



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:49 PM UTC

PDB ID : 7K01 / pdb_00007k01
EMDB ID : EMD-22587
Title : Structure of TFIID in TFIID/Rad4-Rad23-Rad33 DNA opening complex
Authors : van Eeuwen, T.; Min, J.H.; Murakami, K.
Deposited on : 2020-09-02
Resolution : 3.90 Å(reported)
Based on initial models : 5OQJ, 6NMI

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
Mogul : 2022.3.0, CSD as543be (2022)
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

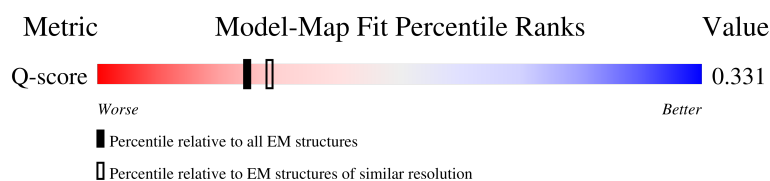
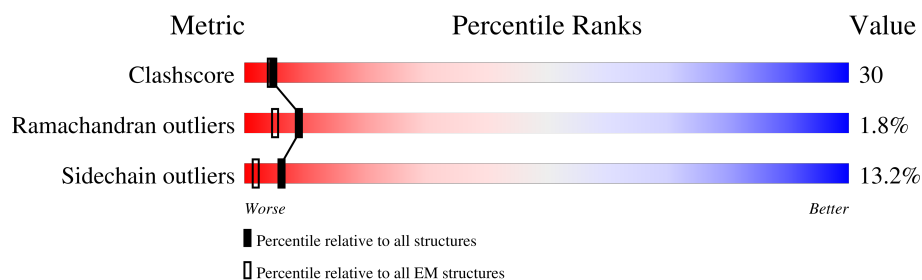
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.



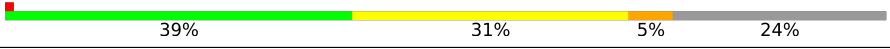
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	1	642	
2	4	338	
3	7	843	
4	5	72	

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Mol	Chain	Length	Quality of chain
5	2	513	
6	0	778	
7	6	461	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21052 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 General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	367	Total	C	N	O	S	0	0
			2408	1533	438	430	7		

- Molecule 2 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	284	Total	C	N	O	S	0	0
			2041	1310	343	376	12		

- Molecule 3 is a protein called DNA repair helicase RAD25.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	634	Total	C	N	O	S	0	0
			4447	2722	827	874	24		

- Molecule 4 is a protein called RNA polymerase II transcription factor B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 5 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	460	Total	C	N	O	S	0	0
			3011	1856	562	584	9		

- Molecule 6 is a protein called DNA repair helicase RAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	0	754	Total	C	N	O	S	0	0
			6108	3891	1032	1147	38		

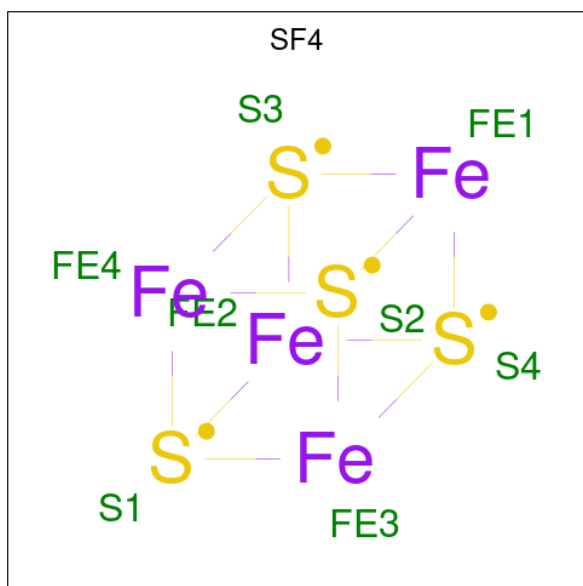
- Molecule 7 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	351	Total	C	N	O	S	0	0
			2526	1589	454	456	27		

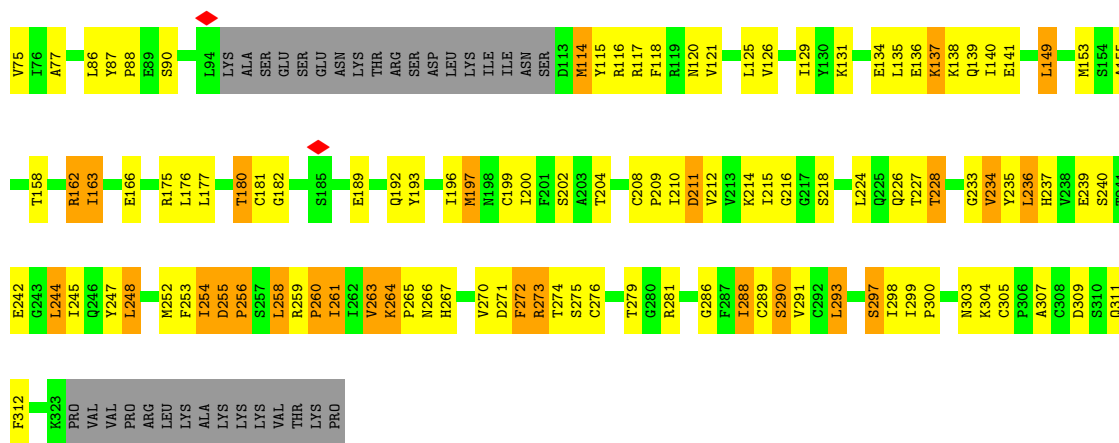
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	4	1	Total	Zn	0
			1	1	
8	6	4	Total	Zn	0
			4	4	

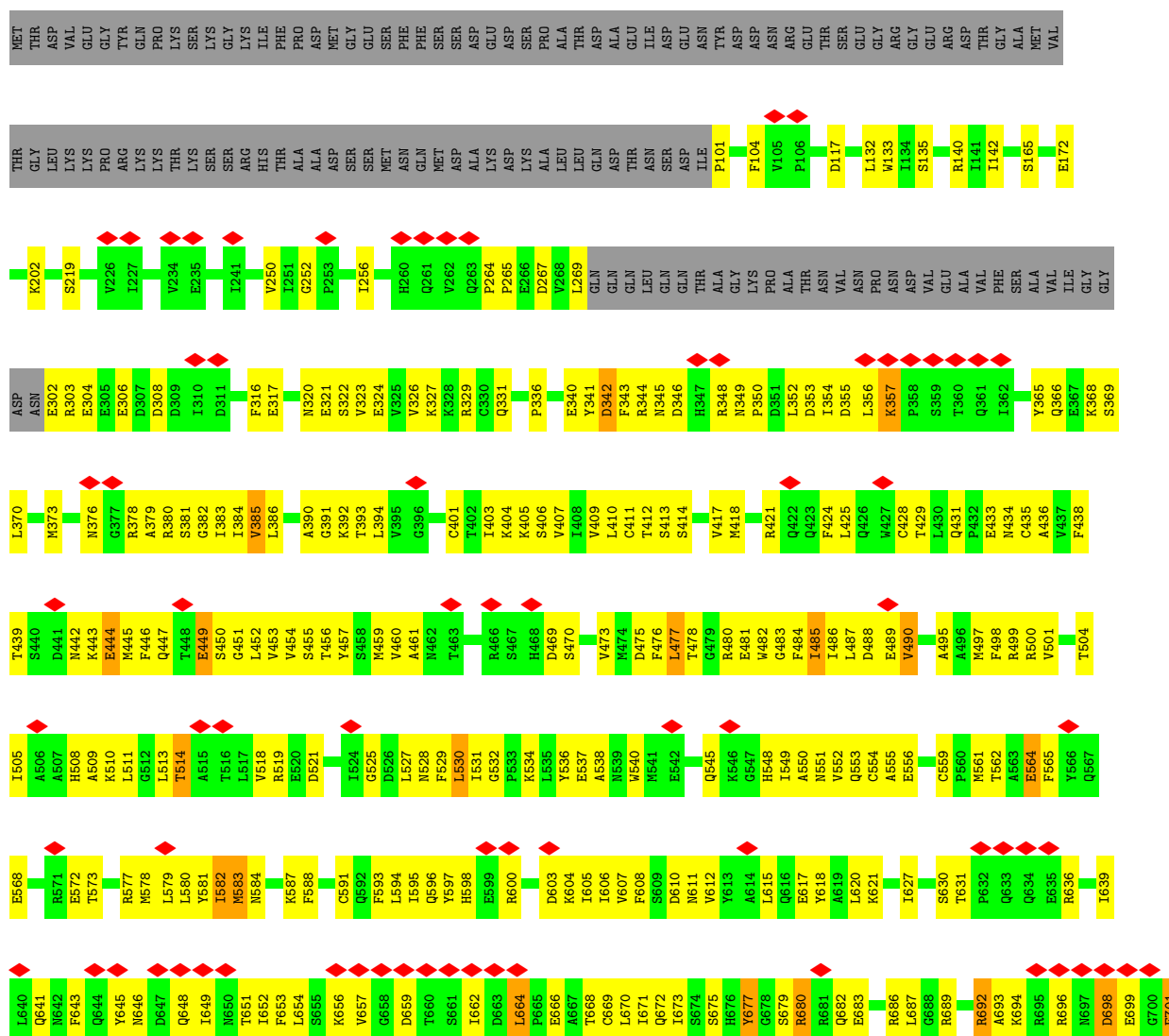
- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

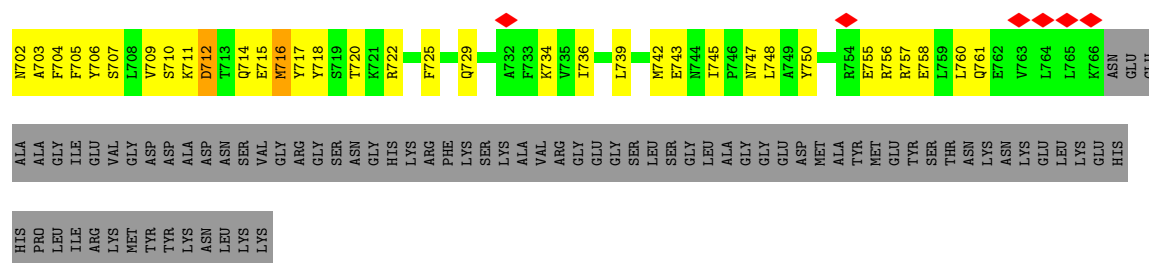


Mol	Chain	Residues	Atoms			AltConf
9	0	1	Total	Fe	S	0
			8	4	4	

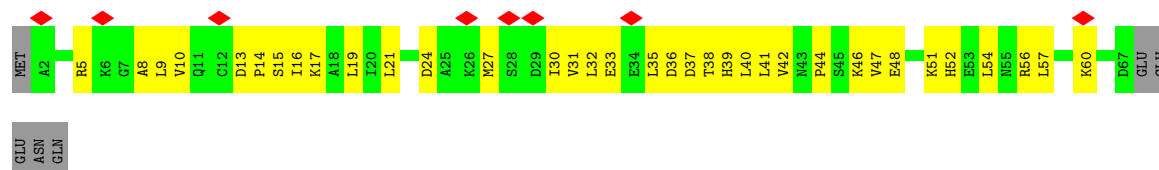


• Molecule 3: DNA repair helicase RAD25

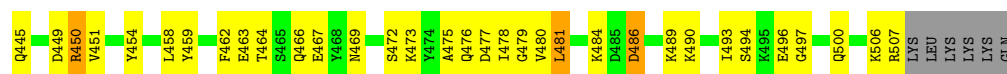
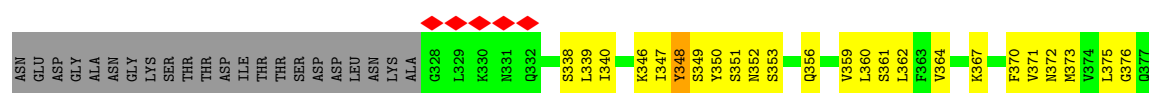
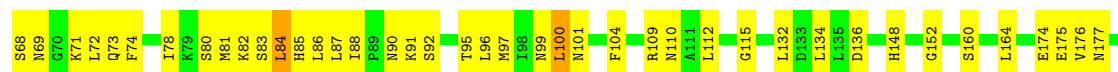




• Molecule 4: RNA polymerase II transcription factor B subunit 5

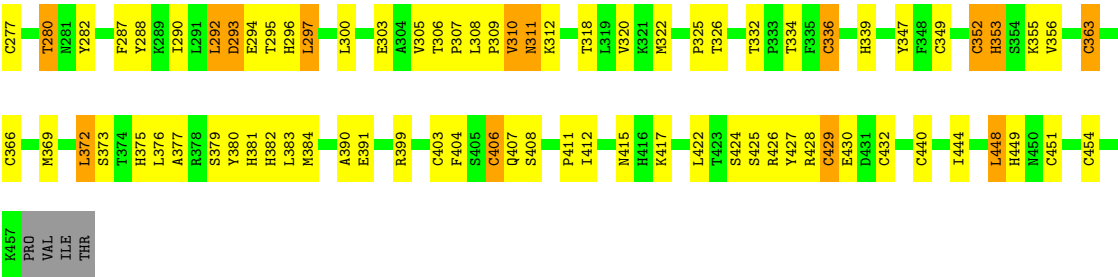


• Molecule 5: General transcription and DNA repair factor IIH subunit TFB2



• Molecule 6: DNA repair helicase RAD3





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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56101	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.016	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00593	Depositor
Map size (Å)	323.69998, 323.69998, 323.69998	wwPDB
Map dimensions	390, 390, 390	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8299999, 0.8299999, 0.8299999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4

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	1	0.45	0/2438	0.69	6/3325 (0.2%)
2	4	0.49	0/2072	0.55	0/2819
3	7	0.12	0/4521	0.34	0/6036
4	5	0.14	0/502	0.37	0/677
5	2	0.28	0/3057	0.41	0/4071
6	0	0.49	0/6226	0.54	0/8407
7	6	0.54	1/2571 (0.0%)	0.60	2/3494 (0.1%)
All	All	0.41	1/21387 (0.0%)	0.51	8/28829 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	6	243	ASP	C-N	-5.38	1.29	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	491	PRO	N-CA-CB	7.81	111.45	103.25
1	1	390	LYS	N-CA-C	-7.61	104.03	113.38
1	1	354	PRO	N-CA-CB	7.22	110.83	103.25
1	1	238	LYS	CA-C-N	-6.12	112.19	119.84
1	1	238	LYS	C-N-CA	-6.12	112.19	119.84
1	1	296	LEU	CB-CA-C	-5.72	109.45	117.23
7	6	163	GLN	CA-C-N	-5.09	117.09	122.28
7	6	163	GLN	C-N-CA	-5.09	117.09	122.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2408	0	1984	166	0
2	4	2041	0	1953	135	0
3	7	4447	0	3905	257	0
4	5	498	0	506	29	0
5	2	3011	0	2600	169	0
6	0	6108	0	6168	389	0
7	6	2526	0	2333	121	0
8	4	1	0	0	0	0
8	6	4	0	0	0	0
9	0	8	0	0	1	0
All	All	21052	0	19449	1223	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 30.

All (1223) 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)
1:1:270:TYR:CE1	1:1:279:LYS:HE3	1.26	1.70
1:1:279:LYS:HA	1:1:283:PHE:CB	1.27	1.56
1:1:270:TYR:CZ	1:1:279:LYS:HE3	1.64	1.33
1:1:279:LYS:CA	1:1:283:PHE:CB	2.13	1.25
1:1:270:TYR:CE1	1:1:279:LYS:CE	2.22	1.22
2:4:255:ASP:H	2:4:256:PRO:CD	1.54	1.19
1:1:279:LYS:HB3	1:1:283:PHE:CG	1.78	1.18
3:7:636:ARG:NH1	3:7:662:ILE:HG21	1.56	1.18
1:1:270:TYR:CE2	1:1:279:LYS:HB2	1.80	1.16
1:1:279:LYS:CA	1:1:283:PHE:HB3	1.75	1.13
1:1:280:GLU:HB3	1:1:281:PRO:HD3	1.28	1.11
2:4:255:ASP:H	2:4:256:PRO:HD3	1.04	1.09
1:1:279:LYS:HA	1:1:283:PHE:HB3	1.19	1.07
1:1:280:GLU:CB	1:1:281:PRO:HD3	1.84	1.06
1:1:270:TYR:CZ	1:1:279:LYS:HB2	1.92	1.05
3:7:630:SER:H	3:7:657:VAL:HG21	1.24	1.01
3:7:636:ARG:HH11	3:7:662:ILE:HG21	1.10	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:270:TYR:CZ	1:1:279:LYS:CE	2.42	1.00
1:1:279:LYS:CA	1:1:283:PHE:HB2	1.87	0.98
1:1:279:LYS:HB3	1:1:283:PHE:CD1	2.00	0.96
1:1:279:LYS:CB	1:1:283:PHE:CG	2.49	0.95
1:1:279:LYS:HA	1:1:283:PHE:HB2	0.94	0.93
1:1:279:LYS:C	1:1:283:PHE:HB3	1.95	0.91
2:4:255:ASP:N	2:4:256:PRO:CD	2.30	0.91
2:4:255:ASP:N	2:4:256:PRO:HD3	1.88	0.88
1:1:280:GLU:HB3	1:1:281:PRO:CD	2.06	0.86
5:2:61:ASP:OD1	5:2:61:ASP:N	2.08	0.86
1:1:343:ILE:O	1:1:345:ASP:N	2.09	0.85
1:1:270:TYR:HE1	1:1:279:LYS:HE3	1.39	0.84
6:0:592:ASN:OD1	6:0:593:GLY:N	2.11	0.82
2:4:289:CYS:SG	2:4:290:SER:N	2.53	0.82
7:6:403:CYS:SG	7:6:404:PHE:N	2.51	0.82
3:7:439:THR:HB	3:7:442:ASN:H	1.45	0.81
1:1:270:TYR:CE2	1:1:279:LYS:CB	2.60	0.81
2:4:254:ILE:CG2	5:2:45:PHE:CE2	2.63	0.81
2:4:254:ILE:HG21	5:2:45:PHE:CE2	2.16	0.81
1:1:198:THR:O	1:1:204:LEU:N	2.12	0.81
7:6:432:CYS:HB3	7:6:454:CYS:SG	2.20	0.81
3:7:699:GLU:HG3	3:7:701:PHE:H	1.46	0.81
1:1:375:LEU:HB3	6:0:571:VAL:HG11	1.63	0.80
6:0:314:GLN:HA	6:0:317:LEU:HD13	1.64	0.79
6:0:275:ARG:HH22	6:0:276:LYS:HG3	1.47	0.78
6:0:297:ASP:O	6:0:386:ARG:NH1	2.16	0.78
3:7:587:LYS:HD3	3:7:673:ILE:HD12	1.66	0.78
6:0:227:SER:HB2	6:0:230:SER:HB2	1.65	0.78
7:6:144:ASN:OD1	7:6:147:ALA:N	2.17	0.77
6:0:166:GLU:OE2	6:0:198:ARG:NH1	2.17	0.77
6:0:63:TYR:O	6:0:67:ARG:NH2	2.17	0.77
1:1:280:GLU:CB	1:1:281:PRO:CD	2.60	0.76
2:4:114:MET:C	2:4:116:ARG:H	1.93	0.76
6:0:674:ASP:N	6:0:674:ASP:OD1	2.17	0.76
7:6:269:GLN:HG3	7:6:288:TYR:HE2	1.51	0.76
4:5:33:GLU:HB2	4:5:41:LEU:HB3	1.66	0.76
2:4:52:LYS:NZ	2:4:240:SER:O	2.19	0.76
2:4:162:ARG:HH21	7:6:408:SER:HA	1.50	0.76
2:4:254:ILE:HG23	5:2:45:PHE:CZ	2.20	0.76
1:1:351:GLY:O	6:0:436:ARG:NH1	2.16	0.75
2:4:162:ARG:NH2	7:6:407:GLN:O	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:460:SER:HB2	6:0:463:ILE:HG13	1.68	0.75
5:2:353:SER:HB2	5:2:356:GLN:HB3	1.69	0.75
7:6:176:ASN:HA	7:6:206:GLY:HA3	1.66	0.75
2:4:290:SER:OG	2:4:291:VAL:N	2.18	0.75
3:7:572:GLU:O	3:7:577:ARG:NH2	2.19	0.74
2:4:304:LYS:HG3	2:4:309:ASP:HA	1.70	0.74
3:7:418:MET:HG3	3:7:421:ARG:HH12	1.53	0.74
5:2:81:MET:HB2	5:2:86:LEU:HD11	1.69	0.74
6:0:608:GLU:O	6:0:668:ARG:NH2	2.17	0.74
5:2:399:TYR:O	5:2:403:HIS:N	2.20	0.74
6:0:288:LYS:O	6:0:291:GLN:NE2	2.20	0.74
5:2:243:SER:O	5:2:247:ARG:N	2.20	0.73
6:0:37:ASN:ND2	6:0:476:LYS:O	2.21	0.73
7:6:139:LYS:NZ	7:6:143:PRO:O	2.19	0.73
4:5:27:MET:HE1	4:5:46:LYS:HB3	1.68	0.73
7:6:294:GLU:OE1	7:6:294:GLU:N	2.20	0.72
6:0:304:GLU:OE1	6:0:386:ARG:NH1	2.22	0.72
6:0:651:ASN:N	6:0:651:ASN:OD1	2.21	0.72
1:1:491:PRO:O	1:1:493:ASN:N	2.19	0.72
5:2:87:LEU:HA	5:2:100:LEU:HA	1.70	0.72
1:1:279:LYS:HA	1:1:283:PHE:CG	2.23	0.72
5:2:86:LEU:O	5:2:101:ASN:N	2.20	0.72
5:2:339:LEU:O	5:2:407:GLN:NE2	2.23	0.72
1:1:188:ASN:HD21	1:1:190:VAL:HB	1.55	0.72
3:7:411:CYS:HA	3:7:488:ASP:HB2	1.70	0.71
6:0:12:PHE:HE1	6:0:14:TYR:HB2	1.54	0.71
4:5:5:ARG:HB2	5:2:458:LEU:HB3	1.72	0.71
1:1:196:GLN:O	1:1:200:ILE:N	2.24	0.71
1:1:479:ASN:O	1:1:483:LYS:N	2.21	0.71
2:4:260:PRO:O	5:2:67:ASN:ND2	2.23	0.71
6:0:439:CYS:SG	6:0:440:LEU:N	2.63	0.71
3:7:669:CYS:HA	3:7:704:PHE:HB2	1.72	0.70
6:0:341:TYR:OH	6:0:362:HIS:ND1	2.23	0.70
6:0:739:TRP:HB3	6:0:745:ILE:HG23	1.70	0.70
6:0:137:THR:HB	6:0:159:HIS:HD2	1.56	0.70
6:0:286:TYR:O	6:0:326:ARG:NH1	2.20	0.70
6:0:117:HIS:HE1	6:0:119:GLU:HB3	1.57	0.70
6:0:378:SER:HG	6:0:407:THR:HG1	1.22	0.70
1:1:174:LEU:O	1:1:181:GLN:NE2	2.24	0.70
7:6:138:GLU:OE2	7:6:145:ARG:NE	2.24	0.70
6:0:610:ILE:O	6:0:668:ARG:NH1	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:380:ARG:NH2	5:2:440:GLN:O	2.26	0.69
6:0:134:ARG:NH2	6:0:303:GLU:O	2.25	0.69
2:4:260:PRO:HD2	2:4:261:ILE:HG22	1.73	0.69
5:2:462:PHE:HB2	5:2:489:LYS:HB3	1.75	0.69
5:2:349:SER:OG	5:2:373:MET:SD	2.50	0.69
1:1:273:ASN:HD22	1:1:283:PHE:HE2	1.40	0.69
6:0:223:SER:O	6:0:226:VAL:N	2.18	0.69
2:4:138:LYS:O	2:4:138:LYS:NZ	2.21	0.69
3:7:421:ARG:HA	3:7:425:LEU:HD23	1.75	0.69
5:2:54:GLU:OE2	5:2:109:ARG:NH2	2.24	0.69
6:0:39:ILE:HD11	6:0:466:LEU:HG	1.74	0.69
6:0:270:ARG:NH2	6:0:388:LEU:O	2.24	0.69
6:0:295:SER:HA	6:0:298:ILE:HG22	1.74	0.69
3:7:556:GLU:HG2	3:7:707:SER:HB3	1.74	0.69
6:0:705:ASP:N	6:0:705:ASP:OD1	2.25	0.69
3:7:425:LEU:HA	3:7:428:CYS:HB3	1.75	0.69
2:4:293:LEU:HD21	7:6:122:ILE:HG13	1.75	0.68
5:2:176:VAL:O	5:2:181:GLU:N	2.26	0.68
1:1:251:LEU:HB3	1:1:254:GLU:HB2	1.74	0.68
3:7:562:THR:HB	3:7:756:ARG:HH11	1.59	0.68
4:5:24:ASP:OD1	4:5:30:ILE:N	2.26	0.68
2:4:182:GLY:N	2:4:215:ILE:O	2.26	0.68
3:7:477:LEU:HB3	3:7:505:ILE:HD12	1.75	0.68
6:0:729:ASP:O	6:0:731:LYS:NZ	2.22	0.68
1:1:279:LYS:CA	1:1:283:PHE:CG	2.76	0.68
2:4:244:LEU:O	2:4:247:TYR:N	2.27	0.68
2:4:254:ILE:CG2	5:2:45:PHE:CZ	2.76	0.68
6:0:683:ASP:OD1	6:0:686:PHE:N	2.26	0.68
6:0:321:ILE:HG13	6:0:323:GLY:H	1.58	0.68
1:1:226:GLN:OE1	7:6:179:ALA:N	2.24	0.68
3:7:646:ASN:ND2	3:7:648:GLN:OE1	2.26	0.67
3:7:477:LEU:HA	3:7:482:TRP:HE1	1.58	0.67
3:7:577:ARG:HH11	3:7:714:GLN:HB2	1.59	0.67
6:0:135:ARG:NH2	6:0:391:THR:O	2.26	0.67
1:1:214:ILE:HG23	1:1:215:PRO:HD3	1.75	0.67
6:0:371:ARG:NH2	6:0:411:THR:O	2.27	0.67
7:6:116:THR:O	7:6:116:THR:OG1	2.10	0.67
2:4:211:ASP:OD1	2:4:211:ASP:N	2.26	0.67
6:0:21:GLN:HE21	6:0:46:THR:HG22	1.60	0.67
6:0:587:ARG:NH2	6:0:611:ASP:O	2.28	0.67
6:0:307:VAL:H	6:0:382:SER:HB3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:160:SER:O	5:2:164:LEU:N	2.19	0.67
4:5:10:VAL:HB	4:5:40:LEU:HB2	1.77	0.66
6:0:507:SER:HG	6:0:685:ARG:HH22	1.40	0.66
3:7:428:CYS:SG	3:7:429:THR:N	2.68	0.66
3:7:551:ASN:HB2	3:7:702:ASN:H	1.60	0.66
6:0:350:HIS:HA	6:0:422:PRO:HG3	1.75	0.66
6:0:572:GLU:OE1	6:0:579:THR:OG1	2.14	0.66
3:7:376:ASN:OD1	3:7:380:ARG:NH2	2.29	0.66
2:4:58:ILE:HD11	2:4:125:LEU:HD22	1.75	0.66
3:7:435:CYS:HB3	3:7:454:VAL:HG12	1.76	0.66
7:6:406:CYS:HB3	7:6:440:CYS:SG	2.35	0.66
7:6:188:ASN:ND2	7:6:191:ASP:OD1	2.28	0.66
3:7:559:CYS:HB2	3:7:710:SER:HA	1.76	0.66
6:0:228:LYS:O	6:0:228:LYS:NZ	2.21	0.66
2:4:137:LYS:HG2	2:4:140:ILE:HG12	1.76	0.66
2:4:244:LEU:HD12	2:4:244:LEU:H	1.60	0.66
2:4:270:VAL:HG22	2:4:272:PHE:H	1.60	0.66
4:5:5:ARG:NH2	4:5:33:GLU:OE2	2.29	0.66
5:2:90:ASN:HB3	5:2:97:MET:HB2	1.77	0.66
6:0:104:ARG:N	6:0:204:ASN:OD1	2.23	0.66
6:0:115:CYS:O	6:0:121:SER:OG	2.08	0.66
3:7:666:GLU:HB3	3:7:694:LYS:HD3	1.78	0.66
7:6:218:ARG:NH1	7:6:257:GLU:OE2	2.27	0.66
6:0:136:MET:HG3	6:0:155:LEU:HA	1.77	0.65
6:0:244:CYS:HB3	6:0:445:ALA:HB3	1.78	0.65
7:6:175:ARG:NH2	7:6:203:GLU:O	2.29	0.65
6:0:224:ASN:OD1	6:0:452:ARG:NH2	2.24	0.65
3:7:671:ILE:HG13	3:7:706:TYR:HB2	1.76	0.65
6:0:722:ARG:NH2	7:6:292:LEU:O	2.28	0.65
5:2:7:LYS:HG2	5:2:9:SER:H	1.61	0.65
6:0:251:ASP:OD1	6:0:436:ARG:NH1	2.25	0.65
6:0:424:GLU:OE1	6:0:432:ASN:ND2	2.29	0.65
6:0:425:ILE:HA	6:0:428:ALA:HB2	1.79	0.65
6:0:645:ASN:O	6:0:647:ARG:NH1	2.29	0.65
1:1:188:ASN:HB3	1:1:191:LEU:HB2	1.79	0.65
3:7:699:GLU:O	3:7:702:ASN:ND2	2.30	0.65
6:0:103:PHE:H	6:0:173:LYS:HZ1	1.44	0.65
2:4:226:GLN:CD	2:4:273:ARG:HE	2.03	0.65
4:5:48:GLU:O	4:5:52:HIS:ND1	2.26	0.65
5:2:185:THR:O	5:2:189:PHE:N	2.24	0.65
5:2:51:VAL:O	5:2:109:ARG:NH2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:327:ARG:HG3	6:0:330:HIS:H	1.62	0.65
6:0:60:GLN:O	6:0:67:ARG:NH2	2.30	0.65
1:1:279:LYS:HE2	1:1:279:LYS:H	1.63	0.64
3:7:528:ASN:O	3:7:532:GLY:N	2.31	0.64
6:0:515:ASP:N	6:0:515:ASP:OD1	2.30	0.64
5:2:475:ALA:O	5:2:479:GLY:N	2.30	0.64
3:7:306:GLU:OE1	3:7:508:HIS:ND1	2.31	0.64
5:2:432:VAL:HG22	5:2:433:LEU:HG	1.80	0.64
6:0:90:MET:O	6:0:94:THR:HG23	1.97	0.64
7:6:221:LEU:HD23	7:6:230:ARG:HB3	1.77	0.64
1:1:346:ASP:HB2	1:1:347:PRO:HD3	1.79	0.64
3:7:409:VAL:HG22	3:7:486:ILE:HD12	1.80	0.64
5:2:42:LEU:HD12	5:2:46:PHE:HE2	1.62	0.64
6:0:109:THR:O	6:0:212:TYR:OH	2.13	0.64
1:1:259:ILE:HD13	1:1:263:TYR:HE2	1.62	0.64
5:2:346:LYS:NZ	5:2:376:GLY:O	2.29	0.64
3:7:341:TYR:N	3:7:379:ALA:O	2.31	0.64
5:2:226:PHE:O	5:2:230:ALA:N	2.31	0.64
5:2:415:LYS:HD3	5:2:434:PRO:HD3	1.80	0.64
6:0:278:ASP:O	6:0:281:LYS:NZ	2.31	0.64
6:0:227:SER:OG	6:0:228:LYS:N	2.30	0.63
1:1:251:LEU:HB2	1:1:255:LYS:HG2	1.80	0.63
6:0:315:ASP:OD1	6:0:315:ASP:N	2.31	0.63
2:4:192:GLN:N	2:4:192:GLN:OE1	2.28	0.63
6:0:750:SER:OG	6:0:751:ARG:NH2	2.31	0.63
5:2:469:ASN:ND2	5:2:486:ASP:OD2	2.32	0.63
6:0:325:ILE:HA	6:0:334:PHE:HE2	1.63	0.63
3:7:617:GLU:OE2	3:7:621:LYS:NZ	2.32	0.63
5:2:348:TYR:O	5:2:407:GLN:NE2	2.31	0.63
2:4:120:ASN:OD1	2:4:121:VAL:N	2.32	0.63
6:0:142:LYS:NZ	6:0:146:GLU:OE2	2.32	0.63
6:0:166:GLU:O	6:0:198:ARG:NH1	2.32	0.63
7:6:191:ASP:OD1	7:6:191:ASP:N	2.29	0.63
1:1:279:LYS:CG	1:1:283:PHE:CD2	2.82	0.62
3:7:495:ALA:HB2	3:7:521:ASP:HB3	1.79	0.62
5:2:481:LEU:HD23	5:2:493:ILE:HG21	1.80	0.62
6:0:71:TYR:HB3	6:0:207:ILE:HG23	1.81	0.62
6:0:744:LEU:O	6:0:748:GLN:HB2	1.98	0.62
3:7:483:GLY:HA2	3:7:508:HIS:HB2	1.80	0.62
6:0:103:PHE:N	6:0:173:LYS:HZ1	1.97	0.62
6:0:531:LYS:HG2	6:0:566:HIS:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:537:MET:HG2	6:0:597:ILE:HG12	1.82	0.62
2:4:189:GLU:O	2:4:192:GLN:NE2	2.33	0.62
3:7:630:SER:N	3:7:657:VAL:HG21	2.06	0.62
6:0:294:HIS:CE1	6:0:297:ASP:HB3	2.34	0.62
1:1:249:VAL:O	1:1:252:SER:OG	2.15	0.62
3:7:352:LEU:O	3:7:404:LYS:NZ	2.31	0.62
6:0:466:LEU:O	6:0:480:GLN:NE2	2.33	0.62
1:1:347:PRO:HB2	1:1:349:VAL:HG13	1.80	0.62
5:2:419:LYS:NZ	5:2:426:CYS:O	2.32	0.62
6:0:227:SER:C	6:0:229:ASP:H	2.08	0.62
3:7:303:ARG:HB2	3:7:323:VAL:H	1.64	0.62
2:4:24:SER:H	2:4:71:ASN:HD22	1.48	0.62
5:2:458:LEU:HD11	5:2:490:LYS:HB3	1.82	0.62
6:0:395:ASP:N	6:0:395:ASP:OD1	2.32	0.62
3:7:581:TYR:CZ	3:7:715:GLU:HB2	2.35	0.61
6:0:157:GLU:HA	6:0:160:GLU:HG2	1.82	0.61
1:1:280:GLU:HB2	1:1:281:PRO:HD3	1.78	0.61
1:1:492:ASN:O	1:1:494:GLU:N	2.33	0.61
3:7:412:THR:HG22	3:7:489:GLU:HB2	1.82	0.61
3:7:435:CYS:HA	3:7:453:VAL:HA	1.82	0.61
5:2:9:SER:O	5:2:12:GLN:N	2.31	0.61
5:2:36:TYR:HE1	5:2:44:LYS:HA	1.64	0.61
6:0:301:ASP:HB3	6:0:304:GLU:HB2	1.80	0.61
7:6:451:CYS:SG	7:6:454:CYS:HB2	2.40	0.61
1:1:185:LEU:HD12	1:1:192:MET:HA	1.82	0.61
2:4:254:ILE:HG21	2:4:261:ILE:CD1	2.30	0.61
6:0:110:SER:OG	6:0:111:ARG:N	2.32	0.61
1:1:194:VAL:O	1:1:198:THR:OG1	2.18	0.61
3:7:381:SER:HB3	3:7:509:ALA:HB1	1.81	0.61
7:6:373:SER:O	7:6:376:LEU:N	2.33	0.61
2:4:218:SER:HA	2:4:237:HIS:HE2	1.66	0.61
6:0:666:LEU:HB3	6:0:679:MET:HE2	1.82	0.61
1:1:337:ILE:O	1:1:339:LEU:N	2.34	0.61
2:4:114:MET:O	2:4:116:ARG:N	2.33	0.61
6:0:528:GLU:OE2	6:0:710:THR:OG1	2.19	0.61
5:2:197:ASN:O	5:2:201:TRP:HB2	2.01	0.61
6:0:643:ARG:HH11	6:0:650:GLU:HG3	1.66	0.61
7:6:406:CYS:SG	7:6:407:GLN:N	2.73	0.61
3:7:303:ARG:HA	3:7:320:ASN:HA	1.83	0.60
6:0:537:MET:HE3	6:0:597:ILE:HD11	1.83	0.60
3:7:101:PRO:O	3:7:331:GLN:NE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:254:ILE:HG21	2:4:261:ILE:HD13	1.83	0.60
3:7:604:LYS:HD3	3:7:694:LYS:HZ1	1.67	0.60
1:1:375:LEU:HD22	6:0:571:VAL:HG21	1.83	0.60
3:7:424:PHE:O	3:7:428:CYS:N	2.23	0.60
5:2:416:LEU:HD12	5:2:432:VAL:HG23	1.82	0.60
5:2:464:THR:OG1	5:2:466:GLN:OE1	2.20	0.60
1:1:235:SER:O	1:1:239:PRO:HD2	2.01	0.60
6:0:619:THR:O	6:0:619:THR:OG1	2.19	0.60
1:1:557:CYS:SG	1:1:585:HIS:NE2	2.68	0.60
3:7:670:LEU:O	3:7:706:TYR:N	2.33	0.60
4:5:31:VAL:HA	4:5:42:VAL:HG13	1.82	0.60
6:0:70:ILE:HB	6:0:232:VAL:HG22	1.82	0.60
6:0:286:TYR:HA	6:0:289:LEU:HD12	1.83	0.60
3:7:436:ALA:HB1	3:7:444:GLU:HB3	1.84	0.60
3:7:549:ILE:HG13	3:7:693:ALA:HA	1.82	0.60
4:5:9:LEU:HD23	5:2:454:TYR:HB2	1.82	0.60
6:0:274:VAL:O	6:0:278:ASP:N	2.30	0.60
7:6:142:ARG:HB2	7:6:143:PRO:HD3	1.84	0.60
3:7:527:LEU:HA	3:7:530:LEU:HB2	1.82	0.60
3:7:561:MET:H	3:7:711:LYS:HE2	1.66	0.60
2:4:271:ASP:C	2:4:273:ARG:HD3	2.27	0.59
3:7:326:VAL:HG22	3:7:329:ARG:HH21	1.67	0.59
3:7:551:ASN:ND2	3:7:702:ASN:OD1	2.35	0.59
5:2:367:LYS:HB2	5:2:375:LEU:HD23	1.84	0.59
2:4:311:GLN:NE2	2:4:312:PHE:O	2.35	0.59
5:2:494:SER:OG	5:2:496:GLU:OE2	2.19	0.59
6:0:77:SER:HA	6:0:80:GLU:OE2	2.02	0.59
7:6:310:VAL:HG13	7:6:311:ASN:H	1.66	0.59
7:6:399:ARG:H	7:6:426:ARG:HH12	1.50	0.59
5:2:475:ALA:HA	5:2:478:ILE:HG12	1.82	0.59
1:1:279:LYS:CE	1:1:279:LYS:H	2.15	0.59
2:4:258:LEU:O	2:4:259:ARG:HG2	2.01	0.59
3:7:269:LEU:HB2	3:7:304:GLU:HA	1.83	0.59
3:7:739:LEU:HB2	3:7:742:MET:HB3	1.84	0.59
5:2:338:SER:O	5:2:356:GLN:NE2	2.31	0.59
7:6:391:GLU:HA	7:6:427:TYR:HA	1.85	0.59
6:0:232:VAL:HG21	6:0:453:PHE:CD2	2.37	0.59
7:6:390:ALA:O	7:6:428:ARG:N	2.36	0.59
1:1:282:GLU:H	1:1:282:GLU:CD	2.09	0.59
6:0:272:SER:OG	6:0:276:LYS:NZ	2.36	0.59
6:0:360:LEU:HD11	6:0:371:ARG:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:507:SER:OG	6:0:508:SER:N	2.34	0.59
1:1:346:ASP:OD1	1:1:346:ASP:N	2.35	0.59
5:2:132:LEU:O	5:2:286:ARG:NH2	2.36	0.59
3:7:411:CYS:SG	3:7:412:THR:N	2.75	0.59
5:2:378:ILE:HD12	5:2:382:SER:HB2	1.85	0.59
3:7:562:THR:OG1	3:7:564:GLU:OE2	2.16	0.58
5:2:68:SER:OG	5:2:69:ASN:N	2.35	0.58
2:4:33:ALA:O	2:4:37:TRP:N	2.27	0.58
6:0:272:SER:O	6:0:275:ARG:NH2	2.36	0.58
6:0:529:PHE:HA	6:0:532:ILE:HG22	1.84	0.58
7:6:243:ASP:OD1	7:6:243:ASP:N	2.36	0.58
1:1:239:PRO:O	1:1:241:ALA:N	2.36	0.58
3:7:607:VAL:O	3:7:654:LEU:N	2.30	0.58
1:1:291:LYS:O	1:1:294:ARG:N	2.36	0.58
1:1:502:ARG:O	1:1:505:THR:OG1	2.16	0.58
6:0:554:TRP:CD1	6:0:559:ILE:HG21	2.38	0.58
6:0:628:GLN:OE1	6:0:628:GLN:N	2.36	0.58
1:1:278:PHE:O	1:1:282:GLU:OE2	2.21	0.58
2:4:291:VAL:HG21	7:6:119:GLN:HG3	1.85	0.58
3:7:352:LEU:HD23	3:7:452:LEU:HD23	1.86	0.58
6:0:252:LEU:HB2	6:0:435:MET:HB3	1.86	0.58
6:0:627:PHE:HD1	6:0:654:LEU:HD12	1.67	0.58
2:4:31:GLU:OE2	2:4:181:CYS:N	2.37	0.58
6:0:747:HIS:O	6:0:751:ARG:HG2	2.04	0.58
1:1:193:LYS:O	1:1:196:GLN:NE2	2.37	0.58
6:0:162:LEU:HD12	6:0:166:GLU:HB3	1.85	0.58
7:6:175:ARG:NH1	7:6:202:GLN:OE1	2.37	0.58
1:1:279:LYS:HB3	1:1:283:PHE:CD2	2.34	0.58
1:1:282:GLU:OE2	1:1:282:GLU:N	2.36	0.58
3:7:366:GLN:HE22	3:7:394:LEU:HD22	1.69	0.58
3:7:357:LYS:NZ	3:7:429:THR:O	2.28	0.58
7:6:336:CYS:SG	7:6:339:HIS:N	2.68	0.58
5:2:18:PRO:HB2	5:2:20:GLN:HE22	1.67	0.57
5:2:349:SER:HA	5:2:407:GLN:HE22	1.69	0.57
1:1:258:ASN:O	1:1:262:ASN:HB2	2.04	0.57
1:1:279:LYS:O	1:1:283:PHE:HB3	2.04	0.57
2:4:239:GLU:OE2	2:4:242:GLU:N	2.37	0.57
3:7:499:ARG:NH1	3:7:525:GLY:O	2.34	0.57
3:7:552:VAL:HA	3:7:703:ALA:HB3	1.86	0.57
5:2:67:ASN:OD1	5:2:68:SER:N	2.37	0.57
6:0:730:PRO:HB2	6:0:732:ASP:OD1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:383:GLU:HG2	6:0:585:THR:HG21	1.84	0.57
1:1:501:LYS:HA	1:1:504:ILE:HD12	1.85	0.57
2:4:52:LYS:NZ	2:4:242:GLU:O	2.36	0.57
2:4:149:LEU:HD22	2:4:153:MET:HE2	1.84	0.57
6:0:311:VAL:HG11	6:0:317:LEU:HD11	1.86	0.57
7:6:168:GLN:OE1	7:6:168:GLN:N	2.37	0.57
7:6:293:ASP:OD2	7:6:296:HIS:N	2.31	0.57
2:4:114:MET:C	2:4:116:ARG:N	2.63	0.57
2:4:254:ILE:HG23	5:2:45:PHE:CE1	2.39	0.57
6:0:308:GLU:CD	6:0:308:GLU:H	2.13	0.57
3:7:267:ASP:O	3:7:348:ARG:NE	2.38	0.57
6:0:379:GLU:OE1	6:0:380:ARG:N	2.38	0.57
3:7:409:VAL:HA	3:7:486:ILE:HB	1.87	0.57
6:0:349:LEU:H	6:0:349:LEU:HD23	1.70	0.57
6:0:519:VAL:HG11	6:0:553:MET:HE1	1.86	0.57
6:0:571:VAL:HA	6:0:599:LEU:HD12	1.87	0.57
2:4:305:CYS:HB3	2:4:312:PHE:HZ	1.70	0.57
6:0:629:TYR:CZ	6:0:636:LYS:HE2	2.40	0.57
5:2:410:ARG:H	5:2:410:ARG:NE	2.03	0.57
1:1:269:ALA:O	1:1:273:ASN:ND2	2.38	0.56
1:1:350:ARG:NH1	6:0:401:ASP:OD1	2.38	0.56
2:4:137:LYS:H	2:4:140:ILE:HB	1.70	0.56
2:4:255:ASP:H	2:4:256:PRO:HD2	1.64	0.56
6:0:719:GLN:OE1	6:0:722:ARG:NH1	2.38	0.56
2:4:202:SER:HB3	7:6:448:LEU:HB3	1.86	0.56
3:7:406:SER:O	3:7:483:GLY:N	2.39	0.56
3:7:577:ARG:HD2	3:7:714:GLN:HB2	1.87	0.56
6:0:11:LEU:HD23	6:0:93:ARG:HA	1.87	0.56
6:0:68:LYS:HB2	6:0:230:SER:OG	2.04	0.56
6:0:440:LEU:HD22	6:0:638:ARG:HA	1.87	0.56
1:1:279:LYS:CB	1:1:283:PHE:CD2	2.87	0.56
2:4:155:ALA:O	2:4:158:THR:OG1	2.18	0.56
3:7:303:ARG:HB3	3:7:323:VAL:HG13	1.88	0.56
6:0:145:LEU:HD13	6:0:153:VAL:HB	1.86	0.56
6:0:615:GLN:OE1	6:0:615:GLN:N	2.36	0.56
3:7:410:LEU:HB2	3:7:487:LEU:HD23	1.86	0.56
6:0:312:LEU:H	6:0:412:TYR:HH	1.50	0.56
3:7:555:ALA:HA	3:7:734:LYS:O	2.06	0.56
7:6:349:CYS:HB3	7:6:352:CYS:SG	2.45	0.56
3:7:577:ARG:HA	3:7:580:LEU:HD12	1.86	0.56
5:2:80:SER:O	5:2:83:SER:OG	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:39:THR:O	2:4:43:GLU:N	2.30	0.56
2:4:40:PHE:HA	2:4:43:GLU:CD	2.31	0.56
2:4:180:THR:HG23	2:4:214:LYS:HA	1.87	0.56
2:4:258:LEU:C	2:4:260:PRO:HD3	2.30	0.56
3:7:677:TYR:HE2	3:7:686:ARG:HB2	1.68	0.56
3:7:594:LEU:O	3:7:598:HIS:ND1	2.33	0.56
3:7:636:ARG:HH11	3:7:662:ILE:CG2	2.01	0.56
3:7:664:LEU:HB3	3:7:692:ARG:HG3	1.88	0.56
5:2:497:GLY:O	5:2:500:GLN:HG2	2.05	0.56
7:6:234:ILE:HB	7:6:263:VAL:HB	1.87	0.56
3:7:554:CYS:HA	3:7:705:PHE:HB3	1.87	0.56
3:7:679:SER:O	3:7:680:ARG:NE	2.39	0.56
6:0:293:LEU:HD22	6:0:319:GLU:HA	1.88	0.55
3:7:410:LEU:HD21	3:7:460:VAL:HG21	1.87	0.55
5:2:12:GLN:N	5:2:12:GLN:OE1	2.39	0.55
6:0:537:MET:HG3	6:0:538:VAL:N	2.21	0.55
7:6:195:ALA:O	7:6:198:SER:OG	2.19	0.55
1:1:551:ARG:O	1:1:555:THR:OG1	2.21	0.55
3:7:579:LEU:HA	3:7:582:ILE:HB	1.88	0.55
3:7:584:ASN:O	3:7:618:TYR:OH	2.24	0.55
3:7:588:PHE:HB2	3:7:618:TYR:CZ	2.42	0.55
5:2:396:ILE:O	5:2:400:LEU:HG	2.07	0.55
1:1:280:GLU:O	1:1:284:TRP:CE3	2.60	0.55
1:1:300:LYS:O	1:1:302:MET:N	2.40	0.55
3:7:365:TYR:OH	3:7:390:ALA:O	2.25	0.55
6:0:270:ARG:HA	6:0:273:GLU:CD	2.31	0.55
1:1:515:LYS:O	1:1:517:ASN:N	2.39	0.55
3:7:554:CYS:O	3:7:734:LYS:N	2.39	0.55
5:2:10:VAL:HG11	5:2:201:TRP:CE3	2.42	0.55
6:0:244:CYS:O	6:0:247:SER:OG	2.22	0.55
4:5:47:VAL:HG12	4:5:51:LYS:HE3	1.89	0.55
5:2:370:PHE:HZ	5:2:375:LEU:HD22	1.72	0.55
3:7:344:ARG:HH12	3:7:404:LYS:HB3	1.71	0.55
1:1:235:SER:C	1:1:239:PRO:HD2	2.32	0.54
3:7:692:ARG:HH11	3:7:692:ARG:HA	1.71	0.54
6:0:258:ARG:O	6:0:261:THR:OG1	2.14	0.54
7:6:372:LEU:H	7:6:375:HIS:CE1	2.25	0.54
1:1:336:ILE:HD13	6:0:80:GLU:HG3	1.87	0.54
6:0:43:PRO:HB3	6:0:696:TRP:CD2	2.42	0.54
6:0:169:ASP:CG	6:0:170:TYR:H	2.14	0.54
1:1:229:GLY:HA3	7:6:242:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:510:ASN:O	1:1:513:GLN:HG3	2.07	0.54
6:0:156:CYS:C	6:0:158:TYR:H	2.15	0.54
3:7:132:LEU:O	3:7:202:LYS:N	2.30	0.54
3:7:757:ARG:O	3:7:761:GLN:HG2	2.07	0.54
5:2:84:LEU:HD11	5:2:86:LEU:HD23	1.89	0.54
5:2:273:LYS:NZ	5:2:285:ILE:O	2.32	0.54
7:6:246:ASP:OD1	7:6:247:ILE:N	2.40	0.54
1:1:279:LYS:HG3	1:1:283:PHE:CD2	2.43	0.54
1:1:597:PHE:CZ	1:1:613:THR:HA	2.43	0.54
3:7:631:THR:HB	3:7:636:ARG:HH21	1.72	0.54
3:7:636:ARG:HH12	3:7:662:ILE:HG21	1.66	0.54
3:7:717:TYR:O	3:7:720:THR:OG1	2.24	0.54
6:0:675:ASP:OD1	6:0:676:TYR:N	2.38	0.54
7:6:376:LEU:O	7:6:379:SER:OG	2.22	0.54
2:4:260:PRO:C	5:2:67:ASN:HD22	2.15	0.54
3:7:607:VAL:HB	3:7:653:PHE:HA	1.90	0.54
5:2:174:GLU:H	5:2:185:THR:N	2.05	0.54
6:0:471:ARG:HH22	6:0:646:TYR:HB3	1.73	0.54
7:6:169:MET:HE2	7:6:171:ILE:HD11	1.89	0.54
2:4:60:PHE:CG	2:4:248:LEU:HD22	2.43	0.54
5:2:17:ILE:HG23	5:2:21:VAL:HG23	1.89	0.54
6:0:255:ASP:O	6:0:259:ARG:HG3	2.08	0.54
7:6:209:SER:OG	7:6:212:ASN:OD1	2.18	0.54
1:1:279:LYS:HE2	1:1:279:LYS:N	2.22	0.54
6:0:325:ILE:HG12	6:0:334:PHE:CE2	2.43	0.54
6:0:535:ASP:OD1	6:0:535:ASP:N	2.38	0.54
6:0:632:SER:OG	6:0:633:ARG:N	2.30	0.54
1:1:490:VAL:O	1:1:492:ASN:N	2.41	0.53
3:7:412:THR:OG1	3:7:413:SER:N	2.42	0.53
7:6:266:LEU:O	7:6:268:ALA:N	2.39	0.53
1:1:593:LEU:HA	1:1:596:LEU:HD12	1.89	0.53
6:0:334:PHE:HD1	6:0:337:ARG:HH21	1.54	0.53
6:0:534:PRO:HA	7:6:239:LEU:HD12	1.89	0.53
6:0:643:ARG:NH1	6:0:650:GLU:H	2.06	0.53
3:7:490:VAL:HB	3:7:519:ARG:HH22	1.73	0.53
1:1:251:LEU:HD22	1:1:255:LYS:HE3	1.90	0.53
2:4:28:VAL:HB	2:4:75:VAL:HG22	1.90	0.53
2:4:38:THR:O	2:4:42:GLU:N	2.35	0.53
3:7:324:GLU:HA	3:7:327:LYS:HE2	1.89	0.53
3:7:438:PHE:HB2	3:7:459:MET:HE2	1.90	0.53
6:0:515:ASP:O	6:0:517:SER:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:352:LEU:HD22	3:7:406:SER:HA	1.91	0.53
5:2:356:GLN:O	5:2:360:LEU:HG	2.08	0.53
2:4:288:ILE:HD11	2:4:293:LEU:HD12	1.89	0.53
3:7:353:ASP:OD2	3:7:434:ASN:ND2	2.34	0.53
4:5:16:ILE:HD13	4:5:19:LEU:HD12	1.90	0.53
5:2:405:HIS:NE2	5:2:409:ARG:HA	2.23	0.53
5:2:486:ASP:N	5:2:486:ASP:OD1	2.42	0.53
1:1:188:ASN:HD22	1:1:191:LEU:HG	1.74	0.53
1:1:224:THR:O	1:1:226:GLN:N	2.42	0.53
2:4:126:VAL:HA	2:4:129:ILE:HG22	1.90	0.53
3:7:256:ILE:N	3:7:317:GLU:O	2.41	0.53
3:7:410:LEU:N	3:7:486:ILE:O	2.41	0.53
5:2:72:LEU:HD23	5:2:72:LEU:H	1.72	0.53
5:2:463:GLU:N	5:2:467:GLU:OE2	2.42	0.53
2:4:303:ASN:HB2	2:4:311:GLN:HG2	1.90	0.53
3:7:582:ILE:HG12	3:7:673:ILE:HG22	1.90	0.53
5:2:445:GLN:O	5:2:449:ASP:CB	2.57	0.53
3:7:578:MET:HA	3:7:581:TYR:CZ	2.44	0.53
3:7:597:TYR:HA	3:7:600:ARG:HE	1.73	0.53
4:5:5:ARG:HD3	5:2:458:LEU:HD23	1.90	0.53
4:5:36:ASP:OD1	4:5:39:HIS:N	2.41	0.53
2:4:293:LEU:HD23	7:6:383:LEU:HD11	1.91	0.53
3:7:349:ASN:ND2	3:7:481:GLU:O	2.42	0.53
3:7:459:MET:O	3:7:470:SER:OG	2.15	0.53
6:0:384:LEU:O	6:0:387:THR:OG1	2.22	0.53
1:1:207:SER:OG	1:1:208:GLU:OE1	2.22	0.52
6:0:12:PHE:CE1	6:0:14:TYR:HB2	2.40	0.52
6:0:510:PHE:CE2	6:0:511:GLU:HB2	2.44	0.52
6:0:573:THR:OG1	6:0:575:ASP:OD1	2.26	0.52
2:4:239:GLU:OE1	2:4:240:SER:N	2.42	0.52
3:7:135:SER:N	3:7:140:ARG:O	2.43	0.52
3:7:564:GLU:H	3:7:564:GLU:CD	2.16	0.52
6:0:169:ASP:OD1	6:0:170:TYR:N	2.41	0.52
1:1:236:THR:HA	1:1:239:PRO:HG2	1.90	0.52
1:1:592:LYS:O	1:1:596:LEU:HG	2.09	0.52
6:0:117:HIS:CE1	6:0:119:GLU:HB3	2.41	0.52
6:0:440:LEU:HD13	6:0:641:PHE:HB2	1.91	0.52
7:6:300:LEU:O	7:6:303:GLU:HG2	2.09	0.52
2:4:228:THR:HG21	2:4:235:TYR:HB2	1.92	0.52
5:2:82:LYS:O	5:2:85:HIS:ND1	2.43	0.52
5:2:174:GLU:H	5:2:185:THR:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:473:LYS:NZ	5:2:477:ASP:OD1	2.37	0.52
7:6:247:ILE:O	7:6:250:THR:OG1	2.22	0.52
1:1:231:TYR:HA	1:1:385:MET:SD	2.50	0.52
3:7:369:SER:HB3	3:7:384:ILE:HD13	1.92	0.52
5:2:95:THR:OG1	5:2:96:LEU:N	2.40	0.52
7:6:217:ALA:O	7:6:220:LEU:N	2.42	0.52
6:0:275:ARG:NH2	6:0:276:LYS:HG3	2.22	0.52
7:6:352:CYS:SG	7:6:353:HIS:N	2.81	0.52
1:1:279:LYS:H	1:1:279:LYS:CD	2.22	0.52
2:4:305:CYS:HB3	2:4:312:PHE:CZ	2.45	0.52
4:5:17:LYS:HE3	4:5:40:LEU:HD21	1.91	0.52
6:0:97:LEU:O	6:0:100:GLN:NE2	2.43	0.52
1:1:510:ASN:HD21	2:4:265:PRO:C	2.18	0.52
2:4:87:TYR:CE1	2:4:121:VAL:HG22	2.45	0.52
3:7:133:TRP:N	3:7:142:ILE:O	2.43	0.52
3:7:457:TYR:HE1	3:7:487:LEU:HD22	1.74	0.52
6:0:119:GLU:OE1	6:0:122:LYS:NZ	2.31	0.52
6:0:183:LYS:O	6:0:187:GLU:HG2	2.09	0.52
3:7:497:MET:HA	3:7:500:ARG:HE	1.74	0.52
3:7:545:GLN:HA	3:7:550:ALA:HA	1.91	0.52
3:7:555:ALA:HB3	3:7:706:TYR:HD1	1.75	0.52
3:7:656:LYS:HE3	3:7:677:TYR:CD1	2.45	0.52
5:2:69:ASN:ND2	5:2:69:ASN:O	2.43	0.52
6:0:343:LYS:HG2	6:0:347:LYS:HZ3	1.75	0.52
6:0:625:ILE:HD11	6:0:658:ALA:HB1	1.92	0.52
3:7:477:LEU:HA	3:7:482:TRP:NE1	2.25	0.51
5:2:32:CYS:HB3	5:2:104:PHE:HE1	1.75	0.51
5:2:381:GLU:O	5:2:385:ARG:HD3	2.11	0.51
6:0:646:TYR:HA	6:0:647:ARG:CZ	2.40	0.51
2:4:64:HIS:HA	2:4:253:PHE:CZ	2.45	0.51
2:4:298:ILE:O	2:4:300:PRO:HD3	2.10	0.51
3:7:489:GLU:OE2	3:7:689:ARG:NH2	2.42	0.51
6:0:12:PHE:HD1	6:0:14:TYR:H	1.56	0.51
6:0:76:MET:HA	6:0:79:ILE:HB	1.93	0.51
6:0:492:PHE:CD2	6:0:494:PRO:HD3	2.46	0.51
6:0:746:LYS:O	6:0:750:SER:HB3	2.10	0.51
3:7:641:GLN:O	3:7:645:TYR:HB3	2.09	0.51
6:0:56:THR:HG21	6:0:233:ILE:HD11	1.92	0.51
6:0:312:LEU:N	6:0:412:TYR:OH	2.25	0.51
4:5:57:LEU:HA	4:5:60:LYS:HD3	1.93	0.51
5:2:56:GLU:OE1	5:2:56:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:500:GLY:HA3	6:0:521:ASN:HD21	1.74	0.51
6:0:639:LEU:HG	6:0:650:GLU:HG2	1.90	0.51
4:5:13:ASP:OD1	4:5:15:SER:OG	2.25	0.51
5:2:32:CYS:HB3	5:2:104:PHE:CE1	2.45	0.51
6:0:123:GLU:HB3	6:0:129:VAL:HG22	1.92	0.51
6:0:217:LYS:HB2	6:0:308:GLU:HG3	1.91	0.51
6:0:742:GLU:OE2	6:0:746:LYS:NZ	2.43	0.51
3:7:715:GLU:HA	3:7:718:TYR:HD2	1.75	0.51
6:0:65:GLU:O	6:0:67:ARG:HG2	2.10	0.51
6:0:375:ARG:HG3	6:0:410:SER:OG	2.11	0.51
6:0:506:ILE:HG21	6:0:521:ASN:HD22	1.75	0.51
2:4:211:ASP:HB3	2:4:234:VAL:HG13	1.93	0.51
3:7:593:PHE:HB2	3:7:745:ILE:HG21	1.92	0.51
7:6:175:ARG:CZ	7:6:202:GLN:HE22	2.23	0.51
3:7:548:HIS:O	3:7:694:LYS:N	2.38	0.51
6:0:241:ASP:OD1	6:0:241:ASP:N	2.42	0.51
7:6:119:GLN:O	7:6:120:ARG:HG2	2.11	0.51
3:7:555:ALA:N	3:7:705:PHE:O	2.43	0.51
3:7:568:GLU:HG2	3:7:580:LEU:HD13	1.93	0.51
3:7:608:PHE:N	3:7:671:ILE:O	2.29	0.51
6:0:18:TYR:HE2	6:0:673:LYS:HD2	1.75	0.51
6:0:94:THR:O	6:0:98:GLY:N	2.40	0.51
2:4:286:GLY:N	7:6:322:MET:O	2.44	0.50
2:4:290:SER:O	2:4:293:LEU:N	2.44	0.50
3:7:434:ASN:OD1	3:7:450:SER:OG	2.25	0.50
3:7:461:ALA:HB3	3:7:497:MET:HB2	1.93	0.50
6:0:316:LEU:C	6:0:317:LEU:HD12	2.37	0.50
6:0:331:PHE:HA	6:0:334:PHE:CD2	2.46	0.50
1:1:279:LYS:CA	1:1:279:LYS:HE2	2.41	0.50
6:0:510:PHE:O	6:0:511:GLU:HG3	2.11	0.50
3:7:712:ASP:OD1	3:7:712:ASP:N	2.44	0.50
5:2:91:LYS:HA	5:2:95:THR:O	2.11	0.50
5:2:382:SER:HA	5:2:385:ARG:NH1	2.26	0.50
6:0:510:PHE:CG	6:0:511:GLU:N	2.80	0.50
3:7:446:PHE:O	3:7:447:GLN:HG2	2.10	0.50
6:0:92:TYR:OH	6:0:96:GLU:OE2	2.25	0.50
7:6:233:LEU:HA	7:6:262:LYS:O	2.12	0.50
7:6:424:SER:O	7:6:426:ARG:N	2.45	0.50
3:7:446:PHE:HB3	3:7:473:VAL:HG22	1.93	0.50
4:5:52:HIS:O	4:5:56:ARG:HG3	2.12	0.50
6:0:270:ARG:O	6:0:273:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:740:SER:H	6:0:744:LEU:HD22	1.77	0.50
7:6:288:TYR:CG	7:6:288:TYR:O	2.65	0.50
2:4:50:ILE:O	2:4:53:VAL:N	2.45	0.50
5:2:51:VAL:HG12	5:2:52:PHE:CD1	2.47	0.50
5:2:90:ASN:ND2	5:2:92:SER:HB2	2.27	0.50
6:0:60:GLN:HE22	6:0:204:ASN:HB3	1.75	0.50
6:0:108:LEU:HD22	6:0:200:ILE:HD11	1.94	0.50
3:7:407:VAL:HG13	3:7:484:PHE:HB3	1.94	0.50
3:7:666:GLU:HB3	3:7:694:LYS:CD	2.42	0.50
5:2:350:TYR:N	5:2:407:GLN:OE1	2.44	0.50
2:4:30:ILE:O	2:4:77:ALA:HA	2.12	0.50
2:4:276:CYS:HB3	2:4:279:THR:HB	1.94	0.50
6:0:65:GLU:N	6:0:65:GLU:OE1	2.45	0.50
6:0:422:PRO:HG2	6:0:423:TYR:CD1	2.47	0.50
6:0:422:PRO:HG2	6:0:423:TYR:HD1	1.76	0.50
1:1:501:LYS:O	1:1:505:THR:HG23	2.12	0.49
1:1:606:GLU:O	1:1:610:ASN:N	2.33	0.49
4:5:8:ALA:HB2	4:5:44:PRO:HG3	1.94	0.49
5:2:347:ILE:HG22	5:2:373:MET:HE1	1.94	0.49
6:0:294:HIS:O	6:0:298:ILE:N	2.32	0.49
6:0:625:ILE:HB	6:0:686:PHE:CZ	2.47	0.49
6:0:694:PRO:HG2	6:0:697:ILE:HG13	1.94	0.49
7:6:254:LEU:O	7:6:257:GLU:N	2.43	0.49
1:1:285:ALA:HA	1:1:288:PHE:CD2	2.47	0.49
6:0:94:THR:HG22	6:0:101:GLU:HG2	1.93	0.49
6:0:708:LEU:HB3	6:0:712:MET:HG3	1.94	0.49
7:6:309:PRO:HA	7:6:312:LYS:NZ	2.27	0.49
3:7:165:SER:O	3:7:172:GLU:N	2.41	0.49
3:7:407:VAL:H	3:7:452:LEU:HD22	1.77	0.49
6:0:138:ASN:O	6:0:142:LYS:HG2	2.11	0.49
1:1:251:LEU:O	1:1:255:LYS:N	2.26	0.49
2:4:25:LEU:HG	2:4:27:THR:HG22	1.94	0.49
3:7:341:TYR:O	3:7:378:ARG:HB3	2.12	0.49
3:7:591:CYS:O	3:7:595:ILE:HG13	2.13	0.49
6:0:318:THR:OG1	6:0:319:GLU:N	2.45	0.49
1:1:235:SER:O	1:1:237:ILE:N	2.46	0.49
1:1:260:PHE:CG	1:1:267:LYS:HD3	2.48	0.49
2:4:200:ILE:HG12	2:4:227:THR:HG23	1.94	0.49
6:0:21:GLN:O	6:0:25:MET:HG2	2.12	0.49
6:0:123:GLU:OE1	6:0:124:ARG:N	2.45	0.49
1:1:270:TYR:CD2	1:1:279:LYS:CB	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:90:SER:HB3	7:6:407:GLN:NE2	2.28	0.49
3:7:606:ILE:HG12	3:7:652:ILE:HD11	1.94	0.49
6:0:254:THR:HA	6:0:257:LEU:HD13	1.95	0.49
6:0:507:SER:OG	6:0:685:ARG:NH2	2.30	0.49
1:1:235:SER:O	1:1:238:LYS:N	2.31	0.49
3:7:608:PHE:HB3	3:7:672:GLN:HA	1.93	0.49
3:7:666:GLU:HG2	3:7:693:ALA:O	2.11	0.49
1:1:204:LEU:HD12	1:1:205:PRO:HD2	1.95	0.49
3:7:303:ARG:HG2	3:7:304:GLU:H	1.77	0.49
3:7:456:THR:HG23	3:7:459:MET:H	1.78	0.49
3:7:712:ASP:N	3:7:716:MET:SD	2.81	0.49
5:2:28:SER:O	5:2:31:THR:OG1	2.24	0.49
5:2:431:GLN:CD	5:2:435:PRO:HD2	2.38	0.49
6:0:496:ILE:HD12	6:0:686:PHE:HB3	1.95	0.49
1:1:306:ARG:O	1:1:308:ASP:N	2.45	0.49
3:7:366:GLN:NE2	3:7:391:GLY:O	2.45	0.49
6:0:529:PHE:O	6:0:533:THR:HG23	2.13	0.49
6:0:629:TYR:CG	6:0:629:TYR:O	2.66	0.49
7:6:139:LYS:NZ	7:6:144:ASN:HB3	2.27	0.49
1:1:199:VAL:HG22	1:1:204:LEU:O	2.13	0.49
3:7:639:ILE:O	3:7:643:PHE:HB3	2.13	0.49
5:2:380:ARG:HG2	5:2:384:ARG:HH22	1.78	0.49
6:0:130:ASP:O	6:0:134:ARG:HG3	2.13	0.49
6:0:492:PHE:HD2	6:0:494:PRO:HD3	1.77	0.49
7:6:212:ASN:HD21	7:6:244:PRO:HG2	1.77	0.49
6:0:306:PHE:CD2	6:0:307:VAL:HG23	2.47	0.48
3:7:250:VAL:H	3:7:329:ARG:CZ	2.27	0.48
4:5:32:LEU:H	4:5:42:VAL:HA	1.78	0.48
6:0:17:ILE:HG22	6:0:739:TRP:O	2.13	0.48
6:0:38:SER:OG	6:0:479:LEU:N	2.32	0.48
6:0:452:ARG:HH21	6:0:453:PHE:HE1	1.61	0.48
3:7:475:ASP:O	3:7:478:THR:OG1	2.27	0.48
5:2:347:ILE:HB	5:2:376:GLY:O	2.13	0.48
6:0:192:PRO:O	6:0:196:VAL:HG12	2.12	0.48
6:0:625:ILE:HD12	6:0:626:PRO:HD2	1.95	0.48
3:7:595:ILE:HG12	3:7:651:THR:OG1	2.13	0.48
5:2:47:ILE:O	5:2:51:VAL:HG23	2.13	0.48
6:0:374:LEU:HD11	6:0:406:ALA:HB1	1.95	0.48
6:0:397:THR:O	6:0:400:LYS:HG2	2.12	0.48
6:0:529:PHE:HB3	6:0:537:MET:HE1	1.96	0.48
3:7:370:LEU:HA	3:7:373:MET:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:386:LEU:HB2	3:7:392:LYS:HG3	1.96	0.48
2:4:254:ILE:CG2	2:4:261:ILE:HD13	2.43	0.48
3:7:133:TRP:O	3:7:142:ILE:N	2.35	0.48
6:0:326:ARG:O	6:0:380:ARG:NH2	2.47	0.48
6:0:486:THR:O	6:0:486:THR:OG1	2.32	0.48
6:0:541:PHE:HD2	6:0:547:MET:HE2	1.78	0.48
6:0:575:ASP:OD1	6:0:575:ASP:N	2.46	0.48
3:7:303:ARG:HB3	3:7:323:VAL:HG22	1.95	0.48
3:7:355:ASP:HB2	3:7:431:GLN:HE22	1.78	0.48
3:7:698:ASP:OD1	3:7:698:ASP:N	2.44	0.48
5:2:110:ASN:O	5:2:115:GLY:N	2.46	0.48
7:6:120:ARG:HD3	7:6:309:PRO:HD3	1.93	0.48
3:7:443:LYS:HE2	3:7:446:PHE:CZ	2.48	0.48
6:0:166:GLU:OE2	6:0:170:TYR:HA	2.14	0.48
6:0:286:TYR:HB3	6:0:326:ARG:NH2	2.29	0.48
6:0:313:PRO:O	6:0:314:GLN:HG2	2.14	0.48
1:1:178:LEU:HA	1:1:181:GLN:OE1	2.14	0.48
3:7:264:PRO:O	3:7:269:LEU:N	2.44	0.48
6:0:446:ILE:O	6:0:449:VAL:HG22	2.13	0.48
6:0:627:PHE:CD1	6:0:654:LEU:HD12	2.47	0.48
5:2:381:GLU:CD	5:2:384:ARG:HE	2.22	0.48
6:0:235:ASP:OD1	6:0:236:GLU:N	2.46	0.48
6:0:255:ASP:N	6:0:255:ASP:OD1	2.44	0.48
6:0:549:SER:O	6:0:553:MET:HG3	2.14	0.48
1:1:254:GLU:OE1	1:1:254:GLU:N	2.36	0.47
3:7:403:ILE:HD12	3:7:405:LYS:HB2	1.95	0.47
5:2:87:LEU:HD23	5:2:87:LEU:H	1.79	0.47
5:2:387:LEU:C	5:2:390:GLY:H	2.22	0.47
7:6:309:PRO:HA	7:6:312:LYS:HE3	1.96	0.47
5:2:397:ILE:O	5:2:401:GLU:HG2	2.13	0.47
6:0:37:ASN:HD22	6:0:475:PHE:HD2	1.63	0.47
6:0:349:LEU:HG	6:0:350:HIS:N	2.29	0.47
7:6:126:LEU:C	7:6:127:ILE:HD12	2.39	0.47
7:6:148:MET:HE2	7:6:148:MET:HB3	1.79	0.47
7:6:253:SER:O	7:6:256:SER:OG	2.16	0.47
7:6:309:PRO:HA	7:6:312:LYS:CE	2.44	0.47
6:0:169:ASP:O	6:0:198:ARG:NH2	2.41	0.47
2:4:263:VAL:C	2:4:265:PRO:HD3	2.40	0.47
3:7:354:ILE:HD12	3:7:404:LYS:HA	1.96	0.47
5:2:238:LYS:H	5:2:269:PHE:N	2.12	0.47
6:0:156:CYS:HB3	6:0:158:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:713:ALA:O	6:0:717:THR:HG22	2.14	0.47
1:1:284:TRP:HA	1:1:287:PHE:HB3	1.95	0.47
1:1:339:LEU:HA	1:1:342:ASN:HB3	1.96	0.47
1:1:517:ASN:O	1:1:519:VAL:N	2.48	0.47
2:4:275:SER:HB2	2:4:281:ARG:C	2.40	0.47
6:0:312:LEU:O	6:0:314:GLN:N	2.48	0.47
7:6:377:ALA:HA	7:6:380:TYR:CD2	2.49	0.47
2:4:276:CYS:SG	2:4:279:THR:N	2.76	0.47
3:7:303:ARG:HA	3:7:321:GLU:N	2.29	0.47
3:7:500:ARG:O	3:7:504:THR:OG1	2.25	0.47
3:7:559:CYS:N	3:7:709:VAL:O	2.35	0.47
3:7:694:LYS:HE2	3:7:696:ARG:HB2	1.96	0.47
5:2:7:LYS:NZ	5:2:9:SER:HA	2.30	0.47
6:0:521:ASN:O	6:0:524:SER:OG	2.30	0.47
3:7:354:ILE:HG21	3:7:401:CYS:HA	1.96	0.47
3:7:670:LEU:N	3:7:704:PHE:O	2.27	0.47
5:2:86:LEU:HD12	5:2:87:LEU:N	2.30	0.47
6:0:132:LYS:HE3	6:0:132:LYS:HB2	1.61	0.47
6:0:494:PRO:HB2	6:0:701:LEU:HD13	1.97	0.47
6:0:533:THR:O	6:0:567:LYS:NZ	2.41	0.47
6:0:628:GLN:O	6:0:630:THR:N	2.48	0.47
6:0:77:SER:O	6:0:80:GLU:HG2	2.14	0.47
6:0:123:GLU:OE1	6:0:125:LYS:N	2.47	0.47
6:0:743:ASP:O	6:0:747:HIS:N	2.44	0.47
7:6:160:PHE:HA	7:6:305:VAL:HG13	1.96	0.47
7:6:269:GLN:HG3	7:6:288:TYR:CE2	2.41	0.47
3:7:303:ARG:NE	3:7:321:GLU:O	2.31	0.47
3:7:341:TYR:HE2	3:7:403:ILE:HB	1.80	0.47
6:0:499:LYS:O	6:0:709:SER:HA	2.14	0.47
3:7:385:VAL:HG13	3:7:537:GLU:HA	1.97	0.47
3:7:413:SER:O	3:7:417:VAL:N	2.40	0.47
6:0:119:GLU:HA	6:0:122:LYS:NZ	2.29	0.47
6:0:142:LYS:HG3	6:0:143:ARG:N	2.30	0.47
7:6:372:LEU:HD22	7:6:375:HIS:HE1	1.79	0.47
1:1:188:ASN:HB3	1:1:191:LEU:HD12	1.97	0.46
1:1:336:ILE:O	6:0:77:SER:OG	2.24	0.46
3:7:117:ASP:C	5:2:370:PHE:HA	2.40	0.46
3:7:383:ILE:HG13	3:7:528:ASN:HA	1.96	0.46
3:7:433:GLU:OE2	3:7:434:ASN:ND2	2.48	0.46
3:7:484:PHE:CZ	3:7:511:LEU:HB2	2.49	0.46
5:2:10:VAL:O	5:2:14:LEU:N	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:20:GLN:O	5:2:24:ARG:HG2	2.15	0.46
6:0:378:SER:O	6:0:382:SER:OG	2.33	0.46
1:1:336:ILE:HG22	1:1:337:ILE:HD13	1.97	0.46
1:1:561:LEU:O	1:1:564:PHE:N	2.48	0.46
5:2:10:VAL:HG12	5:2:205:LEU:HD11	1.96	0.46
6:0:191:CYS:HB2	9:0:801:SF4:S2	2.56	0.46
6:0:201:SER:HA	6:0:225:GLU:CD	2.41	0.46
6:0:259:ARG:NH1	6:0:398:ALA:HB2	2.30	0.46
6:0:586:TYR:OH	6:0:616:TYR:O	2.19	0.46
7:6:227:HIS:HB3	7:6:318:THR:OG1	2.16	0.46
7:6:349:CYS:HB3	7:6:353:HIS:H	1.80	0.46
3:7:540:TRP:HH2	3:7:692:ARG:HH12	1.62	0.46
5:2:17:ILE:HG12	5:2:18:PRO:HD2	1.97	0.46
5:2:222:LEU:HD13	5:2:225:ILE:HD12	1.98	0.46
6:0:257:LEU:O	6:0:261:THR:HG23	2.14	0.46
6:0:297:ASP:HB3	6:0:386:ARG:HH22	1.81	0.46
7:6:108:LYS:O	7:6:109:ARG:NE	2.48	0.46
7:6:130:LEU:O	7:6:174:MET:HE2	2.15	0.46
1:1:465:SER:O	1:1:470:LEU:N	2.48	0.46
2:4:135:LEU:HA	2:4:137:LYS:NZ	2.31	0.46
3:7:410:LEU:HA	3:7:455:SER:O	2.15	0.46
5:2:7:LYS:HG2	5:2:9:SER:N	2.30	0.46
5:2:18:PRO:HB2	5:2:20:GLN:NE2	2.30	0.46
6:0:97:LEU:HB3	6:0:100:GLN:OE1	2.15	0.46
6:0:252:LEU:HA	6:0:252:LEU:HD23	1.69	0.46
7:6:144:ASN:OD1	7:6:146:HIS:N	2.48	0.46
1:1:208:GLU:OE1	1:1:208:GLU:N	2.23	0.46
1:1:390:LYS:HD2	6:0:588:LYS:HZ3	1.80	0.46
2:4:261:ILE:HD11	5:2:65:TRP:CE3	2.50	0.46
6:0:193:TYR:OH	6:0:197:ARG:NH2	2.49	0.46
6:0:481:LYS:HA	6:0:481:LYS:HD3	1.72	0.46
1:1:492:ASN:O	1:1:495:VAL:N	2.48	0.46
3:7:607:VAL:N	3:7:652:ILE:O	2.46	0.46
5:2:449:ASP:O	5:2:450:ARG:HG3	2.16	0.46
6:0:109:THR:OG1	6:0:113:ASN:ND2	2.48	0.46
7:6:182:VAL:HG11	7:6:199:ILE:HD11	1.98	0.46
7:6:293:ASP:CG	7:6:295:THR:HG1	2.17	0.46
3:7:343:PHE:HE2	3:7:379:ALA:H	1.64	0.46
6:0:287:GLU:O	6:0:290:VAL:HG12	2.16	0.46
6:0:489:LYS:HE3	6:0:724:MET:HE1	1.97	0.46
7:6:263:VAL:HG22	7:6:288:TYR:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:373:MET:O	3:7:380:ARG:HG2	2.15	0.46
5:2:20:GLN:OE1	5:2:20:GLN:N	2.43	0.46
6:0:338:LEU:HD22	6:0:338:LEU:HA	1.81	0.46
2:4:236:LEU:HA	2:4:236:LEU:HD23	1.50	0.46
3:7:605:ILE:HA	3:7:669:CYS:HB3	1.98	0.46
5:2:10:VAL:HG11	5:2:201:TRP:CD2	2.50	0.46
6:0:104:ARG:NH1	6:0:171:LEU:O	2.33	0.46
6:0:162:LEU:HG	6:0:167:VAL:HG23	1.98	0.46
6:0:731:LYS:HB2	6:0:731:LYS:HE2	1.78	0.46
7:6:165:PRO:HG2	7:6:375:HIS:HB3	1.96	0.46
1:1:236:THR:HA	1:1:240:VAL:H	1.81	0.46
1:1:389:LEU:HD21	7:6:243:ASP:O	2.16	0.46
3:7:501:VAL:O	3:7:505:ILE:HG12	2.16	0.46
3:7:565:PHE:HZ	3:7:583:MET:HE2	1.80	0.46
3:7:565:PHE:CE2	3:7:581:TYR:HA	2.51	0.46
6:0:380:ARG:O	6:0:383:LEU:HD23	2.16	0.46
2:4:117:ARG:HA	2:4:120:ASN:ND2	2.31	0.45
3:7:252:GLY:HA2	3:7:316:PHE:CZ	2.51	0.45
5:2:409:ARG:HB2	5:2:410:ARG:NH1	2.31	0.45
6:0:327:ARG:HD2	6:0:329:GLU:HG2	1.98	0.45
7:6:263:VAL:HG13	7:6:277:CYS:SG	2.56	0.45
2:4:254:ILE:HG21	5:2:45:PHE:CZ	2.48	0.45
3:7:406:SER:HB2	3:7:482:TRP:CE3	2.52	0.45
3:7:565:PHE:CZ	3:7:583:MET:HE2	2.52	0.45
5:2:382:SER:HA	5:2:385:ARG:HH11	1.81	0.45
6:0:273:GLU:HA	6:0:276:LYS:HE2	1.97	0.45
6:0:311:VAL:CG1	6:0:317:LEU:HD11	2.45	0.45
7:6:322:MET:HE2	7:6:369:MET:HB3	1.98	0.45
3:7:675:SER:HB3	3:7:715:GLU:CD	2.42	0.45
4:5:27:MET:HB2	4:5:27:MET:HE2	1.76	0.45
7:6:145:ARG:HD3	7:6:266:LEU:HD12	1.98	0.45
3:7:308:ASP:O	3:7:340:GLU:N	2.42	0.45
3:7:385:VAL:HB	3:7:514:THR:HB	1.98	0.45
3:7:675:SER:HB2	3:7:722:ARG:HH12	1.81	0.45
5:2:389:ASN:HB3	5:2:391:ILE:HG12	1.97	0.45
6:0:309:THR:O	6:0:309:THR:OG1	2.33	0.45
3:7:621:LYS:O	3:7:747:ASN:ND2	2.49	0.45
5:2:100:LEU:H	5:2:100:LEU:HG	1.52	0.45
6:0:158:TYR:HB3	6:0:191:CYS:N	2.31	0.45
6:0:730:PRO:C	6:0:732:ASP:H	2.24	0.45
7:6:276:LEU:O	7:6:280:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:40:PHE:O	2:4:43:GLU:HG2	2.16	0.45
2:4:90:SER:HB3	7:6:407:GLN:CD	2.41	0.45
3:7:687:LEU:HD22	3:7:729:GLN:HG3	1.99	0.45
5:2:359:VAL:HA	5:2:362:LEU:HG	1.99	0.45
5:2:459:TYR:OH	5:2:493:ILE:O	2.13	0.45
6:0:681:LEU:HD23	6:0:686:PHE:CE1	2.52	0.45
7:6:164:ASN:O	7:6:166:ILE:N	2.49	0.45
1:1:188:ASN:CG	1:1:191:LEU:H	2.24	0.45
3:7:303:ARG:HA	3:7:320:ASN:CA	2.46	0.45
4:5:10:VAL:O	4:5:40:LEU:N	2.39	0.45
4:5:14:PRO:HA	4:5:17:LYS:HB3	1.98	0.45
5:2:346:LYS:HB3	5:2:348:TYR:HE1	1.81	0.45
7:6:127:ILE:HG12	7:6:221:LEU:HD11	1.99	0.45
1:1:342:ASN:OD1	6:0:75:THR:HB	2.17	0.45
1:1:378:MET:HE2	1:1:378:MET:HB3	1.80	0.45
3:7:498:PHE:CD2	3:7:527:LEU:HD22	2.51	0.45
5:2:16:GLU:OE1	5:2:17:ILE:N	2.50	0.45
5:2:340:ILE:CA	5:2:348:TYR:H	2.30	0.45
5:2:350:TYR:HA	5:2:372:ASN:HB2	1.98	0.45
6:0:119:GLU:HA	6:0:122:LYS:HZ2	1.82	0.45
6:0:140:GLN:HA	6:0:143:ARG:HE	1.81	0.45
6:0:341:TYR:CE2	6:0:345:ARG:HG3	2.52	0.45
6:0:680:VAL:C	6:0:681:LEU:HD12	2.41	0.45
7:6:429:CYS:SG	7:6:430:GLU:N	2.89	0.45
1:1:194:VAL:HA	1:1:197:GLU:CD	2.41	0.45
1:1:201:ASN:OD1	1:1:201:ASN:N	2.49	0.45
1:1:270:TYR:CZ	1:1:279:LYS:HE2	2.41	0.45
2:4:293:LEU:HD13	2:4:293:LEU:HA	1.82	0.45
5:2:43:ALA:O	5:2:47:ILE:HG12	2.17	0.45
5:2:380:ARG:HG2	5:2:384:ARG:HH12	1.81	0.45
6:0:227:SER:C	6:0:229:ASP:N	2.74	0.45
6:0:279:SER:HA	6:0:282:LEU:HG	1.99	0.45
6:0:343:LYS:HZ3	6:0:347:LYS:HD2	1.81	0.45
7:6:241:THR:OG1	7:6:243:ASP:OD1	2.19	0.45
3:7:581:TYR:HE2	3:7:714:GLN:HB3	1.82	0.45
5:2:351:SER:N	5:2:407:GLN:OE1	2.50	0.45
6:0:25:MET:SD	6:0:55:LEU:HB2	2.57	0.45
6:0:341:TYR:HE1	6:0:366:LEU:HD12	1.81	0.45
6:0:628:GLN:HE22	6:0:657:ASP:CG	2.25	0.45
1:1:254:GLU:O	1:1:257:LEU:HG	2.18	0.44
2:4:60:PHE:CD1	2:4:248:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:175:ARG:HB3	2:4:209:PRO:HD2	1.99	0.44
3:7:104:PHE:H	3:7:529:PHE:HB2	1.82	0.44
3:7:598:HIS:HB3	3:7:603:ASP:HB2	1.99	0.44
3:7:643:PHE:HA	3:7:649:ILE:O	2.16	0.44
4:5:35:LEU:HB2	4:5:39:HIS:HB2	1.98	0.44
6:0:435:MET:HE2	6:0:435:MET:HB2	1.74	0.44
6:0:594:ARG:HB3	6:0:594:ARG:NH1	2.32	0.44
4:5:17:LYS:NZ	4:5:37:ASP:HA	2.32	0.44
6:0:471:ARG:NH2	6:0:646:TYR:HB3	2.31	0.44
6:0:572:GLU:OE2	6:0:579:THR:HG23	2.17	0.44
6:0:607:SER:OG	6:0:664:GLN:OE1	2.20	0.44
3:7:407:VAL:HB	3:7:452:LEU:HD13	1.99	0.44
6:0:223:SER:O	6:0:225:GLU:N	2.50	0.44
1:1:192:MET:O	1:1:196:GLN:HG3	2.17	0.44
1:1:562:LYS:HA	1:1:562:LYS:HD2	1.80	0.44
3:7:414:SER:HB3	3:7:456:THR:HG21	2.00	0.44
5:2:411:LEU:O	5:2:414:GLU:HG2	2.16	0.44
6:0:338:LEU:O	6:0:342:LEU:HG	2.17	0.44
6:0:668:ARG:HD3	6:0:668:ARG:HA	1.74	0.44
3:7:385:VAL:HG13	3:7:538:ALA:H	1.83	0.44
5:2:340:ILE:O	5:2:347:ILE:HA	2.17	0.44
6:0:209:SER:OG	6:0:210:TYR:N	2.51	0.44
2:4:64:HIS:HA	2:4:253:PHE:HZ	1.81	0.44
2:4:266:ASN:CG	2:4:267:HIS:H	2.24	0.44
2:4:288:ILE:HD11	2:4:293:LEU:CD1	2.47	0.44
5:2:67:ASN:CG	5:2:68:SER:N	2.76	0.44
6:0:298:ILE:O	6:0:299:LEU:HD23	2.17	0.44
6:0:478:VAL:HB	6:0:479:LEU:HD12	1.97	0.44
6:0:702:SER:N	6:0:705:ASP:OD2	2.51	0.44
7:6:282:TYR:CD1	7:6:282:TYR:N	2.84	0.44
2:4:224:LEU:O	2:4:228:THR:HG22	2.18	0.44
3:7:583:MET:O	3:7:618:TYR:OH	2.26	0.44
3:7:595:ILE:HA	3:7:605:ILE:HD12	1.98	0.44
6:0:294:HIS:O	6:0:294:HIS:CG	2.71	0.44
6:0:581:LEU:O	6:0:584:GLU:HG3	2.17	0.44
7:6:251:ILE:O	7:6:255:VAL:HG12	2.18	0.44
2:4:31:GLU:HG3	2:4:180:THR:HA	1.99	0.44
2:4:255:ASP:N	2:4:256:PRO:HD2	2.24	0.44
3:7:350:PRO:O	3:7:480:ARG:NH2	2.49	0.44
3:7:510:LYS:HB2	3:7:531:ILE:HG23	1.99	0.44
5:2:56:GLU:HG3	5:2:97:MET:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:177:ASN:C	5:2:180:GLY:H	2.25	0.44
5:2:384:ARG:HA	5:2:387:LEU:HB2	2.00	0.44
5:2:497:GLY:HA2	5:2:500:GLN:NE2	2.32	0.44
6:0:571:VAL:HG22	6:0:572:GLU:H	1.83	0.44
1:1:188:ASN:ND2	1:1:190:VAL:HB	2.26	0.44
5:2:13:TYR:O	5:2:16:GLU:HB3	2.18	0.44
5:2:99:ASN:N	5:2:99:ASN:OD1	2.51	0.44
6:0:66:HIS:NE2	6:0:229:ASP:O	2.51	0.44
6:0:248:LEU:HD22	6:0:248:LEU:HA	1.72	0.44
2:4:60:PHE:CE1	2:4:253:PHE:HD1	2.35	0.43
3:7:302:GLU:C	3:7:322:SER:H	2.25	0.43
3:7:477:LEU:HD23	3:7:505:ILE:HG13	2.00	0.43
3:7:668:THR:OG1	3:7:694:LYS:NZ	2.30	0.43
5:2:71:LYS:HD2	5:2:72:LEU:N	2.33	0.43
5:2:74:PHE:O	5:2:78:ILE:HG12	2.18	0.43
6:0:272:SER:HA	6:0:275:ARG:HH21	1.83	0.43
6:0:500:GLY:HA3	6:0:521:ASN:OD1	2.18	0.43
6:0:745:ILE:HD12	6:0:746:LYS:N	2.33	0.43
7:6:130:LEU:HD23	7:6:130:LEU:HA	1.80	0.43
7:6:267:SER:O	7:6:267:SER:OG	2.23	0.43
1:1:264:PRO:O	1:1:268:LYS:HG2	2.19	0.43
1:1:279:LYS:CB	1:1:283:PHE:CB	2.76	0.43
3:7:383:ILE:HD11	3:7:531:ILE:HB	2.00	0.43
3:7:757:ARG:NH1	3:7:758:GLU:OE2	2.51	0.43
6:0:379:GLU:H	6:0:379:GLU:HG3	1.54	0.43
6:0:732:ASP:OD1	6:0:733:GLN:N	2.51	0.43
2:4:193:TYR:CE2	2:4:197:MET:HE1	2.54	0.43
3:7:386:LEU:HD12	3:7:513:LEU:HD22	2.01	0.43
5:2:364:VAL:HA	5:2:382:SER:HB3	1.99	0.43
6:0:171:LEU:HB3	6:0:172:PRO:HD2	2.00	0.43
1:1:556:THR:O	1:1:560:PHE:HD1	2.01	0.43
3:7:352:LEU:HD12	3:7:352:LEU:HA	1.90	0.43
3:7:555:ALA:HB3	3:7:706:TYR:CD1	2.52	0.43
5:2:405:HIS:CE1	5:2:409:ARG:HA	2.53	0.43
6:0:525:MET:O	6:0:528:GLU:HG2	2.17	0.43
6:0:568:LEU:HD13	6:0:594:ARG:NH1	2.33	0.43
2:4:138:LYS:HA	2:4:138:LYS:HD2	1.93	0.43
3:7:252:GLY:HA2	3:7:316:PHE:HZ	1.84	0.43
3:7:588:PHE:HB2	3:7:618:TYR:CE2	2.53	0.43
3:7:725:PHE:O	3:7:729:GLN:HG2	2.19	0.43
5:2:78:ILE:HA	5:2:81:MET:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:506:LYS:HD2	5:2:507:ARG:HH21	1.83	0.43
6:0:140:GLN:O	6:0:144:LYS:HG3	2.19	0.43
1:1:265:ILE:HG13	1:1:266:VAL:N	2.33	0.43
3:7:342:ASP:HB2	3:7:345:ASN:HB2	1.99	0.43
3:7:352:LEU:HG	3:7:451:GLY:HA2	2.00	0.43
3:7:656:LYS:HE3	3:7:677:TYR:CE1	2.53	0.43
4:5:17:LYS:O	4:5:21:LEU:HG	2.19	0.43
5:2:31:THR:O	5:2:35:ILE:HG23	2.18	0.43
5:2:175:GLU:CA	5:2:183:LYS:H	2.31	0.43
6:0:161:ASN:HA	6:0:164:ASN:OD1	2.19	0.43
6:0:263:GLY:O	6:0:267:LEU:HG	2.19	0.43
6:0:306:PHE:CE2	6:0:307:VAL:HG23	2.53	0.43
6:0:432:ASN:OD1	6:0:432:ASN:N	2.51	0.43
6:0:497:ILE:HD12	6:0:713:ALA:HB2	2.00	0.43
6:0:737:SER:O	6:0:737:SER:OG	2.28	0.43
7:6:325:PRO:HB2	7:6:347:TYR:HB3	2.01	0.43
1:1:278:PHE:O	1:1:282:GLU:CD	2.61	0.43
1:1:348:VAL:HG12	6:0:127:THR:HG22	2.00	0.43
6:0:68:LYS:NZ	6:0:203:CYS:O	2.34	0.43
6:0:250:LEU:HD12	6:0:251:ASP:H	1.83	0.43
6:0:689:LYS:O	6:0:692:GLN:N	2.47	0.43
1:1:210:TRP:O	1:1:213:ARG:N	2.52	0.43
1:1:288:PHE:O	1:1:292:LEU:HB2	2.19	0.43
1:1:374:ILE:O	1:1:378:MET:HG2	2.19	0.43
3:7:303:ARG:HA	3:7:320:ASN:C	2.44	0.43
3:7:459:MET:HG2	3:7:470:SER:HB2	2.00	0.43
5:2:148:HIS:O	5:2:152:GLY:N	2.45	0.43
6:0:237:ALA:N	6:0:460:SER:OG	2.45	0.43
7:6:243:ASP:HA	7:6:244:PRO:HD3	1.91	0.43
1:1:254:GLU:H	1:1:254:GLU:CD	2.25	0.43
2:4:218:SER:HA	2:4:237:HIS:NE2	2.33	0.43
3:7:383:ILE:O	3:7:534:LYS:HA	2.19	0.43
3:7:449:GLU:H	3:7:449:GLU:HG2	1.54	0.43
3:7:460:VAL:HG12	3:7:501:VAL:HG11	2.01	0.43
3:7:584:ASN:O	3:7:587:LYS:HB3	2.18	0.43
3:7:743:GLU:O	3:7:748:LEU:HD11	2.19	0.43
6:0:104:ARG:HH22	6:0:171:LEU:HB2	1.83	0.43
6:0:223:SER:O	6:0:226:VAL:HG22	2.19	0.43
6:0:333:SER:HB2	6:0:337:ARG:NH1	2.34	0.43
6:0:620:VAL:C	6:0:621:LEU:HD12	2.44	0.43
7:6:432:CYS:N	7:6:454:CYS:SG	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:177:LEU:HD12	2:4:211:ASP:O	2.17	0.43
2:4:197:MET:HE3	2:4:197:MET:HB2	1.57	0.43
3:7:577:ARG:HA	3:7:580:LEU:HB2	2.01	0.43
3:7:610:ASP:HB3	3:7:656:LYS:HB2	2.00	0.43
5:2:273:LYS:O	5:2:277:MET:HG2	2.19	0.43
6:0:253:THR:HG22	6:0:255:ASP:H	1.84	0.43
6:0:553:MET:HB2	6:0:553:MET:HE2	1.53	0.43
6:0:685:ARG:HB3	6:0:689:LYS:NZ	2.34	0.43
7:6:137:LEU:HD23	7:6:137:LEU:HA	1.79	0.43
7:6:137:LEU:HG	7:6:204:PRO:HG2	2.01	0.43
7:6:152:TYR:CG	7:6:297:LEU:HD21	2.54	0.43
1:1:273:ASN:HA	1:1:276:LYS:NZ	2.34	0.42
3:7:219:SER:O	3:7:336:PRO:HG2	2.19	0.42
3:7:425:LEU:HA	3:7:425:LEU:HD13	1.82	0.42
3:7:519:ARG:NE	3:7:521:ASP:HB2	2.34	0.42
4:5:17:LYS:HG3	4:5:40:LEU:HD21	2.00	0.42
5:2:273:LYS:O	5:2:276:LEU:HB3	2.19	0.42
6:0:265:ASN:O	6:0:269:GLU:HG2	2.19	0.42
6:0:419:ILE:HG23	6:0:436:ARG:HB3	2.00	0.42
6:0:494:PRO:HA	6:0:679:MET:O	2.19	0.42
6:0:507:SER:HG	6:0:508:SER:H	1.67	0.42
6:0:594:ARG:HB3	6:0:594:ARG:HH11	1.83	0.42
6:0:706:LEU:HD13	6:0:706:LEU:HA	1.90	0.42
7:6:293:ASP:OD1	7:6:295:THR:N	2.44	0.42
1:1:197:GLU:HA	1:1:201:ASN:OD1	2.19	0.42
1:1:321:PHE:O	1:1:324:LYS:HG2	2.19	0.42
2:4:216:GLY:O	2:4:237:HIS:HE1	2.02	0.42
2:4:244:LEU:O	2:4:245:ILE:C	2.61	0.42
5:2:286:ARG:O	5:2:286:ARG:NE	2.52	0.42
6:0:533:THR:OG1	6:0:567:LYS:NZ	2.52	0.42
2:4:305:CYS:O	2:4:307:ALA:N	2.52	0.42
3:7:593:PHE:O	3:7:596:GLN:HG2	2.20	0.42
3:7:701:PHE:HB2	3:7:704:PHE:CE1	2.54	0.42
5:2:80:SER:O	5:2:84:LEU:HD23	2.19	0.42
6:0:154:GLU:OE1	6:0:154:GLU:N	2.52	0.42
6:0:544:TYR:OH	6:0:574:PRO:HD3	2.19	0.42
7:6:126:LEU:O	7:6:169:MET:HA	2.19	0.42
1:1:194:VAL:O	1:1:197:GLU:HG2	2.18	0.42
2:4:137:LYS:O	2:4:140:ILE:HB	2.18	0.42
2:4:137:LYS:HG3	2:4:139:GLN:HG3	2.01	0.42
3:7:551:ASN:HB3	3:7:701:PHE:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:0:143:ARG:O	6:0:147:GLU:HG2	2.20	0.42
6:0:213:LEU:HD12	6:0:213:LEU:HA	1.79	0.42
6:0:289:LEU:HB2	6:0:326:ARG:NH1	2.34	0.42
6:0:394:GLU:HA	6:0:397:THR:HG23	2.01	0.42
6:0:527:VAL:HB	6:0:559:ILE:HD11	2.01	0.42
6:0:709:SER:OG	6:0:710:THR:N	2.52	0.42
1:1:259:ILE:HD13	1:1:263:TYR:CE2	2.50	0.42
1:1:345:ASP:OD2	6:0:112:LYS:HG2	2.19	0.42
1:1:511:ALA:HB2	2:4:264:LYS:HD2	2.02	0.42
2:4:43:GLU:OE2	2:4:240:SER:OG	2.34	0.42
2:4:126:VAL:O	2:4:129:ILE:HG22	2.20	0.42
3:7:581:TYR:CE2	3:7:714:GLN:HB3	2.55	0.42
3:7:750:TYR:CD2	3:7:755:GLU:HB3	2.54	0.42
6:0:97:LEU:HD23	6:0:97:LEU:HA	1.75	0.42
6:0:188:LYS:O	6:0:190:LEU:HD23	2.20	0.42
6:0:424:GLU:H	6:0:432:ASN:HD21	1.67	0.42
6:0:625:ILE:HB	6:0:686:PHE:CE1	2.54	0.42
7:6:107:LYS:HG2	7:6:109:ARG:HH12	1.84	0.42
1:1:270:TYR:OH	1:1:279:LYS:CE	2.65	0.42
1:1:371:THR:O	1:1:374:ILE:HB	2.20	0.42
5:2:72:LEU:HG	5:2:73:GLN:OE1	2.20	0.42
6:0:20:GLU:OE1	6:0:20:GLU:N	2.37	0.42
6:0:53:LEU:HD12	6:0:85:GLU:OE2	2.20	0.42
6:0:383:LEU:O	6:0:387:THR:HG23	2.19	0.42
7:6:220:LEU:HD12	7:6:220:LEU:HA	1.87	0.42
2:4:163:ILE:O	2:4:166:GLU:HG3	2.18	0.42
3:7:611:ASN:OD1	3:7:615:LEU:HB2	2.20	0.42
5:2:394:ASP:OD1	5:2:395:GLN:N	2.46	0.42
5:2:415:LYS:NZ	5:2:434:PRO:HB3	2.35	0.42
6:0:18:TYR:CE2	6:0:673:LYS:HD2	2.54	0.42
6:0:249:SER:OG	6:0:250:LEU:N	2.51	0.42
6:0:409:ILE:HD12	6:0:409:ILE:HA	1.78	0.42
6:0:541:PHE:HE1	6:0:623:ILE:HG13	1.84	0.42
2:4:254:ILE:HD12	2:4:254:ILE:O	2.19	0.42
3:7:365:TYR:HA	3:7:368:LYS:HG2	2.01	0.42
6:0:48:LYS:HE3	6:0:48:LYS:HB3	1.83	0.42
6:0:545:LEU:HA	6:0:545:LEU:HD13	1.79	0.42
1:1:207:SER:HG	1:1:208:GLU:H	1.68	0.42
1:1:339:LEU:HD12	1:1:342:ASN:HD22	1.85	0.42
5:2:39:LEU:O	5:2:44:LYS:HE3	2.20	0.42
6:0:312:LEU:HB3	6:0:315:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:224:VAL:O	7:6:230:ARG:NH2	2.53	0.42
1:1:259:ILE:O	1:1:263:TYR:N	2.40	0.42
1:1:274:VAL:N	1:1:275:PRO:HD2	2.35	0.42
2:4:66:ALA:HB2	2:4:118:PHE:HZ	1.85	0.42
2:4:273:ARG:CG	2:4:273:ARG:HH21	2.33	0.42
3:7:346:ASP:OD2	3:7:349:ASN:ND2	2.53	0.42
3:7:392:LYS:HG2	3:7:513:LEU:HD13	2.01	0.42
5:2:22:GLN:NE2	5:2:84:LEU:O	2.53	0.42
6:0:53:LEU:HD23	6:0:53:LEU:HA	1.69	0.42
6:0:136:MET:HE2	6:0:154:GLU:HG2	2.01	0.42
7:6:141:LEU:HD23	7:6:145:ARG:HG2	2.02	0.42
7:6:246:ASP:OD1	7:6:248:HIS:N	2.53	0.42
1:1:262:ASN:HB3	1:1:263:TYR:CE2	2.55	0.41
1:1:344:GLN:C	1:1:347:PRO:HD2	2.45	0.41
2:4:228:THR:OG1	2:4:234:VAL:N	2.52	0.41
2:4:273:ARG:HD2	2:4:273:ARG:HA	1.74	0.41
3:7:411:CYS:HB3	3:7:417:VAL:HG22	2.01	0.41
6:0:505:ALA:HB1	6:0:684:ARG:HB3	2.02	0.41
6:0:514:ASN:ND2	6:0:553:MET:HG2	2.34	0.41
1:1:253:ARG:HA	1:1:256:ILE:HG12	2.01	0.41
2:4:175:ARG:HA	2:4:208:CYS:SG	2.60	0.41
3:7:341:TYR:HE1	3:7:508:HIS:HB3	1.85	0.41
3:7:680:ARG:C	3:7:682:GLN:H	2.28	0.41
5:2:472:SER:HA	5:2:481:LEU:HD12	2.01	0.41
6:0:553:MET:O	6:0:556:THR:HB	2.21	0.41
1:1:382:SER:OG	6:0:570:LEU:HD21	2.20	0.41
3:7:382:GLY:HA2	3:7:532:GLY:HA3	2.03	0.41
3:7:573:THR:HA	3:7:577:ARG:NH2	2.35	0.41
5:2:71:LYS:O	5:2:74:PHE:HB3	2.20	0.41
5:2:486:ASP:O	5:2:489:LYS:NZ	2.33	0.41
6:0:471:ARG:HH22	6:0:647:ARG:H	1.69	0.41
6:0:500:GLY:HA3	6:0:521:ASN:ND2	2.36	0.41
6:0:568:LEU:HA	6:0:568:LEU:HD12	1.66	0.41
1:1:184:LEU:HA	1:1:184:LEU:HD12	1.66	0.41
2:4:131:LYS:HE3	2:4:131:LYS:HB3	1.86	0.41
5:2:66:VAL:HG12	5:2:67:ASN:O	2.20	0.41
6:0:27:ASP:OD1	6:0:27:ASP:N	2.53	0.41
1:1:259:ILE:HG23	1:1:263:TYR:CD2	2.56	0.41
1:1:552:MET:O	1:1:556:THR:HG22	2.20	0.41
2:4:254:ILE:CG2	5:2:45:PHE:CD2	3.04	0.41
3:7:497:MET:SD	3:7:498:PHE:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:361:SER:HA	5:2:364:VAL:HG12	2.02	0.41
6:0:444:ILE:HD13	6:0:444:ILE:HA	1.83	0.41
3:7:306:GLU:OE2	3:7:346:ASP:HB2	2.21	0.41
3:7:341:TYR:CE2	3:7:343:PHE:HB3	2.55	0.41
3:7:495:ALA:HB1	3:7:527:LEU:HD21	2.01	0.41
6:0:83:LEU:HD23	6:0:83:LEU:HA	1.56	0.41
6:0:158:TYR:HB3	6:0:190:LEU:C	2.45	0.41
6:0:227:SER:HA	6:0:230:SER:OG	2.21	0.41
6:0:418:LEU:HD23	6:0:418:LEU:HA	1.85	0.41
1:1:257:LEU:HA	1:1:260:PHE:CD2	2.56	0.41
3:7:346:ASP:HB3	3:7:405:LYS:HE2	2.03	0.41
3:7:417:VAL:HG21	3:7:456:THR:HB	2.02	0.41
4:5:36:ASP:CG	4:5:38:THR:H	2.29	0.41
5:2:53:ASN:OD1	5:2:53:ASN:N	2.53	0.41
6:0:50:VAL:O	6:0:54:SER:OG	2.24	0.41
6:0:322:PRO:O	6:0:325:ILE:HG13	2.20	0.41
6:0:695:LYS:HG2	6:0:699:GLN:HE21	1.85	0.41
1:1:270:TYR:HE2	1:1:284:TRP:NE1	2.19	0.41
3:7:438:PHE:CG	3:7:473:VAL:HG21	2.56	0.41
3:7:498:PHE:CE2	3:7:527:LEU:HD22	2.56	0.41
5:2:450:ARG:HG3	5:2:451:VAL:HG23	2.03	0.41
6:0:570:LEU:HD23	6:0:570:LEU:HA	1.83	0.41
6:0:710:THR:O	6:0:714:ILE:HG12	2.21	0.41
6:0:718:LYS:HE3	6:0:718:LYS:HB2	1.89	0.41
7:6:143:PRO:HB2	7:6:147:ALA:HB3	2.02	0.41
7:6:332:THR:C	7:6:334:THR:H	2.29	0.41
1:1:281:PRO:HD2	1:1:282:GLU:OE2	2.20	0.41
1:1:389:LEU:HA	1:1:389:LEU:HD23	1.60	0.41
2:4:33:ALA:HB3	2:4:36:LEU:CB	2.50	0.41
2:4:62:ASN:OD1	2:4:118:PHE:HB3	2.20	0.41
2:4:87:TYR:HB3	2:4:88:PRO:HD3	2.02	0.41
2:4:118:PHE:N	2:4:118:PHE:CD1	2.89	0.41
2:4:228:THR:O	2:4:233:GLY:N	2.51	0.41
2:4:233:GLY:O	2:4:263:VAL:HG11	2.21	0.41
2:4:297:SER:C	2:4:299:ILE:H	2.29	0.41
3:7:469:ASP:O	3:7:473:VAL:HG23	2.20	0.41
3:7:476:PHE:CE2	3:7:482:TRP:HZ2	2.39	0.41
3:7:553:GLN:O	3:7:705:PHE:N	2.44	0.41
4:5:15:SER:O	4:5:19:LEU:HG	2.21	0.41
5:2:58:PRO:HG2	5:2:61:ASP:OD2	2.21	0.41
5:2:350:TYR:H	5:2:407:GLN:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:410:ARG:HE	5:2:410:ARG:HB2	1.71	0.41
6:0:241:ASP:OD1	6:0:242:ASN:N	2.53	0.41
6:0:583:LEU:HA	6:0:583:LEU:HD12	1.79	0.41
6:0:654:LEU:HD13	6:0:654:LEU:HA	1.90	0.41
7:6:145:ARG:O	7:6:149:ILE:HG12	2.21	0.41
2:4:271:ASP:HB3	2:4:273:ARG:NH2	2.36	0.41
3:7:564:GLU:HB2	3:7:760:LEU:HD13	2.03	0.41
5:2:14:LEU:HD13	5:2:14:LEU:HA	1.78	0.41
6:0:37:ASN:HA	6:0:456:VAL:O	2.21	0.41
6:0:78:GLU:HA	6:0:81:LYS:HB2	2.03	0.41
6:0:113:ASN:O	6:0:114:LEU:HD23	2.21	0.41
6:0:124:ARG:HD3	6:0:124:ARG:HA	1.81	0.41
6:0:136:MET:HE3	6:0:136:MET:HB2	1.87	0.41
6:0:408:LEU:HB3	6:0:437:PHE:HE2	1.86	0.41
7:6:120:ARG:HB3	7:6:307:PRO:HB2	2.03	0.41
7:6:161:PHE:CG	7:6:189:PRO:HG3	2.56	0.41
7:6:308:LEU:HD23	7:6:308:LEU:H	1.86	0.41
7:6:363:CYS:SG	7:6:366:CYS:N	2.83	0.41
2:4:137:LYS:O	2:4:141:GLU:HG3	2.21	0.40
2:4:305:CYS:H	2:4:312:PHE:HE1	1.69	0.40
3:7:664:LEU:CB	3:7:692:ARG:HG3	2.52	0.40
6:0:408:LEU:HA	6:0:408:LEU:HD23	1.72	0.40
1:1:205:PRO:HA	1:1:206:PRO:HD3	1.95	0.40
2:4:291:VAL:O	7:6:383:LEU:HD11	2.21	0.40
3:7:265:PRO:O	3:7:269:LEU:HG	2.21	0.40
3:7:384:ILE:HG12	3:7:536:TYR:H	1.86	0.40
3:7:484:PHE:C	3:7:485:ILE:HD12	2.46	0.40
3:7:627:ILE:HD13	3:7:636:ARG:HG3	2.03	0.40
4:5:36:ASP:CG	4:5:39:HIS:HD1	2.28	0.40
5:2:356:GLN:NE2	5:2:360:LEU:HD11	2.36	0.40
6:0:131:GLU:OE1	6:0:132:LYS:N	2.55	0.40
6:0:341:TYR:CE1	6:0:366:LEU:HD12	2.56	0.40
6:0:377:CYS:SG	6:0:406:ALA:HB3	2.62	0.40
6:0:745:ILE:H	6:0:745:ILE:HG13	1.51	0.40
6:0:754:GLN:H	6:0:754:GLN:HG3	1.64	0.40
2:4:304:LYS:O	2:4:305:CYS:C	2.64	0.40
3:7:256:ILE:O	3:7:316:PHE:HB2	2.21	0.40
5:2:134:LEU:C	5:2:136:ASP:H	2.29	0.40
6:0:271:ILE:HA	6:0:274:VAL:HG22	2.03	0.40
6:0:493:LEU:HD11	6:0:720:PHE:HB2	2.03	0.40
7:6:227:HIS:CD2	7:6:320:VAL:HG11	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:347:TYR:O	7:6:355:LYS:HA	2.20	0.40
1:1:370:GLY:C	1:1:372:VAL:H	2.28	0.40
2:4:196:ILE:O	2:4:199:CYS:HB2	2.22	0.40
3:7:321:GLU:HG3	3:7:322:SER:OG	2.20	0.40
3:7:736:ILE:HG22	3:7:739:LEU:HD13	2.03	0.40
5:2:63:ASP:HA	5:2:74:PHE:CE2	2.55	0.40
6:0:385:VAL:O	6:0:389:GLU:N	2.55	0.40
1:1:236:THR:C	1:1:238:LYS:N	2.79	0.40
5:2:10:VAL:HG21	5:2:201:TRP:CZ2	2.56	0.40
5:2:481:LEU:HD13	5:2:484:LYS:HG2	2.04	0.40
6:0:24:TYR:O	6:0:28:ILE:HG22	2.22	0.40
6:0:158:TYR:HB2	6:0:191:CYS:HB3	2.04	0.40
6:0:294:HIS:NE2	6:0:297:ASP:HB3	2.35	0.40
6:0:519:VAL:HG11	6:0:553:MET:SD	2.62	0.40
7:6:132:CYS:O	7:6:175:ARG:HG2	2.21	0.40
7:6:287:PHE:N	7:6:287:PHE:CD1	2.89	0.40
7:6:449:HIS:ND1	7:6:449:HIS:N	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	357/642 (56%)	280 (78%)	40 (11%)	37 (10%)	0	7
2	4	280/338 (83%)	209 (75%)	66 (24%)	5 (2%)	6	34
3	7	630/843 (75%)	566 (90%)	63 (10%)	1 (0%)	43	74
4	5	64/72 (89%)	58 (91%)	6 (9%)	0	100	100
5	2	456/513 (89%)	384 (84%)	72 (16%)	0	100	100
6	0	752/778 (97%)	632 (84%)	118 (16%)	2 (0%)	36	69
7	6	349/461 (76%)	284 (81%)	59 (17%)	6 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2888/3647 (79%)	2413 (84%)	424 (15%)	51 (2%)	9	34

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	230	PRO
1	1	236	THR
1	1	239	PRO
1	1	338	ASP
1	1	344	GLN
1	1	354	PRO
1	1	518	ASN
2	4	255	ASP
7	6	411	PRO
7	6	425	SER
1	1	225	SER
1	1	240	VAL
1	1	241	ALA
1	1	247	VAL
1	1	277	ASN
1	1	301	ILE
1	1	307	GLY
1	1	352	ASN
1	1	389	LEU
1	1	492	ASN
1	1	516	HIS
2	4	115	TYR
1	1	235	SER
1	1	244	GLU
1	1	246	LYS
1	1	281	PRO
1	1	493	ASN
1	1	494	GLU
1	1	517	ASN
3	7	659	ASP
7	6	417	LYS
7	6	422	LEU
1	1	243	SER
1	1	309	VAL
1	1	353	ARG
1	1	467	GLN
1	1	495	VAL

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Mol	Chain	Res	Type
2	4	114	MET
6	0	228	LYS
7	6	412	ILE
7	6	415	ASN
1	1	487	ASN
6	0	172	PRO
1	1	232	ASN
1	1	238	LYS
1	1	249	VAL
1	1	484	LEU
2	4	290	SER
1	1	280	GLU
2	4	256	PRO
1	1	491	PRO

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	1	169/589 (29%)	144 (85%)	25 (15%)	3	16
2	4	198/300 (66%)	163 (82%)	35 (18%)	2	12
3	7	414/737 (56%)	386 (93%)	28 (7%)	14	41
4	5	53/66 (80%)	52 (98%)	1 (2%)	50	66
5	2	258/468 (55%)	222 (86%)	36 (14%)	3	17
6	0	686/707 (97%)	587 (86%)	99 (14%)	3	17
7	6	247/418 (59%)	204 (83%)	43 (17%)	2	12
All	All	2025/3285 (62%)	1758 (87%)	267 (13%)	6	19

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	185	LEU
1	1	198	THR
1	1	201	ASN

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Mol	Chain	Res	Type
1	1	214	ILE
1	1	216	LEU
1	1	263	TYR
1	1	266	VAL
1	1	276	LYS
1	1	279	LYS
1	1	280	GLU
1	1	282	GLU
1	1	287	PHE
1	1	315	LEU
1	1	329	LEU
1	1	339	LEU
1	1	346	ASP
1	1	372	VAL
1	1	378	MET
1	1	382	SER
1	1	389	LEU
1	1	516	HIS
1	1	551	ARG
1	1	553	LEU
1	1	558	CYS
1	1	597	PHE
2	4	26	LEU
2	4	27	THR
2	4	30	ILE
2	4	86	LEU
2	4	134	GLU
2	4	136	GLU
2	4	137	LYS
2	4	149	LEU
2	4	162	ARG
2	4	163	ILE
2	4	176	LEU
2	4	180	THR
2	4	197	MET
2	4	204	THR
2	4	210	ILE
2	4	211	ASP
2	4	212	VAL
2	4	228	THR
2	4	234	VAL
2	4	236	LEU

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Mol	Chain	Res	Type
2	4	244	LEU
2	4	248	LEU
2	4	252	MET
2	4	254	ILE
2	4	258	LEU
2	4	260	PRO
2	4	261	ILE
2	4	263	VAL
2	4	264	LYS
2	4	272	PHE
2	4	273	ARG
2	4	274	THR
2	4	288	ILE
2	4	293	LEU
2	4	297	SER
3	7	342	ASP
3	7	356	LEU
3	7	357	LYS
3	7	385	VAL
3	7	393	THR
3	7	444	GLU
3	7	445	MET
3	7	449	GLU
3	7	477	LEU
3	7	485	ILE
3	7	490	VAL
3	7	514	THR
3	7	518	VAL
3	7	530	LEU
3	7	564	GLU
3	7	582	ILE
3	7	583	MET
3	7	612	VAL
3	7	620	LEU
3	7	664	LEU
3	7	677	TYR
3	7	680	ARG
3	7	683	GLU
3	7	692	ARG
3	7	698	ASP
3	7	701	PHE
3	7	712	ASP

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Mol	Chain	Res	Type
3	7	716	MET
4	5	54	LEU
5	2	8	HIS
5	2	10	VAL
5	2	11	THR
5	2	14	LEU
5	2	16	GLU
5	2	17	ILE
5	2	27	THR
5	2	28	SER
5	2	60	LEU
5	2	61	ASP
5	2	63	ASP
5	2	67	ASN
5	2	84	LEU
5	2	88	ILE
5	2	100	LEU
5	2	112	LEU
5	2	201	TRP
5	2	208	LEU
5	2	279	THR
5	2	286	ARG
5	2	348	TYR
5	2	352	ASN
5	2	371	VAL
5	2	383	ILE
5	2	387	LEU
5	2	407	GLN
5	2	410	ARG
5	2	411	LEU
5	2	413	GLU
5	2	416	LEU
5	2	432	VAL
5	2	450	ARG
5	2	476	GLN
5	2	480	VAL
5	2	481	LEU
5	2	486	ASP
6	0	6	ASP
6	0	11	LEU
6	0	17	ILE
6	0	28	ILE

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Mol	Chain	Res	Type
6	0	32	LEU
6	0	34	VAL
6	0	39	ILE
6	0	46	THR
6	0	48	LYS
6	0	66	HIS
6	0	72	CYS
6	0	80	GLU
6	0	109	THR
6	0	110	SER
6	0	124	ARG
6	0	127	THR
6	0	130	ASP
6	0	131	GLU
6	0	148	ASP
6	0	155	LEU
6	0	157	GLU
6	0	162	LEU
6	0	170	TYR
6	0	173	LYS
6	0	190	LEU
6	0	196	VAL
6	0	198	ARG
6	0	206	ILE
6	0	207	ILE
6	0	208	TYR
6	0	218	ILE
6	0	221	ARG
6	0	222	VAL
6	0	227	SER
6	0	231	ILE
6	0	239	ASN
6	0	248	LEU
6	0	249	SER
6	0	254	THR
6	0	255	ASP
6	0	273	GLU
6	0	280	GLN
6	0	284	ASP
6	0	290	VAL
6	0	298	ILE
6	0	312	LEU

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Mol	Chain	Res	Type
6	0	318	THR
6	0	329	GLU
6	0	338	LEU
6	0	350	HIS
6	0	355	THR
6	0	379	GLU
6	0	382	SER
6	0	383	LEU
6	0	413	GLU
6	0	417	LEU
6	0	438	THR
6	0	462	THR
6	0	477	THR
6	0	486	THR
6	0	487	LEU
6	0	498	THR
6	0	506	ILE
6	0	512	ILE
6	0	515	ASP
6	0	533	THR
6	0	537	MET
6	0	538	VAL
6	0	539	VAL
6	0	545	LEU
6	0	556	THR
6	0	560	LEU
6	0	563	VAL
6	0	568	LEU
6	0	573	THR
6	0	597	ILE
6	0	598	LEU
6	0	599	LEU
6	0	614	HIS
6	0	620	VAL
6	0	625	ILE
6	0	639	LEU
6	0	649	ARG
6	0	651	ASN
6	0	654	LEU
6	0	657	ASP
6	0	659	MET
6	0	674	ASP

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Mol	Chain	Res	Type
6	0	680	VAL
6	0	683	ASP
6	0	705	ASP
6	0	710	THR
6	0	711	ASP
6	0	715	SER
6	0	721	LEU
6	0	729	ASP
6	0	741	TYR
6	0	745	ILE
6	0	747	HIS
7	6	116	THR
7	6	118	TYR
7	6	119	GLN
7	6	125	SER
7	6	136	MET
7	6	150	ILE
7	6	158	HIS
7	6	161	PHE
7	6	164	ASN
7	6	166	ILE
7	6	185	VAL
7	6	191	ASP
7	6	194	ASP
7	6	202	GLN
7	6	214	LEU
7	6	222	LEU
7	6	243	ASP
7	6	254	LEU
7	6	263	VAL
7	6	267	SER
7	6	274	LYS
7	6	280	THR
7	6	290	ILE
7	6	292	LEU
7	6	293	ASP
7	6	297	LEU
7	6	306	THR
7	6	310	VAL
7	6	311	ASN
7	6	326	THR
7	6	336	CYS

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Mol	Chain	Res	Type
7	6	352	CYS
7	6	353	HIS
7	6	356	VAL
7	6	363	CYS
7	6	372	LEU
7	6	381	HIS
7	6	382	HIS
7	6	384	MET
7	6	406	CYS
7	6	429	CYS
7	6	444	ILE
7	6	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	258	ASN
2	4	161	ASN
2	4	198	ASN
3	7	539	ASN
3	7	592	GLN
3	7	747	ASN
5	2	90	ASN
5	2	431	GLN
6	0	21	GLN
6	0	60	GLN
6	0	239	ASN
7	6	151	GLN
7	6	190	GLN
7	6	281	ASN
7	6	375	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	SF4	0	801	6	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	0	801	6	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	0	801	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

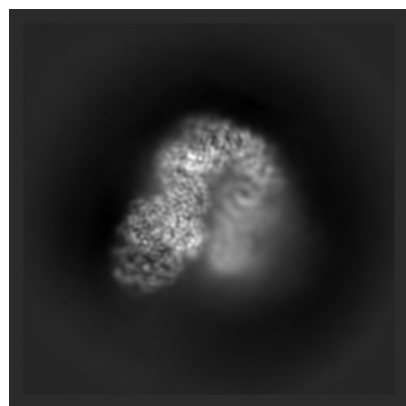
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22587. These allow visual inspection of the internal detail of the map and identification of artifacts.

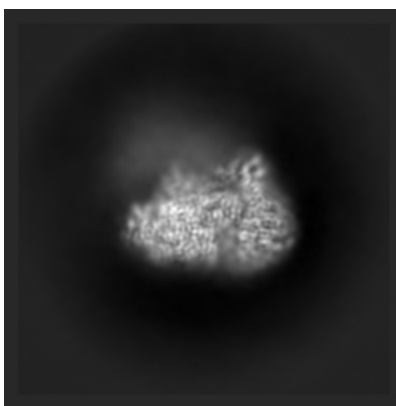
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

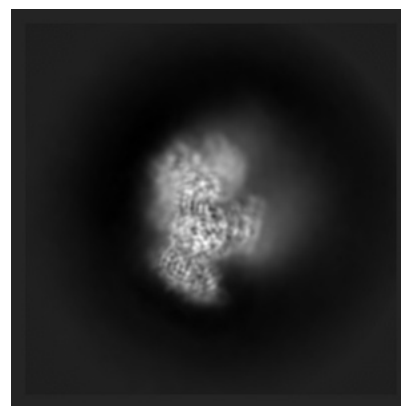
6.1.1 Primary map



X

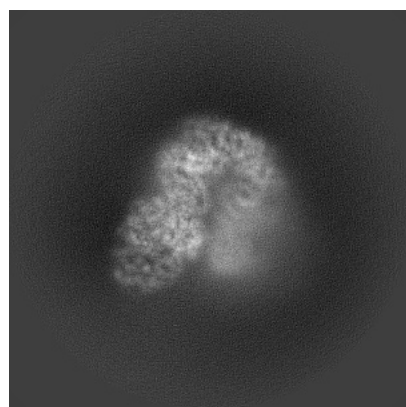


Y

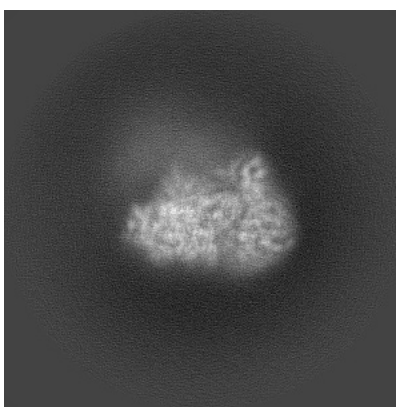


Z

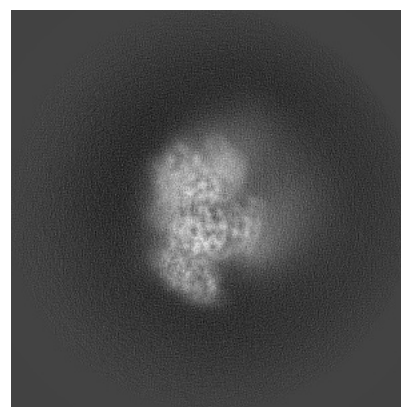
6.1.2 Raw map



X



Y

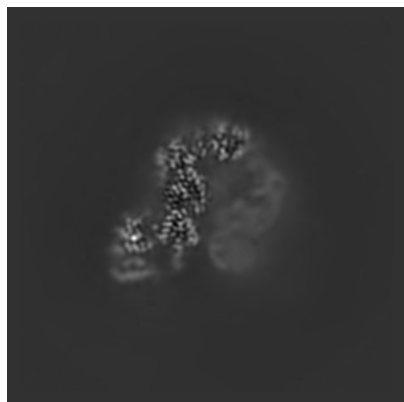


Z

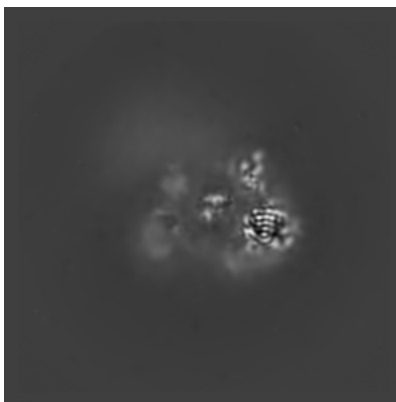
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

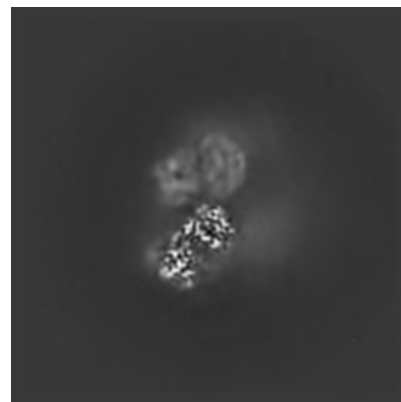
6.2.1 Primary map



X Index: 195

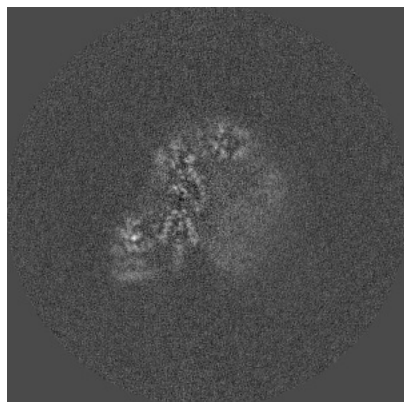


Y Index: 195

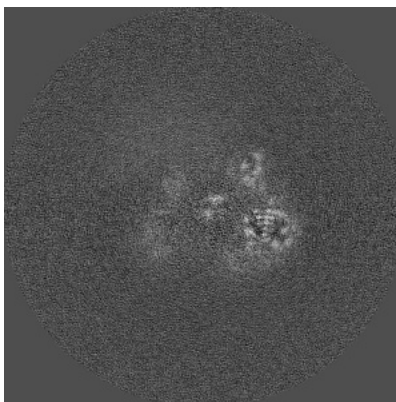


Z Index: 195

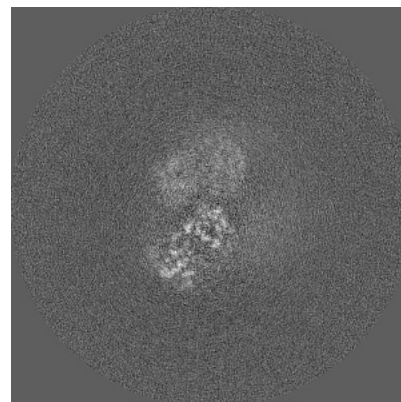
6.2.2 Raw map



X Index: 195



Y Index: 195

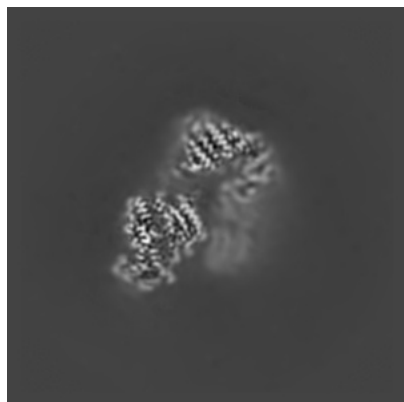


Z Index: 195

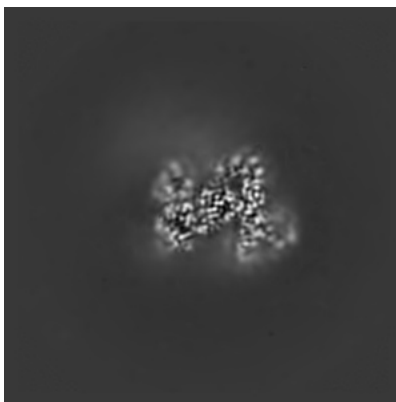
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

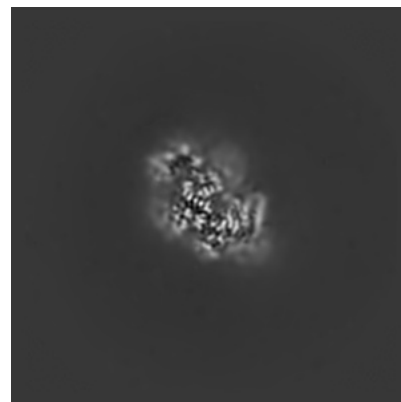
6.3.1 Primary map



X Index: 172

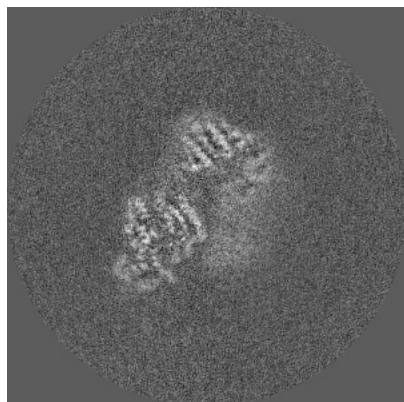


Y Index: 177

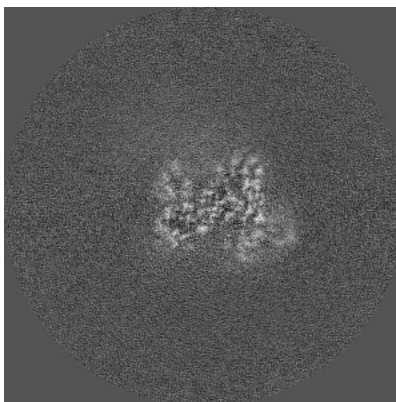


Z Index: 245

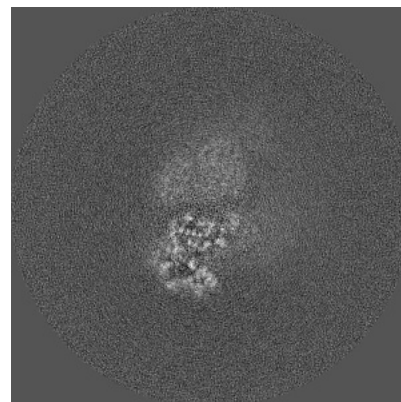
6.3.2 Raw map



X Index: 172



Y Index: 176

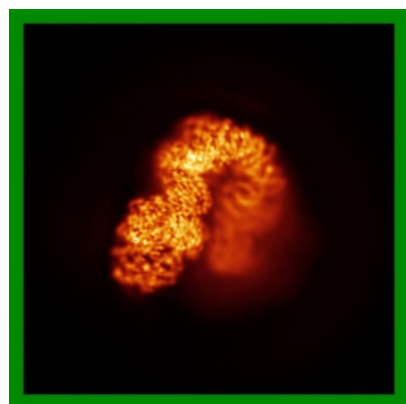


Z Index: 181

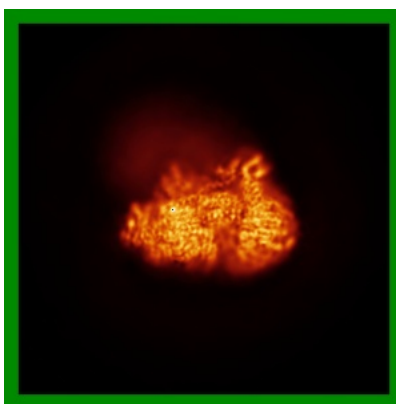
The images above show the largest variance slices of the map in three orthogonal directions.

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

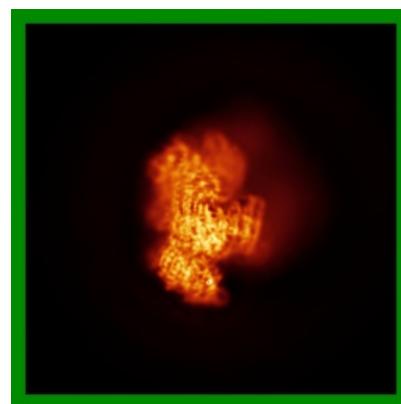
6.4.1 Primary map



X

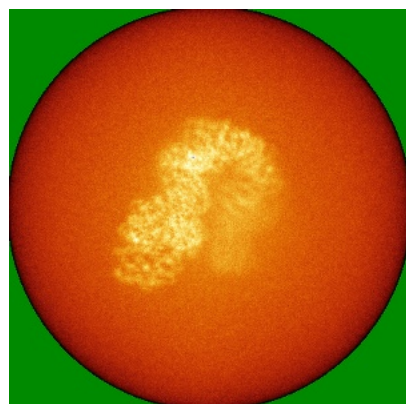


Y

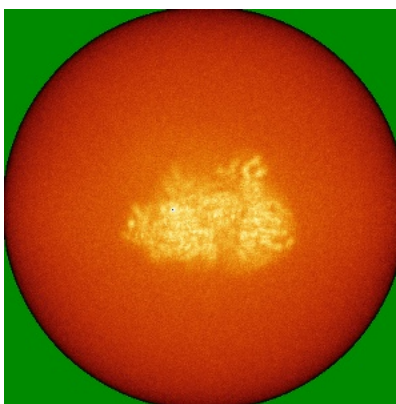


Z

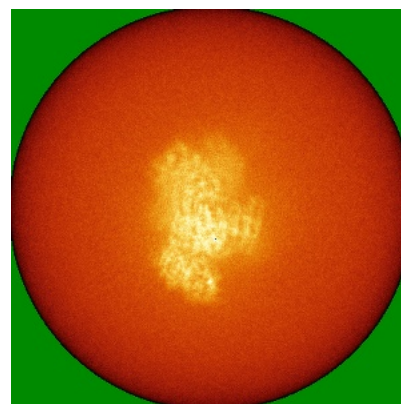
6.4.2 Raw map



X



Y

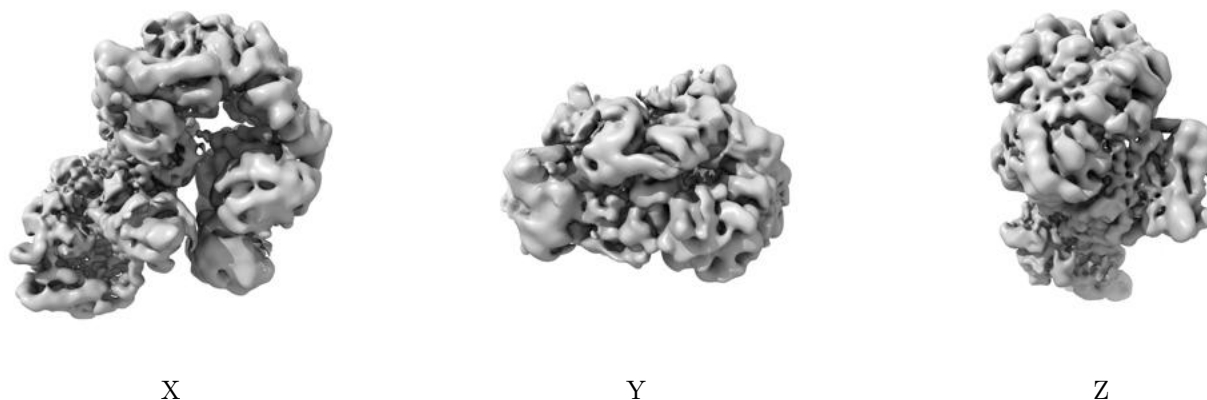


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00593. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

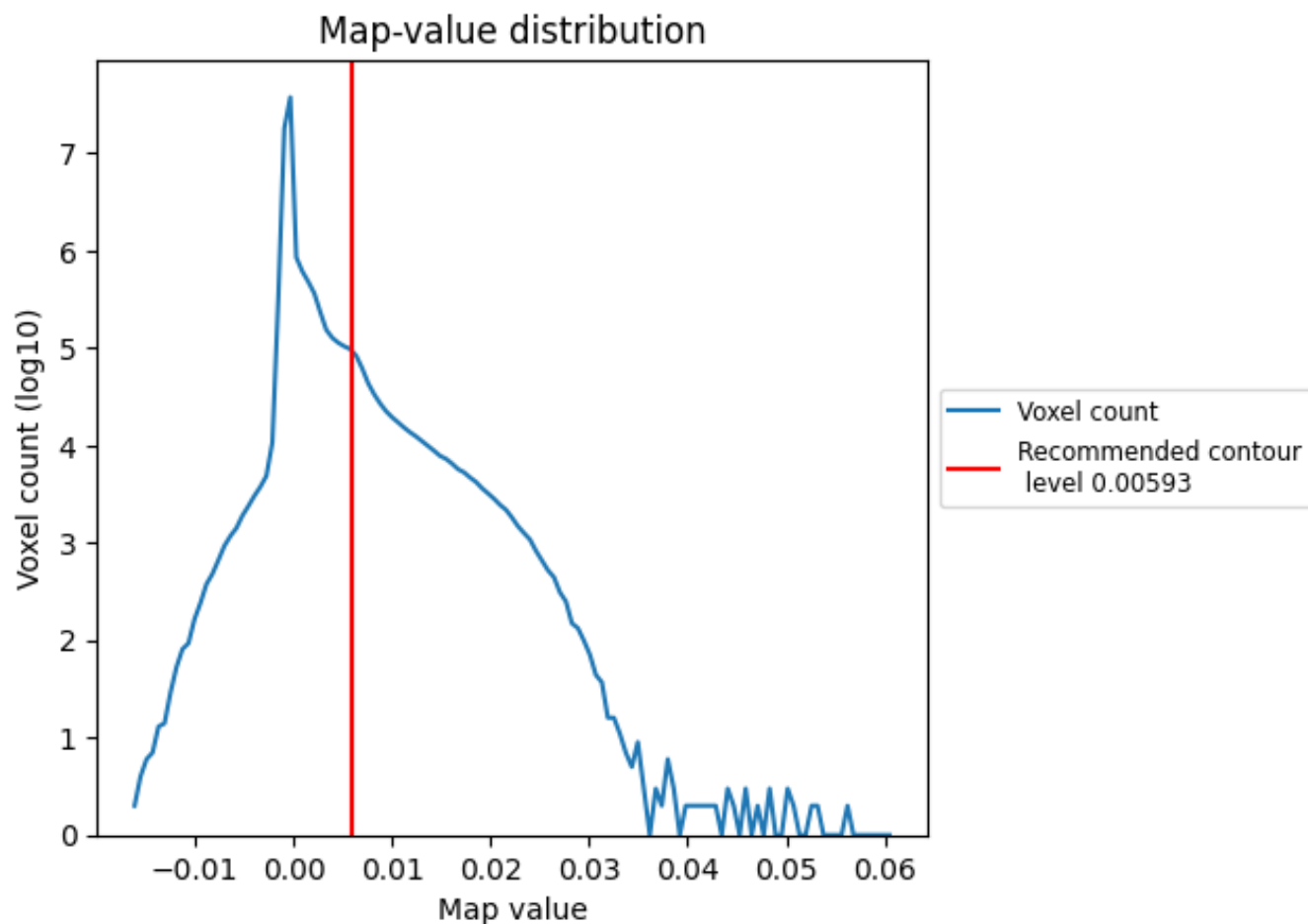
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

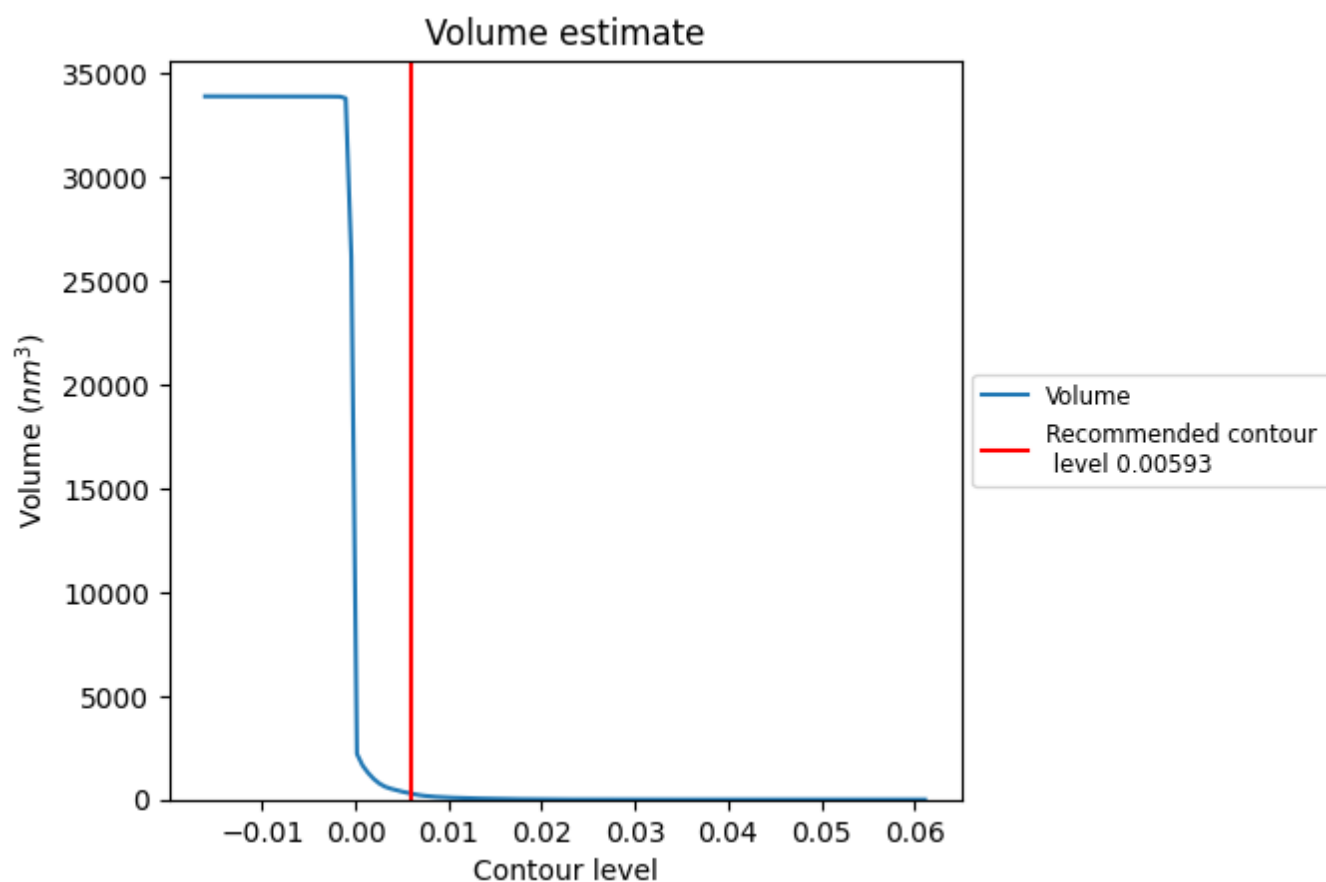
This section contains the results of statistical analysis of the map.

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.

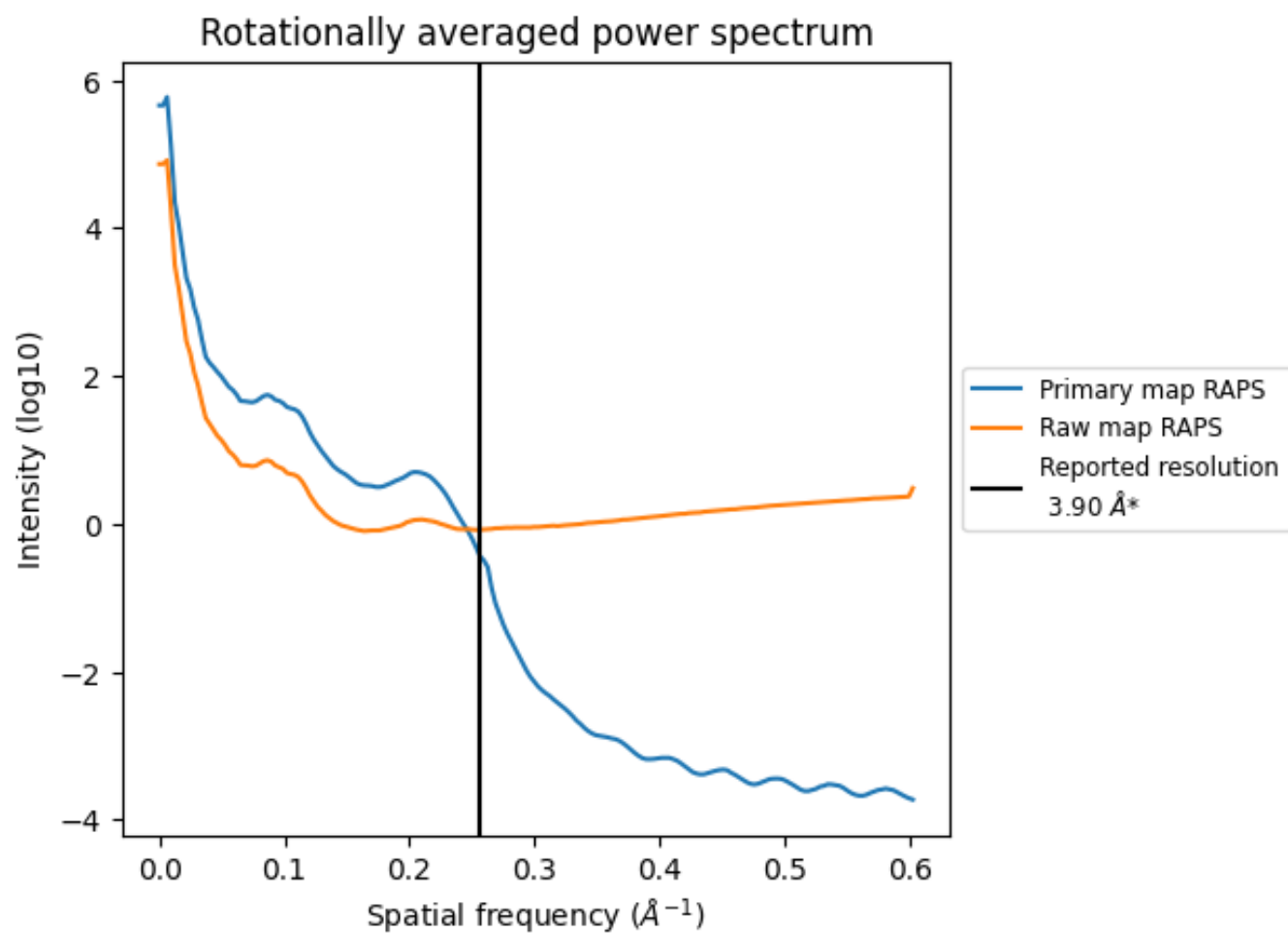
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 295 nm^3 ; this corresponds to an approximate mass of 267 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 ⓘ

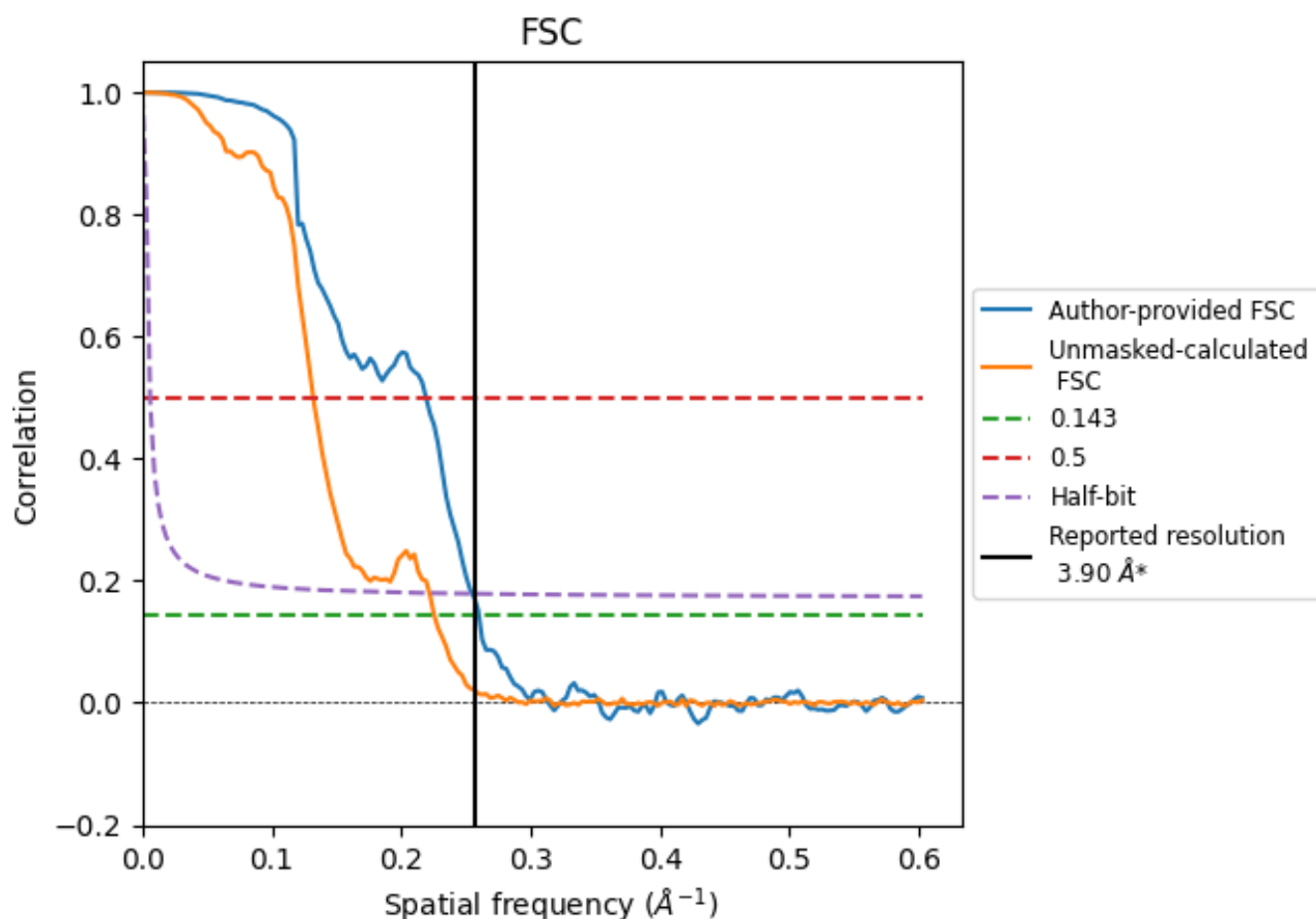


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

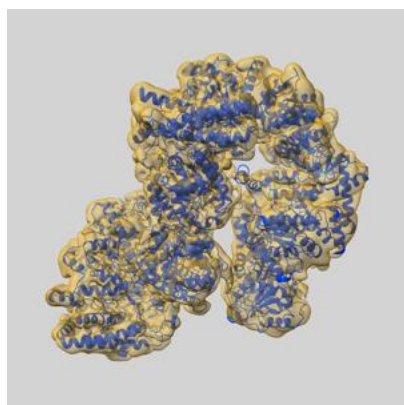
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.84	4.56	3.92
Unmasked-calculated*	4.43	7.56	4.51

*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 4.43 differs from the reported value 3.9 by more than 10 %

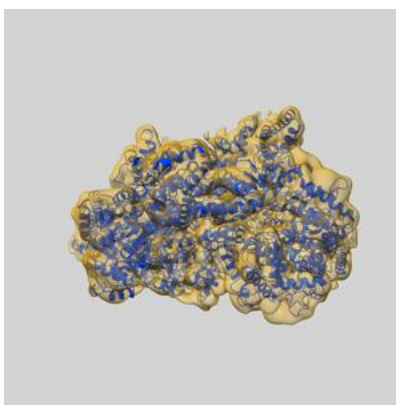
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22587 and PDB model 7K01. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

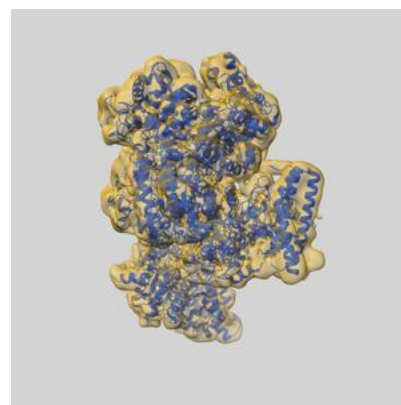
9.1 Map-model overlay [i](#)



X



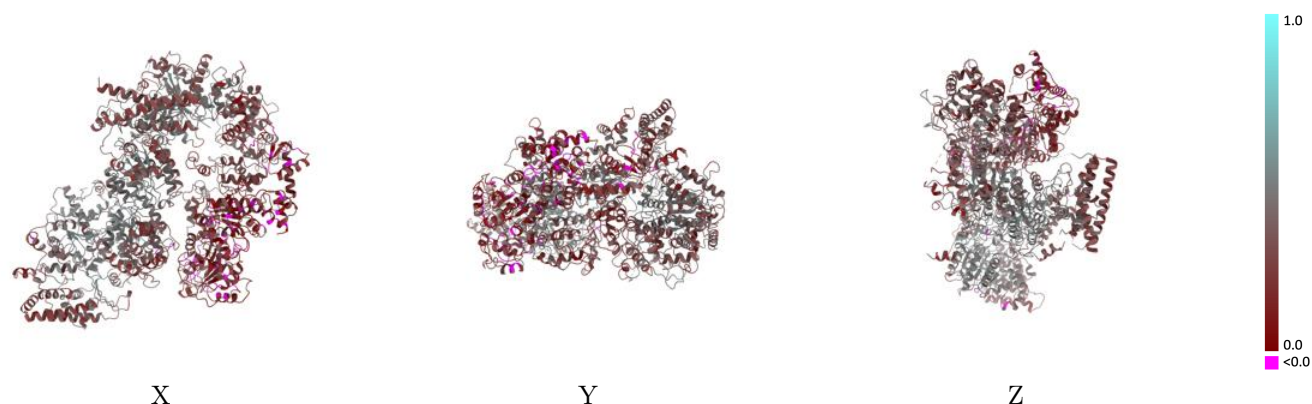
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00593 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

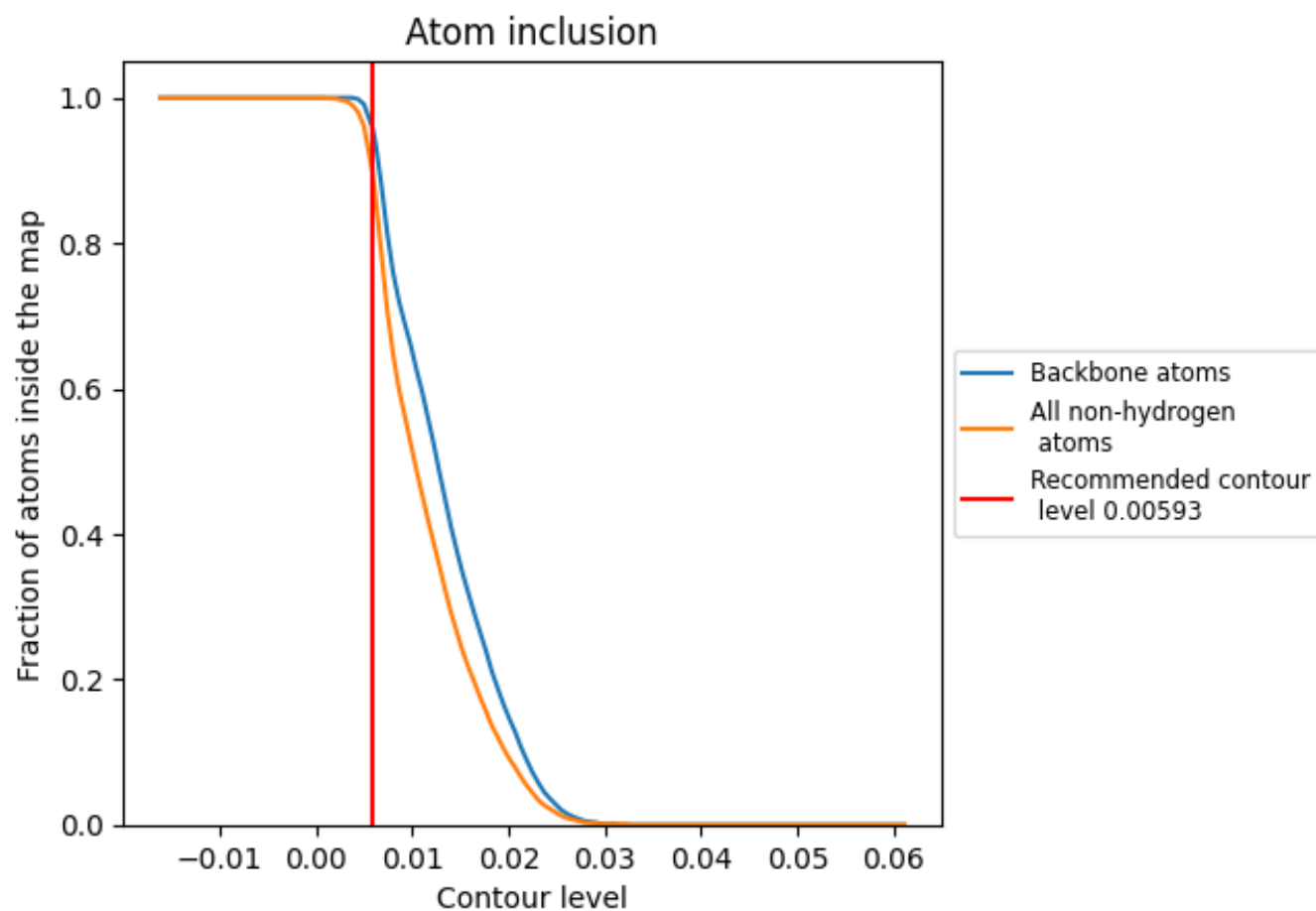


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.00593) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.3310
0	0.9290	0.4060
1	0.9530	0.3410
2	0.9030	0.2950
4	0.9490	0.4190
5	0.7970	0.1820
6	0.9380	0.4500
7	0.7700	0.1570

1.0

0.0

<0.0