Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 09:21 PM EST

PDB ID	:	3J40
EMDB ID	:	EMD-5678
Title	:	Validated Near-Atomic Resolution Structure of Bacteriophage Epsilon15 Derived from Cryo-EM and Modeling
Authors	:	Baker, M.L.; Hryc, C.F.; Zhang, Q.; Wu, W.; Jakana, J.; Haase-Pettingell, C.; Afonine, P.V.; Adams, P.D.; King, J.A.; Jiang, W.; Chiu, W.
Deposited on	:	2013-05-30
Resolution	:	4.50 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:

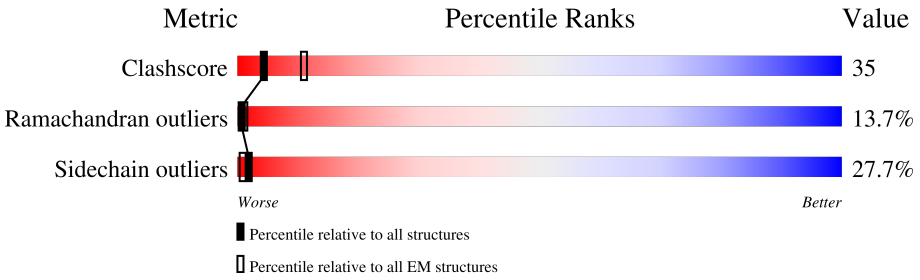
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.50 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 <=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	H	111	35% 25% 49% 23% •
1	I	111	35% 25% 42% 28% 5%
1	J	111	40% 25% 41% 29% 5%
1	K	111	37% 23% 52% 22% •
1	L	111	44% 23% 41% 28% 7%
1	M	111	61% 21% 46% 29% 5%
1	N	111	60% 27% 43% 26% •
2	A	335	35% 29% 50% 19% •

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Mol	Chain	Length	Quality of chain
2	B	335	31% 38% 38% 22%
2	C	335	31% 37% 39% 21%
2	D	335	33% 28% 49% 20%
2	E	335	34% 37% 39% 22%
2	F	335	37% 37% 42% 19%
2	G	335	49% 38% 44% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24066 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 gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	111	Total	C	N	O	S	0	0
			850	521	143	181	5		
1	M	111	Total	C	N	O	S	0	0
			850	521	143	181	5		
1	H	111	Total	C	N	O	S	0	0
			850	521	143	181	5		
1	K	111	Total	C	N	O	S	0	0
			850	521	143	181	5		
1	I	111	Total	C	N	O	S	0	0
			850	521	143	181	5		
1	J	111	Total	C	N	O	S	0	0
			850	521	143	181	5		
1	L	111	Total	C	N	O	S	0	0
			850	521	143	181	5		

- Molecule 2 is a protein called gp7.

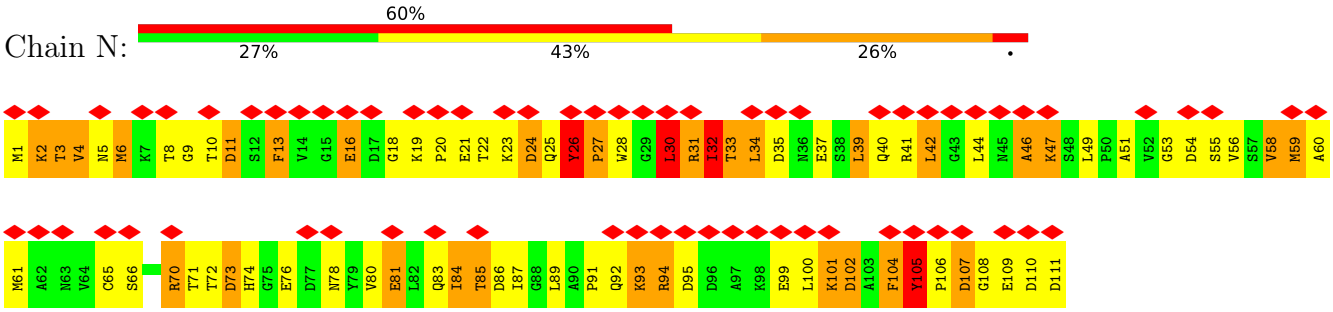
Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	335	Total	C	N	O	S	0	0
			2588	1620	453	502	13		
2	F	335	Total	C	N	O	S	0	0
			2588	1620	453	502	13		
2	B	335	Total	C	N	O	S	0	0
			2588	1620	453	502	13		
2	G	335	Total	C	N	O	S	0	0
			2588	1620	453	502	13		
2	D	335	Total	C	N	O	S	0	0
			2588	1620	453	502	13		
2	C	335	Total	C	N	O	S	0	0
			2588	1620	453	502	13		
2	E	335	Total	C	N	O	S	0	0
			2588	1620	453	502	13		

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.

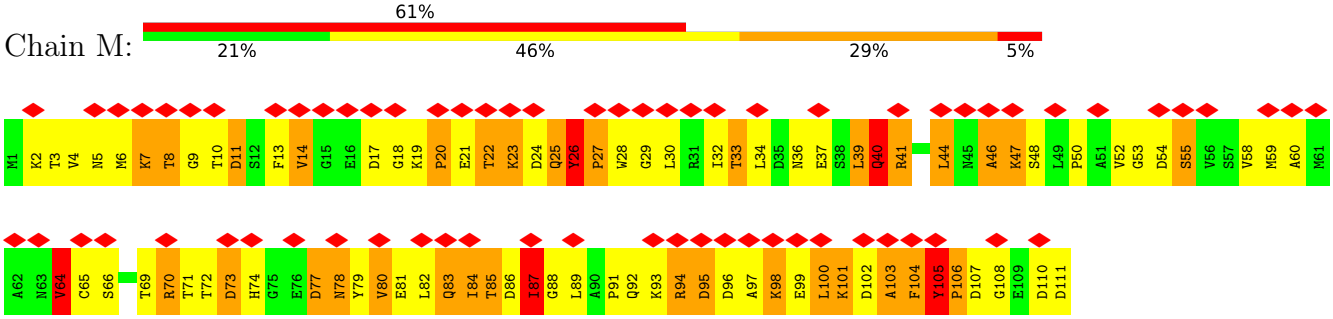
• Molecule 1: gp10

Chain N:



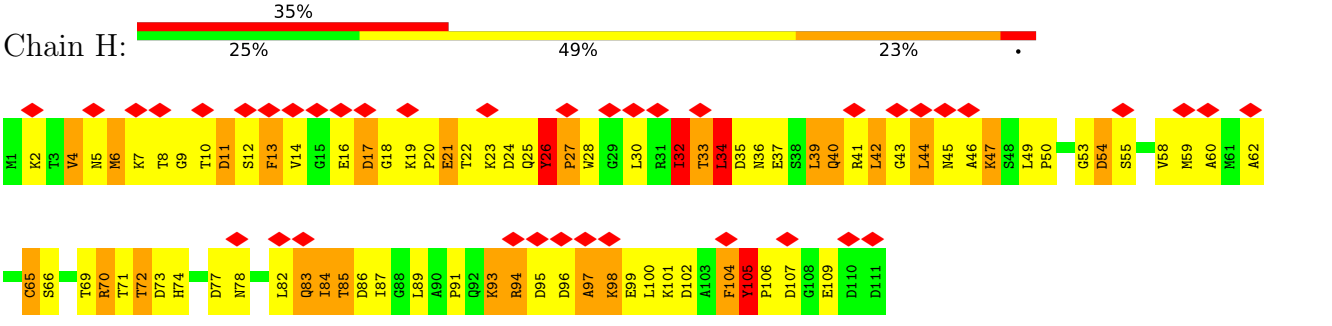
• Molecule 1: gp10

Chain M:



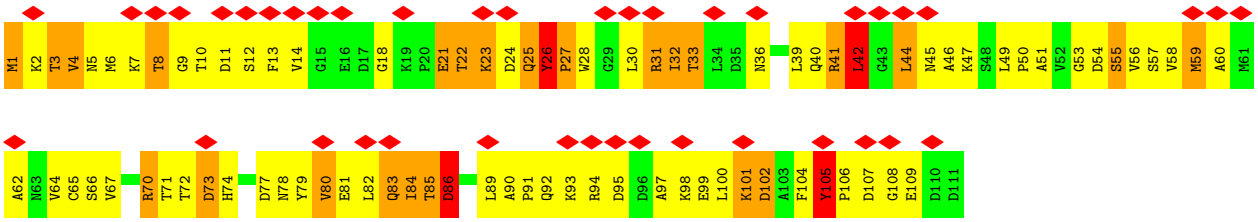
• Molecule 1: gp10

Chain H:



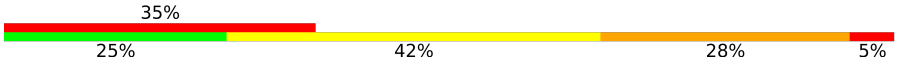
• Molecule 1: gp10

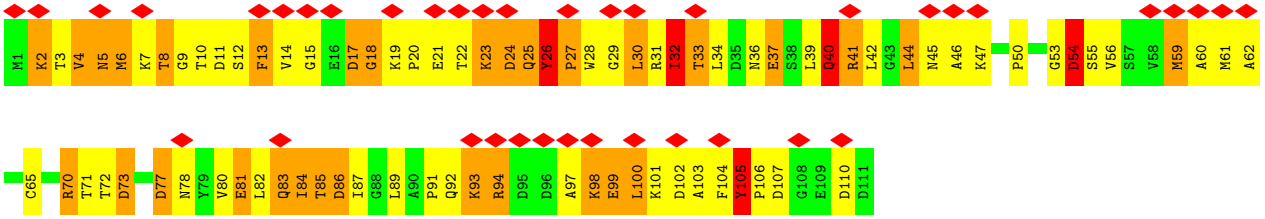
Chain K:



• Molecule 1: gp10

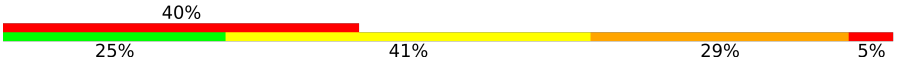
Chain I:

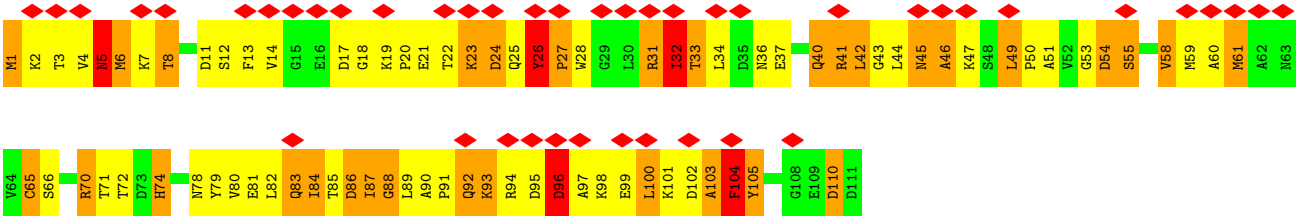




• Molecule 1: gp10

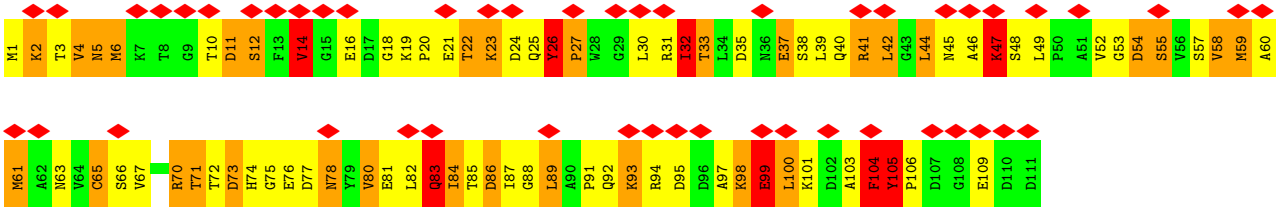
Chain J:





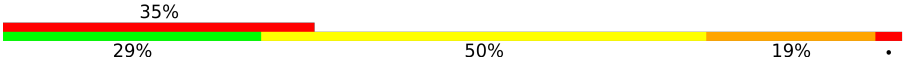
• Molecule 1: gp10

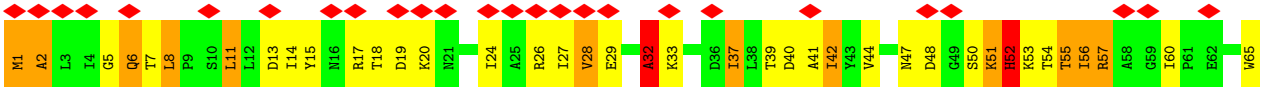
Chain L:

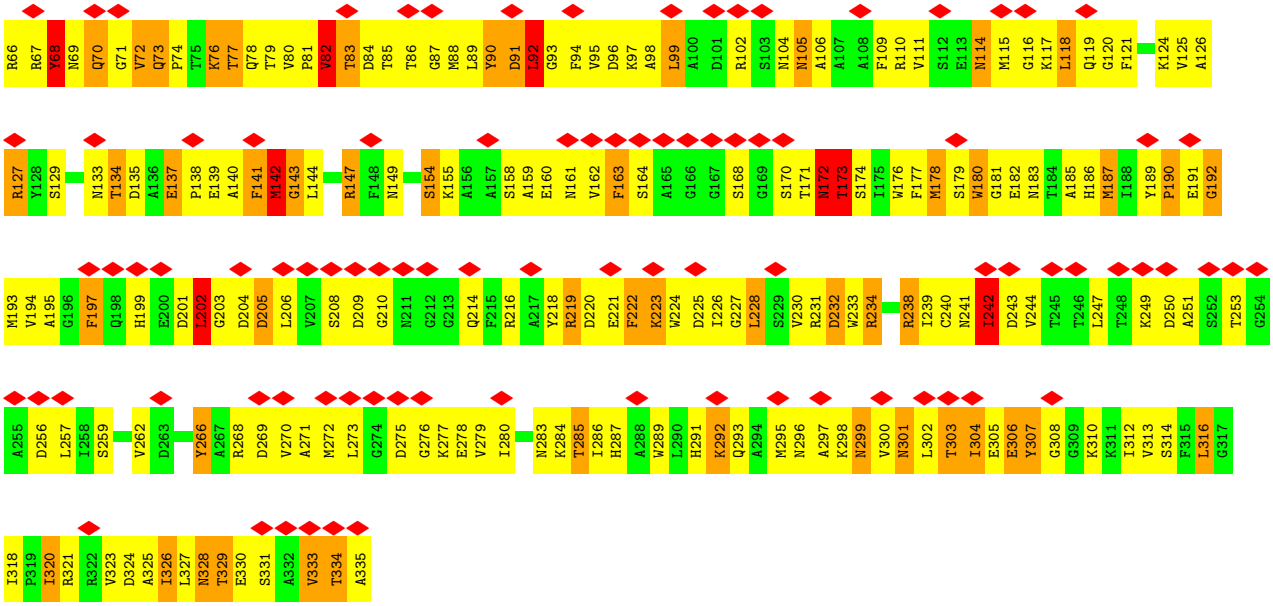


• Molecule 2: gp7

Chain A:

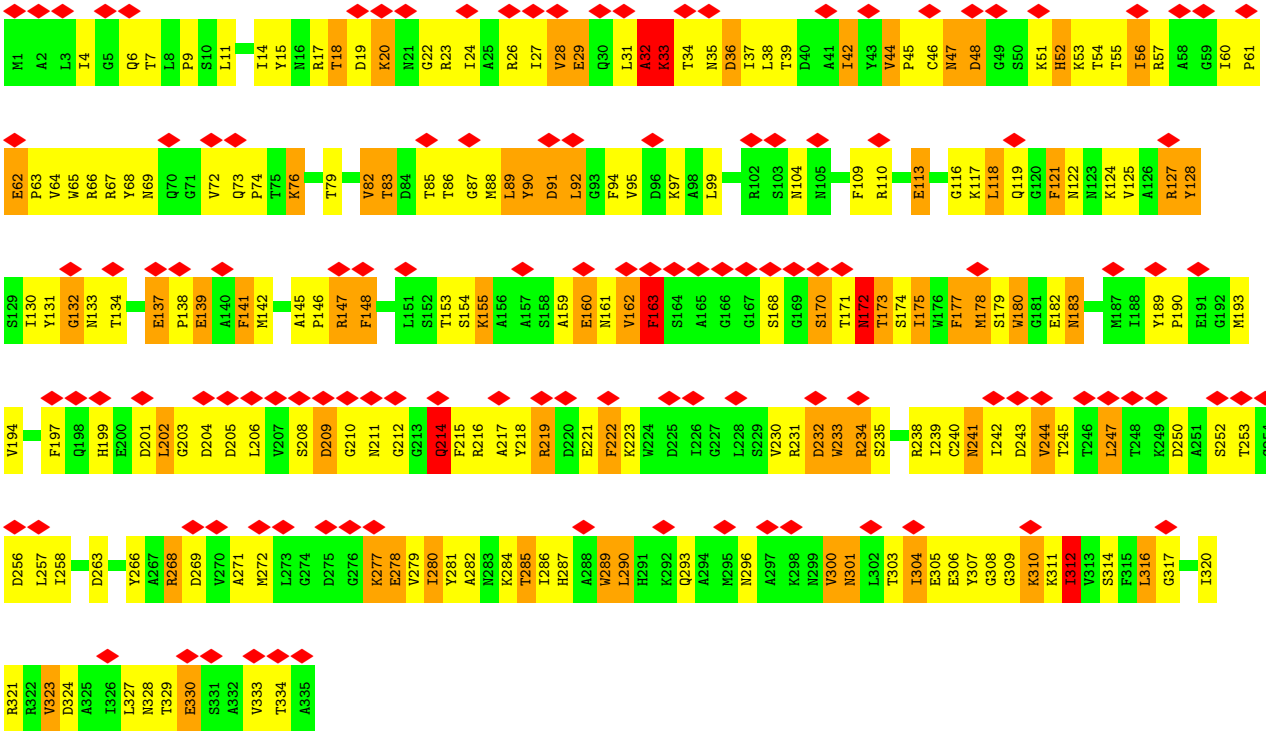






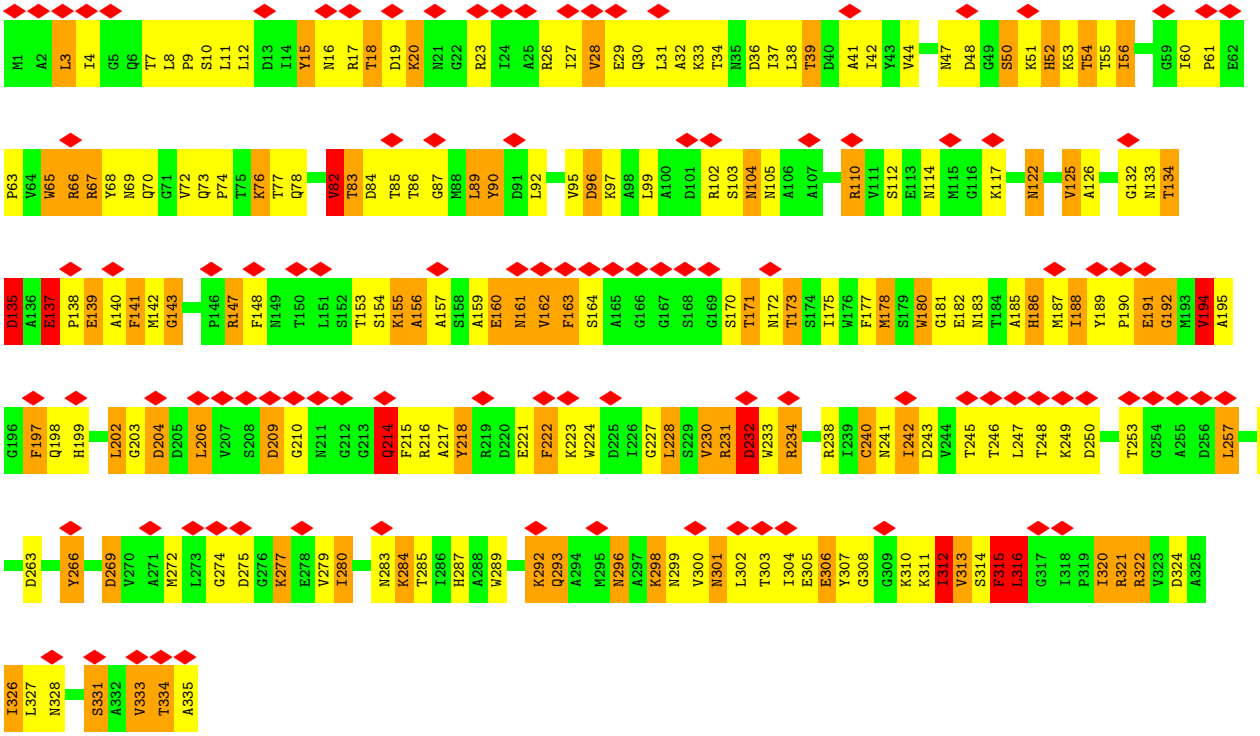
• Molecule 2: gp7

Chain F:



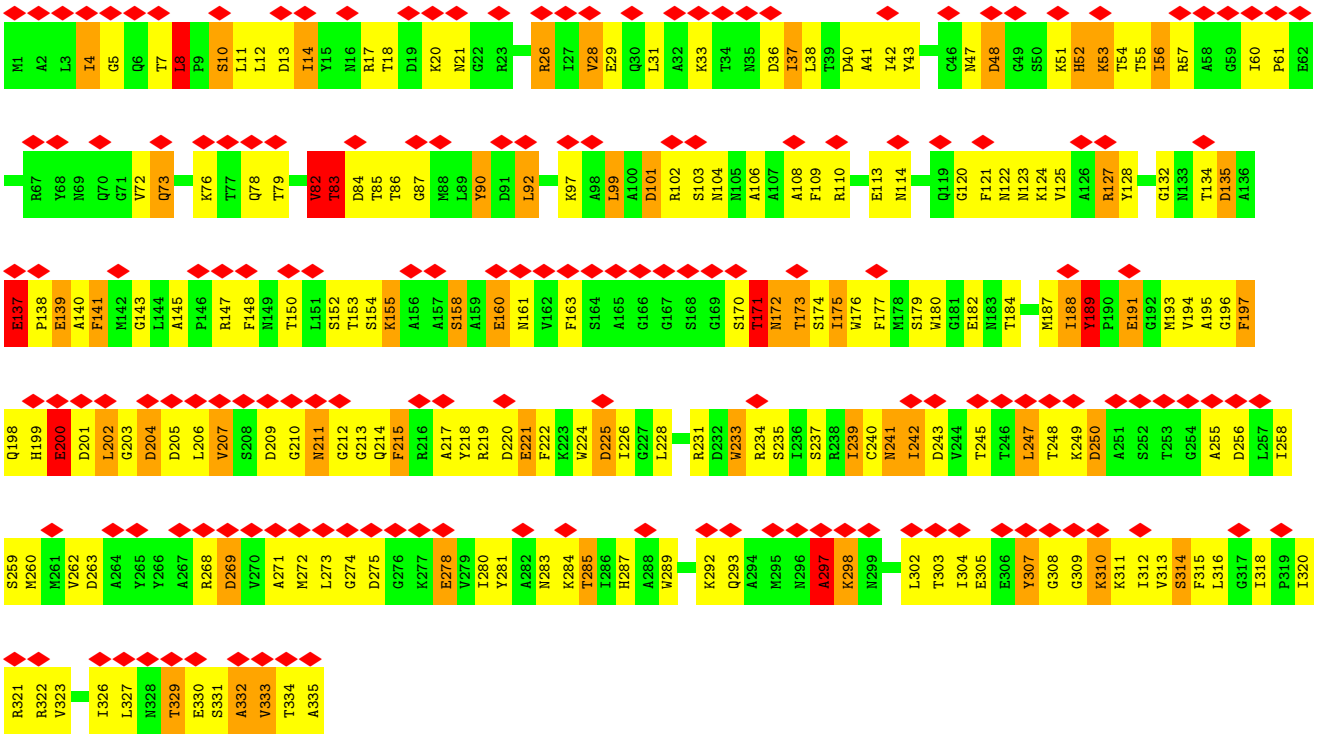
• Molecule 2: gp7

Chain B:



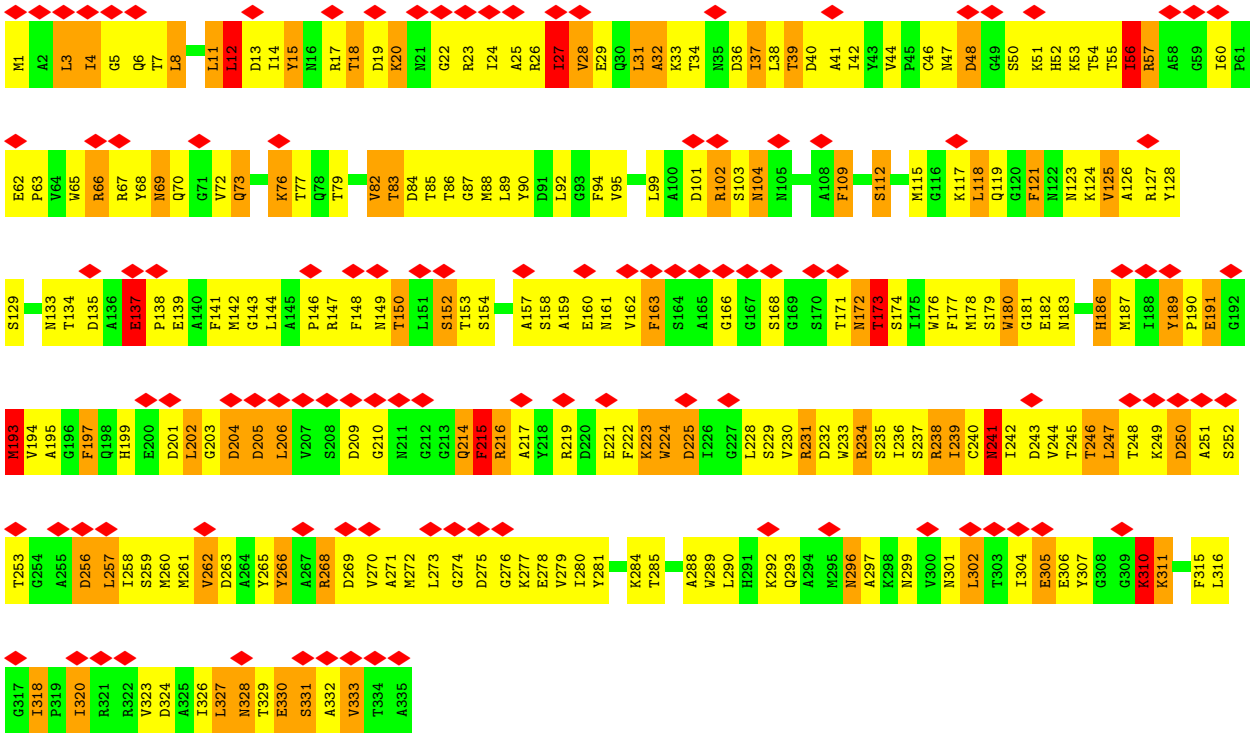
• Molecule 2: gp7

Chain G:



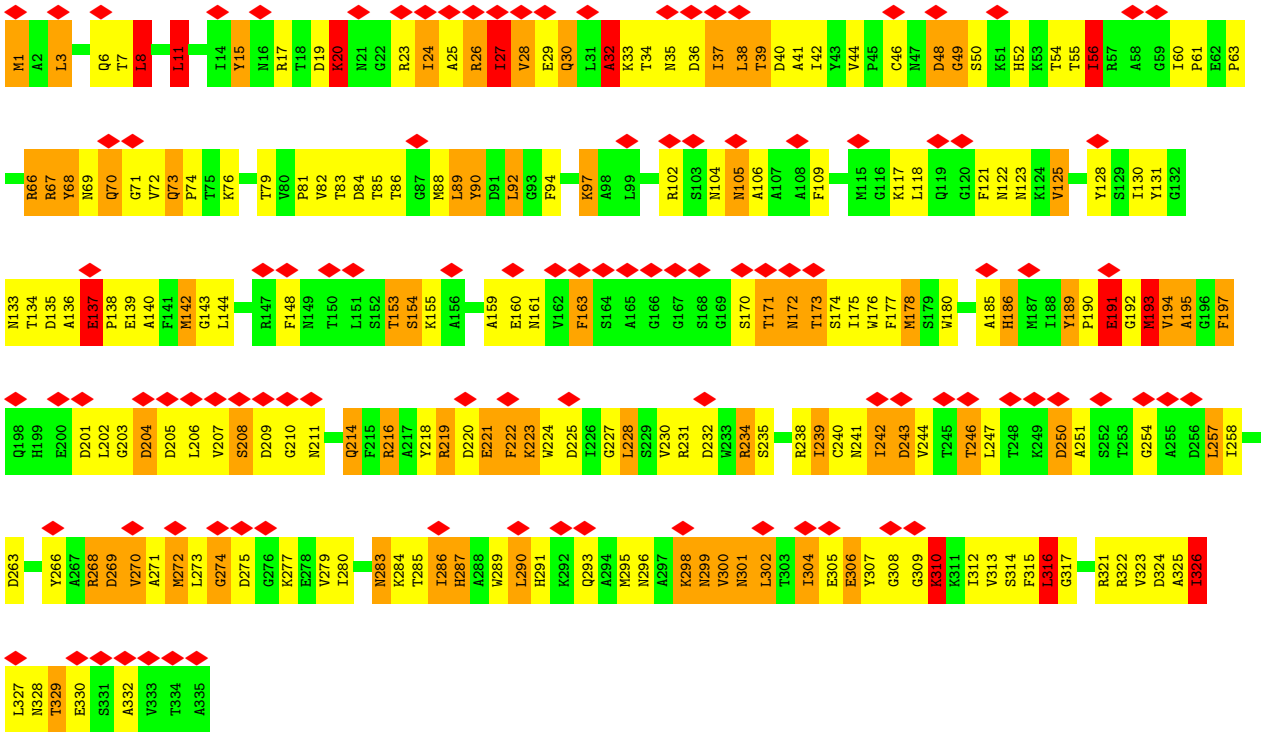
• Molecule 2: gp7

Chain D:



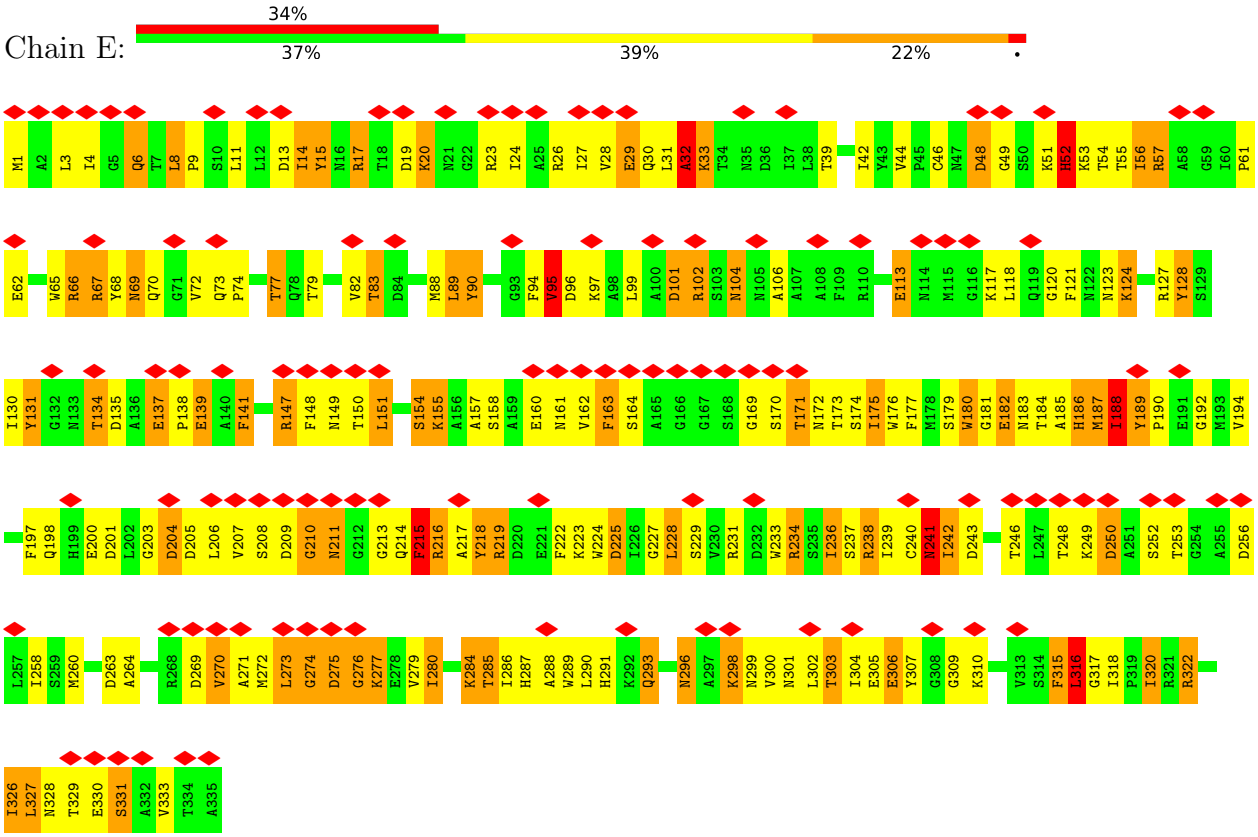
• Molecule 2: gp7

Chain C:



• Molecule 2: gp7

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	14000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	per particle	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	17	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	53361	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	24.633	Depositor
Minimum map value	-15.007	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.422	Depositor
Recommended contour level	5.2	Depositor
Map size (Å)	859.82404, 859.82404, 859.82404	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1942, 1.1942, 1.1942	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	H	0.29	0/862	0.81	1/1166 (0.1%)
1	I	0.31	0/862	0.79	0/1166
1	J	0.31	0/862	0.81	1/1166 (0.1%)
1	K	0.31	0/862	0.81	1/1166 (0.1%)
1	L	0.32	0/862	0.76	0/1166
1	M	0.31	0/862	0.80	0/1166
1	N	0.30	0/862	0.75	1/1166 (0.1%)
2	A	0.31	0/2637	0.72	3/3573 (0.1%)
2	B	0.31	0/2637	0.69	1/3573 (0.0%)
2	C	0.30	0/2637	0.70	1/3573 (0.0%)
2	D	0.31	0/2637	0.71	1/3573 (0.0%)
2	E	0.31	0/2637	0.69	1/3573 (0.0%)
2	F	0.31	0/2637	0.69	0/3573
2	G	0.30	0/2637	0.69	1/3573 (0.0%)
All	All	0.31	0/24493	0.72	12/33173 (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	H	0	2
1	I	0	2
1	J	0	3
1	K	0	1
1	L	0	2
1	M	0	2
1	N	0	1
2	A	0	4
2	B	0	1
2	C	0	3
2	D	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	4
2	F	0	5
2	G	0	5
All	All	0	39

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	92	LEU	CA-CB-CG	6.04	129.19	115.30
2	G	99	LEU	CA-CB-CG	6.00	129.09	115.30
2	A	202	LEU	CA-CB-CG	5.63	128.25	115.30
2	B	316	LEU	CA-CB-CG	5.58	128.14	115.30
2	D	12	LEU	CA-CB-CG	5.55	128.06	115.30
1	J	104	PHE	N-CA-C	5.24	125.14	111.00
2	C	316	LEU	CA-CB-CG	5.23	127.33	115.30
2	A	316	LEU	CA-CB-CG	5.17	127.18	115.30
1	K	42	LEU	CA-CB-CG	5.17	127.18	115.30
1	H	34	LEU	CA-CB-CG	5.13	127.10	115.30
2	E	316	LEU	CA-CB-CG	5.12	127.08	115.30
1	N	30	LEU	CA-CB-CG	5.09	127.02	115.30

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	137	GLU	Peptide
2	A	182	GLU	Peptide
2	A	241	ASN	Peptide
2	A	32	ALA	Peptide
2	B	137	GLU	Peptide
2	C	137	GLU	Peptide
2	C	195	ALA	Peptide
2	C	32	ALA	Peptide
2	D	137	GLU	Peptide
2	D	305	GLU	Peptide
2	D	31	LEU	Peptide
2	D	32	ALA	Peptide
2	E	137	GLU	Peptide
2	E	180	TRP	Peptide
2	E	31	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	E	32	ALA	Peptide
2	F	137	GLU	Peptide
2	F	241	ASN	Peptide
2	F	31	LEU	Peptide
2	F	32	ALA	Peptide
2	F	48	ASP	Peptide
2	G	137	GLU	Peptide
2	G	171	THR	Peptide
2	G	189	TYR	Peptide
2	G	297	ALA	Peptide
2	G	82	VAL	Peptide
1	H	105	TYR	Peptide
1	H	34	LEU	Peptide
1	I	105	TYR	Peptide
1	I	34	LEU	Peptide
1	J	103	ALA	Peptide
1	J	45	ASN	Peptide
1	J	5	ASN	Peptide
1	K	105	TYR	Peptide
1	L	103	ALA	Peptide
1	L	83	GLN	Peptide
1	M	103	ALA	Peptide
1	M	77	ASP	Peptide
1	N	105	TYR	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	H	850	0	820	78	0
1	I	850	0	820	83	0
1	J	850	0	820	74	0
1	K	850	0	820	84	0
1	L	850	0	820	68	0
1	M	850	0	820	74	0
1	N	850	0	820	82	0
2	A	2588	0	2542	194	0
2	B	2588	0	2542	181	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2588	0	2542	169	0
2	D	2588	0	2542	211	0
2	E	2588	0	2542	180	0
2	F	2588	0	2542	195	0
2	G	2588	0	2542	146	0
All	All	24066	0	23534	1682	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 35.

All (1682) 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:L:89:LEU:HG	1:L:91:PRO:HD3	1.48	0.94
2:D:101:ASP:HB2	2:D:104:ASN:HA	1.52	0.91
2:G:200:GLU:HG2	2:G:219:ARG:H	1.34	0.90
2:D:147:ARG:HH22	2:D:162:VAL:HG13	1.34	0.90
2:A:312:ILE:O	2:A:314:SER:N	2.06	0.89
2:E:90:TYR:HB2	2:E:223:LYS:HA	1.55	0.88
2:A:234:ARG:HH12	2:B:33:LYS:HG3	1.38	0.88
2:E:299:ASN:OD1	2:E:301:ASN:ND2	2.08	0.87
2:F:172:ASN:HB3	2:F:243:ASP:HB3	1.57	0.86
2:G:187:MET:SD	2:G:187:MET:N	2.50	0.85
2:C:291:HIS:HB2	2:C:312:ILE:HD11	1.58	0.85
2:A:76:LYS:HE2	2:B:7:THR:HB	1.56	0.85
2:F:132:GLY:H	2:F:142:MET:HG3	1.41	0.84
2:A:301:ASN:HB2	2:F:300:VAL:HG23	1.57	0.84
2:A:307:TYR:HB2	2:A:308:GLY:HA2	1.61	0.83
2:C:1:MET:SD	2:C:1:MET:N	2.51	0.82
2:E:174:SER:HA	2:E:241:ASN:HD21	1.45	0.82
1:N:58:VAL:HG22	1:N:59:MET:HG3	1.62	0.82
2:F:47:ASN:ND2	2:F:48:ASP:OD2	2.13	0.82
2:D:66:ARG:NH1	2:E:88:MET:SD	2.53	0.81
2:G:145:ALA:HA	2:G:333:VAL:HG12	1.63	0.81
1:M:18:GLY:HA3	1:M:91:PRO:HD2	1.62	0.80
2:F:307:TYR:HB2	2:F:308:GLY:HA2	1.61	0.80
2:B:92:LEU:HB3	2:B:221:GLU:HB2	1.61	0.80
2:E:95:VAL:HG23	2:E:218:TYR:HB3	1.64	0.80
2:G:241:ASN:HD22	2:G:242:ILE:HG13	1.47	0.80
2:D:173:THR:OG1	2:D:174:SER:N	2.14	0.80
2:E:284:LYS:HA	2:E:322:ARG:HH21	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:97:LYS:HZ2	2:F:216:ARG:HE	1.28	0.79
1:N:89:LEU:HG	1:N:91:PRO:HD3	1.65	0.79
2:C:329:THR:OG1	2:C:330:GLU:N	2.15	0.79
1:J:45:ASN:HB3	1:J:96:ASP:HB3	1.65	0.78
1:I:89:LEU:HG	1:I:91:PRO:HD3	1.64	0.78
2:G:307:TYR:O	2:G:309:GLY:N	2.16	0.78
2:B:70:GLN:HG2	1:J:3:THR:HG21	1.66	0.77
2:D:234:ARG:HH12	2:E:32:ALA:HB1	1.48	0.77
2:E:187:MET:SD	2:E:187:MET:N	2.55	0.77
2:C:209:ASP:N	2:C:210:GLY:HA2	2.00	0.76
1:M:8:THR:HG22	1:M:9:GLY:HA2	1.66	0.76
2:G:161:ASN:ND2	2:G:256:ASP:OD1	2.12	0.76
1:I:2:LYS:HE2	1:I:106:PRO:HG2	1.66	0.76
2:F:14:ILE:O	2:F:18:THR:OG1	2.02	0.76
2:G:90:TYR:HB2	2:G:222:PHE:O	1.85	0.76
1:I:59:MET:HB2	1:I:60:ALA:HB2	1.68	0.76
1:I:92:GLN:HB3	1:I:93:LYS:HB3	1.68	0.76
2:E:252:SER:OG	2:E:296:ASN:OD1	2.03	0.76
2:F:300:VAL:HG13	2:F:301:ASN:H	1.51	0.76
2:A:209:ASP:N	2:A:210:GLY:HA2	2.01	0.75
1:H:59:MET:HB2	1:H:60:ALA:HB2	1.67	0.75
2:B:209:ASP:N	2:B:210:GLY:HA2	2.00	0.75
2:F:242:ILE:HB	2:F:244:VAL:H	1.51	0.75
2:A:141:PHE:O	2:A:143:GLY:N	2.19	0.75
1:J:20:PRO:HB3	1:J:21:GLU:HG3	1.68	0.75
1:K:1:MET:HB3	1:K:2:LYS:HE3	1.67	0.75
2:D:247:LEU:O	2:D:289:TRP:NE1	2.18	0.74
2:D:327:LEU:O	2:D:328:ASN:ND2	2.20	0.74
2:C:173:THR:OG1	2:C:174:SER:N	2.15	0.74
2:E:296:ASN:O	2:E:299:ASN:ND2	2.20	0.74
1:L:42:LEU:HD11	1:L:101:LYS:HG2	1.68	0.74
2:A:90:TYR:HB3	2:A:223:LYS:HA	1.68	0.74
1:I:28:TRP:HA	1:I:84:ILE:HG21	1.69	0.74
2:A:149:ASN:HB3	2:A:155:LYS:HB2	1.70	0.74
1:H:89:LEU:HG	1:H:91:PRO:HD3	1.69	0.74
1:H:28:TRP:HA	1:H:84:ILE:HG21	1.69	0.74
2:D:92:LEU:HB3	2:D:221:GLU:HG3	1.69	0.74
1:M:8:THR:HG21	1:M:101:LYS:HB3	1.69	0.74
2:F:173:THR:OG1	2:F:174:SER:N	2.21	0.74
1:K:46:ALA:HB3	1:K:95:ASP:HB2	1.69	0.73
2:B:197:PHE:HE2	2:B:221:GLU:HB3	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:164:SER:HB3	2:E:331:SER:HB2	1.69	0.73
2:G:26:ARG:O	2:G:26:ARG:NE	2.21	0.73
2:A:297:ALA:O	2:A:301:ASN:ND2	2.20	0.73
2:G:329:THR:OG1	2:G:330:GLU:N	2.21	0.73
1:L:5:ASN:OD1	1:L:5:ASN:N	2.22	0.73
2:A:17:ARG:HH11	2:F:57:ARG:HH21	1.37	0.73
2:B:32:ALA:HB1	2:B:33:LYS:HB2	1.71	0.73
2:B:155:LYS:O	2:B:157:ALA:N	2.22	0.73
2:A:69:ASN:HB2	1:I:3:THR:HG21	1.69	0.73
2:A:244:VAL:HA	2:A:247:LEU:HB3	1.70	0.73
2:A:326:ILE:HD13	2:A:327:LEU:H	1.54	0.73
1:K:9:GLY:HA2	1:K:101:LYS:HD2	1.70	0.73
2:A:291:HIS:HB2	2:A:312:ILE:HD11	1.71	0.72
2:D:17:ARG:NH1	2:D:112:SER:OG	2.22	0.72
2:D:238:ARG:HH11	2:D:333:VAL:HG22	1.54	0.72
2:G:209:ASP:H	2:G:211:ASN:H	1.35	0.72
2:E:181:GLY:O	2:E:231:ARG:NH2	2.22	0.72
2:B:160:GLU:HB2	2:B:240:CYS:H	1.54	0.72
1:K:18:GLY:HA3	1:K:91:PRO:HD2	1.72	0.72
1:N:24:ASP:N	1:N:24:ASP:OD1	2.23	0.72
2:D:60:ILE:HD13	2:D:77:THR:HG23	1.71	0.72
2:E:23:ARG:O	2:E:26:ARG:NH2	2.23	0.72
1:N:22:THR:OG1	2:A:1:MET:O	2.07	0.71
2:F:95:VAL:HG22	2:F:218:TYR:HB2	1.71	0.71
2:D:57:ARG:HB3	2:D:79:THR:HG22	1.72	0.71
1:L:94:ARG:NH2	1:L:95:ASP:O	2.23	0.71
2:F:171:THR:O	2:F:328:ASN:HA	1.90	0.71
2:F:160:GLU:HB2	2:F:240:CYS:H	1.55	0.71
2:D:186:HIS:HD2	2:D:191:GLU:HA	1.55	0.71
2:E:275:ASP:OD1	2:E:276:GLY:N	2.22	0.71
1:M:89:LEU:HG	1:M:91:PRO:HD3	1.72	0.71
2:G:241:ASN:HB2	2:G:242:ILE:HG13	1.73	0.71
2:C:189:TYR:HB2	2:C:190:PRO:HD2	1.71	0.71
2:F:209:ASP:N	2:F:210:GLY:HA2	2.06	0.71
2:F:72:VAL:HG12	2:F:73:GLN:HG2	1.72	0.70
2:G:175:ILE:HG12	2:G:239:ILE:HD11	1.73	0.70
2:D:202:LEU:HA	2:D:216:ARG:HA	1.71	0.70
2:D:252:SER:HA	2:D:296:ASN:HB2	1.72	0.70
2:A:92:LEU:HD22	2:F:74:PRO:HB3	1.74	0.70
2:A:240:CYS:HB2	2:A:333:VAL:HG11	1.72	0.70
1:H:44:LEU:HB2	1:H:97:ALA:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:TYR:HB3	2:B:223:LYS:HA	1.73	0.70
2:B:117:LYS:HD2	2:B:222:PHE:HE1	1.55	0.70
2:E:97:LYS:HE2	2:E:200:GLU:HB2	1.73	0.70
2:B:299:ASN:HA	2:C:301:ASN:HD21	1.56	0.70
1:H:14:VAL:HA	1:H:96:ASP:HA	1.73	0.70
2:F:172:ASN:HB2	2:F:241:ASN:O	1.91	0.70
2:A:187:MET:SD	2:A:187:MET:N	2.65	0.69
1:L:59:MET:HB2	1:L:60:ALA:HB2	1.74	0.69
2:A:127:ARG:O	2:A:127:ARG:NH1	2.25	0.69
2:B:241:ASN:HB2	2:B:242:ILE:HG23	1.72	0.69
2:A:110:ARG:O	2:A:114:ASN:ND2	2.25	0.69
2:D:245:THR:O	2:D:248:THR:OG1	2.07	0.69
1:N:6:MET:HG2	2:A:1:MET:HB2	1.73	0.69
2:E:224:TRP:HD1	2:E:225:ASP:H	1.39	0.69
2:D:63:PRO:HB2	2:E:89:LEU:HD11	1.74	0.69
1:N:18:GLY:H	1:N:91:PRO:HD2	1.57	0.69
2:D:248:THR:HA	2:D:289:TRP:CZ2	2.28	0.69
1:I:42:LEU:HD13	1:I:101:LYS:HG3	1.75	0.69
2:E:101:ASP:N	2:E:101:ASP:OD1	2.26	0.69
1:J:41:ARG:H	1:J:41:ARG:HD2	1.56	0.69
1:J:51:ALA:HB3	1:J:90:ALA:HB3	1.74	0.69
1:N:92:GLN:HB3	1:N:93:LYS:HB3	1.73	0.69
2:A:66:ARG:HD2	2:A:68:TYR:H	1.58	0.69
1:L:52:VAL:HA	1:L:88:GLY:HA3	1.74	0.69
2:E:241:ASN:HB2	2:E:242:ILE:HG23	1.75	0.68
1:N:30:LEU:O	1:N:31:ARG:NE	2.23	0.68
2:B:247:LEU:O	2:B:289:TRP:NE1	2.24	0.68
2:B:187:MET:O	2:B:189:TYR:N	2.25	0.68
2:C:24:ILE:O	2:C:26:ARG:NH2	2.27	0.68
2:E:182:GLU:HG3	2:E:231:ARG:HB3	1.74	0.68
1:K:21:GLU:OE2	1:K:23:LYS:NZ	2.26	0.68
2:F:68:TYR:O	2:F:69:ASN:ND2	2.26	0.68
2:G:271:ALA:HA	2:G:273:LEU:H	1.58	0.68
2:C:247:LEU:HB3	2:C:289:TRP:NE1	2.09	0.68
2:A:19:ASP:OD2	2:A:26:ARG:NH2	2.27	0.68
2:C:193:MET:O	2:C:195:ALA:N	2.26	0.68
1:J:46:ALA:HB3	1:J:96:ASP:HB2	1.74	0.68
1:N:10:THR:H	1:N:11:ASP:HA	1.59	0.68
2:A:68:TYR:HB2	1:I:2:LYS:HB2	1.76	0.68
2:F:171:THR:OG1	2:F:172:ASN:N	2.26	0.68
2:C:315:PHE:HA	2:C:316:LEU:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:77:ASP:OD1	1:I:78:ASN:ND2	2.26	0.68
1:K:101:LYS:HE3	1:K:101:LYS:H	1.59	0.68
1:N:101:LYS:HD3	1:N:102:ASP:H	1.58	0.67
2:A:158:SER:O	2:A:160:GLU:N	2.27	0.67
2:A:173:THR:OG1	2:A:174:SER:N	2.26	0.67
2:B:289:TRP:O	2:B:292:LYS:NZ	2.27	0.67
1:K:101:LYS:HG2	1:K:102:ASP:H	1.60	0.67
1:I:2:LYS:NZ	1:I:3:THR:O	2.25	0.67
2:A:242:ILE:HG21	2:A:247:LEU:HD13	1.76	0.67
2:C:37:ILE:HG22	2:C:38:LEU:H	1.59	0.67
2:G:195:ALA:HA	2:G:197:PHE:H	1.60	0.67
1:K:59:MET:HB2	1:K:60:ALA:HB2	1.77	0.67
2:E:55:THR:O	2:E:56:ILE:HG13	1.95	0.67
2:D:252:SER:OG	2:C:299:ASN:ND2	2.27	0.67
2:E:8:LEU:HD22	2:E:9:PRO:HD2	1.75	0.67
1:K:80:VAL:HG13	1:K:81:GLU:H	1.60	0.67
2:B:173:THR:HG22	2:B:327:LEU:HA	1.75	0.67
1:I:24:ASP:N	1:I:24:ASP:OD1	2.28	0.66
2:A:17:ARG:HG3	2:F:79:THR:HG21	1.77	0.66
2:F:87:GLY:HA3	2:F:138:PRO:HG3	1.76	0.66
1:J:89:LEU:HG	1:J:91:PRO:HD3	1.76	0.66
1:N:65:CYS:SG	1:N:66:SER:N	2.69	0.66
2:F:124:LYS:NZ	2:F:124:LYS:O	2.28	0.66
2:D:162:VAL:HG12	2:D:163:PHE:H	1.60	0.66
2:A:178:MET:SD	2:A:178:MET:N	2.68	0.66
2:F:177:PHE:HB3	2:F:280:ILE:HA	1.77	0.66
2:F:271:ALA:HA	2:F:272:MET:HB3	1.77	0.66
2:D:249:LYS:NZ	2:D:253:THR:OG1	2.28	0.66
2:E:160:GLU:H	2:E:239:ILE:HG22	1.60	0.66
1:M:21:GLU:HG3	1:M:22:THR:H	1.61	0.66
2:A:326:ILE:HG23	2:A:328:ASN:H	1.61	0.66
2:B:12:LEU:O	2:B:16:ASN:ND2	2.28	0.66
2:B:296:ASN:OD1	2:B:296:ASN:N	2.28	0.66
1:H:6:MET:H	1:H:104:PHE:HE2	1.42	0.66
2:G:187:MET:O	2:G:189:TYR:N	2.28	0.66
2:C:283:ASN:HD21	2:C:286:ILE:HB	1.60	0.66
1:I:40:GLN:NE2	1:I:41:ARG:H	1.93	0.66
2:B:172:ASN:HB2	2:B:242:ILE:N	2.11	0.66
2:E:250:ASP:HA	2:E:253:THR:HG22	1.77	0.66
2:F:9:PRO:HG3	2:F:95:VAL:HA	1.78	0.66
2:F:90:TYR:OH	2:E:66:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:PHE:HD1	2:B:316:LEU:HD13	1.61	0.66
2:D:90:TYR:OH	2:C:66:ARG:NH2	2.29	0.66
2:E:263:ASP:OD1	2:E:264:ALA:N	2.29	0.66
1:N:59:MET:HB2	1:N:60:ALA:HB2	1.78	0.66
2:F:258:ILE:HG21	2:F:290:LEU:HD23	1.78	0.66
2:A:13:ASP:OD2	2:A:17:ARG:NH2	2.29	0.65
2:C:195:ALA:HB3	2:C:222:PHE:HA	1.77	0.65
1:I:14:VAL:HA	1:I:97:ALA:O	1.95	0.65
2:A:1:MET:SD	2:A:1:MET:N	2.53	0.65
2:A:57:ARG:NH2	2:A:77:THR:OG1	2.28	0.65
2:B:284:LYS:O	2:B:287:HIS:N	2.30	0.65
2:G:110:ARG:O	2:G:114:ASN:ND2	2.23	0.65
2:C:258:ILE:HG12	2:C:290:LEU:HD23	1.78	0.65
1:K:40:GLN:HG3	1:K:41:ARG:H	1.61	0.65
2:C:203:GLY:HA3	2:C:204:ASP:HB3	1.79	0.65
2:A:271:ALA:HA	2:A:272:MET:HB2	1.79	0.65
1:H:54:ASP:HB2	1:H:83:GLN:HB3	1.78	0.65
2:C:230:VAL:O	2:C:232:ASP:N	2.29	0.65
2:D:288:ALA:HA	2:C:266:TYR:HD1	1.60	0.65
2:C:23:ARG:HD2	2:C:24:ILE:H	1.62	0.65
1:J:8:THR:OG1	1:J:102:ASP:O	2.11	0.65
2:A:171:THR:OG1	2:A:172:ASN:N	2.28	0.65
2:C:283:ASN:HB3	2:C:325:ALA:HB3	1.79	0.65
1:N:80:VAL:HG22	1:N:81:GLU:H	1.62	0.65
2:G:214:GLN:HG3	2:G:215:PHE:H	1.60	0.65
1:H:7:LYS:HG3	2:F:67:ARG:HH12	1.62	0.65
1:I:44:LEU:HD13	1:I:45:ASN:H	1.60	0.65
1:H:22:THR:O	1:H:25:GLN:NE2	2.30	0.65
2:G:147:ARG:HB2	2:G:335:ALA:HA	1.79	0.65
1:N:55:SER:OG	1:N:56:VAL:N	2.30	0.64
1:M:33:THR:OG1	2:G:53:LYS:NZ	2.30	0.64
2:A:270:VAL:HG13	2:B:36:ASP:OD1	1.97	0.64
1:N:51:ALA:HA	1:N:65:CYS:HA	1.78	0.64
2:G:37:ILE:HG13	2:G:323:VAL:HG13	1.78	0.64
2:E:248:THR:HA	2:E:289:TRP:CZ2	2.32	0.64
1:M:59:MET:HB2	1:M:60:ALA:HB2	1.78	0.64
2:G:179:SER:HA	2:G:278:GLU:HA	1.80	0.64
1:L:22:THR:OG1	1:L:23:LYS:N	2.31	0.64
2:A:304:ILE:HG12	2:A:305:GLU:H	1.63	0.64
2:D:203:GLY:HA2	2:D:204:ASP:CG	2.18	0.64
2:A:70:GLN:HE22	1:I:3:THR:HB	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:96:ASP:OD1	2:E:99:LEU:N	2.30	0.64
2:A:53:LYS:O	2:A:83:THR:OG1	2.16	0.64
2:B:76:LYS:NZ	2:C:6:GLN:O	2.30	0.64
2:A:51:LYS:NZ	2:A:83:THR:O	2.31	0.64
2:G:4:ILE:HG22	2:G:5:GLY:H	1.63	0.64
2:D:215:PHE:HE2	2:D:217:ALA:HB2	1.63	0.64
2:E:274:GLY:O	2:E:276:GLY:N	2.31	0.64
2:D:88:MET:SD	2:C:66:ARG:NH1	2.70	0.63
2:E:177:PHE:CB	2:E:280:ILE:HA	2.29	0.63
2:A:142:MET:O	2:A:144:LEU:N	2.22	0.63
1:K:5:ASN:HD21	1:K:22:THR:HB	1.62	0.63
2:F:97:LYS:HB2	2:F:217:ALA:HA	1.79	0.63
2:D:17:ARG:HG3	2:C:79:THR:HG21	1.80	0.63
2:D:171:THR:HG1	2:D:244:VAL:H	1.46	0.63
1:J:70:ARG:H	1:J:70:ARG:HE	1.46	0.63
2:G:55:THR:OG1	2:G:56:ILE:N	2.29	0.63
2:E:326:ILE:HG13	2:E:328:ASN:H	1.63	0.63
2:D:14:ILE:HG21	2:D:99:LEU:HD11	1.79	0.63
1:M:29:GLY:H	1:M:84:ILE:HG21	1.64	0.63
1:H:10:THR:HB	1:H:101:LYS:HG3	1.80	0.63
2:D:121:PHE:HE1	2:C:63:PRO:HB3	1.64	0.63
2:E:185:ALA:N	2:E:227:GLY:O	2.32	0.63
2:F:37:ILE:HD11	2:F:323:VAL:HA	1.79	0.63
2:F:154:SER:OG	2:F:155:LYS:N	2.32	0.63
2:B:298:LYS:H	2:B:298:LYS:HD2	1.63	0.63
2:G:14:ILE:HG12	2:G:109:PHE:HZ	1.62	0.63
2:G:92:LEU:HA	2:G:221:GLU:HA	1.80	0.63
2:C:154:SER:O	2:C:154:SER:OG	2.17	0.63
2:C:241:ASN:HB2	2:C:242:ILE:HA	1.80	0.63
2:B:198:GLN:HG2	2:B:199:HIS:H	1.64	0.62
2:D:329:THR:OG1	2:D:330:GLU:N	2.32	0.62
2:F:278:GLU:OE1	2:F:279:VAL:N	2.31	0.62
2:B:206:LEU:HD22	2:B:210:GLY:HA3	1.81	0.62
2:D:241:ASN:ND2	2:D:242:ILE:O	2.32	0.62
1:N:13:PHE:N	1:N:16:GLU:OE1	2.29	0.62
1:M:23:LYS:HA	1:M:24:ASP:HB2	1.80	0.62
2:D:152:SER:OG	2:D:153:THR:N	2.33	0.62
2:D:278:GLU:N	2:D:278:GLU:OE1	2.31	0.62
2:E:173:THR:O	2:E:241:ASN:ND2	2.32	0.62
1:I:41:ARG:HG2	1:I:42:LEU:HD12	1.81	0.62
1:J:2:LYS:HZ3	1:J:5:ASN:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:133:ASN:ND2	2:F:139:GLU:O	2.32	0.62
2:E:11:LEU:HA	2:E:14:ILE:HG22	1.82	0.62
1:N:58:VAL:HG13	1:N:59:MET:H	1.65	0.62
2:F:90:TYR:HB3	2:F:223:LYS:HA	1.80	0.62
1:N:13:PHE:H	1:N:13:PHE:HD2	1.46	0.62
1:H:34:LEU:HD22	1:H:35:ASP:H	1.65	0.62
2:G:52:HIS:HB3	2:G:83:THR:HG21	1.82	0.62
2:E:51:LYS:HB3	2:E:83:THR:HG21	1.81	0.62
2:B:202:LEU:HB2	2:B:214:GLN:HA	1.80	0.62
1:K:73:ASP:O	1:K:74:HIS:ND1	2.32	0.62
1:N:46:ALA:HB1	1:N:47:LYS:HD3	1.81	0.61
2:A:133:ASN:O	2:A:134:THR:OG1	2.17	0.61
2:F:116:GLY:HA3	2:E:57:ARG:HH21	1.64	0.61
2:G:171:THR:OG1	2:G:172:ASN:N	2.34	0.61
2:F:285:THR:HG21	2:F:327:LEU:HD21	1.82	0.61
2:F:92:LEU:HA	2:F:221:GLU:HB2	1.81	0.61
2:F:179:SER:H	2:F:235:SER:HB3	1.64	0.61
1:K:2:LYS:HD3	2:C:67:ARG:HB2	1.82	0.61
2:A:65:TRP:CD1	2:B:89:LEU:HD12	2.35	0.61
2:G:101:ASP:HA	2:G:104:ASN:HA	1.81	0.61
2:C:7:THR:O	2:C:8:LEU:HB2	2.00	0.61
1:M:50:PRO:HG2	1:M:66:SER:HB3	1.82	0.61
2:A:55:THR:O	2:A:56:ILE:HG13	2.01	0.61
2:F:284:LYS:O	2:F:287:HIS:N	2.28	0.61
2:G:209:ASP:HB3	2:G:213:GLY:H	1.65	0.61
2:E:161:ASN:ND2	2:E:256:ASP:OD2	2.34	0.61
1:M:47:LYS:H	1:M:47:LYS:HD2	1.65	0.61
2:A:96:ASP:HB3	2:A:99:LEU:HD23	1.82	0.61
2:D:82:VAL:HG13	2:D:83:THR:H	1.65	0.61
1:J:54:ASP:HB2	1:J:83:GLN:HB3	1.82	0.61
2:D:310:LYS:HB3	2:D:311:LYS:HD3	1.82	0.60
1:K:22:THR:OG1	1:K:25:GLN:OE1	2.17	0.60
1:H:65:CYS:SG	1:H:66:SER:N	2.74	0.60
2:F:44:VAL:HG21	2:F:183:ASN:HD22	1.64	0.60
2:C:241:ASN:HB2	2:C:242:ILE:HG23	1.83	0.60
1:J:2:LYS:NZ	1:J:5:ASN:H	1.99	0.60
2:A:52:HIS:HB3	2:A:83:THR:HG21	1.83	0.60
2:F:38:LEU:HD13	2:F:321:ARG:HH11	1.65	0.60
2:B:314:SER:O	2:B:315:PHE:HB3	2.01	0.60
2:E:169:GLY:HA2	2:E:330:GLU:HB3	1.84	0.60
1:N:2:LYS:HD2	2:A:11:LEU:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:THR:O	2:C:153:THR:OG1	2.19	0.60
1:I:5:ASN:OD1	1:I:5:ASN:N	2.34	0.60
1:L:47:LYS:HB3	1:L:93:LYS:HE3	1.83	0.60
2:G:56:ILE:HG22	2:G:57:ARG:H	1.66	0.60
2:D:84:ASP:OD2	2:D:85:THR:N	2.27	0.60
1:J:26:TYR:O	1:J:84:ILE:HG13	2.02	0.60
2:F:33:LYS:HD2	2:E:56:ILE:HD13	1.83	0.60
2:B:232:ASP:HB2	2:C:32:ALA:HB2	1.84	0.60
2:E:242:ILE:H	2:E:243:ASP:HA	1.66	0.60
2:G:38:LEU:HG	2:G:321:ARG:HD2	1.83	0.60
2:D:183:ASN:O	2:D:229:SER:OG	2.17	0.60
2:D:209:ASP:N	2:D:210:GLY:HA2	2.16	0.60
1:N:24:ASP:O	2:A:5:GLY:HA2	2.01	0.60
2:B:192:GLY:HA2	2:B:224:TRP:NE1	2.16	0.60
1:N:70:ARG:O	1:N:70:ARG:NH1	2.32	0.60
2:F:97:LYS:HZ2	2:F:216:ARG:NE	1.99	0.60
2:C:37:ILE:HG23	2:C:323:VAL:HA	1.84	0.60
2:A:203:GLY:HA2	2:A:204:ASP:CG	2.22	0.60
2:G:195:ALA:HB1	2:G:222:PHE:HA	1.84	0.60
2:G:220:ASP:OD2	2:G:221:GLU:N	2.34	0.60
2:G:284:LYS:HD2	2:G:322:ARG:HH21	1.66	0.60
1:M:80:VAL:HG13	1:M:81:GLU:H	1.64	0.59
2:A:284:LYS:O	2:A:287:HIS:N	2.23	0.59
2:F:55:THR:O	2:F:56:ILE:HG13	2.02	0.59
1:K:53:GLY:O	1:K:86:ASP:HA	2.02	0.59
1:K:70:ARG:O	1:K:71:THR:OG1	2.18	0.59
1:K:89:LEU:HG	1:K:91:PRO:HD3	1.84	0.59
1:H:27:PRO:HA	1:H:84:ILE:HG13	1.83	0.59
1:H:83:GLN:OE1	1:H:84:ILE:N	2.35	0.59
2:D:193:MET:H	2:D:224:TRP:HE3	1.50	0.59
1:N:26:TYR:O	1:N:84:ILE:HG13	2.03	0.59
2:B:312:ILE:HD12	2:B:313:VAL:H	1.66	0.59
2:G:271:ALA:HA	2:G:273:LEU:N	2.16	0.59
2:D:103:SER:OG	2:D:104:ASN:N	2.35	0.59
2:C:301:ASN:OD1	2:C:302:LEU:N	2.35	0.59
2:D:15:TYR:O	2:D:18:THR:OG1	2.14	0.59
2:D:19:ASP:OD2	2:D:23:ARG:N	2.30	0.59
2:D:142:MET:O	2:D:144:LEU:N	2.35	0.59
2:A:284:LYS:O	2:A:286:ILE:N	2.35	0.59
1:K:89:LEU:HD23	1:K:89:LEU:H	1.67	0.59
2:C:195:ALA:HB2	2:C:223:LYS:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:13:PHE:N	1:N:13:PHE:CD2	2.69	0.59
2:A:60:ILE:HD13	2:A:77:THR:HB	1.85	0.59
2:A:197:PHE:CE2	2:A:221:GLU:HG3	2.37	0.59
1:I:2:LYS:HG2	1:I:3:THR:O	2.03	0.59
2:A:65:TRP:HA	2:B:89:LEU:HB3	1.85	0.59
2:F:250:ASP:OD1	2:F:257:LEU:HA	2.03	0.59
2:D:230:VAL:O	2:D:232:ASP:N	2.30	0.59
2:E:301:ASN:CG	2:E:302:LEU:H	2.06	0.59
1:L:24:ASP:N	1:L:24:ASP:OD1	2.35	0.59
2:A:91:ASP:N	2:A:91:ASP:OD2	2.36	0.59
2:D:241:ASN:OD1	2:D:241:ASN:N	2.36	0.59
1:K:40:GLN:OE1	1:K:41:ARG:NH2	2.36	0.59
2:A:177:PHE:CB	2:A:280:ILE:HA	2.33	0.58
2:G:160:GLU:N	2:G:239:ILE:HG22	2.17	0.58
2:D:7:THR:HG21	2:C:74:PRO:C	2.23	0.58
2:C:195:ALA:HB3	2:C:223:LYS:H	1.67	0.58
1:J:93:LYS:HD2	1:J:94:ARG:H	1.68	0.58
1:N:32:ILE:O	1:N:33:THR:OG1	2.20	0.58
1:M:83:GLN:OE1	1:M:84:ILE:N	2.33	0.58
2:A:42:ILE:HD11	2:A:183:ASN:HB3	1.84	0.58
2:A:278:GLU:OE2	2:A:279:VAL:N	2.36	0.58
2:D:315:PHE:CD1	2:D:316:LEU:HB2	2.38	0.58
2:E:204:ASP:OD1	2:E:204:ASP:N	2.35	0.58
2:G:209:ASP:N	2:G:210:GLY:HA2	2.18	0.58
1:H:47:LYS:H	1:H:47:LYS:HD3	1.67	0.58
2:F:209:ASP:H	2:F:211:ASN:H	1.50	0.58
2:B:198:GLN:N	2:B:198:GLN:OE1	2.35	0.58
1:L:40:GLN:CD	1:L:41:ARG:H	2.06	0.58
1:M:10:THR:HG23	1:M:20:PRO:HB2	1.86	0.58
2:A:89:LEU:HB3	2:F:65:TRP:CD1	2.39	0.58
2:F:199:HIS:HB2	2:F:219:ARG:HD2	1.85	0.58
2:B:274:GLY:H	2:B:275:ASP:HB3	1.67	0.58
2:G:86:THR:OG1	2:G:87:GLY:N	2.37	0.58
2:A:70:GLN:H	2:A:70:GLN:NE2	2.02	0.58
2:C:170:SER:O	2:C:172:ASN:N	2.34	0.58
1:M:40:GLN:O	1:M:73:ASP:HA	2.02	0.58
2:F:280:ILE:HG12	2:F:320:ILE:HG22	1.84	0.58
1:L:19:LYS:HG3	1:L:20:PRO:HD3	1.84	0.58
2:F:82:VAL:HG13	2:F:83:THR:H	1.69	0.58
2:F:203:GLY:HA2	2:F:204:ASP:HB2	1.84	0.58
2:G:298:LYS:N	2:G:298:LYS:HD2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:41:ARG:HH11	1:K:100:LEU:HD13	1.69	0.58
2:E:19:ASP:OD2	2:E:26:ARG:NH2	2.36	0.58
1:N:10:THR:N	1:N:11:ASP:HA	2.18	0.58
2:D:176:TRP:CZ2	2:D:238:ARG:HD3	2.38	0.58
1:H:40:GLN:HE22	1:H:41:ARG:NE	2.02	0.58
2:F:287:HIS:CE1	2:F:312:ILE:HD11	2.38	0.58
2:B:164:SER:HB2	2:B:331:SER:HB2	1.84	0.58
2:G:297:ALA:HB1	2:G:298:LYS:HD2	1.86	0.58
2:D:230:VAL:C	2:D:232:ASP:H	2.07	0.58
2:B:52:HIS:N	2:B:83:THR:OG1	2.37	0.57
1:H:17:ASP:OD1	1:H:18:GLY:N	2.37	0.57
2:F:91:ASP:N	2:F:221:GLU:OE2	2.37	0.57
2:C:272:MET:SD	2:C:273:LEU:N	2.78	0.57
2:B:50:SER:OG	2:B:51:LYS:N	2.37	0.57
2:B:299:ASN:OD1	2:B:301:ASN:ND2	2.37	0.57
2:E:158:SER:HA	2:E:238:ARG:O	2.04	0.57
1:I:80:VAL:HG13	1:I:81:GLU:H	1.69	0.57
2:F:243:ASP:O	2:F:245:THR:N	2.35	0.57
2:F:304:ILE:HG23	2:F:305:GLU:H	1.67	0.57
2:D:69:ASN:ND2	1:L:3:THR:O	2.37	0.57
1:K:5:ASN:OD1	1:K:6:MET:HB2	2.04	0.57
2:C:133:ASN:HB2	2:C:140:ALA:HA	1.85	0.57
2:C:185:ALA:N	2:C:227:GLY:O	2.33	0.57
2:E:177:PHE:O	2:E:237:SER:OG	2.17	0.57
1:N:18:GLY:N	1:N:91:PRO:HD2	2.19	0.57
1:H:40:GLN:HE22	1:H:41:ARG:HE	1.52	0.57
2:G:271:ALA:CA	2:G:273:LEU:H	2.16	0.57
2:E:271:ALA:HA	2:E:272:MET:HB3	1.85	0.57
1:J:5:ASN:CG	1:J:6:MET:H	2.07	0.57
2:A:72:VAL:HG13	2:A:73:GLN:H	1.68	0.57
2:A:202:LEU:HA	2:A:216:ARG:HA	1.85	0.57
2:B:162:VAL:HG12	2:B:163:PHE:H	1.67	0.57
2:B:206:LEU:HD13	2:B:206:LEU:H	1.70	0.57
2:A:37:ILE:HD13	2:A:126:ALA:HB2	1.87	0.57
1:J:41:ARG:HD2	1:J:41:ARG:N	2.19	0.57
1:N:76:GLU:HA	1:M:80:VAL:HG11	1.87	0.57
2:A:247:LEU:O	2:A:289:TRP:NE1	2.37	0.57
2:B:10:SER:O	2:B:12:LEU:N	2.37	0.57
2:D:11:LEU:HA	2:D:14:ILE:HG22	1.87	0.57
1:K:5:ASN:ND2	1:K:22:THR:HB	2.20	0.57
2:A:106:ALA:O	2:A:110:ARG:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:183:ASN:OD1	2:F:183:ASN:N	2.22	0.57
2:B:55:THR:O	2:B:56:ILE:HG13	2.05	0.57
2:C:142:MET:O	2:C:144:LEU:N	2.37	0.57
2:E:298:LYS:O	2:E:298:LYS:NZ	2.31	0.57
1:J:1:MET:SD	1:J:1:MET:N	2.77	0.57
1:H:32:ILE:O	1:H:33:THR:OG1	2.18	0.57
2:F:241:ASN:HB2	2:F:242:ILE:HG12	1.85	0.57
2:D:121:PHE:CE1	2:C:63:PRO:HB3	2.39	0.57
2:E:177:PHE:HB3	2:E:280:ILE:HA	1.86	0.57
1:J:41:ARG:HD3	1:J:42:LEU:HG	1.86	0.57
2:A:185:ALA:N	2:A:227:GLY:O	2.36	0.56
2:D:36:ASP:HB2	2:C:270:VAL:O	2.05	0.56
2:D:55:THR:O	2:D:56:ILE:HG13	2.04	0.56
1:L:98:LYS:O	1:L:99:GLU:HB2	2.04	0.56
1:N:25:GLN:N	1:N:25:GLN:OE1	2.35	0.56
1:H:45:ASN:ND2	1:H:95:ASP:OD1	2.37	0.56
2:F:130:ILE:HG23	2:F:131:TYR:CD1	2.40	0.56
2:B:221:GLU:OE1	2:B:222:PHE:N	2.35	0.56
1:I:46:ALA:HB2	1:I:70:ARG:HB3	1.86	0.56
1:M:25:GLN:NE2	1:M:86:ASP:O	2.38	0.56
1:M:44:LEU:HB2	1:M:97:ALA:HB2	1.86	0.56
2:B:292:LYS:HZ3	2:B:293:GLN:HB3	1.69	0.56
2:G:206:LEU:HG	2:G:207:VAL:H	1.68	0.56
2:C:26:ARG:N	2:C:26:ARG:HE	2.02	0.56
1:J:78:ASN:ND2	1:J:79:TYR:H	2.03	0.56
2:D:186:HIS:CD2	2:D:191:GLU:HA	2.38	0.56
1:K:2:LYS:HG3	1:K:3:THR:O	2.04	0.56
1:J:70:ARG:H	1:J:70:ARG:NE	2.03	0.56
1:N:41:ARG:HG3	1:N:42:LEU:H	1.71	0.56
1:M:40:GLN:HG3	1:M:101:LYS:C	2.26	0.56
2:A:177:PHE:HB2	2:A:280:ILE:HA	1.88	0.56
2:F:235:SER:HA	2:F:268:ARG:NH2	2.20	0.56
1:I:22:THR:HG21	1:I:87:ILE:HG23	1.88	0.56
1:N:84:ILE:O	1:N:85:THR:OG1	2.23	0.56
1:M:99:GLU:HG2	1:M:101:LYS:NZ	2.19	0.56
2:D:41:ALA:HB1	2:D:180:TRP:HE1	1.70	0.56
1:L:27:PRO:HA	1:L:84:ILE:HG23	1.86	0.56
2:A:231:ARG:HE	2:B:31:LEU:HD11	1.70	0.56
2:F:85:THR:OG1	2:F:86:THR:N	2.38	0.56
2:G:83:THR:OG1	2:G:84:ASP:N	2.36	0.56
2:C:177:PHE:HB2	2:C:279:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:186:HIS:O	2:C:186:HIS:ND1	2.39	0.56
1:N:28:TRP:CA	1:N:84:ILE:HG21	2.35	0.56
2:A:104:ASN:OD1	2:A:105:ASN:N	2.39	0.56
2:F:201:ASP:OD1	2:F:219:ARG:NH2	2.31	0.56
2:B:17:ARG:O	2:B:26:ARG:NH1	2.39	0.56
2:B:234:ARG:NH1	2:C:32:ALA:HA	2.20	0.56
2:G:315:PHE:CD1	2:G:316:LEU:HB3	2.40	0.56
1:L:89:LEU:HD22	1:L:104:PHE:CZ	2.41	0.56
2:D:172:ASN:OD1	2:D:172:ASN:N	2.39	0.56
2:D:189:TYR:HD1	2:D:189:TYR:H	1.51	0.56
2:C:284:LYS:O	2:C:287:HIS:N	2.25	0.56
1:J:65:CYS:SG	1:J:66:SER:N	2.78	0.56
1:J:78:ASN:HD22	1:J:79:TYR:H	1.53	0.56
1:L:60:ALA:N	1:L:61:MET:SD	2.73	0.56
2:A:160:GLU:HB3	2:A:333:VAL:HB	1.88	0.56
2:A:160:GLU:HB3	2:A:334:THR:H	1.71	0.56
2:B:171:THR:HB	2:B:328:ASN:ND2	2.21	0.56
2:G:187:MET:C	2:G:189:TYR:H	2.09	0.56
2:D:17:ARG:HH11	2:D:112:SER:HG	1.53	0.56
2:C:137:GLU:OE1	1:J:1:MET:N	2.35	0.56
1:H:40:GLN:HB2	1:H:101:LYS:O	2.06	0.55
2:C:89:LEU:HD21	2:C:125:VAL:HG23	1.88	0.55
2:E:187:MET:HE3	2:E:225:ASP:HB2	1.86	0.55
1:J:22:THR:HB	1:J:87:ILE:HG23	1.88	0.55
2:B:42:ILE:HG21	2:B:181:GLY:H	1.71	0.55
2:B:245:THR:O	2:B:248:THR:OG1	2.15	0.55
1:N:34:LEU:O	1:N:78:ASN:ND2	2.39	0.55
2:D:67:ARG:O	1:L:2:LYS:HB3	2.07	0.55
1:I:12:SER:HB3	1:I:100:LEU:HB2	1.88	0.55
1:N:70:ARG:O	1:N:71:THR:OG1	2.25	0.55
1:M:3:THR:HG22	2:E:69:ASN:HD21	1.71	0.55
2:A:147:ARG:HB2	2:A:333:VAL:O	2.06	0.55
2:A:228:LEU:HD13	2:A:228:LEU:H	1.72	0.55
2:A:230:VAL:O	2:A:232:ASP:N	2.28	0.55
1:N:110:ASP:OD2	1:N:111:ASP:N	2.40	0.55
2:A:176:TRP:CZ2	2:A:238:ARG:HD3	2.41	0.55
1:K:13:PHE:HD2	1:K:14:VAL:H	1.54	0.55
2:A:70:GLN:HG2	2:A:71:GLY:N	2.22	0.55
1:H:41:ARG:HG3	1:H:42:LEU:H	1.71	0.55
2:D:157:ALA:HB2	2:D:236:ILE:HG13	1.86	0.55
2:D:157:ALA:O	2:D:238:ARG:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:21:GLU:O	1:K:23:LYS:NZ	2.31	0.55
2:G:10:SER:O	2:G:12:LEU:N	2.36	0.55
2:G:110:ARG:HH22	2:G:198:GLN:HB3	1.72	0.55
1:K:55:SER:OG	1:K:56:VAL:N	2.37	0.55
1:M:46:ALA:HB1	1:M:47:LYS:HD2	1.89	0.55
2:A:133:ASN:HB2	2:A:140:ALA:HA	1.89	0.55
2:A:249:LYS:O	2:A:253:THR:OG1	2.18	0.55
1:H:18:GLY:O	1:H:91:PRO:HD2	2.06	0.55
2:F:171:THR:C	2:F:172:ASN:HD22	2.10	0.55
2:A:8:LEU:HD12	2:A:94:PHE:HB2	1.89	0.55
2:A:115:MET:HA	2:A:118:LEU:HD23	1.89	0.55
2:G:84:ASP:OD1	2:G:85:THR:N	2.29	0.55
2:C:299:ASN:OD1	2:C:300:VAL:N	2.36	0.55
2:E:17:ARG:NH1	2:E:113:GLU:OE1	2.27	0.55
1:H:6:MET:HG2	1:H:7:LYS:N	2.20	0.55
2:F:279:VAL:HG13	2:F:281:TYR:HE2	1.72	0.55
2:F:296:ASN:OD1	2:F:296:ASN:N	2.38	0.55
2:D:302:LEU:HA	2:C:302:LEU:HD21	1.89	0.55
2:E:293:GLN:O	2:E:293:GLN:NE2	2.36	0.55
1:L:22:THR:OG1	1:L:25:GLN:OE1	2.22	0.55
2:F:52:HIS:N	2:F:83:THR:OG1	2.40	0.54
2:B:32:ALA:HB1	2:B:33:LYS:CB	2.36	0.54
2:G:172:ASN:HB3	2:G:241:ASN:O	2.06	0.54
2:D:48:ASP:HB3	2:E:20:LYS:NZ	2.22	0.54
2:D:63:PRO:HB2	2:E:89:LEU:CD1	2.37	0.54
2:D:221:GLU:HG2	2:D:222:PHE:H	1.72	0.54
2:F:88:MET:SD	2:E:66:ARG:NH1	2.81	0.54
2:B:17:ARG:NH2	2:B:112:SER:OG	2.38	0.54
2:B:203:GLY:HA2	2:B:204:ASP:CG	2.28	0.54
1:K:21:GLU:O	1:K:23:LYS:HG3	2.06	0.54
1:H:105:TYR:HB3	1:H:106:PRO:CD	2.37	0.54
2:F:202:LEU:HB3	2:F:215:PHE:H	1.72	0.54
2:B:132:GLY:HA3	2:B:140:ALA:HA	1.87	0.54
2:B:178:MET:SD	2:B:178:MET:N	2.80	0.54
2:D:296:ASN:OD1	2:D:296:ASN:N	2.40	0.54
1:K:78:ASN:CG	1:K:79:TYR:H	2.11	0.54
2:E:224:TRP:HD1	2:E:225:ASP:N	2.06	0.54
1:I:105:TYR:HB2	1:I:106:PRO:HD3	1.88	0.54
1:H:8:THR:OG1	1:H:9:GLY:HA2	2.07	0.54
2:F:76:LYS:HE2	2:F:76:LYS:H	1.73	0.54
2:B:147:ARG:NE	2:B:333:VAL:O	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:42:ILE:HG23	2:A:180:TRP:HD1	1.73	0.54
2:A:86:THR:OG1	2:A:226:ILE:O	2.18	0.54
2:D:37:ILE:HG21	2:D:126:ALA:HB1	1.90	0.54
1:K:3:THR:HG23	2:C:69:ASN:HB2	1.90	0.54
2:C:33:LYS:O	2:C:34:THR:OG1	2.25	0.54
2:A:181:GLY:O	2:A:231:ARG:NH2	2.41	0.54
2:F:284:LYS:O	2:F:286:ILE:N	2.41	0.54
2:G:298:LYS:HD2	2:G:298:LYS:H	1.72	0.54
2:G:86:THR:HG21	2:G:187:MET:SD	2.48	0.54
2:G:87:GLY:HA3	2:G:138:PRO:HB3	1.90	0.54
2:D:37:ILE:HG23	2:D:324:ASP:HB3	1.90	0.54
2:D:247:LEU:HD21	2:D:256:ASP:O	2.07	0.54
1:I:83:GLN:OE1	1:I:84:ILE:N	2.41	0.54
1:M:69:THR:HA	1:M:70:ARG:NH2	2.22	0.54
2:A:155:LYS:O	2:A:158:SER:OG	2.25	0.54
2:G:86:THR:OG1	2:G:226:ILE:O	2.16	0.54
2:G:173:THR:HG22	2:G:327:LEU:HA	1.89	0.54
1:K:46:ALA:HA	1:K:70:ARG:HH12	1.73	0.54
2:E:233:TRP:O	2:E:234:ARG:HB2	2.08	0.54
2:B:284:LYS:HG3	2:B:322:ARG:HH21	1.73	0.54
2:G:56:ILE:HD11	2:G:82:VAL:HG21	1.90	0.54
2:D:177:PHE:HB2	2:D:279:VAL:O	2.08	0.54
1:I:54:ASP:HB2	1:I:83:GLN:HB3	1.90	0.54
2:G:37:ILE:HG13	2:G:323:VAL:HA	1.90	0.54
1:K:70:ARG:H	1:K:70:ARG:NE	2.05	0.54
2:E:316:LEU:H	2:E:318:ILE:HG12	1.73	0.54
1:I:8:THR:OG1	1:I:102:ASP:O	2.20	0.54
1:M:27:PRO:HA	1:M:84:ILE:HG13	1.90	0.53
2:A:224:TRP:HD1	2:A:225:ASP:N	2.06	0.53
2:G:195:ALA:CB	2:G:222:PHE:HA	2.37	0.53
2:C:160:GLU:HB2	2:C:240:CYS:H	1.74	0.53
1:L:37:GLU:HG3	1:L:105:TYR:HA	1.90	0.53
2:F:333:VAL:HG13	2:F:334:THR:H	1.73	0.53
2:D:65:TRP:HA	2:E:89:LEU:HB2	1.91	0.53
1:K:3:THR:HG21	2:C:70:GLN:HB2	1.90	0.53
2:F:180:TRP:CE3	2:F:180:TRP:HA	2.44	0.53
2:D:3:LEU:O	2:D:6:GLN:N	2.41	0.53
2:D:275:ASP:OD1	2:D:276:GLY:N	2.41	0.53
2:C:214:GLN:CD	2:C:214:GLN:H	2.11	0.53
2:E:228:LEU:HD13	2:E:228:LEU:H	1.73	0.53
2:F:118:LEU:O	2:F:122:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:202:LEU:HA	2:F:215:PHE:O	2.09	0.53
2:F:243:ASP:C	2:F:245:THR:H	2.11	0.53
1:J:60:ALA:N	1:J:61:MET:SD	2.82	0.53
2:A:70:GLN:NE2	1:I:3:THR:HB	2.23	0.53
2:F:42:ILE:HD11	2:F:183:ASN:HA	1.89	0.53
2:F:177:PHE:HD2	2:F:177:PHE:N	2.06	0.53
2:D:33:LYS:O	2:D:34:THR:OG1	2.23	0.53
1:K:2:LYS:HE2	2:C:68:TYR:H	1.73	0.53
2:E:147:ARG:H	2:E:147:ARG:NE	2.07	0.53
2:E:258:ILE:HG12	2:E:290:LEU:HD23	1.90	0.53
1:N:73:ASP:O	1:N:74:HIS:ND1	2.42	0.53
2:A:179:SER:HB3	2:A:278:GLU:HG2	1.90	0.53
2:F:52:HIS:O	2:F:52:HIS:ND1	2.38	0.53
2:F:289:TRP:HA	2:F:289:TRP:CE3	2.43	0.53
2:G:214:GLN:HG3	2:G:215:PHE:N	2.24	0.53
2:D:3:LEU:HB3	2:D:6:GLN:HA	1.90	0.53
2:D:249:LYS:HZ2	2:D:250:ASP:H	1.57	0.53
2:E:177:PHE:HB2	2:E:280:ILE:HA	1.90	0.53
1:I:26:TYR:CE2	1:I:84:ILE:HD11	2.43	0.53
1:L:99:GLU:O	1:L:100:LEU:HB2	2.08	0.53
2:A:205:ASP:OD2	2:A:205:ASP:N	2.41	0.53
1:K:1:MET:HB3	1:K:2:LYS:HB2	1.91	0.53
1:H:36:ASN:HB3	1:H:78:ASN:HA	1.91	0.53
2:F:116:GLY:HA3	2:E:57:ARG:NH2	2.24	0.53
2:F:214:GLN:O	2:F:214:GLN:NE2	2.42	0.53
2:F:278:GLU:CD	2:F:279:VAL:H	2.12	0.53
2:G:154:SER:OG	2:G:155:LYS:N	2.39	0.53
1:I:70:ARG:O	1:I:71:THR:OG1	2.27	0.53
1:L:47:LYS:HD3	1:L:93:LYS:NZ	2.23	0.53
1:L:71:THR:HB	1:L:74:HIS:HE1	1.74	0.53
2:B:292:LYS:HB3	2:B:292:LYS:HZ2	1.74	0.53
2:D:288:ALA:HA	2:C:266:TYR:CD1	2.42	0.53
1:J:89:LEU:HB3	1:J:104:PHE:CZ	2.44	0.53
2:A:266:TYR:HE2	2:B:287:HIS:HD1	1.58	0.52
1:H:7:LYS:HD2	2:F:67:ARG:HH22	1.74	0.52
2:F:177:PHE:N	2:F:177:PHE:CD2	2.76	0.52
2:C:172:ASN:HB3	2:C:243:ASP:HA	1.91	0.52
2:E:134:THR:O	1:L:41:ARG:NE	2.29	0.52
2:F:130:ILE:HG23	2:F:131:TYR:HD1	1.72	0.52
2:B:20:LYS:HE2	2:B:20:LYS:HA	1.91	0.52
1:L:20:PRO:HB3	1:L:21:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ASN:HB2	2:E:20:LYS:HE2	1.92	0.52
2:D:149:ASN:OD1	2:D:150:THR:N	2.37	0.52
2:E:210:GLY:O	2:E:211:ASN:HB2	2.08	0.52
1:I:17:ASP:O	1:I:19:LYS:N	2.28	0.52
1:I:39:LEU:O	1:I:103:ALA:N	2.43	0.52
1:I:84:ILE:O	1:I:85:THR:OG1	2.27	0.52
1:I:105:TYR:HB2	1:I:106:PRO:CD	2.39	0.52
2:F:90:TYR:CE1	2:E:66:ARG:HG3	2.45	0.52
2:B:177:PHE:HB3	2:B:280:ILE:HA	1.90	0.52
2:D:34:THR:HG21	2:D:119:GLN:HG2	1.90	0.52
2:D:260:MET:HA	2:D:263:ASP:HB3	1.91	0.52
2:C:135:ASP:O	2:C:137:GLU:N	2.42	0.52
1:M:39:LEU:HD22	1:M:40:GLN:HA	1.91	0.52
2:A:102:ARG:NH1	2:G:225:ASP:OD2	2.42	0.52
1:H:23:LYS:HG3	1:H:24:ASP:HA	1.91	0.52
2:F:20:LYS:HD2	2:E:53:LYS:HE3	1.91	0.52
2:F:170:SER:HB3	2:F:171:THR:HG22	1.92	0.52
2:F:205:ASP:HB2	2:F:210:GLY:H	1.74	0.52
2:D:248:THR:HA	2:D:289:TRP:HZ2	1.74	0.52
2:D:280:ILE:HD13	2:D:320:ILE:HB	1.92	0.52
2:A:303:THR:HG22	2:F:300:VAL:HG22	1.92	0.52
2:F:307:TYR:CB	2:F:308:GLY:HA2	2.34	0.52
2:B:164:SER:HA	2:B:170:SER:HB2	1.92	0.52
2:D:157:ALA:HA	2:D:237:SER:HA	1.91	0.52
2:C:105:ASN:O	2:C:105:ASN:ND2	2.43	0.52
2:A:120:GLY:HA3	2:F:60:ILE:HG13	1.91	0.52
2:F:89:LEU:HD12	2:E:65:TRP:CZ3	2.45	0.52
2:F:205:ASP:CB	2:F:210:GLY:H	2.23	0.52
2:B:185:ALA:N	2:B:227:GLY:O	2.43	0.52
2:G:173:THR:OG1	2:G:174:SER:N	2.40	0.52
2:D:189:TYR:CG	2:D:190:PRO:HD3	2.45	0.52
1:I:19:LYS:NZ	1:I:87:ILE:HG21	2.24	0.52
2:F:241:ASN:HB2	2:F:242:ILE:CD1	2.40	0.52
2:F:242:ILE:HB	2:F:244:VAL:N	2.22	0.52
2:F:289:TRP:HA	2:F:289:TRP:HE3	1.74	0.52
2:B:65:TRP:HB3	2:C:88:MET:O	2.10	0.52
2:G:250:ASP:OD1	2:G:250:ASP:N	2.43	0.52
2:C:66:ARG:HG3	2:C:71:GLY:HA2	1.91	0.52
1:I:2:LYS:HE3	1:I:2:LYS:H	1.75	0.52
1:K:54:ASP:OD2	1:K:62:ALA:HB3	2.10	0.52
2:C:302:LEU:C	2:C:304:ILE:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:36:ASN:HB3	1:K:79:TYR:HE2	1.75	0.51
2:D:66:ARG:CZ	2:D:68:TYR:HA	2.40	0.51
1:N:35:ASP:HA	1:N:78:ASN:OD1	2.11	0.51
1:H:96:ASP:OD2	1:H:97:ALA:N	2.43	0.51
2:F:175:ILE:HG13	2:F:239:ILE:HD13	1.93	0.51
2:B:9:PRO:HG3	2:B:95:VAL:HG12	1.92	0.51
2:G:78:GLN:N	2:G:78:GLN:OE1	2.42	0.51
2:G:248:THR:HA	2:G:289:TRP:HZ2	1.74	0.51
2:D:14:ILE:HD13	2:D:109:PHE:CE2	2.45	0.51
2:D:142:MET:C	2:D:144:LEU:H	2.13	0.51
2:C:284:LYS:O	2:C:286:ILE:N	2.44	0.51
1:I:44:LEU:HG	1:I:98:LYS:O	2.10	0.51
2:B:97:LYS:H	2:B:217:ALA:HA	1.75	0.51
2:E:173:THR:HB	2:E:327:LEU:HD12	1.93	0.51
1:I:22:THR:HA	1:I:25:GLN:HE22	1.75	0.51
1:K:100:LEU:HB3	1:K:101:LYS:HE3	1.92	0.51
1:J:28:TRP:CA	1:J:84:ILE:HG21	2.40	0.51
1:M:3:THR:N	2:E:67:ARG:HG2	2.26	0.51
2:A:83:THR:HG22	2:A:84:ASP:H	1.74	0.51
2:A:328:ASN:ND2	2:A:328:ASN:O	2.43	0.51
2:B:247:LEU:HD22	2:B:289:TRP:CD1	2.44	0.51
2:B:277:LYS:HZ3	2:B:277:LYS:HB2	1.76	0.51
2:E:192:GLY:HA2	2:E:224:TRP:NE1	2.26	0.51
1:J:17:ASP:OD1	1:J:18:GLY:N	2.44	0.51
2:A:70:GLN:H	2:A:70:GLN:HE21	1.59	0.51
2:A:275:ASP:OD2	2:A:276:GLY:N	2.44	0.51
1:H:34:LEU:O	1:H:78:ASN:ND2	2.44	0.51
2:D:7:THR:HG21	2:C:74:PRO:HB2	1.92	0.51
2:D:41:ALA:CB	2:D:180:TRP:HE1	2.24	0.51
1:N:34:LEU:HD22	1:N:35:ASP:H	1.76	0.51
1:M:8:THR:HG21	1:M:101:LYS:CB	2.39	0.51
1:M:98:LYS:C	1:M:100:LEU:H	2.14	0.51
1:I:18:GLY:HA3	1:I:91:PRO:HG2	1.92	0.51
1:L:44:LEU:N	1:L:100:LEU:HD11	2.25	0.51
1:H:7:LYS:CD	2:F:67:ARG:HH22	2.23	0.51
2:F:36:ASP:OD2	2:F:36:ASP:N	2.44	0.51
2:F:208:SER:N	2:F:209:ASP:HA	2.26	0.51
2:E:90:TYR:CB	2:E:223:LYS:HA	2.36	0.51
2:E:94:PHE:CD1	2:E:219:ARG:HB3	2.45	0.51
2:E:246:THR:HA	2:E:249:LYS:HD3	1.92	0.51
1:N:105:TYR:CD1	2:A:11:LEU:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:333:VAL:O	2:A:335:ALA:N	2.44	0.51
2:G:209:ASP:H	2:G:210:GLY:HA2	1.75	0.51
2:D:137:GLU:OE1	1:K:1:MET:N	2.44	0.51
2:D:199:HIS:O	2:D:219:ARG:HB2	2.11	0.51
2:D:296:ASN:HB3	2:C:299:ASN:ND2	2.26	0.51
2:E:326:ILE:HG13	2:E:327:LEU:H	1.76	0.51
2:A:86:THR:OG1	2:A:87:GLY:N	2.43	0.50
2:F:60:ILE:N	2:F:61:PRO:HD3	2.26	0.50
2:F:241:ASN:HB2	2:F:242:ILE:CG1	2.41	0.50
1:K:31:ARG:HH21	1:K:31:ARG:C	2.14	0.50
2:C:305:GLU:HG3	2:C:306:GLU:CD	2.31	0.50
2:E:97:LYS:HG3	2:E:216:ARG:HB2	1.91	0.50
2:E:241:ASN:N	2:E:241:ASN:HD22	2.09	0.50
2:E:300:VAL:HG13	2:E:301:ASN:H	1.74	0.50
1:N:6:MET:HA	2:A:2:ALA:HB2	1.93	0.50
1:H:19:LYS:NZ	1:H:87:ILE:HG21	2.25	0.50
2:F:209:ASP:H	2:F:210:GLY:HA2	1.74	0.50
2:B:60:ILE:HD11	2:C:117:LYS:HG2	1.91	0.50
2:G:195:ALA:HA	2:G:197:PHE:N	2.26	0.50
2:G:209:ASP:H	2:G:211:ASN:N	2.06	0.50
2:G:298:LYS:NZ	2:G:298:LYS:HA	2.26	0.50
2:A:41:ALA:CB	2:A:180:TRP:HE1	2.24	0.50
2:A:160:GLU:CB	2:A:334:THR:H	2.25	0.50
2:A:314:SER:OG	2:B:306:GLU:OE1	2.28	0.50
1:H:6:MET:N	1:H:104:PHE:HE2	2.09	0.50
2:B:16:ASN:O	2:B:18:THR:OG1	2.28	0.50
2:B:19:ASP:OD1	2:B:23:ARG:N	2.37	0.50
1:K:104:PHE:O	1:K:105:TYR:HB2	2.10	0.50
2:C:243:ASP:O	2:C:246:THR:HG22	2.11	0.50
1:I:102:ASP:OD1	1:I:103:ALA:N	2.44	0.50
2:A:93:GLY:O	2:A:219:ARG:HB2	2.12	0.50
2:A:178:MET:HG2	2:A:180:TRP:HZ3	1.75	0.50
2:D:154:SER:HB2	2:D:158:SER:OG	2.10	0.50
2:C:25:ALA:C	2:C:26:ARG:HE	2.14	0.50
2:C:189:TYR:HB2	2:C:190:PRO:CD	2.41	0.50
2:E:224:TRP:CD1	2:E:225:ASP:N	2.79	0.50
2:A:53:LYS:O	2:A:82:VAL:HG13	2.10	0.50
1:H:25:GLN:HB2	1:H:85:THR:O	2.11	0.50
2:G:209:ASP:HB2	2:G:212:GLY:H	1.76	0.50
1:J:14:VAL:HG22	1:J:98:LYS:HA	1.94	0.50
2:F:320:ILE:O	2:F:321:ARG:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:6:MET:HG3	1:K:22:THR:HG22	1.94	0.50
1:K:28:TRP:N	1:K:84:ILE:HG12	2.25	0.50
2:C:19:ASP:O	2:C:20:LYS:HB3	2.11	0.50
1:J:89:LEU:HD23	1:J:89:LEU:H	1.77	0.50
1:N:2:LYS:HD3	1:N:3:THR:O	2.12	0.50
2:A:70:GLN:HG2	2:A:71:GLY:H	1.76	0.50
2:B:67:ARG:O	1:J:3:THR:HG22	2.12	0.50
2:G:283:ASN:OD1	2:G:284:LYS:N	2.40	0.50
2:D:94:PHE:CD1	2:D:219:ARG:HA	2.46	0.50
2:D:299:ASN:HB2	2:E:303:THR:HG22	1.94	0.50
1:N:25:GLN:NE2	1:N:86:ASP:O	2.45	0.50
1:M:110:ASP:OD2	1:M:111:ASP:N	2.38	0.50
2:A:86:THR:HG21	2:A:187:MET:SD	2.52	0.50
2:A:242:ILE:HG12	2:A:243:ASP:HA	1.94	0.50
1:H:69:THR:HB	1:H:70:ARG:NH2	2.27	0.50
2:B:163:PHE:CG	2:B:164:SER:N	2.80	0.50
2:G:235:SER:O	2:G:268:ARG:HG3	2.12	0.50
1:K:105:TYR:HB3	1:K:106:PRO:HD3	1.94	0.50
1:I:6:MET:HG2	1:I:104:PHE:CD2	2.47	0.50
1:J:36:ASN:OD1	1:J:37:GLU:N	2.43	0.50
1:H:10:THR:H	1:H:11:ASP:HA	1.75	0.49
2:B:110:ARG:O	2:B:114:ASN:HB2	2.12	0.49
2:B:171:THR:HB	2:B:328:ASN:HD22	1.78	0.49
2:D:256:ASP:OD1	2:D:256:ASP:N	2.45	0.49
1:I:70:ARG:O	1:I:70:ARG:NE	2.44	0.49
2:A:72:VAL:HG21	2:B:92:LEU:HG	1.93	0.49
1:H:2:LYS:HG3	2:F:68:TYR:HB2	1.95	0.49
1:H:33:THR:HG22	1:H:34:LEU:HB3	1.95	0.49
2:F:247:LEU:HD22	2:F:250:ASP:OD1	2.11	0.49
2:B:249:LYS:HA	2:B:253:THR:HG21	1.94	0.49
2:B:307:TYR:HB2	2:B:308:GLY:HA2	1.93	0.49
2:G:182:GLU:OE1	2:G:231:ARG:HB3	2.12	0.49
2:G:303:THR:OG1	2:G:304:ILE:N	2.46	0.49
1:K:7:LYS:HG2	2:C:67:ARG:HH12	1.76	0.49
2:C:178:MET:HA	2:C:235:SER:O	2.12	0.49
1:L:23:LYS:HD2	1:L:24:ASP:HB3	1.93	0.49
1:M:54:ASP:HB3	1:M:86:ASP:H	1.77	0.49
2:A:53:LYS:O	2:A:54:THR:OG1	2.27	0.49
2:F:18:THR:HG22	2:F:19:ASP:H	1.76	0.49
2:B:37:ILE:HD11	2:B:324:ASP:HB3	1.93	0.49
2:B:242:ILE:HG22	2:B:246:THR:HB	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:ARG:NH2	2:D:162:VAL:HG13	2.16	0.49
1:N:71:THR:HB	1:N:74:HIS:HE1	1.76	0.49
1:M:88:GLY:HA2	1:M:89:LEU:C	2.33	0.49
2:A:230:VAL:C	2:A:232:ASP:H	2.15	0.49
2:B:186:HIS:CD2	2:B:191:GLU:HG3	2.47	0.49
2:G:13:ASP:O	2:G:17:ARG:N	2.45	0.49
2:G:180:TRP:C	2:G:182:GLU:H	2.16	0.49
2:G:241:ASN:ND2	2:G:242:ILE:HG13	2.22	0.49
2:D:250:ASP:O	2:D:293:GLN:HG3	2.12	0.49
2:C:254:GLY:HA2	2:C:257:LEU:HD11	1.93	0.49
2:E:172:ASN:HB2	2:E:241:ASN:O	2.12	0.49
2:E:315:PHE:HA	2:E:316:LEU:HB3	1.94	0.49
1:L:5:ASN:OD1	1:L:106:PRO:HG3	2.12	0.49
1:N:71:THR:HB	1:N:74:HIS:CE1	2.48	0.49
1:N:105:TYR:HB3	1:N:106:PRO:CD	2.42	0.49
1:M:28:TRP:HA	1:M:84:ILE:HG21	1.94	0.49
2:A:97:LYS:HE2	2:A:218:TYR:HB2	1.94	0.49
1:H:91:PRO:HG3	1:H:101:LYS:NZ	2.27	0.49
2:F:242:ILE:HB	2:F:243:ASP:HA	1.93	0.49
2:B:189:TYR:HB2	2:B:190:PRO:HD2	1.95	0.49
2:G:195:ALA:N	2:G:196:GLY:HA3	2.27	0.49
2:D:69:ASN:ND2	1:L:3:THR:OG1	2.46	0.49
1:I:20:PRO:HB3	1:I:21:GLU:HG3	1.95	0.49
1:L:47:LYS:HG2	1:L:70:ARG:HH21	1.77	0.49
2:A:323:VAL:HG22	2:A:324:ASP:H	1.78	0.49
2:F:89:LEU:HD23	2:F:121:PHE:CE2	2.47	0.49
2:D:176:TRP:HZ2	2:D:238:ARG:HH21	1.61	0.49
2:C:27:ILE:HG12	2:C:27:ILE:O	2.12	0.49
2:E:279:VAL:HG12	2:E:280:ILE:H	1.78	0.49
2:E:296:ASN:N	2:E:296:ASN:HD22	2.11	0.49
1:J:5:ASN:ND2	1:J:6:MET:H	2.09	0.49
1:J:83:GLN:OE1	1:J:84:ILE:N	2.44	0.49
2:A:92:LEU:HB3	2:A:221:GLU:CB	2.43	0.49
2:B:37:ILE:HD13	2:B:126:ALA:HB3	1.94	0.49
2:B:54:THR:HA	2:C:27:ILE:HD11	1.94	0.49
2:E:163:PHE:CG	2:E:164:SER:N	2.80	0.49
2:E:186:HIS:O	2:E:186:HIS:ND1	2.46	0.49
2:E:206:LEU:N	2:E:210:GLY:HA2	2.28	0.49
2:E:291:HIS:NE2	2:E:309:GLY:HA3	2.27	0.49
1:J:41:ARG:HD3	1:J:42:LEU:H	1.78	0.49
1:M:40:GLN:OE1	1:M:41:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:ASN:HB2	2:B:242:ILE:H	1.77	0.49
2:E:94:PHE:HD1	2:E:219:ARG:HB3	1.78	0.49
2:E:214:GLN:O	2:E:215:PHE:HB3	2.13	0.49
1:I:10:THR:HB	1:I:11:ASP:HA	1.94	0.49
1:I:92:GLN:HB3	1:I:93:LYS:CB	2.39	0.49
1:L:48:SER:HA	1:L:92:GLN:O	2.13	0.49
1:H:5:ASN:OD1	1:H:6:MET:N	2.45	0.49
2:B:54:THR:HG22	2:B:55:THR:H	1.77	0.49
2:D:258:ILE:O	2:D:260:MET:N	2.45	0.49
1:K:51:ALA:HB3	1:K:90:ALA:HB3	1.95	0.49
2:F:11:LEU:HA	2:F:14:ILE:HG22	1.95	0.49
2:D:42:ILE:HG12	2:D:180:TRP:CD1	2.48	0.49
2:D:233:TRP:O	2:D:234:ARG:HB2	2.13	0.49
2:E:174:SER:HA	2:E:241:ASN:ND2	2.20	0.49
1:I:6:MET:H	1:I:105:TYR:HE1	1.61	0.49
2:A:42:ILE:HG23	2:A:180:TRP:CD1	2.49	0.48
1:H:5:ASN:HB3	1:H:104:PHE:CE2	2.48	0.48
1:K:24:ASP:OD2	1:K:25:GLN:N	2.45	0.48
2:E:287:HIS:CE1	2:E:320:ILE:HD12	2.47	0.48
1:I:6:MET:HG3	1:I:7:LYS:N	2.27	0.48
1:J:94:ARG:C	1:J:96:ASP:H	2.16	0.48
1:M:40:GLN:NE2	1:M:101:LYS:HB2	2.28	0.48
2:A:299:ASN:O	2:A:301:ASN:ND2	2.45	0.48
1:H:47:LYS:HE3	1:H:94:ARG:HB3	1.95	0.48
2:F:95:VAL:O	2:F:217:ALA:HB1	2.13	0.48
2:B:177:PHE:CB	2:B:280:ILE:HA	2.44	0.48
2:G:191:GLU:N	2:G:191:GLU:OE2	2.44	0.48
2:G:285:THR:HG21	2:G:327:LEU:HD13	1.95	0.48
2:A:240:CYS:HB2	2:A:333:VAL:CG1	2.42	0.48
2:B:246:THR:HA	2:B:249:LYS:HD2	1.95	0.48
2:D:249:LYS:NZ	2:D:250:ASP:H	2.11	0.48
1:K:10:THR:HB	1:K:101:LYS:HB2	1.95	0.48
1:K:101:LYS:H	1:K:101:LYS:CE	2.25	0.48
2:C:247:LEU:HD13	2:C:289:TRP:CD1	2.49	0.48
2:E:171:THR:HG23	2:E:243:ASP:HB2	1.96	0.48
2:A:283:ASN:HB3	2:A:325:ALA:HB3	1.96	0.48
1:H:54:ASP:OD1	1:H:54:ASP:N	2.46	0.48
2:B:147:ARG:HG3	2:B:334:THR:HA	1.95	0.48
2:G:40:ASP:CG	2:G:41:ALA:H	2.16	0.48
2:D:20:LYS:HZ2	2:C:48:ASP:HB3	1.79	0.48
2:D:72:VAL:O	2:D:73:GLN:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:LEU:O	2:E:15:TYR:HB2	2.13	0.48
2:E:67:ARG:HH21	2:E:67:ARG:HB2	1.79	0.48
1:L:6:MET:HE1	1:L:10:THR:HA	1.95	0.48
2:A:177:PHE:HB3	2:A:280:ILE:HA	1.95	0.48
2:F:90:TYR:HE1	2:E:66:ARG:HG3	1.79	0.48
2:B:69:ASN:HB2	1:J:3:THR:HG23	1.95	0.48
2:B:250:ASP:O	2:B:293:GLN:HB2	2.13	0.48
2:C:94:PHE:CD1	2:C:219:ARG:HB3	2.48	0.48
2:C:160:GLU:HG2	2:C:161:ASN:O	2.14	0.48
1:N:20:PRO:HB3	1:N:21:GLU:HG3	1.95	0.48
2:A:154:SER:OG	2:A:155:LYS:N	2.46	0.48
2:F:86:THR:OG1	2:F:87:GLY:N	2.46	0.48
2:F:215:PHE:CE2	2:F:217:ALA:HB2	2.49	0.48
2:B:230:VAL:HG23	2:B:231:ARG:H	1.78	0.48
2:D:86:THR:OG1	2:D:87:GLY:N	2.46	0.48
2:C:224:TRP:HD1	2:C:225:ASP:H	1.62	0.48
2:A:208:SER:N	2:A:209:ASP:HA	2.27	0.48
2:D:65:TRP:CZ2	2:E:128:TYR:HD1	2.31	0.48
2:E:46:CYS:SG	2:E:185:ALA:HB1	2.53	0.48
2:A:272:MET:HE1	2:B:33:LYS:HA	1.95	0.48
2:A:300:VAL:HB	2:B:303:THR:OG1	2.13	0.48
2:F:241:ASN:HB2	2:F:242:ILE:HD13	1.95	0.48
2:B:326:ILE:HG23	2:B:328:ASN:H	1.77	0.48
2:C:26:ARG:O	2:C:28:VAL:N	2.46	0.48
2:C:50:SER:O	2:C:52:HIS:N	2.42	0.48
2:C:186:HIS:HD2	2:C:191:GLU:HA	1.79	0.48
1:N:94:ARG:HG3	1:N:95:ASP:H	1.79	0.48
2:A:307:TYR:CB	2:A:308:GLY:HA2	2.34	0.48
1:H:49:LEU:O	1:H:91:PRO:HA	2.13	0.48
2:F:33:LYS:HE2	2:E:233:TRP:HE1	1.79	0.48
2:F:189:TYR:HB2	2:F:190:PRO:HD2	1.96	0.48
2:F:242:ILE:HD12	2:F:247:LEU:CD2	2.43	0.48
2:G:241:ASN:CB	2:G:242:ILE:HG13	2.44	0.48
1:K:102:ASP:N	1:K:102:ASP:OD1	2.47	0.48
2:E:154:SER:OG	2:E:155:LYS:N	2.45	0.48
1:I:54:ASP:HB2	1:I:55:SER:H	1.51	0.48
1:M:36:ASN:CG	1:M:37:GLU:H	2.16	0.48
2:A:90:TYR:CB	2:A:223:LYS:HA	2.42	0.48
2:A:94:PHE:HE1	2:A:219:ARG:HG3	1.78	0.48
2:A:271:ALA:HB3	2:A:273:LEU:HG	1.95	0.48
2:B:177:PHE:HB2	2:B:279:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:72:VAL:HG12	2:G:73:GLN:HG2	1.96	0.48
2:C:55:THR:HA	2:C:81:PRO:HA	1.96	0.48
1:L:23:LYS:HA	1:L:24:ASP:HA	1.53	0.48
2:A:125:VAL:O	2:A:129:SER:OG	2.26	0.47
2:F:287:HIS:NE2	2:F:320:ILE:HD13	2.29	0.47
2:D:3:LEU:HD12	2:D:4:ILE:HG22	1.95	0.47
2:D:23:ARG:HG2	2:D:24:ILE:H	1.79	0.47
2:D:215:PHE:HD2	2:D:215:PHE:C	2.18	0.47
1:K:23:LYS:HA	1:K:24:ASP:HA	1.44	0.47
2:A:91:ASP:O	2:A:221:GLU:HB2	2.14	0.47
1:H:47:LYS:HG3	1:H:93:LYS:HE3	1.95	0.47
2:B:66:ARG:HG3	2:B:70:GLN:HB2	1.97	0.47
2:B:95:VAL:HG22	2:B:218:TYR:HB2	1.94	0.47
2:D:174:SER:HA	2:D:242:ILE:HD11	1.95	0.47
1:I:6:MET:HG3	1:I:8:THR:H	1.79	0.47
2:D:42:ILE:HD11	2:D:181:GLY:H	1.78	0.47
1:J:88:GLY:HA2	1:J:89:LEU:HA	1.59	0.47
1:N:40:GLN:HB2	1:N:101:LYS:O	2.15	0.47
2:A:50:SER:OG	2:A:51:LYS:N	2.46	0.47
1:H:41:ARG:HG3	1:H:42:LEU:HG	1.96	0.47
2:F:305:GLU:HA	2:F:306:GLU:HA	1.49	0.47
2:B:160:GLU:HB2	2:B:240:CYS:N	2.25	0.47
2:B:242:ILE:HB	2:B:243:ASP:O	2.14	0.47
2:D:37:ILE:HG23	2:D:324:ASP:H	1.79	0.47
2:E:39:THR:O	2:E:39:THR:OG1	2.31	0.47
2:E:48:ASP:O	2:E:188:ILE:HD11	2.14	0.47
1:J:5:ASN:HD21	1:J:105:TYR:HE1	1.60	0.47
2:B:246:THR:HA	2:B:249:LYS:HB2	1.97	0.47
2:G:280:ILE:HD13	2:G:320:ILE:HG12	1.95	0.47
2:E:69:ASN:OD1	2:E:70:GLN:N	2.48	0.47
2:A:271:ALA:HB1	2:A:273:LEU:N	2.29	0.47
2:G:242:ILE:H	2:G:243:ASP:HA	1.78	0.47
2:C:92:LEU:HD13	2:C:92:LEU:H	1.78	0.47
2:C:160:GLU:HB2	2:C:239:ILE:HA	1.96	0.47
1:L:70:ARG:O	1:L:71:THR:OG1	2.26	0.47
1:N:42:LEU:O	1:N:99:GLU:HG3	2.15	0.47
1:N:54:ASP:HB3	1:N:86:ASP:H	1.80	0.47
1:M:5:ASN:HD21	1:M:104:PHE:HE1	1.61	0.47
1:M:7:LYS:HZ3	1:M:8:THR:H	1.63	0.47
1:M:36:ASN:OD1	1:M:37:GLU:N	2.45	0.47
1:M:36:ASN:H	1:M:78:ASN:HD21	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:195:ALA:CB	2:A:222:PHE:HA	2.44	0.47
1:H:26:TYR:CE2	1:H:84:ILE:HD11	2.49	0.47
2:F:282:ALA:O	2:F:323:VAL:N	2.34	0.47
2:B:38:LEU:HD22	2:B:321:ARG:HG3	1.97	0.47
2:B:66:ARG:HG3	2:B:70:GLN:H	1.79	0.47
2:G:7:THR:O	2:G:8:LEU:HB2	2.14	0.47
2:G:20:LYS:O	2:G:20:LYS:HG3	2.15	0.47
2:G:122:ASN:HA	2:G:125:VAL:HG12	1.97	0.47
2:D:90:TYR:CZ	2:C:66:ARG:HD3	2.50	0.47
2:D:250:ASP:HA	2:D:253:THR:OG1	2.15	0.47
1:K:5:ASN:HB3	1:K:104:PHE:O	2.15	0.47
1:K:21:GLU:O	1:K:23:LYS:N	2.40	0.47
1:K:41:ARG:HG2	1:K:42:LEU:HD22	1.97	0.47
2:C:84:ASP:HA	1:J:110:ASP:HA	1.96	0.47
2:C:92:LEU:HB3	2:C:221:GLU:HB3	1.97	0.47
2:C:176:TRP:CZ2	2:C:238:ARG:HD3	2.50	0.47
2:C:191:GLU:OE1	2:C:192:GLY:N	2.42	0.47
1:J:32:ILE:O	1:J:33:THR:OG1	2.26	0.47
1:M:84:ILE:O	1:M:85:THR:OG1	2.24	0.47
1:H:7:LYS:HG2	1:H:8:THR:N	2.29	0.47
2:B:172:ASN:HA	2:B:243:ASP:HB2	1.96	0.47
2:C:172:ASN:O	2:C:328:ASN:HA	2.15	0.47
2:E:4:ILE:C	2:E:6:GLN:H	2.18	0.47
1:L:89:LEU:HD13	1:L:104:PHE:HE2	1.80	0.47
1:N:23:LYS:HA	1:N:24:ASP:HA	1.57	0.47
2:F:177:PHE:HB3	2:F:280:ILE:HB	1.97	0.47
2:F:178:MET:O	2:F:178:MET:HG2	2.14	0.47
2:B:180:TRP:HA	2:B:180:TRP:CE3	2.50	0.47
2:D:23:ARG:HB3	2:D:25:ALA:O	2.15	0.47
2:C:11:LEU:HD23	2:C:102:ARG:HH12	1.80	0.47
2:E:66:ARG:HE	2:E:68:TYR:H	1.61	0.47
1:I:44:LEU:HD21	1:I:97:ALA:HA	1.97	0.47
2:A:51:LYS:O	2:A:52:HIS:HB2	2.15	0.47
2:A:74:PRO:HA	2:B:92:LEU:O	2.15	0.47
2:A:89:LEU:HB3	2:F:65:TRP:HD1	1.78	0.47
2:D:234:ARG:O	2:D:268:ARG:HG3	2.14	0.47
2:D:277:LYS:HD3	2:D:277:LYS:HA	1.79	0.47
1:J:41:ARG:CD	1:J:42:LEU:H	2.28	0.47
1:N:94:ARG:HA	1:N:94:ARG:HD2	1.60	0.46
2:F:124:LYS:HZ3	2:F:127:ARG:HB3	1.80	0.46
2:G:331:SER:O	2:G:333:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:172:ASN:ND2	2:E:241:ASN:O	2.40	0.46
2:E:184:THR:HA	2:E:228:LEU:HA	1.96	0.46
1:I:28:TRP:C	1:I:84:ILE:HG12	2.35	0.46
1:I:54:ASP:N	1:I:54:ASP:OD1	2.48	0.46
1:J:28:TRP:HA	1:J:84:ILE:HG21	1.97	0.46
1:M:44:LEU:HB2	1:M:97:ALA:CB	2.45	0.46
2:A:92:LEU:HB3	2:A:221:GLU:HB3	1.98	0.46
2:F:92:LEU:HD12	2:E:72:VAL:HG22	1.96	0.46
2:F:271:ALA:HB1	2:F:272:MET:C	2.35	0.46
2:B:122:ASN:O	2:B:125:VAL:HG12	2.15	0.46
2:D:92:LEU:HA	2:D:221:GLU:HA	1.97	0.46
1:K:1:MET:N	1:K:1:MET:SD	2.88	0.46
2:C:90:TYR:CB	2:C:223:LYS:HA	2.45	0.46
1:L:66:SER:OG	1:L:67:VAL:N	2.47	0.46
1:H:36:ASN:OD1	1:H:37:GLU:N	2.49	0.46
2:F:286:ILE:HD13	2:F:286:ILE:HA	1.85	0.46
2:G:28:VAL:HG13	2:G:29:GLU:HG3	1.97	0.46
1:J:27:PRO:HA	1:J:84:ILE:HG23	1.96	0.46
1:J:59:MET:HB2	1:J:60:ALA:HB2	1.97	0.46
1:L:35:ASP:HA	1:L:78:ASN:OD1	2.14	0.46
1:N:71:THR:HG22	1:N:72:THR:H	1.80	0.46
1:M:40:GLN:CD	1:M:101:LYS:HB2	2.36	0.46
1:M:64:VAL:HG23	1:M:65:CYS:H	1.79	0.46
2:A:79:THR:OG1	2:A:80:VAL:N	2.45	0.46
2:D:76:LYS:HZ1	2:E:6:GLN:C	2.19	0.46
2:D:201:ASP:OD2	2:D:219:ARG:NH2	2.49	0.46
2:D:215:PHE:C	2:D:215:PHE:CD2	2.89	0.46
2:C:307:TYR:HB2	2:C:308:GLY:HA3	1.96	0.46
1:I:22:THR:OG1	1:I:25:GLN:NE2	2.49	0.46
1:J:20:PRO:HA	1:J:21:GLU:HA	1.45	0.46
2:A:88:MET:HG2	2:A:225:ASP:HB2	1.96	0.46
1:K:8:THR:HB	1:K:101:LYS:NZ	2.31	0.46
2:C:142:MET:C	2:C:144:LEU:H	2.19	0.46
1:L:14:VAL:C	1:L:16:GLU:H	2.19	0.46
1:L:80:VAL:HG13	1:L:81:GLU:H	1.81	0.46
2:A:47:ASN:O	2:A:52:HIS:HA	2.16	0.46
1:H:46:ALA:H	1:H:70:ARG:HB3	1.79	0.46
2:F:87:GLY:HA3	2:F:138:PRO:CG	2.44	0.46
2:G:106:ALA:O	2:G:110:ARG:HG2	2.16	0.46
1:K:26:TYR:CE2	1:K:84:ILE:HD11	2.50	0.46
2:C:94:PHE:HD1	2:C:219:ARG:HB3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:209:ASP:N	2:C:209:ASP:OD1	2.49	0.46
2:E:305:GLU:HA	2:E:306:GLU:HA	1.48	0.46
1:J:23:LYS:HA	1:J:24:ASP:HA	1.43	0.46
1:L:63:ASN:HD21	1:L:65:CYS:HB3	1.80	0.46
1:M:17:ASP:OD1	1:M:18:GLY:N	2.49	0.46
2:F:39:THR:O	2:F:39:THR:OG1	2.28	0.46
2:F:160:GLU:HG2	2:F:161:ASN:N	2.30	0.46
2:F:180:TRP:HB2	2:F:277:LYS:HE2	1.97	0.46
2:G:203:GLY:HA2	2:G:204:ASP:HB2	1.96	0.46
1:K:10:THR:H	1:K:11:ASP:HA	1.80	0.46
2:C:37:ILE:HD12	2:C:323:VAL:C	2.36	0.46
2:C:208:SER:HA	2:C:209:ASP:HA	1.43	0.46
1:I:23:LYS:HA	1:I:24:ASP:HA	1.51	0.46
1:I:92:GLN:OE1	1:I:93:LYS:HA	2.16	0.46
1:J:80:VAL:HG13	1:J:81:GLU:H	1.81	0.46
1:M:11:ASP:C	1:M:13:PHE:H	2.19	0.46
2:A:57:ARG:HH22	2:B:17:ARG:NH1	2.14	0.46
1:H:39:LEU:N	1:H:102:ASP:OD2	2.49	0.46
2:F:178:MET:HA	2:F:235:SER:O	2.15	0.46
2:B:192:GLY:O	2:B:194:VAL:N	2.49	0.46
2:B:197:PHE:CE2	2:B:221:GLU:HB3	2.41	0.46
2:G:28:VAL:HG22	2:G:29:GLU:HG3	1.97	0.46
2:G:90:TYR:HD2	2:G:90:TYR:O	1.99	0.46
2:D:112:SER:O	2:D:115:MET:HG2	2.15	0.46
2:D:195:ALA:HB1	2:D:222:PHE:HD2	1.80	0.46
1:I:4:VAL:HA	1:I:5:ASN:HA	1.55	0.46
1:N:9:GLY:HA2	1:N:101:LYS:HD2	1.97	0.46
1:H:11:ASP:OD1	1:H:101:LYS:HB2	2.16	0.46
1:H:26:TYR:HA	1:H:27:PRO:HD3	1.77	0.46
2:G:26:ARG:NE	2:G:28:VAL:HG23	2.30	0.46
2:D:166:GLY:O	2:D:331:SER:OG	2.30	0.46
1:I:94:ARG:HD3	1:I:94:ARG:HA	1.52	0.46
1:N:9:GLY:HA3	1:N:11:ASP:OD1	2.15	0.46
1:M:48:SER:HA	1:M:92:GLN:O	2.16	0.46
2:F:138:PRO:HA	2:F:139:GLU:HA	1.49	0.46
2:F:179:SER:HB2	2:F:278:GLU:HG2	1.98	0.46
2:F:180:TRP:HA	2:F:180:TRP:HE3	1.81	0.46
2:B:85:THR:OG1	2:B:86:THR:N	2.49	0.46
2:B:154:SER:O	2:B:233:TRP:HH2	1.98	0.46
2:G:141:PHE:HD2	2:G:141:PHE:O	1.99	0.46
2:D:31:LEU:HB2	2:C:56:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:SER:OG	2:D:51:LYS:N	2.49	0.46
2:D:274:GLY:HA2	2:D:275:ASP:HA	1.51	0.46
1:L:12:SER:O	1:L:12:SER:OG	2.32	0.46
1:N:21:GLU:N	2:A:1:MET:SD	2.90	0.45
2:F:147:ARG:HB2	2:F:147:ARG:HH11	1.81	0.45
2:F:250:ASP:HA	2:F:253:THR:OG1	2.16	0.45
2:D:102:ARG:O	2:D:102:ARG:NE	2.49	0.45
2:D:124:LYS:HD2	2:D:128:TYR:CD2	2.51	0.45
2:E:13:ASP:OD2	2:E:17:ARG:NH2	2.48	0.45
2:A:39:THR:HA	2:A:40:ASP:C	2.36	0.45
2:B:60:ILE:HD11	2:C:117:LYS:NZ	2.31	0.45
2:D:65:TRP:CH2	2:E:128:TYR:HD1	2.34	0.45
1:K:44:LEU:HB2	1:K:99:GLU:OE2	2.15	0.45
2:E:161:ASN:N	2:E:240:CYS:O	2.43	0.45
1:M:19:LYS:N	1:M:20:PRO:HD2	2.32	0.45
1:M:64:VAL:O	1:M:65:CYS:HB2	2.16	0.45
2:A:141:PHE:C	2:A:141:PHE:CD1	2.89	0.45
2:B:67:ARG:NH1	1:J:7:LYS:HD2	2.31	0.45
2:G:187:MET:HB3	2:G:189:TYR:CE1	2.51	0.45
1:K:25:GLN:HG3	1:K:85:THR:O	2.17	0.45
1:J:61:MET:SD	1:J:61:MET:N	2.88	0.45
1:L:46:ALA:HB2	1:L:70:ARG:HB3	1.98	0.45
1:H:98:LYS:H	1:H:98:LYS:HG2	1.58	0.45
2:G:242:ILE:HD12	2:G:243:ASP:HA	1.98	0.45
2:G:305:GLU:O	2:G:312:ILE:HA	2.16	0.45
1:K:71:THR:HB	1:K:74:HIS:CE1	2.52	0.45
2:C:192:GLY:O	2:C:194:VAL:N	2.46	0.45
2:E:203:GLY:N	2:E:215:PHE:O	2.49	0.45
2:B:233:TRP:O	2:B:233:TRP:CG	2.69	0.45
2:G:260:MET:O	2:G:263:ASP:HB3	2.17	0.45
2:D:27:ILE:HG12	2:D:27:ILE:O	2.15	0.45
2:D:124:LYS:O	2:D:127:ARG:HB2	2.16	0.45
2:D:160:GLU:HG3	2:D:240:CYS:HB3	1.98	0.45
1:K:7:LYS:HD2	1:K:8:THR:H	1.82	0.45
1:K:46:ALA:CA	1:K:70:ARG:HH12	2.29	0.45
2:C:159:ALA:HB1	2:C:263:ASP:OD2	2.15	0.45
2:C:163:PHE:HD2	2:C:243:ASP:H	1.65	0.45
2:C:170:SER:O	2:C:328:ASN:HB2	2.17	0.45
2:E:1:MET:HG3	2:E:1:MET:O	2.17	0.45
1:I:53:GLY:O	1:I:86:ASP:HA	2.17	0.45
1:L:16:GLU:OE2	1:L:18:GLY:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:70:ARG:HB3	1:L:70:ARG:HE	1.60	0.45
1:N:109:GLU:CD	1:N:110:ASP:H	2.20	0.45
1:M:53:GLY:O	1:M:86:ASP:HA	2.16	0.45
1:M:94:ARG:HE	1:M:94:ARG:HA	1.80	0.45
1:H:50:PRO:HG2	1:H:66:SER:HB3	1.97	0.45
2:B:92:LEU:HB3	2:B:221:GLU:CB	2.39	0.45
2:D:88:MET:HG2	2:D:225:ASP:OD1	2.17	0.45
2:E:53:LYS:O	2:E:54:THR:OG1	2.25	0.45
2:E:205:ASP:HB2	2:E:210:GLY:CA	2.47	0.45
1:J:24:ASP:OD2	1:J:24:ASP:N	2.50	0.45
1:L:38:SER:O	1:L:75:GLY:HA2	2.17	0.45
2:A:117:LYS:HE2	2:A:222:PHE:HE1	1.81	0.45
2:B:299:ASN:O	2:B:301:ASN:N	2.50	0.45
2:G:250:ASP:OD1	2:G:255:ALA:HB3	2.16	0.45
2:D:189:TYR:CD1	2:D:189:TYR:N	2.84	0.45
2:E:147:ARG:HB3	2:E:333:VAL:HG22	1.99	0.45
1:I:55:SER:OG	1:I:56:VAL:N	2.49	0.45
1:J:92:GLN:CD	1:J:93:LYS:HB3	2.37	0.45
1:L:53:GLY:O	1:L:86:ASP:HA	2.17	0.45
1:N:28:TRP:HA	1:N:84:ILE:HG21	1.98	0.45
1:N:42:LEU:H	1:N:42:LEU:HG	1.61	0.45
1:M:19:LYS:HE3	1:M:87:ILE:HG21	1.98	0.45
2:F:37:ILE:HG23	2:F:38:LEU:O	2.17	0.45
2:B:60:ILE:HD11	2:C:117:LYS:HZ2	1.81	0.45
2:G:152:SER:OG	2:G:153:THR:N	2.49	0.45
2:D:115:MET:HA	2:D:118:LEU:HD23	1.98	0.45
1:K:45:ASN:HB3	1:K:95:ASP:CG	2.37	0.45
1:J:49:LEU:O	1:J:91:PRO:HA	2.16	0.45
1:M:47:LYS:HA	1:M:70:ARG:NH2	2.32	0.45
2:F:38:LEU:HD23	2:F:38:LEU:HA	1.83	0.45
2:F:47:ASN:HA	2:F:48:ASP:HA	1.63	0.45
2:F:141:PHE:HZ	2:F:178:MET:SD	2.39	0.45
2:F:230:VAL:O	2:F:232:ASP:N	2.49	0.45
2:F:241:ASN:CB	2:F:242:ILE:HG12	2.46	0.45
2:B:76:LYS:HD3	2:B:76:LYS:H	1.82	0.45
2:B:160:GLU:HG2	2:B:161:ASN:O	2.16	0.45
2:G:182:GLU:OE2	2:G:231:ARG:NH1	2.50	0.45
2:D:62:GLU:N	2:D:62:GLU:OE1	2.50	0.45
2:D:247:LEU:HD22	2:D:247:LEU:HA	1.76	0.45
1:K:92:GLN:HB3	1:K:93:LYS:HB3	1.99	0.45
2:C:35:ASN:OD1	2:C:123:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:TRP:CE2	2:C:238:ARG:HD3	2.52	0.45
1:N:107:ASP:HA	1:N:108:GLY:HA3	1.77	0.45
1:M:27:PRO:HB3	1:M:85:THR:OG1	2.17	0.45
2:A:85:THR:OG1	2:A:86:THR:N	2.49	0.45
2:A:201:ASP:HB3	2:A:202:LEU:H	1.57	0.45
2:F:28:VAL:HA	2:F:29:GLU:HA	1.65	0.45
2:B:17:ARG:O	2:B:26:ARG:HD2	2.16	0.45
2:G:274:GLY:HA3	2:G:275:ASP:HA	1.67	0.45
2:D:4:ILE:HG12	2:D:5:GLY:H	1.81	0.45
1:K:107:ASP:HA	1:K:108:GLY:HA3	1.60	0.45
2:E:238:ARG:HG2	2:E:239:ILE:N	2.32	0.45
1:L:5:ASN:HB2	1:L:105:TYR:CZ	2.52	0.45
1:L:94:ARG:HD2	1:L:94:ARG:HA	1.75	0.45
1:M:54:ASP:O	1:M:55:SER:HB2	2.17	0.44
2:A:84:ASP:OD2	2:A:85:THR:HG22	2.17	0.44
2:F:119:GLN:HA	2:F:122:ASN:HD21	1.81	0.44
2:D:69:ASN:HB3	1:L:2:LYS:HG3	1.98	0.44
2:D:179:SER:HB2	2:D:278:GLU:HG3	1.98	0.44
2:C:121:PHE:HE1	2:C:224:TRP:HE3	1.64	0.44
2:C:171:THR:OG1	2:C:243:ASP:OD1	2.27	0.44
2:C:268:ARG:O	2:C:269:ASP:HB3	2.17	0.44
1:I:8:THR:OG1	1:I:9:GLY:HA2	2.17	0.44
1:I:25:GLN:HG3	1:I:86:ASP:OD2	2.17	0.44
1:J:53:GLY:O	1:J:86:ASP:HA	2.16	0.44
1:L:70:ARG:H	1:L:70:ARG:NE	2.15	0.44
2:A:41:ALA:HB1	2:A:180:TRP:HE1	1.82	0.44
2:A:66:ARG:HD2	2:A:68:TYR:N	2.31	0.44
1:H:40:GLN:NE2	1:H:41:ARG:HG2	2.32	0.44
2:F:110:ARG:HH12	2:F:218:TYR:HD1	1.65	0.44
2:B:51:LYS:O	2:B:52:HIS:HB2	2.17	0.44
2:B:280:ILE:HG23	2:B:320:ILE:HA	1.98	0.44
2:D:318:ILE:H	2:D:318:ILE:HG13	1.45	0.44
2:C:37:ILE:HD11	2:C:324:ASP:HB2	1.99	0.44
2:C:326:ILE:HD13	2:C:327:LEU:H	1.81	0.44
1:I:20:PRO:HA	1:I:21:GLU:HA	1.57	0.44
1:I:32:ILE:O	1:I:33:THR:OG1	2.27	0.44
1:I:93:LYS:HG3	1:I:94:ARG:H	1.82	0.44
1:L:11:ASP:CG	1:L:101:LYS:HD2	2.38	0.44
1:H:37:GLU:OE2	1:H:39:LEU:HG	2.17	0.44
2:F:113:GLU:OE1	2:E:77:THR:HG21	2.17	0.44
2:G:247:LEU:HD13	2:G:293:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:LYS:HB3	2:D:83:THR:HG21	2.00	0.44
2:D:205:ASP:OD2	2:D:214:GLN:N	2.50	0.44
1:K:40:GLN:HB2	1:K:102:ASP:HA	1.98	0.44
2:C:29:GLU:HB2	2:C:30:GLN:H	1.57	0.44
2:E:8:LEU:HD23	2:E:94:PHE:HB2	1.99	0.44
2:E:147:ARG:NE	2:E:148:PHE:HD2	2.14	0.44
1:I:30:LEU:O	1:I:31:ARG:NE	2.50	0.44
1:L:105:TYR:HB2	1:L:106:PRO:CA	2.48	0.44
2:B:63:PRO:HG3	2:C:121:PHE:CD2	2.53	0.44
2:B:274:GLY:HA3	2:B:275:ASP:HA	1.88	0.44
2:D:48:ASP:HB3	2:E:20:LYS:HZ3	1.82	0.44
2:D:249:LYS:O	2:D:251:ALA:N	2.50	0.44
2:C:326:ILE:HD13	2:C:328:ASN:H	1.82	0.44
1:J:94:ARG:HA	1:J:94:ARG:HD2	1.59	0.44
2:A:163:PHE:CG	2:A:164:SER:N	2.85	0.44
2:A:266:TYR:HE1	2:B:311:LYS:HG2	1.83	0.44
2:B:74:PRO:HG3	2:C:94:PHE:CD2	2.53	0.44
2:B:141:PHE:C	2:B:143:GLY:H	2.21	0.44
2:G:47:ASN:HA	2:G:48:ASP:HA	1.59	0.44
2:G:193:MET:HA	2:G:224:TRP:HE3	1.82	0.44
2:D:33:LYS:HA	2:C:234:ARG:HH22	1.82	0.44
1:H:4:VAL:HA	1:H:5:ASN:HA	1.69	0.44
1:H:53:GLY:O	1:H:86:ASP:HA	2.18	0.44
2:B:162:VAL:HG12	2:B:335:ALA:HB2	1.99	0.44
2:B:315:PHE:HA	2:B:316:LEU:HA	1.65	0.44
2:D:19:ASP:OD2	2:D:26:ARG:NH2	2.51	0.44
2:D:161:ASN:HB3	2:D:241:ASN:ND2	2.33	0.44
2:D:271:ALA:HA	2:D:272:MET:HB3	1.99	0.44
1:J:5:ASN:CG	1:J:6:MET:N	2.70	0.44
2:A:11:LEU:HA	2:A:14:ILE:HG22	2.00	0.44
2:A:190:PRO:HB2	2:A:194:VAL:HG11	2.00	0.44
1:H:13:PHE:H	1:H:16:GLU:CG	2.31	0.44
1:H:40:GLN:HE21	1:H:100:LEU:HB3	1.82	0.44
2:F:128:TYR:CD1	2:E:65:TRP:HZ2	2.35	0.44
2:F:147:ARG:HG2	2:F:334:THR:HB	1.99	0.44
2:F:170:SER:HA	2:F:171:THR:HA	1.83	0.44
2:B:180:TRP:HA	2:B:180:TRP:HE3	1.82	0.44
2:C:130:ILE:HG13	2:C:131:TYR:CD2	2.52	0.44
2:E:51:LYS:O	2:E:52:HIS:HB2	2.18	0.44
1:M:93:LYS:HG3	1:M:94:ARG:H	1.83	0.44
2:F:202:LEU:HD13	2:F:214:GLN:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ILE:HD13	2:B:328:ASN:H	1.83	0.44
2:G:259:SER:O	2:G:262:VAL:HG12	2.18	0.44
2:G:280:ILE:HB	2:G:320:ILE:HG12	1.98	0.44
2:D:223:LYS:NZ	2:D:223:LYS:HB3	2.32	0.44
1:K:70:ARG:O	1:K:70:ARG:HG2	2.18	0.44
2:C:283:ASN:HD21	2:C:286:ILE:H	1.64	0.44
2:E:316:LEU:HA	2:E:317:GLY:HA2	1.66	0.44
1:J:40:GLN:HE22	1:J:41:ARG:NH2	2.15	0.44
1:L:5:ASN:HB2	1:L:6:MET:H	1.71	0.44
1:L:23:LYS:HD2	1:L:23:LYS:HA	1.86	0.44
2:B:280:ILE:HG12	2:B:320:ILE:HD13	2.00	0.44
2:B:305:GLU:HA	2:B:306:GLU:HA	1.66	0.44
2:G:150:THR:N	2:G:152:SER:O	2.51	0.44
2:D:244:VAL:O	2:D:248:THR:HG23	2.17	0.44
1:K:4:VAL:HA	1:K:5:ASN:HA	1.69	0.44
2:C:206:LEU:HG	2:C:207:VAL:H	1.83	0.44
2:C:329:THR:HG1	2:C:330:GLU:H	1.62	0.44
2:E:170:SER:HA	2:E:171:THR:HA	1.78	0.44
2:E:175:ILE:HG13	2:E:239:ILE:HG13	2.00	0.44
2:E:217:ALA:O	2:E:218:TYR:HB2	2.16	0.44
1:J:89:LEU:HD11	1:J:102:ASP:OD2	2.18	0.44
1:L:4:VAL:HA	1:L:5:ASN:HA	1.73	0.44
2:A:251:ALA:HA	2:A:292:LYS:NZ	2.33	0.43
2:F:257:LEU:H	2:F:257:LEU:HD23	1.82	0.43
2:D:242:ILE:N	2:D:243:ASP:HA	2.33	0.43
2:D:316:LEU:H	2:D:318:ILE:HG13	1.82	0.43
2:C:48:ASP:OD2	2:C:48:ASP:N	2.29	0.43
2:E:97:LYS:HE3	2:E:218:TYR:N	2.33	0.43
2:E:182:GLU:HG3	2:E:231:ARG:HD3	1.99	0.43
1:L:54:ASP:HB2	1:L:83:GLN:HB3	1.99	0.43
1:M:27:PRO:HB3	1:M:85:THR:HG1	1.84	0.43
2:A:28:VAL:HA	2:A:29:GLU:HA	1.66	0.43
2:A:161:ASN:HB3	2:A:240:CYS:HB3	2.00	0.43
2:A:170:SER:HA	2:A:171:THR:HA	1.67	0.43
2:F:209:ASP:N	2:F:210:GLY:CA	2.79	0.43
2:G:124:LYS:O	2:G:127:ARG:HB2	2.18	0.43
2:G:268:ARG:HG2	2:G:272:MET:HE1	1.98	0.43
2:D:230:VAL:C	2:D:232:ASP:N	2.71	0.43
2:C:84:ASP:OD2	2:C:85:THR:N	2.46	0.43
2:E:149:ASN:O	2:E:151:LEU:N	2.47	0.43
2:E:273:LEU:HD23	2:E:273:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:286:ILE:HD13	2:E:286:ILE:HA	1.80	0.43
1:J:43:GLY:HA2	1:J:100:LEU:HG	1.99	0.43
1:M:98:LYS:HE3	1:M:98:LYS:HB3	1.77	0.43
2:F:37:ILE:HD11	2:F:324:ASP:N	2.33	0.43
2:B:160:GLU:HG2	2:B:161:ASN:N	2.33	0.43
2:G:97:LYS:HB2	2:G:217:ALA:O	2.17	0.43
1:K:71:THR:HB	1:K:74:HIS:HE1	1.83	0.43
2:C:291:HIS:NE2	2:C:309:GLY:HA3	2.33	0.43
2:E:134:THR:O	2:E:134:THR:OG1	2.36	0.43
1:J:47:LYS:HE3	1:J:70:ARG:HH21	1.82	0.43
2:A:69:ASN:CB	1:I:3:THR:HG21	2.41	0.43
1:H:23:LYS:CG	1:H:24:ASP:HA	2.49	0.43
2:F:97:LYS:HE2	2:F:218:TYR:CD2	2.53	0.43
2:B:170:SER:HA	2:B:171:THR:OG1	2.18	0.43
2:D:4:ILE:HG12	2:D:5:GLY:N	2.34	0.43
2:D:12:LEU:HD13	2:D:13:ASP:N	2.33	0.43
2:D:182:GLU:OE2	2:D:231:ARG:NH1	2.51	0.43
2:C:39:THR:HA	2:C:40:ASP:O	2.19	0.43
2:C:85:THR:OG1	2:C:86:THR:N	2.51	0.43
2:C:203:GLY:HA3	2:C:204:ASP:CB	2.47	0.43
1:L:1:MET:HA	1:L:2:LYS:HA	1.58	0.43
1:L:46:ALA:CB	1:L:70:ARG:HB3	2.47	0.43
1:N:53:GLY:O	1:N:86:ASP:HA	2.18	0.43
1:M:28:TRP:C	1:M:84:ILE:HG12	2.38	0.43
1:H:93:LYS:HG3	1:H:94:ARG:H	1.83	0.43
2:F:148:PHE:O	2:F:154:SER:OG	2.15	0.43
2:F:209:ASP:OD1	2:F:212:GLY:N	2.51	0.43
2:D:138:PRO:HA	2:D:139:GLU:HA	1.55	0.43
1:K:50:PRO:HA	1:K:91:PRO:HA	1.99	0.43
1:N:26:TYR:HA	1:N:27:PRO:HD3	1.85	0.43
2:A:192:GLY:O	2:A:194:VAL:N	2.52	0.43
2:B:250:ASP:OD1	2:B:293:GLN:HG2	2.19	0.43
2:G:250:ASP:HB2	2:G:293:GLN:NE2	2.34	0.43
2:D:22:GLY:HA3	2:D:23:ARG:HA	1.48	0.43
2:D:171:THR:HG21	2:D:245:THR:HG23	2.00	0.43
2:D:197:PHE:N	2:D:197:PHE:CD2	2.87	0.43
2:D:301:ASN:CG	2:C:300:VAL:HG23	2.39	0.43
1:K:57:SER:HA	1:K:85:THR:HG21	1.99	0.43
1:K:105:TYR:HB3	1:K:106:PRO:CD	2.49	0.43
2:E:246:THR:O	2:E:249:LYS:HG2	2.18	0.43
1:J:94:ARG:HG3	1:J:95:ASP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:47:LYS:HA	1:M:70:ARG:HH21	1.82	0.43
2:A:242:ILE:HB	2:A:243:ASP:O	2.19	0.43
2:F:180:TRP:C	2:F:182:GLU:H	2.22	0.43
2:B:28:VAL:HA	2:B:29:GLU:HA	1.77	0.43
2:G:240:CYS:HB3	2:G:334:THR:HA	2.01	0.43
2:G:313:VAL:O	2:G:314:SER:OG	2.32	0.43
2:D:178:MET:HG3	2:D:180:TRP:HZ3	1.84	0.43
1:J:70:ARG:O	1:J:71:THR:OG1	2.34	0.43
1:L:72:THR:HG22	1:L:73:ASP:OD1	2.18	0.43
1:N:4:VAL:HA	1:N:5:ASN:HA	1.53	0.43
1:N:8:THR:HA	1:N:9:GLY:HA2	1.78	0.43
2:A:95:VAL:HG22	2:A:218:TYR:O	2.18	0.43
2:B:189:TYR:HB2	2:B:190:PRO:CD	2.49	0.43
2:G:309:GLY:HA2	2:G:310:LYS:O	2.19	0.43
2:C:244:VAL:O	2:C:247:LEU:HB2	2.19	0.43
2:E:95:VAL:HB	2:E:96:ASP:H	1.61	0.43
2:E:97:LYS:HE3	2:E:218:TYR:H	1.84	0.43
2:E:157:ALA:HB1	2:E:236:ILE:HG23	2.01	0.43
2:E:189:TYR:HB2	2:E:190:PRO:CD	2.49	0.43
1:J:101:LYS:HD2	1:J:101:LYS:N	2.33	0.43
1:L:55:SER:HA	1:L:83:GLN:NE2	2.33	0.43
1:M:94:ARG:HG3	1:M:95:ASP:N	2.34	0.43
2:A:155:LYS:HD2	2:A:155:LYS:HA	1.89	0.43
2:A:280:ILE:HB	2:A:320:ILE:HB	2.00	0.43
2:F:22:GLY:HA3	2:F:23:ARG:HA	1.58	0.43
2:F:242:ILE:HD12	2:F:247:LEU:HD23	1.99	0.43
2:B:15:TYR:HD2	2:B:15:TYR:HA	1.73	0.43
2:B:138:PRO:HA	2:B:139:GLU:HA	1.55	0.43
2:G:138:PRO:HA	2:G:139:GLU:HA	1.51	0.43
2:D:7:THR:CG2	2:C:74:PRO:HB2	2.48	0.43
2:D:182:GLU:OE1	2:D:231:ARG:HB3	2.19	0.43
2:C:17:ARG:HD3	2:C:17:ARG:HA	1.75	0.43
2:C:60:ILE:N	2:C:61:PRO:HD3	2.33	0.43
2:C:139:GLU:HG3	2:C:228:LEU:HD12	2.01	0.43
2:C:314:SER:HB3	2:C:315:PHE:H	1.58	0.43
2:E:104:ASN:O	2:E:106:ALA:N	2.52	0.43
1:I:5:ASN:HB2	1:I:6:MET:H	1.48	0.43
1:L:49:LEU:O	1:L:91:PRO:HA	2.19	0.43
1:L:73:ASP:O	1:L:74:HIS:ND1	2.51	0.43
1:N:37:GLU:O	1:N:104:PHE:HB3	2.18	0.43
1:N:105:TYR:HB3	1:N:106:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:26:TYR:HA	1:M:27:PRO:HD3	1.74	0.43
1:H:42:LEU:H	1:H:42:LEU:HG	1.68	0.43
2:F:172:ASN:HB2	2:F:241:ASN:C	2.39	0.43
2:F:241:ASN:CG	2:F:242:ILE:HG12	2.40	0.43
2:F:285:THR:O	2:F:289:TRP:HB2	2.19	0.43
2:B:172:ASN:HB2	2:B:241:ASN:C	2.39	0.43
2:G:158:SER:O	2:G:158:SER:OG	2.24	0.43
2:G:176:TRP:HB2	2:G:281:TYR:HB2	2.00	0.43
2:G:245:THR:O	2:G:249:LYS:HD3	2.19	0.43
2:G:332:ALA:C	2:G:334:THR:H	2.22	0.43
2:D:315:PHE:HA	2:D:316:LEU:HA	1.80	0.43
1:K:5:ASN:HD21	1:K:22:THR:CB	2.31	0.43
1:K:26:TYR:HA	1:K:27:PRO:HD3	1.72	0.43
1:I:54:ASP:OD1	1:I:62:ALA:HB3	2.18	0.43
1:N:10:THR:HB	1:N:101:LYS:HG2	2.01	0.42
2:A:32:ALA:HA	2:F:234:ARG:NH1	2.34	0.42
2:A:88:MET:SD	2:F:66:ARG:NH2	2.92	0.42
1:H:71:THR:HG22	1:H:72:THR:H	1.84	0.42
2:F:36:ASP:OD1	2:E:270:VAL:HG23	2.18	0.42
2:B:66:ARG:HG2	2:B:68:TYR:H	1.84	0.42
2:D:86:THR:HG1	2:D:87:GLY:H	1.67	0.42
2:D:281:TYR:HD1	2:D:323:VAL:HB	1.83	0.42
1:K:26:TYR:O	1:K:84:ILE:HG13	2.19	0.42
2:C:197:PHE:HE2	2:C:221:GLU:HG3	1.83	0.42
2:C:201:ASP:OD2	2:C:219:ARG:NH1	2.52	0.42
2:E:172:ASN:N	2:E:172:ASN:OD1	2.51	0.42
1:I:17:ASP:C	1:I:19:LYS:H	2.18	0.42
1:I:29:GLY:O	1:I:30:LEU:HD13	2.18	0.42
1:L:47:LYS:HG2	1:L:70:ARG:NH2	2.32	0.42
1:N:28:TRP:N	1:N:84:ILE:HG21	2.34	0.42
2:A:68:TYR:HD2	2:A:68:TYR:HA	1.53	0.42
2:A:76:LYS:HE3	2:A:76:LYS:N	2.34	0.42
2:A:170:SER:HB3	2:A:171:THR:HG22	2.00	0.42
1:H:28:TRP:C	1:H:84:ILE:HG12	2.40	0.42
2:F:90:TYR:HB2	2:F:221:GLU:OE2	2.18	0.42
2:D:70:GLN:OE1	1:L:3:THR:HG21	2.19	0.42
2:D:160:GLU:HB2	2:D:239:ILE:HG22	2.01	0.42
2:D:326:ILE:HD12	2:D:326:ILE:HA	1.85	0.42
1:K:22:THR:HG21	1:K:104:PHE:CZ	2.53	0.42
2:C:82:VAL:HG22	2:C:83:THR:H	1.85	0.42
2:C:246:THR:O	2:C:250:ASP:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:180:TRP:HB2	2:E:277:LYS:HG2	2.01	0.42
2:E:300:VAL:O	2:E:302:LEU:HG	2.18	0.42
1:I:42:LEU:O	1:I:100:LEU:HD23	2.19	0.42
1:M:99:GLU:HG2	1:M:101:LYS:HZ1	1.83	0.42
2:A:7:THR:O	2:A:8:LEU:HB2	2.19	0.42
2:A:233:TRP:O	2:A:233:TRP:CG	2.72	0.42
2:F:94:PHE:CD1	2:F:219:ARG:HB3	2.54	0.42
2:F:279:VAL:CG2	2:F:321:ARG:HG2	2.49	0.42
2:D:20:LYS:NZ	2:C:48:ASP:HB3	2.34	0.42
2:D:125:VAL:O	2:D:129:SER:OG	2.33	0.42
2:E:15:TYR:HD2	2:E:15:TYR:HA	1.61	0.42
1:I:55:SER:H	1:I:83:GLN:HB3	1.84	0.42
1:N:93:LYS:HG2	1:N:94:ARG:H	1.83	0.42
2:F:94:PHE:CE2	2:E:74:PRO:HG3	2.54	0.42
2:F:162:VAL:O	2:F:163:PHE:HB2	2.19	0.42
2:B:38:LEU:HB3	2:B:39:THR:H	1.63	0.42
2:B:87:GLY:HA3	2:B:138:PRO:HB3	2.02	0.42
2:B:117:LYS:HD2	2:B:222:PHE:CE1	2.44	0.42
2:B:155:LYS:HB3	2:B:156:ALA:H	1.67	0.42
2:D:121:PHE:HD1	2:D:121:PHE:HA	1.74	0.42
2:D:249:LYS:HE3	2:D:249:LYS:HB3	1.76	0.42
2:D:265:TYR:O	2:D:268:ARG:NH2	2.52	0.42
2:C:72:VAL:HG12	2:C:73:GLN:HB2	2.02	0.42
2:C:247:LEU:HB3	2:C:289:TRP:CE2	2.54	0.42
2:E:29:GLU:HB3	2:E:30:GLN:H	1.57	0.42
1:J:96:ASP:O	1:J:98:LYS:NZ	2.36	0.42
1:N:101:LYS:CD	1:N:102:ASP:H	2.28	0.42
1:M:65:CYS:SG	1:M:66:SER:N	2.92	0.42
2:G:155:LYS:HD2	2:G:155:LYS:HA	1.69	0.42
2:G:240:CYS:CB	2:G:334:THR:HA	2.50	0.42
2:D:94:PHE:HE1	2:D:219:ARG:HG2	1.84	0.42
2:D:123:ASN:O	2:D:127:ARG:HG3	2.20	0.42
1:K:94:ARG:HA	1:K:94:ARG:HD2	1.91	0.42
1:M:14:VAL:HG13	1:M:96:ASP:CB	2.49	0.42
2:A:199:HIS:HB3	2:A:219:ARG:NH1	2.35	0.42
1:H:12:SER:O	1:H:98:LYS:HA	2.20	0.42
2:G:160:GLU:H	2:G:239:ILE:HG22	1.84	0.42
2:D:37:ILE:HG22	2:D:323:VAL:HG22	2.00	0.42
1:K:83:GLN:O	1:K:84:ILE:HB	2.19	0.42
2:C:172:ASN:HB3	2:C:242:ILE:H	1.85	0.42
2:E:61:PRO:CB	2:E:62:GLU:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:183:ASN:O	2:E:229:SER:OG	2.30	0.42
1:I:104:PHE:HB3	1:I:105:TYR:H	1.68	0.42
1:N:6:MET:HB2	1:N:104:PHE:CZ	2.54	0.42
1:N:19:LYS:HG3	1:N:87:ILE:HD12	2.01	0.42
2:A:161:ASN:CG	2:A:162:VAL:H	2.22	0.42
2:A:250:ASP:HB2	2:A:293:GLN:NE2	2.34	0.42
2:A:266:TYR:HE2	2:B:287:HIS:ND1	2.16	0.42
1:H:6:MET:HB3	1:H:104:PHE:CZ	2.54	0.42
1:H:20:PRO:HA	1:H:21:GLU:HA	1.80	0.42
1:H:94:ARG:HA	1:H:94:ARG:HD2	1.71	0.42
2:F:172:ASN:ND2	2:F:330:GLU:O	2.52	0.42
2:B:102:ARG:HA	2:B:103:SER:HA	1.82	0.42
2:B:218:TYR:HD1	2:B:218:TYR:HA	1.78	0.42
2:B:274:GLY:H	2:B:275:ASP:CB	2.32	0.42
2:G:173:THR:CG2	2:G:327:LEU:HA	2.49	0.42
2:G:260:MET:SD	2:G:260:MET:N	2.91	0.42
2:D:42:ILE:HG12	2:D:180:TRP:HD1	1.84	0.42
2:C:195:ALA:CB	2:C:222:PHE:HA	2.48	0.42
2:C:298:LYS:H	2:C:298:LYS:HG3	1.60	0.42
2:E:208:SER:N	2:E:209:ASP:HA	2.34	0.42
2:E:315:PHE:HD1	2:E:316:LEU:HB3	1.84	0.42
2:F:6:GLN:HG2	2:F:7:THR:N	2.34	0.42
2:B:82:VAL:HB	2:B:83:THR:H	1.54	0.42
2:B:292:LYS:NZ	2:B:292:LYS:HB3	2.34	0.42
2:G:197:PHE:HD2	2:G:197:PHE:O	2.03	0.42
1:K:2:LYS:HE2	2:C:68:TYR:CG	2.55	0.42
1:M:21:GLU:HG3	1:M:22:THR:N	2.33	0.42
1:M:52:VAL:HG22	1:M:64:VAL:HG22	2.02	0.42
2:A:124:LYS:HG2	2:F:63:PRO:HG2	2.01	0.42
2:B:51:LYS:HZ2	2:B:51:LYS:HB2	1.85	0.42
2:D:82:VAL:O	2:D:83:THR:HG22	2.20	0.42
2:D:153:THR:O	2:D:153:THR:OG1	2.37	0.42
2:D:209:ASP:N	2:D:210:GLY:CA	2.81	0.42
1:K:49:LEU:O	1:K:91:PRO:HA	2.19	0.42
2:C:138:PRO:HA	2:C:139:GLU:HA	1.57	0.42
2:E:130:ILE:O	2:E:131:TYR:HB2	2.20	0.42
1:I:13:PHE:HD2	1:I:13:PHE:HA	1.72	0.42
1:N:101:LYS:HB2	1:N:101:LYS:HE2	1.83	0.42
2:A:259:SER:O	2:A:262:VAL:HG22	2.20	0.42
2:F:20:LYS:HB2	2:F:20:LYS:HE2	1.85	0.42
2:F:32:ALA:CA	2:E:234:ARG:HH12	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:92:LEU:HD13	2:E:74:PRO:HA	2.01	0.42
2:F:124:LYS:NZ	2:F:127:ARG:HB3	2.34	0.42
2:B:60:ILE:HD13	2:B:77:THR:HG23	2.02	0.42
2:B:266:TYR:HD1	2:B:266:TYR:HA	1.64	0.42
2:G:204:ASP:HA	2:G:205:ASP:HB2	2.02	0.42
2:D:102:ARG:HA	2:D:103:SER:HA	1.78	0.42
2:C:97:LYS:HG2	2:C:216:ARG:HH12	1.85	0.42
2:E:53:LYS:HD3	2:E:53:LYS:HA	1.82	0.42
2:E:97:LYS:HZ2	2:E:216:ARG:HE	1.67	0.42
1:L:3:THR:HA	1:L:5:ASN:O	2.20	0.42
2:A:94:PHE:CE1	2:A:219:ARG:HG3	2.54	0.41
2:A:161:ASN:ND2	2:A:162:VAL:H	2.18	0.41
2:A:305:GLU:HA	2:A:306:GLU:HA	1.75	0.41
2:F:300:VAL:HG13	2:F:301:ASN:N	2.28	0.41
2:B:51:LYS:HA	2:B:84:ASP:O	2.20	0.41
2:B:234:ARG:NH1	2:B:272:MET:HB2	2.35	0.41
2:B:260:MET:HE2	2:B:260:MET:HB2	1.94	0.41
2:G:28:VAL:HA	2:G:29:GLU:HA	1.62	0.41
2:G:233:TRP:NE1	2:G:234:ARG:HG2	2.35	0.41
2:G:280:ILE:HD11	2:G:318:ILE:CG1	2.50	0.41
2:C:15:TYR:HD2	2:C:15:TYR:HA	1.57	0.41
2:C:274:GLY:HA3	2:C:275:ASP:HA	1.62	0.41
1:J:23:LYS:HD3	1:J:24:ASP:HA	2.02	0.41
2:A:39:THR:O	2:A:39:THR:OG1	2.39	0.41
2:A:80:VAL:HG22	2:A:81:PRO:O	2.20	0.41
2:D:53:LYS:O	2:D:54:THR:OG1	2.33	0.41
2:C:140:ALA:O	2:C:228:LEU:HD11	2.19	0.41
2:E:177:PHE:HB2	2:E:279:VAL:O	2.20	0.41
1:I:7:LYS:HB3	1:I:7:LYS:HE2	1.74	0.41
1:N:47:LYS:HD3	1:N:47:LYS:H	1.86	0.41
1:M:8:THR:CG2	1:M:102:ASP:H	2.33	0.41
2:A:173:THR:HB	2:A:326:ILE:O	2.20	0.41
2:A:302:LEU:HD12	2:B:302:LEU:HB3	2.01	0.41
2:F:199:HIS:HB2	2:F:219:ARG:CD	2.49	0.41
2:F:252:SER:OG	2:F:296:ASN:HB2	2.21	0.41
2:F:272:MET:O	2:F:272:MET:HG3	2.21	0.41
2:B:7:THR:O	2:B:8:LEU:HB2	2.19	0.41
2:D:178:MET:HA	2:D:235:SER:O	2.20	0.41
2:C:316:LEU:HA	2:C:317:GLY:HA2	1.70	0.41
2:E:49:GLY:HA2	2:E:188:ILE:HD11	2.02	0.41
2:E:205:ASP:C	2:E:210:GLY:HA2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:26:TYR:HA	1:I:27:PRO:HD3	1.85	0.41
1:I:55:SER:O	1:I:85:THR:OG1	2.32	0.41
2:F:233:TRP:CE3	2:F:234:ARG:HA	2.56	0.41
2:F:309:GLY:O	2:F:311:LYS:N	2.53	0.41
2:B:41:ALA:HA	2:B:180:TRP:CD1	2.55	0.41
2:B:103:SER:OG	2:B:104:ASN:N	2.54	0.41
2:B:247:LEU:HD23	2:B:247:LEU:HA	1.90	0.41
2:G:202:LEU:HD13	2:G:202:LEU:H	1.84	0.41
2:D:28:VAL:HA	2:D:29:GLU:HA	1.79	0.41
2:D:261:MET:HG3	2:D:262:VAL:HG13	2.02	0.41
1:J:54:ASP:HB2	1:J:55:SER:H	1.60	0.41
1:L:16:GLU:CD	1:L:18:GLY:H	2.24	0.41
2:A:32:ALA:HA	2:F:234:ARG:HH12	1.85	0.41
2:B:147:ARG:CD	2:B:147:ARG:H	2.34	0.41
2:G:258:ILE:HD12	2:G:258:ILE:HA	1.89	0.41
2:E:61:PRO:HB3	2:E:62:GLU:HB3	2.02	0.41
2:E:97:LYS:NZ	2:E:201:ASP:O	2.43	0.41
2:E:138:PRO:HA	2:E:139:GLU:HA	1.63	0.41
1:I:36:ASN:OD1	1:I:37:GLU:N	2.53	0.41
1:L:26:TYR:HA	1:L:27:PRO:HD3	1.79	0.41
1:M:20:PRO:HA	1:M:21:GLU:HA	1.60	0.41
2:D:266:TYR:HB3	2:E:288:ALA:CB	2.50	0.41
1:K:66:SER:OG	1:K:67:VAL:N	2.53	0.41
1:J:71:THR:HG22	1:J:72:THR:H	1.85	0.41
1:N:1:MET:HA	1:N:2:LYS:HA	1.61	0.41
2:A:111:VAL:HA	2:A:114:ASN:HD21	1.85	0.41
2:A:234:ARG:NH1	2:A:272:MET:HE1	2.36	0.41
2:A:329:THR:HG23	2:A:330:GLU:H	1.86	0.41
1:H:54:ASP:OD1	1:H:62:ALA:HB3	2.21	0.41
2:F:66:ARG:HD3	2:F:68:TYR:HA	2.03	0.41
2:F:145:ALA:N	2:F:146:PRO:HD2	2.35	0.41
2:B:202:LEU:HA	2:B:215:PHE:O	2.21	0.41
2:D:38:LEU:O	2:D:39:THR:OG1	2.32	0.41
2:D:305:GLU:HG3	2:C:310:LYS:HE3	2.02	0.41
2:C:48:ASP:HB2	2:C:49:GLY:H	1.59	0.41
2:E:173:THR:OG1	2:E:174:SER:N	2.49	0.41
1:I:6:MET:HG2	1:I:104:PHE:CG	2.56	0.41
1:I:26:TYR:HE2	1:I:84:ILE:HD11	1.85	0.41
1:N:37:GLU:OE2	1:N:39:LEU:HD23	2.21	0.41
1:N:54:ASP:O	1:N:61:MET:HB2	2.21	0.41
1:M:29:GLY:N	1:M:84:ILE:HG12	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:266:TYR:OH	2:B:311:LYS:HB3	2.20	0.41
1:H:43:GLY:HA2	1:H:99:GLU:OE1	2.20	0.41
2:B:47:ASN:HA	2:B:48:ASP:HA	1.75	0.41
2:B:134:THR:HB	2:B:135:ASP:H	1.70	0.41
2:B:137:GLU:HB3	2:B:138:PRO:CD	2.50	0.41
2:D:311:LYS:HD3	2:D:311:LYS:H	1.86	0.41
2:C:106:ALA:O	2:C:109:PHE:HB3	2.21	0.41
2:E:102:ARG:O	2:E:102:ARG:HG2	2.21	0.41
2:E:225:ASP:N	2:E:225:ASP:OD2	2.51	0.41
2:E:285:THR:HG21	2:E:327:LEU:HD13	2.02	0.41
1:I:105:TYR:CD1	1:I:105:TYR:N	2.84	0.41
1:N:10:THR:CB	1:N:101:LYS:HG2	2.51	0.41
1:M:70:ARG:H	1:M:70:ARG:HG2	1.63	0.41
2:A:300:VAL:HA	2:B:301:ASN:O	2.20	0.41
1:H:84:ILE:O	1:H:85:THR:OG1	2.34	0.41
1:H:94:ARG:HG3	1:H:95:ASP:H	1.86	0.41
1:H:97:ALA:HB1	1:H:99:GLU:OE1	2.20	0.41
1:H:104:PHE:O	1:H:105:TYR:HB2	2.21	0.41
2:F:32:ALA:HA	2:E:234:ARG:HH12	1.86	0.41
2:G:280:ILE:HD11	2:G:318:ILE:HD12	2.03	0.41
2:D:3:LEU:O	2:D:6:GLN:HG3	2.21	0.41
2:D:60:ILE:HD11	2:E:117:LYS:HE2	2.03	0.41
2:D:146:PRO:CG	2:D:152:SER:HB3	2.51	0.41
2:D:206:LEU:HD22	2:D:206:LEU:HA	1.89	0.41
2:C:271:ALA:HB1	2:C:273:LEU:N	2.36	0.41
2:C:295:MET:HG3	2:C:296:ASN:OD1	2.21	0.41
2:E:26:ARG:O	2:E:29:GLU:HA	2.21	0.41
2:E:66:ARG:NE	2:E:68:TYR:H	2.18	0.41
2:E:120:GLY:O	2:E:123:ASN:HB3	2.21	0.41
2:E:138:PRO:HB2	2:E:139:GLU:CD	2.41	0.41
2:E:309:GLY:O	2:E:310:LYS:HG2	2.21	0.41
1:I:31:ARG:HA	1:I:31:ARG:CZ	2.50	0.41
1:J:71:THR:HB	1:J:74:HIS:CE1	2.56	0.41
2:G:60:ILE:N	2:G:61:PRO:HD3	2.36	0.41
2:G:113:GLU:OE1	2:G:113:GLU:N	2.53	0.41
2:G:120:GLY:O	2:G:123:ASN:HB3	2.21	0.41
2:G:135:ASP:C	2:G:137:GLU:H	2.25	0.41
2:D:39:THR:HA	2:D:40:ASP:O	2.21	0.41
2:E:242:ILE:HB	2:E:243:ASP:O	2.20	0.41
2:E:326:ILE:HG23	2:E:327:LEU:H	1.85	0.41
1:N:49:LEU:O	1:N:91:PRO:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:25:GLN:HB3	1:M:105:TYR:OH	2.22	0.40
1:M:105:TYR:HD1	1:M:106:PRO:HD3	1.86	0.40
2:F:97:LYS:NZ	2:F:216:ARG:HE	2.08	0.40
2:B:241:ASN:ND2	2:B:242:ILE:HD13	2.37	0.40
2:B:301:ASN:HB2	2:C:304:ILE:O	2.20	0.40
2:G:102:ARG:HA	2:G:103:SER:HA	1.77	0.40
2:G:272:MET:O	2:G:275:ASP:HB3	2.21	0.40
2:D:280:ILE:HD11	2:D:318:ILE:CD1	2.51	0.40
1:K:18:GLY:CA	1:K:91:PRO:HD2	2.48	0.40
2:C:27:ILE:HD13	2:C:27:ILE:H	1.85	0.40
2:C:55:THR:O	2:C:56:ILE:HG12	2.21	0.40
2:C:270:VAL:HG13	2:C:271:ALA:HA	2.03	0.40
1:I:40:GLN:HE22	1:I:42:LEU:HD12	1.87	0.40
1:J:31:ARG:CZ	1:J:31:ARG:HB3	2.50	0.40
1:L:45:ASN:HB2	1:L:97:ALA:HA	2.02	0.40
1:N:49:LEU:HB2	1:N:66:SER:O	2.21	0.40
1:M:87:ILE:H	1:M:87:ILE:HG12	1.60	0.40
2:F:293:GLN:O	2:F:293:GLN:NE2	2.53	0.40
2:F:316:LEU:HA	2:F:317:GLY:HA2	1.71	0.40
2:B:73:GLN:H	2:B:73:GLN:HG2	1.56	0.40
2:D:29:GLU:N	2:D:29:GLU:OE1	2.54	0.40
2:D:246:THR:H	2:D:246:THR:HG1	1.49	0.40
1:J:40:GLN:NE2	1:J:101:LYS:HB2	2.36	0.40
1:N:34:LEU:HD22	1:N:35:ASP:N	2.36	0.40
2:B:30:GLN:OE1	2:B:30:GLN:N	2.54	0.40
2:B:96:ASP:O	2:B:99:LEU:N	2.54	0.40
2:B:247:LEU:HB3	2:B:289:TRP:CE2	2.57	0.40
2:G:43:TYR:HD2	2:G:184:THR:OG1	2.03	0.40
2:G:97:LYS:H	2:G:217:ALA:HA	1.86	0.40
2:D:19:ASP:OD1	2:D:26:ARG:HA	2.21	0.40
2:D:172:ASN:HB3	2:D:241:ASN:O	2.21	0.40
1:J:26:TYR:HA	1:J:27:PRO:HD3	1.86	0.40
1:J:40:GLN:HG3	1:J:101:LYS:C	2.41	0.40
1:J:47:LYS:HE3	1:J:70:ARG:NH2	2.36	0.40
1:L:32:ILE:O	1:L:33:THR:OG1	2.32	0.40
2:A:116:GLY:O	2:A:119:GLN:HG2	2.22	0.40
2:F:61:PRO:CB	2:F:62:GLU:HB3	2.51	0.40
2:B:42:ILE:HG22	2:B:180:TRP:HB3	2.04	0.40
2:G:109:PHE:O	2:G:113:GLU:HB2	2.21	0.40
2:G:132:GLY:O	2:G:140:ALA:HA	2.21	0.40
2:G:268:ARG:HG2	2:G:269:ASP:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:305:GLU:HG3	2:G:307:TYR:H	1.85	0.40
2:D:39:THR:HA	2:D:40:ASP:C	2.42	0.40
2:D:160:GLU:OE1	2:D:160:GLU:N	2.55	0.40
1:I:59:MET:HA	1:I:60:ALA:HA	1.90	0.40
1:J:89:LEU:HG	1:J:91:PRO:CD	2.47	0.40
1:N:2:LYS:NZ	2:A:11:LEU:HB3	2.37	0.40
1:M:107:ASP:OD2	1:M:108:GLY:N	2.54	0.40
2:A:96:ASP:OD2	2:A:98:ALA:HB3	2.22	0.40
1:H:47:LYS:H	1:H:47:LYS:CD	2.32	0.40
2:F:221:GLU:CD	2:F:222:PHE:H	2.24	0.40
2:D:301:ASN:OD1	2:C:300:VAL:HG23	2.21	0.40
1:K:31:ARG:HH22	1:K:33:THR:H	1.69	0.40
1:K:32:ILE:O	1:K:33:THR:OG1	2.31	0.40
2:E:124:LYS:HA	2:E:124:LYS:HD3	1.89	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	H	109/111 (98%)	56 (51%)	38 (35%)	15 (14%)	0 4
1	I	109/111 (98%)	54 (50%)	34 (31%)	21 (19%)	0 2
1	J	109/111 (98%)	54 (50%)	33 (30%)	22 (20%)	0 2
1	K	109/111 (98%)	63 (58%)	27 (25%)	19 (17%)	0 3
1	L	109/111 (98%)	54 (50%)	31 (28%)	24 (22%)	0 1
1	M	109/111 (98%)	49 (45%)	34 (31%)	26 (24%)	0 1
1	N	109/111 (98%)	60 (55%)	34 (31%)	15 (14%)	0 4
2	A	333/335 (99%)	211 (63%)	82 (25%)	40 (12%)	0 6
2	B	333/335 (99%)	207 (62%)	85 (26%)	41 (12%)	0 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	333/335 (99%)	205 (62%)	80 (24%)	48 (14%)	0 4
2	D	333/335 (99%)	200 (60%)	92 (28%)	41 (12%)	0 6
2	E	333/335 (99%)	215 (65%)	79 (24%)	39 (12%)	0 6
2	F	333/335 (99%)	199 (60%)	93 (28%)	41 (12%)	0 6
2	G	333/335 (99%)	215 (65%)	87 (26%)	31 (9%)	0 12
All	All	3094/3122 (99%)	1842 (60%)	829 (27%)	423 (14%)	1 5

All (423) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	27	PRO
1	N	83	GLN
1	N	105	TYR
1	M	23	LYS
1	M	27	PRO
1	M	55	SER
1	M	73	ASP
1	M	83	GLN
1	M	84	ILE
1	M	103	ALA
2	A	28	VAL
2	A	32	ALA
2	A	52	HIS
2	A	56	ILE
2	A	134	THR
2	A	137	GLU
2	A	142	MET
2	A	143	GLY
2	A	154	SER
2	A	172	ASN
2	A	206	LEU
2	A	242	ILE
2	A	269	ASP
2	A	285	THR
2	A	301	ASN
2	A	313	VAL
2	A	331	SER
2	A	334	THR
1	H	27	PRO
1	H	84	ILE

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Mol	Chain	Res	Type
1	H	105	TYR
2	F	4	ILE
2	F	27	ILE
2	F	28	VAL
2	F	33	LYS
2	F	56	ILE
2	F	137	GLU
2	F	148	PHE
2	F	172	ASN
2	F	234	ARG
2	F	244	VAL
2	F	269	ASP
2	F	285	THR
2	F	300	VAL
2	F	301	ASN
2	F	304	ILE
2	F	310	LYS
2	B	3	LEU
2	B	11	LEU
2	B	28	VAL
2	B	52	HIS
2	B	56	ILE
2	B	137	GLU
2	B	156	ALA
2	B	188	ILE
2	B	195	ALA
2	B	257	LEU
2	B	315	PHE
2	B	331	SER
2	B	333	VAL
2	G	4	ILE
2	G	8	LEU
2	G	56	ILE
2	G	137	GLU
2	G	155	LYS
2	G	172	ASN
2	G	308	GLY
2	G	326	ILE
2	D	4	ILE
2	D	8	LEU
2	D	28	VAL
2	D	52	HIS

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Mol	Chain	Res	Type
2	D	56	ILE
2	D	82	VAL
2	D	133	ASN
2	D	137	GLU
2	D	163	PHE
2	D	214	GLN
2	D	215	PHE
2	D	216	ARG
2	D	234	ARG
2	D	250	ASP
2	D	302	LEU
1	K	22	THR
1	K	26	TYR
1	K	55	SER
1	K	83	GLN
1	K	86	ASP
2	C	20	LYS
2	C	28	VAL
2	C	32	ALA
2	C	37	ILE
2	C	56	ILE
2	C	137	GLU
2	C	171	THR
2	C	191	GLU
2	C	194	VAL
2	C	269	ASP
2	C	285	THR
2	E	28	VAL
2	E	32	ALA
2	E	52	HIS
2	E	56	ILE
2	E	83	THR
2	E	104	ASN
2	E	131	TYR
2	E	137	GLU
2	E	154	SER
2	E	163	PHE
2	E	215	PHE
2	E	275	ASP
2	E	327	LEU
1	I	26	TYR
1	I	84	ILE

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Mol	Chain	Res	Type
1	I	105	TYR
1	J	27	PRO
1	J	46	ALA
1	J	84	ILE
1	J	97	ALA
1	J	103	ALA
1	L	12	SER
1	L	22	THR
1	L	84	ILE
1	L	99	GLU
1	L	104	PHE
1	L	105	TYR
1	N	4	VAL
1	N	32	ILE
1	N	84	ILE
1	N	85	THR
1	N	100	LEU
1	M	14	VAL
1	M	85	THR
2	A	2	ALA
2	A	27	ILE
2	A	159	ALA
2	A	234	ARG
2	A	303	THR
1	H	33	THR
1	H	55	SER
1	H	83	GLN
1	H	85	THR
2	F	24	ILE
2	F	32	ALA
2	F	132	GLY
2	F	163	PHE
2	F	197	PHE
2	F	231	ARG
2	F	303	THR
2	F	330	GLU
2	B	163	PHE
2	B	192	GLY
2	B	194	VAL
2	B	228	LEU
2	B	234	ARG
2	B	269	ASP

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Mol	Chain	Res	Type
2	B	284	LYS
2	B	300	VAL
2	B	312	ILE
2	G	21	ASN
2	G	53	LYS
2	G	171	THR
2	G	188	ILE
2	G	200	GLU
2	G	241	ASN
2	G	297	ALA
2	G	332	ALA
2	D	32	ALA
2	D	104	ASN
2	D	143	GLY
2	D	159	ALA
2	D	194	VAL
2	D	204	ASP
2	D	259	SER
2	D	269	ASP
2	D	284	LYS
2	D	328	ASN
2	D	332	ALA
1	K	42	LEU
2	C	3	LEU
2	C	27	ILE
2	C	136	ALA
2	C	143	GLY
2	C	163	PHE
2	C	208	SER
2	C	211	ASN
2	C	251	ALA
2	C	304	ILE
2	C	310	LYS
2	C	326	ILE
2	C	332	ALA
2	E	17	ARG
2	E	27	ILE
2	E	33	LYS
2	E	77	THR
2	E	82	VAL
2	E	95	VAL
2	E	234	ARG

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Mol	Chain	Res	Type
2	E	269	ASP
2	E	276	GLY
1	I	6	MET
1	I	18	GLY
1	I	23	LYS
1	I	32	ILE
1	I	83	GLN
1	I	85	THR
1	J	4	VAL
1	J	23	LYS
1	J	33	THR
1	J	55	SER
1	J	83	GLN
1	J	86	ASP
1	J	88	GLY
1	J	96	ASP
1	L	23	LYS
1	L	55	SER
1	L	85	THR
1	N	33	THR
1	N	107	ASP
1	M	33	THR
1	M	104	PHE
2	A	6	GLN
2	A	18	THR
2	A	82	VAL
2	A	105	ASN
2	A	163	PHE
2	A	173	THR
2	A	193	MET
2	A	214	GLN
1	H	4	VAL
1	H	77	ASP
2	F	45	PRO
2	F	52	HIS
2	F	54	THR
2	F	83	THR
2	F	155	LYS
2	F	193	MET
2	F	206	LEU
2	F	214	GLN
2	B	104	ASN

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Mol	Chain	Res	Type
2	B	135	ASP
2	B	141	PHE
2	B	142	MET
2	B	301	ASN
2	B	304	ILE
2	G	52	HIS
2	G	83	THR
2	G	108	ALA
2	G	194	VAL
2	G	201	ASP
2	G	221	GLU
2	G	269	ASP
2	G	307	TYR
2	D	20	LYS
2	D	172	ASN
2	D	173	THR
2	D	193	MET
2	D	231	ARG
2	D	257	LEU
2	D	297	ALA
2	D	310	LYS
2	D	330	GLU
1	K	4	VAL
1	K	27	PRO
1	K	33	THR
1	K	73	ASP
1	K	97	ALA
2	C	38	LEU
2	C	49	GLY
2	C	104	ASN
2	C	257	LEU
2	C	274	GLY
2	C	302	LEU
2	E	3	LEU
2	E	69	ASN
2	E	141	PHE
2	E	326	ILE
1	I	27	PRO
1	I	99	GLU
1	J	12	SER
1	J	54	ASP
1	J	85	THR

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Mol	Chain	Res	Type
1	J	92	GLN
1	L	33	THR
1	L	100	LEU
1	N	46	ALA
1	N	58	VAL
1	M	20	PRO
1	M	41	ARG
1	M	46	ALA
1	M	95	ASP
1	M	106	PRO
2	A	33	LYS
2	A	68	TYR
1	H	32	ILE
2	F	46	CYS
2	F	47	ASN
2	F	159	ALA
2	F	170	SER
2	B	50	SER
2	B	53	LYS
2	B	82	VAL
2	B	134	THR
2	B	232	ASP
2	G	73	GLN
2	G	333	VAL
2	D	73	GLN
2	D	141	PHE
2	D	304	ILE
1	K	105	TYR
2	C	39	THR
2	C	68	TYR
2	C	73	GLN
2	C	105	ASN
2	C	231	ARG
2	C	287	HIS
2	C	301	ASN
2	E	8	LEU
2	E	24	ILE
2	E	73	GLN
2	E	155	LYS
2	E	274	GLY
2	E	304	ILE
2	E	331	SER

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Mol	Chain	Res	Type
1	I	73	ASP
1	I	77	ASP
1	I	86	ASP
1	I	107	ASP
1	L	44	LEU
1	L	47	LYS
1	L	73	ASP
1	L	83	GLN
1	N	73	ASP
1	N	102	ASP
1	M	4	VAL
1	M	40	GLN
1	M	77	ASP
2	A	138	PRO
1	H	73	ASP
1	H	97	ALA
2	F	82	VAL
2	B	39	THR
2	B	61	PRO
2	B	231	ARG
2	B	313	VAL
2	G	199	HIS
2	G	314	SER
2	D	39	THR
2	D	241	ASN
1	K	12	SER
1	K	84	ILE
1	K	102	ASP
2	C	70	GLN
2	C	154	SER
2	C	193	MET
2	C	204	ASP
2	C	234	ARG
2	C	272	MET
2	E	210	GLY
2	E	211	ASN
2	E	241	ASN
2	E	315	PHE
1	I	4	VAL
1	I	33	THR
1	I	54	ASP
1	L	26	TYR

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Mol	Chain	Res	Type
1	L	27	PRO
1	L	54	ASP
1	L	77	ASP
1	H	17	ASP
1	H	26	TYR
2	F	53	LYS
2	B	27	ILE
2	B	159	ALA
2	B	214	GLN
1	K	77	ASP
2	C	11	LEU
2	C	41	ALA
2	C	299	ASN
1	I	40	GLN
1	L	4	VAL
1	L	14	VAL
1	L	86	ASP
1	M	32	ILE
1	M	80	VAL
1	M	105	TYR
2	A	72	VAL
2	A	304	ILE
2	A	318	ILE
2	F	194	VAL
1	L	32	ILE
1	M	26	TYR
2	A	73	GLN
2	A	192	GLY
1	H	58	VAL
2	B	143	GLY
2	G	82	VAL
2	G	207	VAL
1	K	58	VAL
1	K	80	VAL
2	C	8	LEU
1	I	15	GLY
1	J	26	TYR
1	J	32	ILE
1	M	64	VAL
2	F	162	VAL
2	G	143	GLY
2	D	27	ILE

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Mol	Chain	Res	Type
2	C	24	ILE
2	E	188	ILE
1	J	58	VAL
1	J	87	ILE
1	L	58	VAL
1	N	26	TYR
1	M	87	ILE
2	A	190	PRO
2	F	312	ILE
1	K	64	VAL
2	C	313	VAL
2	E	213	GLY
1	M	58	VAL
1	I	50	PRO
1	J	50	PRO

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	H	95/95 (100%)	70 (74%)	25 (26%)	0 4
1	I	95/95 (100%)	64 (67%)	31 (33%)	0 2
1	J	95/95 (100%)	64 (67%)	31 (33%)	0 2
1	K	95/95 (100%)	70 (74%)	25 (26%)	0 4
1	L	95/95 (100%)	62 (65%)	33 (35%)	0 1
1	M	95/95 (100%)	67 (70%)	28 (30%)	0 2
1	N	95/95 (100%)	72 (76%)	23 (24%)	0 5
2	A	274/274 (100%)	195 (71%)	79 (29%)	0 3
2	B	274/274 (100%)	193 (70%)	81 (30%)	0 2
2	C	274/274 (100%)	199 (73%)	75 (27%)	0 3
2	D	274/274 (100%)	200 (73%)	74 (27%)	0 4
2	E	274/274 (100%)	198 (72%)	76 (28%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	274/274 (100%)	205 (75%)	69 (25%)	0 4
2	G	274/274 (100%)	209 (76%)	65 (24%)	1 5
All	All	2583/2583 (100%)	1868 (72%)	715 (28%)	2 3

All (715) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	2	LYS
1	N	3	THR
1	N	6	MET
1	N	11	ASP
1	N	13	PHE
1	N	16	GLU
1	N	24	ASP
1	N	26	TYR
1	N	30	LEU
1	N	31	ARG
1	N	32	ILE
1	N	34	LEU
1	N	39	LEU
1	N	42	LEU
1	N	44	LEU
1	N	47	LYS
1	N	59	MET
1	N	70	ARG
1	N	81	GLU
1	N	93	LYS
1	N	94	ARG
1	N	101	LYS
1	N	104	PHE
1	M	2	LYS
1	M	6	MET
1	M	7	LYS
1	M	8	THR
1	M	11	ASP
1	M	22	THR
1	M	25	GLN
1	M	26	TYR
1	M	30	LEU
1	M	34	LEU
1	M	39	LEU

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Mol	Chain	Res	Type
1	M	40	GLN
1	M	44	LEU
1	M	47	LYS
1	M	64	VAL
1	M	70	ARG
1	M	71	THR
1	M	72	THR
1	M	74	HIS
1	M	78	ASN
1	M	79	TYR
1	M	82	LEU
1	M	87	ILE
1	M	94	ARG
1	M	98	LYS
1	M	100	LEU
1	M	101	LYS
1	M	105	TYR
2	A	1	MET
2	A	6	GLN
2	A	8	LEU
2	A	11	LEU
2	A	15	TYR
2	A	20	LYS
2	A	24	ILE
2	A	37	ILE
2	A	42	ILE
2	A	44	VAL
2	A	48	ASP
2	A	51	LYS
2	A	52	HIS
2	A	55	THR
2	A	57	ARG
2	A	67	ARG
2	A	68	TYR
2	A	70	GLN
2	A	76	LYS
2	A	77	THR
2	A	78	GLN
2	A	82	VAL
2	A	83	THR
2	A	90	TYR
2	A	91	ASP

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Mol	Chain	Res	Type
2	A	92	LEU
2	A	99	LEU
2	A	109	PHE
2	A	114	ASN
2	A	118	LEU
2	A	121	PHE
2	A	127	ARG
2	A	135	ASP
2	A	139	GLU
2	A	141	PHE
2	A	142	MET
2	A	147	ARG
2	A	168	SER
2	A	172	ASN
2	A	173	THR
2	A	178	MET
2	A	180	TRP
2	A	186	HIS
2	A	187	MET
2	A	189	TYR
2	A	191	GLU
2	A	197	PHE
2	A	202	LEU
2	A	205	ASP
2	A	219	ARG
2	A	220	ASP
2	A	222	PHE
2	A	223	LYS
2	A	228	LEU
2	A	232	ASP
2	A	238	ARG
2	A	239	ILE
2	A	242	ILE
2	A	256	ASP
2	A	257	LEU
2	A	266	TYR
2	A	268	ARG
2	A	277	LYS
2	A	285	THR
2	A	292	LYS
2	A	295	MET
2	A	296	ASN

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Mol	Chain	Res	Type
2	A	298	LYS
2	A	299	ASN
2	A	306	GLU
2	A	307	TYR
2	A	310	LYS
2	A	316	LEU
2	A	320	ILE
2	A	321	ARG
2	A	326	ILE
2	A	328	ASN
2	A	329	THR
2	A	333	VAL
1	H	6	MET
1	H	11	ASP
1	H	13	PHE
1	H	21	GLU
1	H	26	TYR
1	H	30	LEU
1	H	32	ILE
1	H	34	LEU
1	H	39	LEU
1	H	40	GLN
1	H	42	LEU
1	H	44	LEU
1	H	47	LYS
1	H	54	ASP
1	H	65	CYS
1	H	70	ARG
1	H	72	THR
1	H	74	HIS
1	H	82	LEU
1	H	93	LYS
1	H	94	ARG
1	H	98	LYS
1	H	104	PHE
1	H	107	ASP
1	H	109	GLU
2	F	15	TYR
2	F	17	ARG
2	F	18	THR
2	F	20	LYS
2	F	26	ARG

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Mol	Chain	Res	Type
2	F	29	GLU
2	F	33	LYS
2	F	34	THR
2	F	35	ASN
2	F	36	ASP
2	F	42	ILE
2	F	44	VAL
2	F	51	LYS
2	F	62	GLU
2	F	64	VAL
2	F	76	LYS
2	F	89	LEU
2	F	90	TYR
2	F	91	ASP
2	F	92	LEU
2	F	99	LEU
2	F	104	ASN
2	F	109	PHE
2	F	113	GLU
2	F	117	LYS
2	F	118	LEU
2	F	121	PHE
2	F	125	VAL
2	F	127	ARG
2	F	128	TYR
2	F	134	THR
2	F	139	GLU
2	F	141	PHE
2	F	147	ARG
2	F	153	THR
2	F	160	GLU
2	F	163	PHE
2	F	168	SER
2	F	172	ASN
2	F	173	THR
2	F	175	ILE
2	F	177	PHE
2	F	178	MET
2	F	180	TRP
2	F	183	ASN
2	F	202	LEU
2	F	209	ASP

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Mol	Chain	Res	Type
2	F	214	GLN
2	F	219	ARG
2	F	222	PHE
2	F	232	ASP
2	F	233	TRP
2	F	238	ARG
2	F	247	LEU
2	F	256	ASP
2	F	263	ASP
2	F	266	TYR
2	F	268	ARG
2	F	277	LYS
2	F	278	GLU
2	F	280	ILE
2	F	289	TRP
2	F	290	LEU
2	F	310	LYS
2	F	312	ILE
2	F	314	SER
2	F	316	LEU
2	F	323	VAL
2	F	329	THR
2	B	3	LEU
2	B	4	ILE
2	B	15	TYR
2	B	18	THR
2	B	20	LYS
2	B	34	THR
2	B	44	VAL
2	B	54	THR
2	B	65	TRP
2	B	66	ARG
2	B	67	ARG
2	B	72	VAL
2	B	76	LYS
2	B	78	GLN
2	B	82	VAL
2	B	83	THR
2	B	89	LEU
2	B	90	TYR
2	B	96	ASP
2	B	105	ASN

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Mol	Chain	Res	Type
2	B	110	ARG
2	B	122	ASN
2	B	125	VAL
2	B	133	ASN
2	B	135	ASP
2	B	139	GLU
2	B	147	ARG
2	B	148	PHE
2	B	153	THR
2	B	155	LYS
2	B	160	GLU
2	B	161	ASN
2	B	162	VAL
2	B	171	THR
2	B	173	THR
2	B	175	ILE
2	B	178	MET
2	B	180	TRP
2	B	182	GLU
2	B	183	ASN
2	B	186	HIS
2	B	188	ILE
2	B	191	GLU
2	B	194	VAL
2	B	197	PHE
2	B	202	LEU
2	B	204	ASP
2	B	206	LEU
2	B	209	ASP
2	B	214	GLN
2	B	216	ARG
2	B	218	TYR
2	B	222	PHE
2	B	228	LEU
2	B	230	VAL
2	B	232	ASP
2	B	238	ARG
2	B	240	CYS
2	B	242	ILE
2	B	257	LEU
2	B	263	ASP
2	B	266	TYR

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Mol	Chain	Res	Type
2	B	269	ASP
2	B	277	LYS
2	B	280	ILE
2	B	283	ASN
2	B	285	THR
2	B	292	LYS
2	B	293	GLN
2	B	296	ASN
2	B	298	LYS
2	B	306	GLU
2	B	310	LYS
2	B	312	ILE
2	B	315	PHE
2	B	316	LEU
2	B	320	ILE
2	B	321	ARG
2	B	322	ARG
2	B	326	ILE
2	B	334	THR
2	G	8	LEU
2	G	10	SER
2	G	11	LEU
2	G	14	ILE
2	G	18	THR
2	G	26	ARG
2	G	28	VAL
2	G	31	LEU
2	G	33	LYS
2	G	36	ASP
2	G	37	ILE
2	G	42	ILE
2	G	48	ASP
2	G	51	LYS
2	G	54	THR
2	G	76	LYS
2	G	79	THR
2	G	83	THR
2	G	90	TYR
2	G	92	LEU
2	G	99	LEU
2	G	101	ASP
2	G	121	PHE

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Mol	Chain	Res	Type
2	G	127	ARG
2	G	128	TYR
2	G	134	THR
2	G	135	ASP
2	G	139	GLU
2	G	141	PHE
2	G	148	PHE
2	G	158	SER
2	G	160	GLU
2	G	163	PHE
2	G	170	SER
2	G	171	THR
2	G	173	THR
2	G	175	ILE
2	G	177	PHE
2	G	188	ILE
2	G	189	TYR
2	G	191	GLU
2	G	197	PHE
2	G	200	GLU
2	G	202	LEU
2	G	204	ASP
2	G	211	ASN
2	G	215	PHE
2	G	218	TYR
2	G	225	ASP
2	G	228	LEU
2	G	233	TRP
2	G	237	SER
2	G	239	ILE
2	G	242	ILE
2	G	247	LEU
2	G	250	ASP
2	G	278	GLU
2	G	285	THR
2	G	287	HIS
2	G	292	LYS
2	G	298	LYS
2	G	302	LEU
2	G	310	LYS
2	G	311	LYS
2	G	329	THR

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Mol	Chain	Res	Type
2	D	1	MET
2	D	3	LEU
2	D	8	LEU
2	D	11	LEU
2	D	12	LEU
2	D	15	TYR
2	D	18	THR
2	D	27	ILE
2	D	37	ILE
2	D	44	VAL
2	D	46	CYS
2	D	48	ASP
2	D	56	ILE
2	D	57	ARG
2	D	66	ARG
2	D	69	ASN
2	D	76	LYS
2	D	83	THR
2	D	89	LEU
2	D	95	VAL
2	D	102	ARG
2	D	109	PHE
2	D	112	SER
2	D	117	LYS
2	D	118	LEU
2	D	121	PHE
2	D	125	VAL
2	D	134	THR
2	D	135	ASP
2	D	148	PHE
2	D	150	THR
2	D	152	SER
2	D	168	SER
2	D	173	THR
2	D	180	TRP
2	D	186	HIS
2	D	187	MET
2	D	189	TYR
2	D	191	GLU
2	D	193	MET
2	D	197	PHE
2	D	202	LEU

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Mol	Chain	Res	Type
2	D	205	ASP
2	D	206	LEU
2	D	215	PHE
2	D	223	LYS
2	D	224	TRP
2	D	225	ASP
2	D	228	LEU
2	D	238	ARG
2	D	239	ILE
2	D	241	ASN
2	D	246	THR
2	D	247	LEU
2	D	256	ASP
2	D	257	LEU
2	D	262	VAL
2	D	266	TYR
2	D	268	ARG
2	D	270	VAL
2	D	273	LEU
2	D	285	THR
2	D	290	LEU
2	D	292	LYS
2	D	296	ASN
2	D	306	GLU
2	D	307	TYR
2	D	310	LYS
2	D	311	LYS
2	D	318	ILE
2	D	320	ILE
2	D	327	LEU
2	D	331	SER
2	D	333	VAL
1	K	1	MET
1	K	3	THR
1	K	8	THR
1	K	21	GLU
1	K	23	LYS
1	K	25	GLN
1	K	26	TYR
1	K	30	LEU
1	K	31	ARG
1	K	32	ILE

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Mol	Chain	Res	Type
1	K	39	LEU
1	K	41	ARG
1	K	44	LEU
1	K	47	LYS
1	K	59	MET
1	K	65	CYS
1	K	70	ARG
1	K	72	THR
1	K	82	LEU
1	K	85	THR
1	K	86	ASP
1	K	98	LYS
1	K	101	LYS
1	K	105	TYR
1	K	109	GLU
2	C	1	MET
2	C	3	LEU
2	C	8	LEU
2	C	11	LEU
2	C	15	TYR
2	C	20	LYS
2	C	26	ARG
2	C	27	ILE
2	C	30	GLN
2	C	36	ASP
2	C	42	ILE
2	C	44	VAL
2	C	46	CYS
2	C	48	ASP
2	C	54	THR
2	C	56	ILE
2	C	66	ARG
2	C	67	ARG
2	C	76	LYS
2	C	89	LEU
2	C	90	TYR
2	C	92	LEU
2	C	97	LYS
2	C	118	LEU
2	C	122	ASN
2	C	125	VAL
2	C	128	TYR

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Mol	Chain	Res	Type
2	C	134	THR
2	C	142	MET
2	C	148	PHE
2	C	153	THR
2	C	155	LYS
2	C	172	ASN
2	C	173	THR
2	C	175	ILE
2	C	178	MET
2	C	180	TRP
2	C	186	HIS
2	C	189	TYR
2	C	191	GLU
2	C	193	MET
2	C	197	PHE
2	C	202	LEU
2	C	205	ASP
2	C	214	GLN
2	C	216	ARG
2	C	218	TYR
2	C	219	ARG
2	C	220	ASP
2	C	221	GLU
2	C	222	PHE
2	C	223	LYS
2	C	228	LEU
2	C	239	ILE
2	C	242	ILE
2	C	243	ASP
2	C	246	THR
2	C	250	ASP
2	C	268	ARG
2	C	270	VAL
2	C	277	LYS
2	C	280	ILE
2	C	283	ASN
2	C	286	ILE
2	C	290	LEU
2	C	293	GLN
2	C	298	LYS
2	C	300	VAL
2	C	306	GLU

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Mol	Chain	Res	Type
2	C	310	LYS
2	C	316	LEU
2	C	321	ARG
2	C	322	ARG
2	C	326	ILE
2	C	329	THR
2	E	6	GLN
2	E	14	ILE
2	E	15	TYR
2	E	20	LYS
2	E	29	GLU
2	E	33	LYS
2	E	42	ILE
2	E	44	VAL
2	E	48	ASP
2	E	52	HIS
2	E	57	ARG
2	E	66	ARG
2	E	67	ARG
2	E	79	THR
2	E	89	LEU
2	E	90	TYR
2	E	95	VAL
2	E	101	ASP
2	E	102	ARG
2	E	113	GLU
2	E	118	LEU
2	E	121	PHE
2	E	124	LYS
2	E	127	ARG
2	E	128	TYR
2	E	134	THR
2	E	135	ASP
2	E	139	GLU
2	E	141	PHE
2	E	147	ARG
2	E	150	THR
2	E	151	LEU
2	E	162	VAL
2	E	171	THR
2	E	175	ILE
2	E	176	TRP

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Mol	Chain	Res	Type
2	E	179	SER
2	E	182	GLU
2	E	186	HIS
2	E	187	MET
2	E	188	ILE
2	E	189	TYR
2	E	194	VAL
2	E	197	PHE
2	E	198	GLN
2	E	204	ASP
2	E	207	VAL
2	E	215	PHE
2	E	216	ARG
2	E	218	TYR
2	E	219	ARG
2	E	222	PHE
2	E	225	ASP
2	E	228	LEU
2	E	236	ILE
2	E	238	ARG
2	E	241	ASN
2	E	242	ILE
2	E	250	ASP
2	E	260	MET
2	E	270	VAL
2	E	273	LEU
2	E	277	LYS
2	E	280	ILE
2	E	284	LYS
2	E	285	THR
2	E	293	GLN
2	E	296	ASN
2	E	298	LYS
2	E	303	THR
2	E	306	GLU
2	E	307	TYR
2	E	316	LEU
2	E	320	ILE
2	E	322	ARG
2	E	329	THR
1	I	2	LYS
1	I	5	ASN

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Mol	Chain	Res	Type
1	I	8	THR
1	I	13	PHE
1	I	17	ASP
1	I	24	ASP
1	I	25	GLN
1	I	26	TYR
1	I	30	LEU
1	I	32	ILE
1	I	37	GLU
1	I	40	GLN
1	I	41	ARG
1	I	44	LEU
1	I	47	LYS
1	I	54	ASP
1	I	59	MET
1	I	61	MET
1	I	65	CYS
1	I	70	ARG
1	I	72	THR
1	I	73	ASP
1	I	81	GLU
1	I	82	LEU
1	I	93	LYS
1	I	94	ARG
1	I	98	LYS
1	I	99	GLU
1	I	100	LEU
1	I	105	TYR
1	I	110	ASP
1	J	1	MET
1	J	5	ASN
1	J	6	MET
1	J	8	THR
1	J	11	ASP
1	J	13	PHE
1	J	19	LYS
1	J	24	ASP
1	J	25	GLN
1	J	26	TYR
1	J	31	ARG
1	J	32	ILE
1	J	34	LEU

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Mol	Chain	Res	Type
1	J	40	GLN
1	J	41	ARG
1	J	42	LEU
1	J	44	LEU
1	J	49	LEU
1	J	58	VAL
1	J	61	MET
1	J	65	CYS
1	J	70	ARG
1	J	74	HIS
1	J	82	LEU
1	J	93	LYS
1	J	96	ASP
1	J	99	GLU
1	J	100	LEU
1	J	104	PHE
1	J	105	TYR
1	J	110	ASP
1	L	2	LYS
1	L	5	ASN
1	L	6	MET
1	L	11	ASP
1	L	14	VAL
1	L	26	TYR
1	L	30	LEU
1	L	31	ARG
1	L	32	ILE
1	L	37	GLU
1	L	39	LEU
1	L	41	ARG
1	L	42	LEU
1	L	47	LYS
1	L	57	SER
1	L	58	VAL
1	L	59	MET
1	L	61	MET
1	L	65	CYS
1	L	70	ARG
1	L	71	THR
1	L	76	GLU
1	L	78	ASN
1	L	80	VAL

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Mol	Chain	Res	Type
1	L	82	LEU
1	L	87	ILE
1	L	89	LEU
1	L	93	LYS
1	L	98	LYS
1	L	99	GLU
1	L	104	PHE
1	L	105	TYR
1	L	109	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	70	GLN
2	A	105	ASN
2	A	114	ASN
2	A	119	GLN
1	H	40	GLN
1	H	45	ASN
1	H	78	ASN
2	F	47	ASN
2	F	69	ASN
2	F	122	ASN
2	F	172	ASN
2	F	214	GLN
2	B	293	GLN
2	B	301	ASN
2	B	328	ASN
2	G	293	GLN
2	D	69	ASN
2	D	122	ASN
1	K	5	ASN
2	C	123	ASN
2	C	199	HIS
2	C	214	GLN
2	E	16	ASN
2	E	241	ASN
1	I	25	GLN
1	I	40	GLN
1	J	78	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

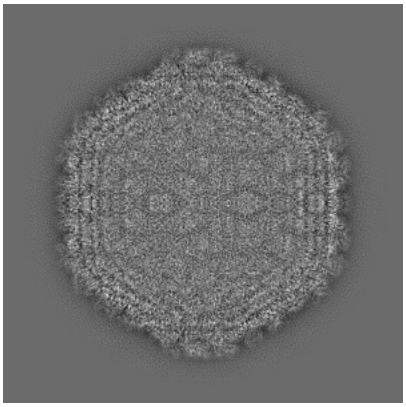
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5678. These allow visual inspection of the internal detail of the map and identification of artifacts.

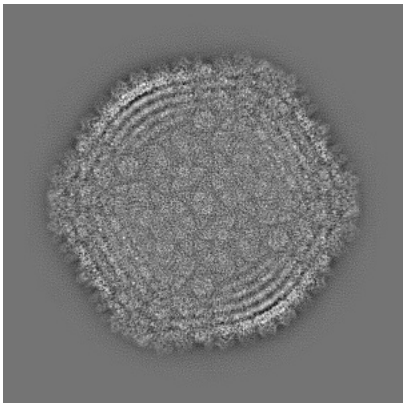
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

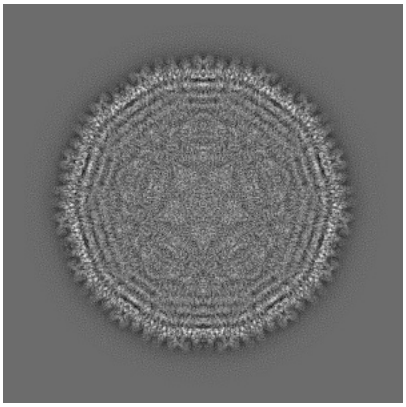
6.1.1 Primary map



X



Y

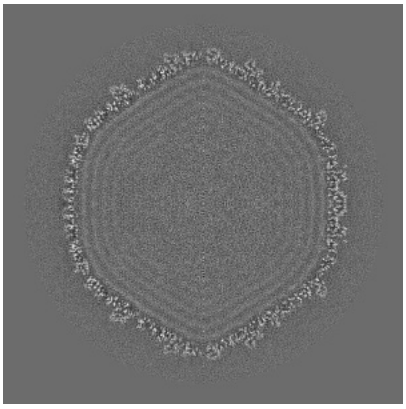


Z

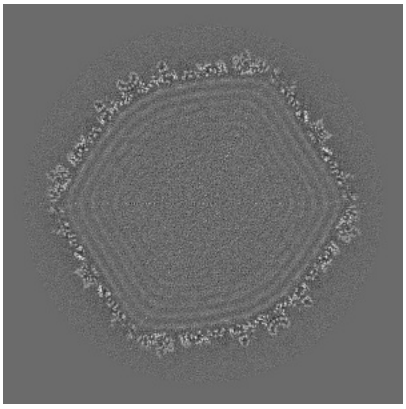
The images above show the map projected in three orthogonal directions.

6.2 Central slices

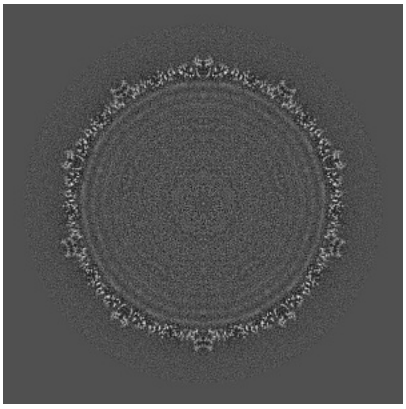
6.2.1 Primary map



X Index: 360



Y Index: 360

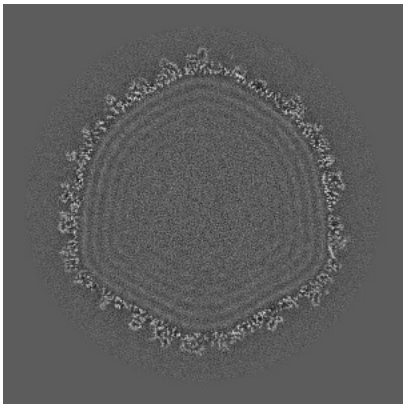


Z Index: 360

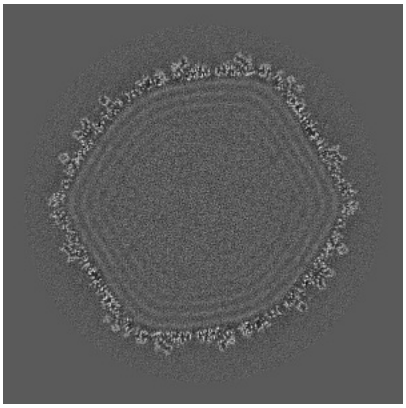
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

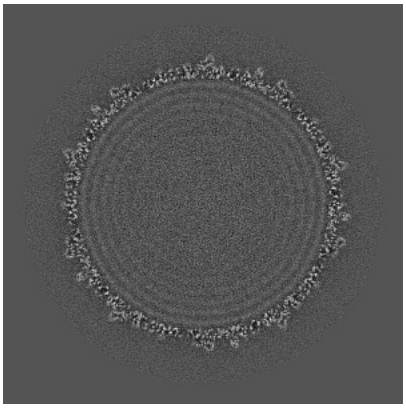
6.3.1 Primary map



X Index: 309



Y Index: 382



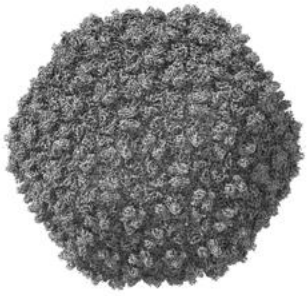
Z Index: 355

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 5.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

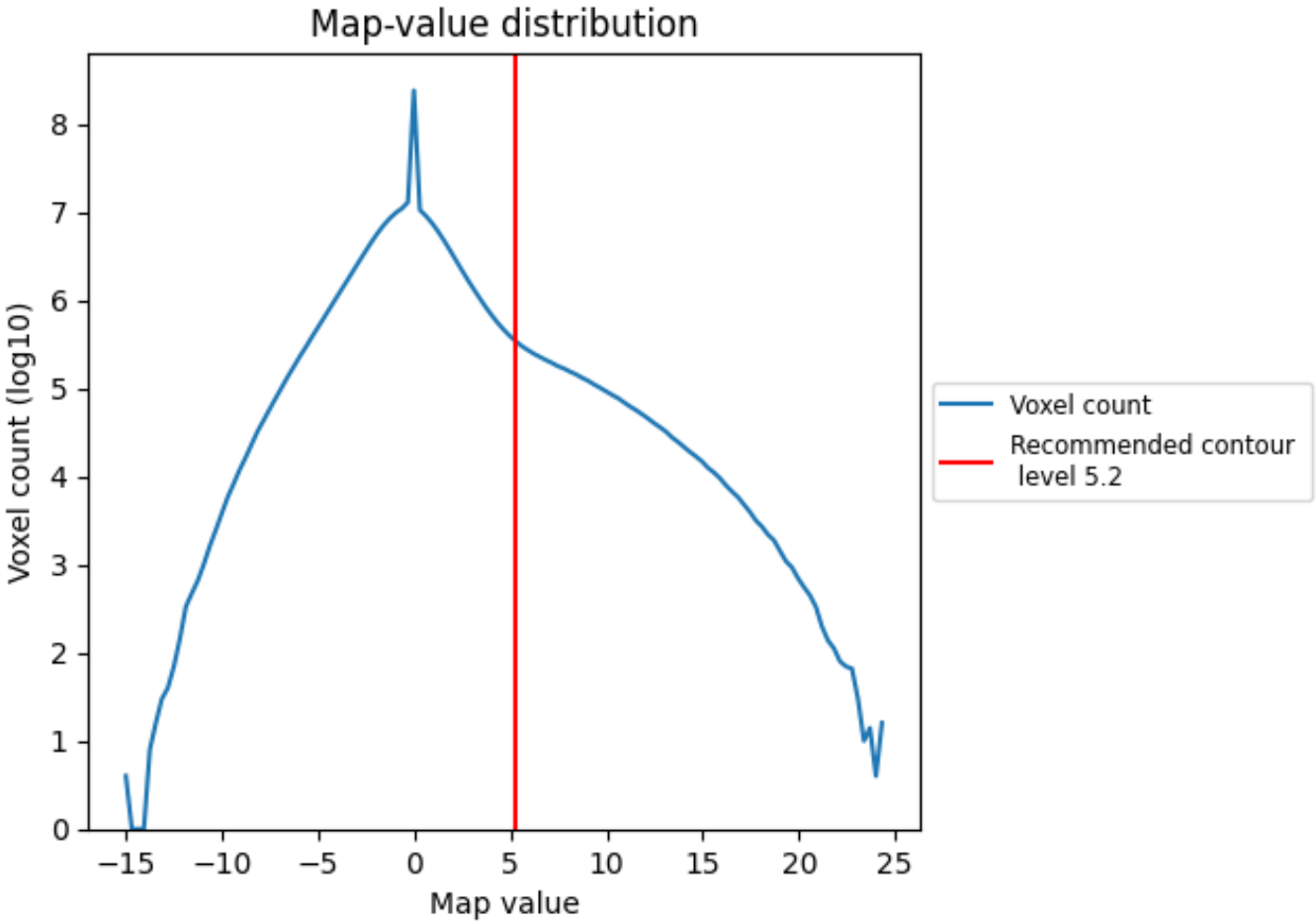
6.5 Mask visualisation (i)

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

7 Map analysis

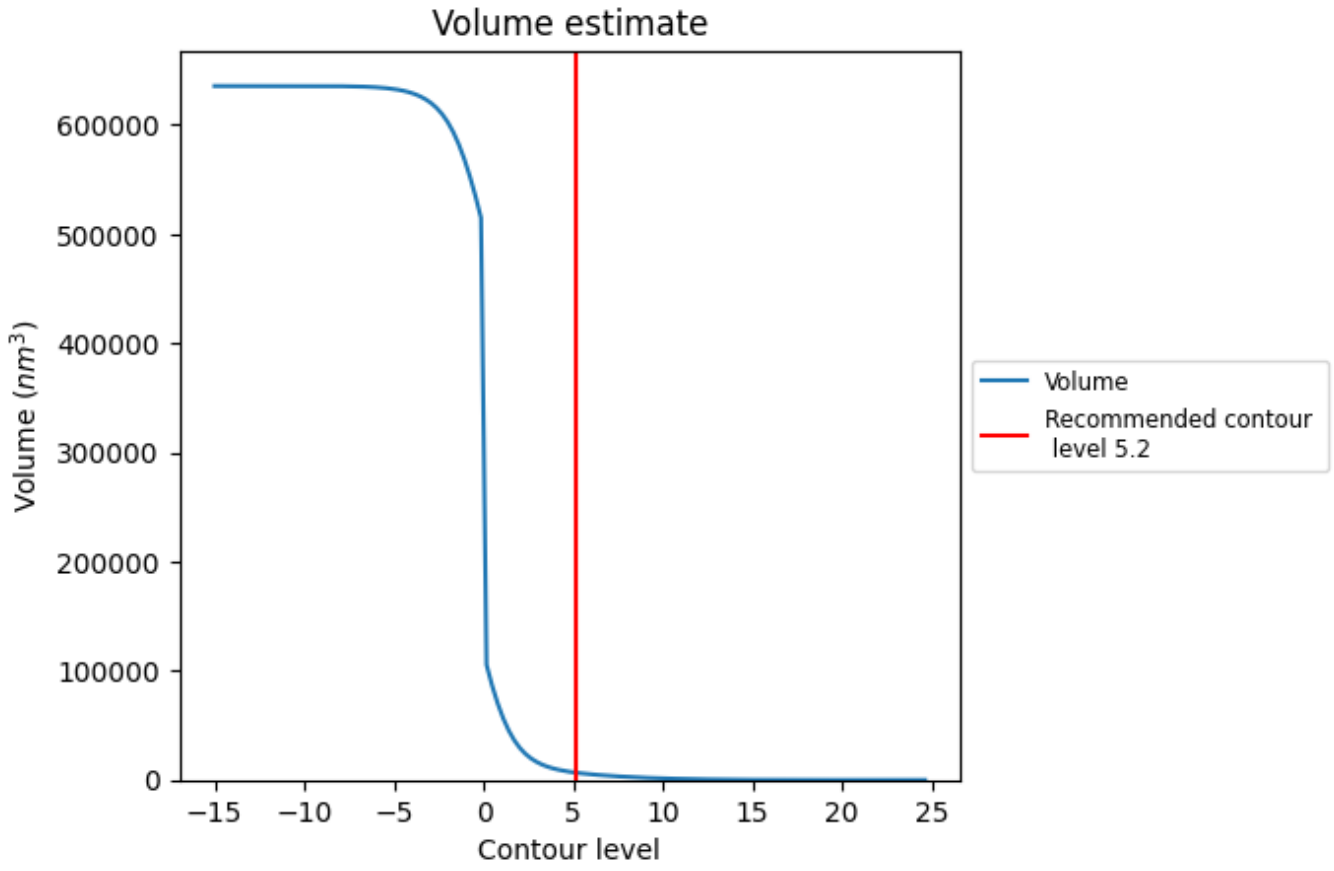
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

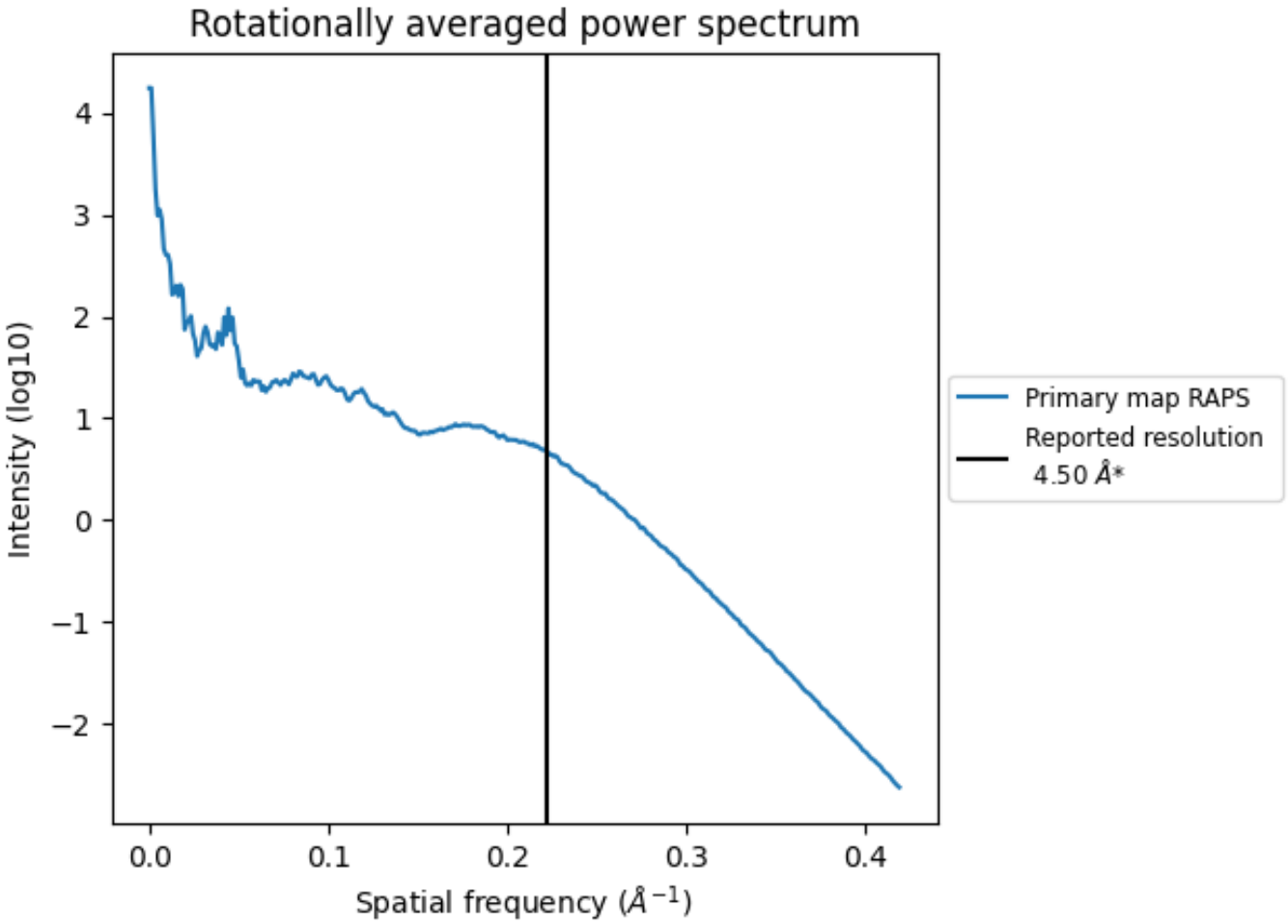
7.2 Volume estimate



The volume at the recommended contour level is 6565 nm^3; this corresponds to an approximate mass of 5931 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 0.222 Å^{-1}

8 Fourier-Shell correlation (i)

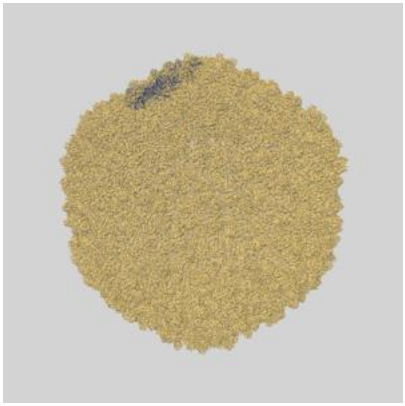
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

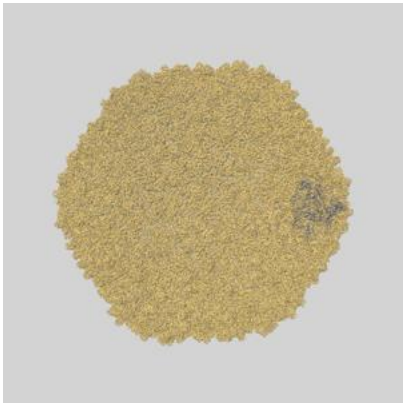
This section contains information regarding the fit between EMDB map EMD-5678 and PDB model 3J40. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

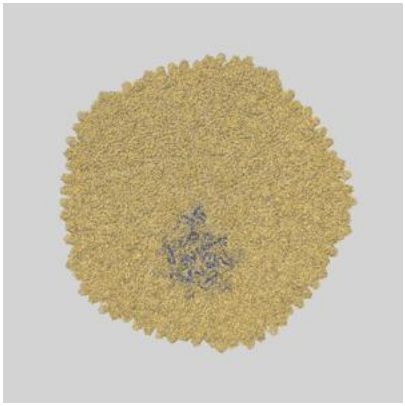
9.1.1 Map-model overlay



X

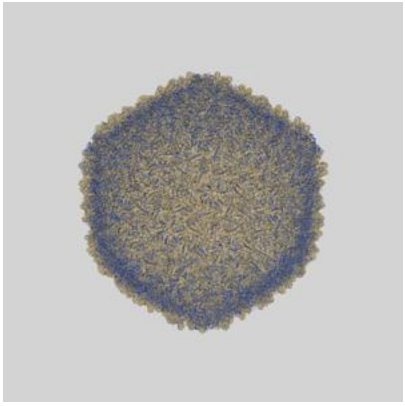


Y

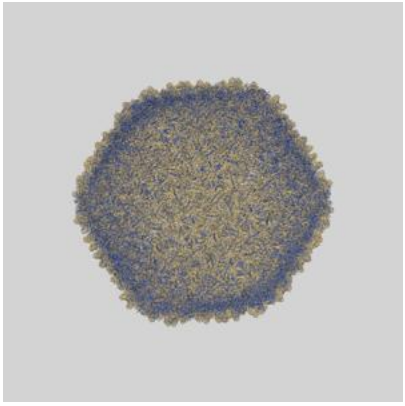


Z

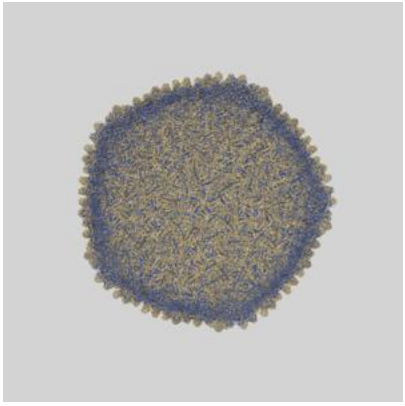
9.1.2 Map-model assembly overlay



X



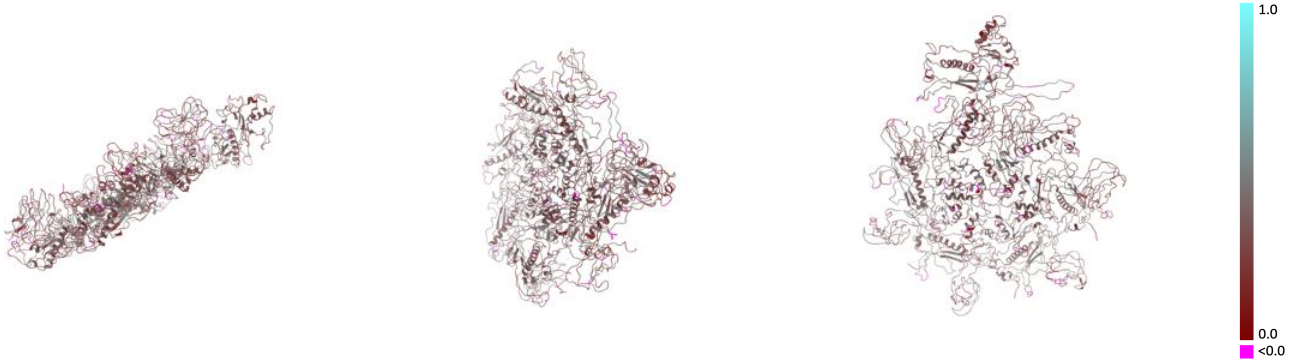
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.2 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.

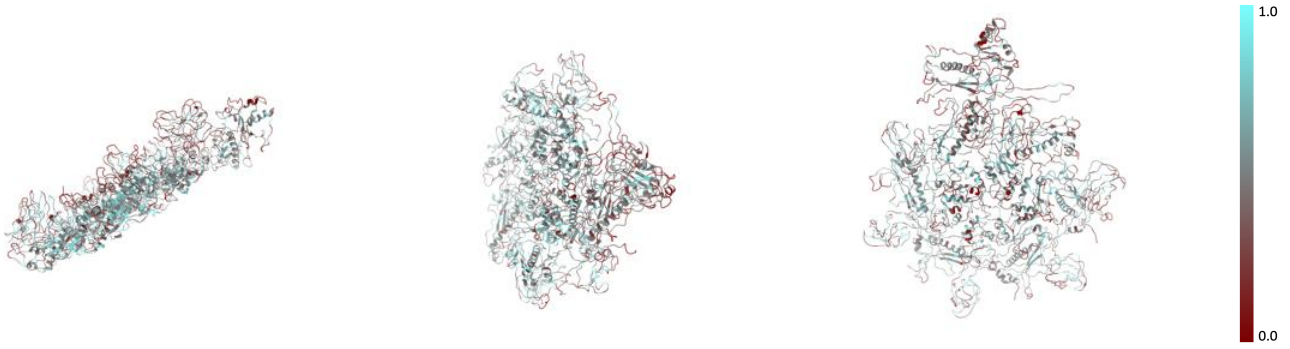
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

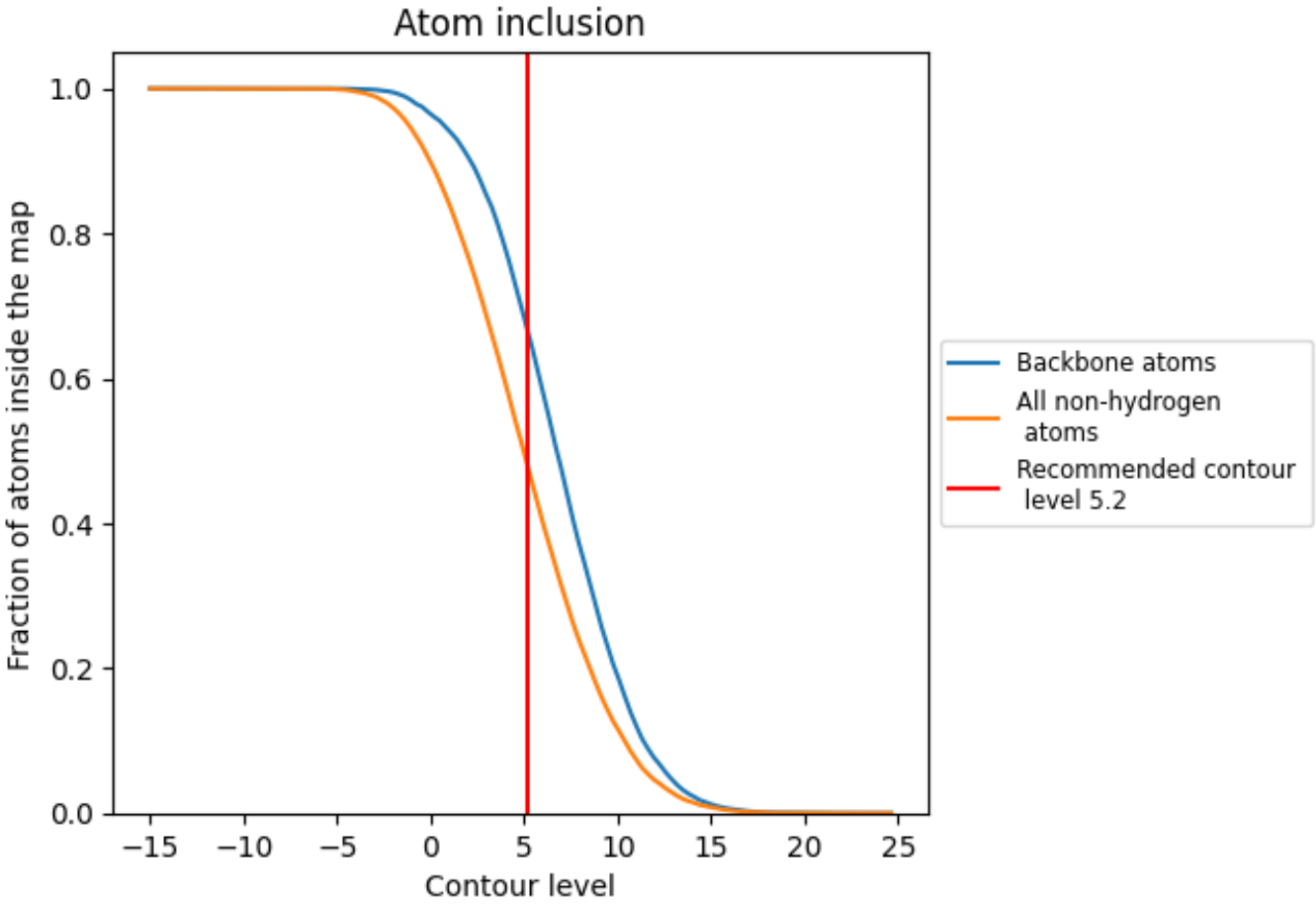
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (5.2).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 48% 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 (5.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4772	0.3230
A	0.4937	0.3300
B	0.5182	0.3440
C	0.5166	0.3450
D	0.5036	0.3310
E	0.5047	0.3300
F	0.4866	0.3340
G	0.4088	0.3220
H	0.4690	0.3030
I	0.5048	0.3110
J	0.4833	0.3060
K	0.4749	0.2830
L	0.4403	0.2840
M	0.3353	0.2740
N	0.3544	0.2790