Full wwPDB EM Validation Report ⓘ

Aug 26, 2024 – 08:50 PM JST

PDB ID	:	8ZVI
EMDB ID	:	EMD-60511
Title	:	Structure of the bacteriophage T5 capsid
Authors	:	Peng, Y.; Liu, H.R.
Deposited on	:	2024-06-11
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

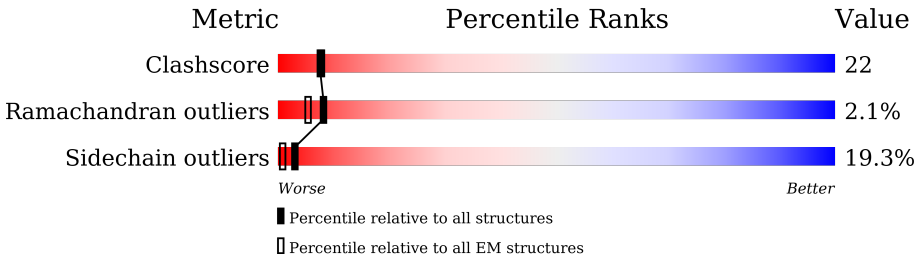
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	458	36% 24% · 35%
1	B	458	33% 26% 5% 35%
1	C	458	37% 23% · 35%
1	D	458	37% 24% · 35%
1	E	458	35% 24% 5% 35%
1	F	458	34% 23% 7% 35%
1	G	458	6% 34% 24% 6% 36%
1	H	458	· 32% 25% 8% 35%

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Mol	Chain	Length	Quality of chain
1	I	458	37% 22% 5% 35%
1	J	458	36% 22% 6% 36%
1	K	458	8% 37% 22% 5% 36%
1	L	458	9% 35% 24% 5% 36%
2	a	164	35% 5% 60%
2	b	164	5% 33% 7% 60%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 28628 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	297	Total	C	N	O	S	0	0
			2305	1460	389	451	5		
1	B	297	Total	C	N	O	S	0	0
			2305	1460	389	451	5		
1	C	297	Total	C	N	O	S	0	0
			2305	1460	389	451	5		
1	D	297	Total	C	N	O	S	0	0
			2305	1460	389	451	5		
1	E	297	Total	C	N	O	S	0	0
			2305	1460	389	451	5		
1	F	297	Total	C	N	O	S	0	0
			2305	1460	389	451	5		
1	G	294	Total	C	N	O	S	0	0
			2281	1446	384	446	5		
1	H	297	Total	C	N	O	S	0	0
			2305	1460	389	451	5		
1	I	297	Total	C	N	O	S	0	0
			2305	1460	389	451	5		
1	J	294	Total	C	N	O	S	0	0
			2281	1446	384	446	5		
1	K	294	Total	C	N	O	S	0	0
			2281	1446	384	446	5		
1	L	294	Total	C	N	O	S	0	0
			2281	1446	384	446	5		

- Molecule 2 is a protein called Decoration protein.

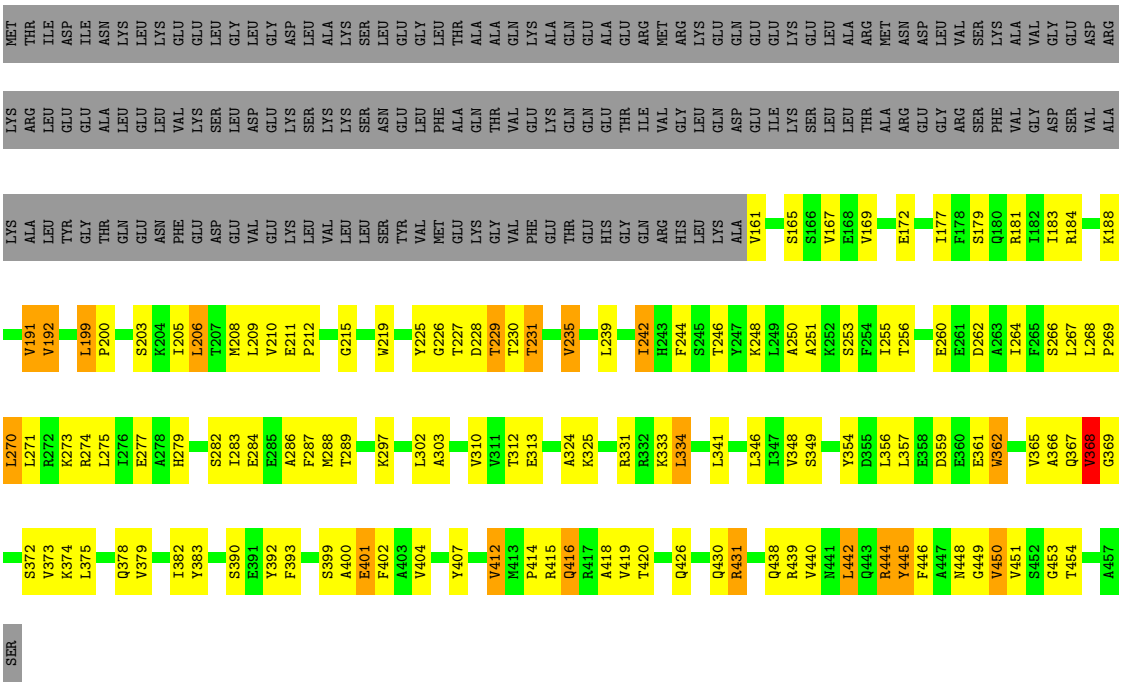
Mol	Chain	Residues	Atoms				AltConf	Trace
2	a	66	Total	C	N	O	0	0
			532	351	92	89		
2	b	66	Total	C	N	O	0	0
			532	351	92	89		

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.

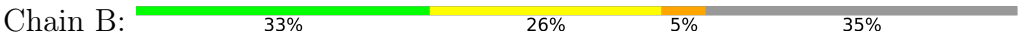
- Molecule 1: Major capsid protein

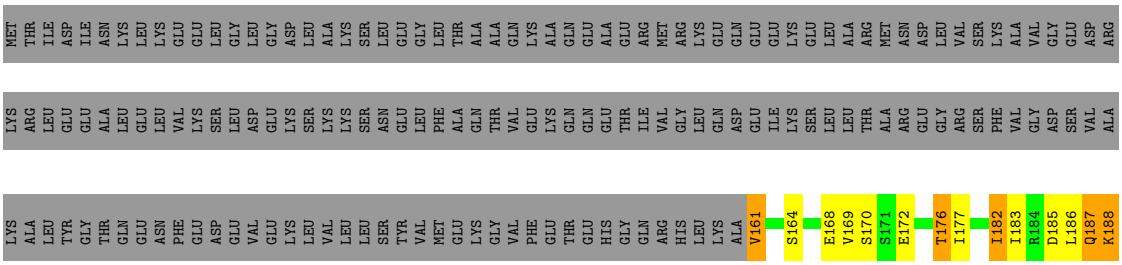
Chain A:

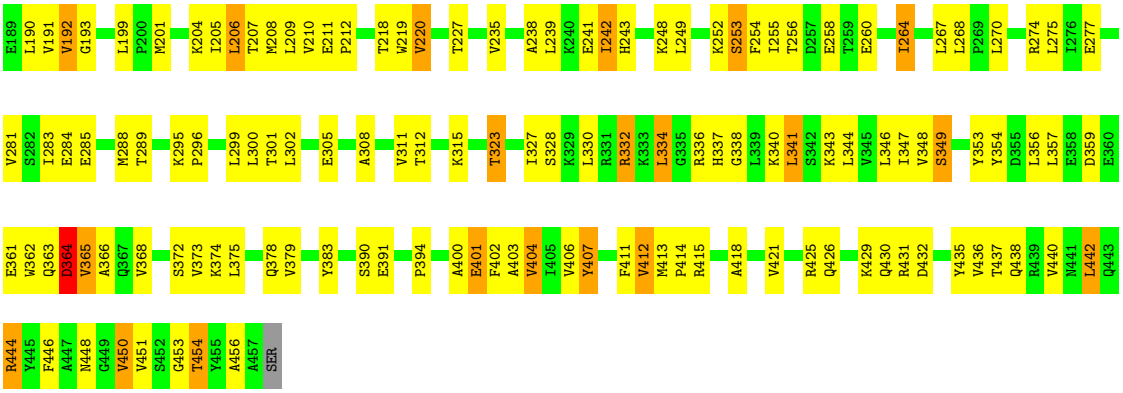


- Molecule 1: Major capsid protein

Chain B:

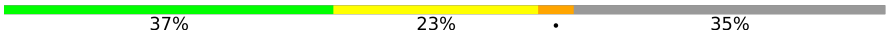


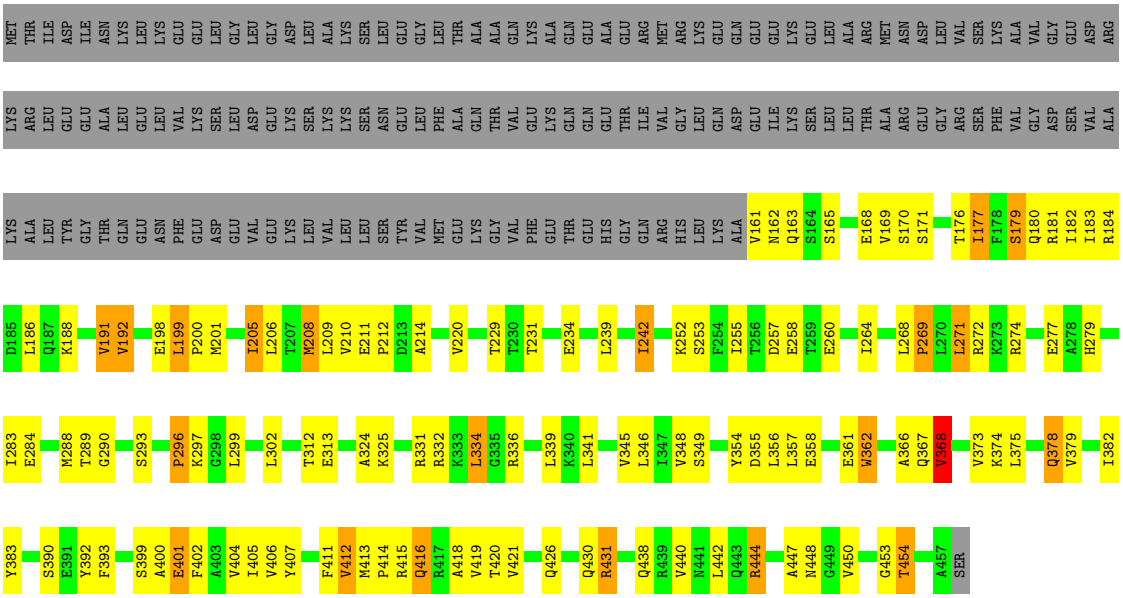




• Molecule 1: Major capsid protein

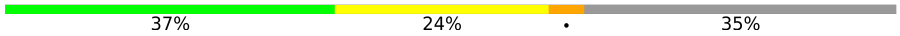
Chain C:

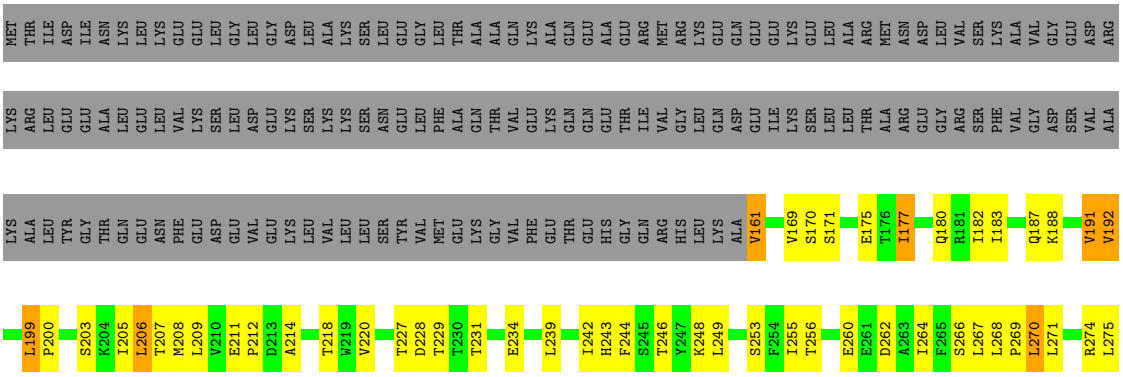


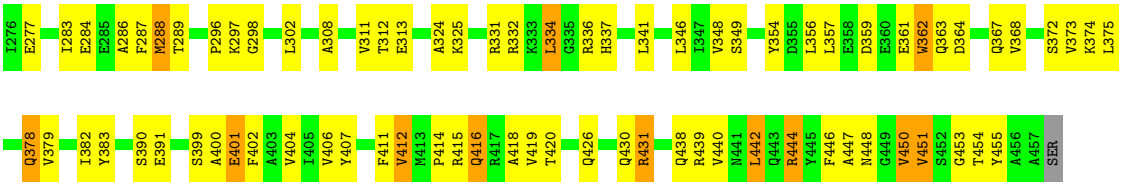


• Molecule 1: Major capsid protein

Chain D:

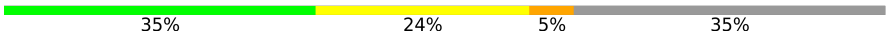


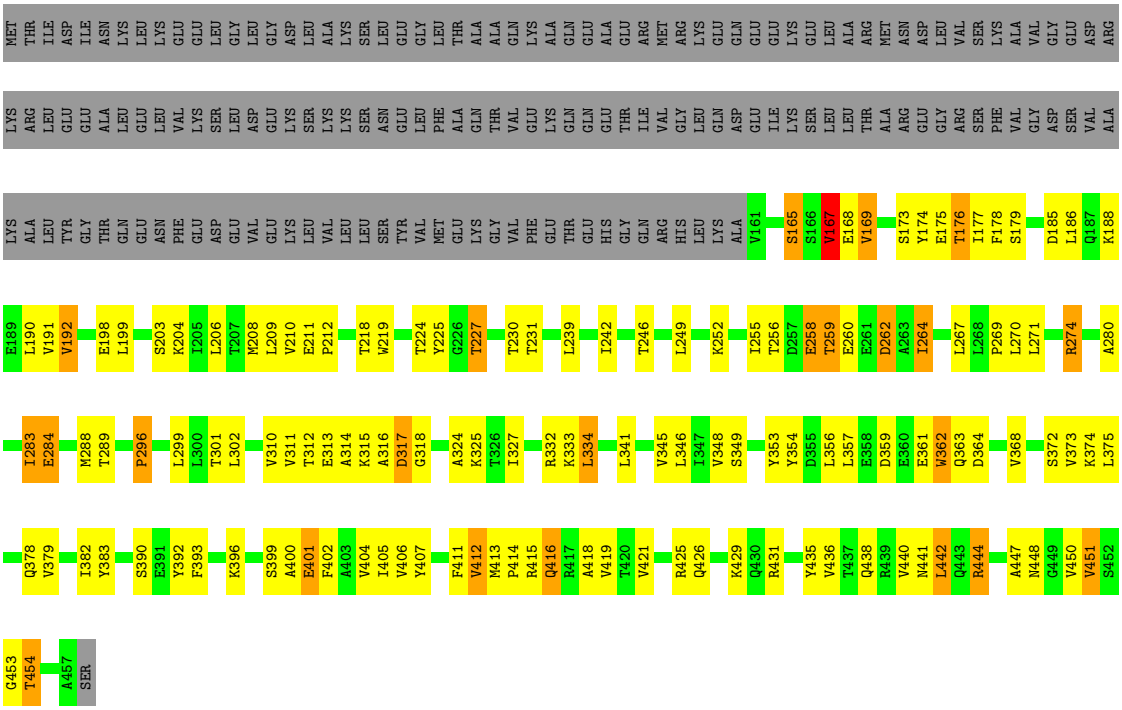




• Molecule 1: Major capsid protein

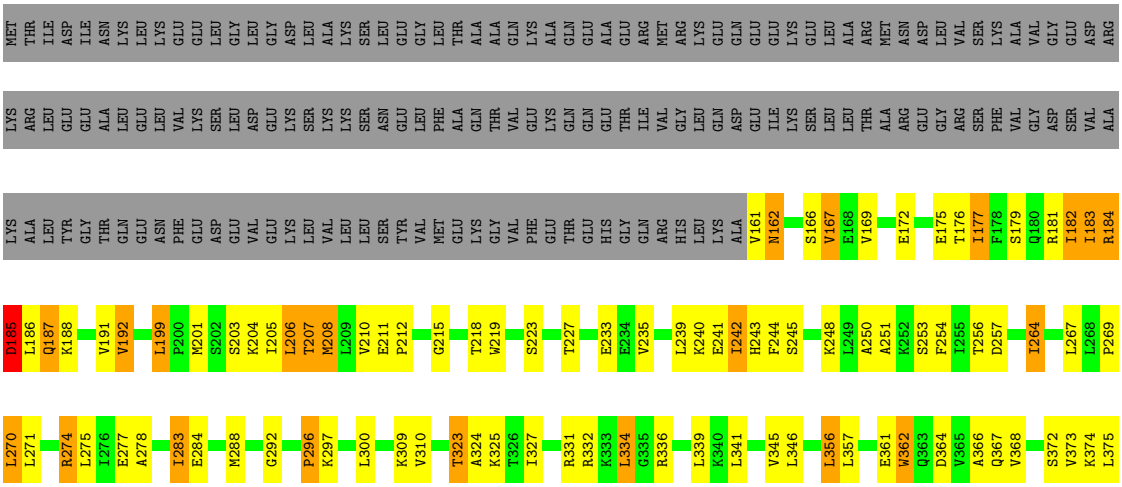
Chain E:

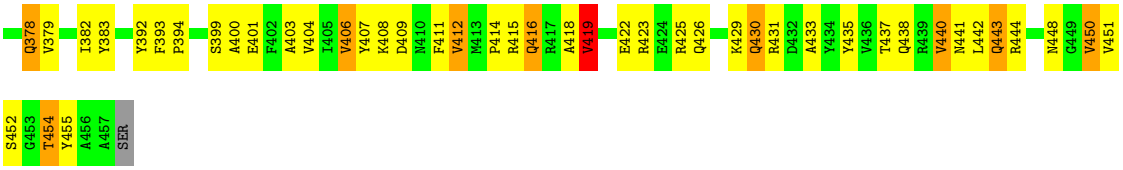




• Molecule 1: Major capsid protein

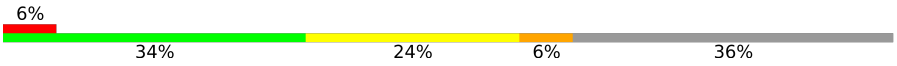
Chain F:

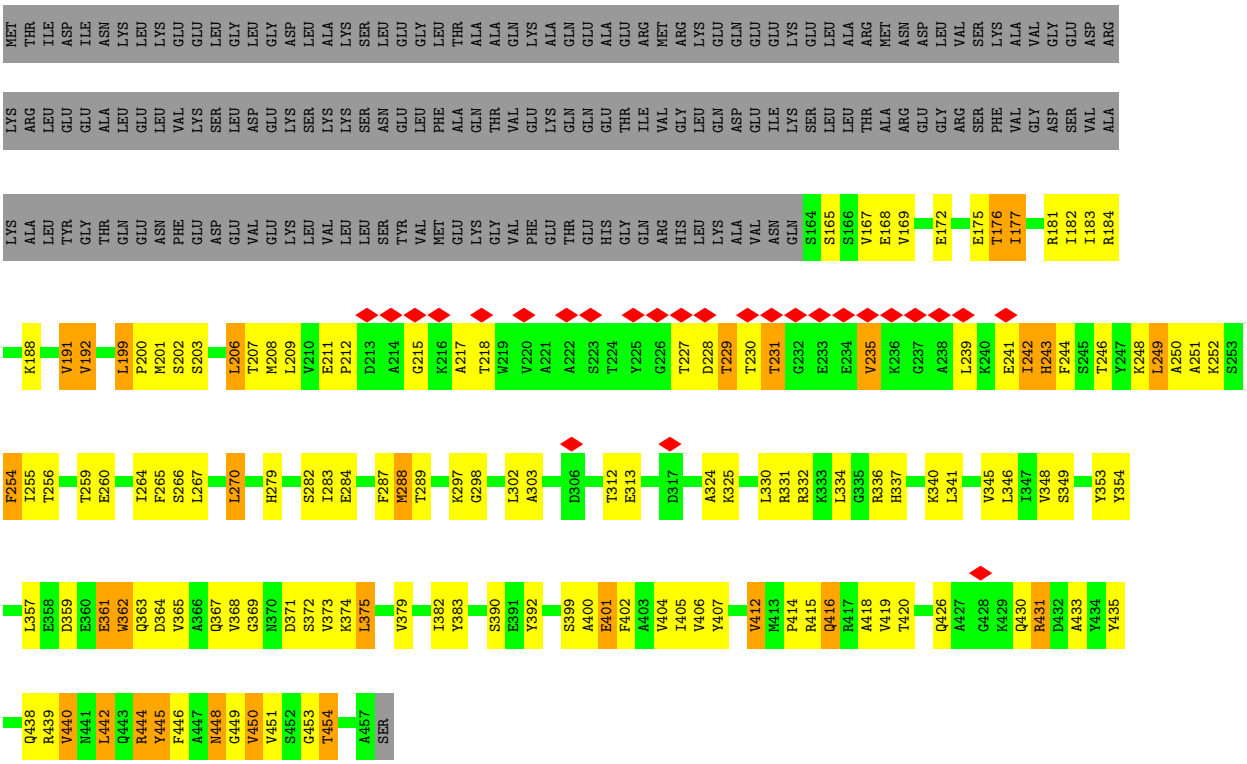




• Molecule 1: Major capsid protein

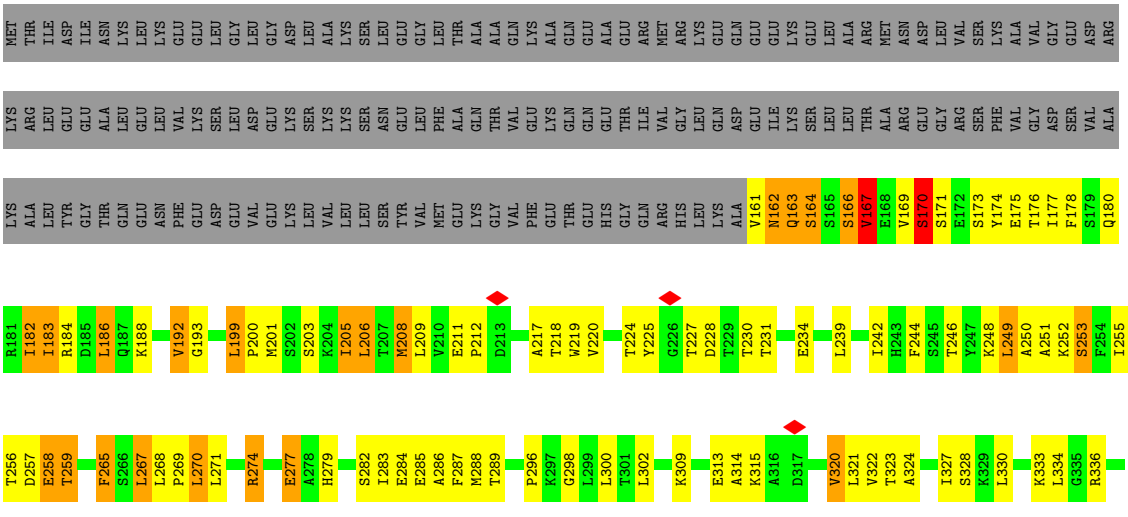
Chain G:

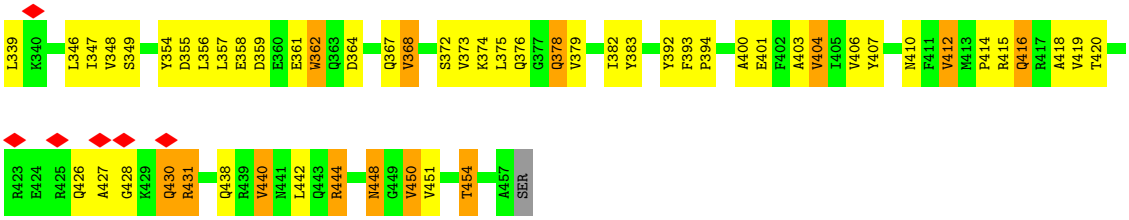




• Molecule 1: Major capsid protein

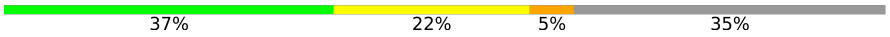
Chain H:

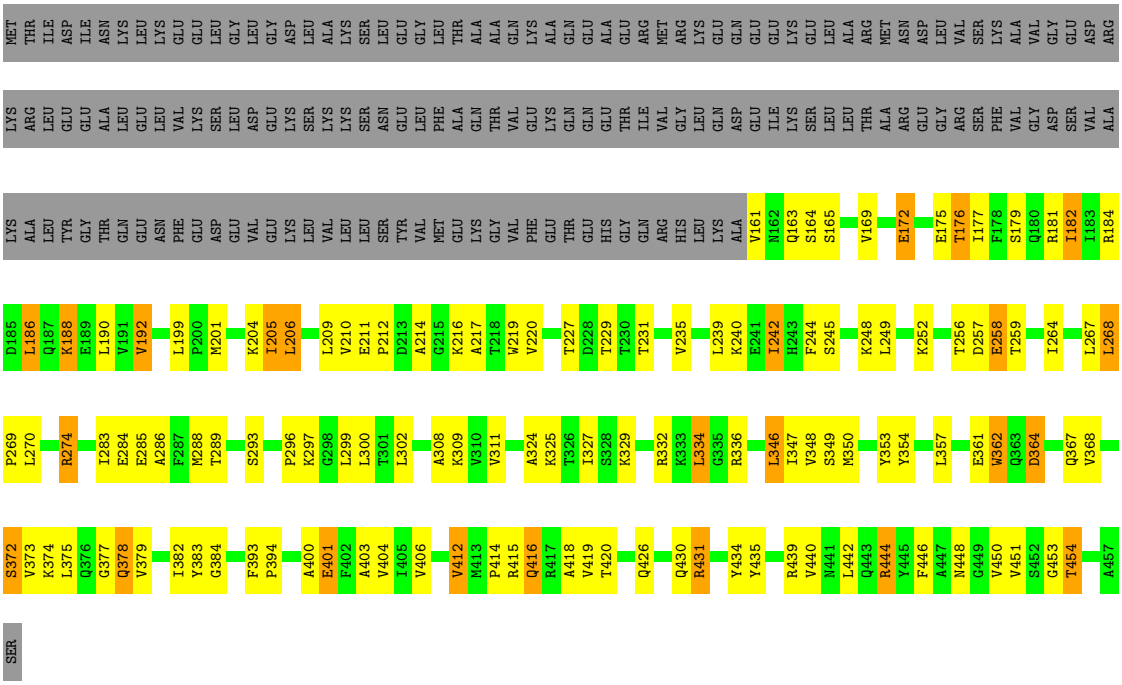




• Molecule 1: Major capsid protein

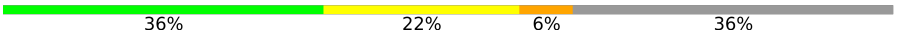
Chain I:

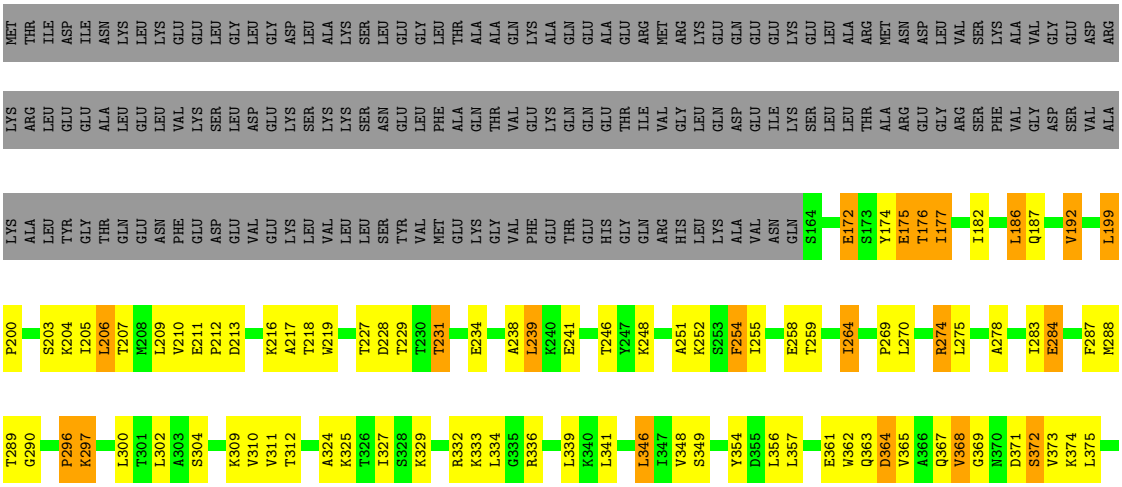


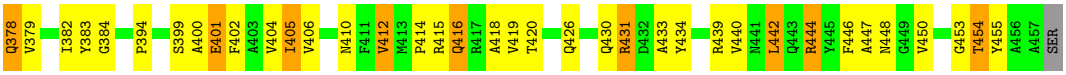


• Molecule 1: Major capsid protein

Chain J:

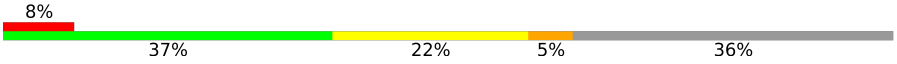


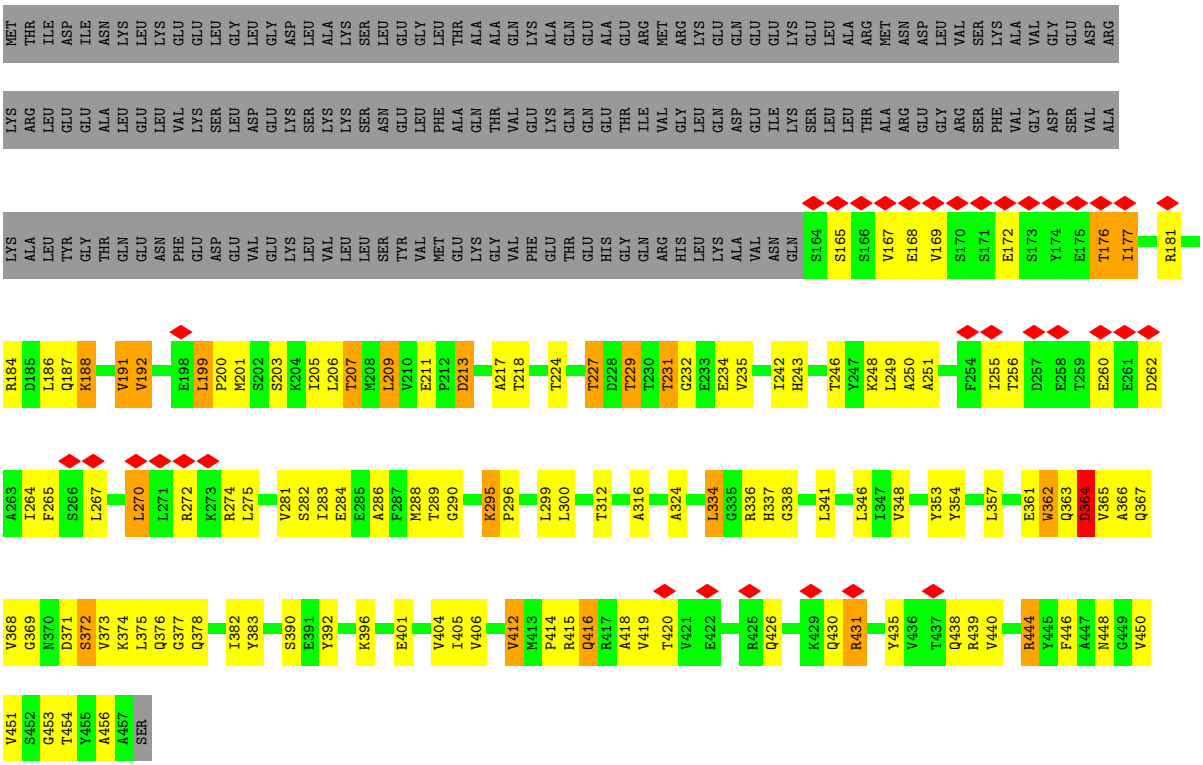




• Molecule 1: Major capsid protein

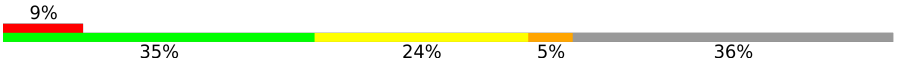
Chain K:

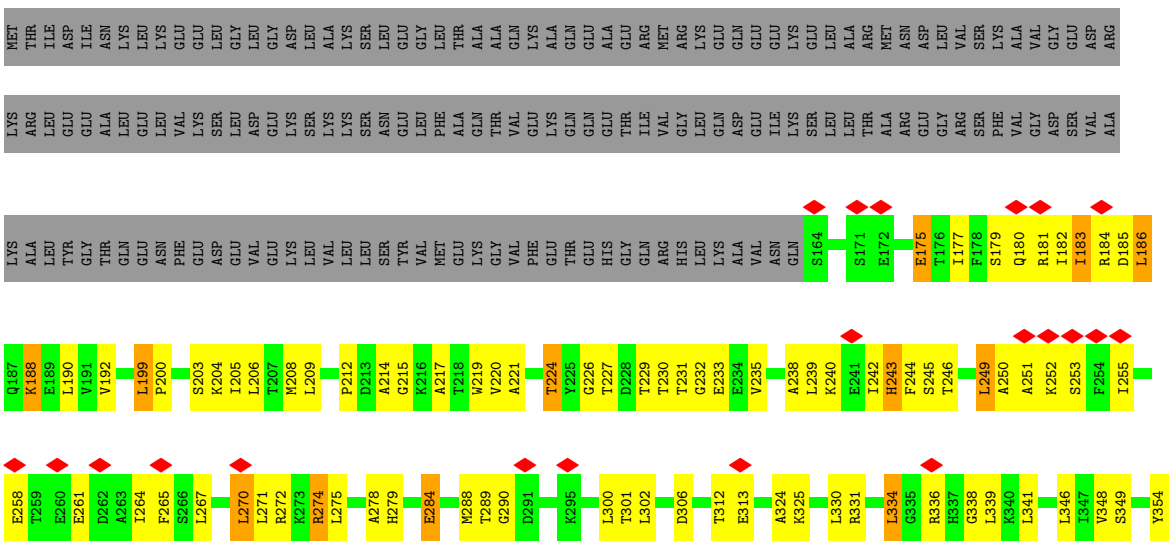


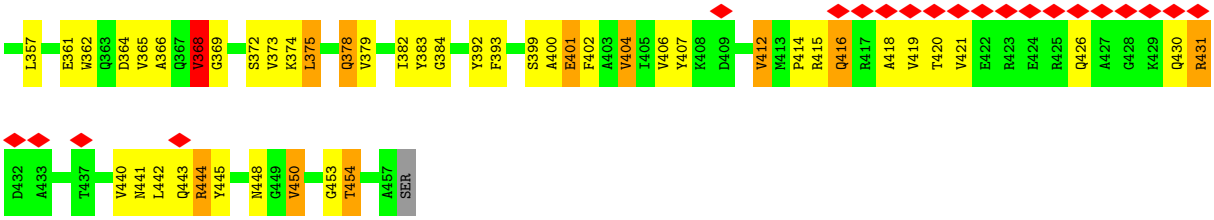


• Molecule 1: Major capsid protein

Chain L:

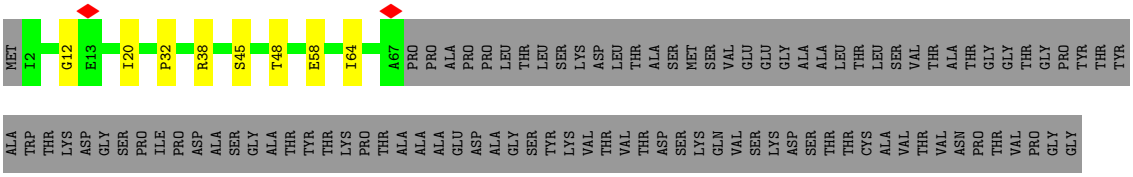






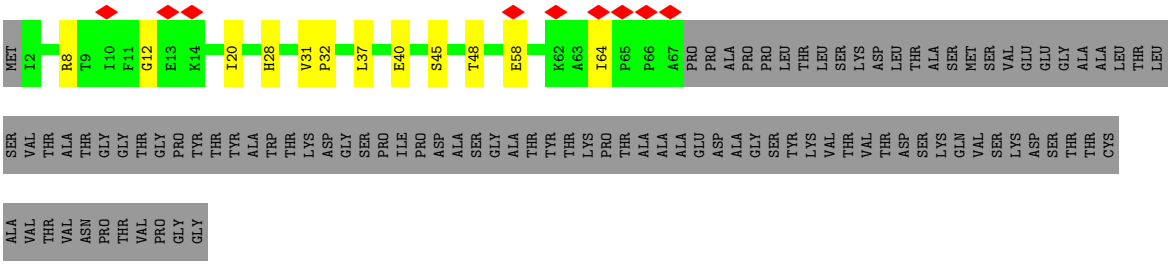
• Molecule 2: Decoration protein

Chain a:



• Molecule 2: Decoration protein

Chain b:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100841	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	43.968	Depositor
Minimum map value	-25.438	Depositor
Average map value	0.014	Depositor
Map value standard deviation	2.129	Depositor
Recommended contour level	3	Depositor
Map size (Å)	467.99997, 467.99997, 467.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.17	0/2340	1.08	0/3163
1	B	1.18	0/2340	1.07	0/3163
1	C	1.25	0/2340	1.11	0/3163
1	D	1.25	0/2340	1.10	0/3163
1	E	1.33	0/2340	1.14	0/3163
1	F	1.20	0/2340	1.12	0/3163
1	G	1.11	0/2316	1.06	0/3130
1	H	1.10	0/2340	1.07	0/3163
1	I	1.16	0/2340	1.08	0/3163
1	J	1.08	0/2316	1.06	0/3130
1	K	0.95	0/2316	0.98	0/3130
1	L	0.98	0/2316	1.02	0/3130
2	a	0.77	0/549	0.77	0/742
2	b	0.70	0/549	0.72	0/742
All	All	1.14	0/29082	1.06	0/39308

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2305	0	2332	132	0
1	B	2305	0	2332	142	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2305	0	2332	130	0
1	D	2305	0	2332	130	0
1	E	2305	0	2332	158	0
1	F	2305	0	2332	144	0
1	G	2281	0	2309	147	0
1	H	2305	0	2332	197	0
1	I	2305	0	2332	145	0
1	J	2281	0	2309	129	0
1	K	2281	0	2309	114	0
1	L	2281	0	2309	133	0
2	a	532	0	536	0	0
2	b	532	0	536	0	0
All	All	28628	0	28964	1255	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 22.

All (1255) 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:C:354:TYR:CG	1:D:332:ARG:HG3	1.63	1.33
1:D:378:GLN:NE2	1:E:341:LEU:HD12	1.46	1.27
1:C:354:TYR:CD2	1:D:332:ARG:HG2	1.72	1.22
1:C:354:TYR:CG	1:D:332:ARG:CG	2.25	1.18
1:B:354:TYR:CD2	1:C:332:ARG:HG2	1.80	1.16
1:J:378:GLN:NE2	1:K:341:LEU:HD12	1.59	1.14
1:C:354:TYR:CB	1:D:332:ARG:CG	2.26	1.14
1:C:354:TYR:HB3	1:D:332:ARG:CD	1.78	1.12
1:A:341:LEU:HD12	1:F:378:GLN:NE2	1.64	1.11
1:C:354:TYR:CD2	1:D:332:ARG:CG	2.36	1.07
1:I:378:GLN:HE21	1:J:341:LEU:HD12	1.14	1.07
1:J:373:VAL:HG12	1:K:383:TYR:CD1	1.89	1.07
1:C:354:TYR:CB	1:D:332:ARG:HG3	1.85	1.06
1:H:249:LEU:HD13	1:I:219:TRP:CD2	1.91	1.06
1:I:378:GLN:HE22	1:J:341:LEU:HB2	1.20	1.04
1:B:354:TYR:HB3	1:C:332:ARG:HD2	1.41	1.02
1:C:354:TYR:HB3	1:D:332:ARG:CG	1.86	1.02
1:E:283:ILE:HD11	1:E:440:VAL:HG11	1.41	1.01
1:B:354:TYR:CG	1:C:332:ARG:CG	2.43	1.00
1:A:341:LEU:HD12	1:F:378:GLN:HE21	1.17	1.00
1:D:378:GLN:NE2	1:E:341:LEU:CD1	2.26	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:192:VAL:HG23	1:K:284:GLU:HG2	1.45	0.98
1:G:341:LEU:HD12	1:L:378:GLN:NE2	1.78	0.98
1:J:373:VAL:HG12	1:K:383:TYR:HD1	1.23	0.98
1:G:374:LYS:HA	1:H:383:TYR:CD1	2.00	0.96
1:H:374:LYS:HA	1:I:383:TYR:CD1	2.01	0.96
1:G:177:ILE:HG22	1:H:203:SER:HB2	1.48	0.95
1:G:373:VAL:HG12	1:H:383:TYR:CD1	2.01	0.95
1:I:378:GLN:NE2	1:J:341:LEU:HD12	1.82	0.94
1:B:354:TYR:CG	1:C:332:ARG:HG3	2.01	0.94
1:C:354:TYR:CB	1:D:332:ARG:CD	2.45	0.94
1:F:357:LEU:HD23	1:F:379:VAL:HG23	1.50	0.93
1:A:341:LEU:CD1	1:F:378:GLN:NE2	2.32	0.93
1:I:378:GLN:HE22	1:J:341:LEU:CB	1.82	0.92
1:G:341:LEU:HD12	1:L:378:GLN:HE21	1.27	0.92
1:J:378:GLN:NE2	1:K:341:LEU:CD1	2.32	0.92
1:C:378:GLN:NE2	1:D:341:LEU:HD12	1.85	0.92
1:J:378:GLN:HE21	1:K:341:LEU:HD12	1.30	0.90
1:A:374:LYS:HA	1:B:383:TYR:CD1	2.06	0.90
1:D:378:GLN:HE21	1:E:341:LEU:HD12	1.22	0.90
1:K:376:GLN:O	1:L:384:GLY:CA	2.20	0.89
1:C:354:TYR:CB	1:D:332:ARG:HD2	2.02	0.89
1:B:354:TYR:HB3	1:C:332:ARG:CD	2.03	0.89
1:I:378:GLN:NE2	1:J:341:LEU:CD1	2.36	0.89
1:A:183:ILE:CG2	1:B:208:MET:CE	2.52	0.87
1:B:354:TYR:CG	1:C:332:ARG:HG2	2.09	0.87
1:E:359:ASP:C	1:E:361:GLU:H	1.77	0.86
1:H:212:PRO:HD3	1:H:239:LEU:HA	1.59	0.85
1:G:341:LEU:CD1	1:L:378:GLN:NE2	2.39	0.85
1:C:354:TYR:HB3	1:D:332:ARG:HG3	1.49	0.85
1:B:212:PRO:HD3	1:B:239:LEU:HA	1.58	0.84
1:J:327:ILE:HG21	1:J:346:LEU:HD21	1.58	0.83
1:A:183:ILE:HG21	1:B:208:MET:HE1	1.58	0.83
1:H:249:LEU:HD22	1:I:219:TRP:CH2	2.13	0.83
1:D:373:VAL:HG12	1:E:383:TYR:CD1	2.12	0.83
1:B:406:VAL:HG12	1:B:450:VAL:HG13	1.60	0.83
1:F:241:GLU:HG3	1:H:170:SER:HB3	1.59	0.83
1:I:378:GLN:NE2	1:J:341:LEU:HB2	1.93	0.83
1:G:383:TYR:HD1	1:L:373:VAL:HG12	1.45	0.82
1:A:383:TYR:HD1	1:F:373:VAL:HG12	1.44	0.82
1:G:374:LYS:HZ3	1:H:361:GLU:HB3	1.44	0.82
1:I:378:GLN:HE21	1:J:341:LEU:CD1	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:TYR:CD2	1:C:332:ARG:CG	2.59	0.81
1:C:177:ILE:HG23	1:D:206:LEU:HD12	1.62	0.81
1:A:183:ILE:HG21	1:B:208:MET:CE	2.11	0.81
1:K:177:ILE:HG21	1:L:203:SER:HB3	1.63	0.81
1:C:354:TYR:HD2	1:D:332:ARG:HG2	1.43	0.80
1:K:373:VAL:HG12	1:L:383:TYR:CD1	2.17	0.80
1:F:199:LEU:HD11	1:F:206:LEU:HD22	1.62	0.80
1:A:199:LEU:HD11	1:A:206:LEU:HD22	1.64	0.79
1:G:199:LEU:HD11	1:G:206:LEU:HD22	1.64	0.79
1:I:311:VAL:HA	1:I:454:THR:HG23	1.65	0.79
1:G:249:LEU:HD11	1:G:282:SER:OG	1.83	0.79
1:I:299:LEU:HD13	1:I:406:VAL:HG11	1.63	0.79
1:H:296:PRO:HD2	1:I:219:TRP:CE2	2.18	0.79
1:A:334:LEU:HG	1:A:451:VAL:HG23	1.64	0.79
1:D:378:GLN:HE22	1:E:341:LEU:HD12	1.47	0.79
1:G:176:THR:HG23	1:H:205:ILE:HB	1.65	0.78
1:C:378:GLN:HE21	1:D:341:LEU:HD12	1.48	0.78
1:D:406:VAL:HG12	1:D:450:VAL:HG13	1.64	0.78
1:D:199:LEU:HD11	1:D:206:LEU:HD22	1.64	0.78
1:G:202:SER:OG	1:L:177:ILE:HD11	1.84	0.78
1:I:354:TYR:HB3	1:J:332:ARG:HD2	1.64	0.78
1:K:376:GLN:O	1:L:384:GLY:HA3	1.84	0.78
1:B:362:TRP:O	1:B:373:VAL:HG23	1.84	0.76
1:B:354:TYR:CD1	1:C:332:ARG:HG3	2.21	0.76
1:I:192:VAL:HG21	1:I:288:MET:HG2	1.68	0.76
1:G:374:LYS:HA	1:H:383:TYR:CE1	2.19	0.76
1:H:250:ALA:HA	1:H:279:HIS:HE1	1.51	0.76
1:J:192:VAL:HG21	1:J:288:MET:HG2	1.68	0.76
1:C:183:ILE:CG2	1:D:208:MET:CE	2.64	0.76
1:G:375:LEU:HD23	1:H:368:VAL:HG12	1.67	0.76
1:H:225:TYR:HA	1:H:230:THR:OG1	1.84	0.76
1:L:302:LEU:HB3	1:L:444:ARG:HH21	1.50	0.76
1:D:308:ALA:HB1	1:D:451:VAL:HG12	1.68	0.75
1:C:192:VAL:HG23	1:C:284:GLU:HG3	1.68	0.75
1:E:271:LEU:CD2	1:H:167:VAL:HB	2.16	0.75
1:H:296:PRO:HD2	1:I:219:TRP:CD2	2.21	0.75
1:A:373:VAL:HG12	1:B:383:TYR:CD1	2.20	0.75
1:G:175:GLU:O	1:H:203:SER:HB3	1.86	0.75
1:J:324:ALA:HB1	1:J:382:ILE:HD12	1.66	0.75
1:G:334:LEU:HG	1:G:451:VAL:HG21	1.68	0.75
1:G:239:LEU:HD11	1:L:270:LEU:HG	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:PHE:HZ	1:B:450:VAL:HG22	1.51	0.74
1:A:205:ILE:HD11	1:F:172:GLU:OE1	1.86	0.74
1:B:248:LYS:HB3	1:C:220:VAL:HG23	1.68	0.74
1:C:253:SER:HB3	1:C:271:LEU:HD13	1.69	0.74
1:J:311:VAL:HA	1:J:454:THR:HG23	1.67	0.74
1:J:362:TRP:NE1	1:J:368:VAL:HG11	2.02	0.74
1:E:374:LYS:HA	1:F:383:TYR:CD1	2.23	0.74
1:G:374:LYS:NZ	1:H:361:GLU:HB3	2.02	0.74
1:I:364:ASP:O	1:I:372:SER:HB2	1.88	0.74
1:C:354:TYR:HB2	1:D:332:ARG:HD2	1.69	0.74
1:F:205:ILE:HA	1:F:244:PHE:O	1.87	0.74
1:J:373:VAL:CG1	1:K:383:TYR:CD1	2.71	0.74
1:J:378:GLN:HE22	1:K:341:LEU:HD12	1.53	0.74
1:K:435:TYR:HD1	1:L:231:THR:HG21	1.53	0.73
1:H:373:VAL:HG12	1:I:383:TYR:CD1	2.23	0.73
1:K:373:VAL:HG12	1:L:383:TYR:HD1	1.52	0.73
1:L:205:ILE:HA	1:L:244:PHE:O	1.88	0.73
1:C:354:TYR:HB3	1:D:332:ARG:HD2	1.59	0.73
1:G:336:ARG:HH22	1:L:188:LYS:HD3	1.54	0.73
1:B:161:VAL:N	1:B:164:SER:HG	1.86	0.72
1:K:299:LEU:HD13	1:K:406:VAL:HG11	1.71	0.72
1:G:248:LYS:HB2	1:G:439:ARG:HD3	1.71	0.72
1:B:354:TYR:CB	1:C:332:ARG:HD2	2.16	0.72
1:H:296:PRO:HG2	1:I:219:TRP:CH2	2.25	0.72
1:B:188:LYS:HD3	1:C:336:ARG:HH12	1.55	0.71
1:E:357:LEU:HD23	1:E:379:VAL:HG23	1.73	0.71
1:K:188:LYS:HD3	1:L:336:ARG:HH12	1.54	0.71
1:B:366:ALA:HB2	1:C:366:ALA:HB1	1.72	0.71
1:F:206:LEU:HB3	1:F:244:PHE:HB2	1.72	0.71
1:G:235:VAL:HG23	1:L:252:LYS:O	1.89	0.71
1:J:357:LEU:HD23	1:J:379:VAL:HG23	1.72	0.71
1:C:374:LYS:NZ	1:D:361:GLU:HB3	2.05	0.71
1:E:252:LYS:HG2	1:E:435:TYR:CD1	2.25	0.71
1:I:357:LEU:HD23	1:I:379:VAL:HG23	1.73	0.71
1:E:190:LEU:HG	1:E:284:GLU:OE1	1.91	0.71
1:H:357:LEU:HD23	1:H:379:VAL:HG23	1.73	0.71
1:J:369:GLY:C	1:J:371:ASP:H	1.94	0.71
1:K:376:GLN:O	1:L:384:GLY:HA2	1.89	0.71
1:L:357:LEU:HD23	1:L:379:VAL:HG23	1.73	0.71
1:A:183:ILE:CG2	1:B:208:MET:HE2	2.20	0.70
1:H:227:THR:HG22	1:H:228:ASP:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:LEU:HD22	1:H:167:VAL:HG13	1.71	0.70
1:A:357:LEU:HD23	1:A:379:VAL:HG23	1.73	0.70
1:D:357:LEU:HD23	1:D:379:VAL:HG23	1.73	0.70
1:A:383:TYR:CD1	1:F:373:VAL:HG12	2.26	0.69
1:C:354:TYR:CE2	1:D:332:ARG:HA	2.27	0.69
1:J:363:GLN:CD	1:K:383:TYR:OH	2.29	0.69
1:G:250:ALA:HA	1:G:279:HIS:HE1	1.54	0.69
1:D:374:LYS:HA	1:E:383:TYR:CD1	2.28	0.69
1:E:174:TYR:HB3	1:H:265:PHE:CE1	2.28	0.69
1:D:373:VAL:HG12	1:E:383:TYR:HD1	1.54	0.69
1:C:183:ILE:CG2	1:D:208:MET:HE2	2.22	0.69
1:C:378:GLN:NE2	1:D:341:LEU:CD1	2.56	0.69
1:G:357:LEU:HD23	1:G:379:VAL:HG23	1.73	0.69
1:A:183:ILE:HG23	1:B:208:MET:HE2	1.74	0.69
1:C:374:LYS:HZ1	1:D:361:GLU:HB3	1.57	0.69
1:F:253:SER:HB3	1:F:271:LEU:HD13	1.75	0.69
1:B:300:LEU:HD13	1:B:401:GLU:HG3	1.75	0.69
1:H:249:LEU:HD13	1:I:219:TRP:CE3	2.27	0.68
1:E:316:ALA:HA	1:E:396:LYS:CE	2.23	0.68
1:I:378:GLN:NE2	1:J:341:LEU:CB	2.51	0.68
1:H:249:LEU:HD22	1:I:219:TRP:CZ2	2.29	0.67
1:J:302:LEU:HB3	1:J:444:ARG:NH2	2.10	0.67
1:C:179:SER:C	1:C:181:ARG:H	1.98	0.67
1:C:192:VAL:HG21	1:C:288:MET:HG2	1.76	0.67
1:B:330:LEU:O	1:B:451:VAL:HG11	1.94	0.67
1:C:183:ILE:HG21	1:D:208:MET:CE	2.25	0.67
1:G:374:LYS:CA	1:H:383:TYR:CE1	2.77	0.67
1:F:435:TYR:CD1	1:H:428:GLY:HA2	2.30	0.67
1:K:199:LEU:HD11	1:K:206:LEU:HD22	1.77	0.66
1:J:199:LEU:HD11	1:J:206:LEU:HD22	1.77	0.66
1:E:359:ASP:C	1:E:361:GLU:N	2.43	0.66
1:E:264:ILE:HD11	1:H:174:TYR:C	2.16	0.66
1:I:327:ILE:HG21	1:I:346:LEU:HD21	1.76	0.66
1:I:373:VAL:HG12	1:J:383:TYR:HD1	1.61	0.66
1:F:414:PRO:HG2	1:F:443:GLN:HG3	1.75	0.66
1:A:183:ILE:CG2	1:B:208:MET:HE1	2.20	0.66
1:H:249:LEU:HD13	1:I:219:TRP:CG	2.30	0.66
1:I:201:MET:CE	1:I:245:SER:HA	2.25	0.66
1:G:446:PHE:CE1	1:L:183:ILE:HB	2.30	0.66
1:G:446:PHE:CE2	1:L:185:ASP:N	2.64	0.66
1:D:411:PHE:HZ	1:D:450:VAL:HG22	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:SER:O	1:F:208:MET:HA	1.95	0.66
1:B:373:VAL:HG12	1:C:383:TYR:CD1	2.31	0.66
1:G:374:LYS:CA	1:H:383:TYR:CD1	2.77	0.66
1:D:359:ASP:C	1:D:361:GLU:H	1.97	0.65
1:F:241:GLU:HG3	1:H:170:SER:CB	2.26	0.65
1:B:192:VAL:HG21	1:B:288:MET:HG2	1.78	0.65
1:F:309:LYS:HG2	1:F:454:THR:CG2	2.26	0.65
1:G:369:GLY:C	1:G:371:ASP:H	1.98	0.65
1:G:177:ILE:HG22	1:H:203:SER:CB	2.26	0.65
1:B:373:VAL:HG12	1:C:383:TYR:HD1	1.61	0.65
1:D:177:ILE:HG22	1:E:203:SER:HB3	1.78	0.65
1:G:374:LYS:HG2	1:H:383:TYR:CZ	2.31	0.65
1:A:226:GLY:O	1:H:431:ARG:NH2	2.30	0.65
1:D:274:ARG:HH21	1:E:212:PRO:HG2	1.61	0.65
1:E:192:VAL:HG21	1:E:288:MET:HG2	1.78	0.65
1:E:415:ARG:HH12	1:E:438:GLN:HG3	1.61	0.65
1:G:212:PRO:HG2	1:L:274:ARG:HH21	1.61	0.65
1:L:302:LEU:HB3	1:L:444:ARG:NH2	2.10	0.65
1:E:316:ALA:HA	1:E:396:LYS:HE3	1.78	0.65
1:F:309:LYS:HG2	1:F:454:THR:HG22	1.78	0.65
1:B:334:LEU:HG	1:B:451:VAL:HG23	1.79	0.65
1:L:215:GLY:HA3	1:L:235:VAL:HG13	1.78	0.65
1:I:374:LYS:HB3	1:J:362:TRP:CZ2	2.32	0.65
1:A:354:TYR:HB3	1:B:332:ARG:HD2	1.78	0.64
1:J:369:GLY:C	1:J:371:ASP:N	2.51	0.64
1:A:374:LYS:NZ	1:B:361:GLU:HB3	2.13	0.64
1:D:283:ILE:HD11	1:D:438:GLN:HE22	1.63	0.64
1:E:318:GLY:H	1:E:396:LYS:NZ	1.95	0.64
1:A:283:ILE:HD11	1:A:438:GLN:HE22	1.63	0.64
1:B:299:LEU:HD23	1:B:442:LEU:HD11	1.80	0.64
1:C:198:GLU:HG2	1:C:413:MET:HE2	1.80	0.64
1:G:331:ARG:HA	1:G:334:LEU:HD12	1.79	0.64
1:B:188:LYS:HB3	1:C:336:ARG:HH12	1.63	0.64
1:H:374:LYS:NZ	1:I:361:GLU:HB3	2.13	0.64
1:E:252:LYS:HG2	1:E:435:TYR:HD1	1.61	0.63
1:A:325:LYS:HA	1:A:383:TYR:HE2	1.64	0.63
1:A:366:ALA:HB1	1:F:366:ALA:HB2	1.79	0.63
1:D:325:LYS:HA	1:D:383:TYR:HE2	1.64	0.63
1:G:334:LEU:HG	1:G:451:VAL:CG2	2.27	0.63
1:H:364:ASP:HB2	1:H:367:GLN:HB2	1.79	0.63
1:K:336:ARG:C	1:K:338:GLY:H	2.01	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LYS:HD2	1:A:302:LEU:HD23	1.79	0.63
1:G:325:LYS:HA	1:G:383:TYR:HE2	1.64	0.63
1:G:446:PHE:HZ	1:L:184:ARG:N	1.96	0.63
1:H:406:VAL:HG12	1:H:450:VAL:HG13	1.79	0.63
1:L:180:GLN:HE21	1:L:265:PHE:HB3	1.64	0.63
1:I:182:ILE:HD11	1:J:239:LEU:HD23	1.79	0.63
1:B:192:VAL:HG23	1:B:284:GLU:HG3	1.78	0.63
1:H:283:ILE:HD11	1:H:438:GLN:HE22	1.63	0.63
1:A:302:LEU:HB3	1:A:444:ARG:HH21	1.64	0.63
1:E:267:LEU:HB3	1:H:167:VAL:HG11	1.81	0.63
1:G:302:LEU:HB3	1:G:444:ARG:HH21	1.64	0.63
1:G:383:TYR:CD1	1:L:373:VAL:HG12	2.30	0.63
1:B:301:THR:O	1:B:305:GLU:HG2	1.99	0.62
1:G:283:ILE:HD11	1:G:438:GLN:HE22	1.63	0.62
1:I:377:GLY:O	1:J:341:LEU:HD11	1.99	0.62
1:J:192:VAL:HG23	1:J:284:GLU:HG2	1.82	0.62
1:K:353:TYR:HD2	1:L:339:LEU:HD22	1.63	0.62
1:G:373:VAL:HG12	1:H:383:TYR:HD1	1.61	0.62
1:K:213:ASP:N	1:K:213:ASP:OD1	2.33	0.62
1:C:325:LYS:HA	1:C:383:TYR:HE2	1.64	0.62
1:J:324:ALA:CB	1:J:382:ILE:HD12	2.29	0.62
1:E:188:LYS:CD	1:F:336:ARG:HH12	2.12	0.62
1:L:272:ARG:HE	1:L:421:VAL:HG21	1.63	0.62
1:A:203:SER:HB3	1:F:177:ILE:HG12	1.82	0.62
1:E:271:LEU:HD21	1:H:166:SER:O	2.00	0.62
1:A:341:LEU:HB2	1:F:378:GLN:HE22	1.63	0.62
1:B:357:LEU:HD23	1:B:379:VAL:HG23	1.80	0.62
1:A:374:LYS:HZ1	1:B:361:GLU:HB3	1.65	0.61
1:B:327:ILE:HD12	1:B:356:LEU:HD11	1.81	0.61
1:D:270:LEU:HD21	1:E:211:GLU:OE2	2.00	0.61
1:G:369:GLY:C	1:G:371:ASP:N	2.53	0.61
1:C:183:ILE:HG23	1:D:208:MET:HE2	1.81	0.61
1:E:373:VAL:HG12	1:F:383:TYR:CD1	2.35	0.61
1:I:300:LEU:HD21	1:I:404:VAL:HG22	1.81	0.61
1:L:206:LEU:HB3	1:L:244:PHE:HB2	1.82	0.61
1:G:353:TYR:CD2	1:H:339:LEU:HD22	2.36	0.61
1:I:177:ILE:HG13	1:J:203:SER:HB3	1.82	0.61
1:A:374:LYS:HA	1:B:383:TYR:CE1	2.36	0.61
1:H:374:LYS:HB3	1:I:362:TRP:CH2	2.34	0.61
1:E:317:ASP:N	1:E:396:LYS:HE2	2.15	0.61
1:L:325:LYS:HA	1:L:383:TYR:HE2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:296:PRO:HG2	1:I:219:TRP:CZ2	2.36	0.61
1:A:192:VAL:HG21	1:A:288:MET:HG2	1.82	0.60
1:E:249:LEU:HD13	1:F:219:TRP:CD2	2.36	0.60
1:E:415:ARG:HG2	1:E:416:GLN:H	1.66	0.60
1:J:325:LYS:HG2	1:J:329:LYS:HE3	1.83	0.60
1:J:362:TRP:CZ2	1:J:382:ILE:HD13	2.36	0.60
1:H:374:LYS:CA	1:I:383:TYR:CD1	2.83	0.60
1:I:201:MET:HE3	1:I:245:SER:HA	1.84	0.60
1:A:446:PHE:HZ	1:F:184:ARG:C	2.04	0.60
1:F:435:TYR:CG	1:H:428:GLY:HA2	2.36	0.60
1:I:353:TYR:CD2	1:J:339:LEU:HD22	2.36	0.60
1:B:353:TYR:CD2	1:C:339:LEU:HD22	2.37	0.60
1:C:183:ILE:HG21	1:D:208:MET:HE1	1.84	0.60
1:E:271:LEU:HD21	1:H:167:VAL:HB	1.82	0.60
1:L:362:TRP:CE2	1:L:382:ILE:HD13	2.37	0.60
1:C:302:LEU:HB3	1:C:444:ARG:NH2	2.17	0.60
1:G:374:LYS:N	1:H:383:TYR:CE1	2.70	0.60
1:K:363:GLN:HB3	1:K:373:VAL:HB	1.84	0.60
1:L:188:LYS:HB3	1:L:392:TYR:HE1	1.65	0.60
1:D:444:ARG:HD3	1:D:447:ALA:HA	1.84	0.60
1:B:415:ARG:HH12	1:B:438:GLN:HE21	1.49	0.59
1:E:188:LYS:HG3	1:F:336:ARG:NH1	2.17	0.59
1:A:183:ILE:HG23	1:B:208:MET:CE	2.30	0.59
1:E:325:LYS:C	1:E:327:ILE:N	2.48	0.59
1:E:174:TYR:HB3	1:H:265:PHE:HE1	1.65	0.59
1:F:241:GLU:CG	1:H:170:SER:HB3	2.32	0.59
1:E:363:GLN:HE22	1:F:325:LYS:HD2	1.67	0.59
1:G:374:LYS:HB3	1:H:362:TRP:CH2	2.37	0.59
1:C:184:ARG:HD3	1:D:211:GLU:HB3	1.85	0.59
1:D:362:TRP:O	1:D:373:VAL:HG23	2.03	0.59
1:E:312:THR:HG21	1:E:402:PHE:HZ	1.66	0.59
1:G:375:LEU:HD23	1:H:368:VAL:CG1	2.32	0.59
1:F:275:LEU:O	1:F:278:ALA:HB3	2.03	0.59
1:A:210:VAL:HG22	1:F:183:ILE:HG13	1.85	0.59
1:K:177:ILE:CG2	1:L:203:SER:HB3	2.33	0.59
1:H:373:VAL:HG12	1:I:383:TYR:HD1	1.68	0.59
1:A:361:GLU:HB3	1:F:374:LYS:HZ1	1.68	0.59
1:B:209:LEU:HD23	1:B:241:GLU:HG2	1.83	0.58
1:C:354:TYR:CD1	1:D:332:ARG:HG3	2.33	0.58
1:F:248:LYS:HZ2	1:H:258:GLU:CD	2.06	0.58
1:G:252:LYS:O	1:H:234:GLU:HA	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:426:GLN:HB2	1:G:431:ARG:HG3	1.85	0.58
1:H:227:THR:CG2	1:H:228:ASP:N	2.66	0.58
1:H:250:ALA:HA	1:H:279:HIS:CE1	2.35	0.58
1:H:362:TRP:CZ2	1:H:382:ILE:HD13	2.38	0.58
1:K:191:VAL:HG21	1:K:390:SER:HB2	1.85	0.58
1:K:426:GLN:HB2	1:K:431:ARG:HG3	1.85	0.58
1:L:188:LYS:HD2	1:L:392:TYR:CE1	2.38	0.58
1:D:191:VAL:HG21	1:D:390:SER:HB2	1.85	0.58
1:F:364:ASP:HB2	1:F:367:GLN:HB2	1.84	0.58
1:K:364:ASP:H	1:K:372:SER:HB2	1.68	0.58
1:B:354:TYR:CB	1:C:332:ARG:CG	2.81	0.58
1:C:355:ASP:OD1	1:D:332:ARG:NH1	2.36	0.58
1:F:211:GLU:HG3	1:F:212:PRO:HD2	1.85	0.58
1:H:330:LEU:HB3	1:H:451:VAL:HG11	1.85	0.58
1:B:357:LEU:C	1:B:359:ASP:H	2.06	0.58
1:H:374:LYS:HA	1:I:383:TYR:CE1	2.36	0.58
1:I:309:LYS:HG2	1:I:454:THR:HG22	1.86	0.58
1:I:393:PHE:CZ	1:I:404:VAL:HG23	2.38	0.58
1:J:324:ALA:HB1	1:J:382:ILE:HG23	1.85	0.58
1:A:191:VAL:HG21	1:A:390:SER:HB2	1.85	0.58
1:D:297:LYS:HD2	1:D:302:LEU:HD23	1.85	0.58
1:G:446:PHE:CZ	1:L:184:ARG:C	2.77	0.58
1:K:282:SER:HB3	1:L:217:ALA:H	1.68	0.58
1:E:264:ILE:CD1	1:H:174:TYR:C	2.72	0.58
1:I:377:GLY:HA3	1:J:384:GLY:HA3	1.84	0.58
1:A:446:PHE:CZ	1:F:184:ARG:C	2.76	0.58
1:B:182:ILE:HA	1:C:209:LEU:O	2.04	0.58
1:G:191:VAL:HG21	1:G:390:SER:HB2	1.85	0.58
1:A:208:MET:HB2	1:A:242:ILE:HD11	1.86	0.58
1:D:359:ASP:C	1:D:361:GLU:N	2.56	0.58
1:H:426:GLN:HB2	1:H:431:ARG:HG3	1.85	0.58
1:I:286:ALA:HB1	1:I:296:PRO:HD2	1.85	0.58
1:L:215:GLY:HA3	1:L:235:VAL:CG1	2.34	0.58
1:L:426:GLN:HB2	1:L:431:ARG:HG3	1.85	0.58
1:D:426:GLN:HB2	1:D:431:ARG:HG3	1.85	0.58
1:F:208:MET:HB2	1:F:242:ILE:HD11	1.86	0.58
1:G:341:LEU:CD1	1:L:378:GLN:HE21	2.05	0.58
1:B:311:VAL:HA	1:B:454:THR:HG23	1.86	0.58
1:C:255:ILE:HD11	1:C:260:GLU:HB2	1.85	0.58
1:K:362:TRP:CD1	1:K:368:VAL:HG21	2.39	0.58
1:G:297:LYS:HD2	1:G:302:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:252:LYS:HE2	1:K:232:GLY:O	2.04	0.57
1:E:400:ALA:O	1:E:454:THR:HB	2.04	0.57
1:H:249:LEU:CD1	1:I:219:TRP:CD2	2.80	0.57
1:H:286:ALA:CB	1:I:219:TRP:HE1	2.17	0.57
1:L:246:THR:HA	1:L:441:ASN:HB2	1.84	0.57
1:K:364:ASP:O	1:K:366:ALA:N	2.37	0.57
1:C:426:GLN:HB2	1:C:431:ARG:HG3	1.85	0.57
1:H:201:MET:HG3	1:H:206:LEU:HB2	1.86	0.57
1:H:220:VAL:HB	1:H:224:THR:HG21	1.86	0.57
1:I:426:GLN:HB2	1:I:431:ARG:HG3	1.85	0.57
1:K:362:TRP:CZ2	1:K:382:ILE:HD13	2.39	0.57
1:C:199:LEU:HB3	1:C:414:PRO:HA	1.87	0.57
1:D:175:GLU:HB3	1:E:204:LYS:HE2	1.86	0.57
1:H:242:ILE:CD1	1:H:244:PHE:CZ	2.87	0.57
1:F:191:VAL:HG23	1:F:192:VAL:N	2.19	0.57
1:I:362:TRP:CZ2	1:I:382:ILE:HD13	2.40	0.57
1:F:207:THR:HA	1:F:242:ILE:O	2.05	0.57
1:J:426:GLN:HB2	1:J:431:ARG:HG3	1.85	0.57
1:A:334:LEU:HG	1:A:451:VAL:CG2	2.32	0.57
1:C:191:VAL:HG21	1:C:390:SER:HB2	1.85	0.57
1:C:192:VAL:CG2	1:C:284:GLU:HG3	2.33	0.57
1:G:218:THR:O	1:L:249:LEU:HA	2.05	0.57
1:H:199:LEU:HD11	1:H:206:LEU:HD22	1.87	0.57
1:C:252:LYS:O	1:D:234:GLU:HA	2.04	0.57
1:F:210:VAL:HG23	1:F:242:ILE:HG12	1.87	0.57
1:I:267:LEU:HD21	1:J:239:LEU:HD11	1.87	0.57
1:K:374:LYS:HA	1:L:383:TYR:CE1	2.39	0.57
1:A:426:GLN:HB2	1:A:431:ARG:HG3	1.85	0.56
1:B:300:LEU:HD23	1:B:404:VAL:HG11	1.87	0.56
1:F:400:ALA:O	1:F:454:THR:HB	2.06	0.56
1:I:188:LYS:HB3	1:J:336:ARG:HH12	1.69	0.56
1:J:252:LYS:O	1:K:234:GLU:HA	2.05	0.56
1:K:274:ARG:NH2	1:L:212:PRO:HG2	2.21	0.56
1:E:212:PRO:HD3	1:E:239:LEU:HA	1.88	0.56
1:J:363:GLN:NE2	1:K:383:TYR:OH	2.38	0.56
1:K:363:GLN:HB2	1:K:374:LYS:HG3	1.88	0.56
1:A:188:LYS:HD2	1:A:392:TYR:CE1	2.40	0.56
1:H:374:LYS:HG2	1:I:383:TYR:CZ	2.40	0.56
1:I:309:LYS:HG2	1:I:454:THR:CG2	2.35	0.56
1:E:333:LYS:HB2	1:E:451:VAL:HG21	1.88	0.56
1:G:188:LYS:HD2	1:G:392:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:327:ILE:CG2	1:J:346:LEU:HD21	2.32	0.56
1:J:362:TRP:CD1	1:J:368:VAL:HG11	2.40	0.56
1:B:354:TYR:HB3	1:C:332:ARG:CG	2.36	0.56
1:C:188:LYS:HD2	1:C:392:TYR:CE1	2.40	0.56
1:E:317:ASP:H	1:E:396:LYS:HE2	1.70	0.56
1:B:415:ARG:HH11	1:B:418:ALA:HA	1.71	0.55
1:I:176:THR:HB	1:J:205:ILE:HB	1.88	0.55
1:B:299:LEU:CD2	1:B:442:LEU:HD11	2.35	0.55
1:F:324:ALA:HB1	1:F:382:ILE:HD12	1.87	0.55
1:K:188:LYS:HD3	1:L:336:ARG:NH1	2.20	0.55
1:A:239:LEU:HD11	1:F:270:LEU:HG	1.89	0.55
1:C:373:VAL:HG12	1:D:383:TYR:CD1	2.42	0.55
1:F:250:ALA:HB2	1:F:437:THR:HG22	1.88	0.55
1:H:161:VAL:O	1:H:162:ASN:C	2.43	0.55
1:K:362:TRP:CG	1:K:368:VAL:HG21	2.41	0.55
1:I:334:LEU:HG	1:I:451:VAL:HG23	1.88	0.55
1:J:310:VAL:HG22	1:J:333:LYS:HG3	1.87	0.55
1:B:374:LYS:HE2	1:C:361:GLU:HB3	1.88	0.55
1:C:177:ILE:HG22	1:D:203:SER:HB3	1.88	0.55
1:G:373:VAL:C	1:H:383:TYR:CD1	2.80	0.55
1:K:369:GLY:C	1:K:371:ASP:H	2.08	0.55
1:A:250:ALA:HA	1:A:279:HIS:HE1	1.71	0.55
1:C:179:SER:O	1:D:208:MET:HA	2.07	0.55
1:A:361:GLU:HB3	1:F:374:LYS:NZ	2.22	0.55
1:B:308:ALA:HB1	1:B:451:VAL:HA	1.88	0.55
1:E:190:LEU:HG	1:E:284:GLU:CD	2.26	0.55
1:G:246:THR:HG21	1:G:415:ARG:O	2.06	0.55
1:H:182:ILE:HA	1:I:209:LEU:O	2.07	0.55
1:E:188:LYS:HD2	1:F:336:ARG:HH12	1.72	0.55
1:E:373:VAL:HG12	1:F:383:TYR:HD1	1.72	0.55
1:J:248:LYS:HB2	1:J:439:ARG:HD3	1.89	0.55
1:L:227:THR:HG23	1:L:229:THR:H	1.71	0.55
1:B:252:LYS:O	1:C:234:GLU:HA	2.07	0.54
1:D:253:SER:HB3	1:D:271:LEU:HD13	1.89	0.54
1:E:178:PHE:HA	1:F:207:THR:HG23	1.88	0.54
1:I:199:LEU:HD21	1:I:206:LEU:HD22	1.88	0.54
1:A:184:ARG:HD3	1:B:211:GLU:HB3	1.87	0.54
1:J:374:LYS:NZ	1:K:361:GLU:HB3	2.22	0.54
1:A:374:LYS:HG2	1:B:383:TYR:CZ	2.42	0.54
1:B:289:THR:HG21	1:B:394:PRO:HG3	1.90	0.54
1:F:422:GLU:CD	1:H:430:GLN:HE21	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:374:LYS:HB3	1:K:362:TRP:CZ2	2.42	0.54
1:L:224:THR:HB	1:L:227:THR:CG2	2.37	0.54
1:A:374:LYS:CA	1:B:383:TYR:CD1	2.87	0.54
1:I:172:GLU:O	1:I:176:THR:HG22	2.08	0.54
1:A:225:TYR:CE2	1:H:258:GLU:HB2	2.42	0.54
1:A:253:SER:HB3	1:A:271:LEU:HD13	1.89	0.54
1:E:256:THR:HA	1:E:431:ARG:HA	1.90	0.54
1:H:376:GLN:O	1:I:384:GLY:HA3	2.07	0.54
1:I:297:LYS:HD2	1:I:302:LEU:HD23	1.90	0.54
1:A:183:ILE:HD11	1:B:242:ILE:HG12	1.90	0.54
1:E:324:ALA:HB1	1:E:382:ILE:HD12	1.89	0.54
1:J:329:LYS:O	1:J:332:ARG:HG3	2.07	0.54
1:K:227:THR:C	1:K:229:THR:H	2.11	0.54
1:L:300:LEU:HD13	1:L:401:GLU:HG3	1.88	0.54
1:B:188:LYS:HB3	1:C:336:ARG:NH1	2.22	0.54
1:E:190:LEU:HA	1:E:284:GLU:OE2	2.07	0.54
1:E:316:ALA:HA	1:E:396:LYS:HE2	1.90	0.54
1:F:324:ALA:CB	1:F:382:ILE:HD12	2.38	0.54
1:H:242:ILE:HD12	1:H:244:PHE:CE2	2.42	0.54
1:C:182:ILE:HA	1:D:209:LEU:O	2.08	0.54
1:C:211:GLU:HG3	1:C:212:PRO:HD2	1.89	0.54
1:J:290:GLY:HA3	1:J:296:PRO:O	2.08	0.54
1:F:192:VAL:HG23	1:F:284:GLU:HG2	1.90	0.54
1:F:426:GLN:HB2	1:F:431:ARG:HG3	1.90	0.53
1:L:275:LEU:O	1:L:278:ALA:HB3	2.08	0.53
1:E:429:LYS:C	1:E:431:ARG:H	2.11	0.53
1:B:191:VAL:HG21	1:B:390:SER:HB2	1.89	0.53
1:B:426:GLN:NE2	1:B:431:ARG:HD2	2.23	0.53
1:D:211:GLU:HG2	1:D:212:PRO:HD2	1.91	0.53
1:D:364:ASP:HB2	1:D:367:GLN:HB2	1.90	0.53
1:E:413:MET:HE3	1:E:440:VAL:HG21	1.89	0.53
1:F:215:GLY:HA3	1:F:235:VAL:HG13	1.90	0.53
1:H:357:LEU:CD2	1:H:379:VAL:HG23	2.38	0.53
1:L:224:THR:HB	1:L:227:THR:HG21	1.91	0.53
1:A:374:LYS:HB3	1:B:362:TRP:CZ2	2.44	0.53
1:C:297:LYS:HD2	1:C:302:LEU:HD23	1.90	0.53
1:D:374:LYS:NZ	1:E:361:GLU:HB3	2.24	0.53
1:F:415:ARG:O	1:F:416:GLN:HB2	2.09	0.53
1:G:177:ILE:CG2	1:H:203:SER:HB2	2.31	0.53
1:A:303:ALA:HB2	1:A:450:VAL:HB	1.91	0.53
1:A:341:LEU:CD1	1:F:378:GLN:HE21	2.03	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LYS:HD3	1:C:336:ARG:NH1	2.22	0.53
1:L:203:SER:HA	1:L:416:GLN:NE2	2.24	0.53
1:C:355:ASP:HA	1:C:358:GLU:HB2	1.91	0.53
1:G:373:VAL:C	1:H:383:TYR:HD1	2.12	0.53
1:K:316:ALA:HA	1:K:396:LYS:HE2	1.91	0.53
1:C:415:ARG:HG2	1:C:416:GLN:H	1.74	0.53
1:E:357:LEU:CD2	1:E:379:VAL:HG23	2.38	0.53
1:G:415:ARG:O	1:G:416:GLN:HB2	2.09	0.53
1:L:357:LEU:CD2	1:L:379:VAL:HG23	2.38	0.53
1:E:318:GLY:H	1:E:396:LYS:HZ3	1.55	0.53
1:G:248:LYS:HB3	1:H:220:VAL:HG22	1.91	0.53
1:H:284:GLU:OE2	1:H:392:TYR:HB2	2.08	0.53
1:I:415:ARG:HG2	1:I:416:GLN:H	1.74	0.53
1:E:173:SER:HB2	1:H:178:PHE:CE2	2.44	0.53
1:E:188:LYS:HG3	1:F:336:ARG:HH12	1.73	0.53
1:E:374:LYS:NZ	1:F:361:GLU:HB3	2.24	0.53
1:I:415:ARG:O	1:I:416:GLN:HB2	2.09	0.53
1:G:357:LEU:C	1:G:359:ASP:H	2.11	0.53
1:G:415:ARG:HG2	1:G:416:GLN:H	1.74	0.53
1:J:302:LEU:HD22	1:J:444:ARG:HE	1.74	0.53
1:D:296:PRO:HD2	1:E:219:TRP:CE2	2.44	0.52
1:D:357:LEU:CD2	1:D:379:VAL:HG23	2.38	0.52
1:E:415:ARG:HH11	1:E:418:ALA:HA	1.73	0.52
1:G:209:LEU:HD23	1:G:241:GLU:HG2	1.90	0.52
1:H:415:ARG:HG2	1:H:416:GLN:H	1.74	0.52
1:J:415:ARG:O	1:J:416:GLN:HB2	2.09	0.52
1:K:176:THR:HG23	1:L:205:ILE:HD12	1.90	0.52
1:E:334:LEU:HG	1:E:451:VAL:HG12	1.92	0.52
1:G:325:LYS:HA	1:G:383:TYR:CE2	2.45	0.52
1:K:251:ALA:HB1	1:K:275:LEU:HD22	1.91	0.52
1:K:374:LYS:HA	1:L:383:TYR:CD1	2.44	0.52
1:E:302:LEU:HB3	1:E:444:ARG:HH21	1.75	0.52
1:F:415:ARG:HG2	1:F:416:GLN:H	1.74	0.52
1:F:433:ALA:HB1	1:F:435:TYR:CE1	2.45	0.52
1:G:303:ALA:HB2	1:G:450:VAL:HB	1.91	0.52
1:I:357:LEU:CD2	1:I:379:VAL:HG23	2.38	0.52
1:J:172:GLU:C	1:J:174:TYR:H	2.11	0.52
1:L:302:LEU:HD22	1:L:444:ARG:HE	1.73	0.52
1:G:215:GLY:O	1:L:278:ALA:HA	2.09	0.52
1:H:242:ILE:HD13	1:H:244:PHE:CZ	2.44	0.52
1:K:415:ARG:O	1:K:416:GLN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ARG:HG2	1:A:416:GLN:H	1.74	0.52
1:E:325:LYS:C	1:E:327:ILE:H	2.12	0.52
1:A:415:ARG:O	1:A:416:GLN:HB2	2.09	0.52
1:C:277:GLU:OE1	1:D:214:ALA:HB2	2.10	0.52
1:E:255:ILE:HD11	1:E:260:GLU:HB2	1.90	0.52
1:G:362:TRP:CZ2	1:G:382:ILE:HD13	2.45	0.52
1:I:190:LEU:HB3	1:I:284:GLU:CD	2.30	0.52
1:B:337:HIS:HD2	1:B:407:TYR:HD2	1.56	0.52
1:L:243:HIS:ND1	1:L:243:HIS:N	2.57	0.52
1:A:288:MET:HE1	1:A:393:PHE:HE1	1.75	0.52
1:A:362:TRP:CZ2	1:F:374:LYS:HB3	2.45	0.52
1:A:373:VAL:HG12	1:B:383:TYR:HD1	1.70	0.52
1:B:429:LYS:HB2	1:B:431:ARG:HG2	1.92	0.52
1:E:362:TRP:CZ2	1:E:382:ILE:HD13	2.45	0.52
1:E:415:ARG:O	1:E:416:GLN:HB2	2.10	0.52
1:G:330:LEU:O	1:G:332:ARG:N	2.43	0.52
1:A:357:LEU:CD2	1:A:379:VAL:HG23	2.38	0.52
1:C:288:MET:HE1	1:C:393:PHE:HE1	1.74	0.52
1:G:341:LEU:HD13	1:L:378:GLN:NE2	2.24	0.52
1:G:357:LEU:CD2	1:G:379:VAL:HG23	2.38	0.52
1:J:357:LEU:CD2	1:J:379:VAL:HG23	2.38	0.52
1:J:415:ARG:HG2	1:J:416:GLN:H	1.74	0.52
1:L:204:LYS:O	1:L:245:SER:HA	2.10	0.52
1:A:212:PRO:HG2	1:F:274:ARG:NH2	2.25	0.52
1:C:415:ARG:O	1:C:416:GLN:HB2	2.09	0.52
1:E:264:ILE:HD11	1:H:175:GLU:N	2.25	0.52
1:H:296:PRO:CD	1:I:219:TRP:CD2	2.91	0.52
1:K:435:TYR:CD1	1:L:231:THR:HG21	2.40	0.52
1:L:415:ARG:HG2	1:L:416:GLN:H	1.74	0.52
1:A:251:ALA:HB1	1:B:235:VAL:HG23	1.92	0.51
1:B:426:GLN:HE21	1:B:431:ARG:HD2	1.74	0.51
1:E:444:ARG:HD3	1:E:447:ALA:HA	1.91	0.51
1:J:374:LYS:HZ1	1:K:361:GLU:HB3	1.73	0.51
1:L:415:ARG:O	1:L:416:GLN:HB2	2.09	0.51
1:A:274:ARG:NH2	1:B:212:PRO:HG2	2.26	0.51
1:D:248:LYS:HG3	1:D:439:ARG:HG2	1.93	0.51
1:I:201:MET:HE1	1:I:245:SER:HA	1.92	0.51
1:K:248:LYS:HG3	1:K:439:ARG:HG2	1.93	0.51
1:A:203:SER:OG	1:F:175:GLU:O	2.27	0.51
1:B:207:THR:HG22	1:B:243:HIS:CD2	2.45	0.51
1:C:272:ARG:HE	1:C:421:VAL:HG11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ARG:O	1:D:416:GLN:HB2	2.09	0.51
1:E:188:LYS:CG	1:F:336:ARG:HH12	2.24	0.51
1:H:227:THR:CG2	1:H:228:ASP:H	2.23	0.51
1:J:175:GLU:C	1:K:203:SER:HB3	2.29	0.51
1:E:354:TYR:CG	1:F:332:ARG:HG2	2.45	0.51
1:H:309:LYS:HG2	1:H:454:THR:HG21	1.93	0.51
1:K:324:ALA:HB1	1:K:382:ILE:HD12	1.91	0.51
1:A:270:LEU:HG	1:B:239:LEU:HD11	1.93	0.51
1:E:227:THR:O	1:E:230:THR:HG22	2.10	0.51
1:H:415:ARG:O	1:H:416:GLN:HB2	2.09	0.51
1:H:358:GLU:OE2	1:I:332:ARG:HD2	2.10	0.51
1:I:350:MET:HG3	1:J:339:LEU:HD11	1.91	0.51
1:L:325:LYS:HA	1:L:383:TYR:CE2	2.45	0.51
1:A:325:LYS:HA	1:A:383:TYR:CE2	2.45	0.51
1:D:378:GLN:HE22	1:E:341:LEU:CD1	2.14	0.51
1:E:271:LEU:HD23	1:H:167:VAL:HB	1.91	0.51
1:G:249:LEU:HG	1:G:279:HIS:ND1	2.26	0.51
1:H:169:VAL:HG23	1:H:170:SER:H	1.76	0.51
1:B:255:ILE:HG12	1:B:260:GLU:HG3	1.93	0.51
1:B:343:LYS:HB3	1:B:407:TYR:CE1	2.46	0.51
1:C:325:LYS:HA	1:C:383:TYR:CE2	2.45	0.51
1:C:357:LEU:HD23	1:C:379:VAL:HG23	1.93	0.51
1:E:190:LEU:HD23	1:E:284:GLU:HG3	1.92	0.51
1:I:325:LYS:HG2	1:I:329:LYS:HE3	1.93	0.51
1:E:224:THR:O	1:E:230:THR:CB	2.59	0.50
1:E:401:GLU:HA	1:E:453:GLY:O	2.11	0.50
1:F:364:ASP:HB2	1:F:367:GLN:OE1	2.11	0.50
1:F:399:SER:O	1:F:455:TYR:HB2	2.11	0.50
1:H:242:ILE:CD1	1:H:244:PHE:CE2	2.93	0.50
1:J:176:THR:HB	1:K:205:ILE:HB	1.93	0.50
1:B:252:LYS:HG2	1:B:435:TYR:CD2	2.46	0.50
1:C:179:SER:C	1:C:181:ARG:N	2.62	0.50
1:I:302:LEU:HB3	1:I:444:ARG:NH2	2.26	0.50
1:A:446:PHE:CE2	1:F:185:ASP:N	2.80	0.50
1:C:177:ILE:CG2	1:D:206:LEU:HD12	2.40	0.50
1:D:415:ARG:HG2	1:D:416:GLN:H	1.74	0.50
1:E:165:SER:HB2	1:H:259:THR:HG21	1.93	0.50
1:G:250:ALA:HA	1:G:279:HIS:CE1	2.42	0.50
1:I:302:LEU:HB3	1:I:444:ARG:HH21	1.76	0.50
1:E:204:LYS:HA	1:E:416:GLN:HE22	1.76	0.50
1:A:341:LEU:CB	1:F:378:GLN:HE22	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:373:VAL:O	1:H:383:TYR:HD1	1.94	0.50
1:I:378:GLN:NE2	1:J:341:LEU:HD13	2.26	0.50
1:K:415:ARG:HG2	1:K:416:GLN:H	1.74	0.50
1:A:211:GLU:HG3	1:F:270:LEU:HD11	1.94	0.50
1:B:185:ASP:O	1:B:187:GLN:N	2.44	0.50
1:C:183:ILE:HG23	1:D:208:MET:CE	2.40	0.50
1:E:316:ALA:CA	1:E:396:LYS:HE2	2.42	0.50
1:H:163:GLN:O	1:H:164:SER:C	2.47	0.50
1:H:374:LYS:HZ1	1:I:361:GLU:HB3	1.76	0.50
1:L:253:SER:HB3	1:L:271:LEU:HD13	1.93	0.50
1:B:421:VAL:HG13	1:B:436:VAL:HG22	1.92	0.50
1:E:354:TYR:CZ	1:F:332:ARG:HA	2.47	0.50
1:A:227:THR:HG22	1:A:228:ASP:H	1.77	0.50
1:E:191:VAL:HG21	1:E:390:SER:HB2	1.94	0.50
1:E:312:THR:HG21	1:E:402:PHE:CZ	2.46	0.50
1:F:248:LYS:NZ	1:H:258:GLU:CD	2.65	0.50
1:F:248:LYS:NZ	1:H:258:GLU:OE2	2.44	0.50
1:F:325:LYS:HA	1:F:383:TYR:HE2	1.76	0.50
1:B:354:TYR:CZ	1:C:332:ARG:HA	2.47	0.50
1:F:324:ALA:HB1	1:F:382:ILE:HG23	1.93	0.50
1:K:369:GLY:C	1:K:371:ASP:N	2.65	0.50
1:D:325:LYS:HA	1:D:383:TYR:CE2	2.45	0.49
1:I:201:MET:HE1	1:I:245:SER:CA	2.42	0.49
1:J:404:VAL:O	1:J:405:ILE:C	2.48	0.49
1:E:178:PHE:CE2	1:H:173:SER:HB2	2.47	0.49
1:G:357:LEU:C	1:G:359:ASP:N	2.66	0.49
1:A:183:ILE:CG1	1:B:210:VAL:HG22	2.42	0.49
1:B:208:MET:HB2	1:B:242:ILE:HD11	1.93	0.49
1:G:211:GLU:HG3	1:L:270:LEU:HD11	1.94	0.49
1:H:169:VAL:HG23	1:H:170:SER:N	2.27	0.49
1:K:249:LEU:N	1:K:438:GLN:O	2.45	0.49
1:B:183:ILE:HG13	1:C:210:VAL:HG22	1.95	0.49
1:B:253:SER:HB2	1:B:275:LEU:HD21	1.93	0.49
1:E:353:TYR:CD2	1:F:339:LEU:HD22	2.47	0.49
1:F:415:ARG:NH2	1:F:440:VAL:HG11	2.28	0.49
1:G:203:SER:HB3	1:L:177:ILE:HG13	1.94	0.49
1:H:183:ILE:HD11	1:I:242:ILE:HD11	1.95	0.49
1:H:249:LEU:CD1	1:I:219:TRP:CG	2.95	0.49
1:K:290:GLY:HA3	1:K:296:PRO:O	2.13	0.49
1:A:362:TRP:CZ2	1:A:382:ILE:HD13	2.47	0.49
1:C:176:THR:HA	1:D:205:ILE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:TYR:HB3	1:D:332:ARG:HD3	1.85	0.49
1:G:249:LEU:CD1	1:G:282:SER:OG	2.58	0.49
1:I:347:ILE:O	1:I:403:ALA:HA	2.13	0.49
1:J:302:LEU:HB3	1:J:444:ARG:HH21	1.76	0.49
1:A:287:PHE:CE2	1:A:442:LEU:HG	2.48	0.49
1:B:412:VAL:O	1:B:414:PRO:HD3	2.13	0.49
1:G:217:ALA:HB1	1:L:250:ALA:C	2.33	0.49
1:J:444:ARG:HH22	1:J:450:VAL:CG1	2.26	0.49
1:A:312:THR:HG21	1:A:402:PHE:HZ	1.78	0.49
1:B:190:LEU:HB3	1:B:284:GLU:CD	2.33	0.49
1:D:354:TYR:HB3	1:E:332:ARG:HD2	1.95	0.49
1:D:374:LYS:HB3	1:E:362:TRP:CH2	2.48	0.49
1:G:287:PHE:CE2	1:G:442:LEU:HG	2.48	0.49
1:I:393:PHE:HZ	1:I:404:VAL:HG23	1.78	0.49
1:L:300:LEU:HD23	1:L:404:VAL:HG13	1.94	0.49
1:C:183:ILE:CG2	1:D:208:MET:HE1	2.38	0.49
1:G:227:THR:HG22	1:G:228:ASP:H	1.77	0.49
1:H:253:SER:HB3	1:H:271:LEU:HD11	1.94	0.49
1:K:188:LYS:HB2	1:K:392:TYR:HE1	1.77	0.49
1:L:288:MET:HE3	1:L:393:PHE:HE1	1.78	0.49
1:E:324:ALA:CB	1:E:382:ILE:HD12	2.42	0.49
1:B:172:GLU:O	1:B:176:THR:HG22	2.12	0.48
1:G:192:VAL:HG23	1:G:284:GLU:HG2	1.95	0.48
1:B:357:LEU:C	1:B:359:ASP:N	2.64	0.48
1:D:287:PHE:CE2	1:D:442:LEU:HG	2.48	0.48
1:E:415:ARG:NH1	1:E:418:ALA:HA	2.28	0.48
1:G:446:PHE:CZ	1:L:183:ILE:HB	2.48	0.48
1:D:161:VAL:HG12	1:E:204:LYS:NZ	2.27	0.48
1:D:192:VAL:HG23	1:D:284:GLU:HG2	1.96	0.48
1:F:206:LEU:N	1:F:244:PHE:O	2.45	0.48
1:F:250:ALA:CB	1:F:437:THR:HG22	2.42	0.48
1:H:208:MET:HG3	1:H:242:ILE:CD1	2.44	0.48
1:I:249:LEU:HD22	1:J:217:ALA:HB3	1.95	0.48
1:I:347:ILE:HG22	1:I:393:PHE:HE1	1.78	0.48
1:A:268:LEU:HB3	1:A:269:PRO:HD3	1.96	0.48
1:B:338:GLY:HA2	1:B:344:LEU:HD11	1.95	0.48
1:C:373:VAL:HG12	1:D:383:TYR:HD1	1.78	0.48
1:F:418:ALA:O	1:F:419:VAL:C	2.52	0.48
1:G:341:LEU:HB2	1:L:378:GLN:HE22	1.78	0.48
1:H:188:LYS:HG3	1:I:336:ARG:HD3	1.96	0.48
1:C:354:TYR:CD2	1:D:332:ARG:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:LYS:HG2	1:E:392:TYR:CE1	2.49	0.48
1:E:249:LEU:HD13	1:F:219:TRP:CE2	2.48	0.48
1:G:312:THR:HG21	1:G:402:PHE:HZ	1.78	0.48
1:K:199:LEU:CD1	1:K:206:LEU:HD13	2.43	0.48
1:B:300:LEU:CD1	1:B:394:PRO:HD3	2.43	0.48
1:E:167:VAL:O	1:H:267:LEU:HG	2.14	0.48
1:J:312:THR:HG21	1:J:402:PHE:HZ	1.78	0.48
1:K:324:ALA:CB	1:K:382:ILE:HD12	2.43	0.48
1:L:306:ASP:OD2	1:L:444:ARG:NH2	2.47	0.48
1:L:324:ALA:HB1	1:L:382:ILE:HD12	1.96	0.48
1:A:248:LYS:O	1:B:219:TRP:HA	2.13	0.48
1:B:190:LEU:HB3	1:B:284:GLU:OE1	2.13	0.48
1:F:433:ALA:HB1	1:F:435:TYR:HE1	1.79	0.48
1:H:277:GLU:OE1	1:I:214:ALA:HA	2.14	0.48
1:A:219:TRP:CZ2	1:F:296:PRO:HD2	2.49	0.48
1:E:311:VAL:HA	1:E:454:THR:OG1	2.13	0.48
1:I:248:LYS:HG3	1:I:439:ARG:HG2	1.95	0.48
1:K:192:VAL:HG21	1:K:288:MET:HG2	1.94	0.48
1:A:362:TRP:O	1:A:373:VAL:HG23	2.13	0.48
1:C:183:ILE:HG21	1:D:208:MET:HE2	1.90	0.48
1:E:267:LEU:HD22	1:H:167:VAL:CG1	2.42	0.48
1:C:206:LEU:HD23	1:C:208:MET:HG2	1.96	0.48
1:H:227:THR:HG22	1:H:228:ASP:H	1.76	0.48
1:H:404:VAL:HA	1:H:451:VAL:O	2.13	0.48
1:J:374:LYS:HZ1	1:K:361:GLU:CB	2.27	0.48
1:D:312:THR:HG21	1:D:402:PHE:HZ	1.78	0.47
1:D:324:ALA:HB1	1:D:382:ILE:HD12	1.96	0.47
1:E:415:ARG:CG	1:E:416:GLN:H	2.27	0.47
1:F:241:GLU:OE2	1:H:171:SER:HB3	2.14	0.47
1:K:354:TYR:OH	1:L:338:GLY:HA3	2.14	0.47
1:B:312:THR:O	1:B:456:ALA:HB2	2.14	0.47
1:E:190:LEU:HA	1:E:284:GLU:CD	2.34	0.47
1:G:330:LEU:C	1:G:332:ARG:N	2.67	0.47
1:A:192:VAL:HG23	1:A:284:GLU:HG2	1.95	0.47
1:B:300:LEU:HD13	1:B:401:GLU:CG	2.43	0.47
1:B:349:SER:HB3	1:B:402:PHE:HA	1.96	0.47
1:C:324:ALA:HB1	1:C:382:ILE:HD12	1.96	0.47
1:H:208:MET:HG3	1:H:242:ILE:HD11	1.96	0.47
1:A:310:VAL:HG22	1:A:333:LYS:HG3	1.95	0.47
1:B:264:ILE:HD12	1:B:264:ILE:H	1.78	0.47
1:C:210:VAL:HG23	1:C:242:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:LYS:HZ1	1:E:361:GLU:HB3	1.77	0.47
1:E:267:LEU:HB3	1:H:167:VAL:CG1	2.43	0.47
1:F:172:GLU:HG3	1:F:175:GLU:OE2	2.15	0.47
1:G:244:PHE:CZ	1:G:445:TYR:HD1	2.33	0.47
1:J:209:LEU:HD23	1:J:241:GLU:HG2	1.95	0.47
1:K:250:ALA:CB	1:L:232:GLY:H	2.28	0.47
1:L:226:GLY:H	1:L:230:THR:HG21	1.79	0.47
1:A:374:LYS:CA	1:B:383:TYR:CE1	2.97	0.47
1:B:206:LEU:HD23	1:B:208:MET:HG3	1.97	0.47
1:C:331:ARG:O	1:C:334:LEU:HB2	2.15	0.47
1:D:399:SER:O	1:D:455:TYR:HB2	2.15	0.47
1:F:191:VAL:CG2	1:F:192:VAL:N	2.78	0.47
1:G:324:ALA:HB1	1:G:382:ILE:HD12	1.96	0.47
1:L:312:THR:HG21	1:L:402:PHE:HZ	1.78	0.47
1:A:206:LEU:HD12	1:F:177:ILE:HG13	1.96	0.47
1:A:341:LEU:HD13	1:F:378:GLN:NE2	2.27	0.47
1:D:274:ARG:NH2	1:E:212:PRO:HG2	2.27	0.47
1:E:274:ARG:NH2	1:F:212:PRO:HG2	2.30	0.47
1:F:212:PRO:HD3	1:F:239:LEU:HA	1.97	0.47
1:F:362:TRP:CZ2	1:F:382:ILE:HD13	2.50	0.47
1:F:411:PHE:HZ	1:F:450:VAL:HG22	1.80	0.47
1:I:274:ARG:NH2	1:J:212:PRO:HG2	2.29	0.47
1:J:364:ASP:HB2	1:J:367:GLN:HG3	1.96	0.47
1:C:312:THR:HG21	1:C:402:PHE:HZ	1.78	0.47
1:H:274:ARG:HH21	1:I:212:PRO:HG2	1.79	0.47
1:H:334:LEU:HG	1:H:451:VAL:CG2	2.44	0.47
1:A:361:GLU:O	1:F:374:LYS:NZ	2.48	0.47
1:B:300:LEU:HD12	1:B:394:PRO:HD3	1.97	0.47
1:D:268:LEU:HB3	1:D:269:PRO:HD3	1.96	0.47
1:G:362:TRP:NE1	1:G:368:VAL:HG21	2.30	0.47
1:H:374:LYS:HG2	1:I:383:TYR:CE1	2.50	0.47
1:I:175:GLU:HB3	1:J:204:LYS:HE2	1.96	0.47
1:K:249:LEU:HD12	1:L:219:TRP:HA	1.97	0.47
1:L:331:ARG:O	1:L:334:LEU:HB2	2.15	0.47
1:H:176:THR:HG23	1:I:205:ILE:HB	1.97	0.47
1:H:183:ILE:HD11	1:I:242:ILE:CD1	2.45	0.47
1:H:410:ASN:ND2	1:H:448:ASN:O	2.48	0.47
1:J:300:LEU:HD13	1:J:394:PRO:HD2	1.97	0.47
1:K:192:VAL:CG2	1:K:284:GLU:HG2	2.31	0.47
1:L:190:LEU:HA	1:L:284:GLU:OE2	2.15	0.47
1:L:199:LEU:HD11	1:L:206:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:400:ALA:O	1:H:454:THR:HB	2.15	0.46
1:I:192:VAL:HG23	1:I:284:GLU:OE1	2.14	0.46
1:I:201:MET:HE3	1:I:244:PHE:O	2.16	0.46
1:I:299:LEU:HA	1:I:302:LEU:HD12	1.97	0.46
1:J:399:SER:O	1:J:400:ALA:HB3	2.15	0.46
1:K:364:ASP:C	1:K:366:ALA:H	2.19	0.46
1:A:446:PHE:CZ	1:F:185:ASP:N	2.83	0.46
1:D:275:LEU:HA	1:D:275:LEU:HD23	1.56	0.46
1:D:331:ARG:O	1:D:334:LEU:HB2	2.15	0.46
1:F:283:ILE:HD11	1:F:440:VAL:HG21	1.97	0.46
1:H:357:LEU:C	1:H:359:ASP:H	2.18	0.46
1:I:300:LEU:HD13	1:I:401:GLU:HG3	1.98	0.46
1:I:374:LYS:NZ	1:J:361:GLU:HB3	2.31	0.46
1:K:373:VAL:O	1:K:374:LYS:C	2.54	0.46
1:A:208:MET:HA	1:F:179:SER:HB2	1.97	0.46
1:D:183:ILE:HG13	1:E:210:VAL:HG22	1.95	0.46
1:H:256:THR:OG1	1:H:259:THR:HG22	2.15	0.46
1:I:400:ALA:O	1:I:454:THR:HB	2.15	0.46
1:K:250:ALA:HB1	1:L:232:GLY:H	1.80	0.46
1:L:180:GLN:NE2	1:L:265:PHE:HB3	2.30	0.46
1:C:188:LYS:HG2	1:D:336:ARG:HD3	1.98	0.46
1:C:208:MET:HE3	1:C:208:MET:HB3	1.57	0.46
1:F:300:LEU:HD11	1:F:393:PHE:CD2	2.50	0.46
1:K:336:ARG:C	1:K:338:GLY:N	2.67	0.46
1:A:244:PHE:HZ	1:A:445:TYR:HD1	1.62	0.46
1:A:324:ALA:HB1	1:A:382:ILE:HD12	1.96	0.46
1:E:444:ARG:HH22	1:E:450:VAL:HG12	1.80	0.46
1:K:444:ARG:HD3	1:K:446:PHE:O	2.16	0.46
1:L:250:ALA:HA	1:L:279:HIS:CE1	2.51	0.46
1:B:315:LYS:HE2	1:B:315:LYS:HB2	1.64	0.46
1:G:251:ALA:HB2	1:H:217:ALA:HB1	1.98	0.46
1:I:210:VAL:HG23	1:I:242:ILE:HG12	1.96	0.46
1:I:364:ASP:HB3	1:J:367:GLN:HA	1.97	0.46
1:K:181:ARG:HB2	1:L:208:MET:HG2	1.96	0.46
1:K:199:LEU:HD13	1:K:206:LEU:HD13	1.97	0.46
1:F:254:PHE:HB3	1:F:431:ARG:HD3	1.98	0.46
1:H:374:LYS:CG	1:I:383:TYR:CE1	2.98	0.46
1:C:212:PRO:HD3	1:C:239:LEU:HA	1.97	0.46
1:H:183:ILE:HB	1:I:446:PHE:CZ	2.50	0.46
1:I:188:LYS:H	1:I:188:LYS:HG3	1.43	0.46
1:I:308:ALA:HB1	1:I:451:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:CG	1:B:383:TYR:CE1	2.99	0.46
1:A:446:PHE:HZ	1:F:184:ARG:CA	2.28	0.46
1:B:323:THR:HB	1:B:361:GLU:OE1	2.16	0.46
1:E:310:VAL:CG2	1:E:333:LYS:HG3	2.46	0.46
1:F:325:LYS:HA	1:F:383:TYR:CE2	2.50	0.46
1:L:368:VAL:HB	1:L:369:GLY:H	1.65	0.46
1:A:229:THR:C	1:A:231:THR:N	2.69	0.46
1:G:336:ARG:NH2	1:L:188:LYS:HD3	2.26	0.46
1:G:340:LYS:O	1:G:341:LEU:HB2	2.16	0.46
1:I:353:TYR:HD2	1:J:339:LEU:HD22	1.79	0.46
1:K:377:GLY:HA3	1:L:383:TYR:O	2.16	0.46
1:L:258:GLU:O	1:L:261:GLU:HG2	2.16	0.46
1:A:248:LYS:HG3	1:A:439:ARG:HG2	1.98	0.45
1:H:180:GLN:HA	1:I:209:LEU:HD12	1.98	0.45
1:I:296:PRO:HD3	1:J:219:TRP:CZ3	2.52	0.45
1:J:309:LYS:HG2	1:J:454:THR:HG22	1.98	0.45
1:L:199:LEU:HD11	1:L:206:LEU:CD2	2.46	0.45
1:E:176:THR:HB	1:F:205:ILE:HB	1.98	0.45
1:F:201:MET:HE2	1:F:201:MET:HB2	1.61	0.45
1:I:289:THR:CG2	1:I:394:PRO:HG3	2.47	0.45
1:J:418:ALA:O	1:J:420:THR:HG23	2.17	0.45
1:A:181:ARG:HB2	1:B:208:MET:HE3	1.98	0.45
1:A:310:VAL:CG2	1:A:333:LYS:HG3	2.46	0.45
1:A:382:ILE:HD13	1:A:382:ILE:HA	1.77	0.45
1:C:331:ARG:HH12	1:C:341:LEU:HD11	1.81	0.45
1:F:345:VAL:HB	1:F:406:VAL:HG23	1.97	0.45
1:H:267:LEU:HD12	1:H:267:LEU:HA	1.76	0.45
1:J:362:TRP:CD1	1:J:368:VAL:HG21	2.51	0.45
1:J:378:GLN:HE22	1:K:341:LEU:CD1	2.17	0.45
1:L:331:ARG:HH12	1:L:341:LEU:HD11	1.81	0.45
1:L:418:ALA:O	1:L:420:THR:HG23	2.17	0.45
1:B:288:MET:CE	1:B:347:ILE:HG21	2.46	0.45
1:C:181:ARG:HH21	1:C:183:ILE:HG22	1.81	0.45
1:D:378:GLN:HE22	1:E:341:LEU:HB2	1.80	0.45
1:F:284:GLU:OE2	1:F:392:TYR:HB2	2.16	0.45
1:H:286:ALA:HB2	1:I:219:TRP:HE1	1.80	0.45
1:I:377:GLY:O	1:J:341:LEU:CD1	2.64	0.45
1:I:418:ALA:O	1:I:420:THR:HG23	2.17	0.45
1:K:418:ALA:O	1:K:420:THR:HG23	2.17	0.45
1:L:212:PRO:HG3	1:L:238:ALA:N	2.32	0.45
1:A:209:LEU:O	1:F:182:ILE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:PHE:O	1:D:298:GLY:HA3	2.17	0.45
1:D:331:ARG:HH12	1:D:341:LEU:HD11	1.81	0.45
1:E:256:THR:HG21	1:H:164:SER:CB	2.46	0.45
1:E:425:ARG:HD2	1:E:425:ARG:HA	1.73	0.45
1:F:205:ILE:HG23	1:F:243:HIS:HB3	1.98	0.45
1:F:414:PRO:HD2	1:F:441:ASN:O	2.16	0.45
1:G:207:THR:HG22	1:G:243:HIS:HD2	1.82	0.45
1:L:220:VAL:HG13	1:L:221:ALA:H	1.81	0.45
1:A:215:GLY:O	1:F:278:ALA:HB1	2.17	0.45
1:B:363:GLN:HB3	1:B:374:LYS:HE3	1.99	0.45
1:E:415:ARG:NH1	1:E:438:GLN:HG3	2.30	0.45
1:H:192:VAL:O	1:H:193:GLY:C	2.54	0.45
1:J:302:LEU:HD22	1:J:444:ARG:NE	2.30	0.45
1:K:176:THR:CG2	1:L:205:ILE:HB	2.46	0.45
1:K:264:ILE:HG22	1:K:265:PHE:N	2.30	0.45
1:A:401:GLU:HA	1:A:453:GLY:O	2.17	0.45
1:B:400:ALA:O	1:B:454:THR:HA	2.17	0.45
1:C:374:LYS:HB3	1:D:362:TRP:CZ2	2.52	0.45
1:E:169:VAL:HG21	1:E:175:GLU:HG3	1.99	0.45
1:H:169:VAL:HG21	1:H:175:GLU:HG3	1.98	0.45
1:H:382:ILE:HD13	1:H:382:ILE:HA	1.77	0.45
1:L:362:TRP:O	1:L:373:VAL:HG23	2.17	0.45
1:D:249:LEU:HD13	1:E:219:TRP:CE2	2.52	0.45
1:E:252:LYS:HE3	1:E:252:LYS:HB2	1.70	0.45
1:E:288:MET:HE1	1:E:393:PHE:HE1	1.82	0.45
1:F:422:GLU:HB3	1:H:427:ALA:HB1	1.99	0.45
1:G:330:LEU:O	1:G:331:ARG:C	2.54	0.45
1:B:415:ARG:NH1	1:B:418:ALA:HA	2.31	0.45
1:E:186:LEU:HD23	1:E:186:LEU:HA	1.53	0.45
1:G:287:PHE:O	1:G:298:GLY:HA3	2.17	0.45
1:H:253:SER:HB3	1:H:271:LEU:CD1	2.47	0.45
1:H:282:SER:HB3	1:I:217:ALA:H	1.82	0.45
1:H:327:ILE:HD12	1:H:356:LEU:HD11	1.98	0.45
1:H:374:LYS:CA	1:I:383:TYR:CE1	3.00	0.45
1:J:248:LYS:HG3	1:J:439:ARG:HG2	1.98	0.45
1:J:364:ASP:H	1:J:372:SER:HB2	1.82	0.45
1:K:281:VAL:HG21	1:L:214:ALA:HB1	1.98	0.45
1:L:401:GLU:HA	1:L:453:GLY:O	2.17	0.45
1:D:418:ALA:O	1:D:420:THR:HG23	2.17	0.45
1:E:374:LYS:HZ1	1:F:361:GLU:HB3	1.80	0.45
1:E:374:LYS:HB3	1:F:362:TRP:CZ2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:418:ALA:O	1:H:420:THR:HG23	2.17	0.45
1:J:254:PHE:HA	1:J:433:ALA:HA	1.99	0.45
1:B:444:ARG:CB	1:B:444:ARG:HH11	2.30	0.44
1:D:207:THR:HG22	1:D:243:HIS:CD2	2.53	0.44
1:D:401:GLU:HA	1:D:453:GLY:O	2.17	0.44
1:G:353:TYR:CE2	1:H:339:LEU:HD22	2.52	0.44
1:G:442:LEU:HD23	1:G:442:LEU:HA	1.82	0.44
1:H:184:ARG:HG2	1:I:211:GLU:HB3	1.99	0.44
1:H:205:ILE:HA	1:H:244:PHE:O	2.16	0.44
1:H:302:LEU:HB3	1:H:444:ARG:NH2	2.32	0.44
1:I:299:LEU:HD13	1:I:406:VAL:CG1	2.42	0.44
1:E:353:TYR:CE2	1:F:339:LEU:HD22	2.53	0.44
1:F:331:ARG:HH12	1:F:341:LEU:HD11	1.81	0.44
1:L:175:GLU:H	1:L:175:GLU:HG3	1.51	0.44
1:A:359:ASP:OD2	1:A:361:GLU:HB2	2.18	0.44
1:A:418:ALA:O	1:A:420:THR:HG23	2.17	0.44
1:B:444:ARG:H	1:B:444:ARG:HG3	1.44	0.44
1:G:181:ARG:HH21	1:G:183:ILE:HG22	1.81	0.44
1:H:300:LEU:CD1	1:H:394:PRO:HD3	2.46	0.44
1:A:331:ARG:HH12	1:A:341:LEU:HD11	1.81	0.44
1:F:412:VAL:O	1:F:414:PRO:HD3	2.18	0.44
1:I:374:LYS:HG2	1:J:362:TRP:CH2	2.51	0.44
1:J:275:LEU:O	1:J:278:ALA:HB3	2.17	0.44
1:K:283:ILE:HG12	1:L:219:TRP:HZ2	1.82	0.44
1:C:401:GLU:HA	1:C:453:GLY:O	2.18	0.44
1:C:412:VAL:O	1:C:414:PRO:HD3	2.18	0.44
1:D:311:VAL:HA	1:D:454:THR:HG23	1.98	0.44
1:E:188:LYS:HD3	1:E:392:TYR:OH	2.18	0.44
1:F:356:LEU:HA	1:F:356:LEU:HD12	1.80	0.44
1:F:438:GLN:HG2	1:F:440:VAL:HG22	1.98	0.44
1:G:206:LEU:HD23	1:G:208:MET:HG3	2.00	0.44
1:G:373:VAL:HG12	1:H:383:TYR:CE1	2.50	0.44
1:H:302:LEU:HD23	1:H:302:LEU:HA	1.84	0.44
1:H:333:LYS:HA	1:H:333:LYS:HD3	1.76	0.44
1:I:361:GLU:O	1:I:367:GLN:HB3	2.18	0.44
1:J:309:LYS:HG2	1:J:454:THR:CG2	2.47	0.44
1:J:400:ALA:O	1:J:454:THR:HB	2.18	0.44
1:B:373:VAL:O	1:B:374:LYS:C	2.55	0.44
1:C:183:ILE:HG13	1:D:446:PHE:CE1	2.52	0.44
1:C:299:LEU:HD13	1:C:406:VAL:HG11	1.99	0.44
1:E:412:VAL:O	1:E:414:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:ILE:HA	1:H:209:LEU:O	2.17	0.44
1:G:184:ARG:HD3	1:H:211:GLU:HB3	1.99	0.44
1:H:251:ALA:HB1	1:I:235:VAL:HG23	1.99	0.44
1:H:287:PHE:O	1:H:298:GLY:HA3	2.17	0.44
1:H:347:ILE:HG22	1:H:393:PHE:HE2	1.82	0.44
1:L:245:SER:H	1:L:443:GLN:HE21	1.65	0.44
1:A:235:VAL:HG22	1:F:251:ALA:HB1	2.00	0.44
1:B:201:MET:HE2	1:B:201:MET:HB2	1.83	0.44
1:D:296:PRO:HG2	1:E:219:TRP:CH2	2.53	0.44
1:E:190:LEU:CD2	1:E:280:ALA:HB1	2.48	0.44
1:E:354:TYR:HB3	1:F:332:ARG:HG2	2.00	0.44
1:E:400:ALA:O	1:E:454:THR:HA	2.17	0.44
1:F:204:LYS:O	1:F:245:SER:HA	2.18	0.44
1:F:323:THR:O	1:F:327:ILE:HG13	2.17	0.44
1:G:374:LYS:CG	1:H:383:TYR:CZ	2.99	0.44
1:G:418:ALA:O	1:G:420:THR:HG23	2.17	0.44
1:H:249:LEU:CD2	1:I:219:TRP:CZ2	3.00	0.44
1:I:268:LEU:HD11	1:I:434:TYR:CE1	2.53	0.44
1:I:435:TYR:CD1	1:J:231:THR:HG21	2.53	0.44
1:J:297:LYS:HB2	1:J:297:LYS:HE2	1.89	0.44
1:J:363:GLN:OE1	1:K:383:TYR:OH	2.35	0.44
1:L:412:VAL:O	1:L:414:PRO:HD3	2.18	0.44
1:A:412:VAL:O	1:A:414:PRO:HD3	2.18	0.44
1:B:268:LEU:HD12	1:B:268:LEU:HA	1.80	0.44
1:C:418:ALA:O	1:C:420:THR:HG23	2.17	0.44
1:G:255:ILE:HD11	1:G:260:GLU:HB2	2.00	0.44
1:K:295:LYS:H	1:K:295:LYS:HG2	1.67	0.44
1:L:224:THR:O	1:L:230:THR:HG22	2.18	0.44
1:L:290:GLY:O	1:L:301:THR:HG21	2.17	0.44
1:A:356:LEU:HD12	1:A:356:LEU:HA	1.82	0.44
1:B:401:GLU:HA	1:B:453:GLY:O	2.18	0.44
1:C:354:TYR:HB2	1:D:332:ARG:CG	2.37	0.44
1:D:188:LYS:HB3	1:D:391:GLU:OE2	2.18	0.44
1:I:186:LEU:HD22	1:I:186:LEU:HA	1.77	0.44
1:J:177:ILE:O	1:J:177:ILE:HG13	2.17	0.44
1:K:412:VAL:O	1:K:414:PRO:HD3	2.18	0.44
1:L:364:ASP:C	1:L:366:ALA:N	2.70	0.44
1:L:444:ARG:H	1:L:444:ARG:HG3	1.48	0.44
1:B:191:VAL:HG23	1:B:192:VAL:H	1.83	0.43
1:G:229:THR:C	1:G:231:THR:N	2.69	0.43
1:G:374:LYS:CG	1:H:383:TYR:CE1	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:LYS:HB2	1:K:392:TYR:CE1	2.53	0.43
1:L:208:MET:HE1	1:L:445:TYR:CE1	2.53	0.43
1:A:191:VAL:CG2	1:A:390:SER:HB2	2.48	0.43
1:E:224:THR:O	1:E:230:THR:HB	2.17	0.43
1:F:264:ILE:H	1:F:264:ILE:HG13	1.43	0.43
1:F:382:ILE:HD12	1:F:382:ILE:HG23	1.78	0.43
1:G:183:ILE:HD11	1:H:242:ILE:HG12	1.99	0.43
1:G:242:ILE:H	1:G:242:ILE:HG13	1.71	0.43
1:H:315:LYS:HB2	1:H:320:VAL:HB	1.99	0.43
1:H:347:ILE:O	1:H:403:ALA:HA	2.19	0.43
1:K:444:ARG:H	1:K:444:ARG:HG3	1.57	0.43
1:A:183:ILE:HG13	1:B:446:PHE:CZ	2.54	0.43
1:A:225:TYR:HE2	1:H:258:GLU:HB2	1.83	0.43
1:C:302:LEU:HD13	1:C:411:PHE:HE2	1.84	0.43
1:D:412:VAL:O	1:D:414:PRO:HD3	2.18	0.43
1:G:412:VAL:O	1:G:414:PRO:HD3	2.18	0.43
1:I:289:THR:HG21	1:I:394:PRO:HG3	2.01	0.43
1:B:347:ILE:O	1:B:403:ALA:HA	2.19	0.43
1:B:400:ALA:O	1:B:454:THR:HB	2.18	0.43
1:C:163:GLN:HA	1:C:168:GLU:HG2	2.00	0.43
1:D:244:PHE:CE2	1:D:412:VAL:HG21	2.53	0.43
1:F:181:ARG:HE	1:F:181:ARG:HB3	1.64	0.43
1:F:407:TYR:O	1:F:409:ASP:N	2.51	0.43
1:I:242:ILE:HD12	1:I:244:PHE:CE2	2.54	0.43
1:G:251:ALA:HB2	1:H:217:ALA:CB	2.49	0.43
1:G:256:THR:HA	1:G:431:ARG:HA	1.99	0.43
1:H:161:VAL:HG13	1:I:204:LYS:NZ	2.33	0.43
1:H:324:ALA:HB1	1:H:382:ILE:HD12	2.01	0.43
1:I:258:GLU:H	1:I:258:GLU:HG3	1.54	0.43
1:J:239:LEU:HD12	1:J:239:LEU:H	1.83	0.43
1:J:255:ILE:HG22	1:J:434:TYR:HE1	1.82	0.43
1:L:186:LEU:HD22	1:L:186:LEU:HA	1.86	0.43
1:E:315:LYS:HB2	1:E:315:LYS:HE3	1.75	0.43
1:G:362:TRP:O	1:G:373:VAL:HG23	2.18	0.43
1:H:378:GLN:HE21	1:H:378:GLN:HB2	1.64	0.43
1:J:412:VAL:O	1:J:414:PRO:HD3	2.18	0.43
1:L:206:LEU:CB	1:L:244:PHE:HB2	2.48	0.43
1:D:191:VAL:CG2	1:D:390:SER:HB2	2.48	0.43
1:E:225:TYR:HD1	1:E:225:TYR:HA	1.71	0.43
1:G:252:LYS:HE2	1:G:252:LYS:HB3	1.73	0.43
1:H:300:LEU:HD13	1:H:394:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:412:VAL:O	1:H:414:PRO:HD3	2.18	0.43
1:I:412:VAL:O	1:I:414:PRO:HD3	2.18	0.43
1:K:374:LYS:HE2	1:L:361:GLU:HB3	2.00	0.43
1:A:206:LEU:HD23	1:A:208:MET:HG3	2.00	0.43
1:C:191:VAL:CG2	1:C:390:SER:HB2	2.48	0.43
1:D:206:LEU:HD23	1:D:208:MET:HG3	2.00	0.43
1:E:382:ILE:HD12	1:E:382:ILE:HG23	1.78	0.43
1:G:211:GLU:HG3	1:G:212:PRO:HD2	2.01	0.43
1:G:401:GLU:HA	1:G:453:GLY:O	2.17	0.43
1:B:191:VAL:HG23	1:B:192:VAL:N	2.34	0.43
1:B:300:LEU:HD21	1:B:404:VAL:CG2	2.49	0.43
1:E:256:THR:HG21	1:H:164:SER:HB2	2.01	0.43
1:E:324:ALA:HB1	1:E:382:ILE:HG23	2.01	0.43
1:E:399:SER:O	1:E:400:ALA:HB3	2.19	0.43
1:H:285:GLU:OE1	1:I:216:LYS:HB3	2.19	0.43
1:H:296:PRO:CG	1:I:219:TRP:CH2	3.00	0.43
1:I:401:GLU:HA	1:I:453:GLY:O	2.19	0.43
1:J:212:PRO:HB3	1:J:238:ALA:O	2.17	0.43
1:J:264:ILE:H	1:J:264:ILE:HG12	1.54	0.43
1:A:399:SER:O	1:A:400:ALA:HB3	2.19	0.43
1:D:374:LYS:HB3	1:E:362:TRP:CZ2	2.54	0.43
1:F:161:VAL:O	1:F:162:ASN:C	2.56	0.43
1:G:191:VAL:CG2	1:G:390:SER:HB2	2.48	0.43
1:J:283:ILE:CG2	1:J:287:PHE:CE2	3.02	0.43
1:A:211:GLU:HG3	1:A:212:PRO:HD2	2.01	0.42
1:A:227:THR:O	1:A:230:THR:HG22	2.19	0.42
1:A:275:LEU:HA	1:A:275:LEU:HD23	1.56	0.42
1:B:212:PRO:HB3	1:B:238:ALA:O	2.18	0.42
1:E:299:LEU:HD13	1:E:406:VAL:HG11	2.00	0.42
1:F:399:SER:O	1:F:400:ALA:HB3	2.19	0.42
1:K:191:VAL:CG2	1:K:390:SER:HB2	2.48	0.42
1:K:270:LEU:HG	1:L:239:LEU:HD11	2.00	0.42
1:K:286:ALA:HB2	1:L:219:TRP:NE1	2.34	0.42
1:K:444:ARG:HH22	1:K:450:VAL:HG12	1.85	0.42
1:A:357:LEU:C	1:A:359:ASP:H	2.21	0.42
1:A:374:LYS:HG2	1:B:383:TYR:CE1	2.54	0.42
1:B:176:THR:HB	1:C:205:ILE:HB	2.02	0.42
1:E:256:THR:HG23	1:E:259:THR:H	1.84	0.42
1:F:161:VAL:HG12	1:F:162:ASN:H	1.84	0.42
1:G:244:PHE:HZ	1:G:445:TYR:HD1	1.68	0.42
1:G:361:GLU:HG3	1:L:374:LYS:HZ1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:382:ILE:HD12	1:H:382:ILE:HG23	1.78	0.42
1:L:399:SER:O	1:L:400:ALA:HB3	2.19	0.42
1:A:231:THR:HB	1:F:435:TYR:HD2	1.84	0.42
1:C:399:SER:O	1:C:400:ALA:HB3	2.19	0.42
1:D:255:ILE:HD11	1:D:260:GLU:HB2	2.02	0.42
1:D:356:LEU:HA	1:D:356:LEU:HD12	1.82	0.42
1:D:439:ARG:NH1	1:E:225:TYR:OH	2.52	0.42
1:E:421:VAL:HG22	1:E:436:VAL:HG22	2.01	0.42
1:F:166:SER:O	1:F:167:VAL:HB	2.19	0.42
1:F:292:GLY:HA3	1:F:297:LYS:HG3	2.00	0.42
1:G:227:THR:O	1:G:230:THR:HG22	2.19	0.42
1:G:270:LEU:HA	1:G:270:LEU:HD22	1.60	0.42
1:I:378:GLN:HE22	1:J:341:LEU:HB3	1.79	0.42
1:J:300:LEU:HD13	1:J:394:PRO:CD	2.48	0.42
1:J:373:VAL:CG1	1:K:383:TYR:CE1	3.03	0.42
1:A:181:ARG:CB	1:B:208:MET:HE3	2.50	0.42
1:A:210:VAL:HG23	1:A:242:ILE:HG12	2.02	0.42
1:C:186:LEU:HD12	1:D:337:HIS:HA	2.01	0.42
1:E:258:GLU:O	1:E:262:ASP:HB2	2.20	0.42
1:G:250:ALA:CA	1:G:279:HIS:HE1	2.28	0.42
1:H:182:ILE:HG23	1:I:211:GLU:HB2	2.02	0.42
1:B:172:GLU:OE1	1:C:205:ILE:HD11	2.19	0.42
1:E:169:VAL:HG21	1:E:175:GLU:CG	2.49	0.42
1:E:177:ILE:HD12	1:F:206:LEU:HD12	2.01	0.42
1:F:429:LYS:HB2	1:F:431:ARG:HG2	2.01	0.42
1:K:177:ILE:HG23	1:L:205:ILE:O	2.19	0.42
1:L:382:ILE:HD12	1:L:382:ILE:HG23	1.78	0.42
1:A:205:ILE:HB	1:F:176:THR:OG1	2.19	0.42
1:A:357:LEU:C	1:A:359:ASP:N	2.70	0.42
1:D:362:TRP:CZ2	1:D:382:ILE:HD13	2.55	0.42
1:G:435:TYR:CD1	1:H:231:THR:HB	2.55	0.42
1:H:186:LEU:HD22	1:H:186:LEU:HA	1.52	0.42
1:J:186:LEU:HD22	1:J:186:LEU:HA	1.89	0.42
1:K:229:THR:C	1:K:231:THR:N	2.68	0.42
1:K:248:LYS:HB3	1:L:221:ALA:HB3	2.01	0.42
1:K:401:GLU:HA	1:K:453:GLY:O	2.19	0.42
1:A:282:SER:O	1:A:283:ILE:C	2.57	0.42
1:B:366:ALA:CB	1:C:366:ALA:HB1	2.46	0.42
1:C:199:LEU:O	1:C:200:PRO:C	2.55	0.42
1:C:362:TRP:CE2	1:C:368:VAL:HG11	2.55	0.42
1:F:334:LEU:HG	1:F:451:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:399:SER:O	1:G:400:ALA:HB3	2.20	0.42
1:H:334:LEU:HG	1:H:451:VAL:HG23	2.01	0.42
1:J:410:ASN:ND2	1:J:448:ASN:O	2.53	0.42
1:K:377:GLY:HA3	1:L:384:GLY:HA3	2.02	0.42
1:A:361:GLU:C	1:F:374:LYS:HZ3	2.23	0.42
1:B:204:LYS:HE2	1:B:204:LYS:HB3	1.47	0.42
1:C:339:LEU:H	1:C:339:LEU:HG	1.69	0.42
1:C:356:LEU:HD12	1:C:356:LEU:HA	1.82	0.42
1:C:444:ARG:HD3	1:C:447:ALA:HA	2.02	0.42
1:I:184:ARG:HG2	1:J:211:GLU:HB3	2.00	0.42
1:J:192:VAL:CG2	1:J:288:MET:HG2	2.46	0.42
1:B:256:THR:HA	1:B:431:ARG:HA	2.00	0.42
1:B:340:LYS:O	1:B:341:LEU:HB2	2.20	0.42
1:D:274:ARG:NH2	1:E:212:PRO:HB2	2.35	0.42
1:I:212:PRO:HD3	1:I:239:LEU:HA	2.01	0.42
1:J:192:VAL:CG2	1:J:284:GLU:HG2	2.49	0.42
1:J:251:ALA:HB2	1:K:217:ALA:HB1	2.01	0.42
1:J:444:ARG:HD3	1:J:447:ALA:HA	2.02	0.42
1:A:212:PRO:HD3	1:A:239:LEU:HA	2.02	0.41
1:A:225:TYR:CD2	1:H:258:GLU:HG3	2.55	0.41
1:B:211:GLU:HG3	1:B:212:PRO:HD2	2.01	0.41
1:B:334:LEU:HG	1:B:451:VAL:CG2	2.48	0.41
1:D:399:SER:O	1:D:400:ALA:HB3	2.19	0.41
1:E:210:VAL:HG23	1:E:242:ILE:HG12	2.02	0.41
1:E:310:VAL:HG21	1:E:333:LYS:HG3	2.02	0.41
1:G:266:SER:O	1:G:267:LEU:HB2	2.20	0.41
1:G:364:ASP:HB2	1:G:367:GLN:HB2	2.02	0.41
1:H:282:SER:OG	1:I:217:ALA:HB3	2.20	0.41
1:H:321:LEU:HB3	1:H:355:ASP:OD2	2.20	0.41
1:H:354:TYR:HA	1:H:357:LEU:HD12	2.02	0.41
1:K:312:THR:O	1:K:456:ALA:HB2	2.19	0.41
1:A:283:ILE:HD11	1:A:438:GLN:NE2	2.32	0.41
1:B:300:LEU:HD23	1:B:404:VAL:CG1	2.49	0.41
1:D:283:ILE:HD11	1:D:438:GLN:NE2	2.32	0.41
1:D:378:GLN:H	1:D:378:GLN:HG2	1.76	0.41
1:I:444:ARG:H	1:I:444:ARG:HG3	1.57	0.41
1:L:212:PRO:HB3	1:L:240:LYS:HE3	2.02	0.41
1:L:354:TYR:HA	1:L:357:LEU:HD12	2.02	0.41
1:D:302:LEU:HB3	1:D:444:ARG:HH21	1.84	0.41
1:D:411:PHE:CZ	1:D:450:VAL:HG22	2.49	0.41
1:G:217:ALA:HB2	1:L:251:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:362:TRP:CD1	1:G:368:VAL:HG11	2.54	0.41
1:I:252:LYS:O	1:J:234:GLU:HA	2.19	0.41
1:J:182:ILE:HA	1:K:209:LEU:O	2.20	0.41
1:L:275:LEU:O	1:L:279:HIS:HD2	2.03	0.41
1:A:248:LYS:HD3	1:B:220:VAL:CG2	2.51	0.41
1:A:297:LYS:HE2	1:A:297:LYS:HB2	1.79	0.41
1:D:192:VAL:HG11	1:D:288:MET:SD	2.61	0.41
1:F:310:VAL:O	1:F:454:THR:HG23	2.20	0.41
1:F:382:ILE:HD13	1:F:382:ILE:HA	1.77	0.41
1:G:362:TRP:CH2	1:L:374:LYS:HG2	2.56	0.41
1:H:314:ALA:HA	1:H:320:VAL:HG12	2.02	0.41
1:L:274:ARG:O	1:L:278:ALA:HB2	2.21	0.41
1:A:354:TYR:HA	1:A:357:LEU:HD12	2.02	0.41
1:A:362:TRP:CD1	1:A:368:VAL:HG11	2.55	0.41
1:C:268:LEU:O	1:C:269:PRO:C	2.57	0.41
1:E:198:GLU:HG2	1:E:413:MET:HB2	2.03	0.41
1:F:403:ALA:O	1:F:452:SER:HA	2.21	0.41
1:G:354:TYR:HA	1:G:357:LEU:HD12	2.02	0.41
1:H:249:LEU:HD22	1:I:219:TRP:CZ3	2.52	0.41
1:I:374:LYS:HZ1	1:J:361:GLU:HB3	1.86	0.41
1:K:255:ILE:HD11	1:K:260:GLU:HB2	2.02	0.41
1:A:368:VAL:HB	1:A:369:GLY:H	1.64	0.41
1:D:382:ILE:HD13	1:D:382:ILE:HA	1.77	0.41
1:G:400:ALA:O	1:G:454:THR:HA	2.21	0.41
1:J:356:LEU:HD12	1:J:356:LEU:HA	1.82	0.41
1:B:188:LYS:H	1:B:188:LYS:HG2	1.28	0.41
1:B:277:GLU:OE1	1:C:214:ALA:HB2	2.20	0.41
1:E:296:PRO:HG3	1:E:441:ASN:HA	2.02	0.41
1:F:400:ALA:O	1:F:454:THR:HA	2.21	0.41
1:G:254:PHE:HB3	1:G:433:ALA:HA	2.02	0.41
1:G:364:ASP:OD1	1:H:367:GLN:HG2	2.21	0.41
1:H:286:ALA:O	1:H:287:PHE:C	2.58	0.41
1:J:176:THR:HA	1:K:205:ILE:O	2.20	0.41
1:J:399:SER:O	1:J:455:TYR:HB2	2.21	0.41
1:K:176:THR:HG22	1:L:205:ILE:HB	2.02	0.41
1:K:187:GLN:O	1:K:188:LYS:C	2.59	0.41
1:B:302:LEU:HD13	1:B:411:PHE:HE1	1.86	0.41
1:C:279:HIS:O	1:C:283:ILE:HG13	2.21	0.41
1:C:290:GLY:HA3	1:C:296:PRO:O	2.20	0.41
1:C:345:VAL:O	1:C:405:ILE:HA	2.21	0.41
1:D:227:THR:C	1:D:229:THR:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:GLU:O	1:E:314:ALA:C	2.58	0.41
1:E:345:VAL:O	1:E:405:ILE:HA	2.21	0.41
1:F:430:GLN:HA	1:F:430:GLN:HE21	1.86	0.41
1:G:249:LEU:HB2	1:H:219:TRP:CE3	2.56	0.41
1:G:283:ILE:HD11	1:G:438:GLN:NE2	2.32	0.41
1:G:382:ILE:HD13	1:G:382:ILE:HA	1.77	0.41
1:G:383:TYR:CD1	1:L:373:VAL:CG1	3.02	0.41
1:A:255:ILE:HD11	1:A:260:GLU:HB2	2.02	0.41
1:A:286:ALA:O	1:A:287:PHE:C	2.58	0.41
1:B:192:VAL:O	1:B:193:GLY:C	2.58	0.41
1:B:254:PHE:HB3	1:B:431:ARG:HD3	2.03	0.41
1:B:281:VAL:O	1:B:285:GLU:HG3	2.21	0.41
1:D:354:TYR:HA	1:D:357:LEU:HD12	2.02	0.41
1:E:354:TYR:CE2	1:F:332:ARG:HA	2.55	0.41
1:G:192:VAL:HG11	1:G:288:MET:SD	2.61	0.41
1:G:208:MET:HE2	1:L:181:ARG:HB3	2.03	0.41
1:G:246:THR:HG22	1:G:414:PRO:O	2.21	0.41
1:G:374:LYS:N	1:H:383:TYR:CD1	2.89	0.41
1:H:211:GLU:OE2	1:H:212:PRO:HD2	2.21	0.41
1:H:224:THR:HG23	1:H:225:TYR:N	2.36	0.41
1:H:357:LEU:C	1:H:359:ASP:N	2.74	0.41
1:I:192:VAL:HG13	1:I:288:MET:HE2	2.02	0.41
1:I:240:LYS:HE3	1:I:240:LYS:HB2	1.78	0.41
1:I:285:GLU:HG3	1:J:216:LYS:NZ	2.35	0.41
1:J:210:VAL:HG13	1:J:446:PHE:HE1	1.85	0.41
1:J:246:THR:HG21	1:J:415:ARG:O	2.19	0.41
1:J:364:ASP:OD1	1:K:367:GLN:HG2	2.20	0.41
1:K:249:LEU:HD12	1:K:249:LEU:HA	1.92	0.41
1:K:283:ILE:HG12	1:L:219:TRP:CZ2	2.55	0.41
1:K:374:LYS:O	1:L:362:TRP:HZ2	2.04	0.41
1:A:383:TYR:CD1	1:F:373:VAL:CG1	3.01	0.41
1:D:286:ALA:O	1:D:287:PHE:C	2.58	0.41
1:H:225:TYR:CA	1:H:230:THR:OG1	2.62	0.41
1:H:248:LYS:O	1:I:219:TRP:HE3	2.04	0.41
1:H:252:LYS:HE3	1:H:252:LYS:HB2	1.79	0.41
1:H:284:GLU:OE2	1:H:392:TYR:CB	2.69	0.41
1:H:322:VAL:H	1:H:322:VAL:HG23	1.54	0.41
1:J:401:GLU:HA	1:J:453:GLY:O	2.20	0.41
1:K:201:MET:HG3	1:K:206:LEU:HB2	2.03	0.41
1:K:207:THR:HA	1:K:242:ILE:O	2.21	0.41
1:K:382:ILE:HD12	1:K:382:ILE:HG23	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:400:ALA:O	1:L:454:THR:HA	2.21	0.41
1:B:212:PRO:HD3	1:B:239:LEU:CA	2.41	0.40
1:E:354:TYR:HA	1:E:357:LEU:HD12	2.02	0.40
1:G:337:HIS:CE1	1:G:448:ASN:HD21	2.39	0.40
1:H:270:LEU:HD22	1:H:270:LEU:HA	1.95	0.40
1:H:283:ILE:HD11	1:H:438:GLN:NE2	2.32	0.40
1:I:300:LEU:CD1	1:I:394:PRO:HD3	2.50	0.40
1:I:374:LYS:NZ	1:J:361:GLU:O	2.52	0.40
1:J:354:TYR:HA	1:J:357:LEU:HD12	2.02	0.40
1:J:442:LEU:HD23	1:J:442:LEU:HA	1.82	0.40
1:K:334:LEU:N	1:K:451:VAL:HG21	2.37	0.40
1:A:273:LYS:C	1:A:275:LEU:N	2.67	0.40
1:C:400:ALA:O	1:C:454:THR:HA	2.21	0.40
1:E:188:LYS:HG2	1:E:392:TYR:HE1	1.86	0.40
1:E:356:LEU:HD12	1:E:356:LEU:HA	1.82	0.40
1:G:415:ARG:HG3	1:G:440:VAL:HG13	2.04	0.40
1:I:297:LYS:HE2	1:I:297:LYS:HB2	1.81	0.40
1:I:373:VAL:HG12	1:J:383:TYR:CD1	2.48	0.40
1:L:330:LEU:O	1:L:331:ARG:C	2.59	0.40
1:A:215:GLY:O	1:F:278:ALA:CB	2.69	0.40
1:B:341:LEU:HA	1:B:341:LEU:HD23	1.62	0.40
1:D:180:GLN:HA	1:E:209:LEU:HD12	2.03	0.40
1:F:400:ALA:HB3	1:F:455:TYR:HD2	1.86	0.40
1:G:207:THR:HG22	1:G:243:HIS:CD2	2.56	0.40
1:G:302:LEU:HB3	1:G:444:ARG:NH2	2.35	0.40
1:G:363:GLN:HG2	1:G:373:VAL:HB	2.03	0.40
1:G:406:VAL:HG12	1:G:450:VAL:HG13	2.03	0.40
1:H:249:LEU:HD12	1:H:249:LEU:HA	1.84	0.40
1:J:274:ARG:NH1	1:K:235:VAL:HG12	2.36	0.40
1:L:375:LEU:HD22	1:L:375:LEU:HA	1.90	0.40
1:B:364:ASP:OD1	1:C:367:GLN:HA	2.22	0.40
1:C:415:ARG:HH22	1:C:438:GLN:HE21	1.69	0.40
1:D:363:GLN:HE22	1:E:325:LYS:HD2	1.86	0.40
1:G:201:MET:CE	1:G:246:THR:HG23	2.52	0.40
1:I:354:TYR:HA	1:I:357:LEU:HD12	2.02	0.40
1:B:188:LYS:CD	1:C:336:ARG:HH12	2.30	0.40
1:E:264:ILE:H	1:E:264:ILE:HD12	1.86	0.40
1:E:302:LEU:HB3	1:E:444:ARG:NH2	2.35	0.40
1:E:411:PHE:HD2	1:E:442:LEU:HD22	1.87	0.40
1:G:267:LEU:HD23	1:G:267:LEU:HA	1.93	0.40
1:G:345:VAL:O	1:G:405:ILE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:415:ARG:HG3	1:H:440:VAL:HG13	2.04	0.40
1:I:324:ALA:HB1	1:I:382:ILE:HD12	2.03	0.40
1:K:353:TYR:O	1:K:357:LEU:HG	2.21	0.40
1:L:406:VAL:HG12	1:L:450:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/458 (64%)	267 (90%)	24 (8%)	4 (1%)	9	31
1	B	295/458 (64%)	272 (92%)	17 (6%)	6 (2%)	6	25
1	C	295/458 (64%)	260 (88%)	30 (10%)	5 (2%)	7	28
1	D	295/458 (64%)	268 (91%)	19 (6%)	8 (3%)	4	21
1	E	295/458 (64%)	267 (90%)	24 (8%)	4 (1%)	9	31
1	F	295/458 (64%)	269 (91%)	16 (5%)	10 (3%)	3	17
1	G	292/458 (64%)	257 (88%)	30 (10%)	5 (2%)	7	28
1	H	295/458 (64%)	261 (88%)	24 (8%)	10 (3%)	3	17
1	I	295/458 (64%)	271 (92%)	20 (7%)	4 (1%)	9	31
1	J	292/458 (64%)	266 (91%)	21 (7%)	5 (2%)	7	28
1	K	292/458 (64%)	258 (88%)	27 (9%)	7 (2%)	5	23
1	L	292/458 (64%)	260 (89%)	27 (9%)	5 (2%)	7	28
2	a	64/164 (39%)	58 (91%)	4 (6%)	2 (3%)	3	18
2	b	64/164 (39%)	58 (91%)	4 (6%)	2 (3%)	3	18
All	All	3656/5824 (63%)	3292 (90%)	287 (8%)	77 (2%)	8	24

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	SER
1	B	365	VAL
1	F	419	VAL
1	F	443	GLN
1	G	168	GLU
1	H	166	SER
1	H	170	SER
1	I	164	SER
1	J	365	VAL
1	K	168	GLU
1	K	364	ASP
1	K	365	VAL
1	A	416	GLN
1	B	168	GLU
1	B	186	LEU
1	C	180	GLN
1	C	416	GLN
1	D	228	ASP
1	D	416	GLN
1	E	416	GLN
1	F	188	LYS
1	F	208	MET
1	F	408	LYS
1	F	416	GLN
1	G	416	GLN
1	H	162	ASN
1	H	167	VAL
1	H	320	VAL
1	H	416	GLN
1	I	293	SER
1	I	368	VAL
1	I	416	GLN
1	J	416	GLN
1	K	224	THR
1	K	416	GLN
1	L	188	LYS
1	L	416	GLN
2	b	12	GLY
1	B	364	ASP
1	D	170	SER
1	E	165	SER
1	E	167	VAL
1	H	164	SER

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Mol	Chain	Res	Type
2	a	12	GLY
2	a	32	PRO
2	b	32	PRO
1	C	171	SER
1	E	368	VAL
1	F	167	VAL
1	F	185	ASP
1	F	187	GLN
1	J	187	GLN
1	J	364	ASP
1	K	337	HIS
1	A	368	VAL
1	B	368	VAL
1	D	187	GLN
1	D	288	MET
1	D	368	VAL
1	F	368	VAL
1	H	288	MET
1	H	368	VAL
1	L	224	THR
1	C	293	SER
1	D	171	SER
1	G	288	MET
1	A	200	PRO
1	D	200	PRO
1	G	200	PRO
1	H	200	PRO
1	J	200	PRO
1	K	200	PRO
1	L	200	PRO
1	L	368	VAL
1	A	449	GLY
1	C	368	VAL
1	G	449	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	249/387 (64%)	199 (80%)	50 (20%)	1 3
1	B	249/387 (64%)	194 (78%)	55 (22%)	1 2
1	C	249/387 (64%)	203 (82%)	46 (18%)	1 4
1	D	249/387 (64%)	205 (82%)	44 (18%)	1 5
1	E	249/387 (64%)	203 (82%)	46 (18%)	1 4
1	F	249/387 (64%)	195 (78%)	54 (22%)	1 2
1	G	246/387 (64%)	201 (82%)	45 (18%)	1 5
1	H	249/387 (64%)	197 (79%)	52 (21%)	1 2
1	I	249/387 (64%)	200 (80%)	49 (20%)	1 3
1	J	246/387 (64%)	199 (81%)	47 (19%)	1 4
1	K	246/387 (64%)	198 (80%)	48 (20%)	1 3
1	L	246/387 (64%)	204 (83%)	42 (17%)	1 6
2	a	54/130 (42%)	48 (89%)	6 (11%)	5 18
2	b	54/130 (42%)	44 (82%)	10 (18%)	1 4
All	All	3084/4904 (63%)	2490 (81%)	594 (19%)	3 3

All (594) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	VAL
1	A	165	SER
1	A	167	VAL
1	A	169	VAL
1	A	172	GLU
1	A	177	ILE
1	A	179	SER
1	A	191	VAL
1	A	192	VAL
1	A	199	LEU
1	A	206	LEU
1	A	229	THR
1	A	231	THR
1	A	235	VAL
1	A	242	ILE
1	A	246	THR
1	A	256	THR
1	A	262	ASP
1	A	264	ILE

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Mol	Chain	Res	Type
1	A	266	SER
1	A	267	LEU
1	A	270	LEU
1	A	277	GLU
1	A	289	THR
1	A	313	GLU
1	A	334	LEU
1	A	346	LEU
1	A	348	VAL
1	A	349	SER
1	A	362	TRP
1	A	365	VAL
1	A	367	GLN
1	A	368	VAL
1	A	372	SER
1	A	375	LEU
1	A	378	GLN
1	A	401	GLU
1	A	404	VAL
1	A	407	TYR
1	A	412	VAL
1	A	419	VAL
1	A	430	GLN
1	A	431	ARG
1	A	440	VAL
1	A	442	LEU
1	A	444	ARG
1	A	445	TYR
1	A	448	ASN
1	A	450	VAL
1	A	454	THR
1	B	161	VAL
1	B	169	VAL
1	B	176	THR
1	B	177	ILE
1	B	182	ILE
1	B	187	GLN
1	B	188	LYS
1	B	192	VAL
1	B	199	LEU
1	B	205	ILE
1	B	206	LEU

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Mol	Chain	Res	Type
1	B	218	THR
1	B	220	VAL
1	B	227	THR
1	B	242	ILE
1	B	249	LEU
1	B	253	SER
1	B	258	GLU
1	B	264	ILE
1	B	267	LEU
1	B	270	LEU
1	B	274	ARG
1	B	283	ILE
1	B	295	LYS
1	B	296	PRO
1	B	323	THR
1	B	328	SER
1	B	332	ARG
1	B	334	LEU
1	B	336	ARG
1	B	341	LEU
1	B	346	LEU
1	B	348	VAL
1	B	349	SER
1	B	364	ASP
1	B	365	VAL
1	B	372	SER
1	B	375	LEU
1	B	378	GLN
1	B	391	GLU
1	B	401	GLU
1	B	404	VAL
1	B	407	TYR
1	B	412	VAL
1	B	413	MET
1	B	425	ARG
1	B	430	GLN
1	B	432	ASP
1	B	437	THR
1	B	440	VAL
1	B	442	LEU
1	B	444	ARG
1	B	448	ASN

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Mol	Chain	Res	Type
1	B	450	VAL
1	B	454	THR
1	C	161	VAL
1	C	162	ASN
1	C	165	SER
1	C	169	VAL
1	C	170	SER
1	C	177	ILE
1	C	179	SER
1	C	191	VAL
1	C	192	VAL
1	C	199	LEU
1	C	201	MET
1	C	205	ILE
1	C	208	MET
1	C	229	THR
1	C	231	THR
1	C	242	ILE
1	C	257	ASP
1	C	258	GLU
1	C	264	ILE
1	C	269	PRO
1	C	271	LEU
1	C	274	ARG
1	C	289	THR
1	C	296	PRO
1	C	313	GLU
1	C	334	LEU
1	C	346	LEU
1	C	348	VAL
1	C	349	SER
1	C	362	TRP
1	C	368	VAL
1	C	375	LEU
1	C	378	GLN
1	C	401	GLU
1	C	404	VAL
1	C	407	TYR
1	C	412	VAL
1	C	419	VAL
1	C	430	GLN
1	C	431	ARG

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Mol	Chain	Res	Type
1	C	440	VAL
1	C	442	LEU
1	C	444	ARG
1	C	448	ASN
1	C	450	VAL
1	C	454	THR
1	D	161	VAL
1	D	169	VAL
1	D	177	ILE
1	D	182	ILE
1	D	191	VAL
1	D	192	VAL
1	D	199	LEU
1	D	206	LEU
1	D	218	THR
1	D	220	VAL
1	D	231	THR
1	D	239	LEU
1	D	242	ILE
1	D	246	THR
1	D	256	THR
1	D	262	ASP
1	D	264	ILE
1	D	266	SER
1	D	267	LEU
1	D	270	LEU
1	D	277	GLU
1	D	289	THR
1	D	313	GLU
1	D	334	LEU
1	D	346	LEU
1	D	348	VAL
1	D	349	SER
1	D	362	TRP
1	D	372	SER
1	D	375	LEU
1	D	378	GLN
1	D	401	GLU
1	D	404	VAL
1	D	407	TYR
1	D	412	VAL
1	D	419	VAL

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Mol	Chain	Res	Type
1	D	430	GLN
1	D	431	ARG
1	D	440	VAL
1	D	442	LEU
1	D	444	ARG
1	D	448	ASN
1	D	450	VAL
1	D	451	VAL
1	E	167	VAL
1	E	168	GLU
1	E	169	VAL
1	E	176	THR
1	E	185	ASP
1	E	192	VAL
1	E	199	LEU
1	E	206	LEU
1	E	208	MET
1	E	218	THR
1	E	227	THR
1	E	231	THR
1	E	246	THR
1	E	258	GLU
1	E	259	THR
1	E	262	ASP
1	E	264	ILE
1	E	269	PRO
1	E	270	LEU
1	E	274	ARG
1	E	283	ILE
1	E	284	GLU
1	E	289	THR
1	E	296	PRO
1	E	301	THR
1	E	317	ASP
1	E	334	LEU
1	E	346	LEU
1	E	348	VAL
1	E	349	SER
1	E	362	TRP
1	E	364	ASP
1	E	372	SER
1	E	375	LEU

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Mol	Chain	Res	Type
1	E	378	GLN
1	E	401	GLU
1	E	404	VAL
1	E	407	TYR
1	E	412	VAL
1	E	419	VAL
1	E	426	GLN
1	E	442	LEU
1	E	444	ARG
1	E	448	ASN
1	E	451	VAL
1	E	454	THR
1	F	162	ASN
1	F	169	VAL
1	F	177	ILE
1	F	182	ILE
1	F	183	ILE
1	F	184	ARG
1	F	185	ASP
1	F	186	LEU
1	F	187	GLN
1	F	192	VAL
1	F	199	LEU
1	F	203	SER
1	F	206	LEU
1	F	207	THR
1	F	218	THR
1	F	223	SER
1	F	227	THR
1	F	233	GLU
1	F	240	LYS
1	F	242	ILE
1	F	256	THR
1	F	257	ASP
1	F	264	ILE
1	F	267	LEU
1	F	269	PRO
1	F	270	LEU
1	F	274	ARG
1	F	277	GLU
1	F	283	ILE
1	F	288	MET

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Mol	Chain	Res	Type
1	F	296	PRO
1	F	323	THR
1	F	334	LEU
1	F	346	LEU
1	F	356	LEU
1	F	362	TRP
1	F	372	SER
1	F	375	LEU
1	F	378	GLN
1	F	394	PRO
1	F	401	GLU
1	F	404	VAL
1	F	406	VAL
1	F	412	VAL
1	F	419	VAL
1	F	423	ARG
1	F	425	ARG
1	F	430	GLN
1	F	440	VAL
1	F	442	LEU
1	F	444	ARG
1	F	448	ASN
1	F	450	VAL
1	F	454	THR
1	G	165	SER
1	G	167	VAL
1	G	169	VAL
1	G	172	GLU
1	G	176	THR
1	G	177	ILE
1	G	191	VAL
1	G	192	VAL
1	G	199	LEU
1	G	206	LEU
1	G	229	THR
1	G	231	THR
1	G	235	VAL
1	G	242	ILE
1	G	243	HIS
1	G	249	LEU
1	G	254	PHE
1	G	259	THR

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Mol	Chain	Res	Type
1	G	264	ILE
1	G	265	PHE
1	G	270	LEU
1	G	289	THR
1	G	313	GLU
1	G	346	LEU
1	G	348	VAL
1	G	349	SER
1	G	361	GLU
1	G	362	TRP
1	G	365	VAL
1	G	372	SER
1	G	375	LEU
1	G	401	GLU
1	G	404	VAL
1	G	407	TYR
1	G	412	VAL
1	G	419	VAL
1	G	430	GLN
1	G	431	ARG
1	G	440	VAL
1	G	442	LEU
1	G	444	ARG
1	G	445	TYR
1	G	448	ASN
1	G	450	VAL
1	G	454	THR
1	H	163	GLN
1	H	167	VAL
1	H	170	SER
1	H	177	ILE
1	H	182	ILE
1	H	183	ILE
1	H	186	LEU
1	H	192	VAL
1	H	199	LEU
1	H	205	ILE
1	H	206	LEU
1	H	208	MET
1	H	218	THR
1	H	246	THR
1	H	249	LEU

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Mol	Chain	Res	Type
1	H	253	SER
1	H	255	ILE
1	H	257	ASP
1	H	258	GLU
1	H	259	THR
1	H	265	PHE
1	H	267	LEU
1	H	268	LEU
1	H	269	PRO
1	H	270	LEU
1	H	274	ARG
1	H	277	GLU
1	H	289	THR
1	H	313	GLU
1	H	323	THR
1	H	328	SER
1	H	336	ARG
1	H	346	LEU
1	H	348	VAL
1	H	349	SER
1	H	362	TRP
1	H	372	SER
1	H	375	LEU
1	H	378	GLN
1	H	401	GLU
1	H	404	VAL
1	H	407	TYR
1	H	412	VAL
1	H	419	VAL
1	H	430	GLN
1	H	431	ARG
1	H	440	VAL
1	H	442	LEU
1	H	444	ARG
1	H	448	ASN
1	H	450	VAL
1	H	454	THR
1	I	161	VAL
1	I	163	GLN
1	I	165	SER
1	I	169	VAL
1	I	172	GLU

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Mol	Chain	Res	Type
1	I	176	THR
1	I	179	SER
1	I	181	ARG
1	I	182	ILE
1	I	186	LEU
1	I	188	LYS
1	I	192	VAL
1	I	205	ILE
1	I	206	LEU
1	I	220	VAL
1	I	227	THR
1	I	229	THR
1	I	231	THR
1	I	242	ILE
1	I	256	THR
1	I	257	ASP
1	I	258	GLU
1	I	259	THR
1	I	264	ILE
1	I	268	LEU
1	I	269	PRO
1	I	270	LEU
1	I	274	ARG
1	I	283	ILE
1	I	334	LEU
1	I	346	LEU
1	I	348	VAL
1	I	349	SER
1	I	362	TRP
1	I	364	ASP
1	I	372	SER
1	I	375	LEU
1	I	378	GLN
1	I	401	GLU
1	I	412	VAL
1	I	419	VAL
1	I	430	GLN
1	I	431	ARG
1	I	440	VAL
1	I	442	LEU
1	I	444	ARG
1	I	448	ASN

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Mol	Chain	Res	Type
1	I	450	VAL
1	I	454	THR
1	J	172	GLU
1	J	175	GLU
1	J	176	THR
1	J	177	ILE
1	J	186	LEU
1	J	192	VAL
1	J	199	LEU
1	J	206	LEU
1	J	207	THR
1	J	213	ASP
1	J	218	THR
1	J	227	THR
1	J	228	ASP
1	J	229	THR
1	J	231	THR
1	J	239	LEU
1	J	254	PHE
1	J	258	GLU
1	J	259	THR
1	J	264	ILE
1	J	269	PRO
1	J	270	LEU
1	J	274	ARG
1	J	284	GLU
1	J	289	THR
1	J	296	PRO
1	J	297	LYS
1	J	304	SER
1	J	334	LEU
1	J	346	LEU
1	J	348	VAL
1	J	349	SER
1	J	368	VAL
1	J	372	SER
1	J	375	LEU
1	J	378	GLN
1	J	401	GLU
1	J	405	ILE
1	J	406	VAL
1	J	412	VAL

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Mol	Chain	Res	Type
1	J	419	VAL
1	J	430	GLN
1	J	431	ARG
1	J	440	VAL
1	J	442	LEU
1	J	444	ARG
1	J	454	THR
1	K	165	SER
1	K	167	VAL
1	K	169	VAL
1	K	172	GLU
1	K	176	THR
1	K	177	ILE
1	K	184	ARG
1	K	186	LEU
1	K	188	LYS
1	K	191	VAL
1	K	192	VAL
1	K	199	LEU
1	K	207	THR
1	K	209	LEU
1	K	211	GLU
1	K	213	ASP
1	K	218	THR
1	K	227	THR
1	K	229	THR
1	K	231	THR
1	K	243	HIS
1	K	246	THR
1	K	256	THR
1	K	262	ASP
1	K	267	LEU
1	K	270	LEU
1	K	272	ARG
1	K	289	THR
1	K	295	LYS
1	K	300	LEU
1	K	334	LEU
1	K	346	LEU
1	K	348	VAL
1	K	362	TRP
1	K	364	ASP

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Mol	Chain	Res	Type
1	K	372	SER
1	K	375	LEU
1	K	378	GLN
1	K	404	VAL
1	K	405	ILE
1	K	412	VAL
1	K	419	VAL
1	K	430	GLN
1	K	431	ARG
1	K	440	VAL
1	K	444	ARG
1	K	448	ASN
1	K	454	THR
1	L	175	GLU
1	L	179	SER
1	L	182	ILE
1	L	183	ILE
1	L	186	LEU
1	L	192	VAL
1	L	199	LEU
1	L	209	LEU
1	L	233	GLU
1	L	242	ILE
1	L	243	HIS
1	L	249	LEU
1	L	255	ILE
1	L	264	ILE
1	L	267	LEU
1	L	270	LEU
1	L	274	ARG
1	L	284	GLU
1	L	289	THR
1	L	313	GLU
1	L	334	LEU
1	L	346	LEU
1	L	348	VAL
1	L	349	SER
1	L	365	VAL
1	L	368	VAL
1	L	372	SER
1	L	375	LEU
1	L	378	GLN

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Mol	Chain	Res	Type
1	L	401	GLU
1	L	404	VAL
1	L	407	TYR
1	L	412	VAL
1	L	419	VAL
1	L	430	GLN
1	L	431	ARG
1	L	440	VAL
1	L	442	LEU
1	L	444	ARG
1	L	448	ASN
1	L	450	VAL
1	L	454	THR
2	a	20	ILE
2	a	38	ARG
2	a	45	SER
2	a	48	THR
2	a	58	GLU
2	a	64	ILE
2	b	8	ARG
2	b	20	ILE
2	b	28	HIS
2	b	31	VAL
2	b	37	LEU
2	b	40	GLU
2	b	45	SER
2	b	48	THR
2	b	58	GLU
2	b	64	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	HIS
1	A	378	GLN
1	A	438	GLN
1	A	448	ASN
1	B	337	HIS
1	B	378	GLN
1	B	426	GLN
1	B	438	GLN
1	B	448	ASN

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Mol	Chain	Res	Type
1	C	378	GLN
1	C	438	GLN
1	D	243	HIS
1	D	378	GLN
1	D	438	GLN
1	D	448	ASN
1	E	163	GLN
1	E	363	GLN
1	E	378	GLN
1	F	162	ASN
1	F	163	GLN
1	F	378	GLN
1	F	430	GLN
1	F	448	ASN
1	G	243	HIS
1	G	438	GLN
1	G	448	ASN
1	H	279	HIS
1	H	378	GLN
1	H	438	GLN
1	H	443	GLN
1	H	448	ASN
1	I	163	GLN
1	I	378	GLN
1	I	398	ASN
1	J	363	GLN
1	J	378	GLN
1	J	438	GLN
1	K	378	GLN
1	K	448	ASN
1	L	180	GLN
1	L	279	HIS
1	L	378	GLN
1	L	448	ASN
2	b	19	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

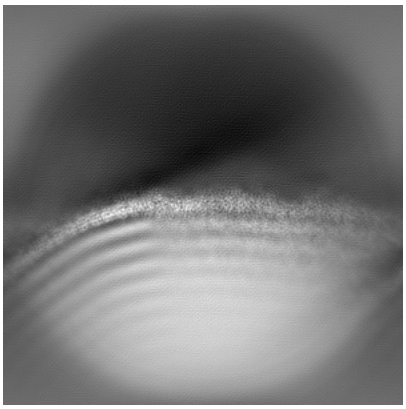
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60511. These allow visual inspection of the internal detail of the map and identification of artifacts.

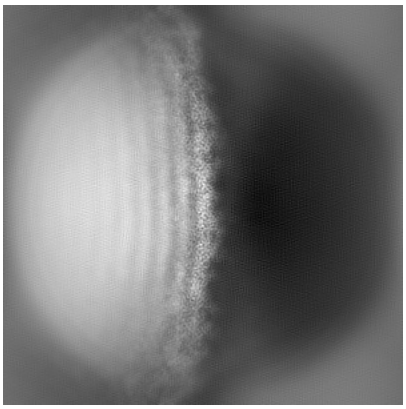
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

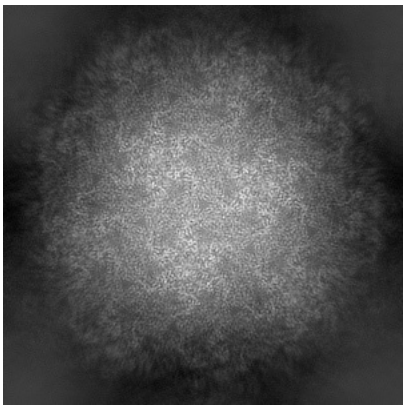
6.1.1 Primary map



X

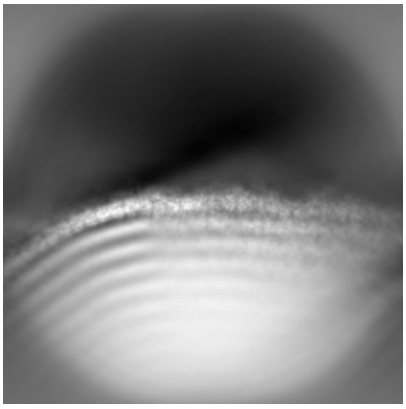


Y

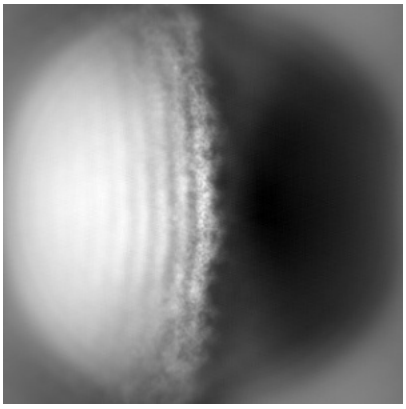


Z

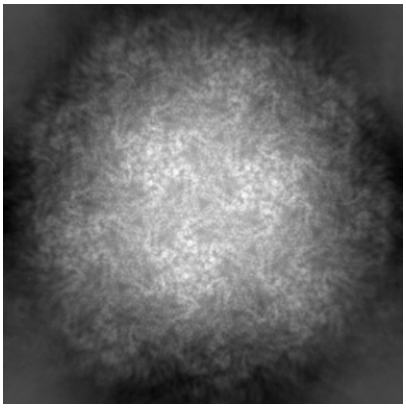
6.1.2 Raw map



X



Y

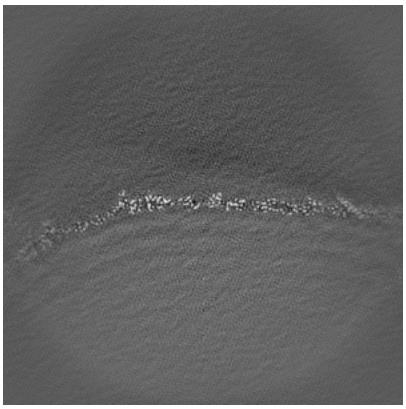


Z

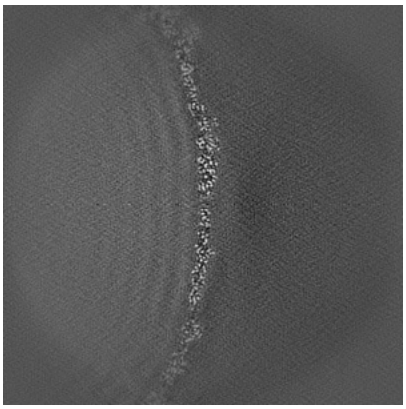
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

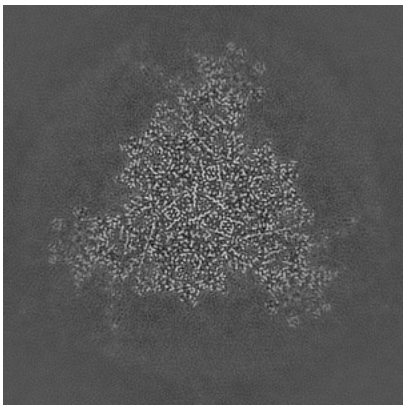
6.2.1 Primary map



X Index: 180

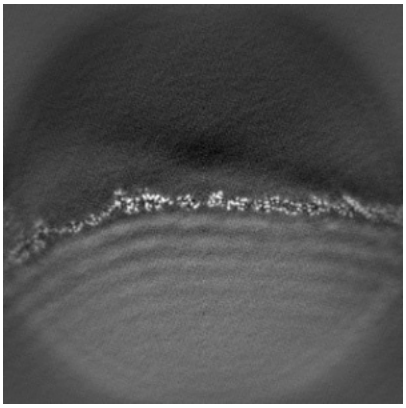


Y Index: 180

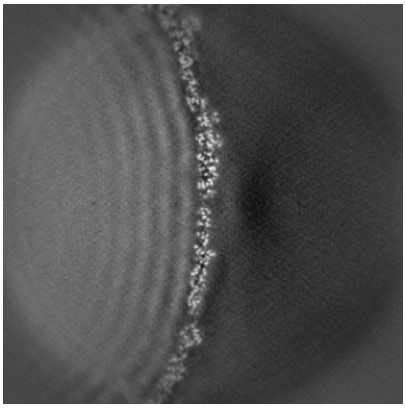


Z Index: 180

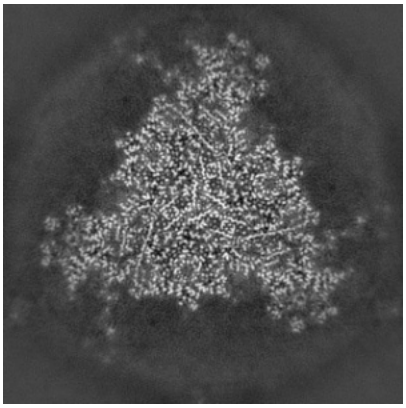
6.2.2 Raw map



X Index: 180



Y Index: 180

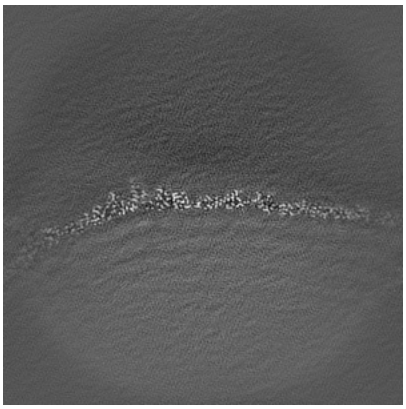


Z Index: 180

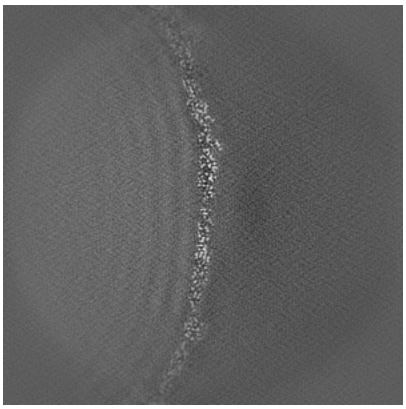
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

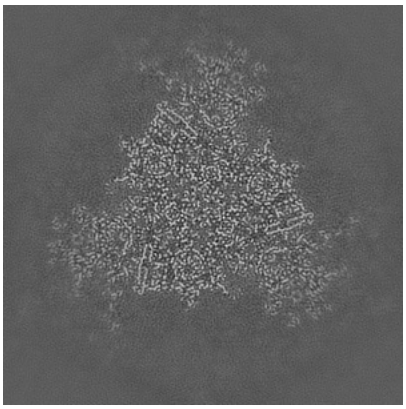
6.3.1 Primary map



X Index: 165

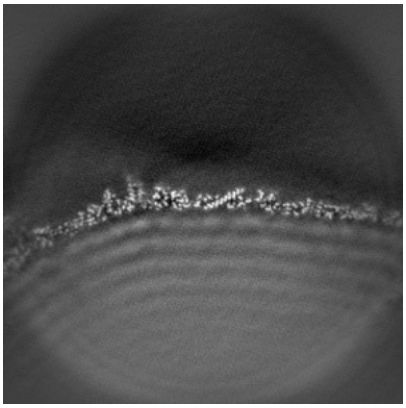


Y Index: 178

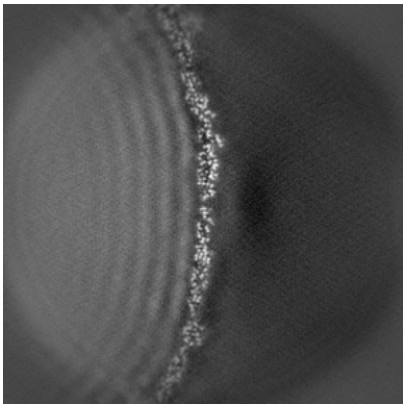


Z Index: 179

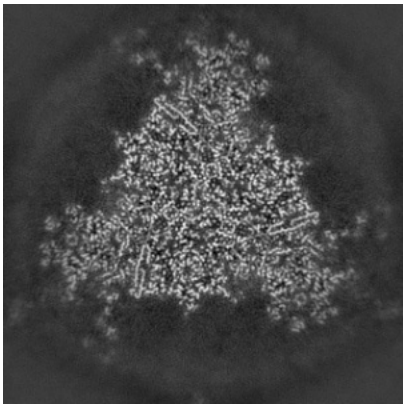
6.3.2 Raw map



X Index: 164



Y Index: 178

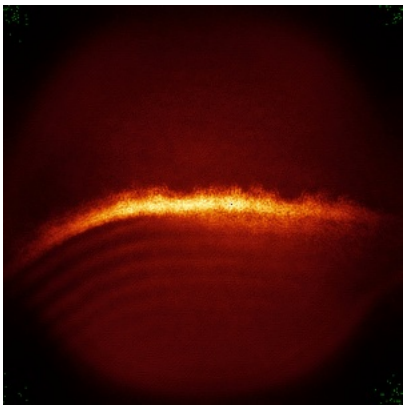


Z Index: 179

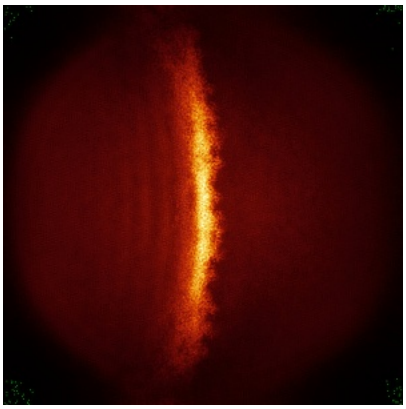
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

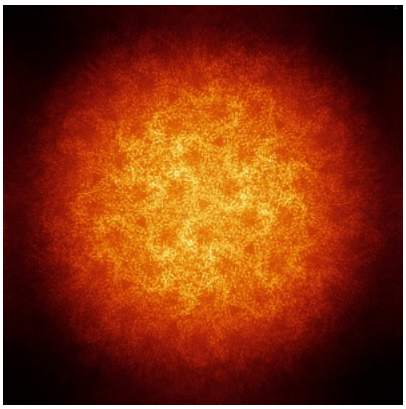
6.4.1 Primary map



X

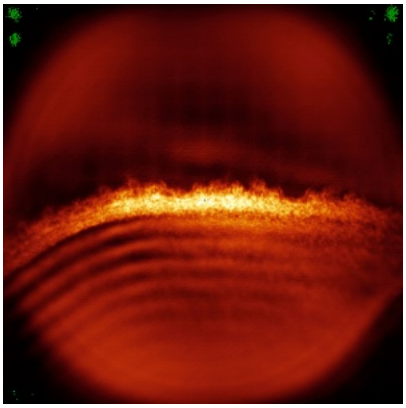


Y

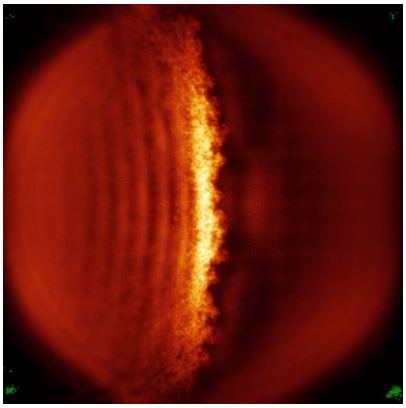


Z

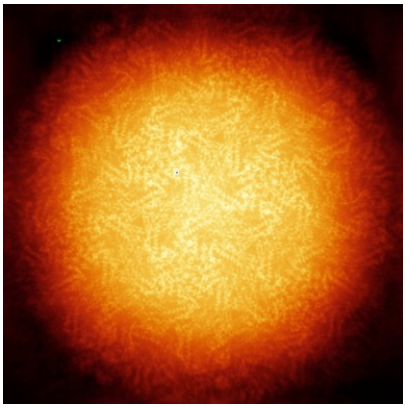
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

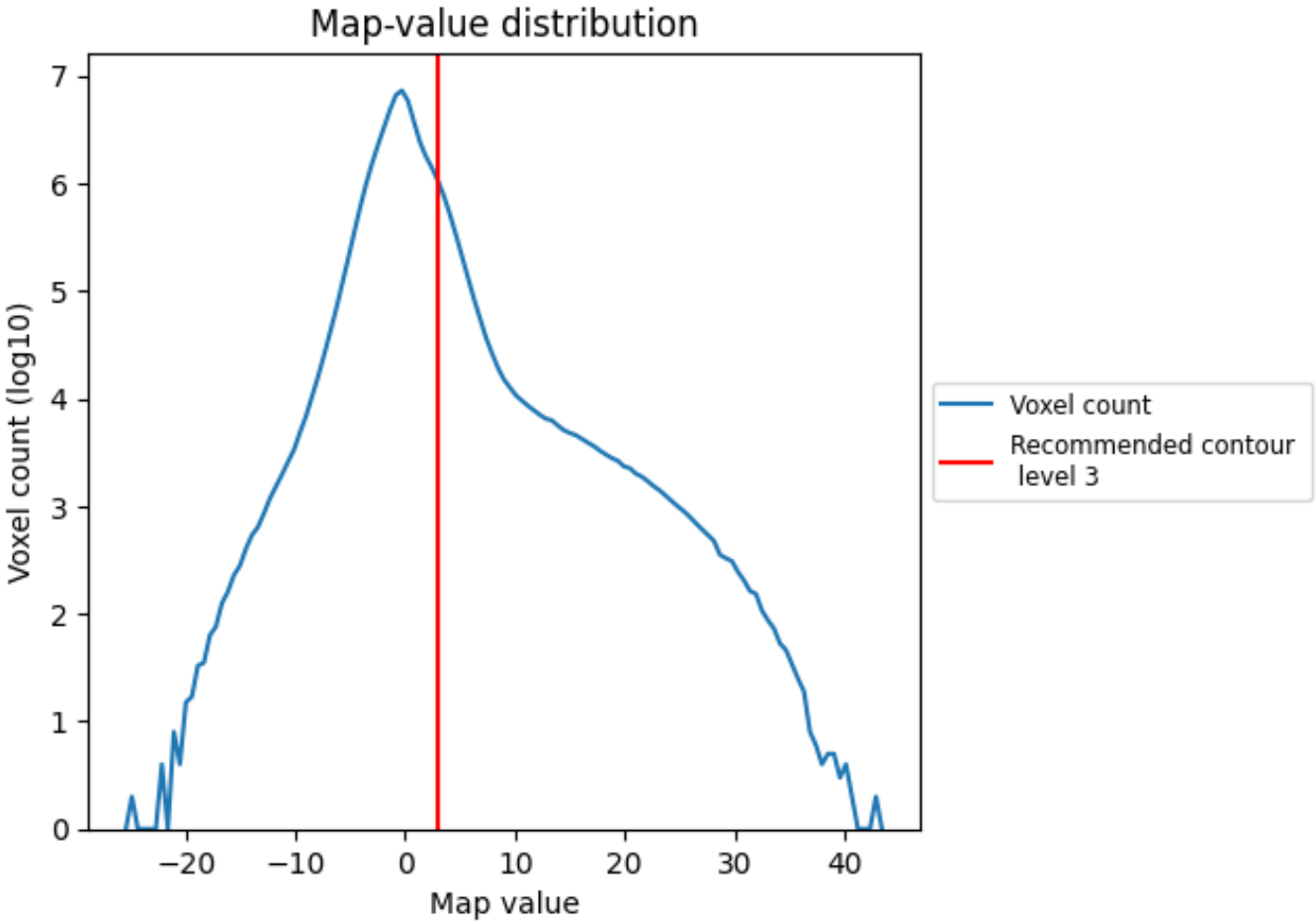
6.6 Mask visualisation (i)

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

7 Map analysis

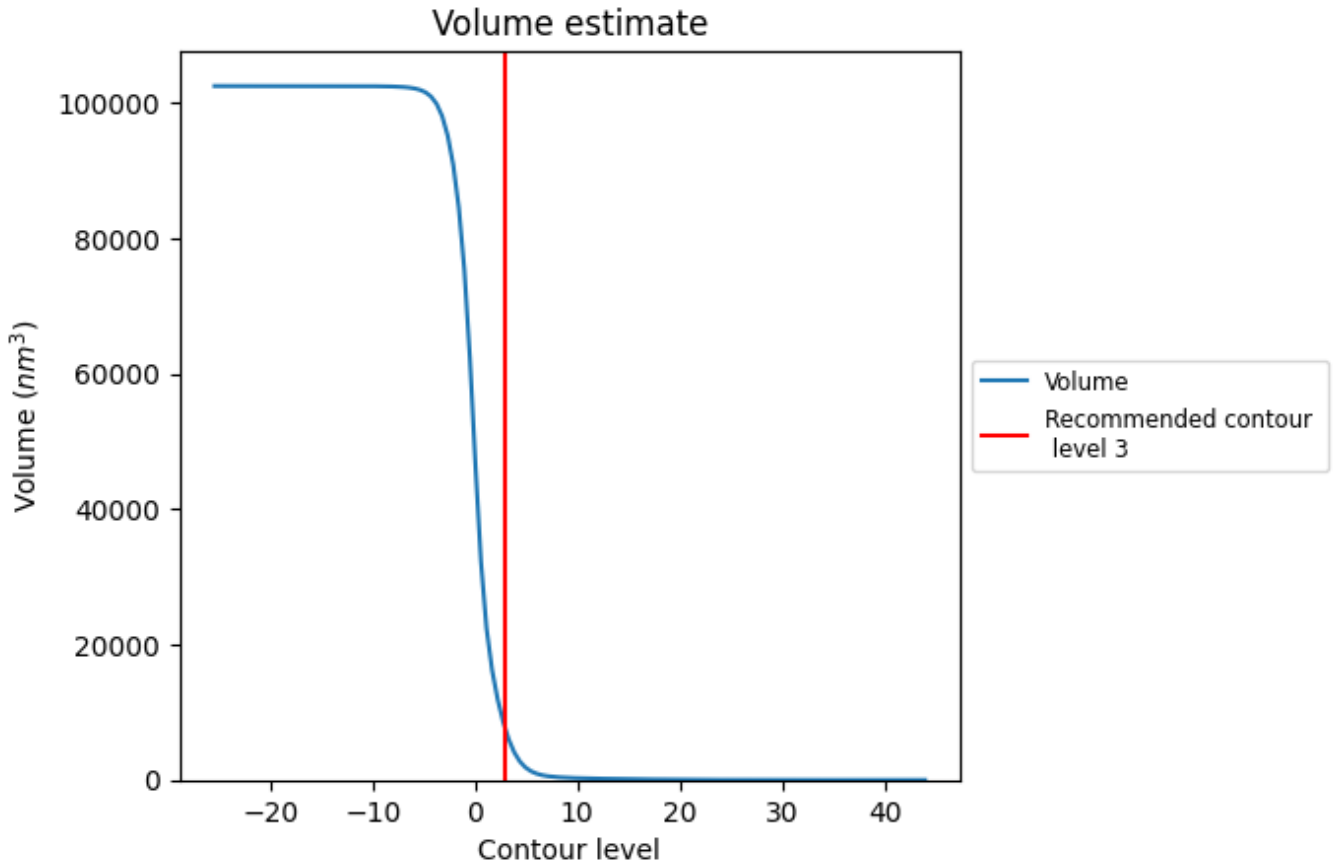
This section contains the results of statistical analysis of the map.

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.

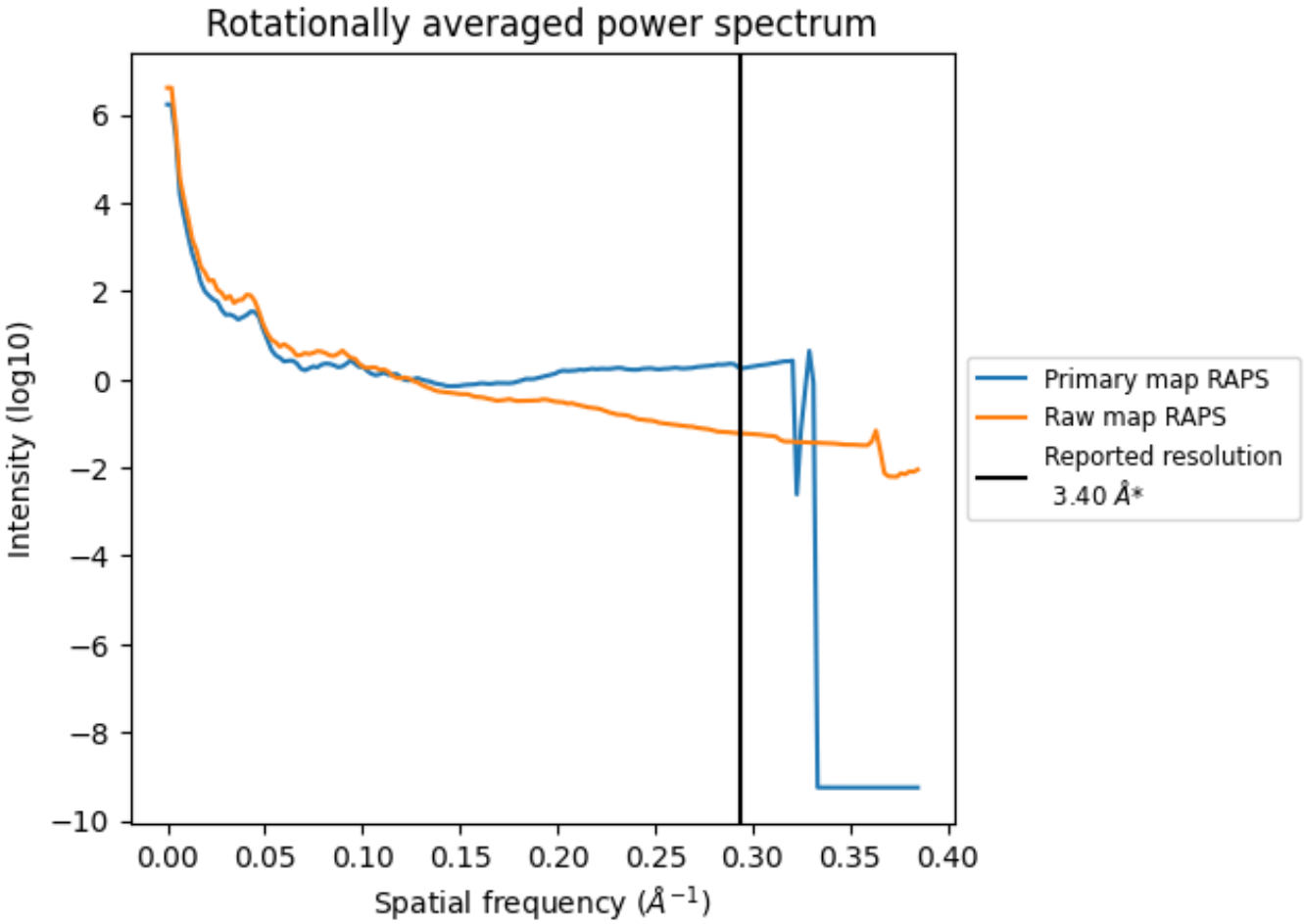
7.2 Volume estimate



The volume at the recommended contour level is 7420 nm^3; this corresponds to an approximate mass of 6703 kDa.

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

7.3 Rotationally averaged power spectrum (i)

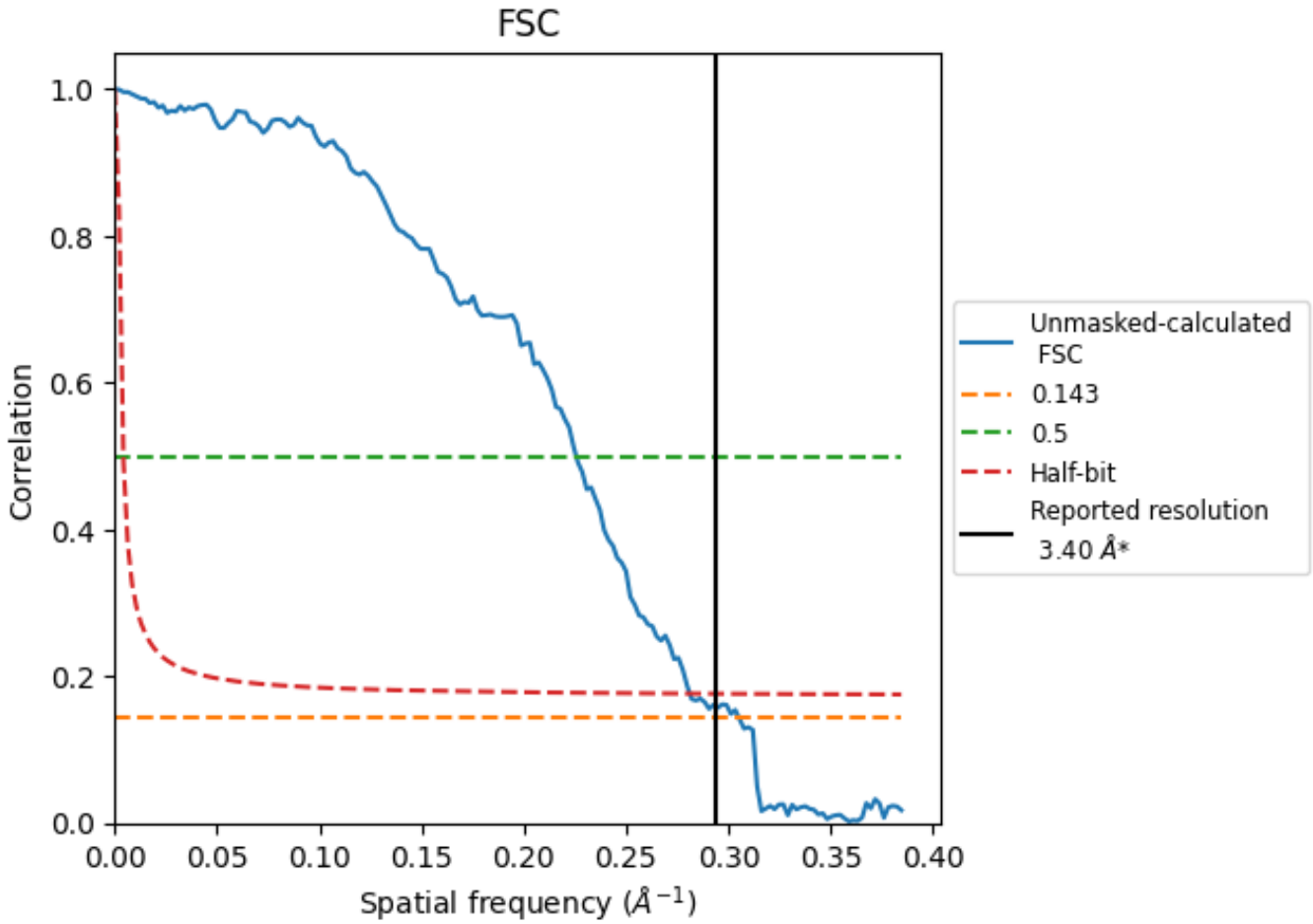


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	4.43	3.56

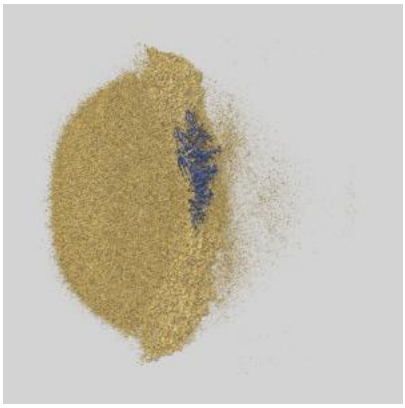
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

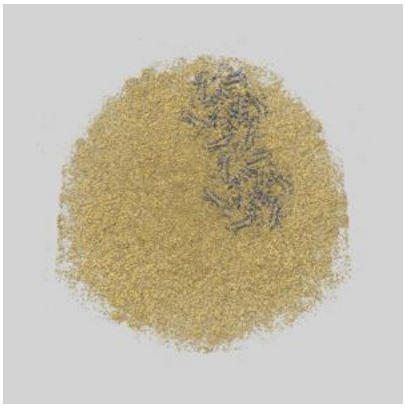
This section contains information regarding the fit between EMDB map EMD-60511 and PDB model 8ZVI. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay

X



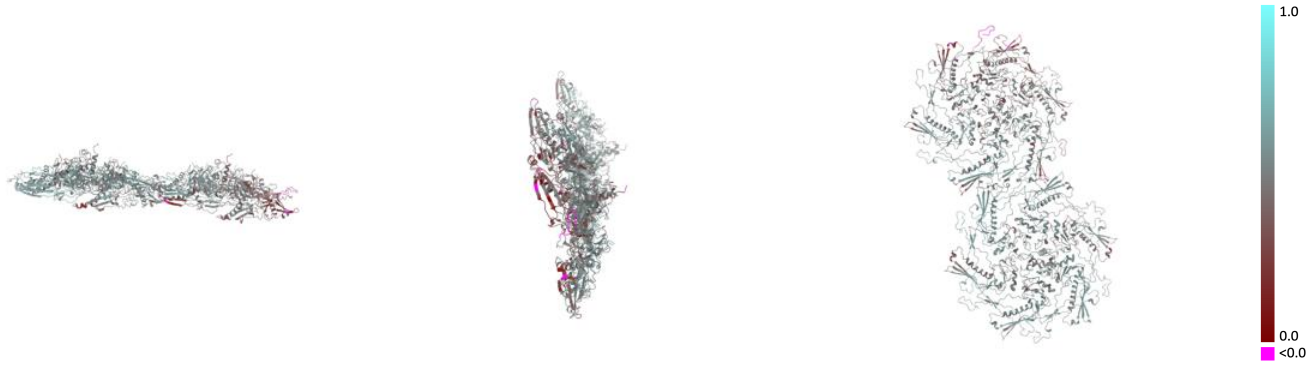
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

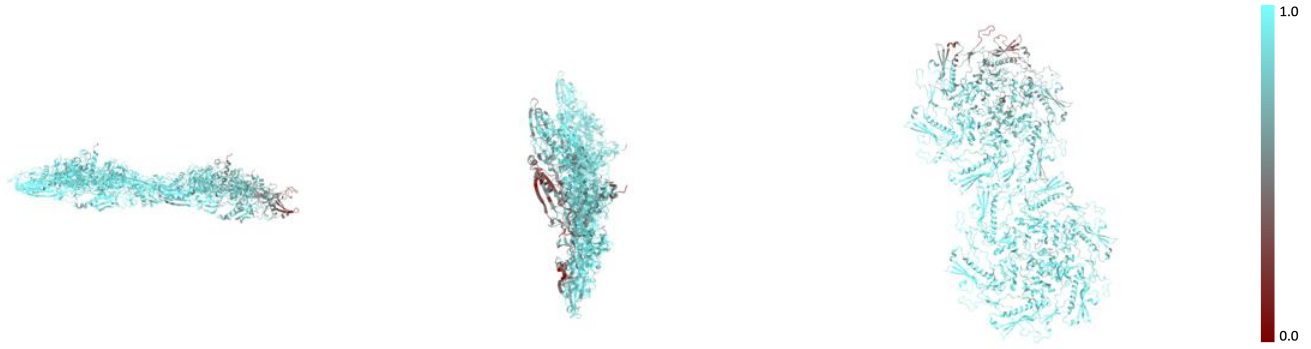
9.2 Q-score mapped to coordinate model (i)



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.

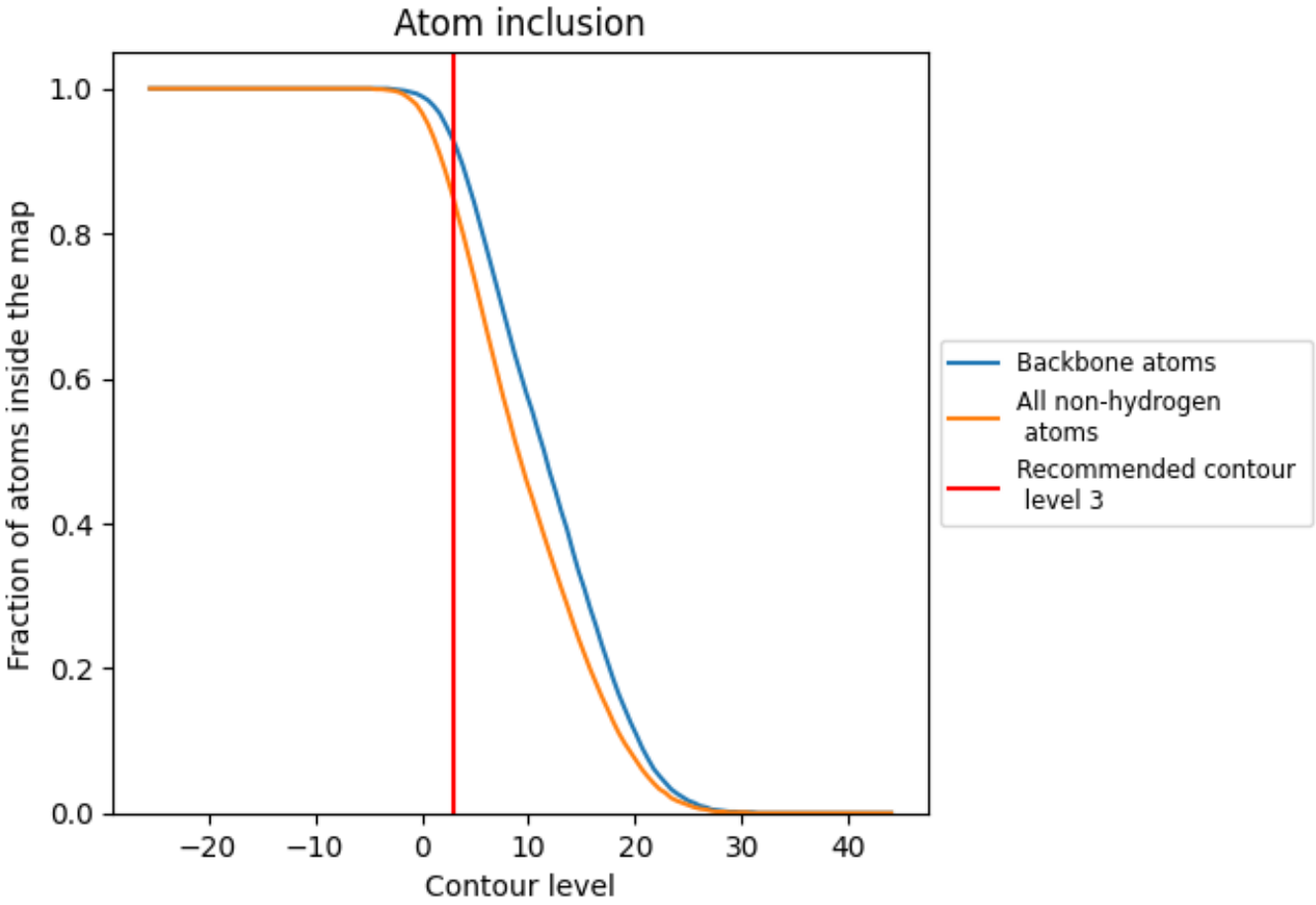
9.3 Atom inclusion mapped to coordinate model (i)



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 (3).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 85% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.4880
A	0.8740	0.4820
B	0.9140	0.5410
C	0.9340	0.5230
D	0.9250	0.5040
E	0.9400	0.5380
F	0.9190	0.5300
G	0.7040	0.4210
H	0.8430	0.4800
I	0.9100	0.5140
J	0.8880	0.5060
K	0.7200	0.4300
L	0.6200	0.3970
a	0.8800	0.4970
b	0.6820	0.4360