



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:27 AM UTC

PDB ID : 8XOT / pdb_00008xot
EMDB ID : EMD-38540
Title : Prohead portal of bacteriophage lambda
Authors : Wang, J.W.; Gu, Z.W.
Deposited on : 2024-01-02
Resolution : 3.51 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

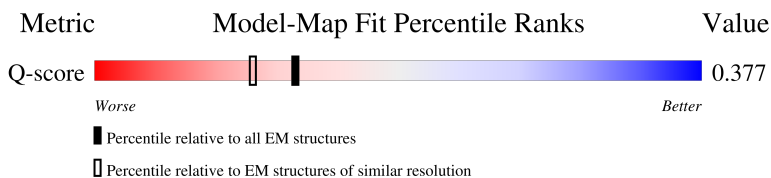
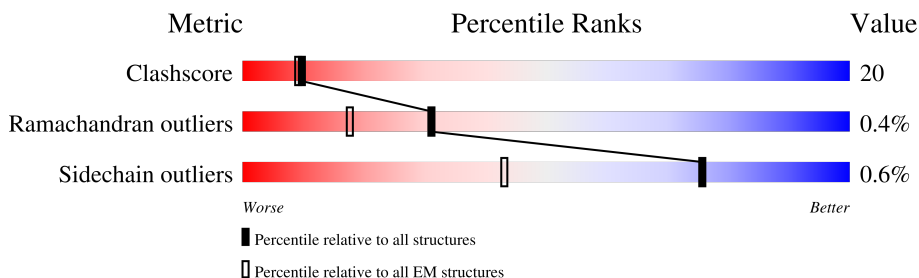
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.51 Å.

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



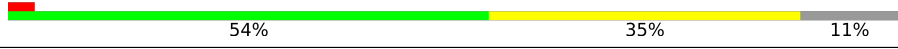
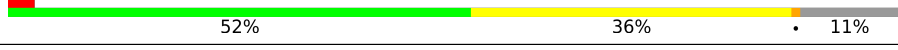
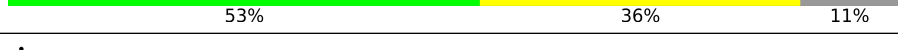
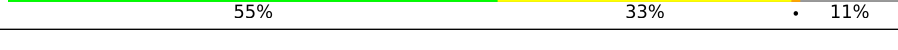
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13085 (3.01 - 4.01)

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

Mol	Chain	Length	Quality of chain
1	B	533	
1	B1	533	
1	B2	533	
1	B3	533	

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Mol	Chain	Length	Quality of chain
1	B4	533	
1	B5	533	
1	b	533	
1	b1	533	
1	b2	533	
1	b3	533	
1	b4	533	
1	b5	533	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 44532 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.

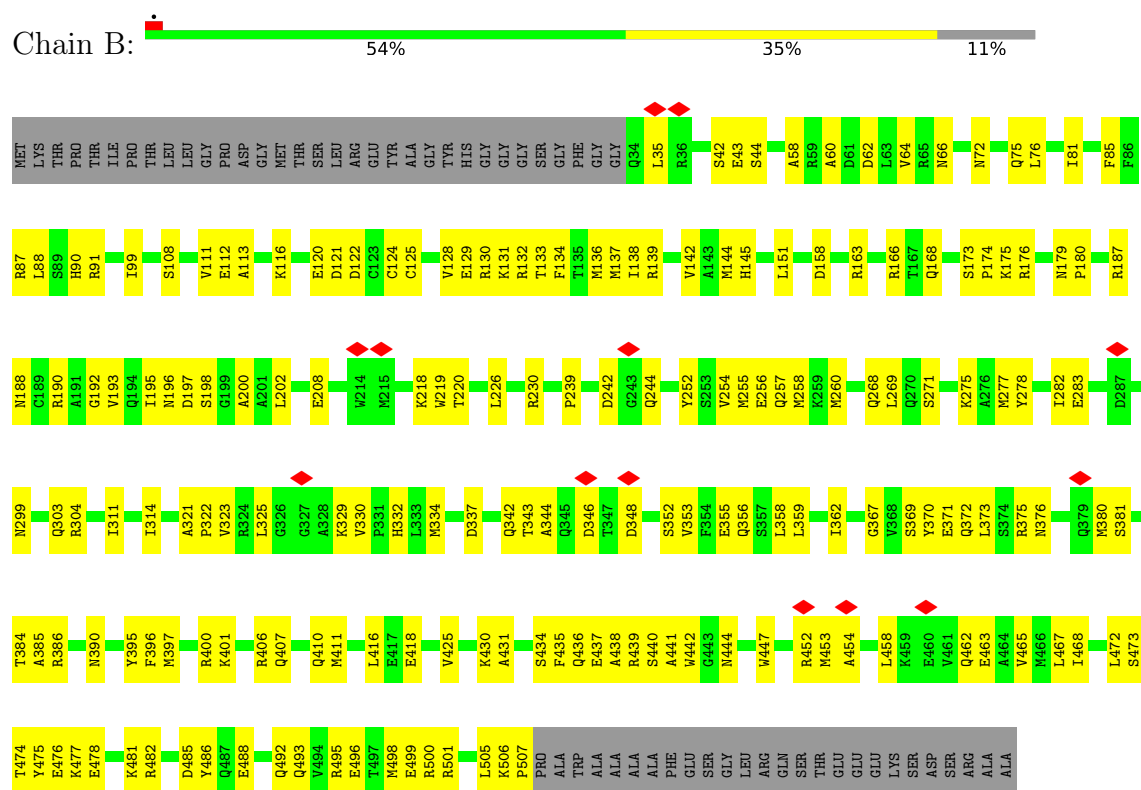
- Molecule 1 is a protein called Portal protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	474	Total 3711	C 2319	N 672	O 697	S 23	0	0
1	b	474	Total 3711	C 2319	N 672	O 697	S 23	0	0
1	B1	474	Total 3711	C 2319	N 672	O 697	S 23	0	0
1	b1	474	Total 3711	C 2319	N 672	O 697	S 23	0	0
1	B2	474	Total 3711	C 2319	N 672	O 697	S 23	0	0
1	b2	474	Total 3711	C 2319	N 672	O 697	S 23	0	0
1	B3	474	Total 3711	C 2319	N 672	O 697	S 23	0	0
1	b3	474	Total 3711	C 2319	N 672	O 697	S 23	0	0
1	B4	474	Total 3711	C 2319	N 672	O 697	S 23	0	0
1	b4	474	Total 3711	C 2319	N 672	O 697	S 23	0	0
1	B5	474	Total 3711	C 2319	N 672	O 697	S 23	0	0
1	b5	474	Total 3711	C 2319	N 672	O 697	S 23	0	0

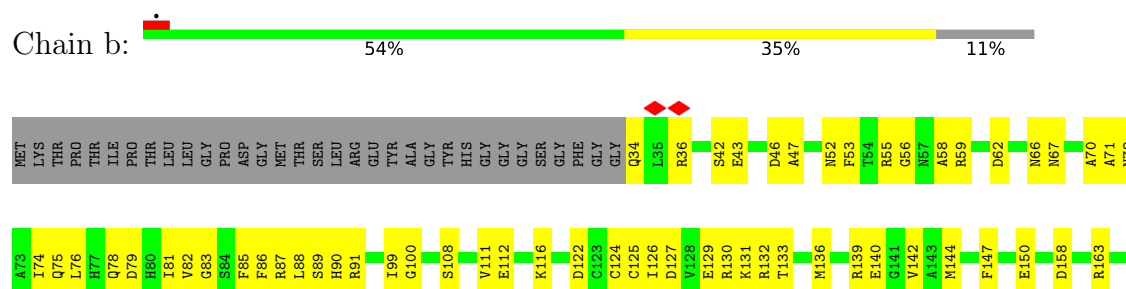
3 Residue-property plots

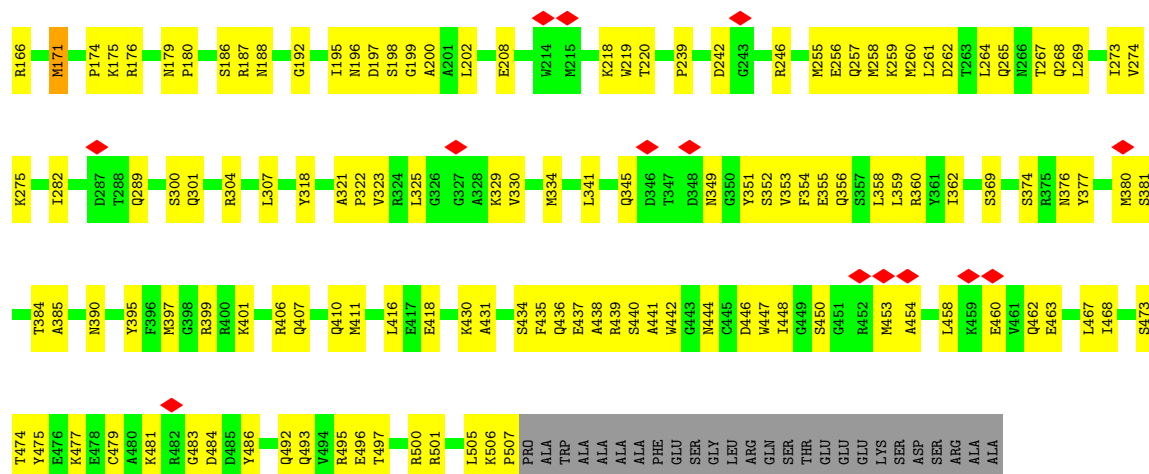
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Portal protein B

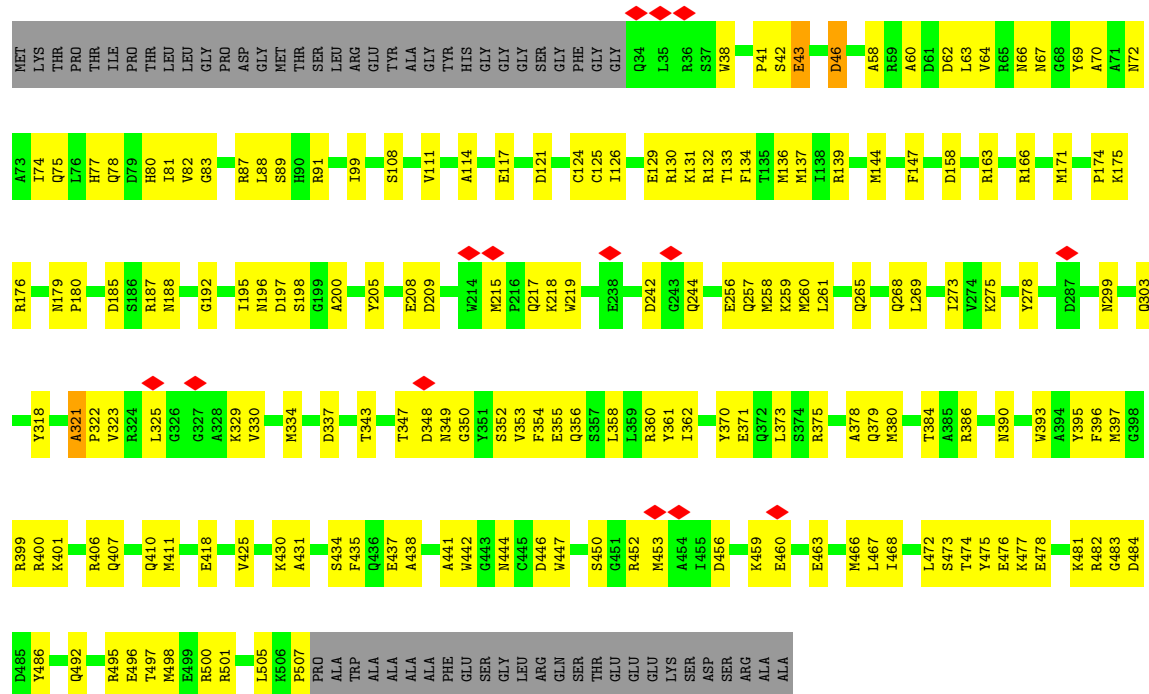


• Molecule 1: Portal protein B

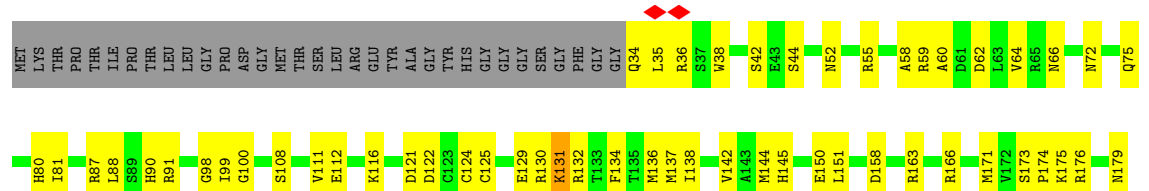


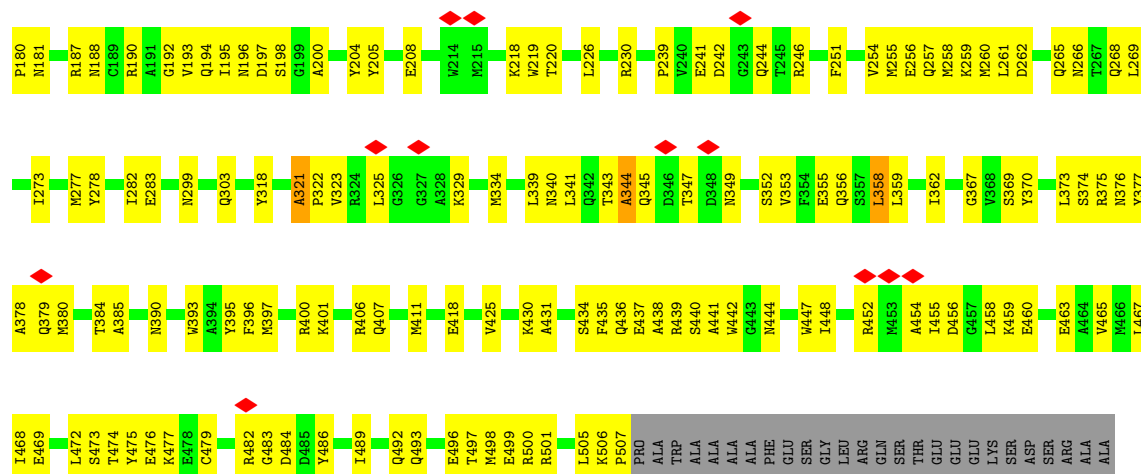


• Molecule 1: Portal protein B

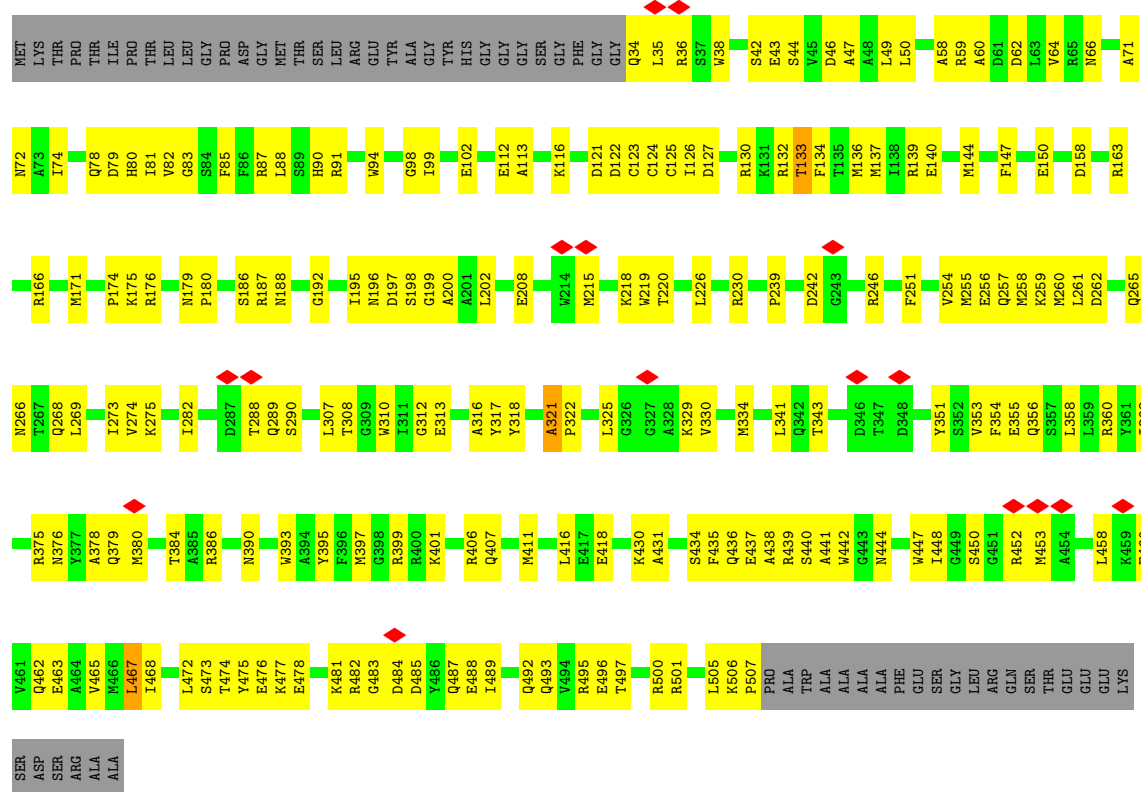


• Molecule 1: Portal protein B

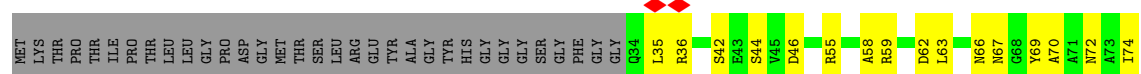


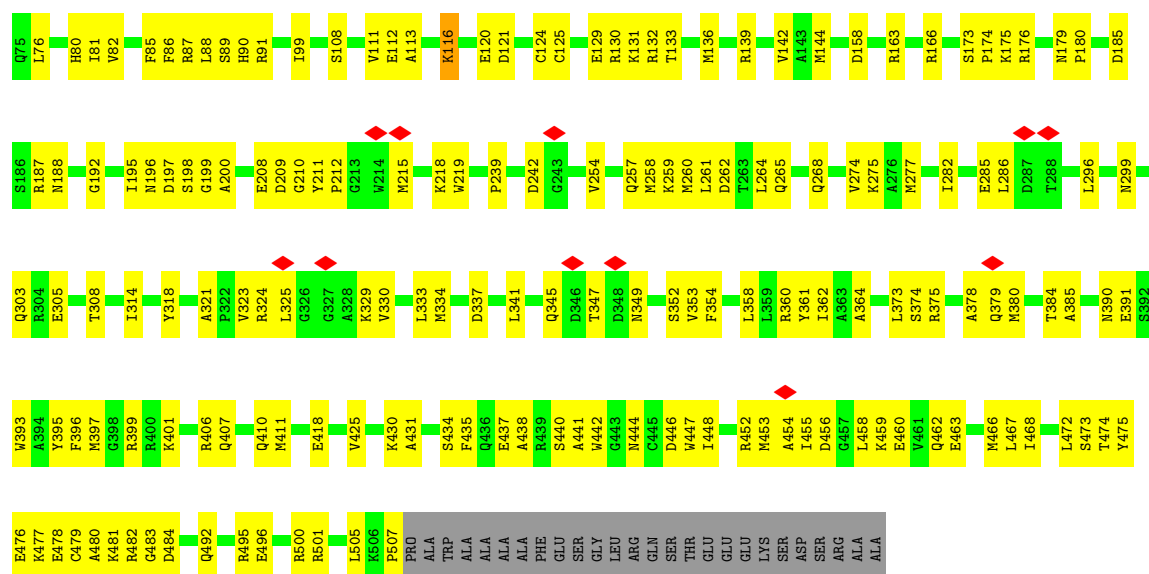


• Molecule 1: Portal protein B

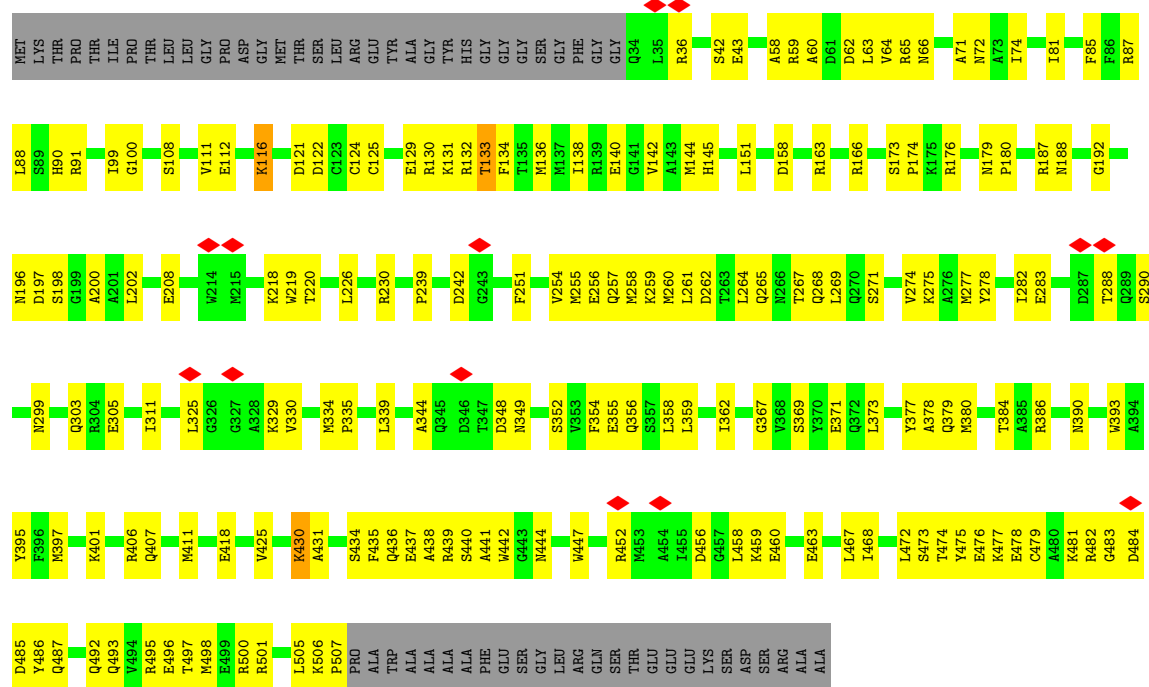


• Molecule 1: Portal protein B

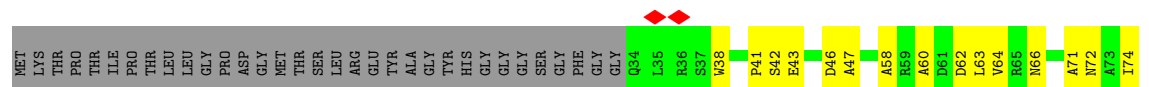


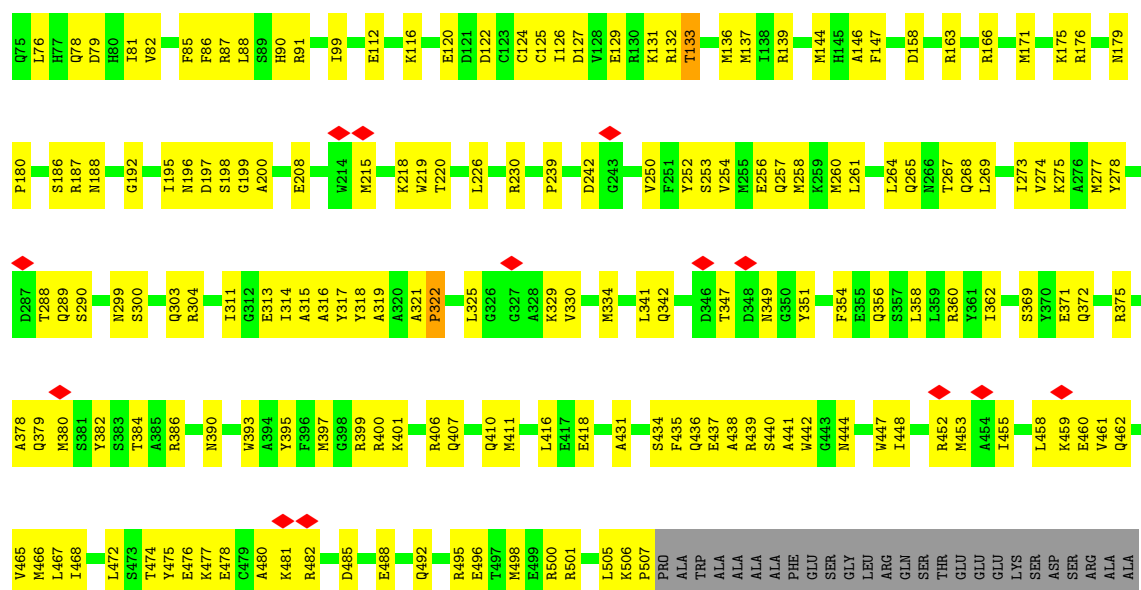


• Molecule 1: Portal protein B



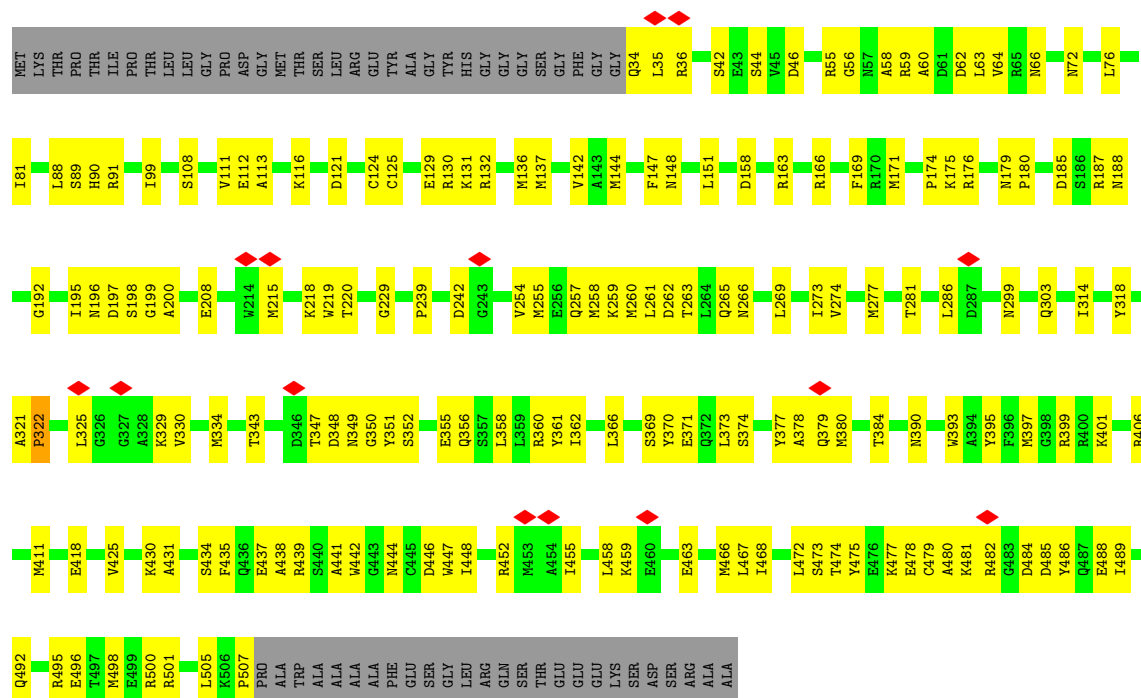
• Molecule 1: Portal protein B





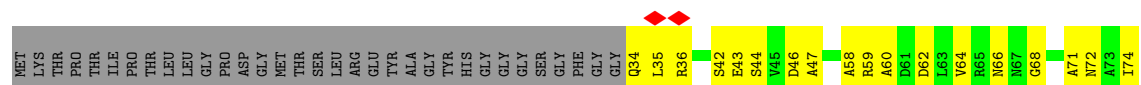
• Molecule 1: Portal protein B

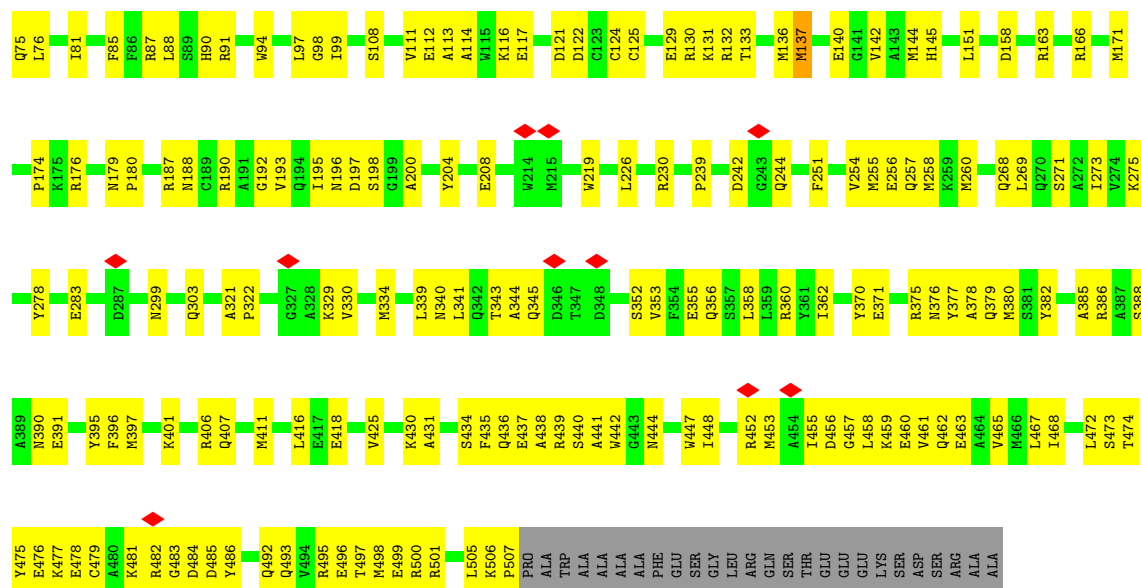
Chain B4: 56% 33% 11%



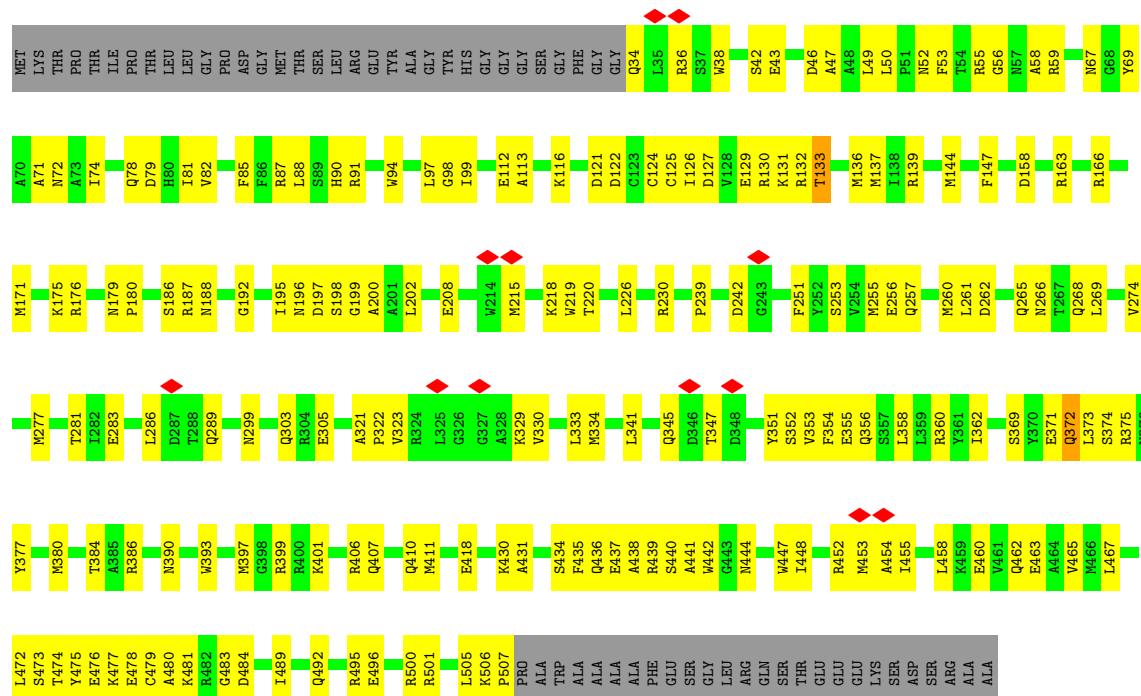
• Molecule 1: Portal protein B

Chain b4: 53% 36% 11%

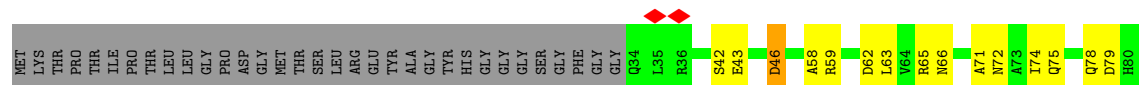




• Molecule 1: Portal protein B



• Molecule 1: Portal protein B



R482	G483	D484	D485	Y486	Q492	R495	E496	T497	M498	E499	R500	R501	L505	K506	P507	PRO	ALA	TRP	ALA	ALA	ALA	ALA	ALA	PHE	GLU	SER	GLY	LEU	ARG	GLN	SER	THR	GLU	GLU	GLU	LYS	SER	SER	ASP	SER	SER	ARG	ALA	ALA						
E391	S392	W393	A394	Y395	F396	M397	G398	R399	K401	R406	Q407	Q410	M411	E418	A431	S434	F435	Q436	E437	A438	R439	S440	A441	W442	G443	N444	W447	I448	R452	M453	A454	I455	L458	K459	E460	E463	L467	I468	S473	T474	Y475	E476	K477	E478	C479	A480	K481			
Q303	Y318	A321	P322	V323	R324	L325	G326	G327	A328	K329	V330	L333	M334	P335	L339	A344	Q345	D346	T347	D348	N349	S352	V353	F354	E355	Q356	S357	L358	L359	R360	Y361	I362	S369	Y370	E371	Q372	L373	S374	R375	M380	S381	Y382	S383	T384	A385	R386	A387	S388	A389	N390
P180	S186	R187	N188	G192	I195	N196	D197	S198	G199	A200	E208	D209	P212	G213	W214	M215	K218	W219	T220	P239	V240	E241	D242	G243	F251	Y252	S253	V254	M255	E256	Q257	M258	K259	M260	L261	Q265	Q268	L269	Q270	I273	V274	K275	Y278	D287	N299					
I81	V82	F86	R87	L88	S89	H90	R91	I99	S108	V111	E112	A113	A114	W115	K116	E117	D121	G124	C125	E129	R130	K131	R132	T133	F134	T135	M136	M137	T138	R139	V142	A143	M144	F147	N148	D158	T159	R163	R166	M171	P174	K175	R176	N179						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50921	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.120	Depositor
Minimum map value	-0.582	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	334.47424, 334.47424, 334.47424	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.30654, 1.30654, 1.30654	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	B	0.21	0/3793	0.42	0/5131
1	B1	0.21	0/3793	0.44	0/5131
1	B2	0.21	0/3793	0.45	0/5131
1	B3	0.22	0/3793	0.44	0/5131
1	B4	0.22	0/3793	0.47	0/5131
1	B5	0.22	0/3793	0.45	0/5131
1	b	0.21	0/3793	0.43	0/5131
1	b1	0.21	0/3793	0.42	0/5131
1	b2	0.22	0/3793	0.46	0/5131
1	b3	0.21	0/3793	0.45	0/5131
1	b4	0.21	0/3793	0.43	0/5131
1	b5	0.21	0/3793	0.42	0/5131
All	All	0.21	0/45516	0.44	0/61572

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	B1	0	1
1	B2	0	1
1	B4	0	1
1	B5	0	1
1	b1	0	1
1	b4	0	1
1	b5	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	321	ALA	Peptide
1	B1	321	ALA	Peptide
1	B2	321	ALA	Peptide
1	B4	321	ALA	Peptide
1	B5	321	ALA	Peptide
1	b1	321	ALA	Peptide
1	b4	321	ALA	Peptide
1	b5	321	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3711	0	3533	176	0
1	B1	3711	0	3533	150	0
1	B2	3711	0	3533	194	0
1	B3	3711	0	3533	156	0
1	B4	3711	0	3533	154	0
1	B5	3711	0	3533	170	0
1	b	3711	0	3533	156	0
1	b1	3711	0	3533	174	0
1	b2	3711	0	3533	174	0
1	b3	3711	0	3533	160	0
1	b4	3711	0	3533	158	0
1	b5	3711	0	3533	160	0
All	All	44532	0	42396	1713	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 20.

All (1713) 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:b3:257:GLN:HA	1:b3:260:MET:HE3	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b4:144:MET:HE3	1:b4:174:PRO:HD3	1.54	0.86
1:b2:501:ARG:HH21	1:b2:507:PRO:HD3	1.41	0.84
1:B1:133:THR:H	1:B1:136:MET:HE3	1.41	0.84
1:B:129:GLU:HG3	1:B:131:LYS:HZ1	1.45	0.81
1:B:133:THR:H	1:B:136:MET:HE3	1.45	0.81
1:B1:129:GLU:HG3	1:B1:131:LYS:HE3	1.64	0.79
1:b4:390:ASN:OD1	1:b4:452:ARG:NH2	2.16	0.78
1:b1:376:ASN:HB2	1:B2:360:ARG:HH22	1.49	0.78
1:B:144:MET:HE3	1:B:174:PRO:HD3	1.66	0.77
1:B:257:GLN:HA	1:B:260:MET:HE3	1.67	0.76
1:B4:257:GLN:HA	1:B4:260:MET:HE3	1.68	0.76
1:b:501:ARG:HH21	1:b:507:PRO:HD3	1.50	0.76
1:B2:87:ARG:HH22	1:B2:484:ASP:HA	1.51	0.76
1:b4:257:GLN:HA	1:b4:260:MET:HE3	1.65	0.75
1:b1:262:ASP:O	1:b1:266:ASN:ND2	2.18	0.75
1:B1:124:CYS:SG	1:b1:406:ARG:NH2	2.61	0.74
1:b1:474:THR:H	1:b1:477:LYS:HZ1	1.36	0.74
1:B5:501:ARG:HH21	1:B5:507:PRO:HD3	1.52	0.74
1:b:100:GLY:H	1:b:430:LYS:HZ1	1.34	0.74
1:B3:497:THR:HG22	1:B3:501:ARG:HE	1.52	0.74
1:B2:256:GLU:N	1:B2:256:GLU:OE2	2.21	0.74
1:B2:497:THR:HG22	1:B2:501:ARG:HE	1.52	0.74
1:B:129:GLU:HG3	1:B:131:LYS:NZ	2.01	0.73
1:B:406:ARG:NH2	1:b5:124:CYS:SG	2.61	0.73
1:b4:113:ALA:HA	1:b4:116:LYS:HE3	1.68	0.73
1:B5:124:CYS:SG	1:b5:406:ARG:NH2	2.62	0.73
1:B2:268:GLN:NE2	1:B2:268:GLN:O	2.21	0.73
1:B3:144:MET:HE3	1:B3:174:PRO:HD3	1.71	0.73
1:b2:268:GLN:OE1	1:b2:349:ASN:ND2	2.22	0.73
1:B5:59:ARG:HD3	1:B5:255:MET:HE1	1.70	0.73
1:b5:133:THR:H	1:b5:136:MET:HE3	1.53	0.73
1:B1:257:GLN:HA	1:B1:260:MET:HE3	1.70	0.73
1:B:87:ARG:HH12	1:B:485:ASP:HB2	1.53	0.72
1:b2:124:CYS:SG	1:B3:406:ARG:NH2	2.62	0.72
1:b:124:CYS:SG	1:B1:406:ARG:NH2	2.62	0.72
1:B4:482:ARG:NH2	1:b4:472:LEU:O	2.23	0.72
1:B:124:CYS:SG	1:b:406:ARG:NH2	2.63	0.72
1:b1:474:THR:H	1:b1:477:LYS:NZ	1.88	0.72
1:B4:124:CYS:SG	1:b4:406:ARG:NH2	2.63	0.72
1:b4:124:CYS:SG	1:B5:406:ARG:NH2	2.63	0.72
1:B2:98:GLY:O	1:B2:430:LYS:NZ	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B2:473:SER:HA	1:B2:477:LYS:HZ1	1.55	0.72
1:b3:474:THR:OG1	1:b3:477:LYS:NZ	2.21	0.72
1:b4:476:GLU:OE1	1:b4:476:GLU:N	2.21	0.72
1:b5:501:ARG:HG2	1:b5:507:PRO:HG3	1.71	0.71
1:b4:482:ARG:NH2	1:B5:472:LEU:O	2.22	0.71
1:b2:268:GLN:HG3	1:B3:354:PHE:CE1	2.25	0.71
1:B5:460:GLU:HA	1:B5:463:GLU:HG2	1.71	0.71
1:B:380:MET:HE1	1:B:384:THR:HB	1.71	0.71
1:B2:257:GLN:HA	1:B2:260:MET:HE3	1.73	0.71
1:b2:257:GLN:HA	1:b2:260:MET:HE3	1.72	0.71
1:b3:124:CYS:SG	1:B4:406:ARG:NH2	2.64	0.71
1:B:482:ARG:HH12	1:b:467:LEU:HD11	1.53	0.71
1:b5:356:GLN:HE21	1:b5:360:ARG:NH2	1.88	0.71
1:b:197:ASP:OD1	1:b:198:SER:N	2.24	0.71
1:b:256:GLU:N	1:b:256:GLU:OE2	2.23	0.71
1:B1:323:VAL:H	1:B1:329:LYS:HZ2	1.37	0.71
1:B2:197:ASP:OD1	1:B2:198:SER:N	2.24	0.71
1:B2:501:ARG:HG2	1:B2:507:PRO:HG3	1.71	0.71
1:b3:275:LYS:NZ	1:B4:347:THR:OG1	2.24	0.70
1:b5:334:MET:HE3	1:b5:335:PRO:HD2	1.71	0.70
1:B1:482:ARG:NH2	1:b1:472:LEU:O	2.24	0.70
1:B1:501:ARG:HG2	1:B1:507:PRO:HG3	1.73	0.70
1:b3:112:GLU:C	1:b3:116:LYS:HZ2	1.98	0.70
1:B3:124:CYS:SG	1:b3:406:ARG:NH2	2.65	0.70
1:B2:218:LYS:NZ	1:B2:220:THR:OG1	2.24	0.70
1:b4:352:SER:HB3	1:B5:353:VAL:HG21	1.74	0.70
1:B3:474:THR:H	1:B3:477:LYS:NZ	1.89	0.70
1:B4:129:GLU:HG3	1:B4:131:LYS:HE3	1.72	0.70
1:B2:125:CYS:SG	1:B2:130:ARG:NH1	2.65	0.70
1:b3:474:THR:H	1:b3:477:LYS:HZ3	1.39	0.70
1:B5:256:GLU:OE2	1:B5:256:GLU:N	2.25	0.70
1:b:85:PHE:HE2	1:b:87:ARG:HE	1.38	0.69
1:b1:374:SER:O	1:B2:360:ARG:NH2	2.26	0.69
1:B1:87:ARG:NH2	1:B1:483:GLY:O	2.25	0.69
1:b3:99:ILE:HD11	1:b3:431:ALA:HA	1.74	0.69
1:b4:356:GLN:HB3	1:b4:360:ARG:HH12	1.57	0.69
1:B:474:THR:H	1:B:477:LYS:HZ2	1.40	0.69
1:b1:454:ALA:O	1:B2:390:ASN:ND2	2.26	0.69
1:b2:458:LEU:HD21	1:B3:459:LYS:HB3	1.73	0.69
1:B2:124:CYS:SG	1:b2:406:ARG:NH2	2.65	0.69
1:b4:497:THR:OG1	1:b4:501:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b1:124:CYS:SG	1:B2:406:ARG:NH2	2.66	0.69
1:b1:257:GLN:HA	1:b1:260:MET:HE3	1.75	0.69
1:B1:269:LEU:HD22	1:b1:260:MET:HB3	1.75	0.68
1:B5:43:GLU:OE1	1:B5:43:GLU:N	2.25	0.68
1:B1:476:GLU:OE2	1:B1:476:GLU:N	2.25	0.68
1:b4:269:LEU:HD22	1:B5:260:MET:HB3	1.75	0.68
1:B1:82:VAL:HG21	1:B1:139:ARG:HG2	1.75	0.68
1:b3:380:MET:SD	1:b3:384:THR:OG1	2.50	0.68
1:b3:278:TYR:HE2	1:B4:277:MET:HE2	1.57	0.68
1:B1:497:THR:HG22	1:B1:501:ARG:HE	1.58	0.68
1:B3:277:MET:HA	1:B3:277:MET:HE3	1.76	0.68
1:b:257:GLN:HA	1:b:260:MET:HE3	1.74	0.68
1:b:474:THR:H	1:b:477:LYS:HZ2	1.40	0.68
1:B3:474:THR:H	1:B3:477:LYS:HZ1	1.40	0.68
1:b:323:VAL:H	1:b:329:LYS:HZ2	1.40	0.67
1:B2:467:LEU:HB3	1:B2:473:SER:HB2	1.74	0.67
1:B4:474:THR:H	1:B4:477:LYS:NZ	1.92	0.67
1:B5:197:ASP:OD1	1:B5:198:SER:N	2.27	0.67
1:B2:79:ASP:OD1	1:B2:139:ARG:NH2	2.22	0.67
1:b4:58:ALA:HB2	1:B5:42:SER:HB3	1.74	0.67
1:B:352:SER:HB3	1:b:353:VAL:HG21	1.77	0.67
1:b2:474:THR:H	1:b2:477:LYS:NZ	1.93	0.67
1:b3:501:ARG:HG2	1:b3:507:PRO:HG3	1.75	0.67
1:B4:197:ASP:OD1	1:B4:198:SER:N	2.27	0.67
1:B4:474:THR:H	1:B4:477:LYS:HZ1	1.40	0.67
1:B:474:THR:H	1:B:477:LYS:NZ	1.93	0.67
1:B1:58:ALA:HB2	1:b1:42:SER:HB3	1.77	0.67
1:b:275:LYS:NZ	1:B1:347:THR:OG1	2.27	0.67
1:B2:196:ASN:OD1	1:B2:200:ALA:N	2.28	0.67
1:b2:197:ASP:OD2	1:b2:198:SER:N	2.28	0.67
1:b3:197:ASP:OD1	1:b3:198:SER:N	2.28	0.67
1:b4:72:ASN:O	1:b4:76:LEU:HD12	1.94	0.67
1:b2:144:MET:HE2	1:b2:174:PRO:HD3	1.76	0.67
1:B:380:MET:HE3	1:B:381:SER:N	2.10	0.66
1:b5:474:THR:H	1:b5:477:LYS:NZ	1.92	0.66
1:b4:493:GLN:O	1:b4:497:THR:HG23	1.96	0.66
1:B5:58:ALA:HB2	1:b5:42:SER:HB3	1.76	0.66
1:b:352:SER:HB3	1:B1:353:VAL:HG21	1.78	0.66
1:B1:132:ARG:HD3	1:b1:239:PRO:HG2	1.77	0.66
1:B2:262:ASP:O	1:B2:266:ASN:ND2	2.28	0.66
1:B:99:ILE:HD11	1:B:431:ALA:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:209:ASP:OD2	1:b1:187:ARG:NH2	2.27	0.66
1:b2:87:ARG:HH22	1:b2:484:ASP:HA	1.60	0.66
1:b:58:ALA:HB2	1:B1:42:SER:HB3	1.77	0.66
1:B2:58:ALA:HB2	1:b2:42:SER:HB3	1.77	0.66
1:B2:356:GLN:O	1:B2:360:ARG:HG3	1.95	0.66
1:B3:58:ALA:HB2	1:b3:42:SER:HB3	1.77	0.66
1:B5:262:ASP:O	1:B5:266:ASN:ND2	2.28	0.66
1:b2:482:ARG:NH2	1:B3:472:LEU:O	2.29	0.66
1:b5:257:GLN:HA	1:b5:260:MET:HE3	1.76	0.66
1:b1:218:LYS:NZ	1:b1:220:THR:OG1	2.29	0.66
1:b2:380:MET:HE2	1:b2:380:MET:HA	1.78	0.66
1:b5:497:THR:HG22	1:b5:501:ARG:HE	1.60	0.66
1:b:72:ASN:O	1:b:76:LEU:HD12	1.95	0.66
1:B1:176:ARG:HH21	1:B1:208:GLU:HA	1.62	0.66
1:B3:401:LYS:O	1:B3:401:LYS:NZ	2.25	0.66
1:b3:356:GLN:HB3	1:b3:360:ARG:HH12	1.59	0.66
1:b3:378:ALA:O	1:b3:379:GLN:NE2	2.29	0.66
1:B:475:TYR:N	1:b5:496:GLU:OE2	2.30	0.65
1:B2:401:LYS:O	1:B2:401:LYS:NZ	2.26	0.65
1:b2:113:ALA:HA	1:b2:116:LYS:NZ	2.12	0.65
1:b3:256:GLU:HG2	1:b3:260:MET:HE2	1.77	0.65
1:b4:275:LYS:NZ	1:B5:347:THR:OG1	2.27	0.65
1:B5:467:LEU:HD12	1:B5:473:SER:HB2	1.76	0.65
1:B:72:ASN:O	1:B:76:LEU:HD12	1.95	0.65
1:b:401:LYS:O	1:b:401:LYS:NZ	2.28	0.65
1:b4:401:LYS:O	1:b4:401:LYS:NZ	2.27	0.65
1:B5:97:LEU:O	1:B5:430:LYS:NZ	2.29	0.65
1:b5:369:SER:OG	1:b5:372:GLN:OE1	2.11	0.65
1:b1:377:TYR:HB3	1:B2:384:THR:HB	1.78	0.65
1:b5:197:ASP:OD1	1:b5:198:SER:N	2.29	0.65
1:B:218:LYS:NZ	1:B:220:THR:OG1	2.28	0.65
1:B3:158:ASP:OD2	1:B3:163:ARG:NH1	2.30	0.65
1:B1:197:ASP:OD2	1:B1:198:SER:N	2.29	0.65
1:B2:378:ALA:O	1:B2:379:GLN:NE2	2.30	0.65
1:b4:474:THR:OG1	1:b4:477:LYS:NZ	2.29	0.65
1:B4:58:ALA:HB2	1:b4:42:SER:HB3	1.78	0.65
1:b1:158:ASP:OD2	1:b1:163:ARG:NH1	2.30	0.65
1:b1:380:MET:HE2	1:b1:380:MET:HA	1.79	0.65
1:b3:176:ARG:HH21	1:b3:208:GLU:HA	1.62	0.65
1:B4:358:LEU:O	1:B4:362:ILE:HD12	1.97	0.65
1:B3:129:GLU:HG3	1:B3:131:LYS:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b5:158:ASP:OD2	1:b5:163:ARG:NH1	2.30	0.64
1:b1:176:ARG:HH21	1:b1:208:GLU:HA	1.62	0.64
1:b4:158:ASP:OD2	1:b4:163:ARG:NH1	2.30	0.64
1:B5:474:THR:H	1:B5:477:LYS:HZ1	1.44	0.64
1:b5:401:LYS:O	1:b5:401:LYS:NZ	2.26	0.64
1:B1:158:ASP:OD2	1:B1:163:ARG:NH1	2.30	0.64
1:B3:257:GLN:HA	1:B3:260:MET:HE3	1.79	0.64
1:B5:274:VAL:HA	1:B5:277:MET:HG2	1.80	0.64
1:B1:401:LYS:O	1:B1:401:LYS:NZ	2.25	0.64
1:B:501:ARG:HH21	1:B:507:PRO:HD3	1.62	0.64
1:b2:467:LEU:HD12	1:b2:473:SER:HB2	1.79	0.64
1:b2:55:ARG:HH12	1:B3:36:ARG:HH12	1.46	0.64
1:b2:434:SER:N	1:b2:437:GLU:OE1	2.30	0.64
1:b3:158:ASP:OD2	1:b3:163:ARG:NH1	2.31	0.64
1:B4:269:LEU:HD22	1:b4:260:MET:HB3	1.79	0.64
1:b4:474:THR:H	1:b4:477:LYS:HZ1	1.45	0.64
1:B:454:ALA:O	1:b:390:ASN:ND2	2.30	0.64
1:b:176:ARG:HH21	1:b:208:GLU:HA	1.63	0.64
1:b2:158:ASP:OD2	1:b2:163:ARG:NH1	2.29	0.64
1:b2:401:LYS:O	1:b2:401:LYS:NZ	2.25	0.64
1:b4:496:GLU:OE2	1:B5:475:TYR:N	2.31	0.64
1:B:58:ALA:HB2	1:b:42:SER:HB3	1.80	0.64
1:B1:91:ARG:O	1:B1:444:ASN:ND2	2.31	0.64
1:b1:397:MET:HA	1:b1:397:MET:HE3	1.80	0.64
1:B4:158:ASP:OD2	1:B4:163:ARG:NH1	2.31	0.64
1:B:472:LEU:O	1:b5:482:ARG:NH2	2.31	0.63
1:B1:46:ASP:OD2	1:B1:46:ASP:N	2.31	0.63
1:B3:99:ILE:HD11	1:B3:431:ALA:HA	1.81	0.63
1:b5:358:LEU:O	1:b5:362:ILE:HD12	1.98	0.63
1:b:196:ASN:OD1	1:b:200:ALA:N	2.30	0.63
1:B5:176:ARG:HH21	1:B5:208:GLU:HA	1.63	0.63
1:B:176:ARG:HH21	1:B:208:GLU:HA	1.63	0.63
1:b1:436:GLN:OE1	1:b1:439:ARG:NH1	2.32	0.63
1:b2:91:ARG:O	1:b2:444:ASN:ND2	2.30	0.63
1:B3:197:ASP:OD1	1:B3:198:SER:N	2.32	0.63
1:B4:218:LYS:NZ	1:B4:220:THR:OG1	2.30	0.63
1:B:436:GLN:OE1	1:B:439:ARG:NH1	2.32	0.63
1:b:218:LYS:NZ	1:b:220:THR:OG1	2.31	0.63
1:B:158:ASP:OD2	1:B:163:ARG:NH1	2.30	0.63
1:b:473:SER:OG	1:b:477:LYS:NZ	2.26	0.63
1:b1:58:ALA:HB2	1:B2:42:SER:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b1:129:GLU:HG3	1:b1:131:LYS:HZ2	1.63	0.63
1:B2:85:PHE:HE1	1:B2:87:ARG:HE	1.46	0.63
1:B5:474:THR:H	1:B5:477:LYS:NZ	1.95	0.63
1:b4:197:ASP:OD1	1:b4:198:SER:N	2.32	0.62
1:B1:275:LYS:HE2	1:b1:349:ASN:HA	1.81	0.62
1:b4:436:GLN:OE1	1:b4:439:ARG:NH1	2.32	0.62
1:b5:91:ARG:O	1:b5:444:ASN:ND2	2.32	0.62
1:B:390:ASN:OD1	1:B:452:ARG:NH2	2.32	0.62
1:B2:158:ASP:OD2	1:B2:163:ARG:NH1	2.32	0.62
1:B3:275:LYS:NZ	1:b3:347:THR:OG1	2.33	0.62
1:b5:323:VAL:H	1:b5:329:LYS:HZ2	1.47	0.62
1:B1:434:SER:N	1:B1:437:GLU:OE1	2.30	0.62
1:B2:188:ASN:HA	1:B2:195:ILE:HG12	1.81	0.62
1:B2:473:SER:HA	1:B2:477:LYS:NZ	2.15	0.62
1:b2:334:MET:HE2	1:b2:334:MET:N	2.15	0.62
1:B4:91:ARG:O	1:B4:444:ASN:ND2	2.33	0.62
1:B:197:ASP:OD1	1:B:198:SER:N	2.33	0.62
1:B1:474:THR:OG1	1:B1:477:LYS:NZ	2.32	0.62
1:B3:339:LEU:O	1:b3:342:GLN:NE2	2.32	0.62
1:B4:401:LYS:O	1:B4:401:LYS:NZ	2.26	0.62
1:b:158:ASP:OD2	1:b:163:ARG:NH1	2.32	0.62
1:b:474:THR:H	1:b:477:LYS:NZ	1.97	0.62
1:b1:197:ASP:OD1	1:b1:198:SER:N	2.33	0.62
1:b4:467:LEU:HD12	1:b4:473:SER:HB2	1.80	0.62
1:B3:436:GLN:OE1	1:B3:439:ARG:NH1	2.32	0.62
1:B4:112:GLU:O	1:B4:116:LYS:NZ	2.28	0.62
1:B:369:SER:OG	1:B:372:GLN:OE1	2.16	0.62
1:b1:91:ARG:O	1:b1:444:ASN:ND2	2.32	0.62
1:b1:458:LEU:HD22	1:B2:463:GLU:OE1	2.00	0.61
1:b1:497:THR:HG22	1:b1:501:ARG:HE	1.63	0.61
1:B3:434:SER:N	1:B3:437:GLU:OE1	2.32	0.61
1:B5:34:GLN:OE1	1:B5:36:ARG:NH1	2.31	0.61
1:b:34:GLN:OE1	1:b:36:ARG:NH1	2.31	0.61
1:b4:176:ARG:HH21	1:b4:208:GLU:HA	1.66	0.61
1:B5:397:MET:HA	1:B5:397:MET:HE3	1.83	0.61
1:b:268:GLN:NE2	1:b:349:ASN:HD21	1.98	0.61
1:B4:459:LYS:O	1:B4:463:GLU:HG2	2.01	0.61
1:B5:268:GLN:HG3	1:b5:354:PHE:CE2	2.35	0.61
1:b1:144:MET:HE3	1:b1:174:PRO:HD3	1.82	0.61
1:B4:371:GLU:HG2	1:B4:377:TYR:CE1	2.35	0.61
1:B:397:MET:HA	1:B:397:MET:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:99:ILE:HD11	1:B1:431:ALA:HA	1.81	0.61
1:B1:397:MET:HA	1:B1:397:MET:HE3	1.82	0.61
1:B4:458:LEU:HD22	1:b4:463:GLU:OE1	2.01	0.61
1:b:282:ILE:HD11	1:B1:337:ASP:HB3	1.81	0.61
1:B5:158:ASP:OD2	1:B5:163:ARG:NH1	2.34	0.61
1:B1:275:LYS:NZ	1:b1:347:THR:OG1	2.33	0.61
1:B3:278:TYR:HB2	1:b3:274:VAL:HG21	1.82	0.61
1:b5:407:GLN:HG2	1:b5:411:MET:HE1	1.83	0.61
1:b1:99:ILE:HD11	1:b1:431:ALA:HA	1.82	0.60
1:B2:62:ASP:OD1	1:B2:66:ASN:ND2	2.34	0.60
1:b2:46:ASP:OD2	1:b2:46:ASP:N	2.31	0.60
1:b:188:ASN:HA	1:b:195:ILE:HG12	1.83	0.60
1:B4:262:ASP:OD1	1:B4:262:ASP:N	2.35	0.60
1:b5:176:ARG:HH21	1:b5:208:GLU:HA	1.67	0.60
1:B:453:MET:SD	1:b:390:ASN:HB3	2.42	0.60
1:B4:90:HIS:O	1:B4:91:ARG:NE	2.34	0.60
1:B4:501:ARG:HG2	1:B4:507:PRO:HG3	1.83	0.60
1:b4:188:ASN:HA	1:b4:195:ILE:HG12	1.84	0.60
1:B:370:TYR:OH	1:B:376:ASN:ND2	2.31	0.60
1:B2:434:SER:N	1:B2:437:GLU:OE1	2.32	0.60
1:B5:87:ARG:HB3	1:B5:448:ILE:HG23	1.83	0.60
1:b1:401:LYS:O	1:b1:401:LYS:NZ	2.26	0.60
1:B5:434:SER:N	1:B5:437:GLU:OE1	2.31	0.60
1:B:343:THR:OG1	1:b:345:GLN:NE2	2.27	0.60
1:B1:83:GLY:HA3	1:B1:450:SER:HB2	1.84	0.60
1:b1:456:ASP:OD2	1:b1:459:LYS:NZ	2.35	0.60
1:B3:43:GLU:N	1:B3:43:GLU:OE1	2.35	0.60
1:B:369:SER:HA	1:b5:375:ARG:HH11	1.66	0.60
1:b1:268:GLN:OE1	1:b1:349:ASN:ND2	2.33	0.60
1:b3:58:ALA:HB2	1:B4:42:SER:HB3	1.82	0.60
1:b3:401:LYS:O	1:b3:401:LYS:NZ	2.31	0.60
1:b5:46:ASP:OD2	1:b5:46:ASP:N	2.31	0.60
1:B1:407:GLN:HG2	1:B1:411:MET:HE1	1.83	0.60
1:B2:132:ARG:HG2	1:B2:136:MET:HG3	1.83	0.60
1:b5:397:MET:HA	1:b5:397:MET:HE3	1.82	0.60
1:b2:501:ARG:NH2	1:b2:507:PRO:HD3	2.15	0.59
1:B3:256:GLU:N	1:B3:256:GLU:OE2	2.34	0.59
1:B4:434:SER:N	1:B4:437:GLU:OE1	2.29	0.59
1:B2:282:ILE:HD11	1:b2:337:ASP:HB3	1.81	0.59
1:b4:407:GLN:O	1:b4:411:MET:HG3	2.02	0.59
1:B:244:GLN:O	1:b5:131:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B4:99:ILE:HD11	1:B4:431:ALA:HA	1.84	0.59
1:b5:218:LYS:NZ	1:b5:220:THR:OG1	2.35	0.59
1:B:401:LYS:O	1:B:401:LYS:NZ	2.28	0.59
1:b:91:ARG:O	1:b:444:ASN:ND2	2.30	0.59
1:B3:355:GLU:OE1	1:B3:356:GLN:NE2	2.36	0.59
1:b4:474:THR:H	1:b4:477:LYS:NZ	2.00	0.59
1:b5:356:GLN:HE21	1:b5:360:ARG:HH21	1.48	0.59
1:b:87:ARG:NH2	1:b:483:GLY:O	2.35	0.59
1:b2:132:ARG:HD3	1:B3:239:PRO:HG2	1.85	0.59
1:B3:371:GLU:HG2	1:B3:377:TYR:CE2	2.37	0.59
1:B4:179:ASN:OD1	1:B4:192:GLY:N	2.36	0.59
1:b:46:ASP:OD1	1:b:47:ALA:N	2.35	0.59
1:b1:179:ASN:OD1	1:b1:192:GLY:N	2.34	0.59
1:b1:378:ALA:O	1:b1:379:GLN:NE2	2.35	0.59
1:b1:352:SER:HB3	1:B2:353:VAL:HG21	1.85	0.59
1:b1:407:GLN:O	1:b1:411:MET:HG3	2.01	0.59
1:b1:434:SER:N	1:b1:437:GLU:OE1	2.30	0.59
1:B2:46:ASP:OD1	1:B2:47:ALA:N	2.35	0.59
1:B3:478:GLU:HA	1:B3:481:LYS:NZ	2.18	0.59
1:b3:87:ARG:HB3	1:b3:448:ILE:HG23	1.83	0.59
1:b3:434:SER:N	1:b3:437:GLU:OE1	2.32	0.59
1:B2:176:ARG:HH21	1:B2:208:GLU:HA	1.66	0.59
1:B4:356:GLN:HB3	1:B4:360:ARG:HH22	1.67	0.59
1:b4:91:ARG:O	1:b4:444:ASN:ND2	2.31	0.59
1:B:91:ARG:O	1:B:444:ASN:ND2	2.32	0.59
1:B1:215:MET:HE2	1:b1:187:ARG:HE	1.67	0.59
1:b2:99:ILE:HD11	1:b2:431:ALA:HA	1.85	0.59
1:B1:343:THR:HG21	1:b1:345:GLN:HG3	1.85	0.59
1:B2:307:LEU:HD12	1:B2:308:THR:HG23	1.85	0.59
1:B5:375:ARG:HH11	1:b5:369:SER:HA	1.68	0.59
1:B4:411:MET:HE3	1:B4:411:MET:HA	1.85	0.58
1:B:187:ARG:NH2	1:b5:215:MET:SD	2.76	0.58
1:B3:493:GLN:O	1:B3:497:THR:OG1	2.19	0.58
1:b3:318:TYR:HA	1:b3:321:ALA:HB3	1.85	0.58
1:B:257:GLN:HB3	1:B:362:ILE:HD11	1.85	0.58
1:B1:496:GLU:OE2	1:b1:475:TYR:N	2.33	0.58
1:B3:133:THR:OG1	1:B3:136:MET:HE3	2.04	0.58
1:B3:501:ARG:HG2	1:B3:507:PRO:HG3	1.83	0.58
1:B4:352:SER:HB3	1:b4:353:VAL:HG21	1.84	0.58
1:b4:90:HIS:O	1:b4:91:ARG:NE	2.34	0.58
1:B:90:HIS:O	1:B:91:ARG:NE	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:356:GLN:OE1	1:B1:370:TYR:OH	2.16	0.58
1:b3:325:LEU:HD23	1:b3:330:VAL:HG22	1.86	0.58
1:b3:329:LYS:HD3	1:b3:330:VAL:N	2.18	0.58
1:B1:378:ALA:O	1:B1:379:GLN:NE2	2.36	0.58
1:B2:99:ILE:HD11	1:B2:431:ALA:HA	1.85	0.58
1:B4:496:GLU:OE2	1:b4:475:TYR:N	2.27	0.58
1:B:430:LYS:HG2	1:B:430:LYS:O	2.04	0.58
1:b1:501:ARG:HG2	1:b1:507:PRO:HG3	1.85	0.58
1:b5:434:SER:N	1:b5:437:GLU:OE1	2.29	0.58
1:B:112:GLU:O	1:B:116:LYS:NZ	2.36	0.58
1:b2:85:PHE:HE2	1:b2:87:ARG:HE	1.50	0.58
1:b2:129:GLU:HG3	1:b2:131:LYS:HG3	1.85	0.58
1:b2:179:ASN:OD1	1:b2:192:GLY:N	2.37	0.58
1:b1:188:ASN:HA	1:b1:195:ILE:HG12	1.86	0.58
1:b2:455:ILE:O	1:B3:386:ARG:NE	2.27	0.58
1:b3:132:ARG:HG2	1:b3:136:MET:HG3	1.85	0.58
1:B5:355:GLU:HG3	1:B5:356:GLN:NE2	2.19	0.58
1:B:196:ASN:OD1	1:B:200:ALA:N	2.37	0.58
1:B3:218:LYS:NZ	1:B3:220:THR:OG1	2.30	0.58
1:b3:390:ASN:HA	1:b3:452:ARG:HH22	1.69	0.58
1:b4:97:LEU:O	1:b4:430:LYS:NZ	2.36	0.58
1:b:434:SER:N	1:b:437:GLU:OE1	2.30	0.57
1:b1:196:ASN:OD1	1:b1:200:ALA:N	2.37	0.57
1:b4:166:ARG:N	1:b4:418:GLU:OE2	2.36	0.57
1:B4:343:THR:HG21	1:b4:345:GLN:HG3	1.86	0.57
1:B5:91:ARG:O	1:B5:444:ASN:ND2	2.33	0.57
1:b5:369:SER:OG	1:b5:371:GLU:OE1	2.22	0.57
1:B:496:GLU:OE2	1:b:475:TYR:N	2.35	0.57
1:b1:463:GLU:O	1:b1:467:LEU:HD23	2.04	0.57
1:b4:460:GLU:HA	1:b4:463:GLU:HG2	1.87	0.57
1:B5:46:ASP:OD1	1:B5:47:ALA:N	2.37	0.57
1:B5:196:ASN:OD1	1:B5:200:ALA:N	2.37	0.57
1:B1:358:LEU:O	1:B1:362:ILE:HD12	2.04	0.57
1:B4:369:SER:OG	1:B4:371:GLU:OE1	2.14	0.57
1:b4:196:ASN:OD1	1:b4:200:ALA:N	2.38	0.57
1:B:239:PRO:HG2	1:b5:132:ARG:HD3	1.87	0.57
1:b:99:ILE:HD11	1:b:431:ALA:HA	1.86	0.57
1:B4:144:MET:HA	1:B4:147:PHE:CD1	2.40	0.57
1:b5:255:MET:SD	1:b5:255:MET:N	2.70	0.57
1:b:467:LEU:HD12	1:b:473:SER:HB2	1.86	0.57
1:B3:176:ARG:HH21	1:B3:208:GLU:HA	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:256:GLU:OE1	1:B5:257:GLN:NE2	2.38	0.57
1:B5:496:GLU:OE2	1:b5:475:TYR:N	2.37	0.57
1:b5:356:GLN:HB3	1:b5:360:ARG:HH22	1.69	0.57
1:b1:218:LYS:HD2	1:b1:219:TRP:N	2.18	0.57
1:B3:196:ASN:OD1	1:B3:200:ALA:N	2.38	0.57
1:b3:188:ASN:HA	1:b3:195:ILE:HG12	1.87	0.57
1:B1:179:ASN:OD1	1:B1:192:GLY:N	2.36	0.57
1:b1:166:ARG:N	1:b1:418:GLU:OE2	2.35	0.57
1:b1:257:GLN:HB3	1:b1:362:ILE:HD11	1.87	0.57
1:b3:129:GLU:HG3	1:b3:131:LYS:HG2	1.87	0.57
1:B:166:ARG:N	1:B:418:GLU:OE2	2.36	0.57
1:B:256:GLU:HG2	1:B:260:MET:HE2	1.87	0.57
1:B:434:SER:N	1:B:437:GLU:OE1	2.32	0.57
1:B1:325:LEU:HD23	1:B1:330:VAL:HG22	1.86	0.57
1:b3:334:MET:N	1:b3:334:MET:SD	2.77	0.57
1:B:85:PHE:CE2	1:B:87:ARG:HD2	2.40	0.56
1:B1:136:MET:HA	1:B1:139:ARG:HB2	1.87	0.56
1:b1:465:VAL:O	1:b1:469:GLU:HG3	2.05	0.56
1:B2:166:ARG:N	1:B2:418:GLU:OE2	2.37	0.56
1:B3:91:ARG:O	1:B3:444:ASN:ND2	2.33	0.56
1:b3:166:ARG:N	1:b3:418:GLU:OE2	2.38	0.56
1:b5:99:ILE:HD11	1:b5:431:ALA:HA	1.86	0.56
1:B:187:ARG:NH2	1:b5:212:PRO:O	2.38	0.56
1:B1:352:SER:HB3	1:b1:353:VAL:HG21	1.85	0.56
1:b1:175:LYS:HZ3	1:B2:44:SER:HA	1.69	0.56
1:B3:166:ARG:N	1:B3:418:GLU:OE2	2.36	0.56
1:b3:46:ASP:OD1	1:b3:47:ALA:N	2.38	0.56
1:b3:371:GLU:OE1	1:b3:371:GLU:N	2.38	0.56
1:b3:382:TYR:CZ	1:b3:386:ARG:HD2	2.41	0.56
1:b4:179:ASN:OD1	1:b4:192:GLY:N	2.35	0.56
1:b4:256:GLU:HG2	1:b4:260:MET:HE2	1.86	0.56
1:b4:479:CYS:HB3	1:b4:484:ASP:HB2	1.87	0.56
1:B5:179:ASN:OD1	1:B5:192:GLY:N	2.38	0.56
1:b:75:GLN:HE21	1:B1:395:TYR:HD1	1.53	0.56
1:b:90:HIS:O	1:b:91:ARG:NE	2.37	0.56
1:B1:334:MET:SD	1:B1:334:MET:N	2.78	0.56
1:b1:125:CYS:SG	1:b1:130:ARG:NH1	2.78	0.56
1:B2:87:ARG:NH2	1:B2:483:GLY:O	2.39	0.56
1:B2:90:HIS:O	1:B2:91:ARG:NE	2.38	0.56
1:b2:176:ARG:HH21	1:b2:208:GLU:HA	1.70	0.56
1:B4:196:ASN:OD1	1:B4:200:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b4:278:TYR:HB2	1:B5:274:VAL:HG21	1.86	0.56
1:B5:453:MET:SD	1:b5:390:ASN:HB3	2.46	0.56
1:B1:362:ILE:HD12	1:B1:362:ILE:H	1.70	0.56
1:b2:275:LYS:NZ	1:B3:348:ASP:O	2.38	0.56
1:b4:35:LEU:HD12	1:b4:36:ARG:HG3	1.86	0.56
1:B5:188:ASN:HA	1:B5:195:ILE:HG12	1.87	0.56
1:b:78:GLN:OE1	1:b:139:ARG:HB3	2.05	0.56
1:b1:132:ARG:HG2	1:b1:136:MET:HG3	1.87	0.56
1:B2:91:ARG:O	1:B2:444:ASN:ND2	2.31	0.56
1:b3:196:ASN:OD1	1:b3:200:ALA:N	2.38	0.56
1:b4:81:ILE:HG21	1:b4:142:VAL:HG21	1.87	0.56
1:B3:269:LEU:HD22	1:b3:260:MET:HB3	1.87	0.56
1:b5:75:GLN:O	1:b5:75:GLN:NE2	2.32	0.56
1:B:218:LYS:HD2	1:B:219:TRP:N	2.21	0.56
1:B:407:GLN:O	1:B:411:MET:HG3	2.05	0.56
1:b3:179:ASN:OD1	1:b3:192:GLY:N	2.38	0.56
1:B4:492:GLN:OE1	1:B4:495:ARG:NH1	2.39	0.56
1:b4:458:LEU:HD22	1:B5:463:GLU:OE2	2.06	0.56
1:B5:401:LYS:O	1:B5:401:LYS:NZ	2.30	0.56
1:b5:179:ASN:OD1	1:b5:192:GLY:N	2.38	0.56
1:b1:90:HIS:O	1:b1:91:ARG:NE	2.33	0.56
1:B5:78:GLN:OE1	1:B5:139:ARG:HB3	2.05	0.56
1:B5:125:CYS:SG	1:B5:130:ARG:NH1	2.79	0.56
1:B:179:ASN:OD1	1:B:192:GLY:N	2.35	0.56
1:B1:256:GLU:OE2	1:B1:256:GLU:N	2.27	0.56
1:B5:458:LEU:HG	1:b5:463:GLU:OE2	2.06	0.56
1:b:179:ASN:OD1	1:b:192:GLY:N	2.38	0.55
1:B2:259:LYS:HA	1:B2:262:ASP:OD1	2.06	0.55
1:b2:380:MET:SD	1:b2:384:THR:HB	2.47	0.55
1:B3:179:ASN:OD1	1:B3:192:GLY:N	2.36	0.55
1:b4:461:VAL:HG13	1:b4:462:GLN:OE1	2.06	0.55
1:B:278:TYR:HB2	1:b:274:VAL:HG21	1.87	0.55
1:b2:259:LYS:HA	1:b2:262:ASP:OD1	2.06	0.55
1:b2:454:ALA:O	1:B3:390:ASN:ND2	2.40	0.55
1:b3:498:MET:HA	1:b3:501:ARG:HE	1.70	0.55
1:b4:125:CYS:SG	1:b4:130:ARG:NH1	2.79	0.55
1:B1:87:ARG:HH22	1:B1:484:ASP:HA	1.71	0.55
1:B1:492:GLN:OE1	1:B1:495:ARG:NH1	2.39	0.55
1:B3:268:GLN:NE2	1:B3:271:SER:OG	2.39	0.55
1:b4:375:ARG:HH11	1:B5:369:SER:HA	1.70	0.55
1:b4:501:ARG:HG2	1:b4:507:PRO:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:268:GLN:HB3	1:B1:354:PHE:CE2	2.42	0.55
1:b2:62:ASP:OD1	1:b2:66:ASN:ND2	2.39	0.55
1:B3:125:CYS:SG	1:B3:130:ARG:NH1	2.80	0.55
1:b4:62:ASP:OD1	1:b4:66:ASN:ND2	2.38	0.55
1:b4:129:GLU:HG3	1:b4:131:LYS:HG2	1.88	0.55
1:b4:334:MET:SD	1:b4:334:MET:N	2.80	0.55
1:B5:352:SER:HB3	1:b5:353:VAL:HG21	1.89	0.55
1:b:166:ARG:N	1:b:418:GLU:OE2	2.38	0.55
1:B2:179:ASN:OD1	1:B2:192:GLY:N	2.37	0.55
1:B:440:SER:OG	1:b5:121:ASP:OD1	2.22	0.55
1:B1:375:ARG:HH11	1:b1:369:SER:HA	1.70	0.55
1:B2:351:TYR:O	1:B2:355:GLU:HG3	2.07	0.55
1:b5:278:TYR:HE2	1:b5:325:LEU:HD13	1.71	0.55
1:B1:268:GLN:OE1	1:B1:349:ASN:ND2	2.39	0.55
1:b1:376:ASN:HA	1:B2:360:ARG:HH12	1.72	0.55
1:b2:90:HIS:O	1:b2:91:ARG:NE	2.34	0.55
1:b3:453:MET:HE1	1:B4:390:ASN:CG	2.31	0.55
1:b4:452:ARG:HD2	1:b4:453:MET:H	1.71	0.55
1:B5:329:LYS:HD3	1:B5:330:VAL:N	2.21	0.55
1:b1:343:THR:OG1	1:b1:344:ALA:N	2.37	0.55
1:B2:133:THR:OG1	1:B2:136:MET:HE3	2.07	0.55
1:b2:196:ASN:OD1	1:b2:200:ALA:N	2.40	0.55
1:b:307:LEU:HD23	1:b:307:LEU:H	1.71	0.54
1:b1:131:LYS:HE2	1:B2:239:PRO:HG3	1.90	0.54
1:b1:277:MET:HE2	1:b1:277:MET:HA	1.89	0.54
1:B3:407:GLN:O	1:B3:411:MET:HG3	2.05	0.54
1:B4:176:ARG:HH21	1:B4:208:GLU:HA	1.71	0.54
1:B:62:ASP:OD1	1:B:66:ASN:ND2	2.40	0.54
1:B:187:ARG:NH1	1:b5:209:ASP:OD2	2.38	0.54
1:B:478:GLU:H	1:B:478:GLU:CD	2.15	0.54
1:B3:393:TRP:NE1	1:B3:397:MET:SD	2.80	0.54
1:b3:275:LYS:HE2	1:B4:349:ASN:HA	1.90	0.54
1:b3:278:TYR:CE2	1:B4:277:MET:HE2	2.42	0.54
1:b4:256:GLU:N	1:b4:256:GLU:OE2	2.40	0.54
1:B5:187:ARG:CZ	1:B5:187:ARG:H	2.19	0.54
1:B3:495:ARG:HA	1:B3:498:MET:SD	2.47	0.54
1:b4:137:MET:O	1:b4:171:MET:HE1	2.08	0.54
1:B5:72:ASN:ND2	1:B5:373:LEU:O	2.40	0.54
1:b5:196:ASN:OD1	1:b5:200:ALA:N	2.41	0.54
1:b1:482:ARG:NH2	1:B2:472:LEU:O	2.40	0.54
1:b3:462:GLN:HA	1:b3:465:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:82:VAL:HG11	1:B5:139:ARG:HG2	1.88	0.54
1:b1:355:GLU:HG2	1:b1:356:GLN:NE2	2.22	0.54
1:B2:268:GLN:HG3	1:b2:354:PHE:CE2	2.43	0.54
1:B2:407:GLN:O	1:B2:411:MET:HG3	2.07	0.54
1:b2:362:ILE:H	1:b2:362:ILE:HD12	1.72	0.54
1:b5:395:TYR:O	1:b5:399:ARG:HG2	2.06	0.54
1:B:475:TYR:H	1:b5:496:GLU:CD	2.15	0.54
1:B5:112:GLU:C	1:B5:116:LYS:HZ2	2.15	0.54
1:b2:166:ARG:N	1:b2:418:GLU:OE2	2.39	0.54
1:b2:393:TRP:O	1:b2:397:MET:HG2	2.08	0.54
1:B4:393:TRP:O	1:B4:397:MET:HG2	2.08	0.54
1:B:463:GLU:OE1	1:b5:458:LEU:HD22	2.08	0.54
1:b2:456:ASP:CG	1:b2:459:LYS:HG2	2.33	0.54
1:b4:397:MET:HA	1:b4:397:MET:HE3	1.89	0.54
1:b4:492:GLN:OE1	1:b4:495:ARG:NH1	2.40	0.54
1:B:252:TYR:OH	1:b5:65:ARG:NH2	2.41	0.54
1:B:492:GLN:OE1	1:B:495:ARG:NH1	2.40	0.54
1:b:501:ARG:NH2	1:b:505:LEU:O	2.41	0.54
1:B3:264:LEU:HA	1:B3:267:THR:HG22	1.89	0.54
1:b3:91:ARG:O	1:b3:444:ASN:ND2	2.35	0.54
1:B4:467:LEU:HD12	1:B4:473:SER:HB2	1.90	0.54
1:b:458:LEU:HD22	1:B1:463:GLU:OE1	2.07	0.54
1:b1:496:GLU:OE2	1:B2:475:TYR:N	2.40	0.53
1:b4:133:THR:OG1	1:b4:136:MET:HE3	2.07	0.53
1:b4:434:SER:N	1:b4:437:GLU:OE1	2.32	0.53
1:b:501:ARG:NH2	1:b:507:PRO:HD3	2.23	0.53
1:B1:435:PHE:HA	1:B1:442:TRP:CD1	2.43	0.53
1:b3:218:LYS:HD2	1:b3:219:TRP:N	2.23	0.53
1:B5:166:ARG:N	1:B5:418:GLU:OE2	2.37	0.53
1:B2:137:MET:HE3	1:B2:137:MET:HA	1.90	0.53
1:B3:144:MET:HE3	1:B3:173:SER:HA	1.90	0.53
1:B4:62:ASP:OD1	1:B4:66:ASN:ND2	2.40	0.53
1:b:62:ASP:OD1	1:b:66:ASN:ND2	2.42	0.53
1:B1:196:ASN:OD1	1:B1:200:ALA:N	2.41	0.53
1:b1:180:PRO:HA	1:b1:219:TRP:CD2	2.44	0.53
1:B2:482:ARG:NH2	1:b2:472:LEU:O	2.42	0.53
1:B4:46:ASP:OD1	1:B4:46:ASP:N	2.41	0.53
1:B4:166:ARG:N	1:B4:418:GLU:OE2	2.41	0.53
1:b:187:ARG:H	1:b:187:ARG:CZ	2.21	0.53
1:b:196:ASN:HB3	1:b:202:LEU:HD21	1.90	0.53
1:b:376:ASN:HB2	1:B1:360:ARG:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:482:ARG:HB3	1:B1:482:ARG:HH11	1.74	0.53
1:b1:323:VAL:H	1:b1:329:LYS:HZ2	1.57	0.53
1:b1:390:ASN:OD1	1:b1:452:ARG:NH2	2.42	0.53
1:B2:218:LYS:HD2	1:B2:219:TRP:N	2.23	0.53
1:b2:132:ARG:HG2	1:b2:136:MET:HG3	1.90	0.53
1:B3:251:PHE:O	1:B3:255:MET:HG3	2.08	0.53
1:b3:187:ARG:H	1:b3:187:ARG:CZ	2.20	0.53
1:B4:169:PHE:CG	1:B4:411:MET:HE1	2.44	0.53
1:B5:218:LYS:HD2	1:B5:219:TRP:N	2.23	0.53
1:b5:269:LEU:O	1:b5:273:ILE:HG12	2.09	0.53
1:b1:498:MET:SD	1:b1:499:GLU:HG3	2.49	0.53
1:B2:307:LEU:HD12	1:B2:308:THR:H	1.72	0.53
1:B3:430:LYS:O	1:B3:430:LYS:HG2	2.09	0.53
1:B3:477:LYS:O	1:B3:481:LYS:HG3	2.09	0.53
1:b4:370:TYR:OH	1:b4:376:ASN:ND2	2.40	0.53
1:b5:188:ASN:HA	1:b5:195:ILE:HG12	1.91	0.53
1:b:269:LEU:O	1:b:273:ILE:HG12	2.09	0.53
1:b:460:GLU:HA	1:b:463:GLU:HG2	1.90	0.53
1:b2:479:CYS:HB3	1:b2:484:ASP:HB2	1.89	0.53
1:B3:492:GLN:OE1	1:B3:495:ARG:NH1	2.40	0.53
1:b3:492:GLN:OE1	1:b3:495:ARG:NH1	2.42	0.53
1:B1:358:LEU:O	1:B1:361:TYR:N	2.42	0.53
1:b1:380:MET:SD	1:b1:384:THR:HB	2.49	0.53
1:B4:81:ILE:HG21	1:B4:142:VAL:HG21	1.91	0.53
1:B4:325:LEU:HD23	1:B4:330:VAL:HB	1.90	0.53
1:B5:478:GLU:HA	1:B5:481:LYS:HZ3	1.73	0.53
1:B1:166:ARG:N	1:B1:418:GLU:OE2	2.40	0.53
1:B1:261:LEU:O	1:B1:265:GLN:HG2	2.08	0.53
1:B3:132:ARG:NH1	1:B3:140:GLU:OE1	2.42	0.53
1:B3:485:ASP:OD1	1:B3:487:GLN:N	2.30	0.53
1:B:256:GLU:OE1	1:B:256:GLU:N	2.43	0.52
1:B:474:THR:OG1	1:B:476:GLU:OE2	2.25	0.52
1:B1:474:THR:H	1:B1:477:LYS:NZ	2.05	0.52
1:b1:257:GLN:HA	1:b1:260:MET:CE	2.39	0.52
1:B2:112:GLU:C	1:B2:116:LYS:HZ2	2.17	0.52
1:B3:145:HIS:HB2	1:B3:151:LEU:HD23	1.91	0.52
1:B4:195:ILE:HD12	1:B4:199:GLY:HA2	1.90	0.52
1:B5:393:TRP:CG	1:B5:452:ARG:HE	2.27	0.52
1:B5:474:THR:OG1	1:B5:477:LYS:NZ	2.42	0.52
1:B:463:GLU:HA	1:B:463:GLU:OE2	2.09	0.52
1:b:112:GLU:C	1:b:116:LYS:HZ2	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:341:LEU:HD12	1:b:341:LEU:O	2.09	0.52
1:b1:467:LEU:HB3	1:b1:473:SER:HB2	1.91	0.52
1:B2:85:PHE:HZ	1:B2:87:ARG:HH21	1.55	0.52
1:b2:180:PRO:HA	1:b2:219:TRP:CD2	2.44	0.52
1:B3:90:HIS:O	1:B3:91:ARG:NE	2.33	0.52
1:b5:467:LEU:HB3	1:b5:473:SER:HB2	1.91	0.52
1:b:242:ASP:N	1:b:242:ASP:OD1	2.42	0.52
1:B2:187:ARG:H	1:B2:187:ARG:CZ	2.22	0.52
1:B2:329:LYS:HD3	1:B2:330:VAL:N	2.25	0.52
1:B2:482:ARG:HH21	1:b2:472:LEU:HB3	1.74	0.52
1:B4:380:MET:HA	1:B4:380:MET:HE2	1.91	0.52
1:b5:166:ARG:N	1:b5:418:GLU:OE2	2.39	0.52
1:B:334:MET:SD	1:B:334:MET:N	2.82	0.52
1:B:467:LEU:HD12	1:B:473:SER:HB2	1.90	0.52
1:b3:62:ASP:OD1	1:b3:66:ASN:ND2	2.42	0.52
1:b3:288:THR:O	1:b3:290:SER:N	2.42	0.52
1:B5:257:GLN:HA	1:B5:260:MET:CE	2.38	0.52
1:B5:501:ARG:NH2	1:B5:505:LEU:O	2.41	0.52
1:b1:218:LYS:HD2	1:b1:218:LYS:C	2.35	0.52
1:b1:251:PHE:O	1:b1:255:MET:HG3	2.10	0.52
1:b2:125:CYS:SG	1:b2:130:ARG:NH1	2.83	0.52
1:B4:132:ARG:HD3	1:b4:239:PRO:HG2	1.92	0.52
1:b5:261:LEU:O	1:b5:265:GLN:HG2	2.08	0.52
1:B2:343:THR:OG1	1:b2:345:GLN:NE2	2.43	0.52
1:b2:58:ALA:HB2	1:B3:42:SER:HB2	1.91	0.52
1:b2:285:GLU:OE2	1:b2:286:LEU:N	2.42	0.52
1:B:180:PRO:HA	1:B:219:TRP:CD2	2.45	0.52
1:B:458:LEU:HD22	1:b:463:GLU:OE2	2.09	0.52
1:B1:467:LEU:HD12	1:B1:473:SER:HB2	1.90	0.52
1:b1:52:ASN:ND2	1:b1:55:ARG:HE	2.08	0.52
1:B2:218:LYS:HD2	1:B2:218:LYS:C	2.35	0.52
1:b5:270:GLN:O	1:b5:274:VAL:HG12	2.10	0.52
1:B3:467:LEU:HB3	1:B3:473:SER:HB2	1.91	0.52
1:b3:436:GLN:OE1	1:b3:439:ARG:NH1	2.43	0.52
1:B4:374:SER:O	1:b4:360:ARG:HG2	2.10	0.52
1:b:500:ARG:NH2	1:b:506:LYS:O	2.42	0.52
1:b1:269:LEU:HD22	1:B2:260:MET:HB3	1.92	0.52
1:b1:455:ILE:O	1:B2:386:ARG:NE	2.33	0.52
1:b3:268:GLN:OE1	1:b3:349:ASN:ND2	2.42	0.52
1:B4:60:ALA:O	1:B4:64:VAL:HG12	2.10	0.52
1:B5:137:MET:O	1:B5:171:MET:HE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ALA:HA	1:B:116:LYS:HZ1	1.75	0.51
1:B:175:LYS:NZ	1:b:43:GLU:O	2.42	0.51
1:b1:460:GLU:HA	1:b1:463:GLU:HG2	1.91	0.51
1:b2:435:PHE:HA	1:b2:442:TRP:CD1	2.45	0.51
1:B3:180:PRO:HA	1:B3:219:TRP:CD2	2.45	0.51
1:b5:492:GLN:OE1	1:b5:495:ARG:NH1	2.43	0.51
1:b:75:GLN:NE2	1:b:79:ASP:OD2	2.43	0.51
1:b:125:CYS:SG	1:b:130:ARG:NH1	2.83	0.51
1:b:351:TYR:O	1:b:355:GLU:HG2	2.10	0.51
1:B1:380:MET:HA	1:B1:380:MET:HE2	1.92	0.51
1:b1:175:LYS:NZ	1:B2:43:GLU:O	2.37	0.51
1:B2:242:ASP:N	1:B2:242:ASP:OD1	2.42	0.51
1:B2:269:LEU:HD22	1:b2:260:MET:HG2	1.91	0.51
1:B3:482:ARG:NH1	1:b3:467:LEU:HD11	2.25	0.51
1:b:436:GLN:OE1	1:b:439:ARG:NH1	2.43	0.51
1:b3:393:TRP:O	1:b3:397:MET:HG2	2.10	0.51
1:b5:460:GLU:HA	1:b5:463:GLU:HG2	1.91	0.51
1:b:462:GLN:HE22	1:B1:466:MET:HE1	1.75	0.51
1:B1:180:PRO:HA	1:B1:219:TRP:CD2	2.46	0.51
1:b3:458:LEU:HD22	1:B4:463:GLU:OE2	2.11	0.51
1:B5:242:ASP:N	1:B5:242:ASP:OD1	2.43	0.51
1:b5:187:ARG:H	1:b5:187:ARG:CZ	2.23	0.51
1:b:492:GLN:OE1	1:b:495:ARG:NH1	2.43	0.51
1:B1:131:LYS:NZ	1:b1:244:GLN:O	2.43	0.51
1:B2:436:GLN:OE1	1:B2:439:ARG:NH1	2.43	0.51
1:b2:460:GLU:HA	1:b2:463:GLU:HG2	1.92	0.51
1:b3:78:GLN:OE1	1:b3:139:ARG:HB3	2.10	0.51
1:b3:435:PHE:HA	1:b3:442:TRP:CD1	2.46	0.51
1:B:380:MET:HE2	1:B:385:ALA:N	2.26	0.51
1:b1:334:MET:SD	1:b1:334:MET:N	2.83	0.51
1:b2:121:ASP:OD1	1:B3:440:SER:OG	2.25	0.51
1:b2:467:LEU:HD13	1:b2:472:LEU:HB2	1.92	0.51
1:B3:393:TRP:CH2	1:B3:452:ARG:HA	2.46	0.51
1:B4:180:PRO:HA	1:B4:219:TRP:CD2	2.45	0.51
1:B4:257:GLN:HG2	1:B4:361:TYR:CD1	2.45	0.51
1:B1:67:ASN:OD1	1:B1:69:TYR:N	2.44	0.51
1:b1:376:ASN:HB2	1:B2:360:ARG:NH2	2.21	0.51
1:B3:496:GLU:OE2	1:b3:475:TYR:N	2.44	0.51
1:B5:281:THR:OG1	1:B5:283:GLU:OE2	2.29	0.51
1:b5:380:MET:HE2	1:b5:380:MET:HA	1.92	0.51
1:B:218:LYS:HD2	1:B:218:LYS:C	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:HD22	1:b:260:MET:HB3	1.92	0.51
1:b5:242:ASP:OD1	1:b5:242:ASP:N	2.42	0.51
1:b5:459:LYS:N	1:b5:459:LYS:HD2	2.26	0.51
1:B:390:ASN:ND2	1:b5:454:ALA:O	2.44	0.51
1:b:218:LYS:HD2	1:b:219:TRP:N	2.25	0.51
1:B1:380:MET:SD	1:B1:384:THR:HB	2.50	0.51
1:b2:341:LEU:HG	1:B3:344:ALA:HB2	1.92	0.51
1:b2:358:LEU:O	1:b2:362:ILE:HD12	2.10	0.51
1:b4:251:PHE:O	1:b4:255:MET:HG3	2.09	0.51
1:b4:457:GLY:O	1:b4:461:VAL:HG12	2.11	0.51
1:B:500:ARG:NH2	1:B:506:LYS:O	2.42	0.51
1:b1:269:LEU:O	1:b1:273:ILE:HG12	2.11	0.51
1:B2:88:LEU:HB2	1:B2:447:TRP:CZ3	2.46	0.51
1:B2:312:GLY:O	1:B2:316:ALA:N	2.42	0.51
1:B2:488:GLU:OE1	1:B2:488:GLU:N	2.42	0.51
1:b2:456:ASP:OD2	1:b2:459:LYS:HG2	2.11	0.51
1:B3:111:VAL:HG12	1:B3:425:VAL:HG11	1.93	0.51
1:b3:137:MET:O	1:b3:171:MET:HE1	2.11	0.51
1:b5:62:ASP:OD1	1:b5:66:ASN:ND2	2.44	0.51
1:b:435:PHE:HA	1:b:442:TRP:CD1	2.46	0.50
1:B1:467:LEU:HD13	1:B1:472:LEU:HB2	1.92	0.50
1:b5:113:ALA:HA	1:b5:116:LYS:HE3	1.93	0.50
1:B:145:HIS:HB2	1:B:151:LEU:HD23	1.93	0.50
1:b2:72:ASN:O	1:b2:76:LEU:HD22	2.11	0.50
1:b3:71:ALA:O	1:b3:74:ILE:HG22	2.11	0.50
1:b4:180:PRO:HA	1:b4:219:TRP:CD2	2.47	0.50
1:B5:501:ARG:NH2	1:B5:507:PRO:HD3	2.23	0.50
1:b:90:HIS:NE2	1:b:442:TRP:O	2.29	0.50
1:b1:278:TYR:HE2	1:b1:325:LEU:HD13	1.76	0.50
1:B4:34:GLN:OE1	1:B4:36:ARG:NH1	2.38	0.50
1:B4:215:MET:HE2	1:b4:187:ARG:HE	1.75	0.50
1:B4:378:ALA:O	1:B4:379:GLN:HG3	2.11	0.50
1:B5:257:GLN:HB3	1:B5:362:ILE:HD11	1.94	0.50
1:b:83:GLY:HA3	1:b:450:SER:HB2	1.94	0.50
1:b:88:LEU:HB2	1:b:447:TRP:CZ3	2.46	0.50
1:B1:62:ASP:OD1	1:B1:66:ASN:ND2	2.44	0.50
1:B1:355:GLU:OE1	1:B1:356:GLN:NE2	2.44	0.50
1:b1:100:GLY:H	1:b1:430:LYS:HZ1	1.60	0.50
1:b1:259:LYS:HE3	1:B2:38:TRP:CE3	2.46	0.50
1:B2:435:PHE:HA	1:B2:442:TRP:CD1	2.46	0.50
1:b2:482:ARG:HB3	1:b2:482:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B3:500:ARG:NH2	1:B3:506:LYS:O	2.44	0.50
1:b4:388:SER:O	1:b4:391:GLU:HG3	2.11	0.50
1:B5:354:PHE:O	1:B5:358:LEU:HD23	2.11	0.50
1:B:268:GLN:NE2	1:B:271:SER:OG	2.43	0.50
1:B1:144:MET:SD	1:B1:174:PRO:HD3	2.51	0.50
1:B2:81:ILE:HD12	1:B2:399:ARG:HB2	1.93	0.50
1:b3:218:LYS:NZ	1:b3:220:THR:OG1	2.45	0.50
1:b4:114:ALA:O	1:b4:117:GLU:HG3	2.12	0.50
1:B5:196:ASN:HB3	1:B5:202:LEU:HD21	1.93	0.50
1:b:460:GLU:H	1:b:460:GLU:CD	2.13	0.50
1:B3:242:ASP:N	1:B3:242:ASP:OD1	2.43	0.50
1:b3:275:LYS:HZ1	1:B4:348:ASP:C	2.20	0.50
1:B:242:ASP:OD1	1:B:242:ASP:N	2.44	0.50
1:B:275:LYS:HD2	1:b:345:GLN:HB2	1.94	0.50
1:b1:393:TRP:CE2	1:b1:452:ARG:HD2	2.47	0.50
1:B2:500:ARG:NH2	1:B2:506:LYS:O	2.43	0.50
1:B4:125:CYS:HB3	1:B4:163:ARG:HD3	1.94	0.50
1:b4:358:LEU:O	1:b4:362:ILE:HG12	2.11	0.50
1:b5:254:VAL:O	1:b5:258:MET:HG2	2.12	0.50
1:b1:137:MET:O	1:b1:171:MET:HE1	2.12	0.50
1:B3:256:GLU:HG2	1:B3:260:MET:HE2	1.92	0.50
1:B3:478:GLU:HA	1:B3:481:LYS:HZ3	1.77	0.50
1:B5:380:MET:HE2	1:B5:380:MET:HA	1.92	0.50
1:b5:387:ALA:HA	1:b5:390:ASN:OD1	2.12	0.50
1:b:460:GLU:OE2	1:b:460:GLU:N	2.28	0.50
1:b1:254:VAL:O	1:b1:258:MET:HG2	2.11	0.50
1:b1:278:TYR:HB2	1:B2:274:VAL:HG21	1.94	0.50
1:b2:257:GLN:HG2	1:b2:361:TYR:CD1	2.46	0.50
1:B3:278:TYR:HE2	1:B3:325:LEU:HD13	1.76	0.50
1:B3:485:ASP:OD1	1:B3:486:TYR:N	2.45	0.50
1:B5:496:GLU:CD	1:b5:475:TYR:H	2.20	0.50
1:B:60:ALA:O	1:B:64:VAL:HG12	2.12	0.49
1:B:343:THR:OG1	1:B:344:ALA:N	2.45	0.49
1:b1:256:GLU:OE1	1:b1:256:GLU:N	2.45	0.49
1:B2:140:GLU:HB3	1:B2:171:MET:CE	2.42	0.49
1:B2:493:GLN:O	1:B2:497:THR:OG1	2.28	0.49
1:b2:87:ARG:HB3	1:b2:448:ILE:HG23	1.94	0.49
1:B3:378:ALA:O	1:B3:379:GLN:NE2	2.45	0.49
1:b3:476:GLU:OE1	1:b3:476:GLU:N	2.34	0.49
1:B5:218:LYS:NZ	1:B5:220:THR:OG1	2.45	0.49
1:b:83:GLY:O	1:b:139:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B2:80:HIS:NE2	1:b2:391:GLU:OE2	2.40	0.49
1:B2:180:PRO:HA	1:B2:219:TRP:CD2	2.47	0.49
1:b2:67:ASN:OD1	1:b2:69:TYR:N	2.45	0.49
1:b2:125:CYS:HB3	1:b2:163:ARG:HD3	1.94	0.49
1:b2:492:GLN:OE1	1:b2:495:ARG:NH1	2.45	0.49
1:b3:85:PHE:HE2	1:b3:87:ARG:HE	1.60	0.49
1:b3:132:ARG:HD3	1:B4:239:PRO:HG2	1.94	0.49
1:b4:452:ARG:N	1:b4:481:LYS:O	2.45	0.49
1:B5:380:MET:SD	1:B5:384:THR:HB	2.52	0.49
1:b5:382:TYR:CZ	1:b5:386:ARG:HD2	2.48	0.49
1:B1:63:LEU:HD11	1:B1:258:MET:HG3	1.94	0.49
1:B1:371:GLU:H	1:B1:371:GLU:CD	2.20	0.49
1:b1:111:VAL:HG12	1:b1:425:VAL:HG11	1.93	0.49
1:B3:479:CYS:HB3	1:B3:484:ASP:C	2.38	0.49
1:b3:300:SER:O	1:b3:304:ARG:NH1	2.45	0.49
1:b3:342:GLN:OE1	1:b3:342:GLN:N	2.27	0.49
1:b5:435:PHE:HA	1:b5:442:TRP:CD1	2.47	0.49
1:B:501:ARG:NH2	1:B:507:PRO:HD3	2.25	0.49
1:b:131:LYS:NZ	1:B1:244:GLN:O	2.45	0.49
1:b:175:LYS:NZ	1:B1:43:GLU:O	2.44	0.49
1:B2:275:LYS:HE2	1:b2:349:ASN:HA	1.94	0.49
1:B2:393:TRP:O	1:B2:397:MET:HG2	2.11	0.49
1:B2:474:THR:OG1	1:B2:476:GLU:OE2	2.28	0.49
1:B2:496:GLU:OE2	1:b2:475:TYR:N	2.46	0.49
1:b3:175:LYS:NZ	1:B4:44:SER:HA	2.28	0.49
1:B5:407:GLN:HG2	1:B5:411:MET:CE	2.43	0.49
1:b5:474:THR:H	1:b5:477:LYS:HZ1	1.57	0.49
1:B1:242:ASP:OD1	1:B1:242:ASP:N	2.44	0.49
1:B2:196:ASN:HB3	1:B2:202:LEU:HD21	1.94	0.49
1:B2:375:ARG:HE	1:b2:364:ALA:HA	1.78	0.49
1:B2:478:GLU:HA	1:B2:481:LYS:HZ3	1.77	0.49
1:B3:352:SER:HA	1:B3:355:GLU:OE2	2.12	0.49
1:B4:435:PHE:HA	1:B4:442:TRP:CD1	2.47	0.49
1:b:257:GLN:HB3	1:b:362:ILE:HD11	1.94	0.49
1:B3:125:CYS:HB3	1:B3:163:ARG:HD3	1.95	0.49
1:B4:137:MET:O	1:B4:171:MET:HE1	2.13	0.49
1:B4:395:TYR:O	1:B4:399:ARG:HG2	2.13	0.49
1:B5:180:PRO:HA	1:B5:219:TRP:CD2	2.47	0.49
1:b5:75:GLN:HE21	1:b5:75:GLN:C	2.18	0.49
1:b5:132:ARG:HG2	1:b5:136:MET:HG3	1.95	0.49
1:B:113:ALA:HA	1:B:116:LYS:NZ	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:MET:HA	1:B:139:ARG:HB2	1.95	0.49
1:b:356:GLN:OE1	1:b:360:ARG:NH1	2.45	0.49
1:b2:261:LEU:O	1:b2:265:GLN:HG2	2.12	0.49
1:B3:380:MET:HE2	1:B3:380:MET:HA	1.95	0.49
1:b3:448:ILE:HD12	1:b3:480:ALA:HA	1.95	0.49
1:b4:68:GLY:HA2	1:B5:253:SER:OG	2.13	0.49
1:B5:436:GLN:OE1	1:B5:439:ARG:NH1	2.45	0.49
1:b5:257:GLN:HG2	1:b5:361:TYR:CD1	2.48	0.49
1:b:180:PRO:HA	1:b:219:TRP:CD2	2.48	0.49
1:B1:121:ASP:OD1	1:b1:440:SER:OG	2.25	0.49
1:B2:254:VAL:O	1:B2:258:MET:HG2	2.11	0.49
1:b2:82:VAL:HG11	1:b2:139:ARG:HG2	1.94	0.49
1:B3:367:GLY:HA3	1:B3:395:TYR:CE1	2.48	0.49
1:b3:60:ALA:O	1:b3:64:VAL:HG12	2.12	0.49
1:b3:180:PRO:HA	1:b3:219:TRP:CD2	2.48	0.49
1:b3:315:ALA:O	1:b3:319:ALA:N	2.46	0.49
1:B4:395:TYR:CE1	1:B4:399:ARG:HD3	2.47	0.49
1:b4:343:THR:OG1	1:b4:344:ALA:N	2.46	0.49
1:B5:87:ARG:NH2	1:B5:483:GLY:O	2.46	0.49
1:B5:369:SER:OG	1:B5:372:GLN:HG2	2.13	0.49
1:b5:72:ASN:ND2	1:b5:373:LEU:O	2.45	0.49
1:B:375:ARG:HH11	1:b:369:SER:HA	1.77	0.49
1:B1:99:ILE:HA	1:B1:430:LYS:HZ2	1.78	0.49
1:b2:329:LYS:HD3	1:b2:330:VAL:N	2.28	0.49
1:b2:501:ARG:O	1:b2:501:ARG:HD3	2.12	0.49
1:B1:72:ASN:ND2	1:B1:373:LEU:O	2.46	0.49
1:B1:459:LYS:N	1:B1:459:LYS:HD2	2.28	0.49
1:B2:175:LYS:NZ	1:b2:44:SER:HA	2.28	0.49
1:B2:307:LEU:HD12	1:B2:308:THR:N	2.28	0.49
1:b2:72:ASN:ND2	1:b2:373:LEU:O	2.46	0.49
1:b3:482:ARG:NH2	1:B4:472:LEU:O	2.46	0.49
1:b4:34:GLN:CD	1:b4:36:ARG:HH22	2.21	0.49
1:b4:242:ASP:OD1	1:b4:242:ASP:N	2.44	0.49
1:B5:377:TYR:HE2	1:b5:388:SER:HA	1.77	0.49
1:B5:500:ARG:NH2	1:B5:506:LYS:O	2.43	0.49
1:b5:334:MET:HE3	1:b5:334:MET:HA	1.95	0.49
1:b:82:VAL:HG23	1:b:86:PHE:CD1	2.48	0.48
1:b:354:PHE:O	1:b:358:LEU:HD23	2.12	0.48
1:B3:100:GLY:H	1:B3:430:LYS:NZ	2.11	0.48
1:B4:261:LEU:O	1:B4:265:GLN:HG2	2.12	0.48
1:b5:137:MET:O	1:b5:171:MET:HE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:323:VAL:N	1:B1:329:LYS:HZ2	2.08	0.48
1:B2:318:TYR:HA	1:B2:321:ALA:HB3	1.95	0.48
1:B3:122:ASP:HA	1:b3:406:ARG:HH12	1.77	0.48
1:b3:81:ILE:HD12	1:b3:399:ARG:HB2	1.95	0.48
1:b3:277:MET:HA	1:b3:277:MET:HE3	1.95	0.48
1:b4:60:ALA:O	1:b4:64:VAL:HG12	2.13	0.48
1:b4:269:LEU:O	1:b4:273:ILE:HG12	2.12	0.48
1:b4:339:LEU:HD12	1:b4:340:ASN:H	1.78	0.48
1:B5:448:ILE:HD11	1:B5:480:ALA:HA	1.95	0.48
1:b5:477:LYS:O	1:b5:481:LYS:NZ	2.44	0.48
1:B:474:THR:HG21	1:b5:492:GLN:HB3	1.95	0.48
1:b1:492:GLN:HB3	1:B2:474:THR:HG21	1.95	0.48
1:B2:133:THR:O	1:B2:137:MET:HG2	2.13	0.48
1:B2:460:GLU:HA	1:B2:463:GLU:HG2	1.95	0.48
1:B4:351:TYR:O	1:B4:355:GLU:HG3	2.13	0.48
1:B5:85:PHE:HE2	1:B5:87:ARG:HE	1.60	0.48
1:b5:180:PRO:HA	1:b5:219:TRP:CD2	2.49	0.48
1:B:122:ASP:O	1:b:406:ARG:NH2	2.43	0.48
1:b:59:ARG:HD3	1:b:255:MET:HE1	1.94	0.48
1:B1:453:MET:SD	1:b1:390:ASN:ND2	2.86	0.48
1:b1:241:GLU:OE1	1:b1:244:GLN:HB2	2.14	0.48
1:b1:242:ASP:OD1	1:b1:242:ASP:N	2.44	0.48
1:b1:395:TYR:HD2	1:b1:396:PHE:CD1	2.31	0.48
1:B2:354:PHE:O	1:B2:358:LEU:HD23	2.14	0.48
1:b2:254:VAL:O	1:b2:258:MET:HG2	2.13	0.48
1:b2:333:LEU:C	1:b2:334:MET:HE2	2.38	0.48
1:b2:378:ALA:O	1:b2:379:GLN:NE2	2.46	0.48
1:b4:125:CYS:HB3	1:b4:163:ARG:HD3	1.95	0.48
1:b5:71:ALA:O	1:b5:74:ILE:HG22	2.13	0.48
1:b:133:THR:H	1:b:136:MET:HE3	1.79	0.48
1:B2:60:ALA:O	1:B2:64:VAL:HG12	2.14	0.48
1:B2:126:ILE:HG13	1:B2:127:ASP:N	2.29	0.48
1:B3:496:GLU:CD	1:b3:475:TYR:H	2.22	0.48
1:B5:277:MET:HA	1:B5:277:MET:HE3	1.95	0.48
1:B1:89:SER:HB3	1:B1:446:ASP:OD2	2.13	0.48
1:B1:395:TYR:CE1	1:B1:399:ARG:HD3	2.48	0.48
1:b1:35:LEU:HD12	1:b1:36:ARG:HG3	1.95	0.48
1:b1:112:GLU:O	1:b1:116:LYS:NZ	2.46	0.48
1:B2:261:LEU:O	1:B2:265:GLN:HG2	2.13	0.48
1:b2:323:VAL:H	1:b2:329:LYS:HZ3	1.61	0.48
1:b2:395:TYR:O	1:b2:399:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b3:125:CYS:HB3	1:b3:163:ARG:HD3	1.96	0.48
1:b3:126:ILE:HG13	1:b3:127:ASP:N	2.28	0.48
1:B4:188:ASN:HA	1:B4:195:ILE:HG12	1.95	0.48
1:B5:99:ILE:HD11	1:B5:431:ALA:HA	1.95	0.48
1:B5:215:MET:N	1:B5:215:MET:SD	2.87	0.48
1:b:325:LEU:HD23	1:b:330:VAL:HG22	1.94	0.48
1:B1:395:TYR:O	1:B1:399:ARG:HG2	2.13	0.48
1:b2:496:GLU:OE2	1:B3:475:TYR:N	2.37	0.48
1:B4:269:LEU:O	1:B4:273:ILE:HG12	2.14	0.48
1:b5:407:GLN:HG2	1:b5:411:MET:CE	2.42	0.48
1:b5:463:GLU:O	1:b5:467:LEU:HD23	2.14	0.48
1:B:343:THR:HG1	1:b:345:GLN:HE21	1.58	0.48
1:B:453:MET:HE2	1:B:453:MET:HB3	1.76	0.48
1:b1:75:GLN:O	1:b1:75:GLN:NE2	2.31	0.48
1:b1:380:MET:HG3	1:b1:385:ALA:HB2	1.96	0.48
1:b1:435:PHE:HA	1:b1:442:TRP:CD1	2.49	0.48
1:B2:125:CYS:HB3	1:B2:163:ARG:HD3	1.95	0.48
1:B2:492:GLN:OE1	1:B2:495:ARG:NH1	2.46	0.48
1:b2:209:ASP:OD1	1:b2:211:TYR:N	2.35	0.48
1:b2:352:SER:OG	1:b2:353:VAL:N	2.46	0.48
1:B3:456:ASP:CG	1:B3:459:LYS:HG3	2.39	0.48
1:B4:242:ASP:OD1	1:B4:242:ASP:N	2.44	0.48
1:B5:371:GLU:HB2	1:B5:377:TYR:CD1	2.49	0.48
1:B5:435:PHE:HA	1:B5:442:TRP:CD1	2.49	0.48
1:B1:500:ARG:NH2	1:B1:505:LEU:HB3	2.29	0.48
1:b1:62:ASP:OD1	1:b1:66:ASN:ND2	2.47	0.48
1:b2:82:VAL:HG23	1:b2:86:PHE:CD1	2.48	0.48
1:b3:256:GLU:OE1	1:b3:256:GLU:N	2.47	0.48
1:b3:407:GLN:HG2	1:b3:411:MET:CE	2.44	0.48
1:b4:75:GLN:HE22	1:B5:399:ARG:NH2	2.12	0.48
1:b5:88:LEU:HB2	1:b5:447:TRP:CZ3	2.49	0.48
1:b5:136:MET:HA	1:b5:139:ARG:HB2	1.95	0.48
1:b5:323:VAL:N	1:b5:329:LYS:HZ2	2.11	0.48
1:b5:482:ARG:HB3	1:b5:482:ARG:NH1	2.29	0.48
1:b:323:VAL:N	1:b:329:LYS:HZ2	2.10	0.48
1:b1:75:GLN:HE21	1:b1:75:GLN:C	2.17	0.48
1:B2:473:SER:OG	1:B2:478:GLU:OE1	2.32	0.48
1:b2:458:LEU:HD13	1:B3:463:GLU:OE1	2.12	0.48
1:b3:82:VAL:HG23	1:b3:86:PHE:CD1	2.49	0.48
1:b4:112:GLU:O	1:b4:116:LYS:HG3	2.13	0.48
1:b4:498:MET:SD	1:b4:499:GLU:N	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b5:129:GLU:HG3	1:b5:131:LYS:HG3	1.95	0.48
1:b3:63:LEU:HD11	1:b3:258:MET:HG3	1.96	0.47
1:B4:88:LEU:HB2	1:B4:447:TRP:CZ3	2.49	0.47
1:B:125:CYS:HB3	1:B:163:ARG:HD3	1.96	0.47
1:B:132:ARG:HG2	1:B:136:MET:HG3	1.95	0.47
1:B:144:MET:CE	1:B:174:PRO:HD3	2.41	0.47
1:b:125:CYS:HB3	1:b:163:ARG:HD3	1.96	0.47
1:b:186:SER:HB2	1:b:187:ARG:NH2	2.30	0.47
1:b:407:GLN:HG2	1:b:411:MET:CE	2.44	0.47
1:b2:80:HIS:HB3	1:b2:396:PHE:CD2	2.48	0.47
1:B4:255:MET:O	1:B4:259:LYS:HG2	2.14	0.47
1:B4:500:ARG:NH2	1:B4:505:LEU:HB3	2.29	0.47
1:b4:85:PHE:HE2	1:b4:87:ARG:HE	1.61	0.47
1:b5:134:PHE:O	1:b5:137:MET:HB2	2.14	0.47
1:B:121:ASP:OD1	1:b:440:SER:OG	2.26	0.47
1:B:353:VAL:HG21	1:b5:352:SER:HB3	1.95	0.47
1:B:355:GLU:HG2	1:B:356:GLN:NE2	2.29	0.47
1:B:369:SER:H	1:B:372:GLN:NE2	2.12	0.47
1:b:82:VAL:HG11	1:b:139:ARG:HG2	1.97	0.47
1:b1:358:LEU:O	1:b1:362:ILE:HD13	2.14	0.47
1:B2:317:TYR:CZ	1:b2:334:MET:HE1	2.49	0.47
1:b2:242:ASP:OD1	1:b2:242:ASP:N	2.44	0.47
1:b4:145:HIS:HB2	1:b4:151:LEU:HD23	1.96	0.47
1:b4:462:GLN:HA	1:b4:465:VAL:HG12	1.96	0.47
1:B5:87:ARG:HH22	1:B5:484:ASP:HA	1.79	0.47
1:B:367:GLY:HA3	1:B:395:TYR:CZ	2.50	0.47
1:b:87:ARG:HB3	1:b:448:ILE:HG23	1.96	0.47
1:B5:375:ARG:HD3	1:b5:369:SER:HA	1.96	0.47
1:b5:87:ARG:HH22	1:b5:484:ASP:HA	1.78	0.47
1:b5:395:TYR:OH	1:b5:399:ARG:NH1	2.47	0.47
1:b1:397:MET:HE1	1:b1:400:ARG:CZ	2.45	0.47
1:b2:482:ARG:HB3	1:b2:482:ARG:HH11	1.79	0.47
1:B3:112:GLU:O	1:B3:116:LYS:HG2	2.14	0.47
1:b3:264:LEU:HD11	1:b3:351:TYR:HD1	1.79	0.47
1:B4:479:CYS:HB3	1:B4:484:ASP:HB2	1.96	0.47
1:b4:376:ASN:HB2	1:B5:360:ARG:HD3	1.97	0.47
1:B5:261:LEU:O	1:B5:265:GLN:HG2	2.14	0.47
1:B:397:MET:HE1	1:B:400:ARG:CZ	2.45	0.47
1:b:71:ALA:O	1:b:74:ILE:HG22	2.14	0.47
1:b1:144:MET:HE3	1:b1:173:SER:HA	1.96	0.47
1:b3:461:VAL:HG12	1:B4:466:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b5:186:SER:HB2	1:b5:187:ARG:NH2	2.29	0.47
1:b5:344:ALA:HB1	1:b5:345:GLN:OE1	2.15	0.47
1:b1:145:HIS:HB2	1:b1:151:LEU:HD23	1.96	0.47
1:b1:479:CYS:HB3	1:b1:484:ASP:C	2.40	0.47
1:b2:395:TYR:CE1	1:b2:399:ARG:HD3	2.49	0.47
1:B3:275:LYS:HZ1	1:b3:347:THR:H	1.61	0.47
1:B3:358:LEU:O	1:B3:362:ILE:HG12	2.13	0.47
1:B3:435:PHE:HA	1:B3:442:TRP:CD1	2.50	0.47
1:B3:456:ASP:OD2	1:B3:459:LYS:HG3	2.15	0.47
1:b3:313:GLU:O	1:b3:316:ALA:HB3	2.15	0.47
1:b3:318:TYR:O	1:b3:322:PRO:HD3	2.14	0.47
1:b3:468:ILE:HD12	1:b3:478:GLU:OE1	2.15	0.47
1:b3:478:GLU:N	1:b3:478:GLU:OE2	2.47	0.47
1:B4:459:LYS:N	1:B4:459:LYS:HD2	2.29	0.47
1:B5:257:GLN:HA	1:B5:260:MET:HE2	1.96	0.47
1:b5:81:ILE:HD12	1:b5:399:ARG:HB2	1.97	0.47
1:b5:369:SER:HG	1:b5:372:GLN:CD	2.16	0.47
1:B:505:LEU:HD21	1:b:493:GLN:HG2	1.96	0.47
1:B1:75:GLN:OE1	1:B1:75:GLN:HA	2.14	0.47
1:B1:144:MET:HE2	1:B1:144:MET:HB3	1.74	0.47
1:B1:386:ARG:NH2	1:B1:390:ASN:HD21	2.13	0.47
1:B2:186:SER:HB2	1:B2:187:ARG:NH2	2.30	0.47
1:B2:258:MET:HE3	1:B2:258:MET:HB3	1.85	0.47
1:b2:275:LYS:HD3	1:B3:349:ASN:HA	1.97	0.47
1:b1:122:ASP:O	1:B2:406:ARG:NH2	2.43	0.47
1:b1:256:GLU:OE2	1:b1:257:GLN:NE2	2.48	0.47
1:B3:112:GLU:HB3	1:B3:116:LYS:NZ	2.30	0.47
1:B3:196:ASN:HB3	1:B3:202:LEU:HD21	1.97	0.47
1:b3:375:ARG:HH11	1:B4:369:SER:HA	1.80	0.47
1:B4:393:TRP:CG	1:B4:452:ARG:HE	2.33	0.47
1:b4:99:ILE:HD11	1:b4:431:ALA:HA	1.96	0.47
1:b4:329:LYS:HD3	1:b4:330:VAL:N	2.29	0.47
1:B5:208:GLU:CD	1:B5:218:LYS:HB3	2.39	0.47
1:B1:460:GLU:OE1	1:B1:460:GLU:N	2.27	0.47
1:b1:125:CYS:HB3	1:b1:163:ARG:HD3	1.97	0.47
1:B4:355:GLU:OE1	1:B4:356:GLN:NE2	2.48	0.47
1:B5:268:GLN:HG2	1:B5:351:TYR:CE2	2.50	0.47
1:b5:500:ARG:NH2	1:b5:505:LEU:HB3	2.30	0.47
1:B:108:SER:HA	1:B:111:VAL:HG22	1.97	0.46
1:B:122:ASP:HA	1:b:406:ARG:HH12	1.79	0.46
1:b:259:LYS:HA	1:b:262:ASP:OD1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b1:493:GLN:O	1:b1:497:THR:OG1	2.33	0.46
1:b1:500:ARG:NH2	1:b1:506:LYS:O	2.47	0.46
1:b2:380:MET:HG3	1:b2:385:ALA:HB2	1.97	0.46
1:B3:60:ALA:O	1:B3:64:VAL:HG12	2.14	0.46
1:b4:435:PHE:HA	1:b4:442:TRP:CD1	2.50	0.46
1:B:268:GLN:NE2	1:B:268:GLN:O	2.38	0.46
1:B:371:GLU:CD	1:B:371:GLU:H	2.23	0.46
1:B1:505:LEU:HD21	1:b1:493:GLN:HG2	1.97	0.46
1:B2:122:ASP:OD1	1:B2:123:CYS:N	2.48	0.46
1:B2:215:MET:HE2	1:b2:187:ARG:HD3	1.97	0.46
1:b2:35:LEU:HG	1:b2:36:ARG:HH11	1.80	0.46
1:B3:187:ARG:HG2	1:B3:188:ASN:OD1	2.15	0.46
1:B3:254:VAL:O	1:B3:258:MET:HG2	2.16	0.46
1:b3:371:GLU:CD	1:b3:371:GLU:H	2.22	0.46
1:B4:136:MET:HE2	1:B4:136:MET:HB3	1.74	0.46
1:B5:455:ILE:O	1:b5:386:ARG:NH1	2.44	0.46
1:B:435:PHE:HA	1:B:442:TRP:CD1	2.50	0.46
1:b:89:SER:HB3	1:b:446:ASP:OD1	2.15	0.46
1:B1:82:VAL:HG21	1:B1:139:ARG:CG	2.45	0.46
1:b3:88:LEU:HB2	1:b3:447:TRP:CZ3	2.51	0.46
1:B4:262:ASP:O	1:B4:266:ASN:ND2	2.48	0.46
1:b4:254:VAL:O	1:b4:258:MET:HG2	2.15	0.46
1:b5:82:VAL:HG23	1:b5:86:PHE:CD1	2.50	0.46
1:B:478:GLU:HA	1:B:481:LYS:NZ	2.29	0.46
1:B:493:GLN:HG2	1:b5:505:LEU:HD21	1.97	0.46
1:b:144:MET:HA	1:b:147:PHE:CE1	2.50	0.46
1:B1:88:LEU:HB2	1:B1:447:TRP:CZ3	2.50	0.46
1:B2:453:MET:HE1	1:b2:390:ASN:CG	2.40	0.46
1:b2:212:PRO:HD2	1:b2:215:MET:HE1	1.97	0.46
1:b2:375:ARG:HH11	1:B3:369:SER:HA	1.79	0.46
1:b2:406:ARG:O	1:b2:410:GLN:HG2	2.15	0.46
1:B3:259:LYS:HA	1:B3:262:ASP:OD1	2.15	0.46
1:B5:112:GLU:O	1:B5:116:LYS:NZ	2.37	0.46
1:B5:492:GLN:OE1	1:B5:495:ARG:NH1	2.48	0.46
1:b:75:GLN:OE1	1:b:75:GLN:HA	2.14	0.46
1:B2:251:PHE:H	1:B2:251:PHE:HD2	1.63	0.46
1:b2:88:LEU:HB2	1:b2:447:TRP:CZ3	2.50	0.46
1:B3:458:LEU:HD12	1:B3:458:LEU:HA	1.77	0.46
1:b3:472:LEU:H	1:b3:472:LEU:HD12	1.81	0.46
1:b3:496:GLU:OE2	1:B4:475:TYR:N	2.49	0.46
1:B4:498:MET:HB3	1:B4:501:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b4:94:TRP:O	1:b4:98:GLY:N	2.48	0.46
1:b4:453:MET:SD	1:B5:390:ASN:HB3	2.56	0.46
1:B5:345:GLN:OE1	1:B5:345:GLN:N	2.35	0.46
1:B5:351:TYR:O	1:B5:355:GLU:HG2	2.15	0.46
1:b:255:MET:HA	1:b:258:MET:HE2	1.98	0.46
1:B1:175:LYS:NZ	1:b1:44:SER:HA	2.30	0.46
1:b1:278:TYR:HE1	1:B2:341:LEU:HD13	1.81	0.46
1:B3:180:PRO:HA	1:B3:219:TRP:CG	2.51	0.46
1:b4:459:LYS:O	1:b4:463:GLU:HG2	2.15	0.46
1:b5:79:ASP:OD1	1:b5:139:ARG:NH2	2.31	0.46
1:b5:268:GLN:NE2	1:b5:349:ASN:HD21	2.13	0.46
1:B:137:MET:HE2	1:B:137:MET:HB2	1.84	0.46
1:b:448:ILE:HD11	1:b:483:GLY:HA2	1.97	0.46
1:b1:72:ASN:ND2	1:b1:373:LEU:O	2.49	0.46
1:b2:108:SER:HA	1:b2:111:VAL:HG22	1.96	0.46
1:b2:500:ARG:NH2	1:b2:505:LEU:HB3	2.29	0.46
1:b3:269:LEU:HD22	1:B4:260:MET:HB3	1.96	0.46
1:b3:485:ASP:HB3	1:b3:488:GLU:HG3	1.98	0.46
1:B5:78:GLN:OE1	1:B5:139:ARG:NE	2.49	0.46
1:b5:144:MET:SD	1:b5:174:PRO:HD3	2.56	0.46
1:B:81:ILE:HG21	1:B:142:VAL:HG21	1.97	0.46
1:b:126:ILE:HG13	1:b:127:ASP:N	2.31	0.46
1:B1:406:ARG:O	1:B1:410:GLN:HG2	2.16	0.46
1:B1:459:LYS:O	1:B1:463:GLU:HG2	2.16	0.46
1:B2:257:GLN:HB3	1:B2:362:ILE:HD11	1.97	0.46
1:B3:354:PHE:O	1:B3:358:LEU:HD23	2.15	0.46
1:B5:88:LEU:HB2	1:B5:447:TRP:CZ3	2.49	0.46
1:b5:380:MET:SD	1:b5:384:THR:HB	2.56	0.46
1:B:348:ASP:O	1:b5:275:LYS:HE2	2.16	0.46
1:b:380:MET:HE3	1:b:381:SER:N	2.31	0.46
1:B2:83:GLY:O	1:B2:139:ARG:NH1	2.48	0.46
1:B2:481:LYS:HE3	1:B2:481:LYS:HB3	1.82	0.46
1:b2:133:THR:H	1:b2:136:MET:HE3	1.80	0.46
1:b4:498:MET:SD	1:b4:499:GLU:HG3	2.55	0.46
1:B5:125:CYS:HB3	1:B5:163:ARG:HD3	1.98	0.46
1:B5:438:ALA:HB1	1:B5:441:ALA:HB3	1.97	0.46
1:b5:500:ARG:NH2	1:b5:506:LYS:O	2.49	0.46
1:B:111:VAL:HG12	1:B:425:VAL:HG11	1.98	0.46
1:b1:60:ALA:O	1:b1:64:VAL:HG12	2.16	0.46
1:b1:134:PHE:O	1:b1:138:ILE:HG12	2.15	0.46
1:B3:59:ARG:HB3	1:b3:38:TRP:CH2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b4:390:ASN:HA	1:b4:452:ARG:HH22	1.81	0.46
1:b:195:ILE:HD12	1:b:199:GLY:HA2	1.97	0.45
1:b1:282:ILE:HD13	1:b1:282:ILE:HA	1.82	0.45
1:B2:175:LYS:HZ1	1:b2:44:SER:HA	1.82	0.45
1:b3:397:MET:SD	1:b3:397:MET:N	2.89	0.45
1:B4:380:MET:SD	1:B4:384:THR:HB	2.57	0.45
1:b4:87:ARG:HB3	1:b4:448:ILE:HG23	1.98	0.45
1:b4:438:ALA:HB1	1:b4:441:ALA:HB3	1.98	0.45
1:B:358:LEU:O	1:B:362:ILE:HD13	2.15	0.45
1:B:386:ARG:NH2	1:B:390:ASN:HD21	2.13	0.45
1:B1:456:ASP:HB3	1:B1:459:LYS:HG2	1.98	0.45
1:B3:208:GLU:OE1	1:B3:218:LYS:HB3	2.16	0.45
1:b3:299:ASN:HA	1:b3:303:GLN:C	2.41	0.45
1:b3:317:TYR:CD2	1:B4:334:MET:HE3	2.51	0.45
1:b4:268:GLN:NE2	1:b4:271:SER:OG	2.49	0.45
1:b5:108:SER:HA	1:b5:111:VAL:HG22	1.98	0.45
1:b1:187:ARG:HB3	1:b1:187:ARG:NH1	2.30	0.45
1:b1:299:ASN:HA	1:b1:303:GLN:C	2.42	0.45
1:b2:358:LEU:O	1:b2:361:TYR:N	2.49	0.45
1:b3:79:ASP:OD2	1:B4:395:TYR:HA	2.16	0.45
1:b3:269:LEU:HD12	1:b3:269:LEU:O	2.17	0.45
1:b3:354:PHE:O	1:b3:358:LEU:HD23	2.17	0.45
1:b3:496:GLU:CD	1:B4:475:TYR:H	2.25	0.45
1:B4:111:VAL:HG12	1:B4:425:VAL:HG11	1.99	0.45
1:B4:144:MET:HA	1:B4:147:PHE:HD1	1.79	0.45
1:B5:112:GLU:C	1:B5:116:LYS:NZ	2.74	0.45
1:B5:467:LEU:HD13	1:B5:472:LEU:HB2	1.98	0.45
1:b5:406:ARG:O	1:b5:410:GLN:HG2	2.16	0.45
1:B:42:SER:HB2	1:b5:58:ALA:HB2	1.98	0.45
1:B:125:CYS:SG	1:B:130:ARG:NH1	2.90	0.45
1:B:329:LYS:HD3	1:B:330:VAL:N	2.31	0.45
1:B:376:ASN:HA	1:b:360:ARG:NH2	2.31	0.45
1:b:129:GLU:OE2	1:b:131:LYS:HE3	2.17	0.45
1:b:359:LEU:HD12	1:b:374:SER:HB3	1.99	0.45
1:B1:125:CYS:HB3	1:B1:163:ARG:HD3	1.98	0.45
1:B2:313:GLU:O	1:B2:316:ALA:HB3	2.16	0.45
1:b2:89:SER:HB3	1:b2:446:ASP:OD2	2.17	0.45
1:b2:175:LYS:H	1:b2:175:LYS:HG2	1.51	0.45
1:b2:274:VAL:HA	1:b2:277:MET:HG2	1.98	0.45
1:B3:81:ILE:HG21	1:B3:142:VAL:HG21	1.98	0.45
1:B3:121:ASP:OD1	1:b3:440:SER:OG	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B4:467:LEU:HD13	1:B4:472:LEU:HB2	1.98	0.45
1:b4:478:GLU:HA	1:b4:481:LYS:NZ	2.32	0.45
1:b4:492:GLN:HG2	1:B5:476:GLU:OE2	2.16	0.45
1:B5:460:GLU:OE1	1:B5:460:GLU:N	2.29	0.45
1:b5:144:MET:HA	1:b5:147:PHE:CE2	2.51	0.45
1:b5:468:ILE:HD12	1:b5:478:GLU:OE1	2.16	0.45
1:B1:407:GLN:HG2	1:B1:411:MET:CE	2.47	0.45
1:B2:59:ARG:HD3	1:B2:255:MET:HE1	1.97	0.45
1:B2:78:GLN:OE1	1:B2:139:ARG:HB3	2.17	0.45
1:B2:397:MET:N	1:B2:397:MET:SD	2.88	0.45
1:b2:136:MET:HA	1:b2:139:ARG:HB2	1.98	0.45
1:B4:281:THR:HA	1:B4:330:VAL:HG23	1.98	0.45
1:b4:122:ASP:O	1:B5:406:ARG:NH2	2.44	0.45
1:B5:195:ILE:HD12	1:B5:199:GLY:HA2	1.98	0.45
1:B5:341:LEU:O	1:B5:341:LEU:HD12	2.16	0.45
1:b5:218:LYS:HD2	1:b5:219:TRP:N	2.31	0.45
1:B:90:HIS:NE2	1:B:442:TRP:O	2.32	0.45
1:B1:188:ASN:HA	1:B1:195:ILE:HG12	1.99	0.45
1:B1:348:ASP:OD1	1:B1:350:GLY:N	2.46	0.45
1:B2:144:MET:HA	1:B2:147:PHE:CE1	2.52	0.45
1:B2:317:TYR:CE1	1:b2:334:MET:HE1	2.51	0.45
1:B2:325:LEU:HD23	1:B2:330:VAL:HG22	1.97	0.45
1:B3:369:SER:OG	1:B3:371:GLU:OE1	2.21	0.45
1:b3:380:MET:HE2	1:b3:380:MET:HA	1.99	0.45
1:B4:356:GLN:OE1	1:B4:370:TYR:OH	2.19	0.45
1:b4:108:SER:HA	1:b4:111:VAL:HG22	1.99	0.45
1:b4:380:MET:HG2	1:b4:385:ALA:HB2	1.98	0.45
1:b2:175:LYS:HZ3	1:B3:43:GLU:C	2.24	0.45
1:b3:90:HIS:C	1:b3:91:ARG:HD2	2.41	0.45
1:b3:466:MET:HE3	1:b3:466:MET:HB2	1.82	0.45
1:B4:144:MET:SD	1:B4:174:PRO:HD3	2.56	0.45
1:B5:175:LYS:NZ	1:b5:43:GLU:O	2.50	0.45
1:B:256:GLU:OE2	1:B:257:GLN:NE2	2.49	0.45
1:b:492:GLN:HE21	1:b:496:GLU:HG3	1.82	0.45
1:B1:144:MET:HA	1:B1:147:PHE:CE2	2.52	0.45
1:b1:266:ASN:H	1:b1:266:ASN:HD22	1.65	0.45
1:B2:334:MET:N	1:B2:334:MET:SD	2.90	0.45
1:B2:500:ARG:NH2	1:B2:505:LEU:HB3	2.32	0.45
1:B3:88:LEU:HB2	1:B3:447:TRP:CZ3	2.52	0.45
1:B3:122:ASP:O	1:b3:406:ARG:NH2	2.42	0.45
1:b4:371:GLU:OE1	1:b4:371:GLU:N	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b4:448:ILE:HD11	1:b4:483:GLY:HA2	1.98	0.45
1:b5:448:ILE:HD12	1:b5:480:ALA:HA	1.99	0.45
1:b:268:GLN:HE21	1:b:349:ASN:HD21	1.65	0.45
1:B1:217:GLN:C	1:B1:218:LYS:HD2	2.42	0.45
1:B2:288:THR:O	1:B2:290:SER:N	2.50	0.45
1:b2:374:SER:C	1:b2:375:ARG:HG2	2.42	0.45
1:b2:463:GLU:HA	1:b2:463:GLU:OE2	2.17	0.45
1:B4:169:PHE:CD1	1:B4:411:MET:HE1	2.52	0.45
1:b4:299:ASN:HA	1:b4:303:GLN:C	2.42	0.45
1:b5:497:THR:O	1:b5:501:ARG:HG3	2.17	0.45
1:b:261:LEU:O	1:b:265:GLN:HG2	2.17	0.45
1:b:264:LEU:HA	1:b:267:THR:HG22	1.99	0.45
1:B2:269:LEU:O	1:B2:273:ILE:HG12	2.17	0.45
1:B2:275:LYS:HZ1	1:b2:347:THR:C	2.25	0.45
1:B4:35:LEU:HD23	1:B4:35:LEU:H	1.82	0.45
1:B4:108:SER:HA	1:B4:111:VAL:HG22	1.99	0.45
1:B4:229:GLY:O	1:B4:439:ARG:NH2	2.50	0.45
1:b4:71:ALA:O	1:b4:74:ILE:HG22	2.17	0.45
1:B5:126:ILE:HG13	1:B5:127:ASP:N	2.32	0.45
1:B5:362:ILE:HD13	1:B5:362:ILE:N	2.32	0.45
1:b5:460:GLU:OE1	1:b5:460:GLU:N	2.37	0.45
1:b5:482:ARG:HB3	1:b5:482:ARG:HH11	1.82	0.45
1:B2:49:LEU:HD23	1:B2:50:LEU:HD23	1.99	0.44
1:B5:393:TRP:CE2	1:B5:452:ARG:HB2	2.51	0.44
1:b5:114:ALA:O	1:b5:117:GLU:HG3	2.17	0.44
1:b5:125:CYS:HB3	1:b5:163:ARG:HD3	1.97	0.44
1:B:188:ASN:HA	1:B:195:ILE:HG12	1.99	0.44
1:B:314:ILE:HG21	1:B:332:HIS:CD2	2.52	0.44
1:b:453:MET:SD	1:b:454:ALA:N	2.90	0.44
1:B1:70:ALA:O	1:B1:74:ILE:HG22	2.17	0.44
1:b1:52:ASN:CG	1:b1:55:ARG:HE	2.25	0.44
1:b1:486:TYR:HA	1:b1:489:ILE:HG22	1.98	0.44
1:B2:132:ARG:NH1	1:B2:140:GLU:OE1	2.48	0.44
1:b2:395:TYR:HD2	1:b2:396:PHE:CD1	2.35	0.44
1:b2:448:ILE:HD11	1:b2:483:GLY:HA2	1.98	0.44
1:b2:448:ILE:HD12	1:b2:480:ALA:HA	1.99	0.44
1:B3:261:LEU:O	1:B3:265:GLN:HG2	2.17	0.44
1:B4:334:MET:HE2	1:B4:334:MET:N	2.32	0.44
1:b4:355:GLU:HG2	1:b4:356:GLN:NE2	2.32	0.44
1:B:501:ARG:NH2	1:B:505:LEU:O	2.50	0.44
1:B2:269:LEU:O	1:B2:269:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B2:462:GLN:HA	1:B2:465:VAL:HG12	1.99	0.44
1:b2:185:ASP:N	1:b2:185:ASP:OD1	2.50	0.44
1:b3:186:SER:HB2	1:b3:187:ARG:NH2	2.32	0.44
1:b3:278:TYR:HB2	1:B4:274:VAL:HG21	2.00	0.44
1:B4:72:ASN:O	1:B4:76:LEU:HD22	2.17	0.44
1:B4:482:ARG:HH21	1:b4:472:LEU:HB3	1.83	0.44
1:B5:90:HIS:C	1:B5:91:ARG:HD2	2.42	0.44
1:B2:318:TYR:HA	1:B2:321:ALA:CB	2.48	0.44
1:B3:278:TYR:HE1	1:b3:341:LEU:HD13	1.82	0.44
1:b3:72:ASN:O	1:b3:76:LEU:HD12	2.17	0.44
1:b3:120:GLU:H	1:b3:120:GLU:HG3	1.64	0.44
1:b3:500:ARG:NH2	1:b3:506:LYS:O	2.47	0.44
1:b4:121:ASP:OD1	1:B5:440:SER:OG	2.25	0.44
1:B5:386:ARG:NH2	1:B5:390:ASN:HD21	2.16	0.44
1:B:356:GLN:OE1	1:B:370:TYR:OH	2.34	0.44
1:b:486:TYR:CD1	1:b:486:TYR:C	2.96	0.44
1:B1:125:CYS:SG	1:B1:130:ARG:NH1	2.91	0.44
1:b1:438:ALA:HB1	1:b1:441:ALA:HB3	2.00	0.44
1:B2:269:LEU:CD2	1:b2:260:MET:HG2	2.48	0.44
1:b2:475:TYR:HA	1:b2:478:GLU:HG2	1.99	0.44
1:B3:479:CYS:O	1:B3:483:GLY:N	2.50	0.44
1:b3:395:TYR:O	1:b3:399:ARG:HG2	2.18	0.44
1:B4:121:ASP:OD1	1:b4:440:SER:OG	2.30	0.44
1:b4:111:VAL:HG12	1:b4:425:VAL:HG11	1.99	0.44
1:b4:382:TYR:CZ	1:b4:386:ARG:HD2	2.52	0.44
1:B5:401:LYS:HD2	1:B5:401:LYS:HA	1.70	0.44
1:b5:59:ARG:O	1:b5:63:LEU:HD23	2.16	0.44
1:b5:252:TYR:HA	1:b5:255:MET:HE1	1.98	0.44
1:B:88:LEU:HB2	1:B:447:TRP:CZ3	2.53	0.44
1:b1:34:GLN:CD	1:b1:36:ARG:HH22	2.24	0.44
1:B4:99:ILE:HA	1:B4:430:LYS:HZ2	1.82	0.44
1:B4:254:VAL:HB	1:B4:362:ILE:HG23	1.98	0.44
1:b4:122:ASP:HA	1:B5:406:ARG:HH12	1.82	0.44
1:b4:467:LEU:HD13	1:b4:472:LEU:HB2	2.00	0.44
1:b4:500:ARG:NH2	1:b4:505:LEU:HB3	2.33	0.44
1:B5:144:MET:HA	1:B5:147:PHE:CD1	2.53	0.44
1:B5:251:PHE:O	1:B5:255:MET:HG3	2.18	0.44
1:B:468:ILE:HD13	1:B:468:ILE:HA	1.86	0.44
1:B:492:GLN:HE21	1:B:496:GLU:HG3	1.83	0.44
1:b1:374:SER:C	1:b1:375:ARG:HG2	2.42	0.44
1:b2:477:LYS:C	1:b2:481:LYS:HZ3	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B3:65:ARG:HH21	1:b3:252:TYR:HE2	1.66	0.44
1:B4:125:CYS:SG	1:B4:130:ARG:NH1	2.91	0.44
1:B4:254:VAL:O	1:B4:258:MET:HG2	2.18	0.44
1:b4:456:ASP:HB3	1:b4:459:LYS:HG2	2.00	0.44
1:B5:36:ARG:H	1:B5:36:ARG:HG2	1.59	0.44
1:B5:122:ASP:HA	1:b5:406:ARG:HH12	1.83	0.44
1:B:371:GLU:OE1	1:B:371:GLU:N	2.50	0.44
1:B:501:ARG:O	1:B:501:ARG:HD3	2.18	0.44
1:b1:498:MET:SD	1:b1:499:GLU:N	2.91	0.44
1:B3:131:LYS:HD3	1:b3:239:PRO:HG3	2.00	0.44
1:B4:144:MET:O	1:B4:148:ASN:HB2	2.18	0.44
1:B:500:ARG:NH2	1:B:505:LEU:HB3	2.33	0.44
1:b:493:GLN:O	1:b:497:THR:OG1	2.33	0.44
1:b2:462:GLN:O	1:b2:466:MET:HG2	2.17	0.44
1:b3:254:VAL:O	1:b3:258:MET:HG2	2.17	0.44
1:B5:475:TYR:O	1:B5:478:GLU:HG2	2.18	0.44
1:b5:81:ILE:HG21	1:b5:142:VAL:HG21	2.00	0.44
1:b5:90:HIS:O	1:b5:91:ARG:HD3	2.18	0.44
1:b:144:MET:SD	1:b:174:PRO:HD3	2.58	0.43
1:B1:269:LEU:O	1:B1:273:ILE:HG12	2.18	0.43
1:B1:278:TYR:HE1	1:b1:341:LEU:HD13	1.83	0.43
1:b1:112:GLU:HB3	1:b1:116:LYS:HZ1	1.83	0.43
1:b1:395:TYR:HD2	1:b1:396:PHE:HD1	1.66	0.43
1:b2:268:GLN:HG3	1:B3:354:PHE:CZ	2.53	0.43
1:b4:132:ARG:HG2	1:b4:136:MET:HG3	1.99	0.43
1:B:395:TYR:HD2	1:B:396:PHE:CD1	2.36	0.43
1:B:485:ASP:HB3	1:B:488:GLU:OE1	2.18	0.43
1:b:140:GLU:HB3	1:b:171:MET:CE	2.48	0.43
1:B1:460:GLU:HA	1:B1:463:GLU:HG2	1.99	0.43
1:b1:318:TYR:HA	1:b1:321:ALA:HB3	1.99	0.43
1:B2:195:ILE:HD12	1:B2:199:GLY:HA2	1.99	0.43
1:B2:317:TYR:CD1	1:B2:317:TYR:C	2.96	0.43
1:B2:376:ASN:HB2	1:b2:360:ARG:HD3	2.00	0.43
1:b2:59:ARG:O	1:b2:63:LEU:HD23	2.18	0.43
1:B3:65:ARG:O	1:b3:253:SER:OG	2.31	0.43
1:b3:401:LYS:HA	1:b3:401:LYS:HD2	1.67	0.43
1:b4:500:ARG:NH2	1:b4:506:LYS:O	2.51	0.43
1:b5:485:ASP:OD2	1:b5:486:TYR:N	2.51	0.43
1:B:359:LEU:HD23	1:B:359:LEU:HA	1.72	0.43
1:B2:496:GLU:CD	1:b2:475:TYR:H	2.26	0.43
1:b2:476:GLU:HG2	1:b2:477:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B3:108:SER:HA	1:B3:111:VAL:HG22	2.00	0.43
1:B3:288:THR:O	1:B3:290:SER:N	2.51	0.43
1:b3:144:MET:HA	1:b3:147:PHE:CE2	2.53	0.43
1:b3:311:ILE:O	1:b3:314:ILE:HB	2.19	0.43
1:B4:488:GLU:OE1	1:B4:488:GLU:N	2.42	0.43
1:b5:255:MET:HE3	1:b5:255:MET:HB3	1.89	0.43
1:B:277:MET:HE3	1:b5:278:TYR:CE2	2.53	0.43
1:b:377:TYR:HB3	1:B1:384:THR:CG2	2.47	0.43
1:b:477:LYS:O	1:b:481:LYS:HG2	2.17	0.43
1:b1:59:ARG:HB3	1:B2:38:TRP:CH2	2.52	0.43
1:B2:134:PHE:O	1:B2:137:MET:HB2	2.18	0.43
1:B2:395:TYR:O	1:B2:399:ARG:HG2	2.18	0.43
1:B2:485:ASP:OD1	1:B2:487:GLN:N	2.43	0.43
1:B3:371:GLU:HG2	1:B3:377:TYR:CD2	2.53	0.43
1:B3:393:TRP:CD1	1:B3:397:MET:HG2	2.54	0.43
1:b3:264:LEU:HA	1:b3:267:THR:HG22	1.99	0.43
1:B4:322:PRO:HA	1:B4:329:LYS:NZ	2.33	0.43
1:b4:59:ARG:HB3	1:B5:38:TRP:CH2	2.53	0.43
1:b4:144:MET:HE2	1:b4:151:LEU:HA	2.00	0.43
1:b4:180:PRO:HA	1:b4:219:TRP:CG	2.53	0.43
1:B5:478:GLU:HA	1:B5:481:LYS:NZ	2.32	0.43
1:B:43:GLU:OE2	1:B:43:GLU:N	2.51	0.43
1:B1:185:ASP:OD1	1:B1:185:ASP:N	2.50	0.43
1:b1:112:GLU:HB3	1:b1:116:LYS:NZ	2.34	0.43
1:B4:185:ASP:OD1	1:B4:185:ASP:N	2.51	0.43
1:B4:299:ASN:HA	1:B4:303:GLN:C	2.44	0.43
1:B4:352:SER:HA	1:B4:355:GLU:OE2	2.18	0.43
1:b4:140:GLU:O	1:b4:144:MET:HB3	2.18	0.43
1:B5:94:TRP:O	1:B5:98:GLY:N	2.51	0.43
1:B:342:GLN:HE22	1:b5:339:LEU:HG	1.84	0.43
1:B:473:SER:OG	1:B:477:LYS:NZ	2.36	0.43
1:b:318:TYR:HA	1:b:321:ALA:HB3	2.00	0.43
1:B1:208:GLU:CD	1:B1:218:LYS:H	2.27	0.43
1:B1:438:ALA:HB1	1:B1:441:ALA:HB3	2.00	0.43
1:B1:478:GLU:H	1:B1:478:GLU:CD	2.27	0.43
1:b1:112:GLU:O	1:b1:116:LYS:HG2	2.19	0.43
1:B2:282:ILE:HG22	1:B2:330:VAL:HG12	1.99	0.43
1:b2:195:ILE:HD12	1:b2:199:GLY:HA2	1.99	0.43
1:b2:323:VAL:H	1:b2:329:LYS:NZ	2.17	0.43
1:b4:44:SER:OG	1:b4:46:ASP:OD1	2.30	0.43
1:b4:88:LEU:HB2	1:b4:447:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b4:132:ARG:HD3	1:B5:239:PRO:HG2	2.01	0.43
1:b4:378:ALA:O	1:b4:379:GLN:NE2	2.52	0.43
1:b4:468:ILE:HG12	1:b4:475:TYR:CE1	2.54	0.43
1:B:283:GLU:OE2	1:B:283:GLU:N	2.51	0.43
1:B1:497:THR:O	1:B1:501:ARG:HG3	2.18	0.43
1:b1:81:ILE:HG21	1:b1:142:VAL:HG21	2.01	0.43
1:b1:496:GLU:CD	1:B2:475:TYR:H	2.26	0.43
1:B2:390:ASN:HA	1:B2:452:ARG:HH22	1.83	0.43
1:B2:460:GLU:OE1	1:B2:460:GLU:N	2.31	0.43
1:b2:453:MET:HB2	1:b2:453:MET:HE3	1.71	0.43
1:b5:371:GLU:OE1	1:b5:371:GLU:N	2.34	0.43
1:b:259:LYS:HE3	1:B1:38:TRP:CE3	2.54	0.43
1:b:380:MET:HE2	1:b:385:ALA:N	2.34	0.43
1:b:492:GLN:HG2	1:B1:476:GLU:OE1	2.19	0.43
1:B1:318:TYR:HA	1:B1:321:ALA:HB3	2.00	0.43
1:B1:468:ILE:HD12	1:B1:478:GLU:OE1	2.19	0.43
1:b1:88:LEU:HB2	1:b1:447:TRP:CZ3	2.53	0.43
1:B2:380:MET:HB3	1:b2:384:THR:HG21	2.00	0.43
1:b2:460:GLU:O	1:b2:463:GLU:HB2	2.19	0.43
1:B3:274:VAL:O	1:B3:277:MET:HG2	2.19	0.43
1:b4:492:GLN:O	1:b4:492:GLN:NE2	2.52	0.43
1:B:132:ARG:HD3	1:b:239:PRO:HG2	2.01	0.43
1:B1:108:SER:HA	1:B1:111:VAL:HG22	2.00	0.43
1:B1:114:ALA:O	1:B1:117:GLU:HG3	2.19	0.43
1:b2:81:ILE:HG21	1:b2:142:VAL:HG21	2.00	0.43
1:B3:72:ASN:ND2	1:B3:373:LEU:O	2.52	0.43
1:B4:348:ASP:CG	1:B4:350:GLY:H	2.27	0.43
1:b4:395:TYR:HD1	1:b4:396:PHE:CD1	2.37	0.43
1:B5:49:LEU:HD23	1:B5:50:LEU:HD23	2.00	0.43
1:B5:81:ILE:HD12	1:B5:399:ARG:HB3	2.01	0.43
1:B:462:GLN:HA	1:B:465:VAL:HG12	2.01	0.43
1:b:496:GLU:CD	1:B1:475:TYR:H	2.26	0.43
1:B2:78:GLN:HE22	1:B2:139:ARG:HB3	1.84	0.43
1:B2:196:ASN:OD1	1:B2:199:GLY:N	2.52	0.43
1:B2:458:LEU:HD22	1:b2:463:GLU:OE1	2.19	0.43
1:b2:324:ARG:NH1	1:b2:324:ARG:HB2	2.34	0.43
1:b3:91:ARG:HD2	1:b3:91:ARG:N	2.33	0.43
1:b3:406:ARG:O	1:b3:410:GLN:HG2	2.19	0.43
1:b4:258:MET:HG2	1:b4:258:MET:H	1.57	0.43
1:B5:133:THR:H	1:B5:136:MET:HE3	1.83	0.43
1:b:397:MET:HA	1:b:397:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b1:359:LEU:HD13	1:b1:359:LEU:HA	1.85	0.42
1:B3:218:LYS:HG2	1:B3:219:TRP:N	2.33	0.42
1:B3:438:ALA:HB1	1:B3:441:ALA:HB3	2.01	0.42
1:b3:129:GLU:OE2	1:b3:131:LYS:NZ	2.52	0.42
1:b3:438:ALA:HB1	1:b3:441:ALA:HB3	2.01	0.42
1:b3:478:GLU:HA	1:b3:481:LYS:NZ	2.34	0.42
1:B4:208:GLU:OE1	1:B4:218:LYS:HE3	2.19	0.42
1:B5:180:PRO:HA	1:B5:219:TRP:CG	2.54	0.42
1:B5:186:SER:HB2	1:B5:187:ARG:NH2	2.33	0.42
1:B5:407:GLN:HG2	1:B5:411:MET:HE2	2.01	0.42
1:B:187:ARG:HD3	1:B:190:ARG:HH21	1.84	0.42
1:B:299:ASN:O	1:B:304:ARG:HG3	2.20	0.42
1:b:399:ARG:HG2	1:b:399:ARG:HH11	1.84	0.42
1:B1:41:PRO:HG2	1:B1:43:GLU:OE1	2.19	0.42
1:b2:111:VAL:HG12	1:b2:425:VAL:HG11	2.01	0.42
1:B3:397:MET:HA	1:B3:397:MET:HE3	2.01	0.42
1:B4:72:ASN:ND2	1:B4:373:LEU:O	2.52	0.42
1:B4:482:ARG:HB3	1:B4:482:ARG:NH1	2.34	0.42
1:B4:489:ILE:HD13	1:B4:489:ILE:HA	1.85	0.42
1:B5:377:TYR:HB3	1:b5:384:THR:CG2	2.49	0.42
1:B:190:ARG:O	1:B:193:VAL:HG12	2.18	0.42
1:B:196:ASN:HB3	1:B:202:LEU:HD21	2.01	0.42
1:b:52:ASN:O	1:b:53:PHE:C	2.62	0.42
1:b:132:ARG:HG2	1:b:136:MET:HG3	1.99	0.42
1:b:406:ARG:O	1:b:410:GLN:HG2	2.18	0.42
1:B1:187:ARG:HD2	1:B1:187:ARG:HA	1.91	0.42
1:B1:486:TYR:CD1	1:B1:486:TYR:C	2.97	0.42
1:B2:268:GLN:HE21	1:B2:268:GLN:C	2.24	0.42
1:b2:209:ASP:OD1	1:b2:210:GLY:N	2.52	0.42
1:B3:226:LEU:HD12	1:B3:230:ARG:HD3	2.02	0.42
1:B3:259:LYS:HA	1:B3:259:LYS:HD3	1.80	0.42
1:b3:122:ASP:O	1:B4:406:ARG:NH2	2.44	0.42
1:b3:226:LEU:HD12	1:b3:230:ARG:HD3	2.02	0.42
1:b3:264:LEU:HD12	1:b3:264:LEU:O	2.19	0.42
1:b4:386:ARG:NH1	1:b4:390:ASN:HD21	2.17	0.42
1:B5:52:ASN:O	1:B5:53:PHE:C	2.62	0.42
1:B:323:VAL:N	1:B:329:LYS:HZ3	2.17	0.42
1:B1:77:HIS:O	1:B1:81:ILE:HG12	2.18	0.42
1:b1:486:TYR:CD1	1:b1:486:TYR:C	2.97	0.42
1:B2:475:TYR:O	1:B2:478:GLU:HG2	2.18	0.42
1:b2:70:ALA:O	1:b2:74:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b2:116:LYS:HE2	1:b2:116:LYS:HB2	1.82	0.42
1:b2:116:LYS:O	1:b2:120:GLU:HG3	2.19	0.42
1:b2:215:MET:HE2	1:B3:187:ARG:HE	1.84	0.42
1:b2:393:TRP:CG	1:b2:452:ARG:HE	2.38	0.42
1:B3:500:ARG:NH2	1:B3:505:LEU:HB3	2.33	0.42
1:b3:369:SER:N	1:b3:372:GLN:OE1	2.32	0.42
1:b4:46:ASP:OD1	1:b4:47:ALA:N	2.52	0.42
1:b4:482:ARG:NH1	1:b4:482:ARG:HB3	2.35	0.42
1:b4:485:ASP:OD2	1:b4:486:TYR:N	2.52	0.42
1:B5:371:GLU:HB2	1:B5:377:TYR:HD1	1.84	0.42
1:b5:393:TRP:CD1	1:b5:452:ARG:HE	2.37	0.42
1:B:452:ARG:N	1:B:481:LYS:O	2.52	0.42
1:B:492:GLN:O	1:B:492:GLN:NE2	2.52	0.42
1:B2:458:LEU:HD21	1:b2:459:LYS:HE2	2.02	0.42
1:b2:113:ALA:HA	1:b2:116:LYS:HZ2	1.80	0.42
1:b2:188:ASN:HA	1:b2:195:ILE:HG12	2.00	0.42
1:B3:460:GLU:H	1:B3:460:GLU:CD	2.17	0.42
1:B3:498:MET:C	1:B3:498:MET:HE2	2.44	0.42
1:b3:126:ILE:HD11	1:b3:137:MET:HE3	2.01	0.42
1:B4:218:LYS:HG2	1:B4:219:TRP:N	2.33	0.42
1:B4:255:MET:H	1:B4:255:MET:HG3	1.66	0.42
1:b4:190:ARG:O	1:b4:193:VAL:HG12	2.20	0.42
1:B:128:VAL:HG22	1:B:168:GLN:HB2	2.01	0.42
1:B:438:ALA:HB1	1:B:441:ALA:HB3	2.01	0.42
1:b:78:GLN:OE1	1:b:139:ARG:NE	2.52	0.42
1:b:318:TYR:OH	1:B1:334:MET:HG2	2.19	0.42
1:b1:261:LEU:O	1:b1:265:GLN:HG2	2.19	0.42
1:b1:339:LEU:HD12	1:b1:340:ASN:N	2.34	0.42
1:b3:195:ILE:HD12	1:b3:199:GLY:HA2	2.01	0.42
1:b3:500:ARG:NH2	1:b3:505:LEU:HB3	2.33	0.42
1:B4:477:LYS:C	1:B4:481:LYS:HZ2	2.25	0.42
1:B5:406:ARG:O	1:B5:410:GLN:HG2	2.19	0.42
1:B5:500:ARG:NH2	1:B5:505:LEU:HB3	2.35	0.42
1:b5:251:PHE:O	1:b5:253:SER:N	2.51	0.42
1:b:67:ASN:OD1	1:b:70:ALA:N	2.39	0.42
1:b:150:GLU:CD	1:b:246:ARG:HE	2.25	0.42
1:b:196:ASN:OD1	1:b:199:GLY:N	2.53	0.42
1:B1:176:ARG:NH2	1:B1:208:GLU:HA	2.33	0.42
1:B1:477:LYS:C	1:B1:481:LYS:HZ2	2.27	0.42
1:b2:318:TYR:HA	1:b2:321:ALA:HB3	2.01	0.42
1:B4:455:ILE:O	1:b4:386:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b4:193:VAL:HG23	1:b4:204:TYR:CD2	2.55	0.42
1:b4:269:LEU:O	1:b4:269:LEU:HD12	2.20	0.42
1:B5:98:GLY:C	1:B5:430:LYS:HZ2	2.28	0.42
1:B5:323:VAL:H	1:B5:329:LYS:HZ1	1.67	0.42
1:b5:438:ALA:HB1	1:b5:441:ALA:HB3	2.02	0.42
1:B:254:VAL:O	1:B:258:MET:HG2	2.19	0.42
1:B:299:ASN:HA	1:B:303:GLN:C	2.44	0.42
1:B:485:ASP:OD1	1:B:486:TYR:N	2.52	0.42
1:B1:299:ASN:HA	1:B1:303:GLN:C	2.44	0.42
1:B1:498:MET:HB3	1:B1:501:ARG:NH2	2.35	0.42
1:b1:226:LEU:HD12	1:b1:230:ARG:HD3	2.01	0.42
1:B2:34:GLN:CD	1:B2:36:ARG:HH22	2.27	0.42
1:B2:393:TRP:CE2	1:B2:452:ARG:HB2	2.55	0.42
1:B2:416:LEU:HD12	1:B2:416:LEU:O	2.20	0.42
1:B2:497:THR:O	1:B2:501:ARG:HG3	2.19	0.42
1:B4:263:THR:HA	1:B4:266:ASN:HD22	1.83	0.42
1:B5:87:ARG:HB3	1:B5:448:ILE:CG2	2.48	0.42
1:B5:132:ARG:HG2	1:B5:136:MET:HG3	2.01	0.42
1:B5:299:ASN:HA	1:B5:303:GLN:C	2.45	0.42
1:b5:333:LEU:HD23	1:b5:333:LEU:HA	1.78	0.42
1:b:122:ASP:HA	1:B1:406:ARG:HH12	1.84	0.42
1:b:334:MET:HA	1:b:334:MET:HE3	2.02	0.42
1:B2:144:MET:SD	1:B2:174:PRO:HD3	2.60	0.42
1:B2:310:TRP:CZ3	1:b2:296:LEU:HA	2.55	0.42
1:b2:264:LEU:HD12	1:b2:264:LEU:O	2.19	0.42
1:b2:323:VAL:N	1:b2:329:LYS:HZ3	2.17	0.42
1:B3:282:ILE:HD13	1:B3:282:ILE:HA	1.86	0.42
1:b3:459:LYS:HE2	1:b3:459:LYS:HA	2.00	0.42
1:B4:358:LEU:HD13	1:B4:358:LEU:HA	1.90	0.42
1:b4:226:LEU:HD12	1:b4:230:ARG:HD3	2.02	0.42
1:B5:55:ARG:HG3	1:B5:56:GLY:N	2.34	0.42
1:B5:72:ASN:HD22	1:B5:373:LEU:HD12	1.85	0.42
1:B5:448:ILE:CD1	1:B5:480:ALA:HA	2.50	0.42
1:B5:489:ILE:HD13	1:B5:489:ILE:HA	1.81	0.42
1:b5:325:LEU:HD23	1:b5:330:VAL:HG22	2.01	0.42
1:B:35:LEU:HD23	1:B:35:LEU:H	1.85	0.42
1:B1:393:TRP:CH2	1:B1:452:ARG:HA	2.54	0.42
1:b1:80:HIS:HB2	1:b1:396:PHE:CE2	2.55	0.42
1:b2:438:ALA:HB1	1:b2:441:ALA:HB3	2.02	0.42
1:B3:90:HIS:NE2	1:B3:442:TRP:O	2.32	0.42
1:b3:81:ILE:O	1:b3:400:ARG:NE	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b3:87:ARG:HB3	1:b3:448:ILE:CG2	2.48	0.42
1:b3:269:LEU:O	1:b3:273:ILE:HG12	2.19	0.42
1:b3:393:TRP:CE2	1:b3:452:ARG:HB2	2.55	0.42
1:b3:460:GLU:H	1:b3:460:GLU:CD	2.17	0.42
1:B4:144:MET:HE3	1:B4:151:LEU:HA	2.02	0.42
1:b4:455:ILE:O	1:B5:386:ARG:NE	2.38	0.42
1:B5:226:LEU:HD12	1:B5:230:ARG:HD3	2.00	0.42
1:B:44:SER:HA	1:b5:175:LYS:NZ	2.33	0.41
1:B2:71:ALA:O	1:B2:74:ILE:HG22	2.20	0.41
1:B2:208:GLU:CD	1:B2:218:LYS:HB3	2.45	0.41
1:B2:255:MET:O	1:B2:259:LYS:HG2	2.20	0.41
1:B3:134:PHE:O	1:B3:138:ILE:HG12	2.20	0.41
1:B3:334:MET:HE2	1:B3:335:PRO:HD2	2.02	0.41
1:B3:468:ILE:HD13	1:B3:468:ILE:HA	1.87	0.41
1:B4:112:GLU:C	1:B4:116:LYS:NZ	2.78	0.41
1:B4:448:ILE:HD12	1:B4:480:ALA:HA	2.02	0.41
1:b4:395:TYR:HD1	1:b4:396:PHE:HD1	1.68	0.41
1:b5:381:SER:O	1:b5:385:ALA:N	2.48	0.41
1:b1:108:SER:HA	1:b1:111:VAL:HG22	2.01	0.41
1:B2:467:LEU:HB3	1:B2:473:SER:CB	2.46	0.41
1:B3:62:ASP:OD1	1:B3:66:ASN:ND2	2.52	0.41
1:B3:380:MET:SD	1:B3:384:THR:OG1	2.64	0.41
1:b3:261:LEU:O	1:b3:265:GLN:HG2	2.20	0.41
1:b4:136:MET:HE2	1:b4:136:MET:HB3	1.82	0.41
1:B1:259:LYS:HE3	1:b1:38:TRP:CE3	2.56	0.41
1:B2:78:GLN:OE1	1:B2:139:ARG:NE	2.53	0.41
1:b2:144:MET:CE	1:b2:173:SER:HA	2.50	0.41
1:B3:63:LEU:HD23	1:B3:63:LEU:HA	1.80	0.41
1:b3:133:THR:O	1:b3:137:MET:HE2	2.21	0.41
1:b3:133:THR:OG1	1:b3:136:MET:HE3	2.20	0.41
1:b3:329:LYS:HD3	1:b3:329:LYS:C	2.45	0.41
1:b3:362:ILE:HD13	1:b3:362:ILE:N	2.35	0.41
1:B4:180:PRO:HA	1:B4:219:TRP:CG	2.55	0.41
1:b4:283:GLU:N	1:b4:283:GLU:OE2	2.53	0.41
1:B5:453:MET:HE2	1:B5:454:ALA:N	2.35	0.41
1:b5:318:TYR:HA	1:b5:321:ALA:HB3	2.02	0.41
1:B:506:LYS:HA	1:B:507:PRO:HD3	1.95	0.41
1:b1:80:HIS:HB3	1:b1:396:PHE:HD2	1.84	0.41
1:b1:87:ARG:NH2	1:b1:483:GLY:O	2.53	0.41
1:b1:98:GLY:O	1:b1:430:LYS:HE2	2.20	0.41
1:b1:323:VAL:N	1:b1:329:LYS:HZ2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b1:476:GLU:N	1:b1:476:GLU:OE1	2.51	0.41
1:B2:121:ASP:OD1	1:b2:440:SER:OG	2.25	0.41
1:B4:113:ALA:HA	1:B4:116:LYS:NZ	2.35	0.41
1:B4:362:ILE:HG22	1:B4:366:LEU:HD23	2.02	0.41
1:B4:475:TYR:HA	1:B4:478:GLU:HG2	2.03	0.41
1:B4:477:LYS:O	1:B4:481:LYS:NZ	2.50	0.41
1:b5:393:TRP:CG	1:b5:452:ARG:HE	2.37	0.41
1:B:278:TYR:HE2	1:B:325:LEU:HD13	1.85	0.41
1:B:346:ASP:HA	1:b:345:GLN:OE1	2.20	0.41
1:B:372:GLN:HG2	1:B:373:LEU:N	2.35	0.41
1:B1:111:VAL:HG12	1:B1:425:VAL:HG11	2.02	0.41
1:B1:492:GLN:HB3	1:b1:474:THR:HG21	2.02	0.41
1:b1:150:GLU:CD	1:b1:246:ARG:HE	2.28	0.41
1:b1:370:TYR:OH	1:b1:376:ASN:ND2	2.54	0.41
1:b1:500:ARG:NH2	1:b1:505:LEU:HB3	2.35	0.41
1:B2:140:GLU:HB3	1:B2:171:MET:HE1	2.03	0.41
1:b2:468:ILE:HD12	1:b2:468:ILE:HA	1.95	0.41
1:B3:299:ASN:HA	1:B3:303:GLN:C	2.45	0.41
1:b3:321:ALA:N	1:b3:322:PRO:HD2	2.35	0.41
1:B4:362:ILE:HD12	1:B4:362:ILE:H	1.86	0.41
1:b4:257:GLN:HA	1:b4:260:MET:CE	2.44	0.41
1:B5:467:LEU:HB3	1:B5:473:SER:HB2	2.02	0.41
1:b5:144:MET:O	1:b5:148:ASN:HB2	2.20	0.41
1:b5:362:ILE:HD12	1:b5:362:ILE:H	1.85	0.41
1:b1:121:ASP:OD1	1:B2:440:SER:OG	2.26	0.41
1:B2:468:ILE:HD13	1:B2:478:GLU:OE2	2.21	0.41
1:b2:299:ASN:HA	1:b2:303:GLN:C	2.45	0.41
1:B3:305:GLU:H	1:B3:305:GLU:HG3	1.69	0.41
1:B3:479:CYS:O	1:B3:484:ASP:N	2.30	0.41
1:B4:59:ARG:O	1:B4:63:LEU:HD23	2.20	0.41
1:B4:131:LYS:NZ	1:b4:244:GLN:O	2.53	0.41
1:B4:486:TYR:HA	1:B4:489:ILE:HB	2.03	0.41
1:b4:482:ARG:HH21	1:B5:472:LEU:HB3	1.86	0.41
1:B5:127:ASP:OD2	1:B5:130:ARG:N	2.54	0.41
1:b5:498:MET:HB3	1:b5:501:ARG:NH2	2.35	0.41
1:B:144:MET:HE1	1:B:173:SER:HA	2.01	0.41
1:B:334:MET:HG2	1:b5:318:TYR:OH	2.20	0.41
1:B:452:ARG:HD2	1:B:453:MET:H	1.86	0.41
1:b:362:ILE:HD13	1:b:362:ILE:N	2.36	0.41
1:b:380:MET:HE1	1:b:384:THR:HB	2.03	0.41
1:b:479:CYS:O	1:b:484:ASP:N	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:134:PHE:HA	1:B1:137:MET:HB2	2.02	0.41
1:B1:482:ARG:HB3	1:B1:482:ARG:NH1	2.35	0.41
1:b1:190:ARG:O	1:b1:193:VAL:HG12	2.20	0.41
1:B2:102:GLU:OE1	1:B2:102:GLU:N	2.43	0.41
1:B2:132:ARG:HD3	1:b2:239:PRO:HG2	2.01	0.41
1:B2:477:LYS:C	1:B2:481:LYS:HZ2	2.28	0.41
1:B2:478:GLU:HA	1:B2:481:LYS:NZ	2.36	0.41
1:b2:496:GLU:CD	1:B3:475:TYR:H	2.24	0.41
1:B3:359:LEU:HD23	1:B3:359:LEU:HA	1.86	0.41
1:B4:314:ILE:HG23	1:B4:318:TYR:CD2	2.56	0.41
1:b4:377:TYR:HB3	1:B5:384:THR:CG2	2.51	0.41
1:B5:79:ASP:OD2	1:b5:395:TYR:HA	2.20	0.41
1:B5:113:ALA:HA	1:B5:116:LYS:HZ3	1.86	0.41
1:B5:121:ASP:OD1	1:b5:440:SER:OG	2.24	0.41
1:B:226:LEU:HD12	1:B:230:ARG:HD3	2.02	0.41
1:b:506:LYS:HA	1:b:507:PRO:HD3	1.94	0.41
1:B1:137:MET:O	1:B1:171:MET:HE1	2.21	0.41
1:B1:477:LYS:HZ2	1:B1:477:LYS:HG3	1.66	0.41
1:b1:188:ASN:O	1:b1:194:GLN:NE2	2.54	0.41
1:B2:72:ASN:OD1	1:B2:375:ARG:NH2	2.54	0.41
1:B2:94:TRP:O	1:B2:98:GLY:N	2.54	0.41
1:B2:438:ALA:HB1	1:B2:441:ALA:HB3	2.03	0.41
1:b2:474:THR:H	1:b2:477:LYS:HZ2	1.65	0.41
1:B3:132:ARG:HG2	1:B3:136:MET:HG3	2.02	0.41
1:B3:311:ILE:HD13	1:B3:311:ILE:HA	1.90	0.41
1:B4:89:SER:HB3	1:B4:446:ASP:OD1	2.20	0.41
1:B5:67:ASN:OD1	1:B5:69:TYR:N	2.54	0.41
1:B5:269:LEU:O	1:B5:269:LEU:HD12	2.20	0.41
1:b5:386:ARG:O	1:b5:390:ASN:ND2	2.54	0.41
1:B:134:PHE:O	1:B:138:ILE:HG12	2.20	0.41
1:B:252:TYR:HA	1:B:255:MET:SD	2.61	0.41
1:B:258:MET:HE3	1:B:258:MET:HB3	2.00	0.41
1:B:498:MET:SD	1:B:499:GLU:N	2.94	0.41
1:b:81:ILE:HG21	1:b:142:VAL:HG21	2.02	0.41
1:b:416:LEU:HD12	1:b:416:LEU:O	2.20	0.41
1:B1:78:GLN:OE1	1:B1:139:ARG:HB3	2.20	0.41
1:B1:192:GLY:O	1:B1:205:TYR:N	2.51	0.41
1:b1:181:ASN:OD1	1:b1:181:ASN:N	2.54	0.41
1:b1:256:GLU:HG2	1:b1:260:MET:HE2	2.03	0.41
1:b1:367:GLY:HA3	1:b1:395:TYR:CZ	2.56	0.41
1:b1:380:MET:HB3	1:B2:384:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b1:458:LEU:HB2	1:b1:459:LYS:NZ	2.35	0.41
1:B2:82:VAL:HG13	1:B2:83:GLY:H	1.86	0.41
1:B2:448:ILE:HG13	1:B2:448:ILE:O	2.20	0.41
1:B2:460:GLU:H	1:B2:460:GLU:CD	2.14	0.41
1:b2:112:GLU:O	1:b2:116:LYS:HG3	2.21	0.41
1:b2:259:LYS:HA	1:b2:259:LYS:HD2	1.60	0.41
1:b2:282:ILE:HD13	1:b2:282:ILE:HA	1.92	0.41
1:b2:314:ILE:HG23	1:b2:318:TYR:CD2	2.55	0.41
1:b2:407:GLN:HG2	1:b2:411:MET:CE	2.51	0.41
1:B3:71:ALA:O	1:B3:74:ILE:HG22	2.21	0.41
1:B3:85:PHE:CE2	1:B3:87:ARG:HD2	2.55	0.41
1:B3:85:PHE:HE2	1:B3:87:ARG:HD2	1.85	0.41
1:B3:112:GLU:O	1:B3:116:LYS:NZ	2.49	0.41
1:B3:283:GLU:N	1:B3:283:GLU:OE1	2.54	0.41
1:b3:41:PRO:HG2	1:b3:43:GLU:OE2	2.21	0.41
1:b3:242:ASP:N	1:b3:242:ASP:OD1	2.53	0.41
1:b3:416:LEU:HD12	1:b3:416:LEU:O	2.20	0.41
1:B4:485:ASP:OD2	1:B4:486:TYR:N	2.53	0.41
1:B5:129:GLU:CD	1:B5:131:LYS:HD3	2.46	0.41
1:B5:479:CYS:O	1:B5:483:GLY:N	2.54	0.41
1:b5:257:GLN:OE1	1:b5:257:GLN:N	2.54	0.41
1:b5:299:ASN:HA	1:b5:303:GLN:C	2.45	0.41
1:B:75:GLN:HE21	1:b:395:TYR:HD1	1.69	0.41
1:B:406:ARG:O	1:B:410:GLN:HG2	2.21	0.41
1:b:55:ARG:HG3	1:b:56:GLY:N	2.36	0.41
1:b:301:GLN:O	1:b:304:ARG:NH2	2.54	0.41
1:B1:397:MET:HE1	1:B1:400:ARG:CZ	2.51	0.41
1:b1:283:GLU:OE1	1:b1:283:GLU:N	2.54	0.41
1:b1:465:VAL:HA	1:b1:468:ILE:HG22	2.03	0.41
1:B2:458:LEU:HD21	1:b2:459:LYS:HB3	2.02	0.41
1:b2:208:GLU:CD	1:b2:218:LYS:H	2.29	0.41
1:b2:397:MET:N	1:b2:397:MET:HE2	2.36	0.41
1:B3:87:ARG:HE	1:B3:87:ARG:HB2	1.66	0.41
1:b3:82:VAL:HG23	1:b3:86:PHE:HD1	1.85	0.41
1:b3:197:ASP:OD1	1:b3:197:ASP:C	2.64	0.41
1:b3:476:GLU:OE2	1:b3:477:LYS:NZ	2.54	0.41
1:B4:263:THR:HA	1:B4:266:ASN:ND2	2.36	0.41
1:B4:438:ALA:HB1	1:B4:441:ALA:HB3	2.03	0.41
1:B4:492:GLN:NE2	1:B4:492:GLN:O	2.54	0.41
1:B5:132:ARG:HD3	1:b5:239:PRO:HG2	2.01	0.41
1:B5:458:LEU:HD11	1:b5:459:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:TYR:CE1	1:b:341:LEU:HD13	2.56	0.40
1:B1:80:HIS:HB3	1:B1:396:PHE:CD1	2.57	0.40
1:B2:113:ALA:HA	1:B2:116:LYS:NZ	2.36	0.40
1:B2:150:GLU:CD	1:B2:246:ARG:HE	2.27	0.40
1:B2:226:LEU:HD12	1:B2:230:ARG:HD3	2.03	0.40
1:B2:362:ILE:N	1:B2:362:ILE:HD13	2.36	0.40
1:B3:329:LYS:HD3	1:B3:330:VAL:O	2.20	0.40
1:b3:448:ILE:CD1	1:b3:480:ALA:HA	2.51	0.40
1:b4:75:GLN:NE2	1:B5:399:ARG:HH22	2.20	0.40
1:b4:416:LEU:O	1:b4:416:LEU:HD12	2.21	0.40
1:b4:474:THR:N	1:b4:477:LYS:HZ1	2.15	0.40
1:B:282:ILE:HD13	1:B:282:ILE:HA	1.83	0.40
1:B:372:GLN:OE1	1:B:372:GLN:N	2.53	0.40
1:B:380:MET:HE3	1:B:381:SER:H	1.84	0.40
1:B:416:LEU:O	1:B:416:LEU:HD12	2.21	0.40
1:b:438:ALA:HB1	1:b:441:ALA:HB3	2.03	0.40
1:B1:60:ALA:O	1:B1:64:VAL:HG12	2.20	0.40
1:B1:492:GLN:HE21	1:B1:496:GLU:HG3	1.85	0.40
1:b1:87:ARG:HB3	1:b1:448:ILE:HG23	2.03	0.40
1:b1:90:HIS:NE2	1:b1:442:TRP:O	2.33	0.40
1:b1:193:VAL:HG23	1:b1:204:TYR:CD2	2.56	0.40
1:b1:376:ASN:CA	1:B2:360:ARG:HH12	2.35	0.40
1:B2:34:GLN:HB2	1:B2:35:LEU:H	1.74	0.40
1:B2:473:SER:OG	1:B2:477:LYS:HE2	2.20	0.40
1:B3:459:LYS:O	1:B3:463:GLU:HG2	2.21	0.40
1:B3:460:GLU:O	1:B3:463:GLU:HB2	2.21	0.40
1:b3:215:MET:HE1	1:B4:187:ARG:HD3	2.03	0.40
1:b4:75:GLN:NE2	1:B5:399:ARG:NH2	2.69	0.40
1:b4:341:LEU:HD23	1:b4:341:LEU:H	1.86	0.40
1:B5:374:SER:C	1:B5:375:ARG:HG2	2.46	0.40
1:b5:261:LEU:HD12	1:b5:261:LEU:HA	1.86	0.40
1:B:256:GLU:O	1:B:260:MET:HG3	2.21	0.40
1:b:300:SER:O	1:b:304:ARG:NH1	2.51	0.40
1:B1:453:MET:C	1:B1:453:MET:HE3	2.46	0.40
1:b1:468:ILE:HG12	1:b1:475:TYR:CE1	2.57	0.40
1:b1:497:THR:HB	1:b1:501:ARG:HH21	1.85	0.40
1:B2:83:GLY:HA3	1:B2:450:SER:OG	2.22	0.40
1:b2:99:ILE:HA	1:b2:430:LYS:HZ2	1.86	0.40
1:b2:305:GLU:HA	1:b2:308:THR:HG1	1.85	0.40
1:B3:485:ASP:OD1	1:B3:485:ASP:C	2.64	0.40
1:B4:208:GLU:OE1	1:B4:218:LYS:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b4:371:GLU:O	1:b4:375:ARG:HA	2.21	0.40
1:B5:334:MET:HE3	1:B5:334:MET:HA	2.03	0.40
1:b5:256:GLU:H	1:b5:256:GLU:CD	2.24	0.40
1:B:120:GLU:H	1:B:120:GLU:HG3	1.63	0.40
1:B:311:ILE:HD13	1:B:311:ILE:HA	1.90	0.40
1:B:334:MET:HB2	1:B:337:ASP:OD1	2.21	0.40
1:B:386:ARG:NE	1:b5:455:ILE:O	2.44	0.40
1:b:175:LYS:HZ1	1:B1:43:GLU:C	2.30	0.40
1:B1:261:LEU:HD12	1:B1:261:LEU:HA	1.81	0.40
1:b1:180:PRO:HA	1:b1:219:TRP:CG	2.57	0.40
1:b1:192:GLY:O	1:b1:205:TYR:N	2.53	0.40
1:B2:275:LYS:NZ	1:b2:347:THR:OG1	2.54	0.40
1:B2:458:LEU:HD13	1:b2:463:GLU:OE1	2.21	0.40
1:B2:458:LEU:CD2	1:b2:459:LYS:HB3	2.52	0.40
1:b2:492:GLN:HG2	1:B3:476:GLU:OE2	2.21	0.40
1:b3:180:PRO:HA	1:b3:219:TRP:CG	2.56	0.40
1:B4:175:LYS:NZ	1:b4:44:SER:HA	2.37	0.40
1:B4:258:MET:HG2	1:B4:258:MET:H	1.64	0.40
1:B5:303:GLN:HA	1:B5:305:GLU:CD	2.46	0.40
1:b5:78:GLN:HB3	1:b5:139:ARG:NH2	2.37	0.40
1:b:108:SER:HA	1:b:111:VAL:HG22	2.03	0.40
1:b2:120:GLU:HG3	1:b2:120:GLU:H	1.69	0.40
1:b3:146:ALA:O	1:b3:250:VAL:HG12	2.21	0.40
1:B4:55:ARG:HG3	1:B4:56:GLY:N	2.35	0.40
1:B4:175:LYS:NZ	1:b4:43:GLU:O	2.50	0.40
1:B4:269:LEU:O	1:B4:269:LEU:HD12	2.21	0.40
1:B5:71:ALA:O	1:B5:74:ILE:HG22	2.21	0.40
1:B5:462:GLN:HA	1:B5:465:VAL:HG12	2.03	0.40
1:b5:158:ASP:OD1	1:b5:159:THR:N	2.54	0.40
1:b5:268:GLN:HE22	1:b5:349:ASN:HD21	1.69	0.40
1:b5:391:GLU:H	1:b5:391:GLU:CD	2.26	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	B	472/533 (89%)	444 (94%)	27 (6%)	1 (0%)	43	74
1	B1	472/533 (89%)	445 (94%)	26 (6%)	1 (0%)	43	74
1	B2	295/533 (55%)	275 (93%)	18 (6%)	2 (1%)	18	52
1	B4	472/533 (89%)	445 (94%)	25 (5%)	2 (0%)	30	62
1	B5	472/533 (89%)	446 (94%)	23 (5%)	3 (1%)	21	55
1	b	472/533 (89%)	442 (94%)	28 (6%)	2 (0%)	30	62
1	b1	472/533 (89%)	446 (94%)	24 (5%)	2 (0%)	30	62
1	b3	412/533 (77%)	388 (94%)	22 (5%)	2 (0%)	24	58
1	b4	472/533 (89%)	446 (94%)	25 (5%)	1 (0%)	43	74
1	b5	472/533 (89%)	451 (96%)	20 (4%)	1 (0%)	43	74
All	All	4483/5330 (84%)	4228 (94%)	238 (5%)	17 (0%)	31	62

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	PRO
1	b	322	PRO
1	B1	322	PRO
1	b1	322	PRO
1	b1	344	ALA
1	B2	322	PRO
1	b3	322	PRO
1	B4	322	PRO
1	b4	322	PRO
1	B5	322	PRO
1	b5	322	PRO
1	B2	289	GLN
1	b3	289	GLN
1	b	289	GLN
1	B5	286	LEU
1	B5	289	GLN
1	B4	286	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	176/428 (41%)	176 (100%)	0	100	100
1	B1	373/428 (87%)	370 (99%)	3 (1%)	73	77
1	B2	373/428 (87%)	370 (99%)	3 (1%)	73	77
1	B3	373/428 (87%)	370 (99%)	3 (1%)	73	77
1	B4	373/428 (87%)	372 (100%)	1 (0%)	86	83
1	B5	373/428 (87%)	370 (99%)	3 (1%)	73	77
1	b	342/428 (80%)	340 (99%)	2 (1%)	78	80
1	b1	373/428 (87%)	371 (100%)	2 (0%)	81	81
1	b2	373/428 (87%)	371 (100%)	2 (0%)	81	81
1	b3	373/428 (87%)	371 (100%)	2 (0%)	81	81
1	b4	373/428 (87%)	372 (100%)	1 (0%)	86	83
1	b5	373/428 (87%)	370 (99%)	3 (1%)	73	77
All	All	4248/5136 (83%)	4223 (99%)	25 (1%)	76	80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	171	MET
1	b	468	ILE
1	B1	43	GLU
1	B1	46	ASP
1	B1	126	ILE
1	b1	131	LYS
1	b1	358	LEU
1	B2	133	THR
1	B2	467	LEU
1	B2	489	ILE
1	b2	116	LYS
1	b2	325	LEU
1	B3	116	LYS
1	B3	133	THR

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Mol	Chain	Res	Type
1	B3	430	LYS
1	b3	133	THR
1	b3	455	ILE
1	B4	468	ILE
1	b4	137	MET
1	B5	133	THR
1	B5	333	LEU
1	B5	372	GLN
1	b5	46	ASP
1	b5	256	GLU
1	b5	356	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	ASN
1	B	379	GLN
1	b	75	GLN
1	b	194	GLN
1	b	268	GLN
1	b	462	GLN
1	B1	34	GLN
1	B1	145	HIS
1	B1	182	ASN
1	B1	268	GLN
1	B1	349	ASN
1	b1	75	GLN
1	b1	182	ASN
1	b1	356	GLN
1	b1	376	ASN
1	b1	407	GLN
1	B2	52	ASN
1	B2	168	GLN
1	B2	194	GLN
1	B2	487	GLN
1	b2	52	ASN
1	b2	72	ASN
1	b2	340	ASN
1	B3	72	ASN
1	B3	194	GLN
1	B3	379	GLN
1	b3	52	ASN

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Mol	Chain	Res	Type
1	b3	66	ASN
1	b3	379	GLN
1	B4	52	ASN
1	B4	145	HIS
1	B4	182	ASN
1	B4	266	ASN
1	b4	75	GLN
1	b4	182	ASN
1	b4	340	ASN
1	b4	356	GLN
1	b4	376	ASN
1	b4	379	GLN
1	B5	349	ASN
1	b5	52	ASN
1	b5	182	ASN
1	b5	349	ASN
1	b5	356	GLN
1	b5	390	ASN
1	b5	487	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

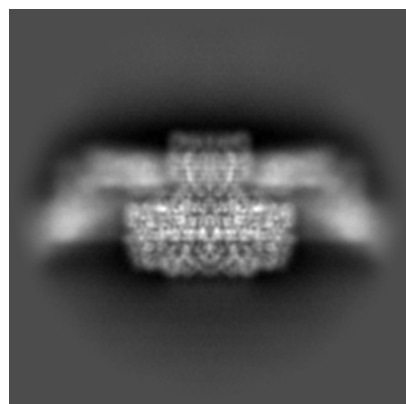
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38540. These allow visual inspection of the internal detail of the map and identification of artifacts.

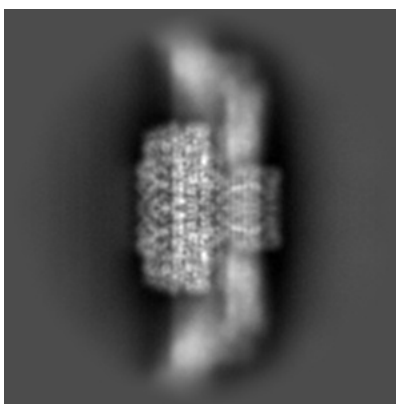
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

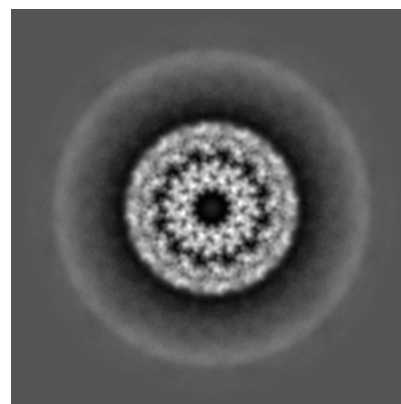
6.1.1 Primary map



X

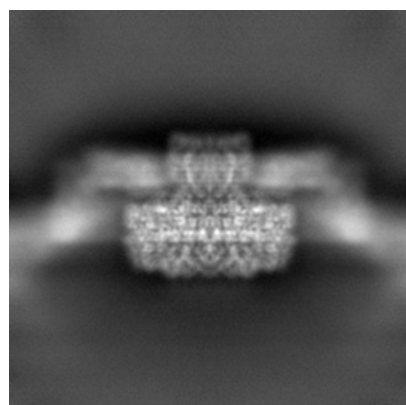


Y

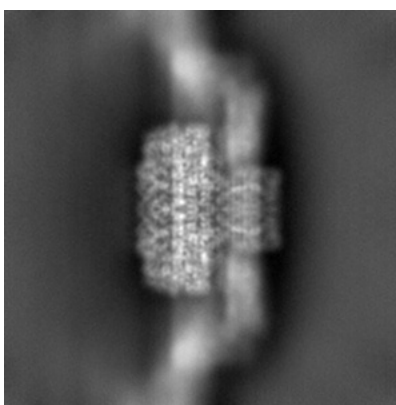


Z

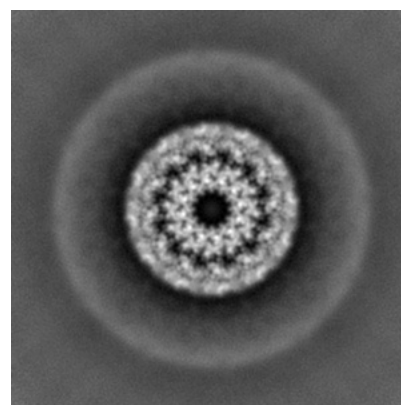
6.1.2 Raw map



X



Y

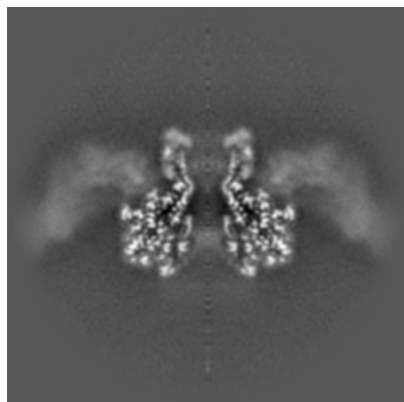


Z

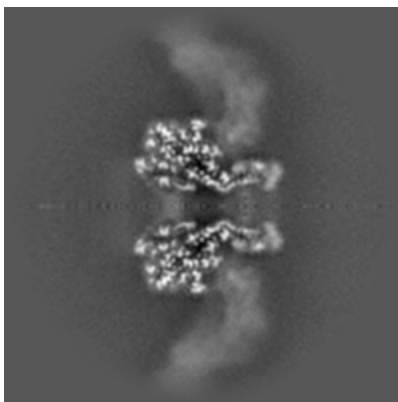
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

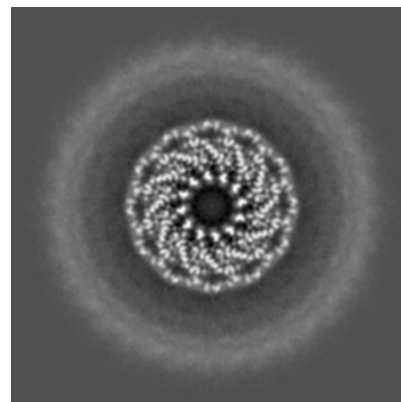
6.2.1 Primary map



X Index: 128

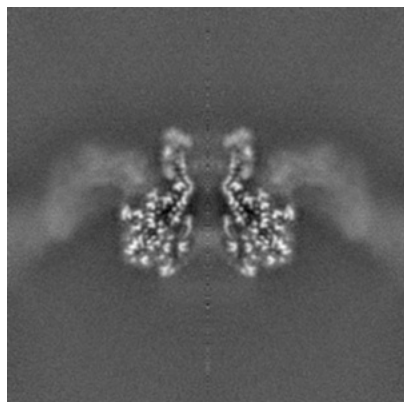


Y Index: 128

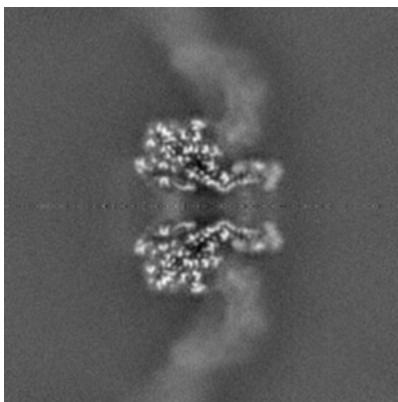


Z Index: 128

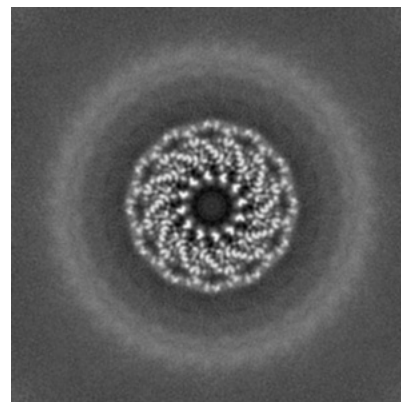
6.2.2 Raw map



X Index: 128



Y Index: 128

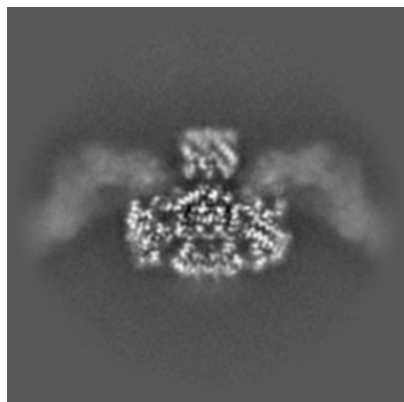


Z Index: 128

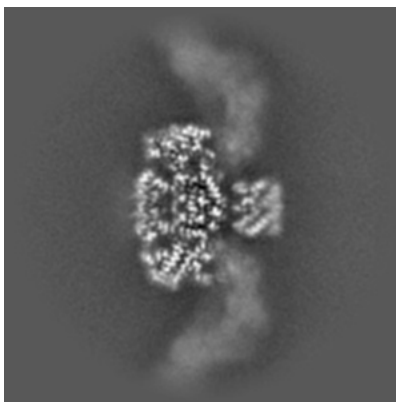
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

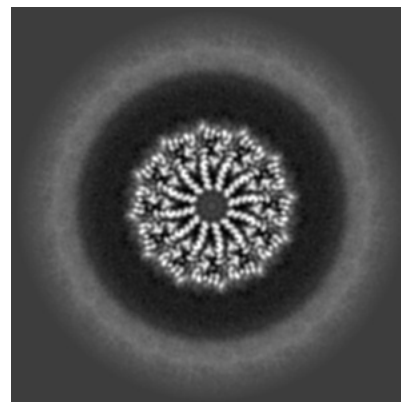
6.3.1 Primary map



X Index: 106

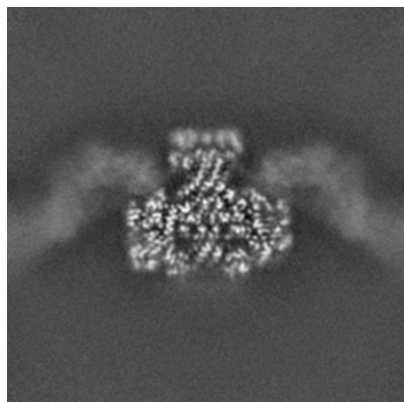


Y Index: 106

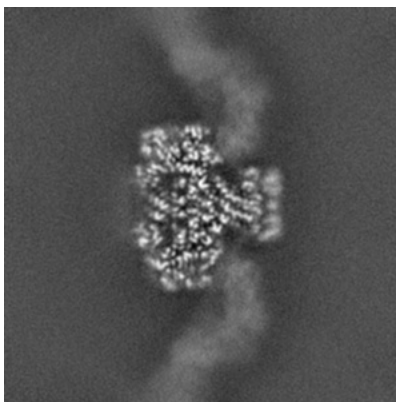


Z Index: 113

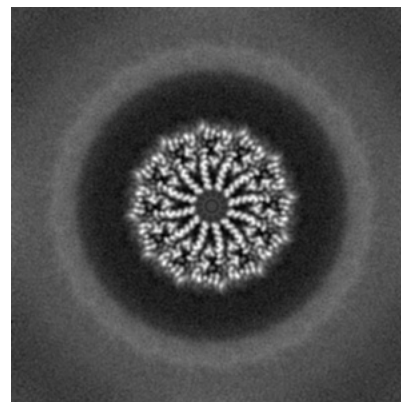
6.3.2 Raw map



X Index: 111



Y Index: 111

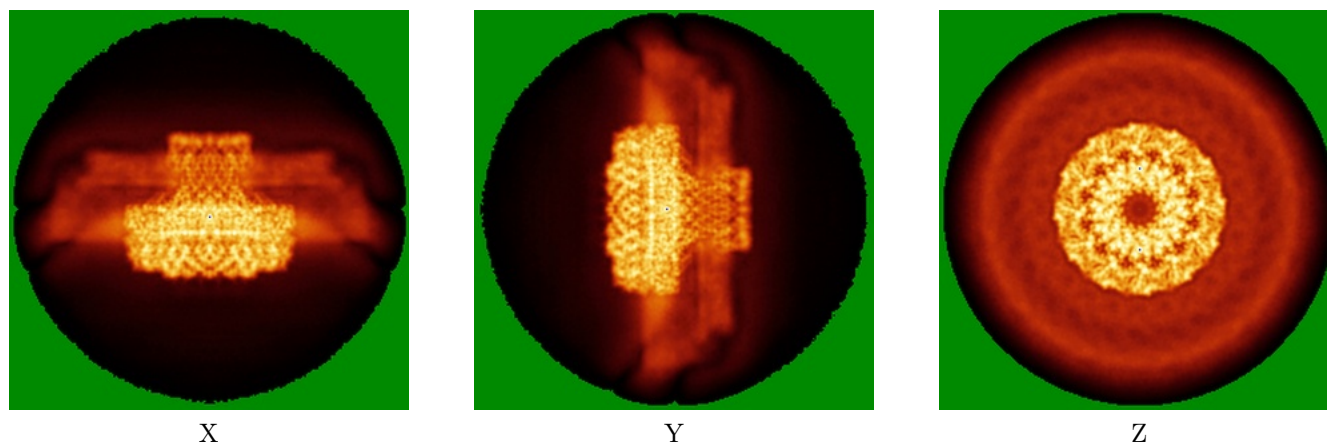


Z Index: 113

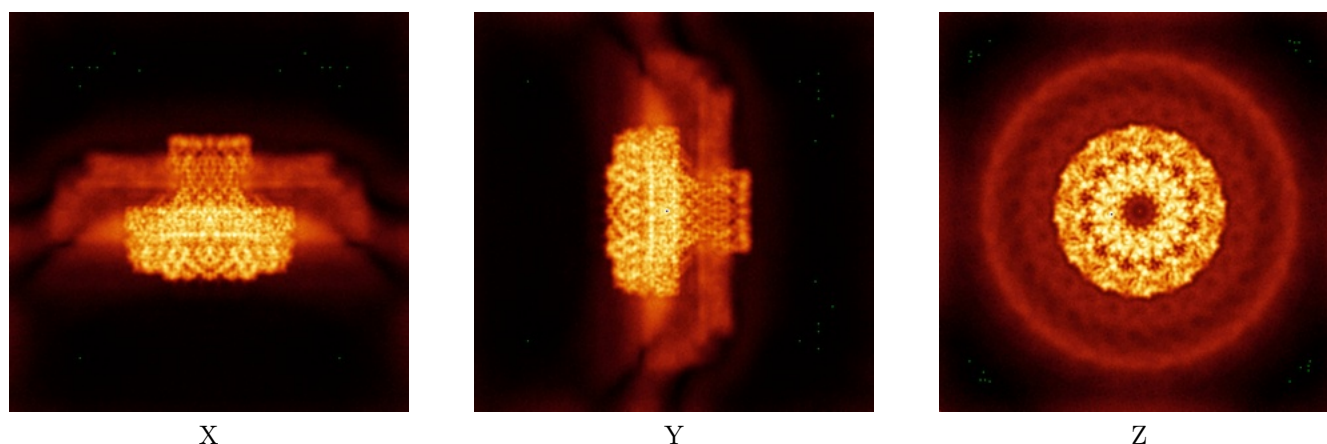
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

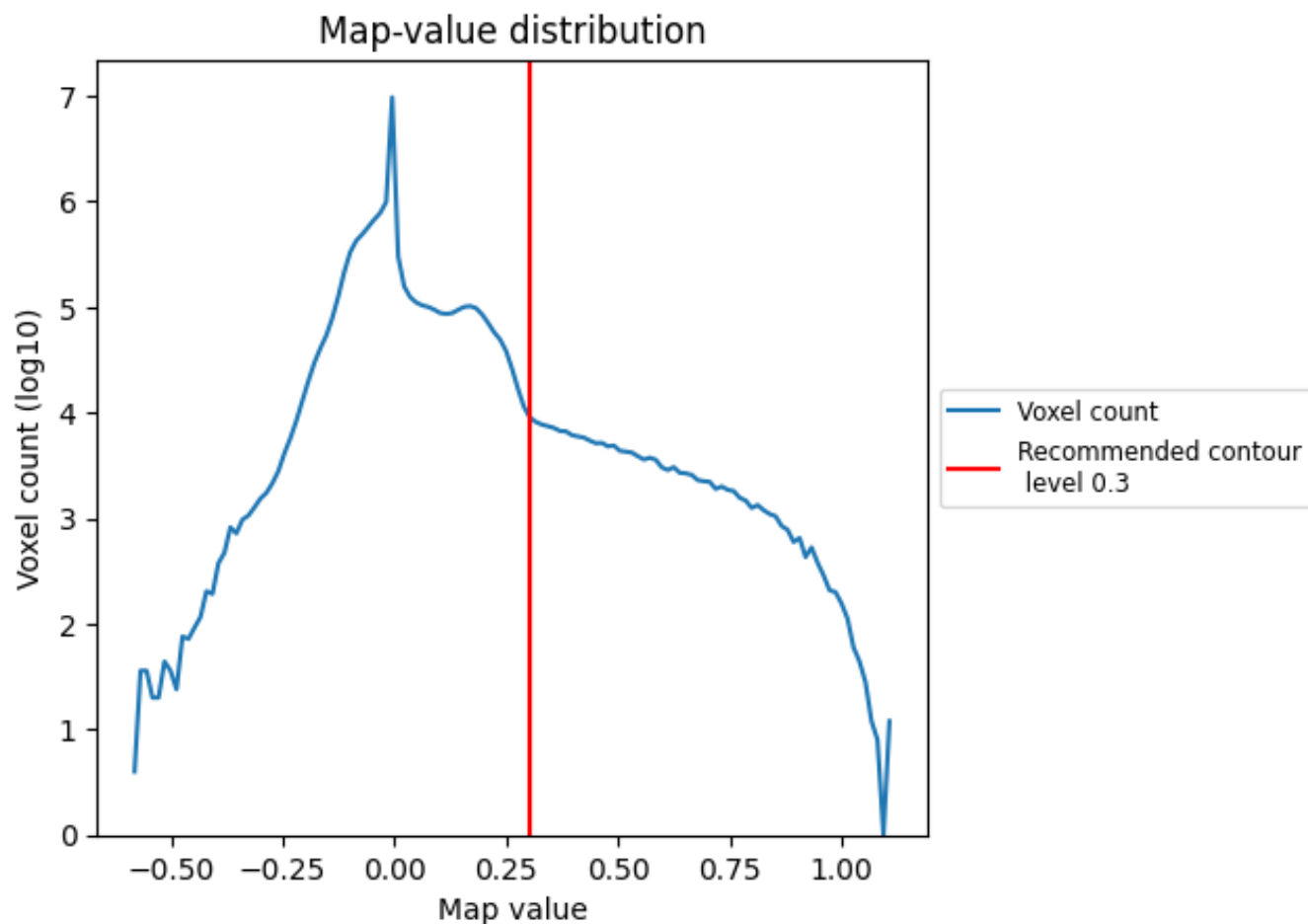
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

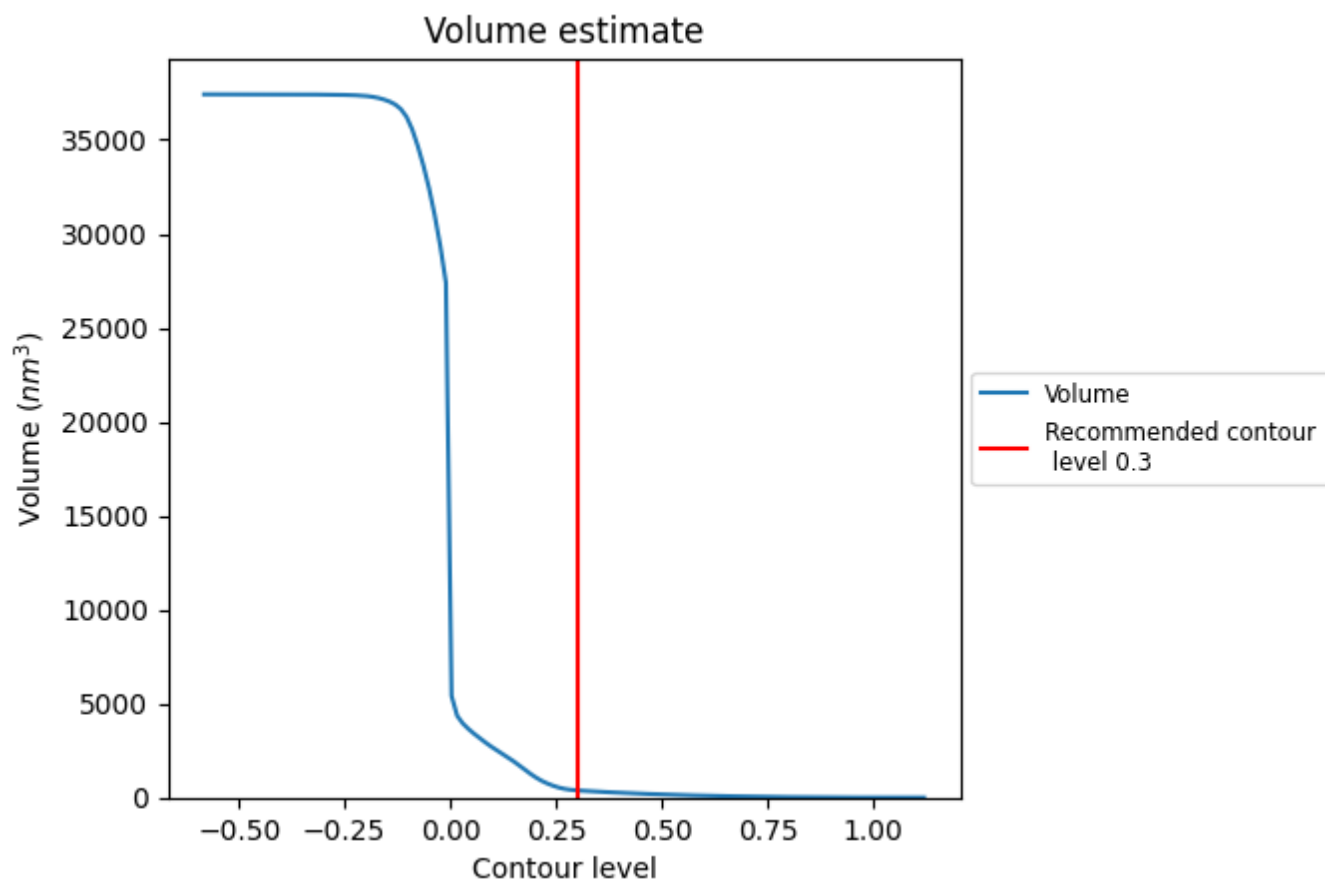
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

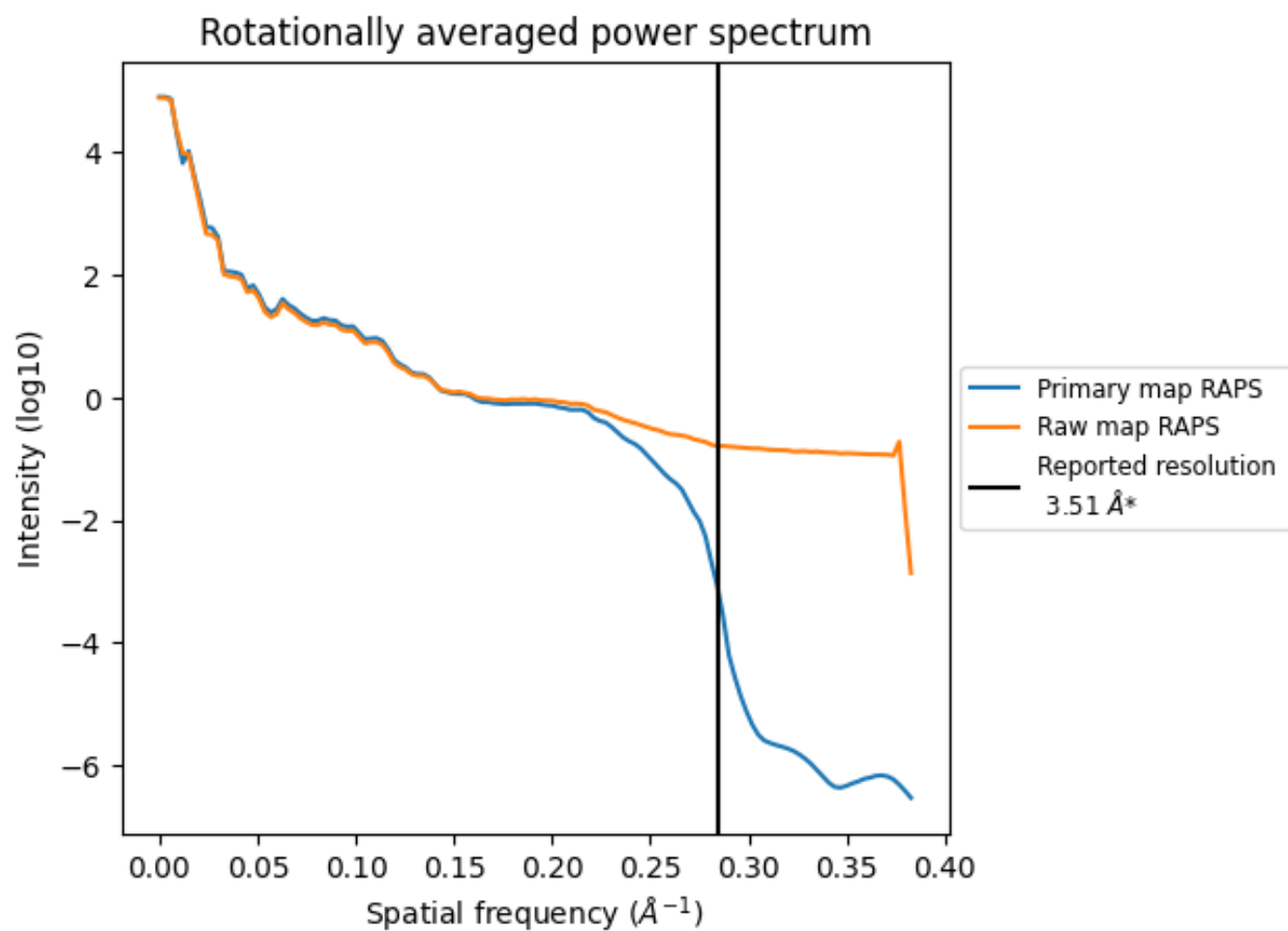
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 383 nm³; this corresponds to an approximate mass of 346 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

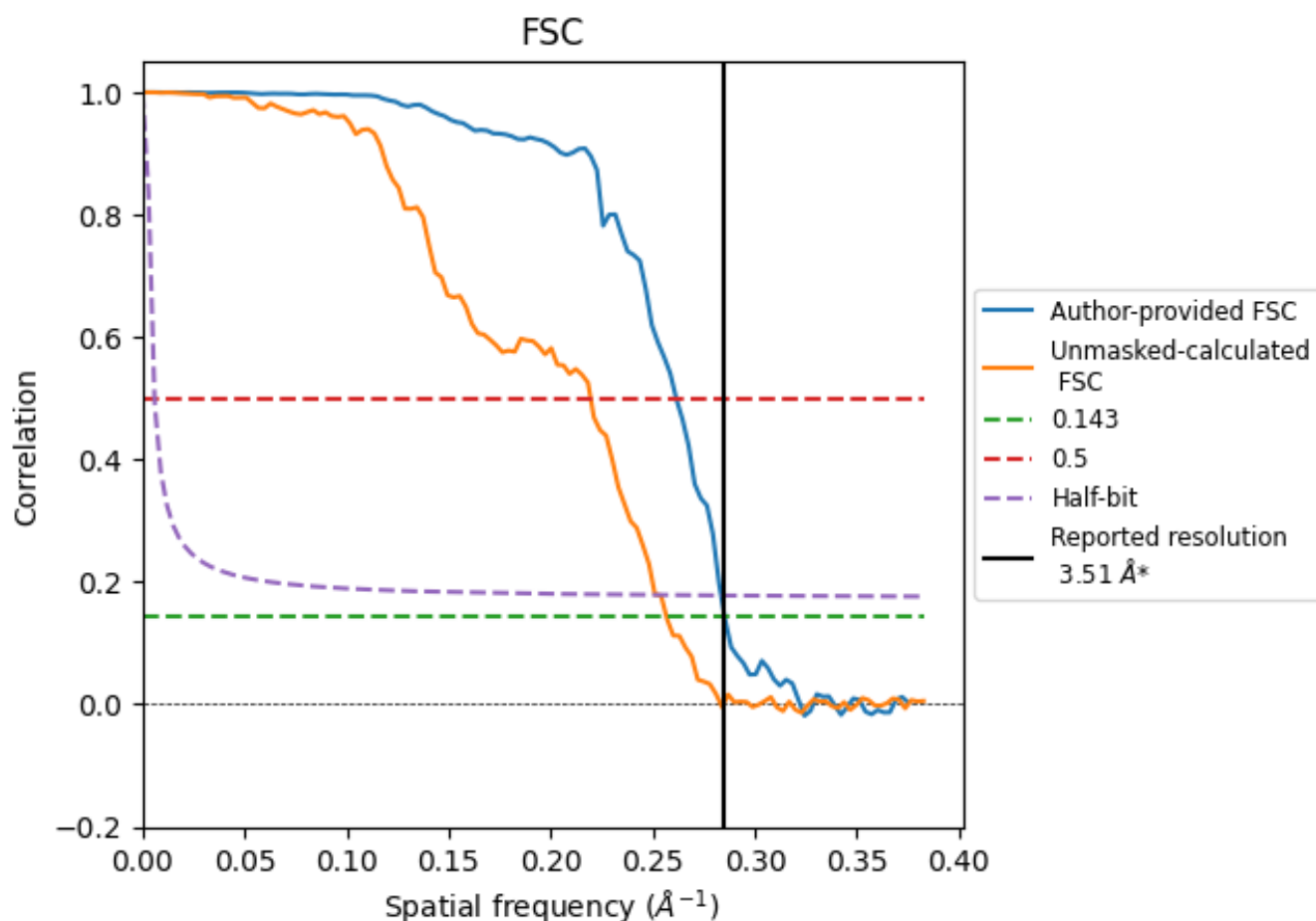


*Reported resolution corresponds to spatial frequency of 0.285 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.285 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.51	-	-
Author-provided FSC curve	3.51	3.82	3.53
Unmasked-calculated*	3.89	4.55	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.51 by more than 10 %

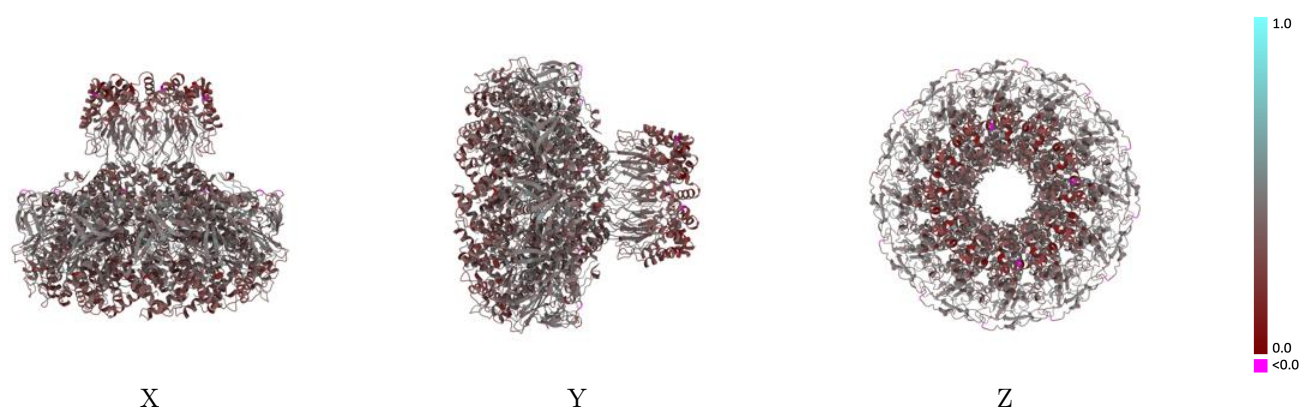
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38540 and PDB model 8XOT. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

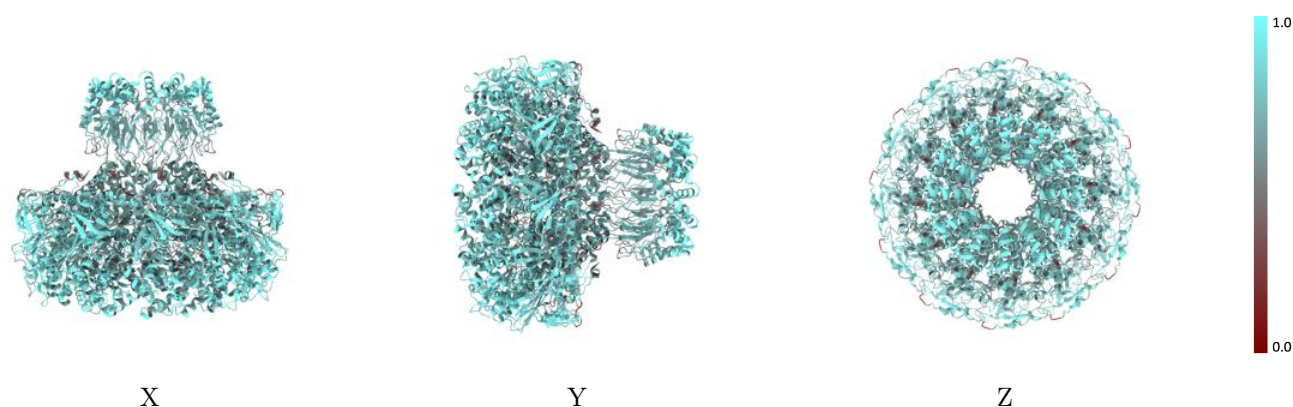
This section was not generated.

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



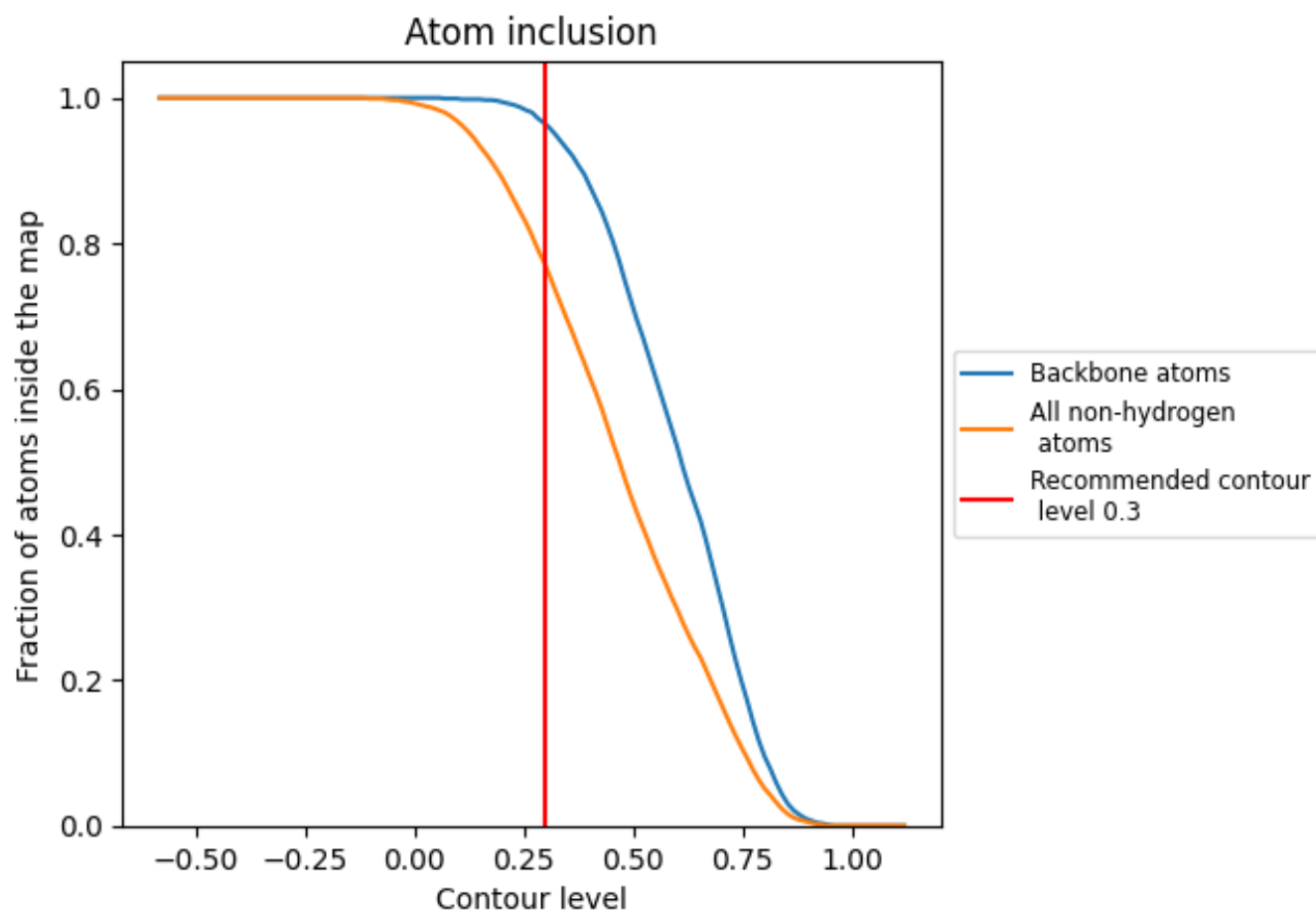
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7700	0.3770
B	0.7690	0.3760
B1	0.7720	0.3770
B2	0.7670	0.3760
B3	0.7690	0.3780
B4	0.7710	0.3780
B5	0.7700	0.3760
b	0.7670	0.3760
b1	0.7700	0.3750
b2	0.7710	0.3780
b3	0.7670	0.3750
b4	0.7700	0.3780
b5	0.7700	0.3770

1.0

0.0

<0.0