



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:51 AM UTC

PDB ID : 6QI5 / pdb_00006qi5
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:

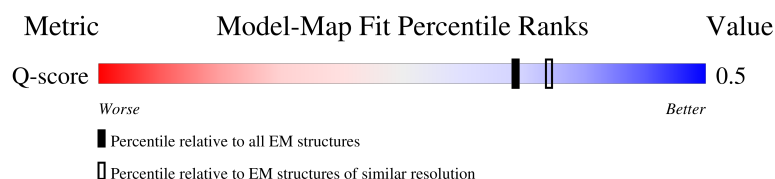
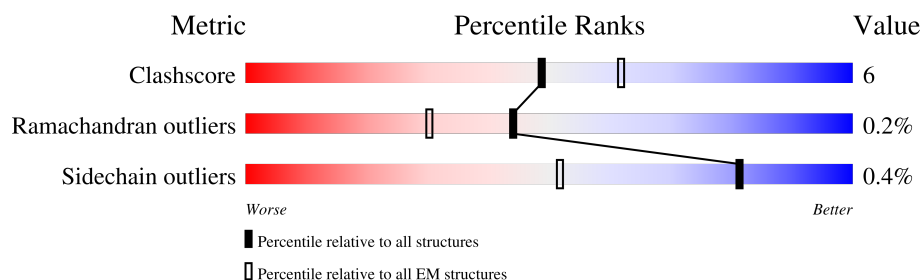
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	 83% 16%
1	B	909	 80% 19% ..
1	C	909	 82% 17%
1	D	909	 81% 18%

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Mol	Chain	Length	Quality of chain
1	E	909	 82% 18%
1	F	909	 84% 15%
1	G	909	 84% 15%
1	H	909	 82% 18%
1	I	909	 82% 17%
1	J	909	 84% 15%
1	K	909	 83% 16%
1	L	909	 83% 16%
2	Q	370	 83% 16% .
2	R	370	 82% 17% .
2	S	370	 82% 17% .
2	T	370	 85% 14% .
3	O	278	 61% 6% 33%
3	P	278	 61% 6% 33%
4	N	609	 38% 58% .
5	M	451	 15% 81% 19%

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
1	A	905	Total	C	N	O	S	0	0
			7168	4547	1226	1366	29		
1	L	906	Total	C	N	O	S	0	0
			7174	4550	1227	1368	29		
1	K	908	Total	C	N	O	S	0	0
			7184	4556	1229	1370	29		
1	J	906	Total	C	N	O	S	0	0
			7171	4548	1227	1368	28		
1	H	905	Total	C	N	O	S	0	0
			7166	4545	1226	1367	28		
1	I	906	Total	C	N	O	S	0	0
			7171	4548	1227	1368	28		
1	G	906	Total	C	N	O	S	0	0
			7171	4548	1227	1368	28		
1	F	906	Total	C	N	O	S	0	0
			7172	4548	1227	1368	29		
1	E	906	Total	C	N	O	S	0	0
			7171	4548	1227	1368	28		
1	D	906	Total	C	N	O	S	0	0
			7174	4550	1227	1368	29		
1	C	907	Total	C	N	O	S	0	0
			7179	4553	1228	1369	29		
1	B	904	Total	C	N	O	S	0	0
			7161	4542	1225	1365	29		

- Molecule 2 is a protein called Protein LH3.

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

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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		

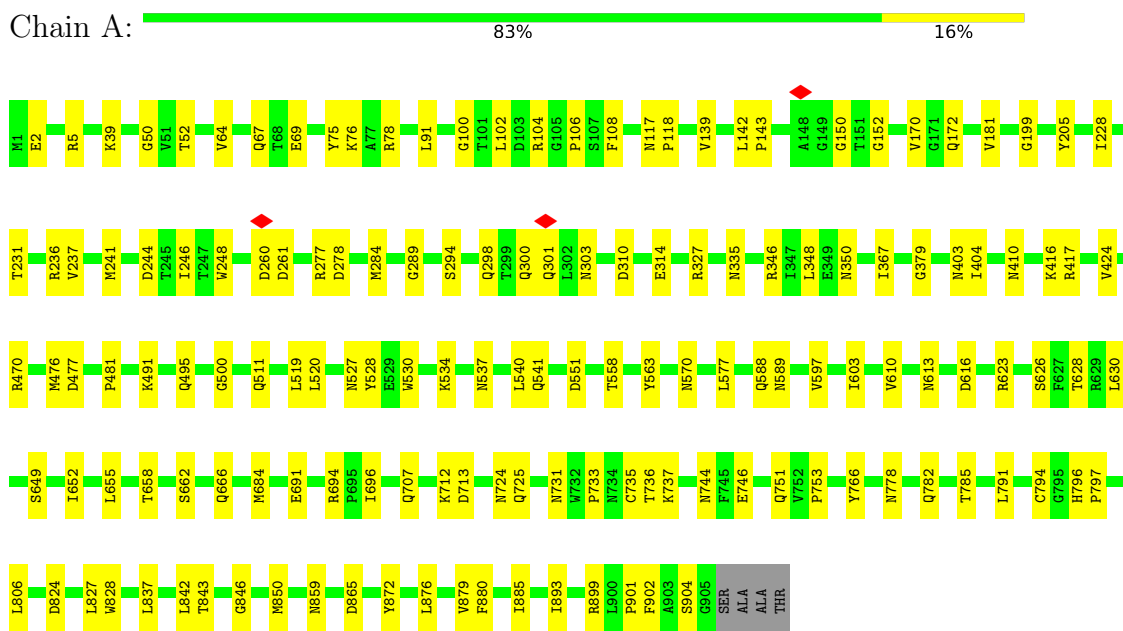
- Molecule 5 is a protein called Penton protein.

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

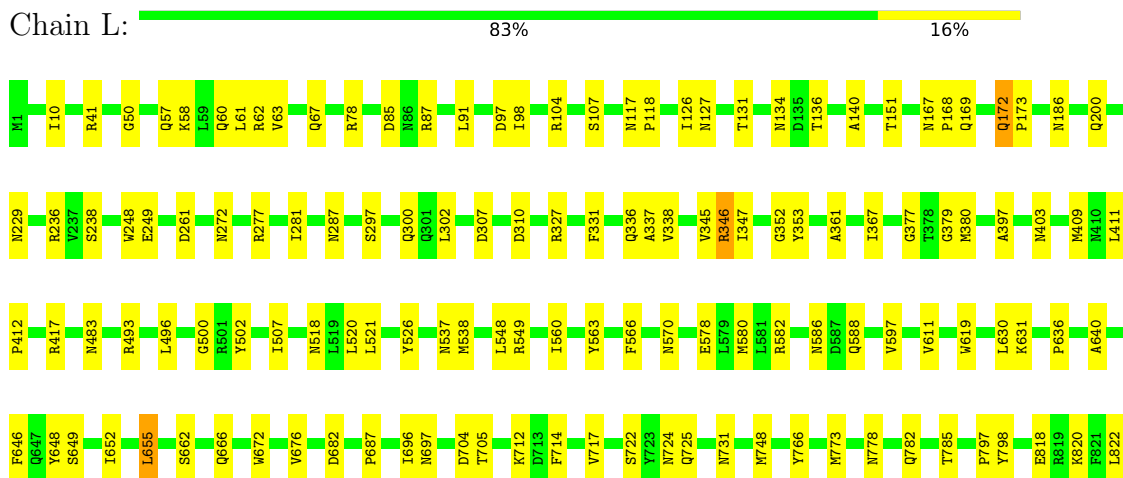
3 Residue-property plots

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



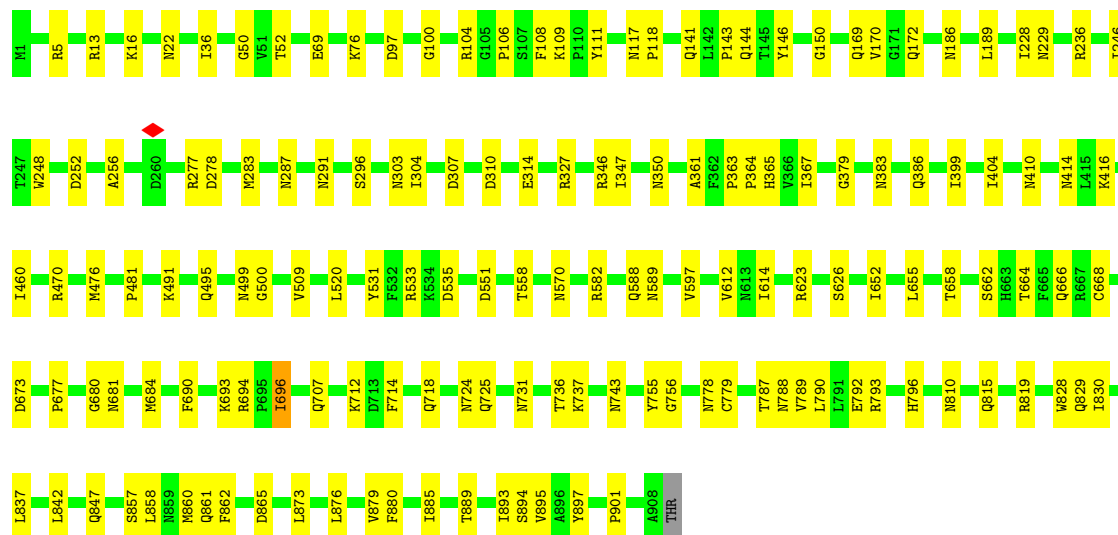
• Molecule 1: Hexon protein





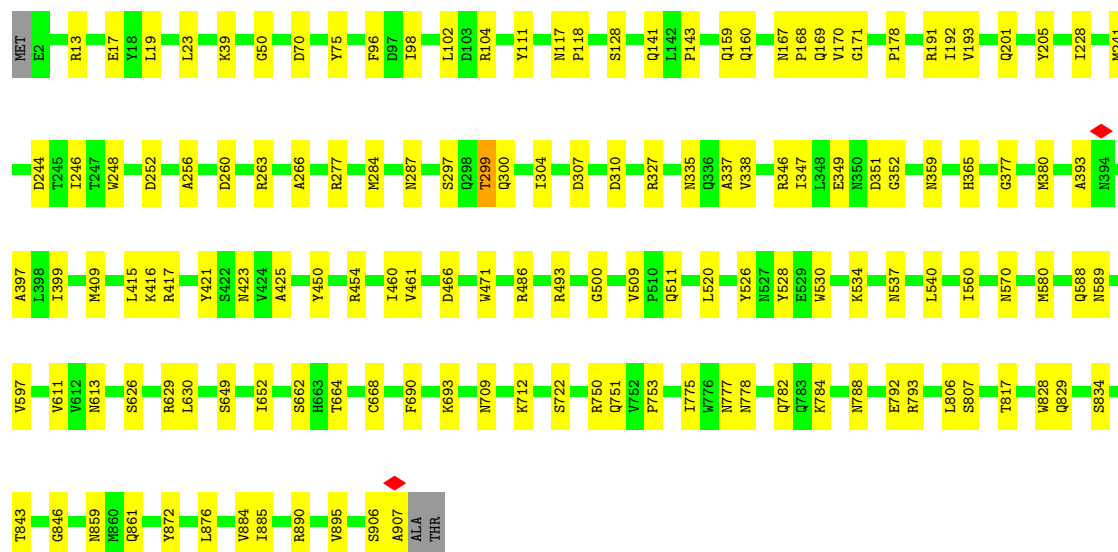
• Molecule 1: Hexon protein

Chain K: 83% 16%



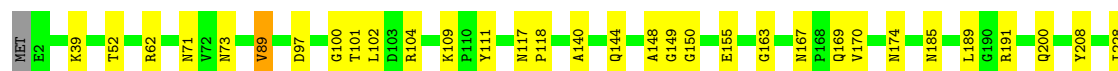
• Molecule 1: Hexon protein

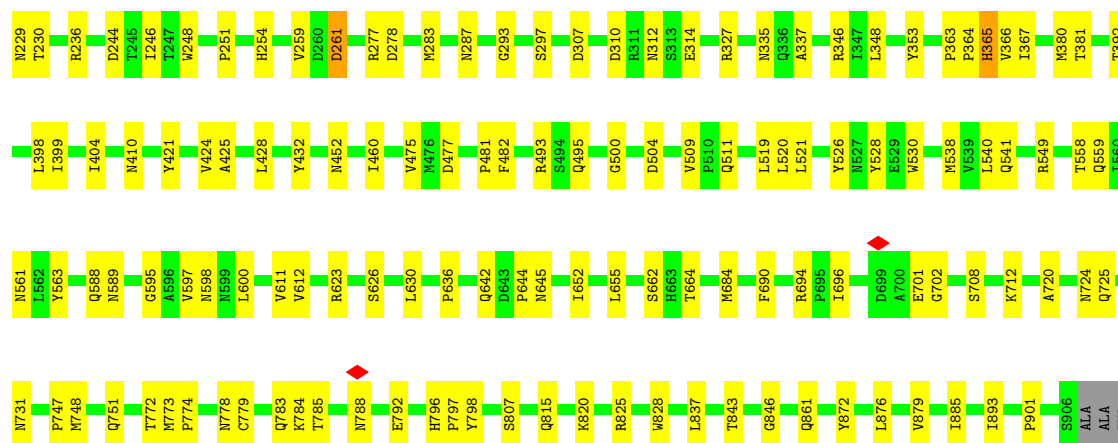
Chain J: 84% 15%



• Molecule 1: Hexon protein

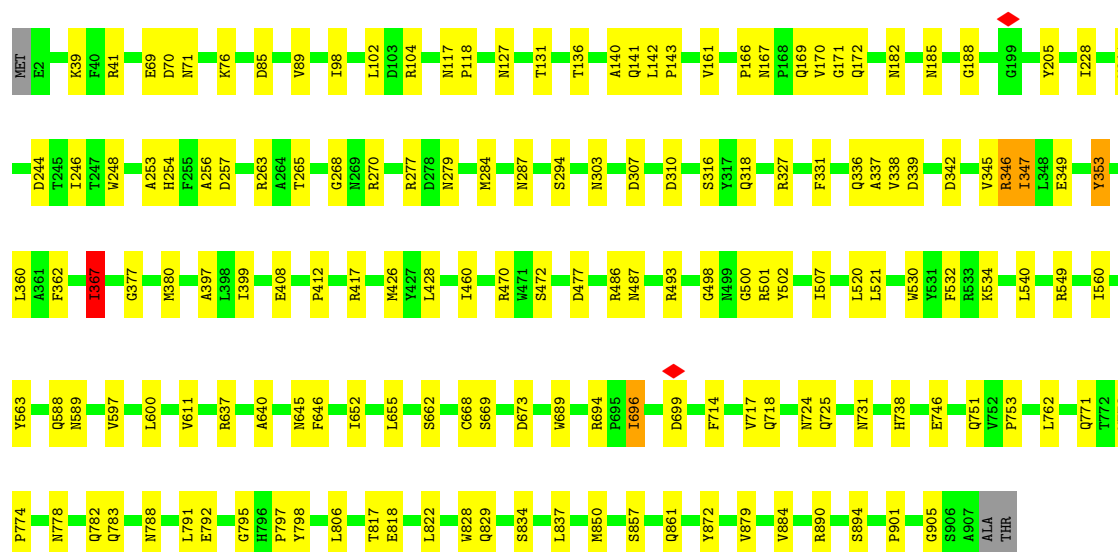
Chain H: 82% 18%





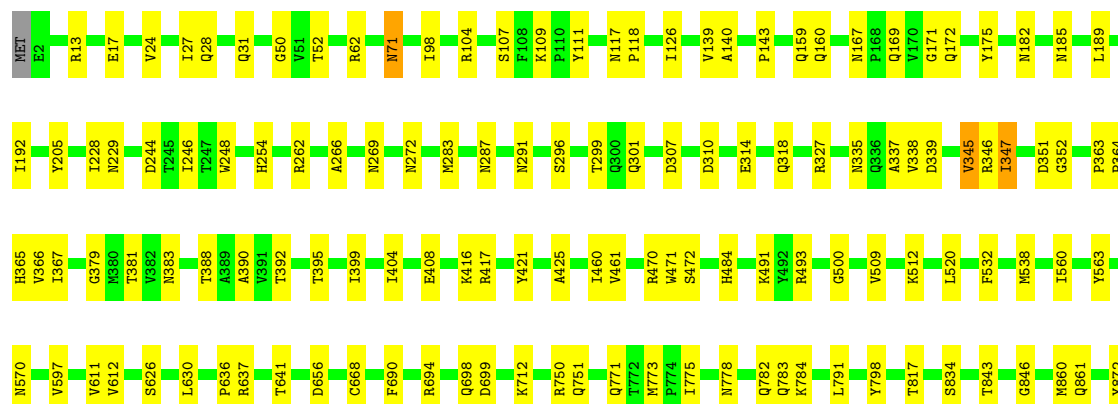
• Molecule 1: Hexon protein

Chain I: 82% 17%



• Molecule 1: Hexon protein

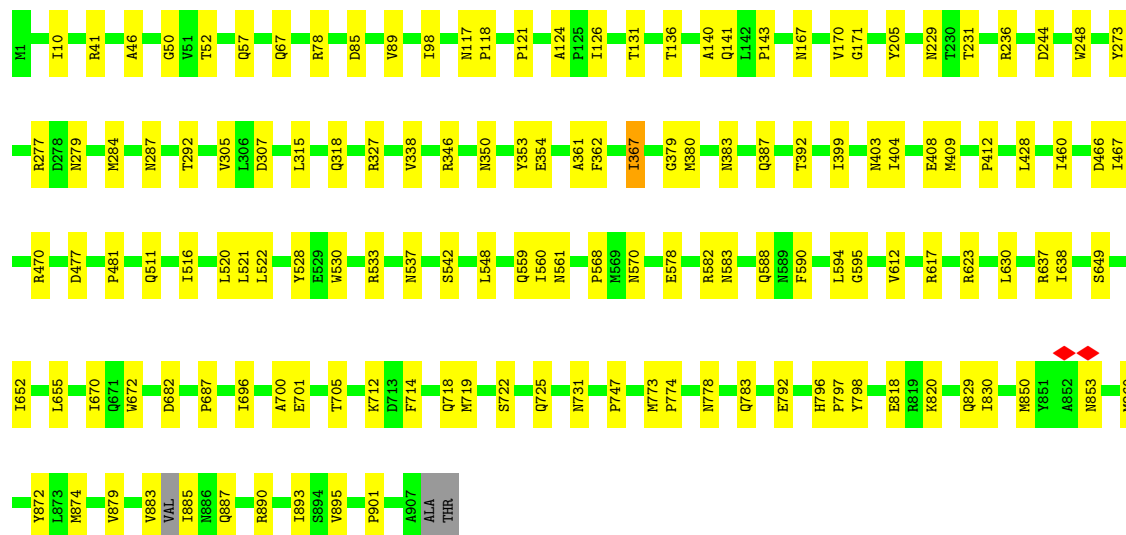
Chain G: 84% 15%





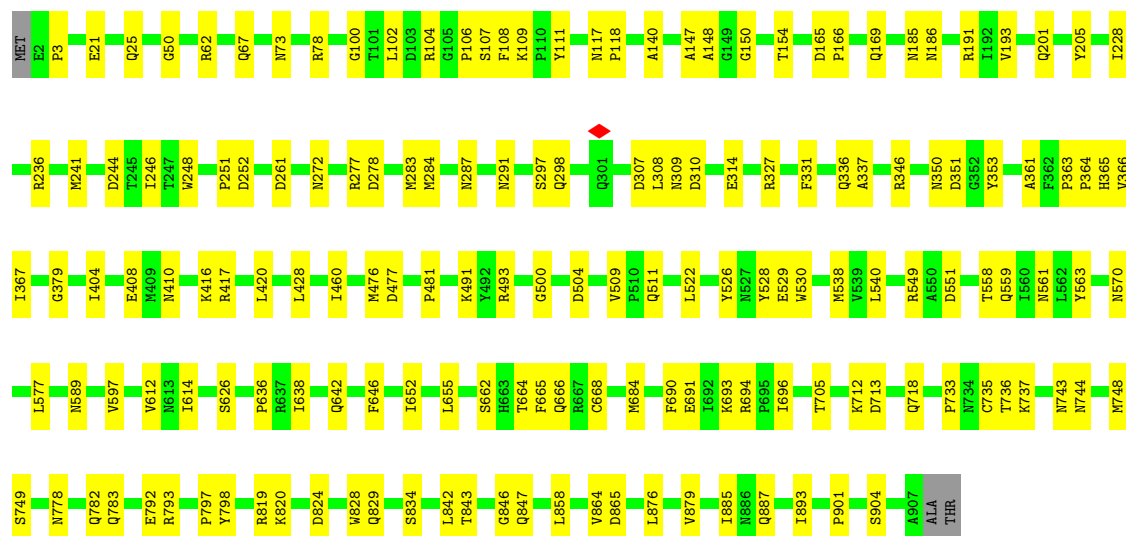
• Molecule 1: Hexon protein

Chain F: 84% 15%



• Molecule 1: Hexon protein

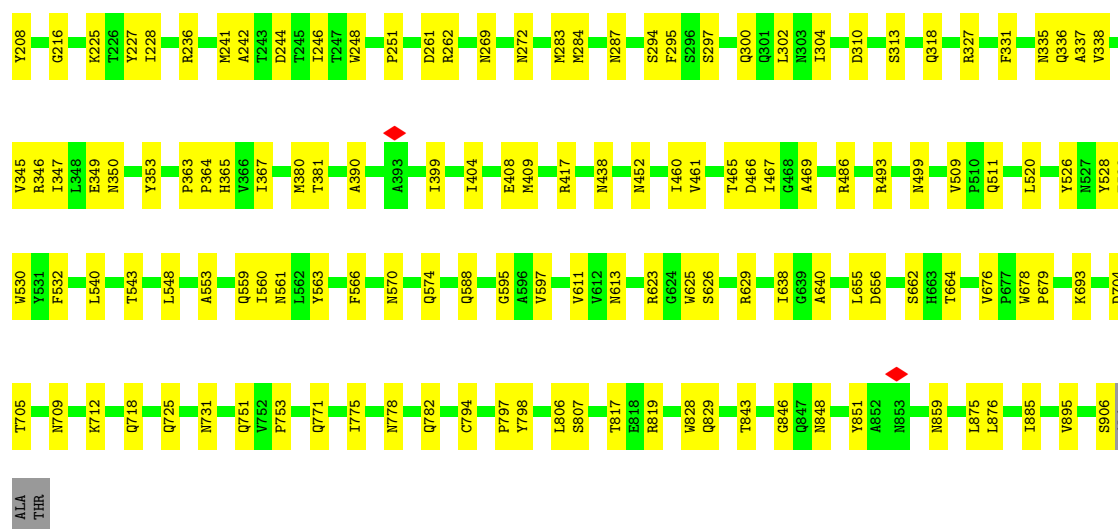
Chain E: 82% 18%



• Molecule 1: Hexon protein

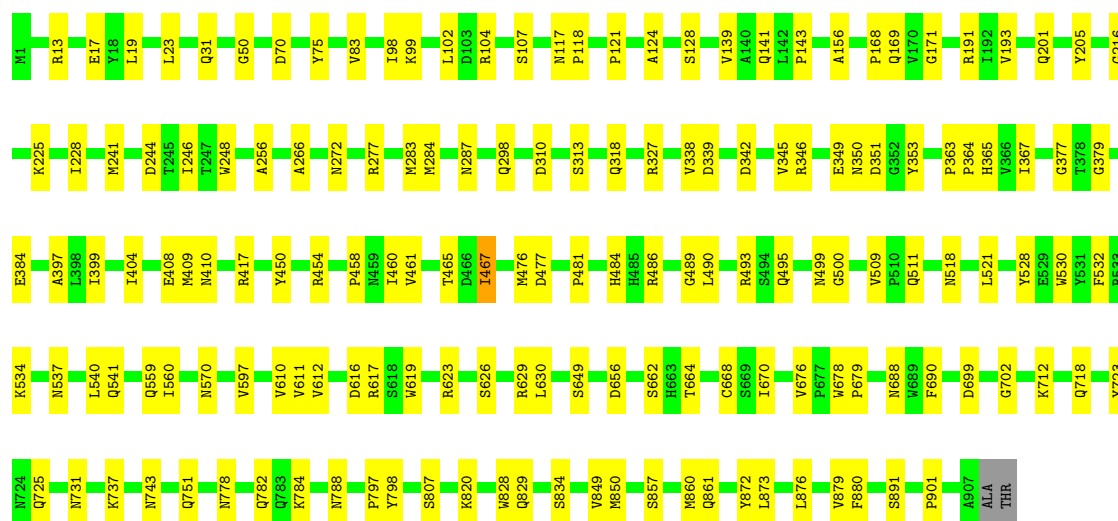
Chain D: 81% 18%





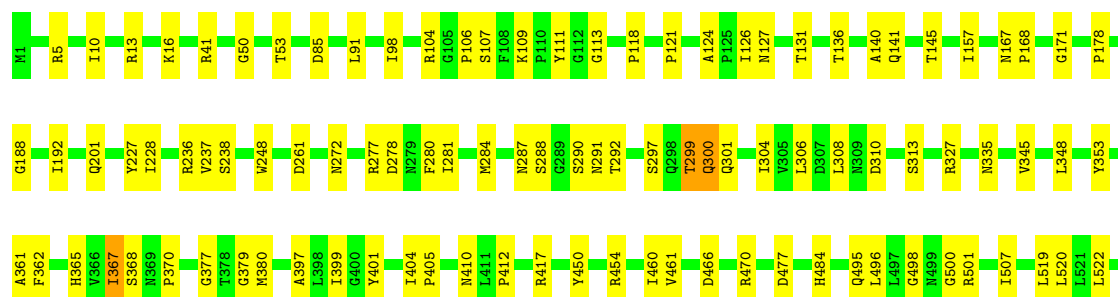
• Molecule 1: Hexon protein

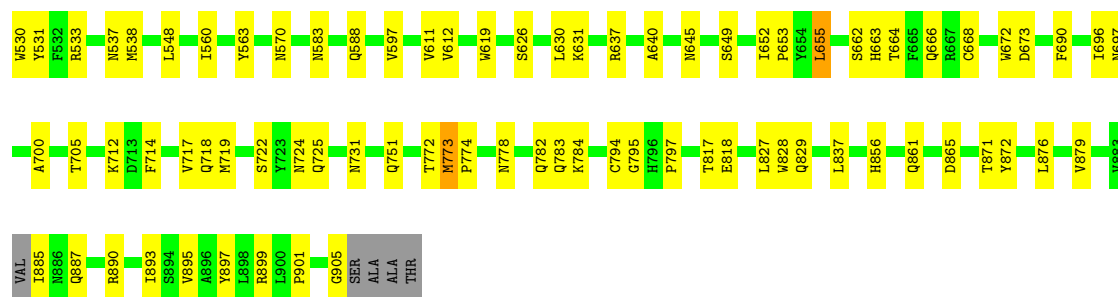
Chain C: 82% 17%



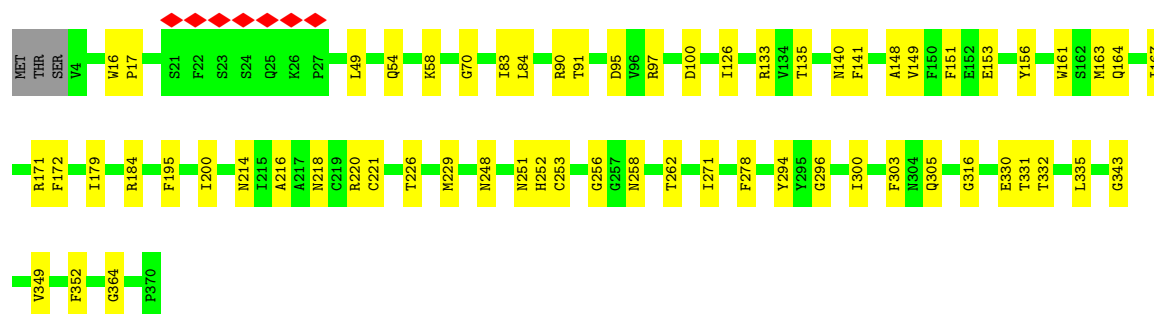
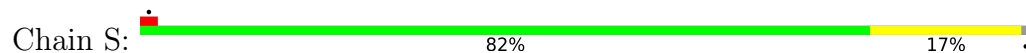
• Molecule 1: Hexon protein

Chain B: 80% 19%

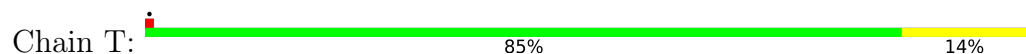




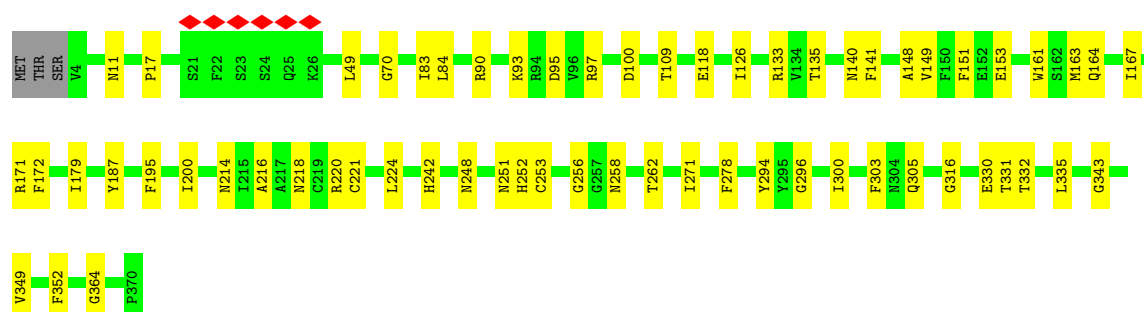
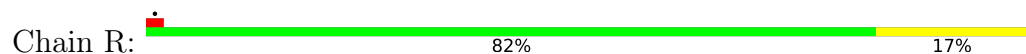
- Molecule 2: Protein LH3



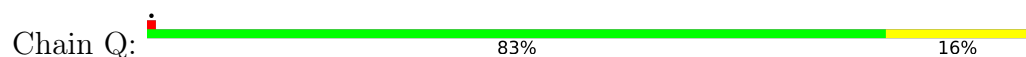
- Molecule 2: Protein LH3



- Molecule 2: Protein LH3

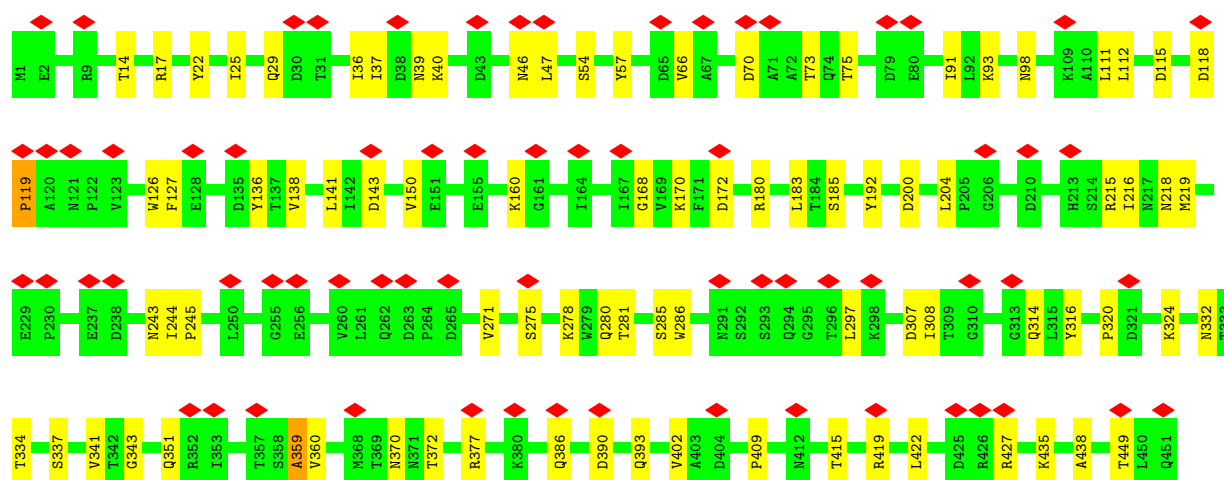


- Molecule 2: Protein LH3



SER SER SER VAL SER SER THR PRO THR PRO PHE GLU LEU PRO PRO GLY PHE ALA SER SER VAL ASN PRO LEU MET ARG PRO GLU GLY ASP ARG ASP VAL SER GLY THR GLY ILE VAL ASN PHE HIS SER LEU LYS PRO ARG ASN GLY LEU LIN

Chain M:



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 ($\text{\AA}$)	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 ($\text{\AA}$)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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	0.28	0/7373	0.58	2/10074 (0.0%)
1	B	0.27	0/7365	0.60	8/10061 (0.1%)
1	C	0.28	0/7384	0.57	2/10089 (0.0%)
1	D	0.30	0/7379	0.58	0/10082
1	E	0.29	0/7376	0.60	4/10079 (0.0%)
1	F	0.29	0/7376	0.59	4/10076 (0.0%)
1	G	0.30	0/7376	0.57	2/10079 (0.0%)
1	H	0.31	0/7371	0.60	2/10072 (0.0%)
1	I	0.30	0/7376	0.62	8/10079 (0.1%)
1	J	0.28	0/7376	0.56	2/10079 (0.0%)
1	K	0.29	0/7389	0.59	3/10096 (0.0%)
1	L	0.30	0/7379	0.59	2/10082 (0.0%)
2	Q	0.28	0/2954	0.54	2/4016 (0.0%)
2	R	0.28	0/2954	0.54	2/4016 (0.0%)
2	S	0.28	0/2954	0.54	2/4016 (0.0%)
2	T	0.28	0/2954	0.54	2/4016 (0.0%)
3	O	0.25	0/1494	0.56	0/2048
3	P	0.25	0/1494	0.56	0/2048
4	N	0.24	0/2014	0.58	0/2741
5	M	0.25	0/3660	0.64	2/5005 (0.0%)
All	All	0.29	0/108998	0.58	49/148854 (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 (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	696	ILE	CA-C-N	7.15	135.20	121.54
1	H	696	ILE	C-N-CA	7.15	135.20	121.54
1	I	367	ILE	N-CA-C	6.42	113.08	106.21
1	I	316	SER	N-CA-C	-5.79	106.76	113.88
1	B	773	MET	C-N-CD	-5.74	107.98	120.60
1	B	773	MET	CA-C-N	5.70	140.68	127.00
1	B	773	MET	C-N-CA	5.70	140.68	127.00
1	I	771	GLN	CA-C-N	5.64	132.32	121.54
1	I	771	GLN	C-N-CA	5.64	132.32	121.54
1	B	348	LEU	CA-CB-CG	5.61	135.93	116.30
1	E	696	ILE	CA-C-N	5.42	135.69	125.66
1	E	696	ILE	C-N-CA	5.42	135.69	125.66
1	J	299	THR	CA-C-N	5.33	131.72	121.54
1	J	299	THR	C-N-CA	5.33	131.72	121.54
1	B	672	TRP	CA-C-N	5.24	131.55	121.54
1	B	672	TRP	C-N-CA	5.24	131.55	121.54
1	A	696	ILE	CA-C-N	5.22	135.40	126.32
1	A	696	ILE	C-N-CA	5.22	135.40	126.32
1	K	681	ASN	N-CA-C	-5.20	104.75	111.71
1	I	696	ILE	CA-C-N	5.19	135.64	126.45
1	I	696	ILE	C-N-CA	5.19	135.64	126.45
1	F	672	TRP	CA-C-N	5.15	131.38	121.54
1	F	672	TRP	C-N-CA	5.15	131.38	121.54
2	T	305	GLN	CA-C-N	5.13	127.11	120.44
2	T	305	GLN	C-N-CA	5.13	127.11	120.44
5	M	359	ALA	CA-C-N	5.13	131.20	121.97
5	M	359	ALA	C-N-CA	5.13	131.20	121.97
2	S	305	GLN	CA-C-N	5.13	127.10	120.44
2	S	305	GLN	C-N-CA	5.13	127.10	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	305	GLN	CA-C-N	5.12	127.10	120.44
2	R	305	GLN	C-N-CA	5.12	127.10	120.44
1	E	251	PRO	CA-C-N	5.11	131.31	121.54
1	E	251	PRO	C-N-CA	5.11	131.31	121.54
2	Q	305	GLN	CA-C-N	5.11	127.09	120.44
2	Q	305	GLN	C-N-CA	5.11	127.09	120.44
1	I	353	TYR	CA-CB-CG	5.11	123.10	113.90
1	C	723	TYR	CA-C-N	5.11	131.29	121.54
1	C	723	TYR	C-N-CA	5.11	131.29	121.54
1	L	672	TRP	CA-C-N	5.08	131.24	121.54
1	L	672	TRP	C-N-CA	5.08	131.24	121.54
1	I	346	ARG	N-CA-C	-5.06	104.19	110.41
1	B	299	THR	CA-C-N	5.06	131.20	121.54
1	B	299	THR	C-N-CA	5.06	131.20	121.54
1	F	383	ASN	CA-C-N	5.05	131.19	121.54
1	F	383	ASN	C-N-CA	5.05	131.19	121.54
1	G	771	GLN	CA-C-N	5.04	131.17	121.54
1	G	771	GLN	C-N-CA	5.04	131.17	121.54
1	K	696	ILE	CA-C-N	5.01	135.03	126.32
1	K	696	ILE	C-N-CA	5.01	135.03	126.32

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

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Mol	Chain	Res	Type	Group
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
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

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	99	0
1	B	7161	0	6790	116	0
1	C	7179	0	6810	102	0
1	D	7174	0	6805	110	0
1	E	7171	0	6798	104	0
1	F	7172	0	6800	92	0
1	G	7171	0	6798	91	0
1	H	7166	0	6793	105	0
1	I	7171	0	6798	109	0
1	J	7171	0	6798	87	0
1	K	7184	0	6815	105	0
1	L	7174	0	6805	99	0
2	Q	2874	0	2742	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	2874	0	2742	44	0
2	S	2874	0	2742	40	0
2	T	2874	0	2742	27	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	54	0
All	All	106009	0	100897	1199	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 (1199) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:228:ILE:HG13	1:I:241:MET:HE2	1.80	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:C:228:ILE:HG12	1:C:241:MET:HE2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:H:380:MET:HE3	1:G:229:ASN:HD22	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:109:LYS:NZ	1:G:111:TYR:O	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:798:TYR:OH	1:G:244:ASP:OD2	2.24	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: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
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:205:TYR:HH	1:E:353:TYR:HH	1.55	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
1:D:1:MET:SD	1:D:1:MET:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:L:361:ALA:HB2	1:J:409:MET:HE2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:409:MET:HE2	1:B:361:ALA:HB2	1.88	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
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:70:ASP:OD1	1:J:534:LYS:NZ	2.40	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:K:22:ASN:HB3	1:J:580:MET:HE2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:563:TYR:HE2	1:K:712:LYS:HZ2	1.56	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:F:798:TYR:OH	1:D:244:ASP:OD2	2.24	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
1:J:417:ARG:NH2	1:J:782:GLN:OE1	2.41	0.53
1:G:538:MET:HE1	1:G:636:PRO:HG3	1.91	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:ILE:HG22	1:I:560:ILE:HG23	1.90	0.52
1:F:229:ASN:HD22	1:D:380:MET:HE3	1.74	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: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:F:850:MET:HE2	1:F:853:ASN:HA	1.90	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: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
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: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: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:A:205:TYR:HH	1:C:353:TYR:HH	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:156:ALA:O	1:C:225:LYS:NZ	2.41	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
1:G:314:GLU:OE2	1:G:512:LYS:NZ	2.43	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:H:684:MET:HE1	1:H:690:PHE:HA	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:K:97:ASP:OD1	1:J:712:LYS:NZ	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:684:MET:HE3	1:E:713:ASP:HB3	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
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:70:ASP:OD1	1:I:534:LYS:NZ	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:353:TYR:OH	1:I:205:TYR:OH	2.30	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
2:T:226:THR:OG1	2:T:229:MET:SD	2.71	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: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
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
1:E:228:ILE:HB	1:E:241:MET:HE1	1.95	0.47
2:R:253:CYS:O	2:R:258:ASN:ND2	2.48	0.47
1:A:684:MET:HE3	1:A:713:ASP:HB2	1.97	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:F:477:ASP:OD2	1:F:820:LYS:NZ	2.40	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:421:TYR:HA	1:H:425:ALA:HB3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:M:141:LEU:HD13	5:M:219:MET:HE1	1.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:381:THR:OG1	1:G:392:THR:OG1	2.34	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
1:A:563:TYR:HE2	1:C:712:LYS:HZ3	1.62	0.46
1:K:111:TYR:OH	1:K:252:ASP:OD2	2.32	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:S:226:THR:OG1	2:S:229:MET:SD	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:126:ILE:HB	2:T:149:VAL:HG12	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
1:E:205:TYR:HH	1:D:353:TYR:HH	1.56	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
1:F:361:ALA:HB2	1:D:409:MET:HE2	1.98	0.45
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:K:858:LEU:HD21	1:K:860:MET:HE3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:619:TRP:HA	1:B:901:PRO:HB3	1.98	0.45
2:Q:226:THR:OG1	2:Q:229:MET:SD	2.71	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: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
1:B:109:LYS:NZ	1:B:111:TYR:O	2.49	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
1:B:297:SER:OG	1:B:300:GLN:O	2.33	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
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:L:229:ASN:HD22	1:J:380:MET:HE3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:689:TRP:CG	2:S:16:TRP:HE1	2.36	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
1:B:380:MET:HB2	1:B:380:MET:HE2	1.80	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:472:SER:OG	1:I:477:ASP:OD1	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:109:LYS:NZ	1:B:113:GLY:O	2.47	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:109:LYS:NZ	1:H:111:TYR:O	2.44	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
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:H:538:MET:HE1	1:H:636:PRO:HG3	2.00	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
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:L:538:MET:HE1	1:L:636:PRO:HG3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:850:MET:HE1	1:D:906:SER:HB2	2.02	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:E:538:MET:HE1	1:E:636:PRO:HG3	2.02	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:39:LYS:NZ	1:C:518:ASN:O	2.46	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:F:315:LEU:HD13	1:F:874:MET:HE1	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:229:ASN:HB2	1:I:380:MET:HE3	2.02	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
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:L:748:MET:HE3	1:L:820:LYS:HG3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:380:MET:HE1	1:K:229:ASN:HB2	2.03	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
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:542:SER:OG	1:F:649:SER:OG	2.33	0.41
1:F:774:PRO:HB2	1:D:216:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:228:ILE:HG12	1:D:241:MET:HE2	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	903/909 (99%)	825 (91%)	77 (8%)	1 (0%)	48 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	900/909 (99%)	816 (91%)	82 (9%)	2 (0%)	43	71
1	C	905/909 (100%)	816 (90%)	87 (10%)	2 (0%)	43	71
1	D	904/909 (99%)	838 (93%)	65 (7%)	1 (0%)	48	78
1	E	904/909 (99%)	835 (92%)	68 (8%)	1 (0%)	48	78
1	F	902/909 (99%)	829 (92%)	73 (8%)	0	100	100
1	G	904/909 (99%)	834 (92%)	68 (8%)	2 (0%)	43	71
1	H	903/909 (99%)	822 (91%)	79 (9%)	2 (0%)	43	71
1	I	904/909 (99%)	829 (92%)	73 (8%)	2 (0%)	43	71
1	J	904/909 (99%)	841 (93%)	61 (7%)	2 (0%)	43	71
1	K	906/909 (100%)	822 (91%)	82 (9%)	2 (0%)	43	71
1	L	904/909 (99%)	833 (92%)	67 (7%)	4 (0%)	30	59
2	Q	365/370 (99%)	325 (89%)	39 (11%)	1 (0%)	36	65
2	R	365/370 (99%)	325 (89%)	39 (11%)	1 (0%)	36	65
2	S	365/370 (99%)	325 (89%)	39 (11%)	1 (0%)	36	65
2	T	365/370 (99%)	326 (89%)	38 (10%)	1 (0%)	36	65
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%)	18	47
All	All	13369/14004 (96%)	12183 (91%)	1158 (9%)	28 (0%)	44	71

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
1	B	673	ASP
5	M	359	ALA
1	A	658	THR

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Mol	Chain	Res	Type
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 ⓘ

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%)	773 (100%)	2 (0%)	86	84
1	B	774/777 (100%)	769 (99%)	5 (1%)	78	80
1	C	776/777 (100%)	773 (100%)	3 (0%)	84	83
1	D	776/777 (100%)	773 (100%)	3 (0%)	84	83
1	E	775/777 (100%)	771 (100%)	4 (0%)	81	81
1	F	775/777 (100%)	771 (100%)	4 (0%)	81	81
1	G	775/777 (100%)	773 (100%)	2 (0%)	86	84
1	H	775/777 (100%)	769 (99%)	6 (1%)	73	77
1	I	775/777 (100%)	771 (100%)	4 (0%)	81	81
1	J	775/777 (100%)	773 (100%)	2 (0%)	86	84
1	K	776/777 (100%)	775 (100%)	1 (0%)	88	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	776/777 (100%)	775 (100%)	1 (0%)	88	89
2	Q	301/304 (99%)	300 (100%)	1 (0%)	86	84
2	R	301/304 (99%)	300 (100%)	1 (0%)	86	84
2	S	301/304 (99%)	300 (100%)	1 (0%)	86	84
2	T	301/304 (99%)	300 (100%)	1 (0%)	86	84
3	O	158/234 (68%)	158 (100%)	0	100	100
3	P	158/234 (68%)	158 (100%)	0	100	100
4	N	226/520 (44%)	226 (100%)	0	100	100
5	M	406/406 (100%)	406 (100%)	0	100	100
All	All	11455/11934 (96%)	11414 (100%)	41 (0%)	81	83

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	A	577	LEU
1	L	655	LEU
1	K	612	VAL
1	J	193	VAL
1	J	335	ASN
1	H	71	ASN
1	H	89	VAL
1	H	259	VAL
1	H	335	ASN
1	H	612	VAL
1	H	664	THR
1	I	71	ASN
1	I	367	ILE
1	I	655	LEU
1	I	788	ASN
1	G	71	ASN
1	G	335	ASN
1	F	367	ILE
1	F	583	ASN
1	F	612	VAL
1	F	655	LEU
1	E	185	ASN
1	E	193	VAL
1	E	577	LEU

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Mol	Chain	Res	Type
1	E	612	VAL
1	D	193	VAL
1	D	335	ASN
1	D	467	ILE
1	C	193	VAL
1	C	467	ILE
1	C	612	VAL
1	B	367	ILE
1	B	583	ASN
1	B	612	VAL
1	B	655	LEU
1	B	664	THR
2	S	271	ILE
2	T	271	ILE
2	R	271	ILE
2	Q	271	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (373) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	86	ASN
1	A	117	ASN
1	A	200	GLN
1	A	234	ASN
1	A	272	ASN
1	A	291	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	588	GLN
1	A	599	ASN
1	A	703	ASN
1	A	724	ASN
1	A	725	GLN
1	A	829	GLN
1	A	838	ASN
1	A	853	ASN

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Mol	Chain	Res	Type
1	A	856	HIS
1	L	35	ASN
1	L	82	ASN
1	L	134	ASN
1	L	141	GLN
1	L	167	ASN
1	L	254	HIS
1	L	335	ASN
1	L	350	ASN
1	L	359	ASN
1	L	403	ASN
1	L	410	ASN
1	L	414	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	771	GLN
1	L	783	GLN
1	L	788	ASN
1	L	829	GLN
1	L	847	GLN
1	K	9	HIS
1	K	82	ASN
1	K	117	ASN
1	K	141	GLN
1	K	167	ASN
1	K	234	ASN
1	K	279	ASN
1	K	318	GLN
1	K	329	HIS
1	K	336	GLN
1	K	359	ASN
1	K	369	ASN
1	K	414	ASN
1	K	423	ASN
1	K	561	ASN
1	K	588	GLN
1	K	598	ASN

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Mol	Chain	Res	Type
1	K	703	ASN
1	K	709	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	K	859	ASN
1	J	22	ASN
1	J	31	GLN
1	J	82	ASN
1	J	117	ASN
1	J	141	GLN
1	J	159	GLN
1	J	169	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
1	J	365	HIS
1	J	537	ASN
1	J	574	GLN
1	J	588	GLN
1	J	599	ASN
1	J	602	GLN
1	J	613	ASN
1	J	671	GLN
1	J	681	ASN
1	J	709	ASN
1	J	725	GLN
1	J	738	HIS
1	J	777	ASN
1	J	783	GLN
1	J	788	ASN
1	J	829	GLN
1	J	853	ASN
1	J	859	ASN

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Mol	Chain	Res	Type
1	J	882	GLN
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	141	GLN
1	H	174	ASN
1	H	200	GLN
1	H	300	GLN
1	H	335	ASN
1	H	359	ASN
1	H	383	ASN
1	H	403	ASN
1	H	487	ASN
1	H	511	GLN
1	H	559	GLN
1	H	574	GLN
1	H	588	GLN
1	H	598	ASN
1	H	707	GLN
1	H	724	ASN
1	H	725	GLN
1	H	751	GLN
1	H	758	ASN
1	H	783	GLN
1	H	853	ASN
1	H	856	HIS
1	I	71	ASN
1	I	117	ASN
1	I	127	ASN
1	I	137	HIS
1	I	141	GLN
1	I	172	GLN
1	I	182	ASN
1	I	185	ASN
1	I	233	ASN
1	I	301	GLN
1	I	303	ASN
1	I	350	ASN
1	I	359	ASN

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Mol	Chain	Res	Type
1	I	445	HIS
1	I	487	ASN
1	I	559	GLN
1	I	561	ASN
1	I	574	GLN
1	I	588	GLN
1	I	642	GLN
1	I	707	GLN
1	I	724	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	60	GLN
1	G	71	ASN
1	G	73	ASN
1	G	82	ASN
1	G	117	ASN
1	G	159	GLN
1	G	169	GLN
1	G	172	GLN
1	G	182	ASN
1	G	185	ASN
1	G	200	GLN
1	G	335	ASN
1	G	350	ASN
1	G	359	ASN
1	G	383	ASN
1	G	414	ASN
1	G	452	ASN
1	G	574	GLN
1	G	598	ASN
1	G	725	GLN
1	G	734	ASN
1	G	738	HIS
1	G	751	GLN
1	G	829	GLN
1	G	856	HIS
1	F	67	GLN

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Mol	Chain	Res	Type
1	F	141	GLN
1	F	169	GLN
1	F	287	ASN
1	F	336	GLN
1	F	343	HIS
1	F	344	HIS
1	F	350	ASN
1	F	383	ASN
1	F	387	GLN
1	F	414	ASN
1	F	445	HIS
1	F	506	HIS
1	F	537	ASN
1	F	561	ASN
1	F	574	GLN
1	F	583	ASN
1	F	586	ASN
1	F	588	GLN
1	F	598	ASN
1	F	671	GLN
1	F	698	GLN
1	F	725	GLN
1	F	738	HIS
1	F	829	GLN
1	F	887	GLN
1	E	25	GLN
1	E	31	GLN
1	E	60	GLN
1	E	82	ASN
1	E	117	ASN
1	E	141	GLN
1	E	167	ASN
1	E	172	GLN
1	E	182	ASN
1	E	185	ASN
1	E	186	ASN
1	E	234	ASN
1	E	272	ASN
1	E	303	ASN
1	E	309	ASN
1	E	336	GLN
1	E	359	ASN

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Mol	Chain	Res	Type
1	E	383	ASN
1	E	403	ASN
1	E	423	ASN
1	E	511	GLN
1	E	599	ASN
1	E	724	ASN
1	E	725	GLN
1	E	777	ASN
1	E	838	ASN
1	E	856	HIS
1	D	117	ASN
1	D	127	ASN
1	D	134	ASN
1	D	144	GLN
1	D	172	GLN
1	D	185	ASN
1	D	287	ASN
1	D	291	ASN
1	D	301	GLN
1	D	335	ASN
1	D	336	GLN
1	D	344	HIS
1	D	387	GLN
1	D	438	ASN
1	D	445	HIS
1	D	452	ASN
1	D	487	ASN
1	D	574	GLN
1	D	588	GLN
1	D	599	ASN
1	D	602	GLN
1	D	709	ASN
1	D	725	GLN
1	D	738	HIS
1	D	751	GLN
1	D	777	ASN
1	D	783	GLN
1	D	829	GLN
1	D	838	ASN
1	D	856	HIS
1	D	882	GLN
1	C	4	GLN

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Mol	Chain	Res	Type
1	C	22	ASN
1	C	35	ASN
1	C	57	GLN
1	C	117	ASN
1	C	141	GLN
1	C	167	ASN
1	C	169	GLN
1	C	172	GLN
1	C	185	ASN
1	C	201	GLN
1	C	229	ASN
1	C	287	ASN
1	C	359	ASN
1	C	369	ASN
1	C	387	GLN
1	C	495	GLN
1	C	537	ASN
1	C	559	GLN
1	C	574	GLN
1	C	599	ASN
1	C	602	GLN
1	C	688	ASN
1	C	709	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	C	887	GLN
1	B	35	ASN
1	B	82	ASN
1	B	141	GLN
1	B	167	ASN
1	B	201	GLN
1	B	287	ASN
1	B	343	HIS
1	B	350	ASN
1	B	387	GLN
1	B	403	ASN
1	B	414	ASN
1	B	445	HIS

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Mol	Chain	Res	Type
1	B	527	ASN
1	B	537	ASN
1	B	588	GLN
1	B	602	GLN
1	B	642	GLN
1	B	724	ASN
1	B	725	GLN
1	B	738	HIS
1	B	769	ASN
1	B	783	GLN
1	B	829	GLN
1	B	838	ASN
1	B	847	GLN
1	B	882	GLN
2	S	14	ASN
2	S	54	GLN
2	S	194	ASN
2	S	218	ASN
2	T	15	GLN
2	T	54	GLN
2	T	194	ASN
2	T	252	HIS
2	R	11	ASN
2	R	54	GLN
2	R	218	ASN
2	Q	11	ASN
2	Q	54	GLN
2	Q	218	ASN
2	Q	280	ASN
3	P	44	GLN
3	P	47	ASN
3	P	79	GLN
3	P	235	ASN
3	O	44	GLN
3	O	47	ASN
3	O	79	GLN
3	O	109	GLN
3	O	235	ASN
4	N	29	GLN
4	N	34	GLN
4	N	99	ASN
4	N	144	GLN

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Mol	Chain	Res	Type
4	N	145	HIS
4	N	176	GLN
4	N	218	ASN
5	M	23	ASN
5	M	29	GLN
5	M	33	HIS
5	M	46	ASN
5	M	74	GLN
5	M	175	ASN
5	M	218	ASN
5	M	270	HIS
5	M	345	HIS
5	M	351	GLN
5	M	363	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 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.

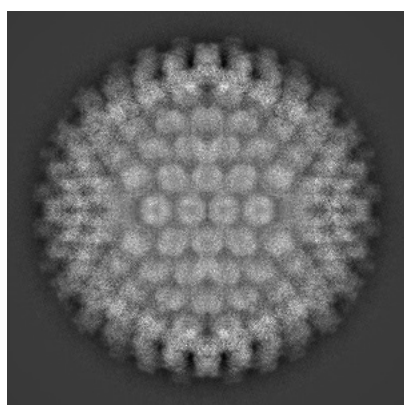
6 Map visualisation [i](#)

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

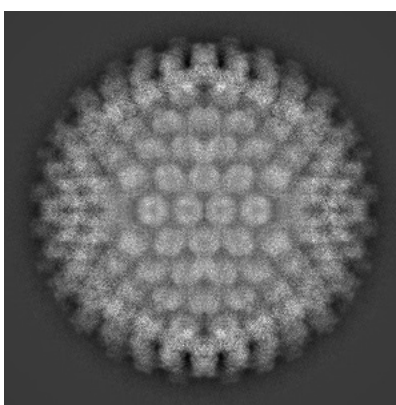
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

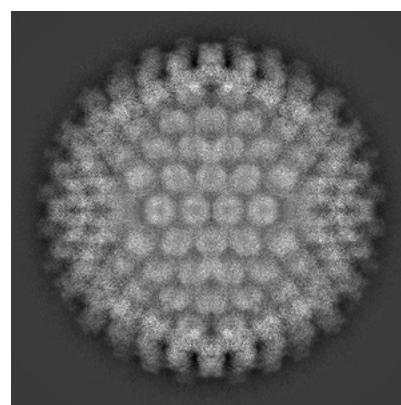
6.1.1 Primary map



X



Y

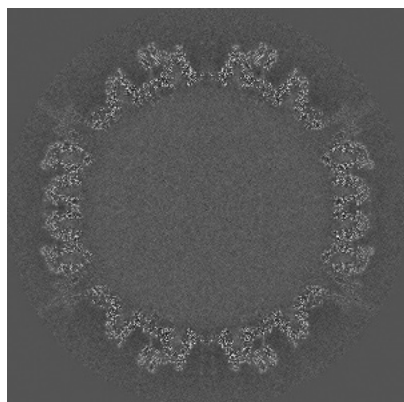


Z

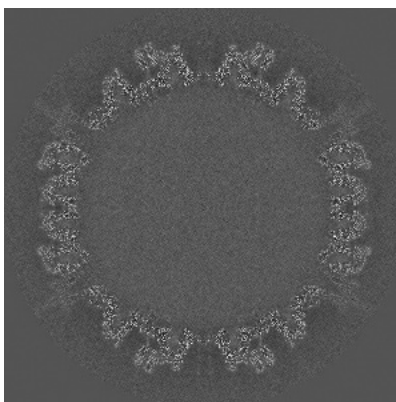
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

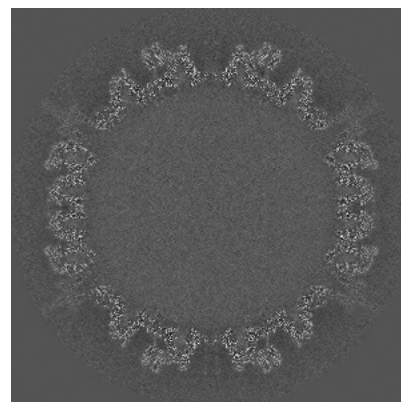
6.2.1 Primary map



X Index: 390



Y Index: 390

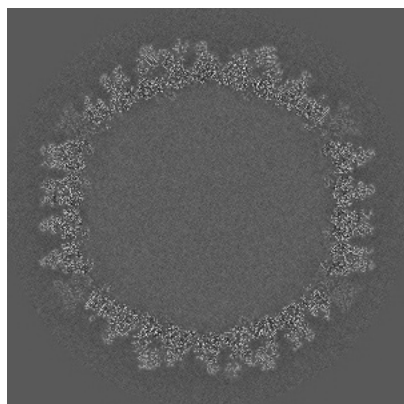


Z Index: 390

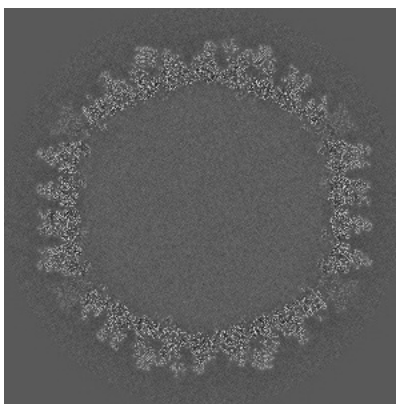
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

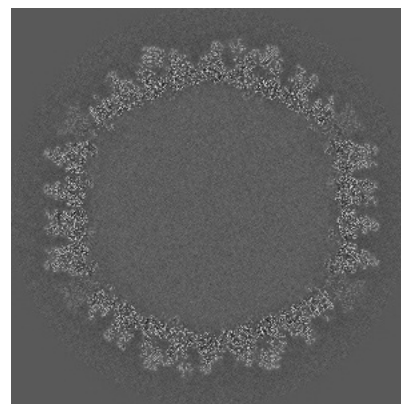
6.3.1 Primary map



X Index: 404



Y Index: 376

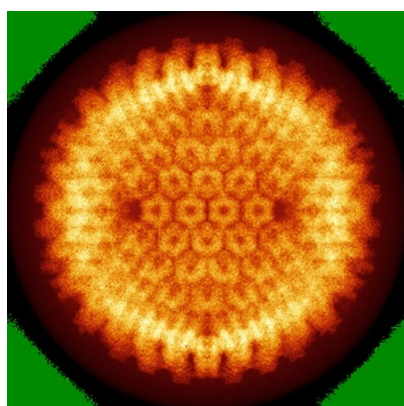


Z Index: 376

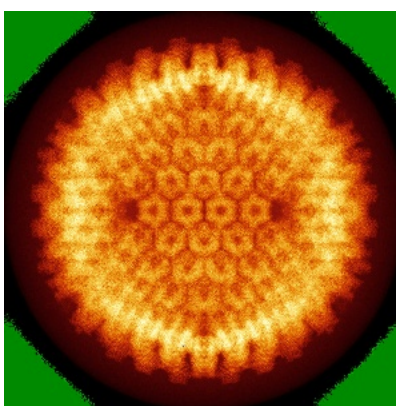
The images above show the largest variance slices of the map in three orthogonal directions.

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

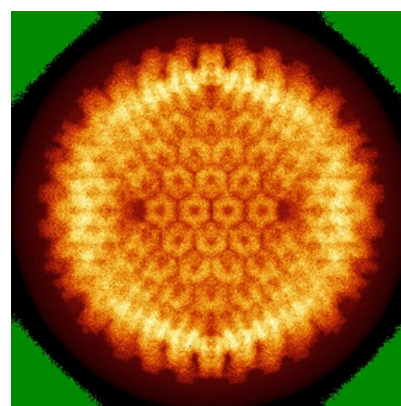
6.4.1 Primary map



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

This section was not generated.

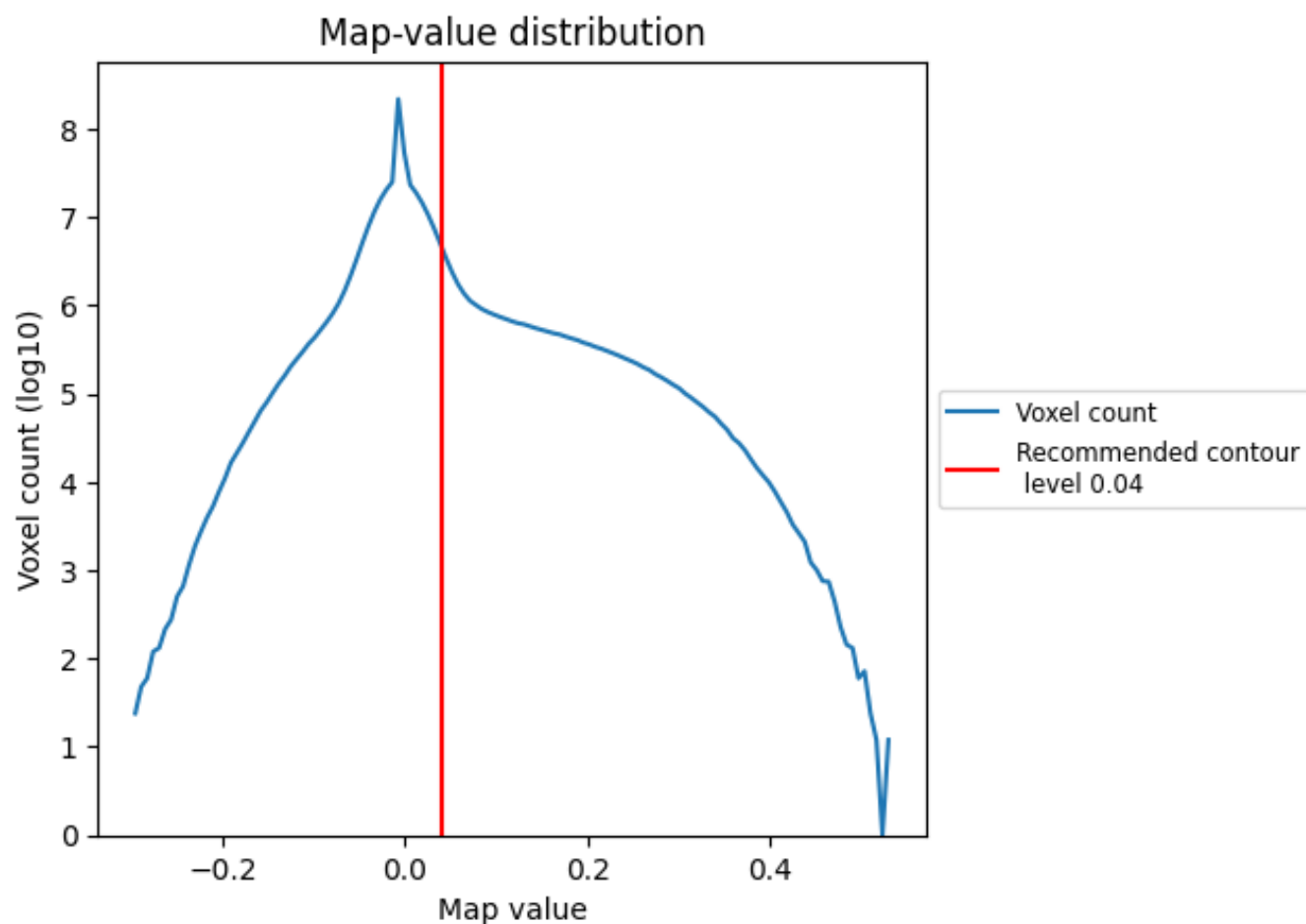
6.6 Mask visualisation

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

7 Map analysis [i](#)

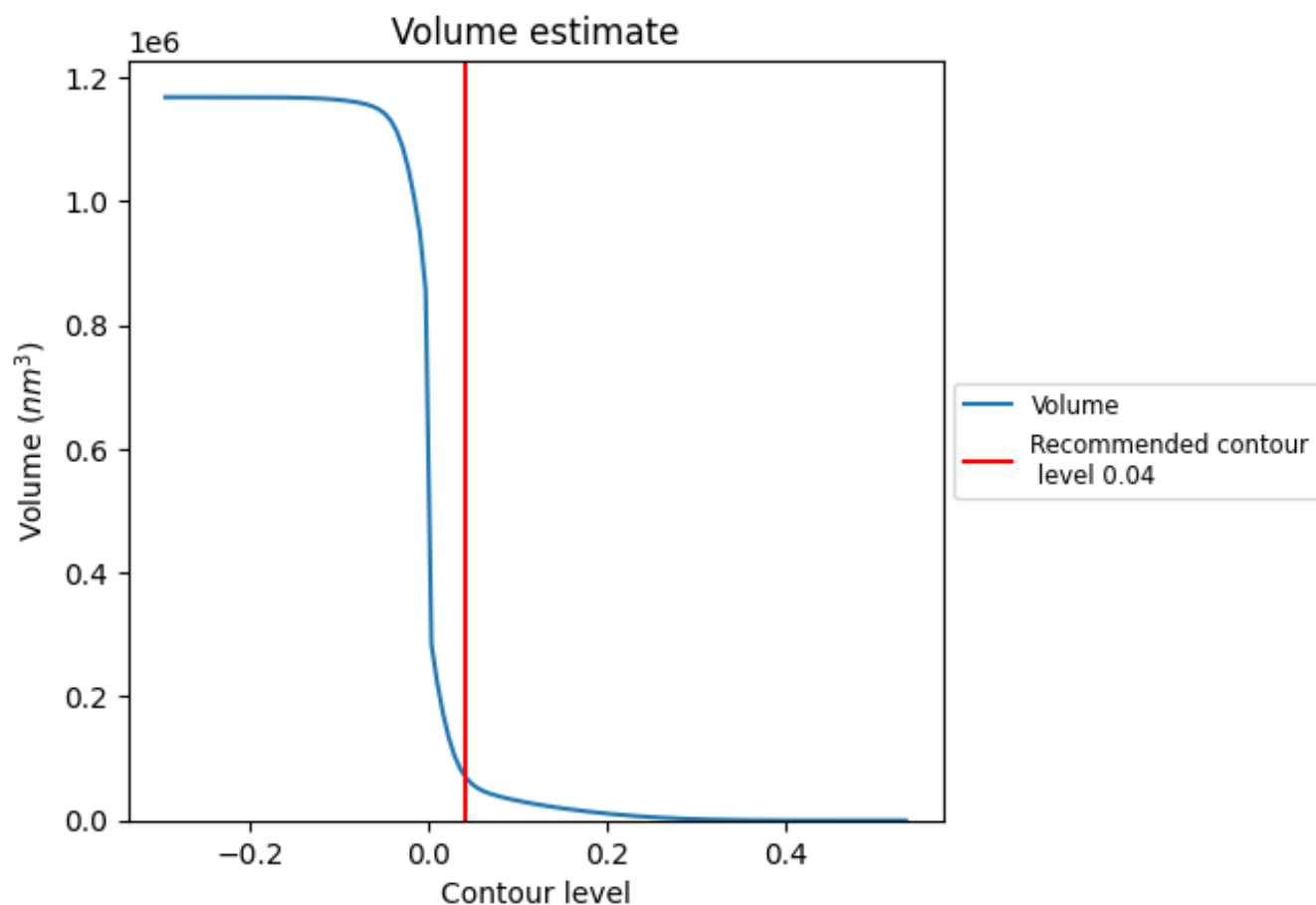
This section contains the results of statistical analysis of the map.

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.

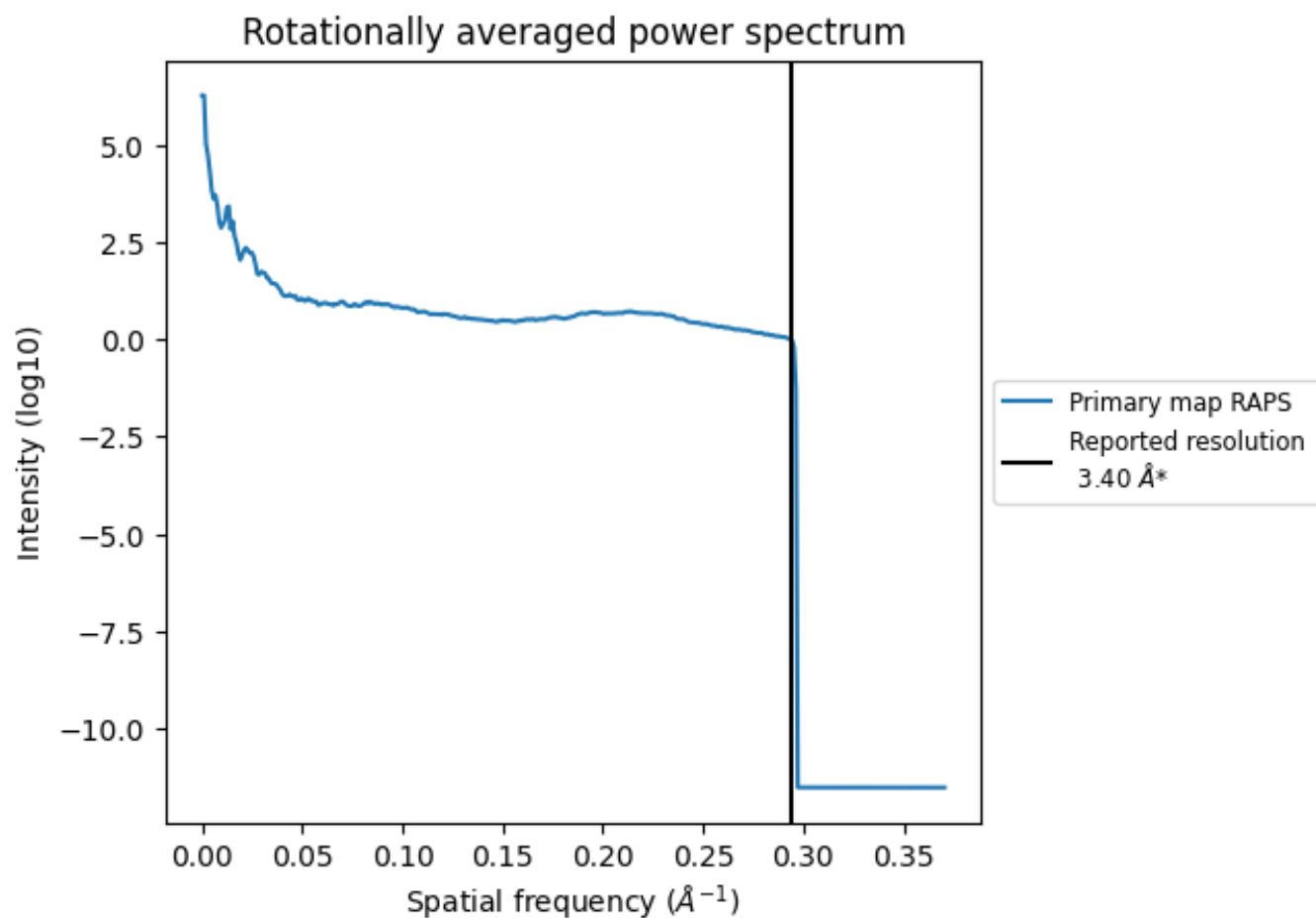
7.2 Volume estimate [i](#)



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 ⓘ

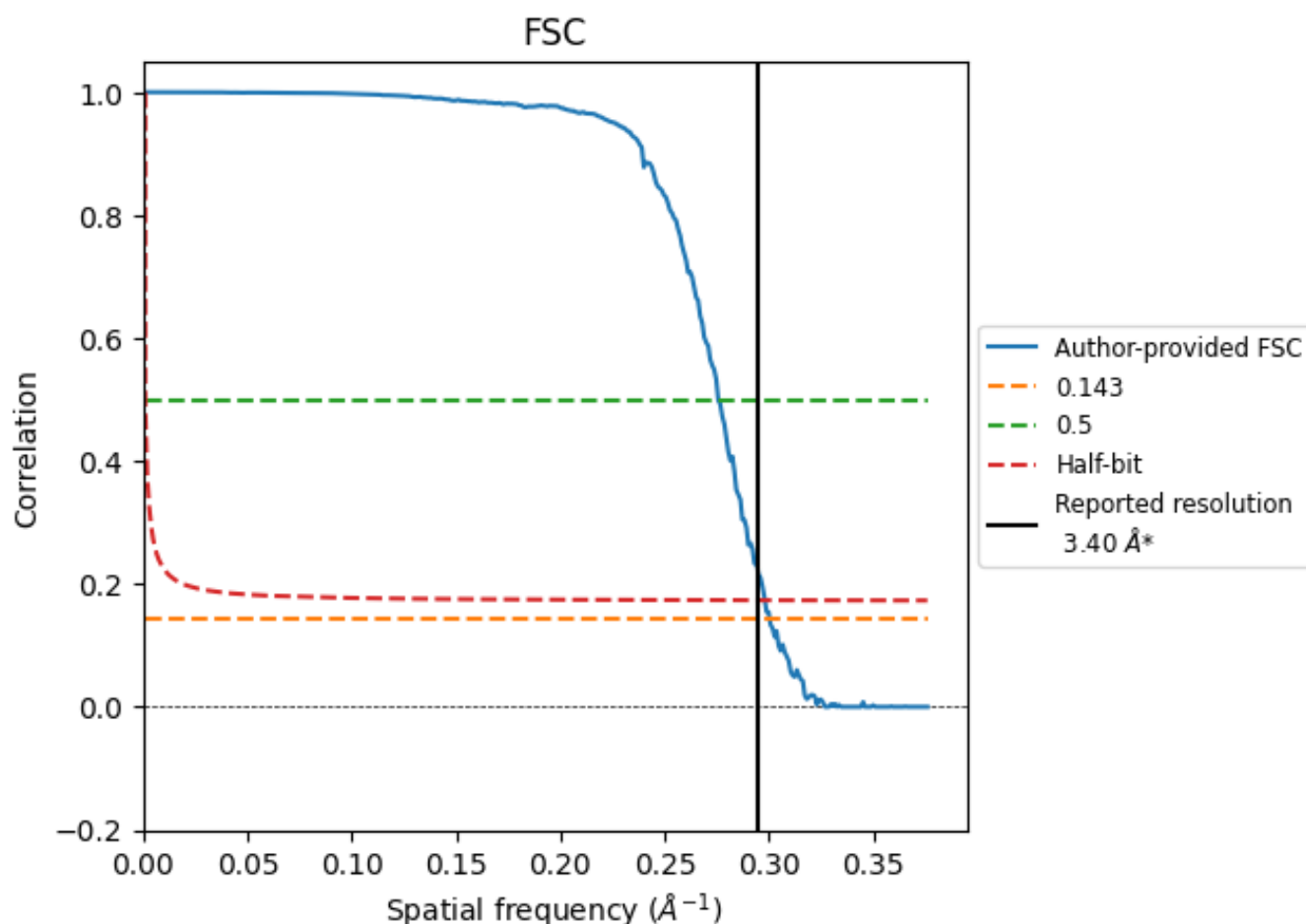


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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.

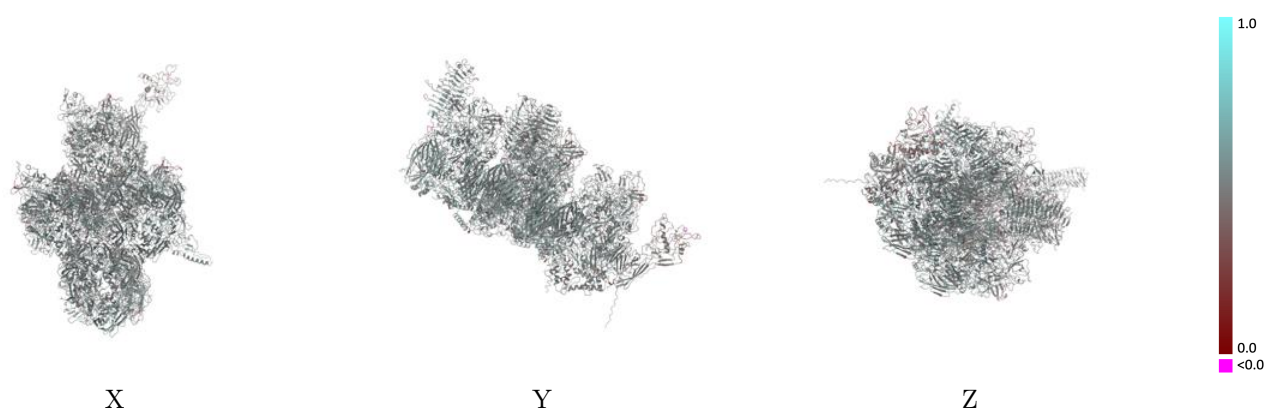
9 Map-model fit [i](#)

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 overlay [i](#)

This section was not generated.

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

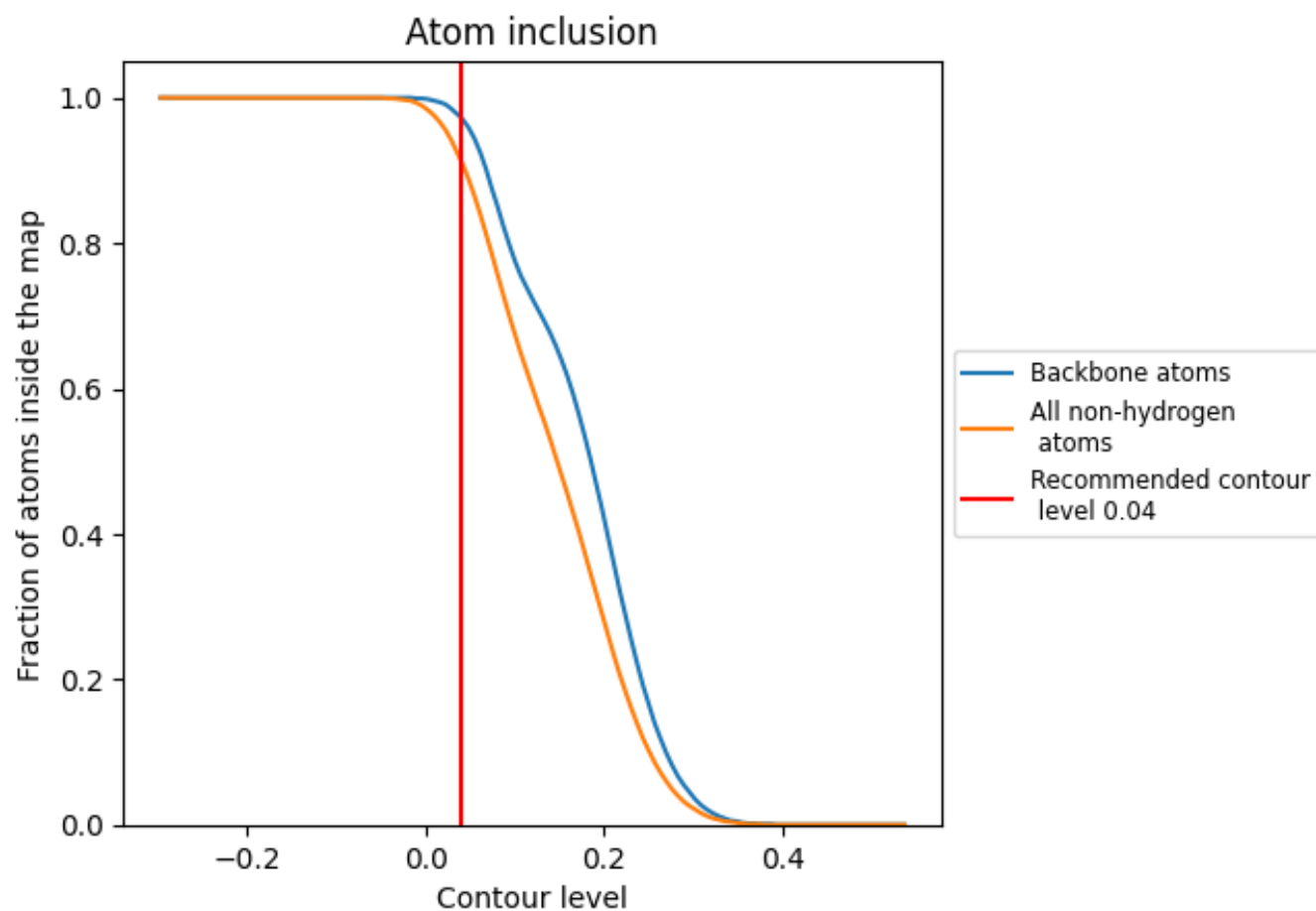


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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	 0.9140	 0.5000
A	 0.9320	 0.4980
B	 0.9380	 0.4970
C	 0.9300	 0.5000
D	 0.9300	 0.5090
E	 0.9340	 0.5110
F	 0.9290	 0.5070
G	 0.9300	 0.5130
H	 0.9280	 0.5100
I	 0.9260	 0.5100
J	 0.9280	 0.5090
K	 0.9350	 0.5090
L	 0.9300	 0.5110
M	 0.5950	 0.4120
N	 0.8300	 0.4720
O	 0.8960	 0.5000
P	 0.8480	 0.4840
Q	 0.9130	 0.4810
R	 0.9180	 0.4850
S	 0.9080	 0.4790
T	 0.9200	 0.4870

