2	S	301/304 (99%)	300 (100%)	1 (0%)	92	97
2	T	301/304 (99%)	300 (100%)	1 (0%)	92	97
3	O	158/234 (68%)	155 (98%)	3 (2%)	57	78
3	P	158/234 (68%)	155 (98%)	3 (2%)	57	78
4	N	226/520 (44%)	221 (98%)	5 (2%)	52	75
5	M	406/406 (100%)	399 (98%)	7 (2%)	60	80
All	All	11455/11934 (96%)	11296 (99%)	159 (1%)	68	83

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	A	234	ASN
1	A	263	ARG
1	A	303	ASN
1	A	335	ASN
1	A	383	ASN
1	A	452	ASN
1	A	470	ARG
1	A	527	ASN
1	A	724	ASN
1	A	793	ARG
1	A	838	ASN
1	L	35	ASN
1	L	82	ASN
1	L	167	ASN
1	L	262	ARG
1	L	263	ARG
1	L	335	ASN
1	L	350	ASN
1	L	380	MET
1	L	410	ASN

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Mol	Chain	Res	Type
1	L	655	LEU
1	L	684	MET
1	L	750	ARG
1	L	769	ASN
1	L	793	ARG
1	K	78	ARG
1	K	82	ASN
1	K	167	ASN
1	K	234	ASN
1	K	383	ASN
1	K	470	ARG
1	K	724	ASN
1	K	793	ARG
1	K	838	ASN
1	J	22	ASN
1	J	35	ASN
1	J	82	ASN
1	J	174	ASN
1	J	262	ARG
1	J	335	ASN
1	J	350	ASN
1	J	452	ASN
1	J	750	ARG
1	J	777	ASN
1	J	793	ARG
1	J	838	ASN
1	H	22	ASN
1	H	35	ASN
1	H	71	ASN
1	H	272	ASN
1	H	335	ASN
1	H	383	ASN
1	H	487	ASN
1	H	724	ASN
1	H	758	ASN
1	H	761	ASN
1	H	793	ARG
1	H	838	ASN
1	I	71	ASN
1	I	262	ARG
1	I	263	ARG
1	I	303	ASN

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Mol	Chain	Res	Type
1	I	350	ASN
1	I	452	ASN
1	I	487	ASN
1	I	598	ASN
1	I	617	ARG
1	I	750	ARG
1	I	769	ASN
1	I	788	ASN
1	I	793	ARG
1	G	22	ASN
1	G	35	ASN
1	G	71	ASN
1	G	82	ASN
1	G	335	ASN
1	G	350	ASN
1	G	470	ARG
1	G	734	ASN
1	G	750	ARG
1	G	793	ARG
1	G	838	ASN
1	G	890	ARG
1	F	263	ARG
1	F	350	ASN
1	F	380	MET
1	F	383	ASN
1	F	527	ASN
1	F	583	ASN
1	F	684	MET
1	F	750	ARG
1	F	769	ASN
1	F	793	ARG
1	F	899	ARG
1	E	82	ASN
1	E	167	ASN
1	E	185	ASN
1	E	234	ASN
1	E	303	ASN
1	E	383	ASN
1	E	470	ARG
1	E	724	ASN
1	E	777	ASN
1	E	793	ARG

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Mol	Chain	Res	Type
1	E	838	ASN
1	D	335	ASN
1	D	470	ARG
1	D	487	ASN
1	D	750	ARG
1	D	777	ASN
1	D	793	ARG
1	D	838	ASN
1	D	890	ARG
1	D	899	ARG
1	C	22	ASN
1	C	167	ASN
1	C	174	ASN
1	C	229	ASN
1	C	452	ASN
1	C	750	ARG
1	C	777	ASN
1	C	793	ARG
1	C	853	ASN
1	C	899	ARG
1	B	35	ASN
1	B	82	ASN
1	B	167	ASN
1	B	262	ARG
1	B	263	ARG
1	B	350	ASN
1	B	583	ASN
1	B	655	LEU
1	B	664	THR
1	B	750	ARG
1	B	769	ASN
1	B	793	ARG
2	S	194	ASN
2	T	194	ASN
2	R	194	ASN
2	Q	194	ASN
3	P	50	ARG
3	P	62	ARG
3	P	235	ASN
3	O	50	ARG
3	O	62	ARG
3	O	235	ASN

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Mol	Chain	Res	Type
4	N	99	ASN
4	N	116	ARG
4	N	135	ARG
4	N	180	ARG
4	N	193	ASN
5	M	23	ASN
5	M	152	ASN
5	M	174	ARG
5	M	175	ASN
5	M	252	LYS
5	M	277	LYS
5	M	427	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (281) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	86	ASN
1	A	117	ASN
1	A	234	ASN
1	A	303	ASN
1	A	335	ASN
1	A	336	GLN
1	A	369	ASN
1	A	423	ASN
1	A	511	GLN
1	A	537	ASN
1	A	724	ASN
1	A	725	GLN
1	A	829	GLN
1	A	838	ASN
1	L	35	ASN
1	L	82	ASN
1	L	86	ASN
1	L	137	HIS
1	L	167	ASN
1	L	301	GLN
1	L	335	ASN
1	L	350	ASN
1	L	359	ASN
1	L	410	ASN
1	L	414	ASN

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Mol	Chain	Res	Type
1	L	423	ASN
1	L	445	HIS
1	L	508	GLN
1	L	527	ASN
1	L	537	ASN
1	L	574	GLN
1	L	645	ASN
1	L	724	ASN
1	L	728	GLN
1	L	769	ASN
1	L	783	GLN
1	L	829	GLN
1	L	856	HIS
1	K	9	HIS
1	K	82	ASN
1	K	117	ASN
1	K	167	ASN
1	K	234	ASN
1	K	359	ASN
1	K	369	ASN
1	K	423	ASN
1	K	559	GLN
1	K	561	ASN
1	K	724	ASN
1	K	725	GLN
1	K	743	ASN
1	K	783	GLN
1	K	815	GLN
1	K	829	GLN
1	K	838	ASN
1	J	22	ASN
1	J	35	ASN
1	J	82	ASN
1	J	117	ASN
1	J	159	GLN
1	J	186	ASN
1	J	201	GLN
1	J	287	ASN
1	J	291	ASN
1	J	335	ASN
1	J	350	ASN
1	J	359	ASN

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Mol	Chain	Res	Type
1	J	495	GLN
1	J	537	ASN
1	J	613	ASN
1	J	777	ASN
1	J	788	ASN
1	J	829	GLN
1	J	838	ASN
1	J	859	ASN
1	H	9	HIS
1	H	22	ASN
1	H	35	ASN
1	H	71	ASN
1	H	86	ASN
1	H	117	ASN
1	H	272	ASN
1	H	335	ASN
1	H	369	ASN
1	H	383	ASN
1	H	487	ASN
1	H	511	GLN
1	H	561	ASN
1	H	574	GLN
1	H	588	GLN
1	H	589	ASN
1	H	598	ASN
1	H	724	ASN
1	H	758	ASN
1	H	761	ASN
1	H	783	GLN
1	H	815	GLN
1	H	829	GLN
1	H	838	ASN
1	I	71	ASN
1	I	86	ASN
1	I	117	ASN
1	I	137	HIS
1	I	141	GLN
1	I	172	GLN
1	I	182	ASN
1	I	185	ASN
1	I	303	ASN
1	I	350	ASN

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Mol	Chain	Res	Type
1	I	445	HIS
1	I	452	ASN
1	I	487	ASN
1	I	574	GLN
1	I	588	GLN
1	I	598	ASN
1	I	724	ASN
1	I	769	ASN
1	I	771	GLN
1	I	788	ASN
1	I	829	GLN
1	I	856	HIS
1	G	22	ASN
1	G	28	GLN
1	G	35	ASN
1	G	71	ASN
1	G	82	ASN
1	G	86	ASN
1	G	117	ASN
1	G	141	GLN
1	G	159	GLN
1	G	172	GLN
1	G	182	ASN
1	G	185	ASN
1	G	201	GLN
1	G	291	ASN
1	G	335	ASN
1	G	350	ASN
1	G	359	ASN
1	G	369	ASN
1	G	414	ASN
1	G	574	GLN
1	G	725	GLN
1	G	734	ASN
1	G	751	GLN
1	G	783	GLN
1	G	829	GLN
1	G	838	ASN
1	F	67	GLN
1	F	86	ASN
1	F	287	ASN
1	F	350	ASN

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Mol	Chain	Res	Type
1	F	383	ASN
1	F	387	GLN
1	F	445	HIS
1	F	527	ASN
1	F	537	ASN
1	F	559	GLN
1	F	561	ASN
1	F	574	GLN
1	F	583	ASN
1	F	598	ASN
1	F	698	GLN
1	F	769	ASN
1	F	829	GLN
1	F	887	GLN
1	E	9	HIS
1	E	31	GLN
1	E	82	ASN
1	E	117	ASN
1	E	167	ASN
1	E	185	ASN
1	E	186	ASN
1	E	234	ASN
1	E	303	ASN
1	E	309	ASN
1	E	369	ASN
1	E	383	ASN
1	E	423	ASN
1	E	511	GLN
1	E	724	ASN
1	E	777	ASN
1	E	838	ASN
1	E	856	HIS
1	D	86	ASN
1	D	117	ASN
1	D	141	GLN
1	D	172	GLN
1	D	201	GLN
1	D	269	ASN
1	D	287	ASN
1	D	301	GLN
1	D	335	ASN
1	D	383	ASN

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Mol	Chain	Res	Type
1	D	438	ASN
1	D	445	HIS
1	D	487	ASN
1	D	645	ASN
1	D	725	GLN
1	D	751	GLN
1	D	777	ASN
1	D	783	GLN
1	D	829	GLN
1	D	838	ASN
1	C	22	ASN
1	C	117	ASN
1	C	167	ASN
1	C	201	GLN
1	C	229	ASN
1	C	287	ASN
1	C	369	ASN
1	C	445	HIS
1	C	495	GLN
1	C	537	ASN
1	C	574	GLN
1	C	688	ASN
1	C	725	GLN
1	C	751	GLN
1	C	777	ASN
1	C	783	GLN
1	C	829	GLN
1	C	853	ASN
1	B	35	ASN
1	B	67	GLN
1	B	82	ASN
1	B	141	GLN
1	B	167	ASN
1	B	287	ASN
1	B	350	ASN
1	B	387	GLN
1	B	527	ASN
1	B	537	ASN
1	B	724	ASN
1	B	725	GLN
1	B	728	GLN
1	B	769	ASN

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Mol	Chain	Res	Type
1	B	783	GLN
1	B	829	GLN
2	S	14	ASN
2	S	194	ASN
2	S	208	ASN
2	S	218	ASN
2	S	272	GLN
2	T	194	ASN
2	T	208	ASN
2	T	252	HIS
2	T	272	GLN
2	R	11	ASN
2	R	194	ASN
2	R	208	ASN
2	R	218	ASN
2	R	272	GLN
2	Q	11	ASN
2	Q	194	ASN
2	Q	208	ASN
2	Q	218	ASN
2	Q	272	GLN
3	P	13	GLN
3	P	44	GLN
3	P	79	GLN
3	P	235	ASN
3	O	13	GLN
3	O	44	GLN
3	O	79	GLN
3	O	109	GLN
3	O	235	ASN
4	N	99	ASN
4	N	144	GLN
4	N	145	HIS
4	N	218	ASN
5	M	23	ASN
5	M	29	GLN
5	M	46	ASN
5	M	152	ASN
5	M	175	ASN
5	M	218	ASN
5	M	294	GLN
5	M	345	HIS

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Mol	Chain	Res	Type
5	M	351	GLN
5	M	367	GLN
5	M	386	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

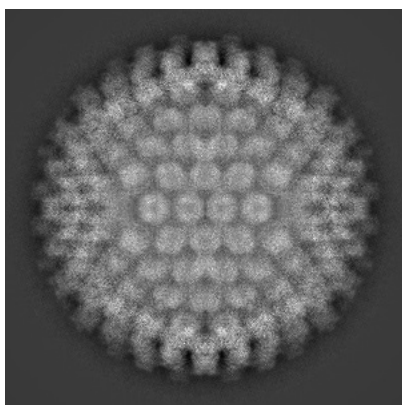
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4551. These allow visual inspection of the internal detail of the map and identification of artifacts.

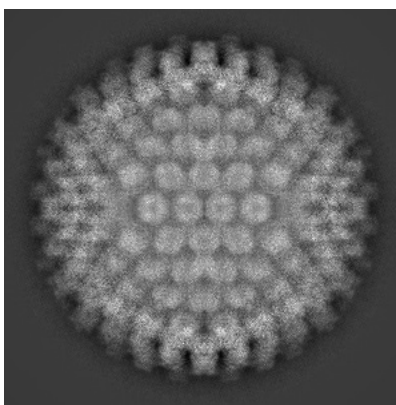
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

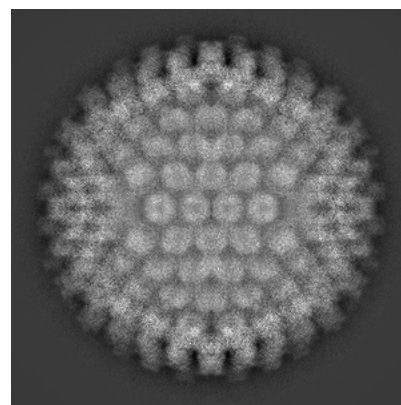
6.1.1 Primary map



X



Y

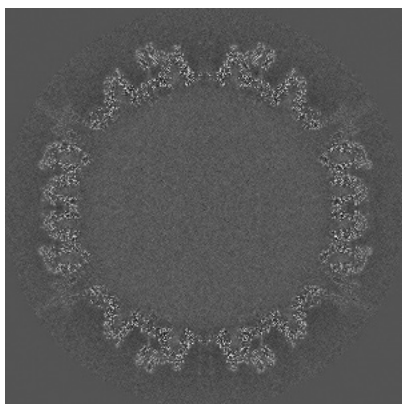


Z

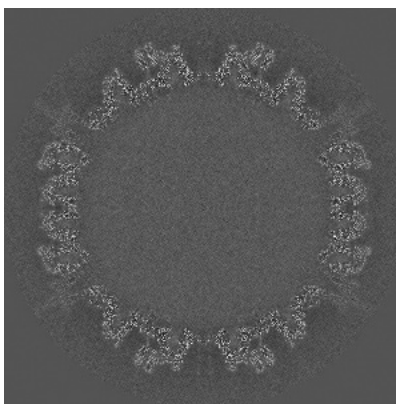
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 390



Y Index: 390

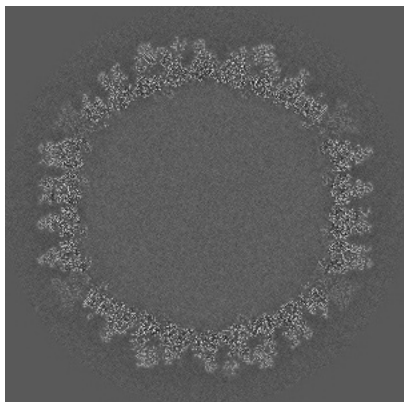


Z Index: 390

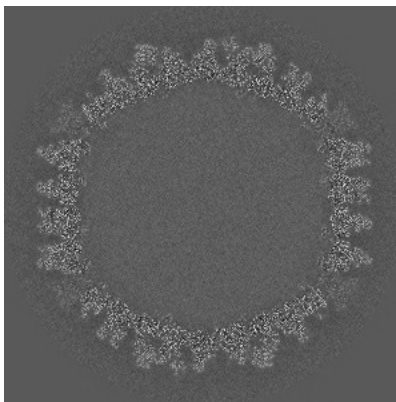
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

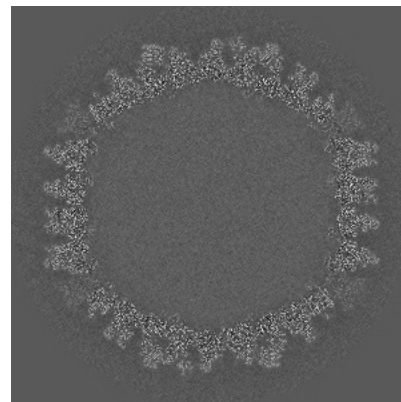
6.3.1 Primary map



X Index: 404



Y Index: 376

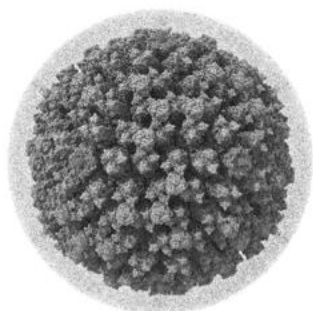


Z Index: 376

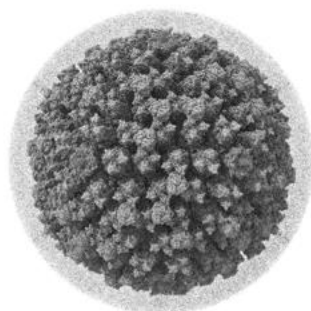
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

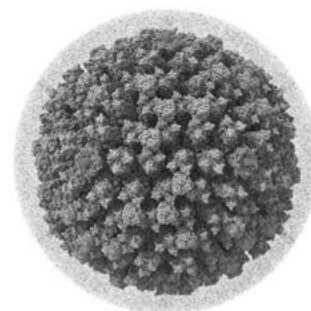
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

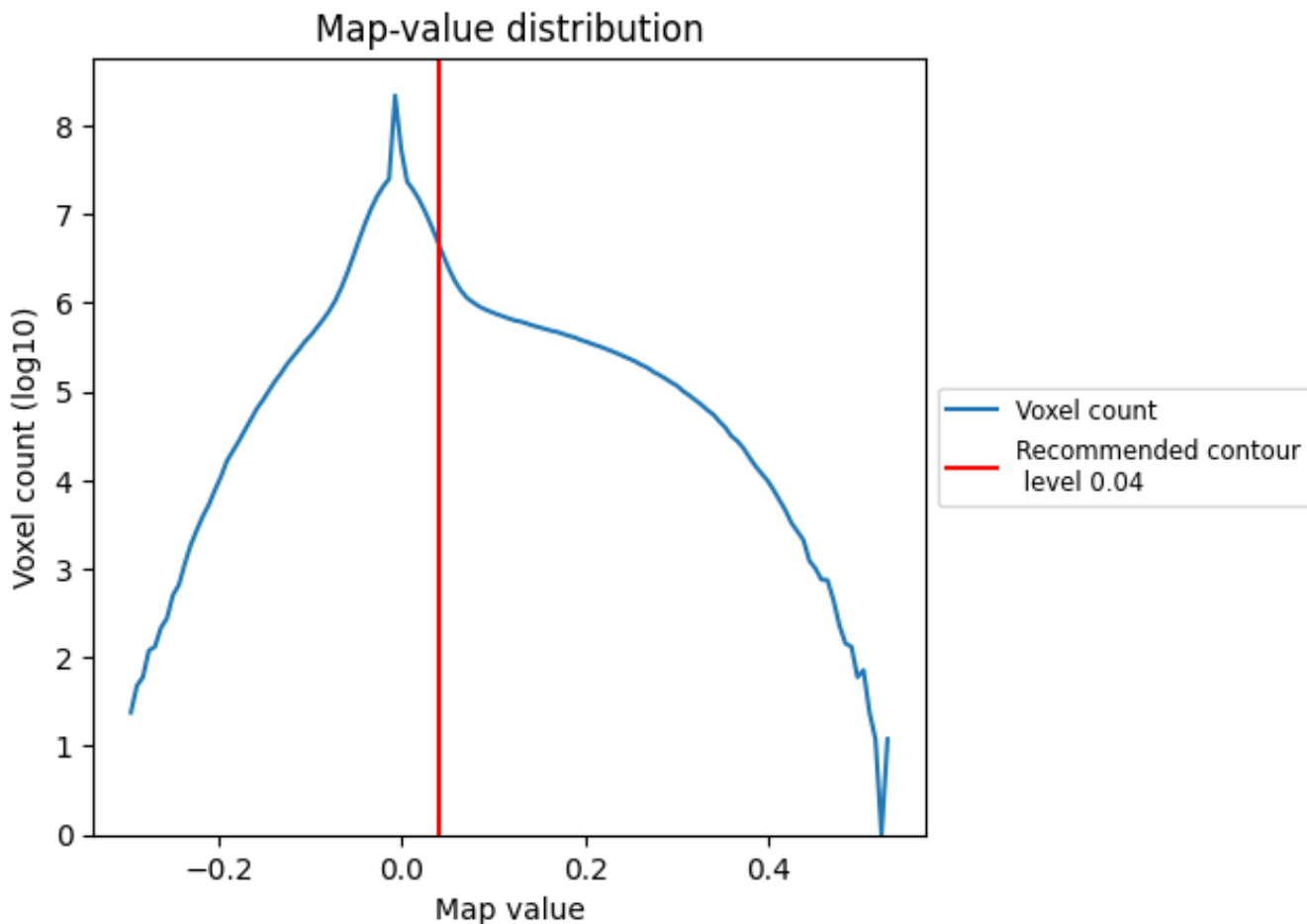
6.5 Mask visualisation

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

7 Map analysis [i](#)

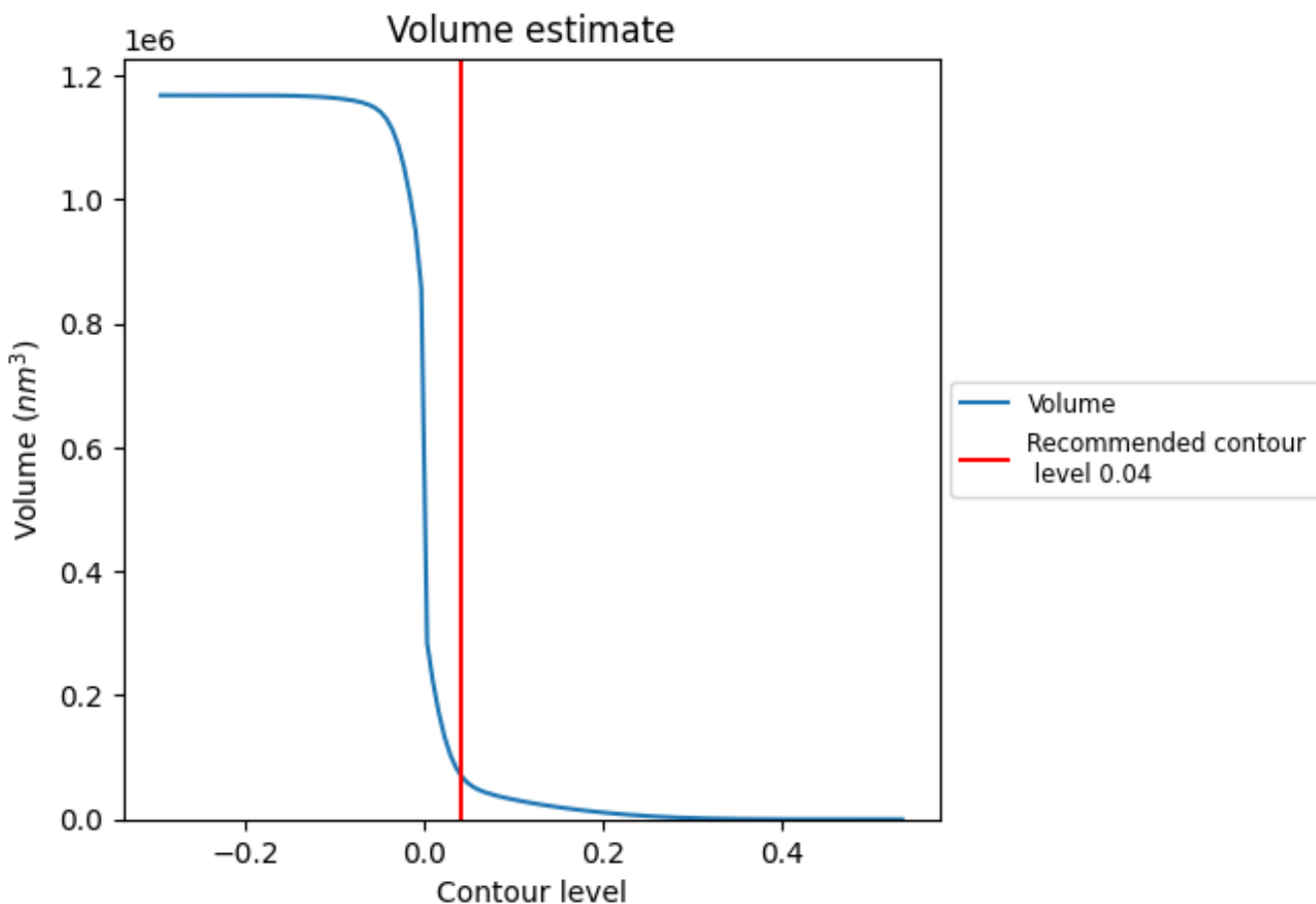
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

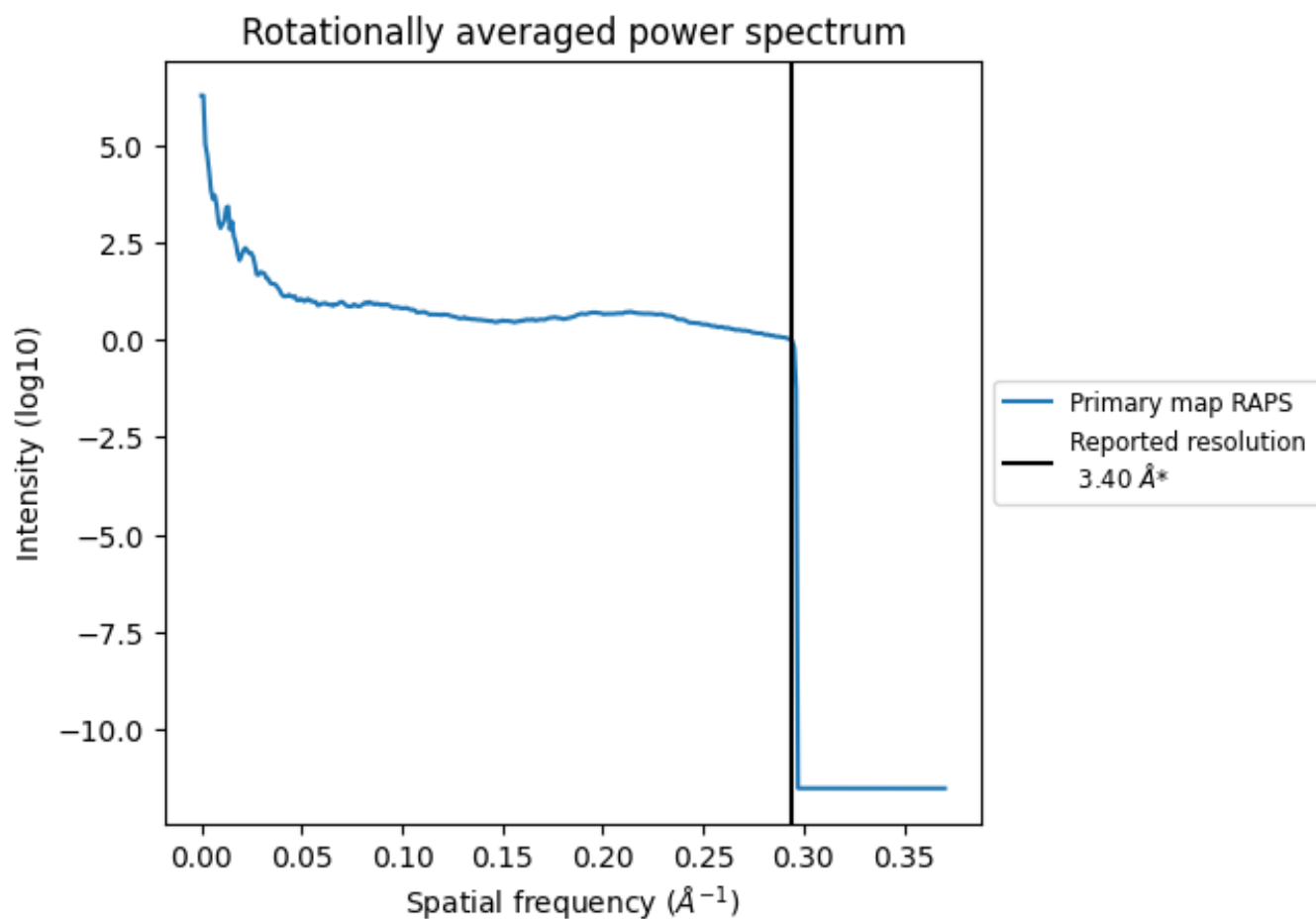
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73404 nm³; this corresponds to an approximate mass of 66308 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 i

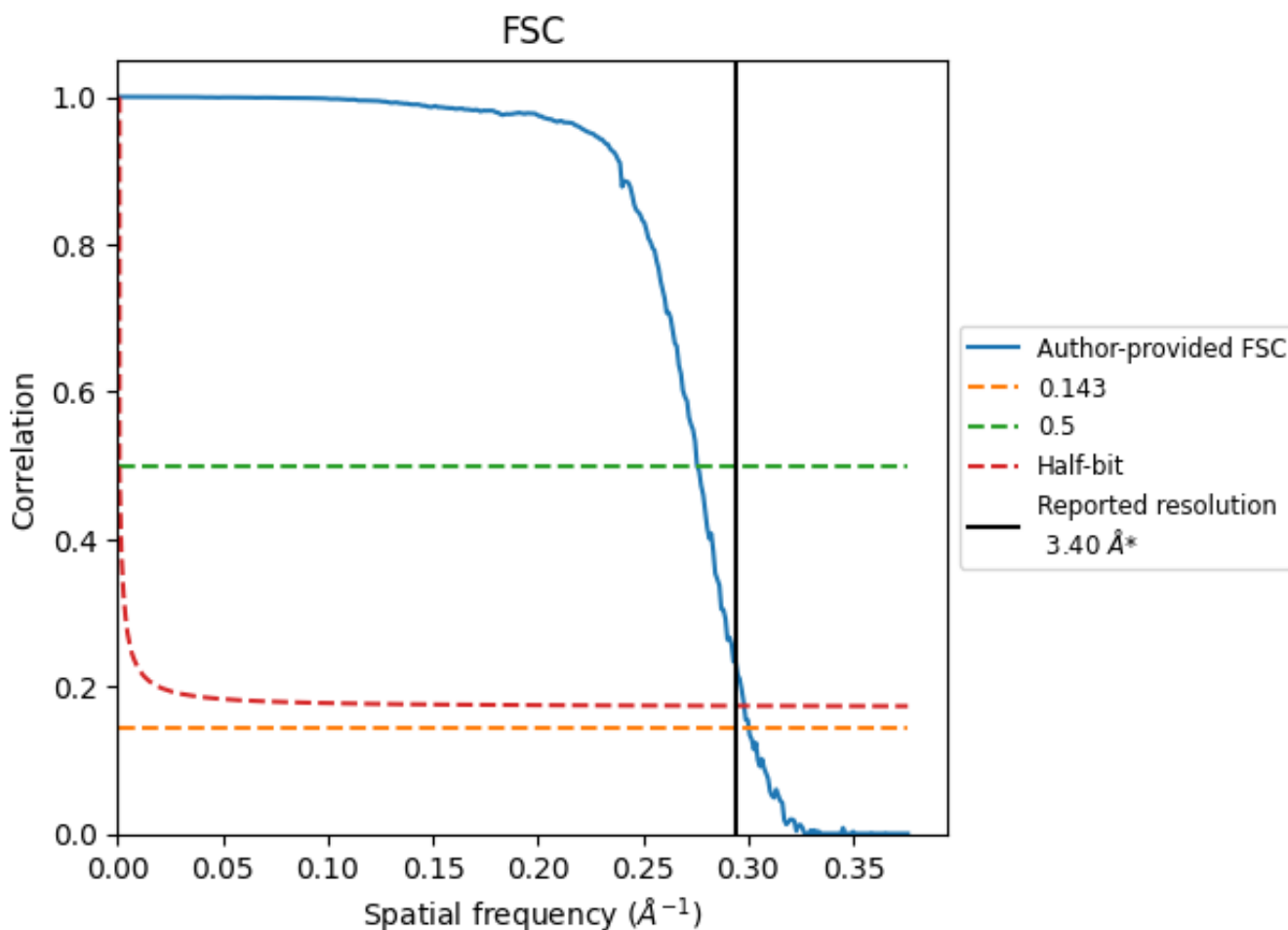


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.33	3.63	3.35
Unmasked-calculated*	-	-	-

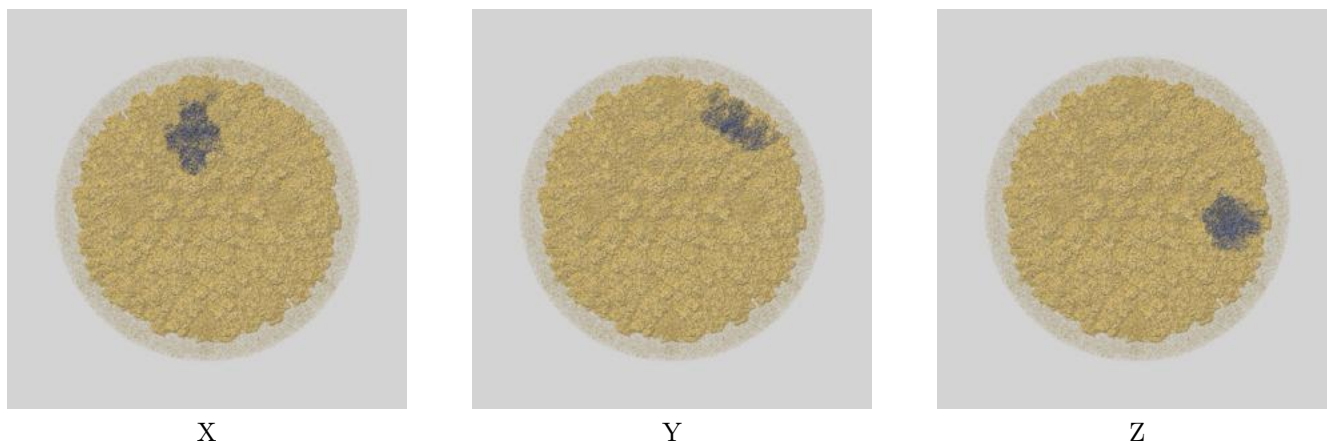
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

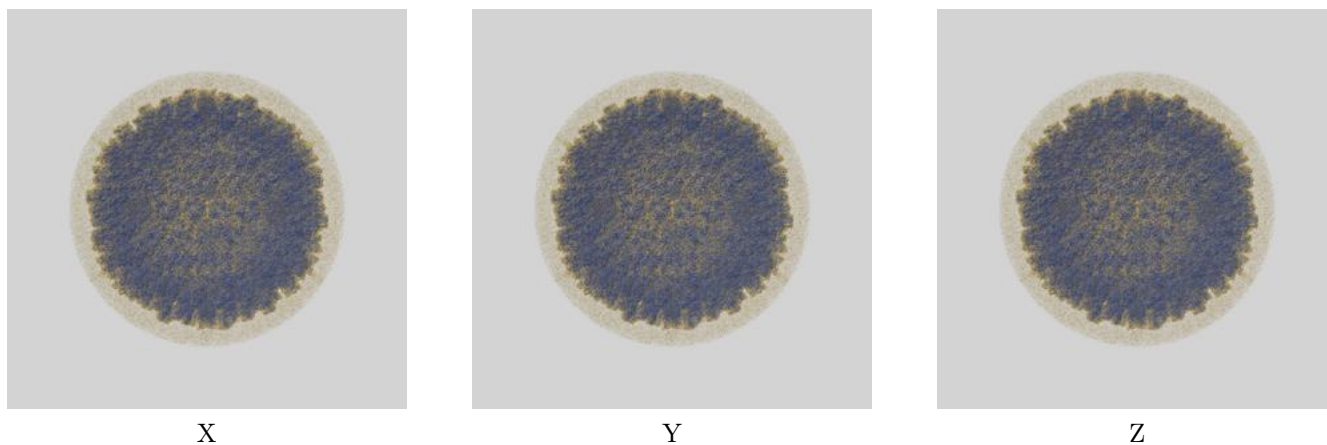
This section contains information regarding the fit between EMDB map EMD-4551 and PDB model 6QI5. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

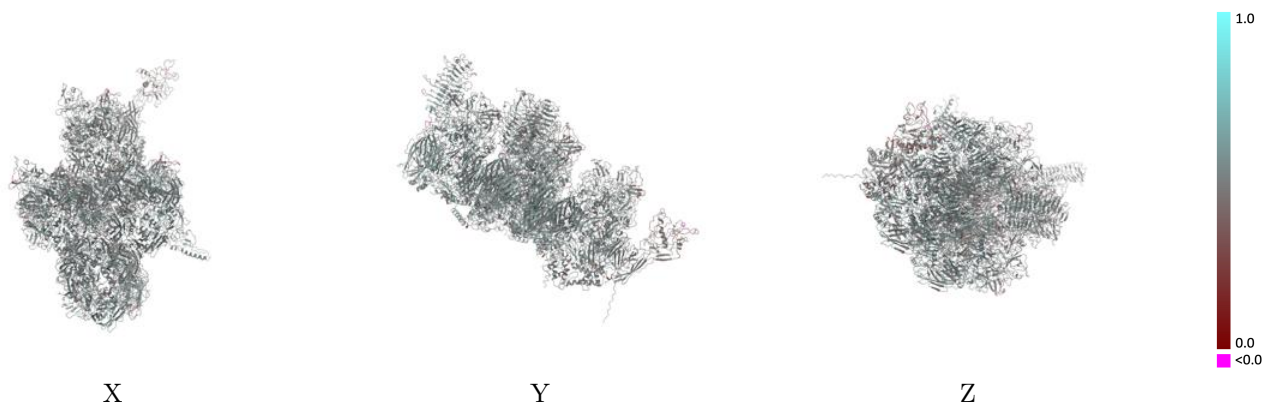


9.1.2 Map-model assembly overlay [i](#)



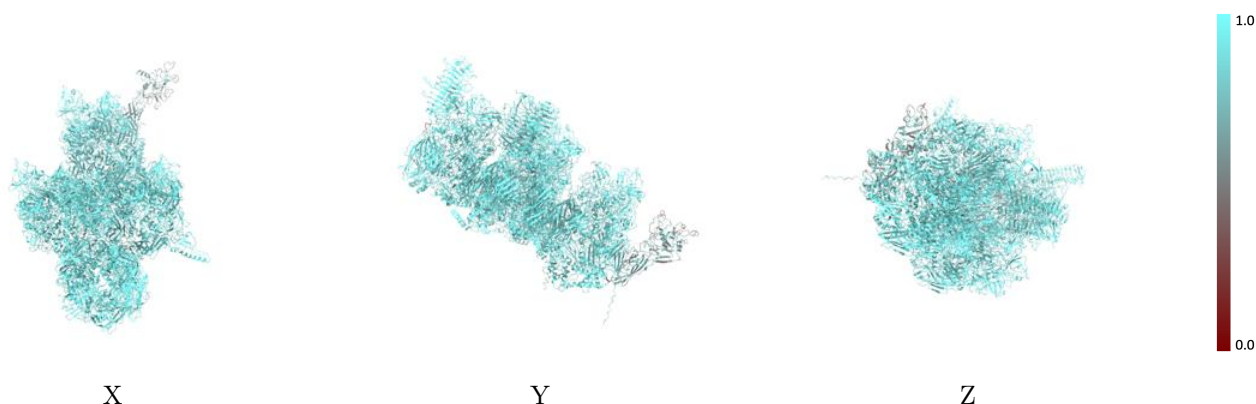
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



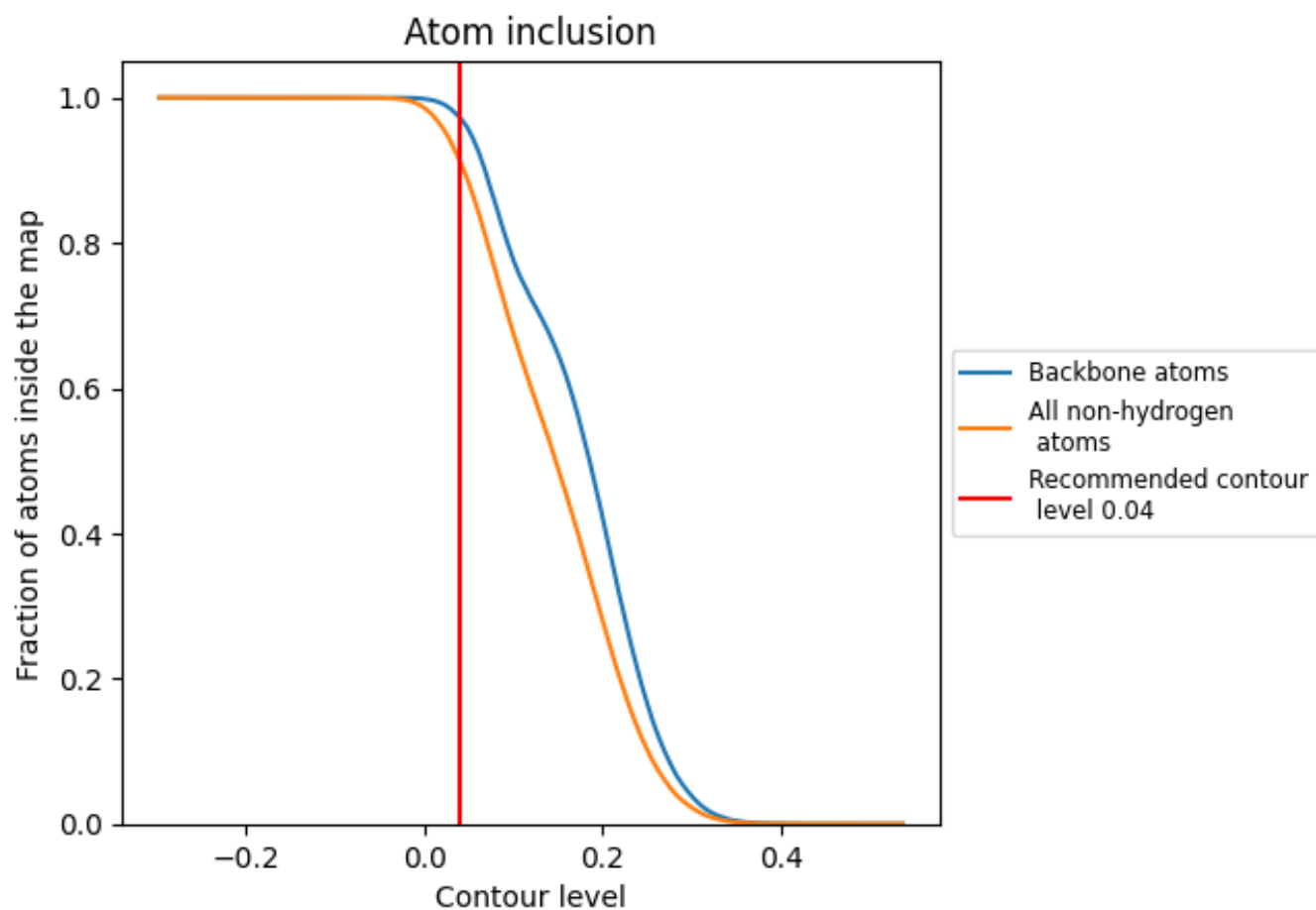
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9143	 0.5000
A	 0.9318	 0.4980
B	 0.9377	 0.4970
C	 0.9300	 0.5000
D	 0.9300	 0.5090
E	 0.9341	 0.5110
F	 0.9295	 0.5070
G	 0.9300	 0.5130
H	 0.9278	 0.5100
I	 0.9265	 0.5100
J	 0.9282	 0.5090
K	 0.9348	 0.5090
L	 0.9298	 0.5110
M	 0.5954	 0.4120
N	 0.8303	 0.4720
O	 0.8959	 0.5000
P	 0.8481	 0.4840
Q	 0.9131	 0.4810
R	 0.9177	 0.4850
S	 0.9082	 0.4790
T	 0.9202	 0.4870

