



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 04:23 PM EDT

PDB ID : 7M2U / pdb_00007m2u
EMDB ID : EMD-22576
Title : Nucleotide Excision Repair complex TFIIH Rad4-33
Authors : van Eeuwen, T.; Murakami, K.
Deposited on : 2021-03-17
Resolution : 8.20 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:

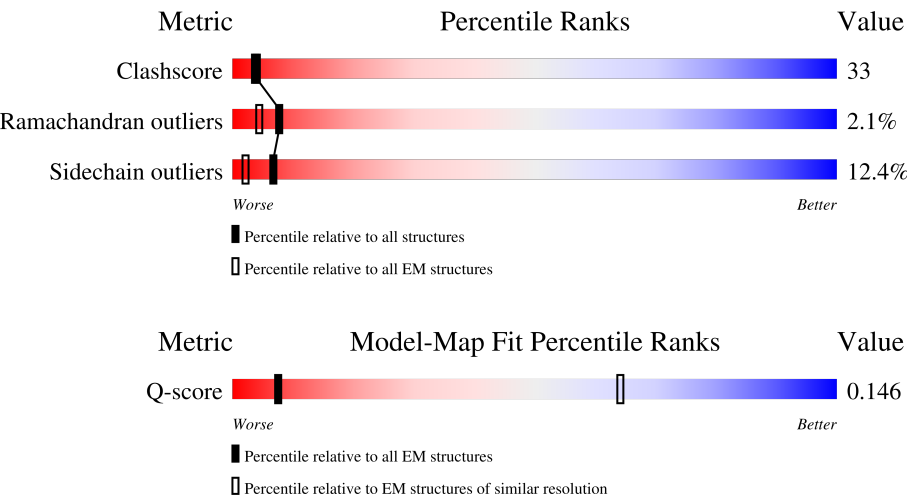
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 8.20 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	361 (7.50 - 8.50)

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	7	843	
2	Y	10	
3	W	14	
4	5	66	

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Mol	Chain	Length	Quality of chain
5	0	778	
6	1	642	
7	4	338	
8	6	461	
9	A	754	
10	E	177	
11	2	513	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	SF4	0	801	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22847 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 DNA repair helicase RAD25.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	7	638	Total	C	N	O	S	0	0
			4478	2739	832	883	24		

- Molecule 2 is a DNA chain called Undamaged DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	10	Total	C	N	O	P	0	0
			202	97	35	60	10		

- Molecule 3 is a DNA chain called Damaged DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	14	Total	C	N	O	P	0	0
			289	137	58	80	14		

- Molecule 4 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

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 DNA repair helicase RAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	0	754	Total	C	N	O	S	0	0
			6108	3891	1032	1147	38		

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	367	Total	C	N	O	S	0	0
			2408	1533	438	430	7		

- Molecule 7 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4	284	Total	C	N	O	S	0	0
			2041	1310	343	376	12		

- Molecule 8 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	351	Total	C	N	O	S	0	0
			2526	1589	454	456	27		

- Molecule 9 is a protein called DNA repair protein RAD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	105	Total	C	N	O	S	0	0
			795	515	135	142	3		

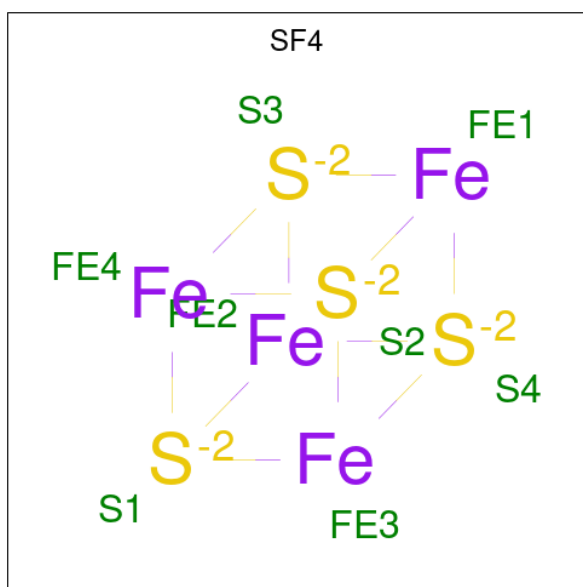
- Molecule 10 is a protein called DNA repair protein RAD33.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	62	Total	C	N	O	S	0	0
			476	301	77	92	6		

- Molecule 11 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	460	Total	C	N	O	S	0	0
			3011	1856	562	584	9		

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
12	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	4	1	Total	Zn	0
			1	1	
13	6	4	Total	Zn	0
			4	4	

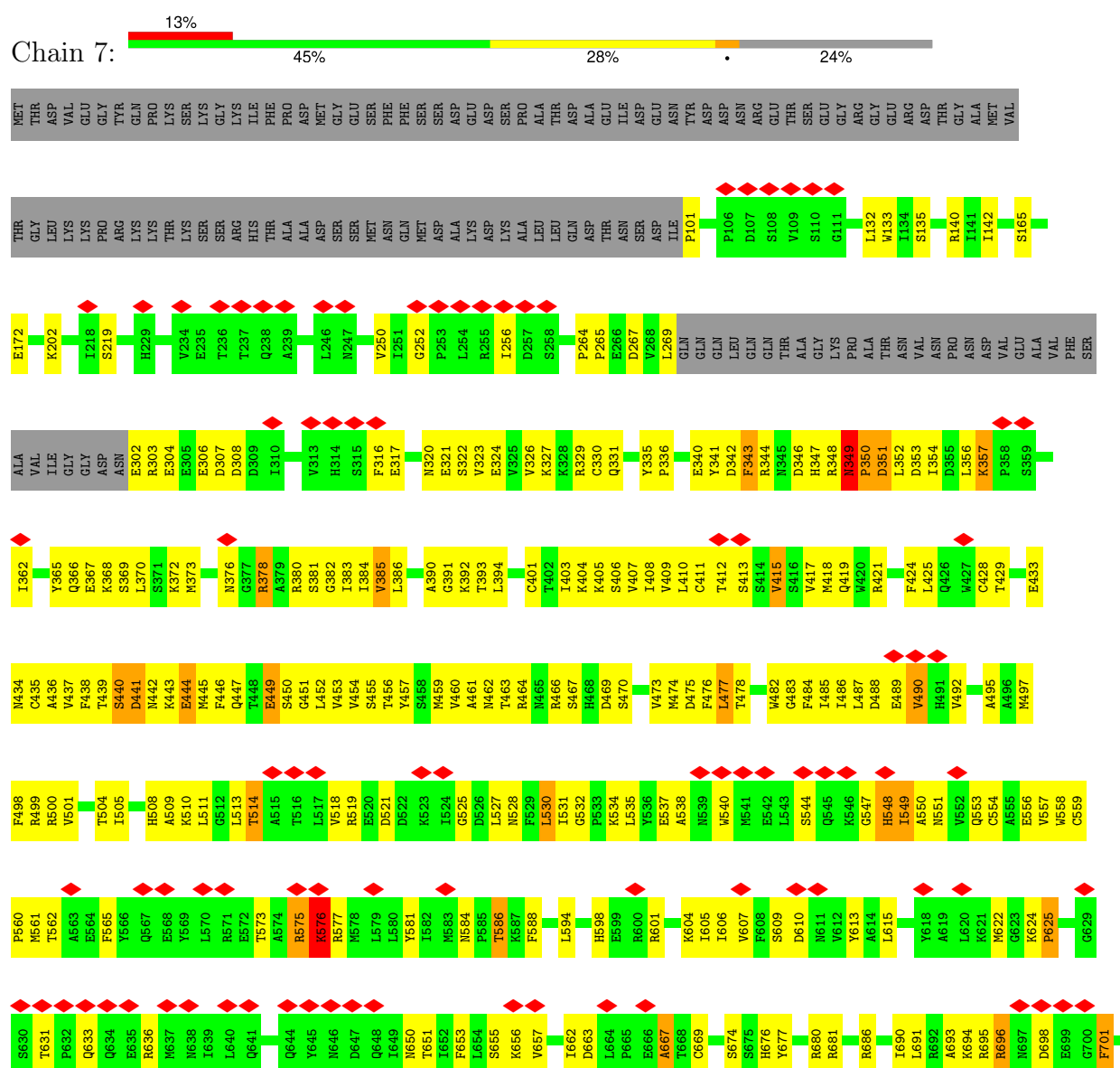
- Molecule 14 is CALCIUM ION (CCD ID: CA) (formula: Ca).

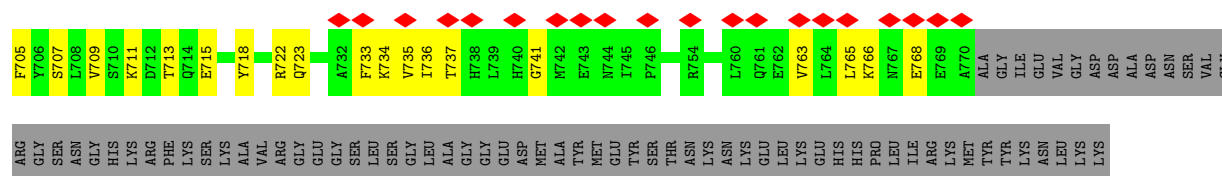
Mol	Chain	Residues	Atoms		AltConf
14	E	2	Total	Ca	0
			2	2	

3 Residue-property plots

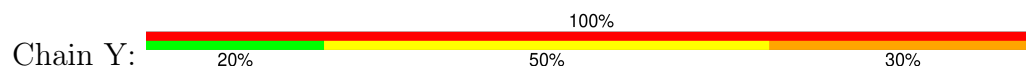
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA repair helicase RAD25

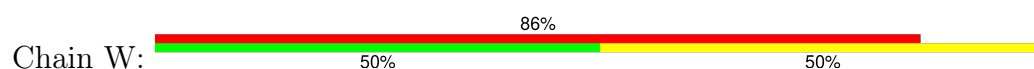




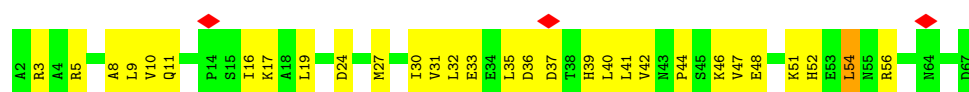
• Molecule 2: Undamaged DNA strand



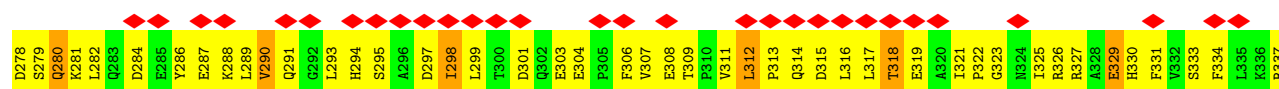
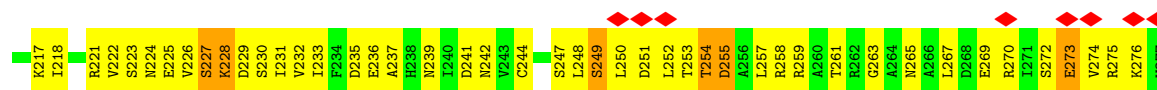
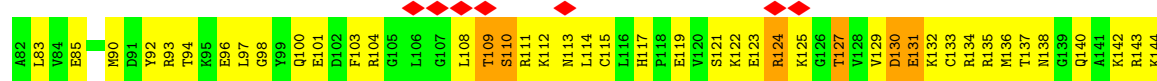
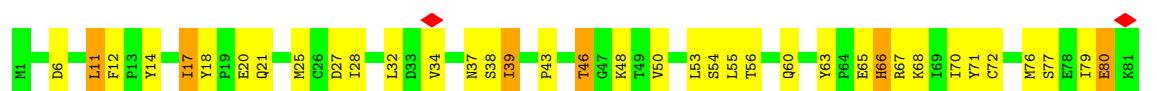
• Molecule 3: Damaged DNA strand

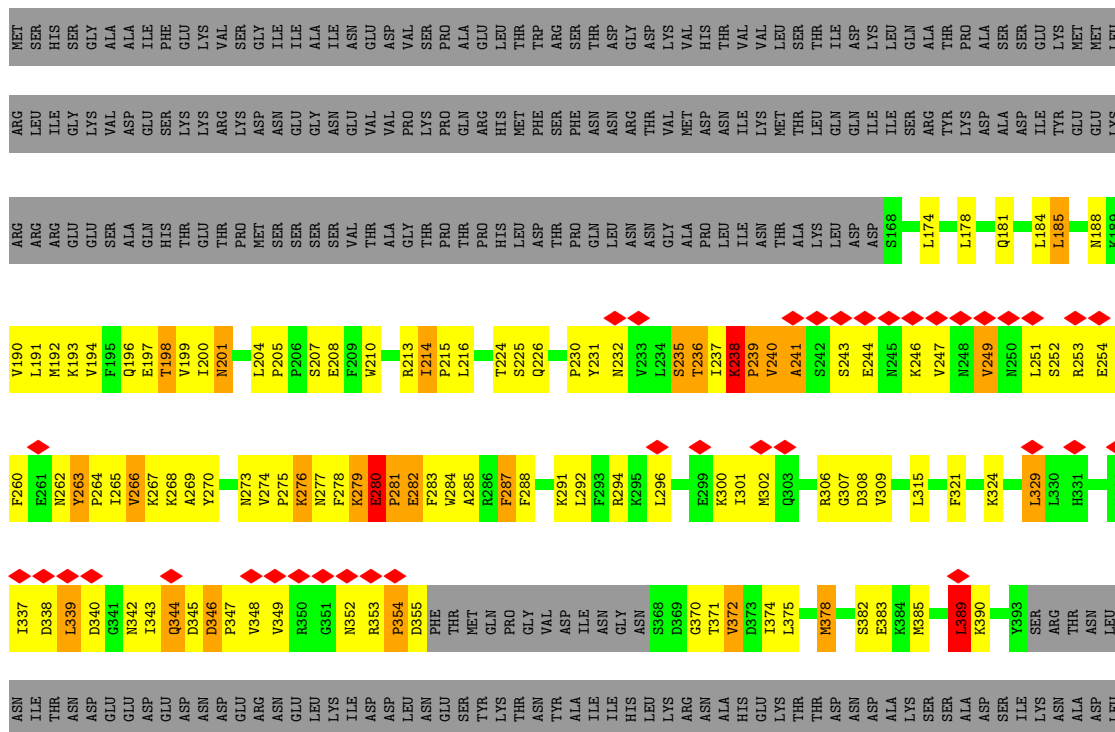


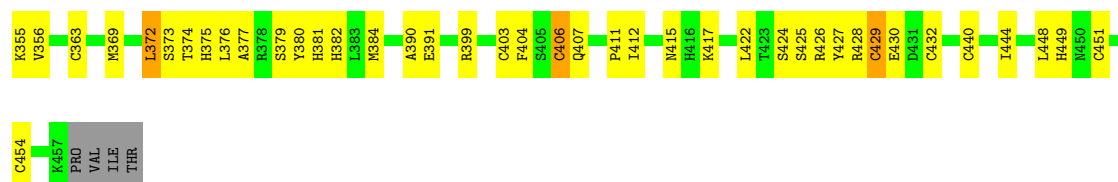
• Molecule 4: General transcription and DNA repair factor IIH subunit TFB5



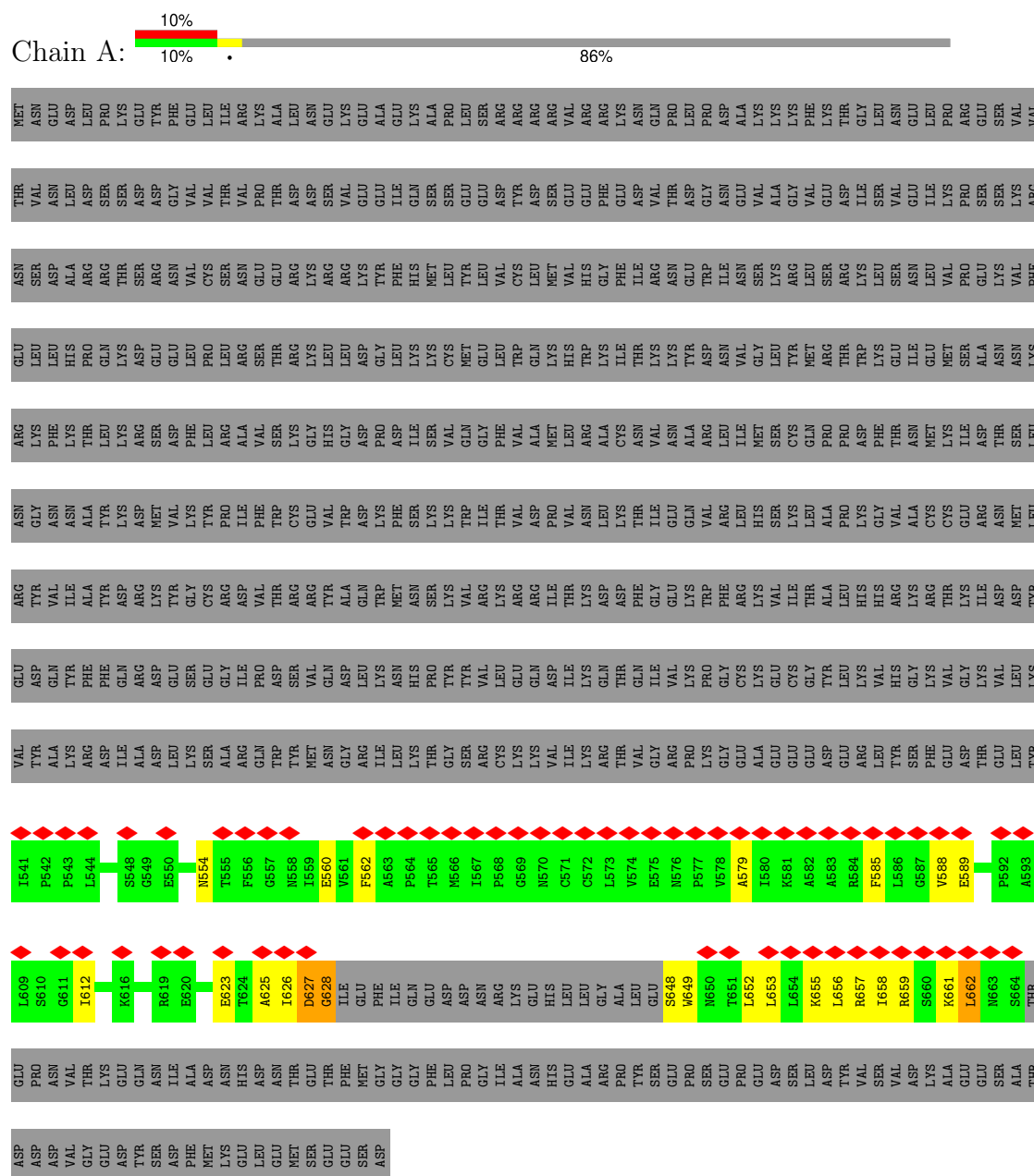
• Molecule 5: DNA repair helicase RAD3



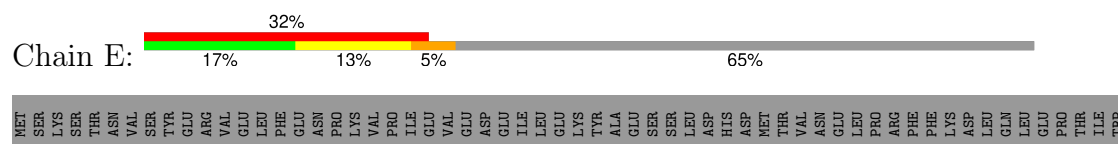


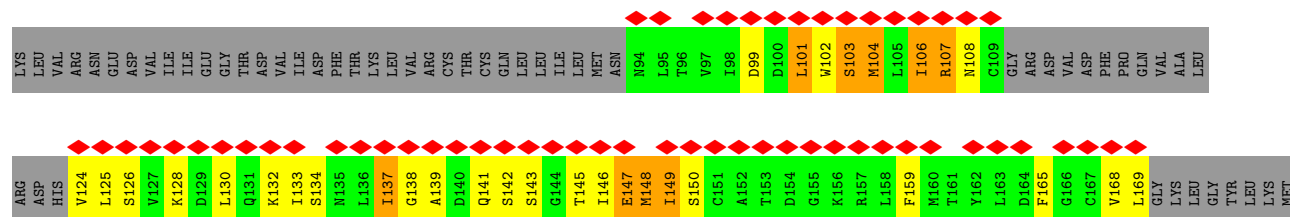


• Molecule 9: DNA repair protein RAD4

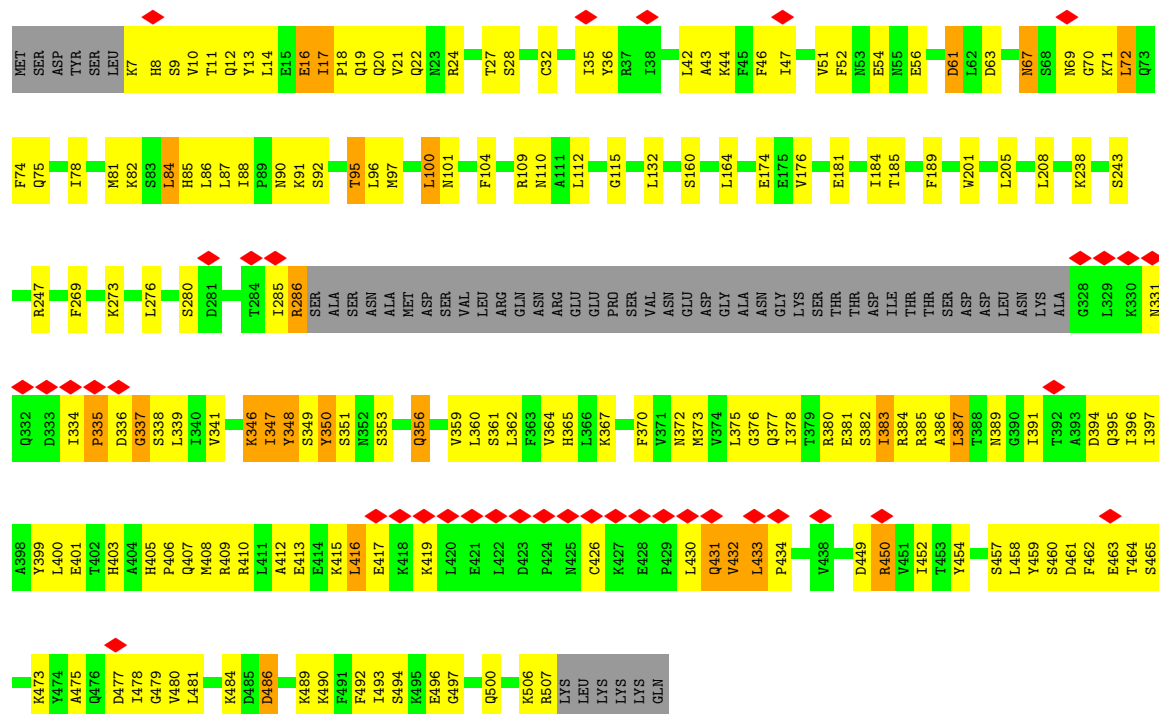


• Molecule 10: DNA repair protein RAD33





• Molecule 11: General transcription and DNA repair factor IIH subunit TFB2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34000	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.007	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00239	Depositor
Map size ($\text{\AA}$)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	7	0.34	2/4552 (0.0%)	0.67	13/6078 (0.2%)
2	Y	0.67	0/225	1.64	3/344 (0.9%)
3	W	0.38	0/325	0.66	0/499
4	5	0.11	0/502	0.36	0/677
5	0	0.49	0/6226	0.54	0/8407
6	1	0.45	0/2438	0.69	6/3325 (0.2%)
7	4	0.49	0/2072	0.55	0/2819
8	6	0.54	1/2571 (0.0%)	0.60	2/3494 (0.1%)
9	A	0.27	0/810	0.83	5/1099 (0.5%)
10	E	0.38	0/479	0.96	2/644 (0.3%)
11	2	0.24	0/3057	0.53	4/4071 (0.1%)
All	All	0.43	3/23257 (0.0%)	0.63	35/31457 (0.1%)

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
2	Y	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7	350	PRO	CA-C	5.53	1.59	1.52
1	7	350	PRO	N-CA	5.43	1.53	1.47
8	6	243	ASP	C-N	-5.32	1.29	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	4	DA	OP2-P-O3'	-15.14	62.59	108.00
2	Y	5	DA	OP1-P-OP2	-13.95	78.15	120.00
1	7	351	ASP	N-CA-C	13.27	129.74	109.96
2	Y	4	DA	OP1-P-O3'	10.76	140.27	108.00
9	A	628	GLY	N-CA-C	9.26	140.15	113.30
1	7	548	HIS	N-CA-C	8.91	120.92	111.03
1	7	351	ASP	CB-CA-C	-8.78	97.52	110.16
1	7	350	PRO	CA-C-N	8.18	133.12	121.02
1	7	350	PRO	C-N-CA	8.18	133.12	121.02
1	7	350	PRO	N-CA-C	7.98	124.06	111.38
6	1	491	PRO	N-CA-CB	7.83	111.47	103.25
6	1	390	LYS	N-CA-C	-7.59	104.04	113.38
9	A	627	ASP	N-CA-C	7.49	120.32	111.71
6	1	354	PRO	N-CA-CB	7.20	110.81	103.25
1	7	547	GLY	N-CA-C	6.67	128.98	113.18
1	7	547	GLY	CA-C-N	6.30	129.20	120.63
1	7	547	GLY	C-N-CA	6.30	129.20	120.63
6	1	238	LYS	CA-C-N	-6.13	112.18	119.84
6	1	238	LYS	C-N-CA	-6.13	112.18	119.84
9	A	601	ARG	CA-C-N	5.98	133.12	121.41
9	A	601	ARG	C-N-CA	5.98	133.12	121.41
1	7	349	ASN	CA-C-N	5.92	125.83	119.85
1	7	349	ASN	C-N-CA	5.92	125.83	119.85
11	2	350	TYR	N-CA-C	-5.79	105.31	112.72
6	1	296	LEU	CB-CA-C	-5.71	109.47	117.23
10	E	137	ILE	CA-CB-CG1	5.20	119.23	110.40
10	E	101	LEU	CA-CB-CG	-5.08	98.52	116.30
1	7	415	VAL	N-CA-CB	5.08	117.44	110.54
8	6	163	GLN	CA-C-N	-5.07	117.11	122.28
8	6	163	GLN	C-N-CA	-5.07	117.11	122.28
1	7	441	ASP	CB-CA-C	-5.06	101.15	109.65
11	2	449	ASP	N-CA-C	5.05	118.70	111.02
11	2	452	ILE	CA-C-N	5.02	130.45	122.62
11	2	452	ILE	C-N-CA	5.02	130.45	122.62
9	A	601	ARG	N-CA-C	5.01	116.99	110.43

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Y	-3	DA	Sidechain

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	7	4478	0	3928	265	0
2	Y	202	0	114	19	0
3	W	289	0	157	12	0
4	5	498	0	506	36	0
5	0	6108	0	6167	420	0
6	1	2408	0	1984	226	0
7	4	2041	0	1953	158	0
8	6	2526	0	2333	128	0
9	A	795	0	833	86	0
10	E	476	0	487	128	0
11	2	3011	0	2600	187	0
12	0	8	0	0	2	0
13	4	1	0	0	0	0
13	6	4	0	0	0	0
14	E	2	0	0	0	0
All	All	22847	0	21062	1453	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 33.

All (1453) 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)
9:A:649:TRP:CZ2	10:E:149:ILE:HG12	1.31	1.65
9:A:649:TRP:CZ2	10:E:149:ILE:HA	1.27	1.65
6:1:270:TYR:CE1	6:1:279:LYS:HE3	1.26	1.62
9:A:649:TRP:CH2	10:E:149:ILE:CG1	1.78	1.60
6:1:279:LYS:HA	6:1:283:PHE:CB	1.27	1.56
9:A:649:TRP:HZ2	10:E:149:ILE:CA	1.19	1.50
9:A:649:TRP:CH2	10:E:149:ILE:HG12	0.96	1.46
9:A:649:TRP:HE1	10:E:148:MET:C	1.27	1.37
10:E:130:LEU:CD2	10:E:149:ILE:HG13	0.89	1.36
10:E:130:LEU:HD22	10:E:149:ILE:CG1	0.89	1.35
11:2:336:ASP:O	11:2:351:SER:HB3	1.20	1.34
9:A:649:TRP:CZ2	10:E:149:ILE:CA	1.97	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:270:TYR:CZ	6:1:279:LYS:HE3	1.64	1.32
6:1:486:LEU:CB	7:4:55:GLU:OE2	1.78	1.31
6:1:491:PRO:CB	7:4:245:ILE:HD11	1.64	1.27
9:A:649:TRP:NE1	10:E:148:MET:C	1.89	1.27
6:1:279:LYS:CA	6:1:283:PHE:CB	2.13	1.24
6:1:491:PRO:O	7:4:245:ILE:HD12	1.33	1.22
9:A:649:TRP:HH2	10:E:149:ILE:CD1	1.51	1.22
6:1:270:TYR:CE1	6:1:279:LYS:CE	2.22	1.21
10:E:130:LEU:HD22	10:E:149:ILE:CD1	1.69	1.21
4:5:11:GLN:HB3	11:2:454:TYR:CE1	1.77	1.20
6:1:486:LEU:CA	7:4:55:GLU:OE2	1.90	1.20
5:0:112:LYS:HE2	6:1:345:ASP:OD2	1.42	1.19
6:1:279:LYS:HB3	6:1:283:PHE:CG	1.78	1.19
9:A:649:TRP:CH2	10:E:149:ILE:CD1	2.26	1.18
6:1:279:LYS:HA	6:1:283:PHE:HB3	1.19	1.18
11:2:347:ILE:O	11:2:373:MET:HE1	1.39	1.18
7:4:255:ASP:H	7:4:256:PRO:CD	1.55	1.17
5:0:545:LEU:HD23	6:1:355:ASP:C	1.70	1.17
6:1:270:TYR:CE2	6:1:279:LYS:HB2	1.80	1.16
6:1:279:LYS:CA	6:1:283:PHE:HB3	1.75	1.15
7:4:255:ASP:H	7:4:256:PRO:HD3	1.04	1.14
10:E:130:LEU:HD21	10:E:149:ILE:HG13	1.27	1.14
5:0:112:LYS:CG	6:1:345:ASP:HB3	1.76	1.14
1:7:610:ASP:OD2	1:7:676:HIS:HB2	1.46	1.13
1:7:765:LEU:HD22	10:E:128:LYS:HD3	1.30	1.12
6:1:280:GLU:HB3	6:1:281:PRO:HD3	1.28	1.12
6:1:491:PRO:CB	7:4:245:ILE:CD1	2.27	1.12
9:A:649:TRP:CZ2	10:E:149:ILE:CG1	2.12	1.11
5:0:576:ALA:CB	6:1:343:ILE:HG12	1.81	1.10
6:1:486:LEU:O	7:4:55:GLU:CD	1.94	1.10
6:1:510:ASN:ND2	7:4:265:PRO:O	1.82	1.10
4:5:54:LEU:HD11	11:2:450:ARG:HD2	1.30	1.09
5:0:112:LYS:HG2	6:1:345:ASP:HB3	1.34	1.09
11:2:338:SER:CA	11:2:407:GLN:OE1	2.00	1.09
11:2:346:LYS:HE2	11:2:377:GLN:HB2	1.24	1.08
6:1:280:GLU:CB	6:1:281:PRO:HD3	1.84	1.07
5:0:580:SER:HA	6:1:339:LEU:HD23	1.12	1.06
11:2:416:LEU:CA	11:2:432:VAL:HG12	1.83	1.05
5:0:127:THR:HG22	6:1:348:VAL:HG12	1.31	1.04
6:1:270:TYR:CZ	6:1:279:LYS:HB2	1.92	1.04
5:0:112:LYS:HG2	6:1:345:ASP:CB	1.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:649:TRP:CD1	10:E:148:MET:CB	2.42	1.03
5:0:545:LEU:HD23	6:1:355:ASP:O	1.56	1.03
4:5:5:ARG:HB2	11:2:458:LEU:HB3	1.37	1.03
9:A:649:TRP:CD1	10:E:148:MET:HB3	1.92	1.02
6:1:270:TYR:CZ	6:1:279:LYS:CE	2.42	1.01
11:2:416:LEU:HA	11:2:432:VAL:CG1	1.91	1.00
5:0:580:SER:HA	6:1:339:LEU:CD2	1.91	1.00
1:7:441:ASP:HB2	2:Y:4:DA:O5'	1.61	0.99
5:0:580:SER:CA	6:1:339:LEU:HD23	1.94	0.98
5:0:726:GLN:CD	8:6:292:LEU:HD23	1.90	0.96
9:A:649:TRP:CZ2	10:E:149:ILE:CB	2.47	0.96
9:A:628:GLY:C	10:E:137:ILE:HG13	1.91	0.96
6:1:279:LYS:HB3	6:1:283:PHE:CD1	2.00	0.96
5:0:545:LEU:CD2	6:1:355:ASP:C	2.38	0.95
1:7:765:LEU:HD22	10:E:128:LYS:CD	1.96	0.95
6:1:279:LYS:CB	6:1:283:PHE:CG	2.49	0.95
4:5:11:GLN:HB3	11:2:454:TYR:HE1	1.16	0.94
9:A:652:LEU:HD12	10:E:148:MET:HE1	1.49	0.94
11:2:334:ILE:O	11:2:409:ARG:NH2	1.99	0.94
1:7:549:ILE:HD13	1:7:549:ILE:H	1.33	0.94
7:4:255:ASP:N	7:4:256:PRO:CD	2.30	0.94
5:0:577:GLN:OE1	6:1:340:ASP:HB2	1.70	0.92
6:1:279:LYS:HA	6:1:283:PHE:HB2	0.94	0.92
11:2:416:LEU:HA	11:2:432:VAL:HG12	0.95	0.92
6:1:279:LYS:C	6:1:283:PHE:HB3	1.95	0.92
1:7:768:GLU:HB3	10:E:107:ARG:NH2	1.83	0.92
6:1:279:LYS:CA	6:1:283:PHE:HB2	1.87	0.91
6:1:491:PRO:O	7:4:245:ILE:CD1	2.19	0.91
6:1:507:ILE:HG23	7:4:264:LYS:HD2	1.51	0.91
9:A:649:TRP:CZ3	10:E:149:ILE:HG12	2.03	0.91
1:7:768:GLU:CB	10:E:107:ARG:HH22	1.83	0.90
9:A:655:LYS:HD3	10:E:137:ILE:HB	1.53	0.90
11:2:72:LEU:HD23	11:2:72:LEU:H	1.36	0.90
1:7:765:LEU:CD2	10:E:128:LYS:HD3	2.01	0.90
11:2:338:SER:CA	11:2:351:SER:HB2	2.02	0.89
9:A:652:LEU:CD1	10:E:148:MET:HE1	2.00	0.89
6:1:492:ASN:CB	7:4:243:GLY:HA3	2.01	0.89
11:2:336:ASP:O	11:2:351:SER:CB	2.16	0.89
9:A:649:TRP:HH2	10:E:149:ILE:HD13	1.39	0.88
6:1:486:LEU:O	7:4:55:GLU:OE1	1.93	0.87
7:4:255:ASP:N	7:4:256:PRO:HD3	1.88	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:130:LEU:CD2	10:E:149:ILE:CB	2.52	0.86
7:4:289:CYS:HA	8:6:319:LEU:HD23	1.56	0.86
9:A:628:GLY:O	10:E:139:ALA:N	2.09	0.86
6:1:270:TYR:HE1	6:1:279:LYS:HE3	1.39	0.86
11:2:347:ILE:O	11:2:373:MET:CE	2.23	0.86
10:E:130:LEU:CD2	10:E:149:ILE:CG1	1.76	0.85
6:1:280:GLU:HB3	6:1:281:PRO:CD	2.06	0.85
6:1:343:ILE:O	6:1:345:ASP:N	2.09	0.85
11:2:346:LYS:HE2	11:2:377:GLN:CB	2.06	0.85
11:2:338:SER:CA	11:2:407:GLN:HB2	2.06	0.85
10:E:146:ILE:HB	10:E:150:SER:HB2	1.57	0.85
6:1:486:LEU:C	7:4:55:GLU:CD	2.43	0.84
1:7:610:ASP:OD2	1:7:676:HIS:CB	2.25	0.84
5:0:112:LYS:HG3	6:1:345:ASP:HB3	1.57	0.84
5:0:112:LYS:HG2	6:1:345:ASP:CG	2.02	0.83
5:0:378:SER:HG	5:0:407:THR:HG1	1.21	0.83
6:1:486:LEU:HA	7:4:55:GLU:OE2	1.78	0.83
8:6:403:CYS:SG	8:6:404:PHE:N	2.51	0.83
5:0:127:THR:HG22	6:1:348:VAL:CG1	2.09	0.82
6:1:270:TYR:CE2	6:1:279:LYS:CB	2.60	0.82
1:7:344:ARG:CZ	1:7:378:ARG:HE	1.92	0.82
5:0:592:ASN:OD1	5:0:593:GLY:N	2.11	0.82
4:5:3:ARG:HD2	11:2:460:SER:HB2	1.61	0.82
10:E:125:LEU:CD2	10:E:149:ILE:HD11	2.10	0.82
10:E:130:LEU:HB2	10:E:149:ILE:HD12	1.59	0.82
7:4:289:CYS:SG	7:4:290:SER:N	2.53	0.81
1:7:768:GLU:CB	10:E:107:ARG:NH2	2.42	0.81
7:4:201:PHE:CE1	8:6:374:THR:HB	2.16	0.81
9:A:628:GLY:O	10:E:138:GLY:N	2.14	0.80
9:A:657:ARG:HG2	10:E:101:LEU:HD22	1.63	0.80
6:1:486:LEU:C	7:4:55:GLU:OE2	2.25	0.80
5:0:576:ALA:HB1	6:1:343:ILE:HG12	1.63	0.80
5:0:577:GLN:OE1	6:1:340:ASP:CB	2.30	0.80
11:2:51:VAL:O	11:2:109:ARG:NH2	2.15	0.80
6:1:280:GLU:CB	6:1:281:PRO:CD	2.60	0.79
8:6:432:CYS:HB3	8:6:454:CYS:SG	2.20	0.79
5:0:297:ASP:O	5:0:386:ARG:NH1	2.16	0.79
5:0:314:GLN:HA	5:0:317:LEU:HD13	1.64	0.79
9:A:649:TRP:CZ2	10:E:149:ILE:N	2.49	0.79
9:A:649:TRP:NE1	10:E:148:MET:O	2.04	0.79
1:7:576:LYS:HB2	1:7:576:LYS:NZ	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:353:SER:HB2	11:2:356:GLN:HB3	1.66	0.78
5:0:674:ASP:N	5:0:674:ASP:OD1	2.17	0.78
5:0:63:TYR:O	5:0:67:ARG:NH2	2.17	0.78
1:7:765:LEU:HD22	10:E:128:LYS:CE	2.13	0.78
7:4:293:LEU:CB	8:6:380:TYR:HE1	1.97	0.78
1:7:351:ASP:OD1	1:7:405:LYS:NZ	2.14	0.78
5:0:166:GLU:OE2	5:0:198:ARG:NH1	2.17	0.78
7:4:114:MET:C	7:4:116:ARG:H	1.93	0.77
8:6:176:ASN:HA	8:6:206:GLY:HA3	1.66	0.77
10:E:130:LEU:HB2	10:E:149:ILE:CD1	2.13	0.77
5:0:227:SER:HB2	5:0:230:SER:HB2	1.66	0.77
5:0:275:ARG:HH22	5:0:276:LYS:HG3	1.47	0.77
1:7:343:PHE:HB2	1:7:378:ARG:NH1	1.98	0.77
6:1:198:THR:O	6:1:204:LEU:N	2.12	0.77
9:A:656:LEU:HB3	10:E:104:MET:HE2	1.67	0.77
4:5:9:LEU:HD23	11:2:454:TYR:HB2	1.67	0.77
6:1:503:VAL:HG13	7:4:247:TYR:CE1	2.20	0.76
9:A:625:ALA:HA	9:A:655:LYS:NZ	2.00	0.76
4:5:9:LEU:HD22	11:2:492:PHE:HB3	1.65	0.76
7:4:52:LYS:NZ	7:4:240:SER:O	2.19	0.76
1:7:343:PHE:CD2	1:7:378:ARG:HB2	2.22	0.75
11:2:349:SER:HA	11:2:407:GLN:HE22	1.51	0.75
8:6:269:GLN:HG3	8:6:288:TYR:HE2	1.51	0.75
9:A:649:TRP:CE2	10:E:149:ILE:HA	2.15	0.75
5:0:460:SER:HB2	5:0:463:ILE:HG13	1.68	0.75
10:E:130:LEU:HD23	10:E:149:ILE:CG1	2.13	0.75
11:2:54:GLU:OE2	11:2:109:ARG:NH2	2.20	0.74
8:6:144:ASN:OD1	8:6:147:ALA:N	2.17	0.74
9:A:649:TRP:CE2	10:E:149:ILE:N	2.55	0.74
10:E:125:LEU:HD23	10:E:149:ILE:HD11	1.69	0.74
5:0:288:LYS:O	5:0:291:GLN:NE2	2.20	0.74
10:E:126:SER:HA	10:E:159:PHE:HD1	1.51	0.74
8:6:139:LYS:NZ	8:6:143:PRO:O	2.19	0.74
1:7:418:MET:HG3	1:7:421:ARG:HH12	1.52	0.74
5:0:110:SER:HB3	6:1:346:ASP:HA	1.68	0.74
5:0:37:ASN:ND2	5:0:476:LYS:O	2.21	0.73
6:1:491:PRO:O	6:1:493:ASN:N	2.19	0.73
7:4:290:SER:OG	7:4:291:VAL:N	2.18	0.73
11:2:338:SER:C	11:2:407:GLN:OE1	2.30	0.73
6:1:491:PRO:C	7:4:245:ILE:HD12	2.12	0.73
5:0:304:GLU:OE1	5:0:386:ARG:NH1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:0:608:GLU:O	5:0:668:ARG:NH2	2.17	0.73
11:2:335:PRO:CA	11:2:409:ARG:HH12	2.02	0.73
5:0:729:ASP:O	5:0:731:LYS:NZ	2.22	0.73
8:6:294:GLU:OE1	8:6:294:GLU:N	2.20	0.73
1:7:376:ASN:OD1	1:7:380:ARG:NH2	2.22	0.72
5:0:651:ASN:N	5:0:651:ASN:OD1	2.21	0.72
6:1:507:ILE:HG23	7:4:264:LYS:CD	2.17	0.72
7:4:304:LYS:HG3	7:4:309:ASP:HA	1.70	0.72
7:4:293:LEU:HB3	8:6:380:TYR:CE1	2.25	0.72
11:2:335:PRO:CA	11:2:406:PRO:HB3	2.20	0.72
1:7:343:PHE:HD1	1:7:344:ARG:H	1.38	0.71
4:5:27:MET:HE1	4:5:46:LYS:HB3	1.72	0.71
5:0:739:TRP:HB3	5:0:745:ILE:HG23	1.71	0.71
6:1:479:ASN:O	6:1:483:LYS:N	2.21	0.71
5:0:507:SER:HG	5:0:685:ARG:HH22	1.38	0.71
4:5:3:ARG:CD	11:2:460:SER:HB2	2.20	0.71
6:1:507:ILE:CG2	7:4:264:LYS:HD2	2.20	0.71
5:0:12:PHE:HE1	5:0:14:TYR:HB2	1.54	0.71
11:2:243:SER:O	11:2:247:ARG:N	2.22	0.71
6:1:279:LYS:HA	6:1:283:PHE:CG	2.23	0.71
7:4:138:LYS:O	7:4:138:LYS:NZ	2.21	0.71
1:7:613:TYR:CE2	1:7:766:LYS:HD3	2.26	0.70
5:0:439:CYS:SG	5:0:440:LEU:N	2.63	0.70
11:2:431:GLN:HG3	11:2:434:PRO:HA	1.73	0.70
5:0:545:LEU:CD2	6:1:355:ASP:O	2.36	0.70
7:4:260:PRO:HD2	7:4:261:ILE:HG22	1.73	0.70
8:6:138:GLU:OE2	8:6:145:ARG:NE	2.24	0.70
5:0:286:TYR:O	5:0:326:ARG:NH1	2.20	0.70
6:1:174:LEU:O	6:1:181:GLN:NE2	2.24	0.70
1:7:421:ARG:HA	1:7:425:LEU:HD23	1.73	0.70
5:0:110:SER:HB2	6:1:346:ASP:O	1.91	0.70
5:0:134:ARG:NH2	5:0:303:GLU:O	2.25	0.70
5:0:224:ASN:OD1	5:0:452:ARG:NH2	2.23	0.70
11:2:350:TYR:HA	11:2:372:ASN:HB2	1.73	0.70
5:0:295:SER:HA	5:0:298:ILE:HG22	1.74	0.70
5:0:705:ASP:N	5:0:705:ASP:OD1	2.25	0.70
6:1:188:ASN:HD21	6:1:190:VAL:HB	1.56	0.70
1:7:604:LYS:NZ	1:7:650:ASN:OD1	2.22	0.70
5:0:117:HIS:HE1	5:0:119:GLU:HB3	1.56	0.70
7:4:293:LEU:HB3	8:6:380:TYR:HE1	1.57	0.70
5:0:137:THR:HB	5:0:159:HIS:HD2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:0:610:ILE:O	5:0:668:ARG:NH1	2.24	0.69
6:1:273:ASN:HD22	6:1:283:PHE:HE2	1.40	0.69
7:4:201:PHE:CZ	8:6:374:THR:HB	2.27	0.69
11:2:81:MET:HB2	11:2:86:LEU:HD11	1.72	0.69
4:5:33:GLU:HB2	4:5:41:LEU:HB3	1.73	0.69
5:0:135:ARG:NH2	5:0:391:THR:O	2.26	0.69
6:1:196:GLN:O	6:1:200:ILE:N	2.24	0.69
1:7:610:ASP:H	1:7:674:SER:HB2	1.56	0.69
9:A:657:ARG:CZ	10:E:101:LEU:HD13	2.22	0.69
1:7:352:LEU:O	1:7:404:LYS:NZ	2.25	0.69
1:7:415:VAL:HG13	2:Y:3:DC:P	2.33	0.69
6:1:214:ILE:HG23	6:1:215:PRO:HD3	1.75	0.69
1:7:492:VAL:CG1	3:W:26:DG:H5''	2.23	0.69
5:0:127:THR:HA	6:1:348:VAL:HG11	1.74	0.69
8:6:116:THR:O	8:6:116:THR:OG1	2.10	0.69
1:7:477:LEU:HA	1:7:482:TRP:HE1	1.57	0.68
5:0:104:ARG:N	5:0:204:ASN:OD1	2.23	0.68
11:2:356:GLN:HG3	11:2:403:HIS:HE1	1.57	0.68
4:5:5:ARG:O	11:2:458:LEU:N	2.21	0.68
1:7:411:CYS:HA	1:7:488:ASP:HB2	1.73	0.68
5:0:228:LYS:O	5:0:228:LYS:NZ	2.21	0.68
5:0:341:TYR:OH	5:0:362:HIS:ND1	2.23	0.68
7:4:58:ILE:HD11	7:4:125:LEU:HD22	1.75	0.68
9:A:649:TRP:NE1	10:E:148:MET:CB	2.56	0.68
5:0:321:ILE:HG13	5:0:323:GLY:H	1.58	0.68
6:1:251:LEU:HB3	6:1:254:GLU:HB2	1.74	0.68
9:A:649:TRP:CD1	10:E:148:MET:HB2	2.27	0.68
5:0:39:ILE:HD11	5:0:466:LEU:HG	1.74	0.68
8:6:218:ARG:NH1	8:6:257:GLU:OE2	2.27	0.68
1:7:439:THR:HB	1:7:442:ASN:H	1.57	0.68
6:1:279:LYS:CA	6:1:283:PHE:CG	2.76	0.68
7:4:244:LEU:O	7:4:247:TYR:N	2.27	0.68
7:4:293:LEU:CB	8:6:380:TYR:CE1	2.77	0.68
10:E:99:ASP:O	10:E:103:SER:HB2	1.93	0.68
4:5:24:ASP:OD1	4:5:30:ILE:N	2.27	0.68
5:0:683:ASP:OD1	5:0:686:PHE:N	2.26	0.68
11:2:481:LEU:HD23	11:2:493:ILE:HG21	1.75	0.68
5:0:571:VAL:HG11	6:1:375:LEU:HB3	1.74	0.67
5:0:223:SER:O	5:0:226:VAL:N	2.18	0.67
5:0:350:HIS:HA	5:0:422:PRO:HG3	1.75	0.67
5:0:371:ARG:NH2	5:0:411:THR:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:399:TYR:O	11:2:403:HIS:N	2.25	0.67
1:7:691:LEU:HD23	1:7:694:LYS:HZ1	1.58	0.67
7:4:137:LYS:HG2	7:4:140:ILE:HG12	1.76	0.67
10:E:143:SER:O	10:E:146:ILE:HD11	1.95	0.67
4:5:5:ARG:NH2	4:5:33:GLU:OE2	2.28	0.67
8:6:221:LEU:HD23	8:6:230:ARG:HB3	1.78	0.66
11:2:469:ASN:ND2	11:2:486:ASP:OD2	2.28	0.66
1:7:306:GLU:CD	1:7:346:ASP:HB2	2.20	0.66
7:4:182:GLY:N	7:4:215:ILE:O	2.26	0.66
9:A:649:TRP:NE1	10:E:148:MET:CA	2.57	0.66
5:0:424:GLU:OE1	5:0:432:ASN:ND2	2.28	0.66
5:0:307:VAL:H	5:0:382:SER:HB3	1.59	0.66
5:0:103:PHE:H	5:0:173:LYS:HZ1	1.42	0.66
5:0:587:ARG:NH2	5:0:611:ASP:O	2.28	0.66
11:2:69:ASN:ND2	11:2:69:ASN:O	2.29	0.66
1:7:428:CYS:SG	1:7:429:THR:N	2.69	0.66
5:0:251:ASP:OD1	5:0:436:ARG:NH1	2.25	0.66
8:6:406:CYS:HB3	8:6:440:CYS:SG	2.35	0.66
5:0:127:THR:CG2	6:1:348:VAL:HG12	2.19	0.66
5:0:244:CYS:HB3	5:0:445:ALA:HB3	1.78	0.66
6:1:280:GLU:HB2	6:1:281:PRO:HD3	1.78	0.66
6:1:507:ILE:HD12	7:4:264:LYS:HG3	1.76	0.66
7:4:33:ALA:O	7:4:37:TRP:N	2.27	0.66
11:2:347:ILE:HB	11:2:376:GLY:O	1.95	0.66
11:2:415:LYS:O	11:2:432:VAL:HA	1.95	0.66
5:0:572:GLU:OE1	5:0:579:THR:OG1	2.14	0.66
5:0:645:ASN:O	5:0:647:ARG:NH1	2.29	0.66
1:7:483:GLY:HA2	1:7:508:HIS:HB2	1.78	0.65
1:7:435:CYS:HB3	1:7:454:VAL:HG12	1.79	0.65
7:4:226:GLN:CD	7:4:273:ARG:HE	2.03	0.65
8:6:188:ASN:ND2	8:6:191:ASP:OD1	2.28	0.65
5:0:21:GLN:HE21	5:0:46:THR:HG22	1.60	0.65
5:0:115:CYS:O	5:0:121:SER:OG	2.08	0.65
8:6:175:ARG:NH2	8:6:203:GLU:O	2.29	0.65
1:7:343:PHE:CG	1:7:378:ARG:HB2	2.31	0.65
10:E:130:LEU:HD23	10:E:149:ILE:HB	1.77	0.65
1:7:698:ASP:HB2	1:7:701:PHE:HB2	1.78	0.65
5:0:425:ILE:HA	5:0:428:ALA:HB2	1.79	0.65
9:A:649:TRP:NE1	10:E:149:ILE:N	2.42	0.65
1:7:425:LEU:HA	1:7:428:CYS:HB3	1.78	0.65
7:4:192:GLN:N	7:4:192:GLN:OE1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:244:LEU:HD12	7:4:244:LEU:H	1.60	0.65
7:4:270:VAL:HG22	7:4:272:PHE:H	1.60	0.65
1:7:477:LEU:HB3	1:7:505:ILE:HD12	1.78	0.65
6:1:346:ASP:HB2	6:1:347:PRO:HD3	1.79	0.65
1:7:550:ALA:HB1	1:7:701:PHE:O	1.96	0.64
5:0:60:GLN:O	5:0:67:ARG:NH2	2.30	0.64
5:0:136:MET:HG3	5:0:155:LEU:HA	1.77	0.64
5:0:270:ARG:NH2	5:0:388:LEU:O	2.24	0.64
5:0:327:ARG:HG3	5:0:330:HIS:H	1.62	0.64
7:4:211:ASP:OD1	7:4:211:ASP:N	2.26	0.64
9:A:649:TRP:CE2	10:E:148:MET:C	2.72	0.64
6:1:557:CYS:SG	6:1:585:HIS:NE2	2.68	0.64
6:1:249:VAL:O	6:1:252:SER:OG	2.15	0.64
5:0:571:VAL:HG21	6:1:375:LEU:HD13	1.79	0.64
9:A:623:GLU:O	9:A:627:ASP:HB2	1.98	0.64
11:2:185:THR:O	11:2:189:PHE:N	2.26	0.64
6:1:259:ILE:HD13	6:1:263:TYR:HE2	1.62	0.64
6:1:188:ASN:HB3	6:1:191:LEU:HB2	1.79	0.64
11:2:87:LEU:HA	11:2:100:LEU:HA	1.78	0.64
1:7:415:VAL:HG13	2:Y:3:DC:OP1	1.98	0.64
5:0:632:SER:OG	5:0:633:ARG:N	2.29	0.64
11:2:458:LEU:HD11	11:2:490:LYS:HB3	1.78	0.64
6:1:491:PRO:C	7:4:245:ILE:CD1	2.70	0.64
9:A:652:LEU:HD12	10:E:148:MET:CE	2.27	0.64
10:E:102:TRP:HB2	10:E:165:PHE:CE2	2.33	0.64
11:2:61:ASP:N	11:2:61:ASP:OD1	2.28	0.64
1:7:495:ALA:HB2	1:7:521:ASP:HB3	1.80	0.64
9:A:585:PHE:CZ	9:A:659:ARG:HD3	2.32	0.64
5:0:90:MET:O	5:0:94:THR:HG23	1.97	0.63
11:2:415:LYS:C	11:2:432:VAL:HA	2.23	0.63
11:2:415:LYS:HB3	11:2:431:GLN:O	1.99	0.63
5:0:278:ASP:O	5:0:281:LYS:NZ	2.31	0.63
5:0:325:ILE:HA	5:0:334:PHE:HE2	1.63	0.63
11:2:475:ALA:O	11:2:479:GLY:N	2.31	0.63
1:7:459:MET:O	1:7:470:SER:OG	2.14	0.63
5:0:744:LEU:O	5:0:748:GLN:HB2	1.98	0.63
11:2:347:ILE:HD13	11:2:364:VAL:HG21	1.80	0.63
1:7:528:ASN:O	1:7:532:GLY:N	2.30	0.63
1:7:435:CYS:HA	1:7:453:VAL:HA	1.81	0.63
5:0:750:SER:OG	5:0:751:ARG:NH2	2.31	0.63
1:7:352:LEU:HD23	1:7:452:LEU:HD23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:0:71:TYR:HB3	5:0:207:ILE:HG23	1.81	0.63
6:1:279:LYS:CG	6:1:283:PHE:CD2	2.82	0.63
9:A:652:LEU:HD23	10:E:137:ILE:HD11	1.81	0.63
1:7:409:VAL:HG22	1:7:486:ILE:HD12	1.81	0.63
7:4:120:ASN:OD1	7:4:121:VAL:N	2.32	0.63
8:6:191:ASP:OD1	8:6:191:ASP:N	2.30	0.63
10:E:125:LEU:HD21	10:E:149:ILE:HD11	1.80	0.63
11:2:67:ASN:ND2	11:2:67:ASN:H	1.97	0.63
5:0:515:ASP:N	5:0:515:ASP:OD1	2.30	0.62
6:1:251:LEU:HB2	6:1:255:LYS:HG2	1.80	0.62
6:1:347:PRO:HB2	6:1:349:VAL:HG13	1.80	0.62
1:7:303:ARG:HA	1:7:320:ASN:HA	1.82	0.62
5:0:294:HIS:CE1	5:0:297:ASP:HB3	2.34	0.62
5:0:301:ASP:HB3	5:0:304:GLU:HB2	1.80	0.62
6:1:279:LYS:HE2	6:1:279:LYS:H	1.63	0.62
7:4:201:PHE:HE1	8:6:374:THR:HB	1.62	0.62
1:7:492:VAL:HG13	3:W:26:DG:H5''	1.81	0.62
9:A:625:ALA:HA	9:A:655:LYS:HZ2	1.62	0.62
9:A:656:LEU:HB3	10:E:104:MET:CE	2.29	0.62
2:Y:-1:DC:H2''	2:Y:0:DT:H5''	1.80	0.62
6:1:488:GLN:CB	7:4:59:VAL:CG2	2.77	0.62
11:2:10:VAL:HG11	11:2:201:TRP:CE3	2.35	0.62
1:7:622:MET:SD	1:7:622:MET:N	2.73	0.62
6:1:507:ILE:HG23	7:4:264:LYS:CG	2.30	0.62
7:4:189:GLU:O	7:4:192:GLN:NE2	2.33	0.62
8:6:373:SER:O	8:6:376:LEU:N	2.33	0.62
5:0:142:LYS:NZ	5:0:146:GLU:OE2	2.32	0.62
7:4:254:ILE:HG21	7:4:261:ILE:CD1	2.30	0.62
11:2:90:ASN:HB3	11:2:97:MET:HB2	1.82	0.62
1:7:441:ASP:CB	2:Y:4:DA:H3'	2.29	0.62
5:0:166:GLU:O	5:0:198:ARG:NH1	2.32	0.62
5:0:274:VAL:O	5:0:278:ASP:N	2.30	0.62
7:4:293:LEU:HB2	8:6:380:TYR:HE1	1.64	0.62
11:2:347:ILE:O	11:2:347:ILE:HG22	2.00	0.62
5:0:70:ILE:HB	5:0:232:VAL:HG22	1.82	0.62
5:0:466:LEU:O	5:0:480:GLN:NE2	2.33	0.62
5:0:531:LYS:HG2	5:0:566:HIS:CE1	2.35	0.62
1:7:576:LYS:HB2	1:7:576:LYS:HZ2	1.62	0.61
5:0:227:SER:C	5:0:229:ASP:H	2.07	0.61
9:A:652:LEU:HD11	10:E:148:MET:HE1	1.82	0.61
8:6:310:VAL:HG13	8:6:311:ASN:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:337:ILE:O	6:1:339:LEU:N	2.34	0.61
1:7:303:ARG:HB2	1:7:323:VAL:H	1.66	0.61
1:7:561:MET:SD	1:7:584:ASN:ND2	2.73	0.61
4:5:31:VAL:HA	4:5:42:VAL:HG13	1.81	0.61
5:0:110:SER:CB	6:1:346:ASP:O	2.49	0.61
5:0:537:MET:HG2	5:0:597:ILE:HG12	1.81	0.61
6:1:492:ASN:O	6:1:494:GLU:N	2.33	0.61
5:0:103:PHE:N	5:0:173:LYS:HZ1	1.98	0.61
6:1:502:ARG:O	6:1:505:THR:OG1	2.16	0.61
11:2:36:TYR:HE1	11:2:44:LYS:HA	1.65	0.61
5:0:157:GLU:HA	5:0:160:GLU:HG2	1.82	0.60
11:2:176:VAL:O	11:2:181:GLU:N	2.32	0.60
11:2:389:ASN:HB3	11:2:391:ILE:HG12	1.83	0.60
9:A:628:GLY:C	10:E:139:ALA:HB2	2.26	0.60
9:A:628:GLY:HA2	10:E:139:ALA:HB2	1.83	0.60
6:1:185:LEU:HD12	6:1:192:MET:HA	1.82	0.60
6:1:486:LEU:O	7:4:55:GLU:OE2	2.15	0.60
7:4:218:SER:HA	7:4:237:HIS:HE2	1.65	0.60
5:0:529:PHE:HA	5:0:532:ILE:HG22	1.84	0.60
5:0:576:ALA:HB2	6:1:343:ILE:HG12	1.80	0.60
5:0:643:ARG:HH11	5:0:650:GLU:HG3	1.66	0.60
9:A:657:ARG:HG2	10:E:101:LEU:CD2	2.29	0.60
10:E:125:LEU:HD23	10:E:149:ILE:CD1	2.30	0.60
5:0:666:LEU:HB3	5:0:679:MET:HE2	1.82	0.60
7:4:254:ILE:HG21	7:4:261:ILE:HD13	1.83	0.60
7:4:289:CYS:HA	8:6:319:LEU:CD2	2.31	0.60
8:6:406:CYS:SG	8:6:407:GLN:N	2.74	0.60
1:7:132:LEU:O	1:7:202:LYS:N	2.31	0.60
4:5:17:LYS:HE3	4:5:40:LEU:HD21	1.84	0.60
6:1:194:VAL:O	6:1:198:THR:OG1	2.18	0.60
10:E:106:ILE:O	10:E:106:ILE:HG12	2.01	0.60
5:0:232:VAL:HG21	5:0:453:PHE:CD2	2.37	0.60
5:0:507:SER:OG	5:0:508:SER:N	2.34	0.60
5:0:528:GLU:OE2	5:0:710:THR:OG1	2.19	0.60
7:4:24:SER:H	7:4:71:ASN:HD22	1.47	0.60
6:1:235:SER:O	6:1:239:PRO:HD2	2.01	0.60
11:2:184:ILE:O	11:2:389:ASN:ND2	2.31	0.60
5:0:258:ARG:O	5:0:261:THR:OG1	2.14	0.60
5:0:537:MET:HE3	5:0:597:ILE:HD11	1.83	0.60
6:1:279:LYS:CE	6:1:279:LYS:H	2.15	0.60
8:6:451:CYS:SG	8:6:454:CYS:HB2	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:99:ASP:O	10:E:103:SER:N	2.35	0.60
1:7:575:ARG:C	1:7:577:ARG:H	2.10	0.59
7:4:271:ASP:C	7:4:273:ARG:HD3	2.27	0.59
5:0:576:ALA:HB3	6:1:343:ILE:HG12	1.81	0.59
6:1:282:GLU:H	6:1:282:GLU:CD	2.09	0.59
8:6:399:ARG:H	8:6:426:ARG:HH12	1.50	0.59
6:1:291:LYS:O	6:1:294:ARG:N	2.36	0.59
8:6:336:CYS:SG	8:6:339:HIS:N	2.68	0.59
8:6:391:GLU:HA	8:6:427:TYR:HA	1.85	0.59
10:E:145:THR:O	10:E:145:THR:HG22	2.00	0.59
1:7:441:ASP:HB2	2:Y:4:DA:H3'	1.83	0.59
4:5:3:ARG:CZ	11:2:461:ASP:HB3	2.32	0.59
5:0:628:GLN:OE1	5:0:628:GLN:N	2.36	0.59
8:6:142:ARG:HB2	8:6:143:PRO:HD3	1.84	0.59
1:7:101:PRO:O	1:7:331:GLN:NE2	2.36	0.59
1:7:326:VAL:HG22	1:7:329:ARG:HH21	1.67	0.59
1:7:631:THR:HB	1:7:636:ARG:HE	1.67	0.59
1:7:696:ARG:NE	1:7:698:ASP:OD2	2.34	0.59
5:0:227:SER:OG	5:0:228:LYS:N	2.30	0.59
9:A:628:GLY:O	10:E:134:SER:O	2.20	0.59
11:2:273:LYS:NZ	11:2:285:ILE:O	2.32	0.59
11:2:464:THR:OG1	11:2:466:GLN:OE1	2.21	0.59
5:0:294:HIS:O	5:0:298:ILE:N	2.32	0.59
7:4:39:THR:O	7:4:43:GLU:N	2.30	0.59
7:4:311:GLN:NE2	7:4:312:PHE:O	2.35	0.59
8:6:195:ALA:O	8:6:198:SER:OG	2.19	0.59
5:0:77:SER:HA	5:0:80:GLU:OE2	2.01	0.59
7:4:258:LEU:O	7:4:259:ARG:HG2	2.01	0.59
1:7:267:ASP:O	1:7:348:ARG:NH2	2.35	0.59
1:7:464:ARG:HA	1:7:466:ARG:CZ	2.32	0.59
1:7:527:LEU:HA	1:7:530:LEU:HB2	1.84	0.59
5:0:272:SER:OG	5:0:276:LYS:NZ	2.36	0.59
5:0:554:TRP:CD1	5:0:559:ILE:HG21	2.38	0.59
5:0:110:SER:OG	5:0:111:ARG:N	2.32	0.59
1:7:768:GLU:HB3	10:E:107:ARG:HH21	1.68	0.58
5:0:272:SER:O	5:0:275:ARG:NH2	2.36	0.58
5:0:286:TYR:HA	5:0:289:LEU:HD12	1.84	0.58
1:7:561:MET:HG3	1:7:562:THR:H	1.65	0.58
5:0:747:HIS:O	5:0:751:ARG:HG2	2.04	0.58
6:1:278:PHE:O	6:1:282:GLU:OE2	2.21	0.58
5:0:360:LEU:HD11	5:0:371:ARG:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:149:LEU:HD22	7:4:153:MET:HE2	1.84	0.58
1:7:269:LEU:HB2	1:7:304:GLU:HA	1.84	0.58
8:6:390:ALA:O	8:6:428:ARG:N	2.36	0.58
9:A:658:ILE:HG22	9:A:662:LEU:HD22	1.84	0.58
11:2:473:LYS:NZ	11:2:477:ASP:OD1	2.36	0.58
5:0:315:ASP:OD1	5:0:315:ASP:N	2.31	0.58
6:1:239:PRO:O	6:1:241:ALA:N	2.36	0.58
6:1:507:ILE:HD12	7:4:264:LYS:CG	2.34	0.58
8:6:168:GLN:OE1	8:6:168:GLN:N	2.37	0.58
11:2:72:LEU:HD23	11:2:72:LEU:N	2.15	0.58
11:2:338:SER:CA	11:2:407:GLN:CD	2.75	0.58
5:0:519:VAL:HG11	5:0:553:MET:HE1	1.86	0.58
5:0:627:PHE:HD1	5:0:654:LEU:HD12	1.67	0.58
8:6:293:ASP:OD2	8:6:296:HIS:N	2.31	0.58
9:A:623:GLU:O	9:A:627:ASP:CB	2.52	0.58
4:5:11:GLN:CB	11:2:454:TYR:HE1	2.05	0.58
4:5:48:GLU:O	4:5:52:HIS:ND1	2.35	0.58
6:1:501:LYS:HA	6:1:504:ILE:HD12	1.85	0.58
7:4:155:ALA:O	7:4:158:THR:OG1	2.18	0.58
7:4:312:PHE:CD2	8:6:319:LEU:HD11	2.38	0.58
8:6:175:ARG:NH1	8:6:202:GLN:OE1	2.37	0.58
8:6:293:ASP:CG	8:6:295:THR:HG1	2.12	0.58
10:E:139:ALA:HB1	10:E:141:GLN:HG3	1.85	0.58
1:7:556:GLU:HG2	1:7:707:SER:HB3	1.85	0.58
11:2:356:GLN:HG3	11:2:403:HIS:CE1	2.39	0.58
6:1:480:LEU:CB	7:4:51:ILE:HG21	2.34	0.58
1:7:424:PHE:O	1:7:428:CYS:N	2.24	0.57
1:7:466:ARG:CB	2:Y:4:DA:H4'	2.33	0.57
9:A:649:TRP:CE2	10:E:149:ILE:CA	2.76	0.57
11:2:415:LYS:NZ	11:2:434:PRO:HG3	2.18	0.57
5:0:145:LEU:HD13	5:0:153:VAL:HB	1.86	0.57
11:2:475:ALA:HA	11:2:478:ILE:HG12	1.85	0.57
8:6:243:ASP:OD1	8:6:243:ASP:N	2.36	0.57
11:2:462:PHE:HB2	11:2:489:LYS:HB3	1.85	0.57
10:E:130:LEU:HD23	10:E:149:ILE:CB	2.29	0.57
1:7:573:THR:HA	1:7:577:ARG:HD2	1.85	0.57
4:5:54:LEU:HG	11:2:450:ARG:HH21	1.70	0.57
5:0:252:LEU:HB2	5:0:435:MET:HB3	1.86	0.57
5:0:730:PRO:HB2	5:0:732:ASP:OD1	2.04	0.57
6:1:193:LYS:O	6:1:196:GLN:NE2	2.37	0.57
7:4:114:MET:O	7:4:116:ARG:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:180:THR:HG23	7:4:214:LYS:HA	1.87	0.57
11:2:132:LEU:O	11:2:286:ARG:NH2	2.37	0.57
5:0:349:LEU:H	5:0:349:LEU:HD23	1.70	0.57
6:1:269:ALA:O	6:1:273:ASN:ND2	2.38	0.57
7:4:305:CYS:HB3	7:4:312:PHE:HZ	1.70	0.57
9:A:655:LYS:HD3	10:E:137:ILE:CB	2.31	0.57
10:E:102:TRP:HD1	10:E:165:PHE:CG	2.23	0.57
11:2:346:LYS:CE	11:2:377:GLN:HB2	2.17	0.57
11:2:494:SER:OG	11:2:496:GLU:OE2	2.21	0.57
5:0:162:LEU:HD12	5:0:166:GLU:HB3	1.85	0.57
5:0:308:GLU:CD	5:0:308:GLU:H	2.13	0.57
1:7:768:GLU:HB2	10:E:107:ARG:HH22	1.70	0.57
5:0:312:LEU:N	5:0:412:TYR:OH	2.24	0.57
6:1:606:GLU:O	6:1:610:ASN:N	2.33	0.57
7:4:114:MET:C	7:4:116:ARG:N	2.63	0.57
5:0:629:TYR:CZ	5:0:636:LYS:HE2	2.40	0.57
6:1:279:LYS:CB	6:1:283:PHE:CD2	2.87	0.57
6:1:282:GLU:OE2	6:1:282:GLU:N	2.36	0.57
6:1:346:ASP:OD1	6:1:346:ASP:N	2.35	0.57
11:2:9:SER:O	11:2:12:GLN:N	2.37	0.57
1:7:381:SER:HB3	1:7:509:ALA:HB1	1.85	0.57
5:0:112:LYS:CG	6:1:345:ASP:CB	2.58	0.57
5:0:379:GLU:OE1	5:0:380:ARG:N	2.38	0.57
9:A:649:TRP:CH2	10:E:149:ILE:HD11	2.32	0.57
11:2:7:LYS:HG2	11:2:9:SER:H	1.69	0.57
11:2:367:LYS:HB2	11:2:375:LEU:HD23	1.87	0.57
5:0:112:LYS:HB3	6:1:345:ASP:O	2.05	0.56
5:0:719:GLN:OE1	5:0:722:ARG:NH1	2.38	0.56
5:0:726:GLN:CG	8:6:292:LEU:HD23	2.35	0.56
7:4:31:GLU:OE2	7:4:181:CYS:N	2.37	0.56
10:E:130:LEU:CD2	10:E:149:ILE:CD1	2.53	0.56
11:2:18:PRO:HB2	11:2:20:GLN:HE22	1.70	0.56
11:2:32:CYS:HB3	11:2:104:PHE:HE1	1.69	0.56
1:7:411:CYS:SG	1:7:412:THR:N	2.77	0.56
7:4:239:GLU:OE2	7:4:242:GLU:N	2.37	0.56
1:7:357:LYS:NZ	1:7:429:THR:O	2.29	0.56
1:7:366:GLN:HE22	1:7:394:LEU:HD22	1.70	0.56
1:7:439:THR:HG22	2:Y:4:DA:OP1	2.05	0.56
3:W:17:DA:C8	9:A:607:PRO:HG3	2.41	0.56
6:1:279:LYS:O	6:1:283:PHE:HB3	2.04	0.56
7:4:137:LYS:H	7:4:140:ILE:HB	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:258:LEU:C	7:4:260:PRO:HD3	2.30	0.56
9:A:579:ALA:HB1	9:A:612:ILE:HG12	1.88	0.56
1:7:406:SER:O	1:7:483:GLY:N	2.39	0.56
1:7:609:SER:HB2	1:7:615:LEU:HD13	1.87	0.56
5:0:577:GLN:OE1	6:1:340:ASP:CG	2.49	0.56
9:A:649:TRP:HZ2	10:E:149:ILE:HA	0.42	0.56
1:7:606:ILE:HG13	1:7:667:ALA:CB	2.35	0.56
5:0:68:LYS:HB2	5:0:230:SER:OG	2.04	0.56
5:0:311:VAL:HG11	5:0:317:LEU:HD11	1.86	0.56
6:1:491:PRO:CA	7:4:245:ILE:HD11	2.34	0.56
7:4:40:PHE:HA	7:4:43:GLU:CD	2.31	0.56
1:7:409:VAL:HA	1:7:486:ILE:HB	1.87	0.56
5:0:537:MET:HG3	5:0:538:VAL:N	2.21	0.56
5:0:395:ASP:N	5:0:395:ASP:OD1	2.32	0.56
5:0:440:LEU:HD22	5:0:638:ARG:HA	1.87	0.56
6:1:258:ASN:O	6:1:262:ASN:HB2	2.04	0.56
1:7:343:PHE:HD1	1:7:344:ARG:N	2.01	0.56
8:6:266:LEU:O	8:6:268:ALA:N	2.39	0.56
8:6:349:CYS:HB3	8:6:352:CYS:SG	2.45	0.56
1:7:306:GLU:O	1:7:341:TYR:HA	2.05	0.56
1:7:324:GLU:HA	1:7:327:LYS:HE2	1.88	0.56
1:7:343:PHE:CD1	1:7:378:ARG:HG3	2.41	0.56
5:0:675:ASP:OD1	5:0:676:TYR:N	2.38	0.56
1:7:352:LEU:HD22	1:7:406:SER:HA	1.87	0.55
5:0:571:VAL:HA	5:0:599:LEU:HD12	1.87	0.55
6:1:279:LYS:HB3	6:1:283:PHE:CD2	2.34	0.55
9:A:649:TRP:NE1	10:E:148:MET:HB2	2.19	0.55
1:7:412:THR:HG22	1:7:489:GLU:HB2	1.87	0.55
9:A:649:TRP:HZ2	10:E:149:ILE:CB	1.96	0.55
4:5:47:VAL:HG12	4:5:51:LYS:HE3	1.87	0.55
5:0:334:PHE:HD1	5:0:337:ARG:HH21	1.54	0.55
6:1:515:LYS:O	6:1:517:ASN:N	2.39	0.55
1:7:341:TYR:O	1:7:343:PHE:CD2	2.60	0.55
5:0:156:CYS:C	5:0:158:TYR:H	2.15	0.55
11:2:42:LEU:HD12	11:2:46:PHE:HE2	1.72	0.55
11:2:463:GLU:N	11:2:467:GLU:OE2	2.39	0.55
5:0:169:ASP:CG	5:0:170:TYR:H	2.14	0.55
5:0:726:GLN:CD	8:6:292:LEU:CD2	2.75	0.55
5:0:11:LEU:HD23	5:0:93:ARG:HA	1.87	0.55
11:2:82:LYS:O	11:2:85:HIS:ND1	2.40	0.55
5:0:619:THR:O	5:0:619:THR:OG1	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:52:LYS:NZ	7:4:242:GLU:O	2.36	0.55
1:7:441:ASP:HB2	2:Y:4:DA:C5'	2.36	0.55
1:7:601:ARG:NH2	1:7:669:CYS:SG	2.80	0.55
5:0:112:LYS:CE	6:1:345:ASP:OD2	2.36	0.55
6:1:474:SER:CB	7:4:34:PRO:HB3	2.37	0.55
8:6:234:ILE:HB	8:6:263:VAL:HB	1.87	0.55
8:6:267:SER:O	8:6:267:SER:OG	2.23	0.55
1:7:303:ARG:HB3	1:7:323:VAL:HG13	1.88	0.55
5:0:119:GLU:OE1	5:0:122:LYS:NZ	2.31	0.55
5:0:270:ARG:HA	5:0:273:GLU:CD	2.31	0.55
5:0:545:LEU:HD22	6:1:355:ASP:C	2.31	0.55
6:1:300:LYS:O	6:1:302:MET:N	2.40	0.55
6:1:510:ASN:O	6:1:513:GLN:HG3	2.07	0.55
8:6:246:ASP:OD1	8:6:247:ILE:N	2.40	0.55
11:2:84:LEU:HD11	11:2:86:LEU:HD23	1.88	0.55
4:5:11:GLN:CB	11:2:454:TYR:CE1	2.71	0.54
6:1:280:GLU:O	6:1:284:TRP:CE3	2.60	0.54
7:4:303:ASN:HB2	7:4:311:GLN:HG2	1.90	0.54
11:2:32:CYS:HB3	11:2:104:PHE:CE1	2.42	0.54
11:2:407:GLN:O	11:2:410:ARG:NH2	2.40	0.54
1:7:622:MET:O	1:7:624:LYS:NZ	2.39	0.54
6:1:279:LYS:HE2	6:1:279:LYS:N	2.22	0.54
11:2:417:GLU:CD	11:2:430:LEU:HD12	2.32	0.54
5:0:535:ASP:OD1	5:0:535:ASP:N	2.38	0.54
6:1:480:LEU:CB	7:4:51:ILE:HD13	2.37	0.54
5:0:117:HIS:CE1	5:0:119:GLU:HB3	2.41	0.54
8:6:169:MET:HE2	8:6:171:ILE:HD11	1.89	0.54
8:6:372:LEU:H	8:6:375:HIS:CE1	2.25	0.54
9:A:653:LEU:HD21	9:A:657:ARG:HH21	1.71	0.54
10:E:130:LEU:CD2	10:E:149:ILE:HB	2.29	0.54
11:2:91:LYS:HA	11:2:95:THR:O	2.06	0.54
11:2:174:GLU:H	11:2:185:THR:N	2.05	0.54
6:1:279:LYS:HG3	6:1:283:PHE:CD2	2.43	0.54
11:2:378:ILE:HD12	11:2:382:SER:HB2	1.90	0.54
1:7:677:TYR:CE1	1:7:715:GLU:HG3	2.43	0.54
5:0:515:ASP:O	5:0:517:SER:N	2.41	0.54
5:0:293:LEU:HD22	5:0:319:GLU:HA	1.88	0.54
11:2:67:ASN:H	11:2:67:ASN:HD22	1.55	0.54
1:7:403:ILE:HD12	1:7:405:LYS:HB2	1.90	0.54
1:7:540:TRP:O	1:7:544:SER:OG	2.20	0.54
6:1:235:SER:C	6:1:239:PRO:HD2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:288:ILE:HD11	7:4:293:LEU:HD12	1.89	0.54
5:0:384:LEU:O	5:0:387:THR:OG1	2.22	0.54
5:0:544:TYR:HB3	6:1:355:ASP:CB	2.38	0.54
6:1:597:PHE:CZ	6:1:613:THR:HA	2.43	0.54
8:6:352:CYS:SG	8:6:353:HIS:N	2.81	0.54
11:2:110:ASN:O	11:2:115:GLY:N	2.41	0.54
11:2:160:SER:O	11:2:164:LEU:N	2.26	0.54
11:2:364:VAL:HA	11:2:382:SER:HB3	1.89	0.54
1:7:412:THR:OG1	1:7:413:SER:N	2.41	0.53
5:0:471:ARG:HH22	5:0:646:TYR:HB3	1.73	0.53
6:1:236:THR:HA	6:1:239:PRO:HG2	1.90	0.53
1:7:365:TYR:OH	1:7:390:ALA:O	2.26	0.53
1:7:410:LEU:HB2	1:7:487:LEU:HD23	1.89	0.53
5:0:325:ILE:HG12	5:0:334:PHE:CE2	2.43	0.53
1:7:436:ALA:HB1	1:7:444:GLU:HB3	1.89	0.53
5:0:639:LEU:HG	5:0:650:GLU:HG2	1.90	0.53
10:E:165:PHE:CE2	10:E:169:LEU:HD11	2.44	0.53
1:7:477:LEU:HA	1:7:482:TRP:NE1	2.24	0.53
5:0:43:PRO:HB3	5:0:696:TRP:CD2	2.42	0.53
5:0:312:LEU:H	5:0:412:TYR:HH	1.49	0.53
5:0:573:THR:OG1	5:0:575:ASP:OD1	2.26	0.53
7:4:60:PHE:CG	7:4:248:LEU:HD22	2.43	0.53
8:6:217:ALA:O	8:6:220:LEU:N	2.42	0.53
11:2:365:HIS:HB3	11:2:385:ARG:HH22	1.73	0.53
5:0:12:PHE:CE1	5:0:14:TYR:HB2	2.40	0.53
5:0:255:ASP:O	5:0:259:ARG:HG3	2.08	0.53
5:0:510:PHE:CE2	5:0:511:GLU:HB2	2.44	0.53
6:1:224:THR:O	6:1:226:GLN:N	2.42	0.53
5:0:643:ARG:NH1	5:0:650:GLU:H	2.06	0.53
6:1:235:SER:O	6:1:238:LYS:N	2.31	0.53
6:1:270:TYR:CZ	6:1:279:LYS:HE2	2.41	0.53
6:1:592:LYS:O	6:1:596:LEU:HG	2.09	0.53
7:4:28:VAL:HB	7:4:75:VAL:HG22	1.90	0.53
7:4:239:GLU:OE1	7:4:240:SER:N	2.42	0.53
10:E:102:TRP:HB2	10:E:165:PHE:CD2	2.43	0.53
11:2:486:ASP:O	11:2:489:LYS:NZ	2.31	0.53
1:7:558:TRP:HB3	1:7:711:LYS:HE2	1.89	0.53
11:2:339:LEU:C	11:2:408:MET:HE1	2.33	0.53
11:2:384:ARG:HA	11:2:387:LEU:HB2	1.89	0.53
1:7:497:MET:HA	1:7:500:ARG:HE	1.74	0.53
5:0:217:LYS:HB2	5:0:308:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:279:LYS:H	6:1:279:LYS:CD	2.22	0.53
9:A:625:ALA:HA	9:A:655:LYS:HZ1	1.71	0.53
11:2:95:THR:OG1	11:2:96:LEU:N	2.42	0.53
1:7:354:ILE:HD12	1:7:404:LYS:HA	1.90	0.52
6:1:188:ASN:HD22	6:1:191:LEU:HG	1.74	0.52
11:2:346:LYS:HD3	11:2:377:GLN:HG3	1.91	0.52
1:7:656:LYS:NZ	1:7:686:ARG:HH21	2.06	0.52
6:1:251:LEU:HD22	6:1:255:LYS:HE3	1.90	0.52
6:1:593:LEU:HA	6:1:596:LEU:HD12	1.89	0.52
10:E:128:LYS:O	10:E:132:LYS:HG3	2.09	0.52
11:2:72:LEU:H	11:2:72:LEU:CD2	2.08	0.52
1:7:560:PRO:HD2	1:7:586:THR:HG21	1.92	0.52
5:0:244:CYS:O	5:0:247:SER:OG	2.22	0.52
5:0:500:GLY:HA3	5:0:521:ASN:HD21	1.74	0.52
11:2:396:ILE:O	11:2:400:LEU:HG	2.10	0.52
11:2:416:LEU:O	11:2:432:VAL:CG1	2.57	0.52
1:7:133:TRP:N	1:7:142:ILE:O	2.42	0.52
7:4:64:HIS:HA	7:4:253:PHE:CZ	2.45	0.52
10:E:130:LEU:CB	10:E:149:ILE:HD12	2.33	0.52
6:1:231:TYR:HA	6:1:385:MET:SD	2.50	0.52
7:4:305:CYS:HB3	7:4:312:PHE:CZ	2.45	0.52
8:6:175:ARG:CZ	8:6:202:GLN:HE22	2.23	0.52
1:7:439:THR:HG22	2:Y:4:DA:P	2.50	0.52
1:7:499:ARG:NH1	1:7:525:GLY:O	2.36	0.52
6:1:551:ARG:O	6:1:555:THR:OG1	2.21	0.52
10:E:142:SER:OG	10:E:145:THR:OG1	2.18	0.52
11:2:346:LYS:HB3	11:2:348:TYR:CE2	2.45	0.52
11:2:419:LYS:NZ	11:2:426:CYS:O	2.40	0.52
1:7:549:ILE:HD13	1:7:549:ILE:N	2.15	0.52
5:0:742:GLU:OE2	5:0:746:LYS:NZ	2.43	0.52
1:7:256:ILE:N	1:7:317:GLU:O	2.43	0.52
3:W:17:DA:N6	9:A:554:ASN:HD21	2.08	0.52
5:0:440:LEU:HD13	5:0:641:PHE:HB2	1.91	0.52
9:A:585:PHE:HZ	9:A:659:ARG:HD3	1.74	0.52
11:2:17:ILE:HG23	11:2:21:VAL:HG23	1.92	0.52
5:0:12:PHE:HD1	5:0:14:TYR:H	1.56	0.51
5:0:183:LYS:O	5:0:187:GLU:HG2	2.09	0.51
7:4:87:TYR:CE1	7:4:121:VAL:HG22	2.45	0.51
7:4:90:SER:HB3	8:6:407:GLN:OE1	2.10	0.51
11:2:10:VAL:HG12	11:2:205:LEU:HD11	1.91	0.51
1:7:354:ILE:HB	1:7:404:LYS:HD2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:768:GLU:OE1	10:E:107:ARG:NH1	2.41	0.51
6:1:490:VAL:O	6:1:492:ASN:N	2.41	0.51
7:4:126:VAL:HA	7:4:129:ILE:HG22	1.90	0.51
7:4:228:THR:HG21	7:4:235:TYR:HB2	1.92	0.51
7:4:298:ILE:O	7:4:300:PRO:HD3	2.10	0.51
10:E:126:SER:HA	10:E:159:PHE:CD1	2.39	0.51
5:0:109:THR:O	5:0:212:TYR:OH	2.13	0.51
5:0:625:ILE:HD11	5:0:658:ALA:HB1	1.92	0.51
8:6:300:LEU:O	8:6:303:GLU:HG2	2.09	0.51
1:7:467:SER:HB3	2:Y:5:DA:OP2	2.11	0.51
5:0:65:GLU:O	5:0:67:ARG:HG2	2.10	0.51
1:7:410:LEU:HD21	1:7:460:VAL:HG21	1.91	0.51
5:0:104:ARG:NH1	5:0:171:LEU:O	2.33	0.51
5:0:375:ARG:HG3	5:0:410:SER:OG	2.11	0.51
8:6:254:LEU:O	8:6:257:GLU:N	2.43	0.51
1:7:369:SER:HB3	1:7:384:ILE:HD13	1.92	0.51
5:0:646:TYR:HA	5:0:647:ARG:CZ	2.40	0.51
8:6:253:SER:O	8:6:256:SER:OG	2.16	0.51
1:7:343:PHE:HB2	1:7:378:ARG:HH11	1.73	0.51
1:7:165:SER:O	1:7:172:GLU:N	2.40	0.51
1:7:264:PRO:O	1:7:269:LEU:N	2.41	0.51
1:7:663:ASP:OD2	1:7:693:ALA:HB2	2.11	0.51
1:7:734:LYS:HE2	1:7:736:ILE:HD11	1.92	0.51
5:0:138:ASN:O	5:0:142:LYS:HG2	2.11	0.51
5:0:169:ASP:OD1	5:0:170:TYR:N	2.41	0.51
6:1:491:PRO:CB	7:4:245:ILE:HD13	2.33	0.51
5:0:56:THR:HG21	5:0:233:ILE:HD11	1.92	0.51
5:0:571:VAL:HG11	6:1:375:LEU:HD13	1.93	0.51
5:0:746:LYS:O	5:0:750:SER:HB3	2.10	0.51
11:2:338:SER:CA	11:2:351:SER:CB	2.85	0.51
11:2:356:GLN:O	11:2:360:LEU:HG	2.11	0.51
11:2:397:ILE:O	11:2:401:GLU:HG2	2.11	0.51
1:7:490:VAL:HB	1:7:519:ARG:HH22	1.76	0.50
5:0:18:TYR:HE2	5:0:673:LYS:HD2	1.76	0.50
5:0:97:LEU:O	5:0:100:GLN:NE2	2.43	0.50
5:0:422:PRO:HG2	5:0:423:TYR:HD1	1.76	0.50
5:0:94:THR:HG22	5:0:101:GLU:HG2	1.93	0.50
5:0:506:ILE:HG21	5:0:521:ASN:HD22	1.75	0.50
5:0:507:SER:OG	5:0:685:ARG:NH2	2.30	0.50
7:4:25:LEU:HG	7:4:27:THR:HG22	1.93	0.50
10:E:165:PHE:CZ	10:E:169:LEU:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:446:PHE:HB3	1:7:473:VAL:HG22	1.93	0.50
4:5:10:VAL:HB	4:5:40:LEU:HB2	1.93	0.50
5:0:331:PHE:HA	5:0:334:PHE:CD2	2.46	0.50
5:0:492:PHE:CD2	5:0:494:PRO:HD3	2.46	0.50
11:2:56:GLU:HG3	11:2:97:MET:HB3	1.92	0.50
11:2:347:ILE:CD1	11:2:364:VAL:HG21	2.42	0.50
11:2:459:TYR:OH	11:2:493:ILE:O	2.25	0.50
11:2:480:VAL:HG13	11:2:493:ILE:HD12	1.93	0.50
1:7:303:ARG:HG2	1:7:304:GLU:H	1.76	0.50
2:Y:-1:DC:H2'	2:Y:0:DT:H71	1.94	0.50
5:0:318:THR:OG1	5:0:319:GLU:N	2.45	0.50
8:6:119:GLN:O	8:6:120:ARG:HG2	2.11	0.50
8:6:120:ARG:HD3	8:6:309:PRO:HD3	1.93	0.50
11:2:497:GLY:O	11:2:500:GLN:HG2	2.11	0.50
1:7:250:VAL:H	1:7:329:ARG:CZ	2.25	0.50
1:7:351:ASP:HA	1:7:405:LYS:HD3	1.94	0.50
5:0:123:GLU:HB3	5:0:129:VAL:HG22	1.92	0.50
5:0:241:ASP:OD1	5:0:241:ASP:N	2.42	0.50
6:1:501:LYS:O	6:1:505:THR:HG23	2.12	0.50
6:1:503:VAL:CG1	7:4:247:TYR:CE1	2.94	0.50
9:A:649:TRP:CD1	10:E:148:MET:CA	2.92	0.50
11:2:347:ILE:HG22	11:2:373:MET:HE1	1.92	0.50
11:2:382:SER:HA	11:2:385:ARG:HH11	1.75	0.50
1:7:624:LYS:HG3	1:7:653:PHE:HE1	1.76	0.50
1:7:768:GLU:CG	10:E:107:ARG:NH2	2.74	0.50
5:0:275:ARG:NH2	5:0:276:LYS:HG3	2.22	0.50
5:0:510:PHE:CG	5:0:511:GLU:N	2.80	0.50
8:6:424:SER:O	8:6:426:ARG:N	2.45	0.50
10:E:107:ARG:O	10:E:108:ASN:HB2	2.12	0.50
1:7:677:TYR:HB3	1:7:718:TYR:CE2	2.46	0.50
5:0:316:LEU:C	5:0:317:LEU:HD12	2.37	0.50
7:4:50:ILE:O	7:4:53:VAL:N	2.45	0.50
1:7:588:PHE:CD1	1:7:622:MET:HE1	2.47	0.50
5:0:60:GLN:HE22	5:0:204:ASN:HB3	1.75	0.50
7:4:211:ASP:HB3	7:4:234:VAL:HG13	1.93	0.50
11:2:486:ASP:N	11:2:486:ASP:OD1	2.44	0.50
1:7:446:PHE:O	1:7:447:GLN:HG2	2.12	0.50
5:0:76:MET:HA	5:0:79:ILE:HB	1.93	0.50
5:0:94:THR:O	5:0:98:GLY:N	2.40	0.50
5:0:585:THR:HG21	6:1:383:GLU:HG2	1.93	0.50
3:W:25:DA:H2''	3:W:26:DG:H5'	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:0:21:GLN:O	5:0:25:MET:HG2	2.12	0.49
5:0:492:PHE:HD2	5:0:494:PRO:HD3	1.77	0.49
5:0:615:GLN:OE1	5:0:615:GLN:N	2.36	0.49
5:0:625:ILE:HB	5:0:686:PHE:CZ	2.47	0.49
5:0:627:PHE:CD1	5:0:654:LEU:HD12	2.47	0.49
8:6:139:LYS:NZ	8:6:144:ASN:HB3	2.27	0.49
8:6:233:LEU:HA	8:6:262:LYS:O	2.12	0.49
1:7:443:LYS:HE2	1:7:446:PHE:CZ	2.46	0.49
1:7:456:THR:HG23	1:7:459:MET:H	1.77	0.49
1:7:550:ALA:HB2	1:7:701:PHE:CD2	2.47	0.49
7:4:38:THR:O	7:4:42:GLU:N	2.35	0.49
7:4:200:ILE:HG12	7:4:227:THR:HG23	1.95	0.49
1:7:306:GLU:OE1	1:7:346:ASP:HB2	2.11	0.49
1:7:407:VAL:HG13	1:7:484:PHE:HB3	1.94	0.49
5:0:270:ARG:O	5:0:273:GLU:HG2	2.12	0.49
7:4:290:SER:O	7:4:293:LEU:N	2.44	0.49
5:0:65:GLU:N	5:0:65:GLU:OE1	2.45	0.49
5:0:123:GLU:OE1	5:0:124:ARG:N	2.45	0.49
5:0:397:THR:O	5:0:400:LYS:HG2	2.12	0.49
5:0:422:PRO:HG2	5:0:423:TYR:CD1	2.47	0.49
5:0:510:PHE:O	5:0:511:GLU:HG3	2.11	0.49
7:4:24:SER:HG	7:4:64:HIS:HE2	1.59	0.49
1:7:705:PHE:HE2	1:7:723:GLN:HE22	1.58	0.49
5:0:374:LEU:HD11	5:0:406:ALA:HB1	1.95	0.49
5:0:496:ILE:HD12	5:0:686:PHE:HB3	1.94	0.49
6:1:306:ARG:O	6:1:308:ASP:N	2.45	0.49
7:4:30:ILE:O	7:4:77:ALA:HA	2.12	0.49
9:A:628:GLY:O	10:E:137:ILE:C	2.55	0.49
1:7:550:ALA:CB	1:7:701:PHE:CG	2.96	0.49
4:5:36:ASP:OD1	4:5:39:HIS:N	2.46	0.49
5:0:108:LEU:HD22	5:0:200:ILE:HD11	1.94	0.49
5:0:586:TYR:OH	5:0:616:TYR:O	2.19	0.49
5:0:694:PRO:HG2	5:0:697:ILE:HG13	1.94	0.49
6:1:270:TYR:CD2	6:1:279:LYS:CB	2.96	0.49
7:4:27:THR:O	7:4:27:THR:OG1	2.14	0.49
11:2:86:LEU:O	11:2:101:ASN:N	2.25	0.49
1:7:457:TYR:HE1	1:7:487:LEU:HD22	1.76	0.49
5:0:575:ASP:OD1	5:0:575:ASP:N	2.46	0.49
5:0:629:TYR:CG	5:0:629:TYR:O	2.66	0.49
8:6:212:ASN:HD21	8:6:244:PRO:HG2	1.77	0.49
11:2:378:ILE:HD11	11:2:383:ILE:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:576:LYS:HB2	1:7:576:LYS:HZ3	1.77	0.49
1:7:765:LEU:HB2	10:E:128:LYS:HZ2	1.77	0.49
4:5:8:ALA:HB2	4:5:44:PRO:HG3	1.94	0.49
5:0:192:PRO:O	5:0:196:VAL:HG12	2.12	0.49
5:0:446:ILE:O	5:0:449:VAL:HG22	2.13	0.49
6:1:235:SER:O	6:1:237:ILE:N	2.46	0.49
6:1:285:ALA:HA	6:1:288:PHE:CD2	2.47	0.49
1:7:553:GLN:HB3	1:7:734:LYS:NZ	2.28	0.49
11:2:382:SER:HA	11:2:385:ARG:NH1	2.28	0.49
3:W:18:DC:H2"	3:W:19:DA:C8	2.48	0.48
4:5:52:HIS:O	4:5:56:ARG:HG3	2.13	0.48
5:0:541:PHE:HD2	5:0:547:MET:HE2	1.78	0.48
5:0:625:ILE:HD12	5:0:626:PRO:HD2	1.95	0.48
6:1:470:LEU:HA	7:4:38:THR:CB	2.42	0.48
8:6:209:SER:OG	8:6:212:ASN:OD1	2.18	0.48
8:6:376:LEU:O	8:6:379:SER:OG	2.22	0.48
6:1:260:PHE:CG	6:1:267:LYS:HD3	2.48	0.48
1:7:588:PHE:HD1	1:7:622:MET:HE1	1.79	0.48
1:7:693:ALA:HA	1:7:695:ARG:HH21	1.77	0.48
4:5:32:LEU:H	4:5:42:VAL:HA	1.76	0.48
5:0:255:ASP:N	5:0:255:ASP:OD1	2.45	0.48
5:0:452:ARG:HH21	5:0:453:PHE:HE1	1.61	0.48
9:A:627:ASP:O	10:E:139:ALA:HA	2.13	0.48
1:7:303:ARG:HA	1:7:321:GLU:N	2.27	0.48
5:0:38:SER:OG	5:0:479:LEU:N	2.32	0.48
5:0:306:PHE:CD2	5:0:307:VAL:HG23	2.47	0.48
5:0:529:PHE:O	5:0:533:THR:HG23	2.13	0.48
5:0:708:LEU:HB3	5:0:712:MET:HG3	1.94	0.48
6:1:199:VAL:HG22	6:1:204:LEU:O	2.13	0.48
6:1:279:LYS:CA	6:1:279:LYS:HE2	2.41	0.48
6:1:477:MET:CB	7:4:49:SER:CB	2.91	0.48
7:4:254:ILE:CG2	7:4:261:ILE:HD13	2.43	0.48
8:6:241:THR:OG1	8:6:243:ASP:OD1	2.19	0.48
8:6:309:PRO:HA	8:6:312:LYS:NZ	2.27	0.48
11:2:56:GLU:OE1	11:2:56:GLU:N	2.46	0.48
1:7:386:LEU:HB2	1:7:392:LYS:HG3	1.96	0.48
5:0:235:ASP:OD1	5:0:236:GLU:N	2.46	0.48
5:0:740:SER:H	5:0:744:LEU:HD22	1.77	0.48
6:1:208:GLU:OE1	6:1:208:GLU:N	2.23	0.48
6:1:178:LEU:HA	6:1:181:GLN:OE1	2.14	0.48
1:7:407:VAL:H	1:7:452:LEU:HD22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:633:GLN:HA	1:7:636:ARG:HB2	1.96	0.48
9:A:648:SER:HA	10:E:148:MET:HG2	1.95	0.48
11:2:346:LYS:HD2	11:2:346:LYS:HA	1.49	0.48
1:7:438:PHE:HB2	1:7:459:MET:HE2	1.96	0.48
1:7:557:VAL:HG21	1:7:594:LEU:HD11	1.96	0.48
4:5:30:ILE:HG21	4:5:46:LYS:HB2	1.95	0.48
6:1:204:LEU:HD12	6:1:205:PRO:HD2	1.95	0.48
1:7:303:ARG:HB3	1:7:323:VAL:HG22	1.94	0.48
1:7:500:ARG:O	1:7:504:THR:OG1	2.25	0.48
1:7:624:LYS:HD2	1:7:651:THR:HB	1.95	0.48
5:0:169:ASP:O	5:0:198:ARG:NH2	2.41	0.48
6:1:207:SER:OG	6:1:208:GLU:OE1	2.22	0.48
7:4:276:CYS:HB3	7:4:279:THR:HB	1.94	0.48
11:2:174:GLU:H	11:2:185:THR:H	1.61	0.48
5:0:326:ARG:O	5:0:380:ARG:NH2	2.47	0.47
8:6:372:LEU:HD22	8:6:375:HIS:HE1	1.79	0.47
5:0:713:ALA:O	5:0:717:THR:HG22	2.14	0.47
6:1:259:ILE:O	6:1:263:TYR:N	2.40	0.47
8:6:126:LEU:C	8:6:127:ILE:HD12	2.39	0.47
11:2:405:HIS:NE2	11:2:409:ARG:HA	2.29	0.47
1:7:366:GLN:NE2	1:7:391:GLY:O	2.47	0.47
1:7:553:GLN:HB3	1:7:734:LYS:HZ2	1.79	0.47
1:7:554:CYS:HB2	1:7:733:PHE:HA	1.96	0.47
1:7:613:TYR:CD2	1:7:766:LYS:HE2	2.47	0.47
5:0:17:ILE:HG22	5:0:739:TRP:O	2.13	0.47
5:0:312:LEU:O	5:0:314:GLN:N	2.48	0.47
5:0:737:SER:O	5:0:737:SER:OG	2.28	0.47
8:6:165:PRO:HG2	8:6:375:HIS:HB3	1.96	0.47
8:6:288:TYR:CG	8:6:288:TYR:O	2.65	0.47
1:7:303:ARG:HA	1:7:320:ASN:CA	2.44	0.47
1:7:411:CYS:HB3	1:7:417:VAL:HG22	1.97	0.47
1:7:466:ARG:HG3	2:Y:4:DA:H5'	1.95	0.47
5:0:119:GLU:HA	5:0:122:LYS:NZ	2.29	0.47
5:0:254:THR:HA	5:0:257:LEU:HD13	1.95	0.47
6:1:339:LEU:HA	6:1:342:ASN:HB3	1.96	0.47
8:6:160:PHE:HA	8:6:305:VAL:HG13	1.96	0.47
8:6:309:PRO:HA	8:6:312:LYS:CE	2.44	0.47
1:7:354:ILE:HG21	1:7:401:CYS:HA	1.97	0.47
1:7:610:ASP:OD2	1:7:676:HIS:N	2.47	0.47
5:0:156:CYS:HB3	5:0:158:TYR:HD2	1.79	0.47
5:0:166:GLU:OE2	5:0:170:TYR:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:0:259:ARG:NH1	5:0:398:ALA:HB2	2.30	0.47
6:1:284:TRP:HA	6:1:287:PHE:HB3	1.95	0.47
1:7:410:LEU:HA	1:7:455:SER:O	2.15	0.47
4:5:54:LEU:HG	11:2:450:ARG:NH2	2.30	0.47
5:0:37:ASN:HD22	5:0:475:PHE:HD2	1.63	0.47
5:0:173:LYS:HD2	5:0:173:LYS:HA	1.75	0.47
5:0:494:PRO:HB2	5:0:701:LEU:HD13	1.97	0.47
11:2:346:LYS:CD	11:2:377:GLN:HG3	2.44	0.47
1:7:462:ASN:ND2	3:W:25:DA:OP1	2.48	0.47
1:7:475:ASP:O	1:7:478:THR:OG1	2.26	0.47
1:7:610:ASP:H	1:7:674:SER:CB	2.27	0.47
4:5:16:ILE:HD13	4:5:19:LEU:HD12	1.96	0.47
5:0:286:TYR:HB3	5:0:326:ARG:NH2	2.29	0.47
5:0:349:LEU:HG	5:0:350:HIS:N	2.29	0.47
5:0:545:LEU:HB2	6:1:355:ASP:O	2.13	0.47
5:0:628:GLN:O	5:0:630:THR:N	2.48	0.47
7:4:236:LEU:HA	7:4:236:LEU:HD23	1.50	0.47
7:4:275:SER:HB2	7:4:281:ARG:C	2.40	0.47
8:6:144:ASN:OD1	8:6:146:HIS:N	2.48	0.47
9:A:625:ALA:O	10:E:137:ILE:O	2.33	0.47
11:2:415:LYS:HZ2	11:2:434:PRO:HG3	1.79	0.47
1:7:461:ALA:HB3	1:7:497:MET:HB2	1.97	0.47
1:7:575:ARG:C	1:7:577:ARG:N	2.73	0.47
5:0:257:LEU:O	5:0:261:THR:HG23	2.14	0.47
5:0:378:SER:O	5:0:382:SER:OG	2.33	0.47
5:0:529:PHE:HB3	5:0:537:MET:HE1	1.96	0.47
5:0:580:SER:CA	6:1:339:LEU:CD2	2.74	0.47
6:1:486:LEU:CA	7:4:55:GLU:CD	2.75	0.47
7:4:263:VAL:C	7:4:265:PRO:HD3	2.40	0.47
8:6:130:LEU:O	8:6:174:MET:HE2	2.15	0.47
8:6:377:ALA:HA	8:6:380:TYR:CD2	2.49	0.47
11:2:90:ASN:ND2	11:2:92:SER:HB2	2.30	0.47
11:2:412:ALA:O	11:2:416:LEU:HB2	2.14	0.47
5:0:489:LYS:HE3	5:0:724:MET:HE1	1.97	0.47
5:0:743:ASP:O	5:0:747:HIS:N	2.44	0.47
11:2:338:SER:CA	11:2:407:GLN:CB	2.85	0.47
2:Y:2:DG:H1'	2:Y:3:DC:H5'	1.97	0.47
5:0:313:PRO:O	5:0:314:GLN:HG2	2.14	0.47
6:1:517:ASN:O	6:1:519:VAL:N	2.48	0.47
6:1:561:LEU:O	6:1:564:PHE:N	2.48	0.47
8:6:148:MET:HE2	8:6:148:MET:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:19:GLN:HG3	11:2:85:HIS:CD2	2.50	0.47
1:7:434:ASN:OD1	1:7:450:SER:OG	2.29	0.46
1:7:680:ARG:HB3	1:7:722:ARG:HB2	1.97	0.46
5:0:201:SER:HA	5:0:225:GLU:CD	2.41	0.46
7:4:255:ASP:N	7:4:256:PRO:HD2	2.24	0.46
8:6:227:HIS:HB3	8:6:318:THR:OG1	2.15	0.46
8:6:309:PRO:HA	8:6:312:LYS:HE3	1.96	0.46
9:A:658:ILE:HA	9:A:661:LYS:HG2	1.97	0.46
1:7:385:VAL:HG13	1:7:537:GLU:HA	1.97	0.46
5:0:77:SER:O	5:0:80:GLU:HG2	2.14	0.46
5:0:478:VAL:HB	5:0:479:LEU:HD12	1.97	0.46
5:0:549:SER:O	5:0:553:MET:HG3	2.14	0.46
6:1:336:ILE:HG22	6:1:337:ILE:HD13	1.97	0.46
8:6:349:CYS:HB3	8:6:353:HIS:H	1.80	0.46
1:7:303:ARG:NE	1:7:321:GLU:O	2.31	0.46
5:0:297:ASP:HB3	5:0:386:ARG:HH22	1.81	0.46
6:1:188:ASN:HB3	6:1:191:LEU:HD12	1.97	0.46
6:1:492:ASN:O	6:1:495:VAL:N	2.48	0.46
9:A:560:GLU:HB3	9:A:562:PHE:CE2	2.49	0.46
1:7:410:LEU:N	1:7:486:ILE:O	2.42	0.46
7:4:197:MET:HE3	7:4:197:MET:HB2	1.57	0.46
9:A:653:LEU:HD21	9:A:657:ARG:NH2	2.30	0.46
1:7:343:PHE:CD1	1:7:344:ARG:N	2.79	0.46
1:7:354:ILE:O	1:7:404:LYS:HE2	2.16	0.46
1:7:550:ALA:O	1:7:701:PHE:O	2.34	0.46
5:0:499:LYS:O	5:0:709:SER:HA	2.14	0.46
9:A:657:ARG:NH2	10:E:101:LEU:HD13	2.30	0.46
11:2:381:GLU:O	11:2:385:ARG:HD3	2.15	0.46
5:0:130:ASP:O	5:0:134:ARG:HG3	2.13	0.46
5:0:607:SER:OG	5:0:664:GLN:OE1	2.20	0.46
6:1:465:SER:O	6:1:470:LEU:N	2.48	0.46
7:4:64:HIS:HA	7:4:253:PHE:HZ	1.81	0.46
1:7:418:MET:HA	1:7:421:ARG:NH1	2.31	0.46
5:0:97:LEU:HB3	5:0:100:GLN:OE1	2.15	0.46
5:0:123:GLU:OE1	5:0:125:LYS:N	2.47	0.46
5:0:193:TYR:OH	5:0:197:ARG:NH2	2.49	0.46
5:0:287:GLU:O	5:0:290:VAL:HG12	2.16	0.46
5:0:680:VAL:C	5:0:681:LEU:HD12	2.41	0.46
6:1:236:THR:HA	6:1:240:VAL:H	1.81	0.46
8:6:276:LEU:O	8:6:280:THR:HG23	2.16	0.46
9:A:628:GLY:CA	10:E:139:ALA:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:383:ILE:HG13	1:7:528:ASN:HA	1.98	0.46
5:0:50:VAL:O	5:0:54:SER:OG	2.24	0.46
1:7:464:ARG:HG2	1:7:466:ARG:NH2	2.31	0.46
5:0:158:TYR:HB3	5:0:191:CYS:N	2.31	0.46
5:0:343:LYS:HZ3	5:0:347:LYS:HD2	1.81	0.46
6:1:188:ASN:CG	6:1:191:LEU:H	2.24	0.46
10:E:165:PHE:O	10:E:169:LEU:HG	2.16	0.46
11:2:13:TYR:O	11:2:16:GLU:HB3	2.15	0.46
11:2:405:HIS:CE1	11:2:409:ARG:HA	2.51	0.46
5:0:127:THR:HA	6:1:348:VAL:CG1	2.42	0.46
5:0:341:TYR:HE1	5:0:366:LEU:HD12	1.81	0.46
6:1:188:ASN:ND2	6:1:190:VAL:HB	2.26	0.46
6:1:192:MET:HE2	6:1:192:MET:HB2	1.86	0.46
8:6:145:ARG:HD3	8:6:266:LEU:HD12	1.98	0.46
5:0:142:LYS:HG3	5:0:143:ARG:N	2.30	0.45
5:0:191:CYS:HB2	12:0:801:SF4:S2	2.56	0.45
5:0:252:LEU:HD23	5:0:252:LEU:HA	1.69	0.45
5:0:681:LEU:HD23	5:0:686:PHE:CE1	2.52	0.45
6:1:184:LEU:HD12	6:1:184:LEU:HA	1.66	0.45
6:1:194:VAL:HA	6:1:197:GLU:CD	2.42	0.45
11:2:334:ILE:C	11:2:409:ARG:HH22	2.13	0.45
11:2:465:SER:HA	11:2:489:LYS:HE3	1.98	0.45
1:7:352:LEU:HD12	1:7:352:LEU:HA	1.76	0.45
5:0:311:VAL:CG1	5:0:317:LEU:HD11	2.45	0.45
8:6:108:LYS:O	8:6:109:ARG:NE	2.48	0.45
8:6:164:ASN:O	8:6:166:ILE:N	2.49	0.45
8:6:429:CYS:SG	8:6:430:GLU:N	2.89	0.45
9:A:657:ARG:NE	10:E:101:LEU:HD13	2.31	0.45
11:2:337:GLY:O	11:2:406:PRO:HB2	2.17	0.45
1:7:135:SER:N	1:7:140:ARG:O	2.50	0.45
1:7:581:TYR:CD1	1:7:713:THR:HB	2.52	0.45
5:0:273:GLU:HA	5:0:276:LYS:HE2	1.97	0.45
5:0:343:LYS:HG2	5:0:347:LYS:HZ3	1.82	0.45
7:4:135:LEU:HA	7:4:137:LYS:NZ	2.31	0.45
7:4:276:CYS:SG	7:4:279:THR:N	2.76	0.45
8:6:127:ILE:HG12	8:6:221:LEU:HD11	1.99	0.45
8:6:182:VAL:HG11	8:6:199:ILE:HD11	1.98	0.45
9:A:658:ILE:HA	9:A:661:LYS:HE2	1.97	0.45
1:7:370:LEU:HA	1:7:373:MET:HG3	1.97	0.45
1:7:501:VAL:O	1:7:505:ILE:HG12	2.17	0.45
5:0:92:TYR:OH	5:0:96:GLU:OE2	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:0:227:SER:C	5:0:229:ASP:N	2.74	0.45
6:1:389:LEU:HD23	6:1:389:LEU:HA	1.60	0.45
9:A:656:LEU:HD11	10:E:133:ILE:HG21	1.99	0.45
1:7:267:ASP:C	1:7:348:ARG:HH21	2.24	0.45
5:0:140:GLN:HA	5:0:143:ARG:HE	1.81	0.45
5:0:380:ARG:O	5:0:383:LEU:HD23	2.16	0.45
5:0:408:LEU:HD23	5:0:408:LEU:HA	1.72	0.45
7:4:31:GLU:HG3	7:4:180:THR:HA	1.99	0.45
7:4:117:ARG:HA	7:4:120:ASN:ND2	2.31	0.45
11:2:381:GLU:CD	11:2:384:ARG:HE	2.24	0.45
1:7:394:LEU:HD21	1:7:424:PHE:CZ	2.52	0.45
1:7:495:ALA:HB1	1:7:527:LEU:HD21	1.98	0.45
6:1:251:LEU:O	6:1:255:LYS:N	2.26	0.45
11:2:7:LYS:NZ	11:2:9:SER:HA	2.32	0.45
1:7:449:GLU:H	1:7:449:GLU:HG2	1.55	0.45
1:7:550:ALA:HB1	1:7:701:PHE:CG	2.51	0.45
1:7:765:LEU:HD22	10:E:128:LYS:NZ	2.32	0.45
2:Y:4:DA:H2''	2:Y:5:DA:O4'	2.17	0.45
7:4:153:MET:HE3	7:4:153:MET:HB2	1.61	0.45
7:4:177:LEU:HD12	7:4:211:ASP:O	2.17	0.45
7:4:266:ASN:CG	7:4:267:HIS:H	2.24	0.45
10:E:130:LEU:HB2	10:E:149:ILE:HD11	1.97	0.45
11:2:43:ALA:O	11:2:47:ILE:HG12	2.17	0.45
1:7:498:PHE:CD2	1:7:527:LEU:HD22	2.52	0.45
5:0:162:LEU:HG	5:0:167:VAL:HG23	1.98	0.45
7:4:60:PHE:CD1	7:4:248:LEU:HD22	2.52	0.45
10:E:124:VAL:CG1	10:E:159:PHE:HB3	2.47	0.45
11:2:47:ILE:O	11:2:51:VAL:HG23	2.17	0.45
11:2:238:LYS:H	11:2:269:PHE:N	2.14	0.45
1:7:417:VAL:HG21	1:7:456:THR:HB	1.98	0.45
5:0:223:SER:O	5:0:225:GLU:N	2.50	0.45
5:0:471:ARG:NH2	5:0:646:TYR:HB3	2.31	0.45
7:4:40:PHE:O	7:4:43:GLU:HG2	2.16	0.45
8:6:263:VAL:HG13	8:6:277:CYS:SG	2.56	0.45
1:7:484:PHE:CZ	1:7:511:LEU:HB2	2.52	0.44
2:Y:1:DC:H2''	2:Y:2:DG:C8	2.52	0.44
5:0:525:MET:O	5:0:528:GLU:HG2	2.17	0.44
5:0:730:PRO:C	5:0:732:ASP:H	2.24	0.44
8:6:293:ASP:OD1	8:6:295:THR:N	2.44	0.44
8:6:322:MET:HE2	8:6:369:MET:HB3	1.98	0.44
9:A:585:PHE:HE2	9:A:655:LYS:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:648:SER:C	10:E:148:MET:HE3	2.42	0.44
1:7:415:VAL:CG1	2:Y:3:DC:P	3.04	0.44
5:0:745:ILE:H	5:0:745:ILE:HG13	1.51	0.44
6:1:201:ASN:OD1	6:1:201:ASN:N	2.49	0.44
7:4:288:ILE:HD11	7:4:293:LEU:CD1	2.47	0.44
9:A:657:ARG:CG	10:E:101:LEU:HD22	2.42	0.44
11:2:67:ASN:ND2	11:2:67:ASN:N	2.64	0.44
1:7:252:GLY:HA2	1:7:316:PHE:CZ	2.52	0.44
5:0:83:LEU:HD23	5:0:83:LEU:HA	1.56	0.44
5:0:327:ARG:HD2	5:0:329:GLU:HG2	1.98	0.44
5:0:341:TYR:CE2	5:0:345:ARG:HG3	2.52	0.44
5:0:594:ARG:HB3	5:0:594:ARG:NH1	2.32	0.44
5:0:668:ARG:HD3	5:0:668:ARG:HA	1.74	0.44
6:1:192:MET:O	6:1:196:GLN:HG3	2.17	0.44
1:7:715:GLU:N	1:7:715:GLU:OE1	2.50	0.44
5:0:209:SER:OG	5:0:210:TYR:N	2.51	0.44
5:0:338:LEU:O	5:0:342:LEU:HG	2.17	0.44
6:1:254:GLU:O	6:1:257:LEU:HG	2.17	0.44
6:1:270:TYR:OH	6:1:279:LYS:CE	2.65	0.44
7:4:175:ARG:HB3	7:4:209:PRO:HD2	1.99	0.44
8:6:247:ILE:O	8:6:250:THR:OG1	2.22	0.44
1:7:303:ARG:HA	1:7:320:ASN:C	2.42	0.44
1:7:353:ASP:HB3	1:7:451:GLY:CA	2.48	0.44
1:7:406:SER:HB2	1:7:482:TRP:CE3	2.52	0.44
5:0:25:MET:SD	5:0:55:LEU:HB2	2.57	0.44
5:0:279:SER:HA	5:0:282:LEU:HG	1.99	0.44
5:0:298:ILE:O	5:0:299:LEU:HD23	2.17	0.44
5:0:702:SER:N	5:0:705:ASP:OD2	2.51	0.44
1:7:307:ASP:HA	1:7:340:GLU:O	2.17	0.44
1:7:347:HIS:O	1:7:347:HIS:CG	2.70	0.44
1:7:463:THR:HB	3:W:24:DG:H4'	1.99	0.44
5:0:272:SER:HA	5:0:275:ARG:HH21	1.83	0.44
7:4:60:PHE:CE1	7:4:253:PHE:HD1	2.35	0.44
7:4:224:LEU:O	7:4:228:THR:HG22	2.18	0.44
11:2:370:PHE:HZ	11:2:375:LEU:HD22	1.82	0.44
1:7:385:VAL:HG13	1:7:538:ALA:H	1.82	0.44
1:7:392:LYS:HG2	1:7:513:LEU:HD13	2.00	0.44
1:7:438:PHE:CG	1:7:473:VAL:HG21	2.53	0.44
5:0:171:LEU:HB3	5:0:172:PRO:HD2	2.00	0.44
5:0:419:ILE:HG23	5:0:436:ARG:HB3	2.00	0.44
5:0:521:ASN:O	5:0:524:SER:OG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:0:610:ILE:HD13	5:0:610:ILE:HA	1.79	0.44
6:1:270:TYR:CD2	6:1:279:LYS:HB2	2.46	0.44
7:4:255:ASP:H	7:4:256:PRO:HD2	1.64	0.44
10:E:102:TRP:CD2	10:E:102:TRP:O	2.70	0.44
11:2:401:GLU:OE1	11:2:433:LEU:HD22	2.18	0.44
1:7:382:GLY:HA2	1:7:532:GLY:HA3	1.99	0.44
1:7:540:TRP:HE3	1:7:544:SER:HB3	1.82	0.44
4:5:35:LEU:HB2	4:5:39:HIS:HB2	2.00	0.44
5:0:250:LEU:HD12	5:0:251:ASP:H	1.83	0.44
5:0:435:MET:HB2	5:0:435:MET:HE2	1.73	0.44
5:0:581:LEU:O	5:0:584:GLU:HG3	2.17	0.44
8:6:263:VAL:HG22	8:6:288:TYR:HD1	1.81	0.44
9:A:656:LEU:HD21	10:E:133:ILE:HG23	2.00	0.44
1:7:440:SER:HB3	1:7:467:SER:H	1.83	0.44
5:0:500:GLY:HA3	5:0:521:ASN:OD1	2.18	0.44
7:4:163:ILE:O	7:4:166:GLU:HG3	2.18	0.44
11:2:338:SER:N	11:2:351:SER:HB2	2.33	0.44
11:2:386:ALA:HB1	11:2:391:ILE:HB	1.99	0.44
5:0:628:GLN:HE22	5:0:657:ASP:CG	2.25	0.43
11:2:409:ARG:HB2	11:2:410:ARG:NH1	2.33	0.43
11:2:506:LYS:HD2	11:2:507:ARG:HH21	1.82	0.43
1:7:302:GLU:C	1:7:322:SER:H	2.26	0.43
1:7:476:PHE:CE2	1:7:482:TRP:HZ2	2.35	0.43
1:7:690:ILE:HG22	1:7:694:LYS:NZ	2.33	0.43
4:5:3:ARG:HD3	11:2:460:SER:HB2	1.99	0.43
4:5:54:LEU:CG	11:2:450:ARG:HH21	2.30	0.43
5:0:18:TYR:HD2	5:0:673:LYS:HZ1	1.65	0.43
5:0:136:MET:HE3	5:0:136:MET:HB2	1.87	0.43
5:0:594:ARG:HB3	5:0:594:ARG:HH11	1.83	0.43
5:0:732:ASP:OD1	5:0:733:GLN:N	2.51	0.43
5:0:745:ILE:HD12	5:0:746:LYS:N	2.33	0.43
6:1:278:PHE:O	6:1:282:GLU:CD	2.61	0.43
8:6:137:LEU:HD23	8:6:137:LEU:HA	1.79	0.43
8:6:251:ILE:O	8:6:255:VAL:HG12	2.18	0.43
1:7:497:MET:SD	1:7:498:PHE:N	2.91	0.43
1:7:681:ARG:HH22	3:W:28:DT:H71	1.83	0.43
5:0:294:HIS:O	5:0:294:HIS:CG	2.71	0.43
5:0:330:HIS:O	5:0:333:SER:OG	2.32	0.43
5:0:541:PHE:HE1	5:0:623:ILE:HG13	1.84	0.43
5:0:568:LEU:HD13	5:0:594:ARG:NH1	2.33	0.43
10:E:130:LEU:CB	10:E:149:ILE:CD1	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:75:GLN:HA	11:2:78:ILE:HG12	2.00	0.43
1:7:413:SER:O	1:7:417:VAL:N	2.42	0.43
4:5:54:LEU:HD21	11:2:450:ARG:HG2	2.01	0.43
5:0:79:ILE:HD13	5:0:79:ILE:HA	1.84	0.43
5:0:113:ASN:OD1	5:0:113:ASN:N	2.48	0.43
5:0:249:SER:OG	5:0:250:LEU:N	2.51	0.43
5:0:306:PHE:CE2	5:0:307:VAL:HG23	2.54	0.43
5:0:338:LEU:HD22	5:0:338:LEU:HA	1.81	0.43
5:0:409:ILE:HA	5:0:409:ILE:HD12	1.78	0.43
5:0:583:LEU:HA	5:0:583:LEU:HD12	1.79	0.43
5:0:726:GLN:CG	8:6:292:LEU:CD2	2.96	0.43
7:4:244:LEU:O	7:4:245:ILE:C	2.61	0.43
8:6:269:GLN:HG3	8:6:288:TYR:CE2	2.41	0.43
9:A:658:ILE:HG12	9:A:661:LYS:HE2	2.00	0.43
11:2:336:ASP:C	11:2:351:SER:HB3	2.22	0.43
1:7:461:ALA:HB3	1:7:497:MET:HE2	2.01	0.43
1:7:624:LYS:O	1:7:625:PRO:C	2.61	0.43
1:7:656:LYS:HZ3	1:7:686:ARG:HH21	1.67	0.43
5:0:66:HIS:NE2	5:0:229:ASP:O	2.51	0.43
5:0:109:THR:OG1	5:0:113:ASN:ND2	2.48	0.43
5:0:110:SER:CB	6:1:346:ASP:HA	2.42	0.43
5:0:731:LYS:HE2	5:0:731:LYS:HB2	1.78	0.43
7:4:193:TYR:CE2	7:4:197:MET:HE1	2.54	0.43
7:4:218:SER:HA	7:4:237:HIS:NE2	2.33	0.43
9:A:649:TRP:CZ3	10:E:149:ILE:CG1	2.78	0.43
1:7:544:SER:C	1:7:549:ILE:HD11	2.43	0.43
1:7:598:HIS:HB2	1:7:605:ILE:HD11	1.99	0.43
5:0:140:GLN:O	5:0:144:LYS:HG3	2.19	0.43
5:0:394:GLU:HA	5:0:397:THR:HG23	2.01	0.43
5:0:497:ILE:HD12	5:0:713:ALA:HB2	2.00	0.43
5:0:572:GLU:OE2	5:0:579:THR:HG23	2.17	0.43
9:A:649:TRP:CG	10:E:168:VAL:HG11	2.53	0.43
10:E:106:ILE:O	10:E:106:ILE:HG23	2.17	0.43
1:7:433:GLU:OE2	1:7:434:ASN:ND2	2.52	0.43
1:7:459:MET:HG2	1:7:470:SER:HB2	2.00	0.43
1:7:548:HIS:O	1:7:694:LYS:O	2.36	0.43
1:7:698:ASP:HB2	1:7:701:PHE:CB	2.46	0.43
4:5:5:ARG:HD3	11:2:458:LEU:HG	1.99	0.43
5:0:424:GLU:H	5:0:432:ASN:HD21	1.67	0.43
5:0:571:VAL:HG22	5:0:572:GLU:H	1.83	0.43
6:1:194:VAL:O	6:1:197:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:6:214:LEU:HA	8:6:214:LEU:HD13	1.82	0.43
8:6:432:CYS:N	8:6:454:CYS:SG	2.91	0.43
1:7:349:ASN:O	1:7:405:LYS:CE	2.66	0.43
5:0:333:SER:HB2	5:0:337:ARG:NH1	2.34	0.43
7:4:137:LYS:O	7:4:140:ILE:HB	2.18	0.43
8:6:126:LEU:O	8:6:169:MET:HA	2.19	0.43
5:0:104:ARG:HH22	5:0:171:LEU:HB2	1.83	0.43
5:0:549:SER:O	5:0:552:SER:OG	2.33	0.43
8:6:124:ARG:NH1	8:6:305:VAL:O	2.39	0.43
8:6:282:TYR:CD1	8:6:282:TYR:N	2.84	0.43
8:6:300:LEU:HD23	8:6:300:LEU:HA	1.87	0.43
11:2:63:ASP:HA	11:2:74:PHE:CE2	2.53	0.43
11:2:201:TRP:CE3	11:2:201:TRP:HA	2.54	0.43
11:2:380:ARG:HG2	11:2:384:ARG:HH22	1.84	0.43
5:0:132:LYS:HE3	5:0:132:LYS:HB2	1.60	0.43
5:0:223:SER:O	5:0:226:VAL:HG22	2.19	0.43
5:0:265:ASN:O	5:0:269:GLU:HG2	2.19	0.43
5:0:568:LEU:HA	5:0:568:LEU:HD12	1.67	0.43
5:0:620:VAL:C	5:0:621:LEU:HD12	2.44	0.43
5:0:625:ILE:HB	5:0:686:PHE:CE1	2.54	0.43
6:1:254:GLU:OE1	6:1:254:GLU:N	2.36	0.43
6:1:374:ILE:O	6:1:378:MET:HG2	2.19	0.43
8:6:149:ILE:HD13	8:6:149:ILE:HA	1.82	0.43
10:E:124:VAL:HG13	10:E:159:PHE:HB3	2.01	0.43
11:2:67:ASN:HD22	11:2:67:ASN:N	2.16	0.43
1:7:267:ASP:C	1:7:348:ARG:NH2	2.77	0.42
1:7:385:VAL:HB	1:7:514:THR:HB	2.00	0.42
1:7:425:LEU:HA	1:7:425:LEU:HD13	1.86	0.42
1:7:609:SER:CB	1:7:674:SER:HB2	2.48	0.42
1:7:690:ILE:HG22	1:7:694:LYS:HZ2	1.84	0.42
5:0:18:TYR:CE2	5:0:673:LYS:HD2	2.54	0.42
5:0:263:GLY:O	5:0:267:LEU:HG	2.19	0.42
6:1:378:MET:HE2	6:1:378:MET:HB3	1.80	0.42
7:4:216:GLY:O	7:4:237:HIS:HE1	2.02	0.42
7:4:305:CYS:O	7:4:307:ALA:N	2.52	0.42
9:A:588:VAL:HG22	9:A:589:GLU:H	1.83	0.42
11:2:71:LYS:H	11:2:71:LYS:HG3	1.63	0.42
11:2:276:LEU:O	11:2:280:SER:OG	2.20	0.42
1:7:252:GLY:HA2	1:7:316:PHE:HZ	1.84	0.42
1:7:407:VAL:HB	1:7:452:LEU:HD13	2.02	0.42
1:7:550:ALA:HB2	1:7:701:PHE:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:0:289:LEU:HB2	5:0:326:ARG:NH1	2.34	0.42
5:0:533:THR:OG1	5:0:567:LYS:NZ	2.53	0.42
5:0:544:TYR:OH	5:0:574:PRO:HD3	2.19	0.42
5:0:570:LEU:HD23	5:0:570:LEU:HA	1.84	0.42
7:4:228:THR:OG1	7:4:234:VAL:N	2.52	0.42
9:A:649:TRP:CE2	10:E:148:MET:HB2	2.53	0.42
11:2:359:VAL:HA	11:2:362:LEU:HG	2.00	0.42
11:2:380:ARG:O	11:2:384:ARG:HB2	2.18	0.42
11:2:381:GLU:HG2	11:2:384:ARG:HH21	1.84	0.42
5:0:241:ASP:OD1	5:0:242:ASN:N	2.53	0.42
5:0:432:ASN:OD1	5:0:432:ASN:N	2.51	0.42
10:E:134:SER:O	10:E:139:ALA:HB3	2.19	0.42
10:E:146:ILE:HG22	10:E:149:ILE:HB	2.01	0.42
11:2:7:LYS:HG2	11:2:9:SER:N	2.34	0.42
11:2:12:GLN:N	11:2:12:GLN:OE1	2.51	0.42
11:2:18:PRO:HB2	11:2:20:GLN:NE2	2.32	0.42
11:2:20:GLN:OE1	11:2:20:GLN:N	2.49	0.42
11:2:481:LEU:HD13	11:2:484:LYS:HG2	2.01	0.42
1:7:308:ASP:O	1:7:340:GLU:N	2.46	0.42
1:7:344:ARG:NH1	1:7:378:ARG:HH21	2.17	0.42
1:7:383:ILE:O	1:7:534:LYS:HA	2.19	0.42
5:0:53:LEU:HD12	5:0:85:GLU:OE2	2.20	0.42
5:0:383:LEU:O	5:0:387:THR:HG23	2.19	0.42
5:0:514:ASN:ND2	5:0:553:MET:HG2	2.34	0.42
6:1:197:GLU:HA	6:1:201:ASN:OD1	2.19	0.42
6:1:259:ILE:HD13	6:1:263:TYR:CE2	2.50	0.42
6:1:265:ILE:HG13	6:1:266:VAL:N	2.33	0.42
6:1:288:PHE:O	6:1:292:LEU:HB2	2.19	0.42
6:1:329:LEU:HA	6:1:329:LEU:HD13	1.83	0.42
9:A:626:ILE:O	10:E:138:GLY:HA3	2.18	0.42
10:E:102:TRP:HD1	10:E:165:PHE:CB	2.32	0.42
11:2:32:CYS:O	11:2:35:ILE:HG12	2.20	0.42
11:2:338:SER:N	11:2:351:SER:CB	2.83	0.42
1:7:308:ASP:O	1:7:340:GLU:HG2	2.19	0.42
6:1:210:TRP:O	6:1:213:ARG:N	2.52	0.42
6:1:262:ASN:HB3	6:1:263:TYR:CE2	2.55	0.42
6:1:552:MET:O	6:1:556:THR:HG22	2.20	0.42
8:6:107:LYS:HG2	8:6:109:ARG:HH12	1.84	0.42
11:2:338:SER:C	11:2:407:GLN:CD	2.87	0.42
1:7:469:ASP:O	1:7:473:VAL:HG23	2.19	0.42
1:7:663:ASP:OD1	1:7:663:ASP:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:0:136:MET:HE2	5:0:154:GLU:HG2	2.01	0.42
5:0:527:VAL:HB	5:0:559:ILE:HD11	2.01	0.42
6:1:264:PRO:O	6:1:268:LYS:HG2	2.19	0.42
6:1:556:THR:O	6:1:560:PHE:HD1	2.01	0.42
5:0:154:GLU:OE1	5:0:154:GLU:N	2.52	0.42
5:0:161:ASN:HA	5:0:164:ASN:OD1	2.19	0.42
5:0:253:THR:HG22	5:0:255:ASP:H	1.84	0.42
5:0:494:PRO:HA	5:0:679:MET:O	2.19	0.42
1:7:306:GLU:OE2	1:7:346:ASP:HB2	2.19	0.42
1:7:498:PHE:CE2	1:7:527:LEU:HD22	2.55	0.42
1:7:559:CYS:HA	1:7:560:PRO:HD3	1.92	0.42
6:1:371:THR:O	6:1:374:ILE:HB	2.20	0.42
11:2:338:SER:O	11:2:407:GLN:OE1	2.38	0.42
1:7:365:TYR:HA	1:7:368:LYS:HG2	2.01	0.42
8:6:143:PRO:HB2	8:6:147:ALA:HB3	2.02	0.42
8:6:325:PRO:HB2	8:6:347:TYR:HB3	2.00	0.42
11:2:51:VAL:HG12	11:2:52:PHE:CD1	2.55	0.42
1:7:460:VAL:HA	1:7:474:MET:HE3	2.02	0.42
1:7:492:VAL:O	3:W:26:DG:OP1	2.37	0.42
1:7:565:PHE:HE2	1:7:763:VAL:HG11	1.84	0.42
5:0:237:ALA:N	5:0:460:SER:OG	2.45	0.42
6:1:370:GLY:C	6:1:372:VAL:H	2.28	0.42
7:4:87:TYR:HB3	7:4:88:PRO:HD3	2.02	0.42
8:6:130:LEU:HD23	8:6:130:LEU:HA	1.80	0.42
8:6:347:TYR:O	8:6:355:LYS:HA	2.20	0.42
11:2:360:LEU:O	11:2:364:VAL:HG12	2.20	0.42
5:0:53:LEU:HD23	5:0:53:LEU:HA	1.69	0.41
5:0:188:LYS:O	5:0:190:LEU:HD23	2.20	0.41
5:0:322:PRO:O	5:0:325:ILE:HG13	2.20	0.41
5:0:553:MET:O	5:0:556:THR:HB	2.20	0.41
6:1:273:ASN:HA	6:1:276:LYS:NZ	2.34	0.41
6:1:281:PRO:HD2	6:1:282:GLU:OE2	2.20	0.41
6:1:344:GLN:C	6:1:347:PRO:HD2	2.45	0.41
8:6:137:LEU:HG	8:6:204:PRO:HG2	2.01	0.41
8:6:152:TYR:CG	8:6:297:LEU:HD21	2.54	0.41
10:E:104:MET:HB3	10:E:104:MET:HE3	1.76	0.41
11:2:457:SER:O	11:2:492:PHE:HA	2.20	0.41
1:7:386:LEU:HD12	1:7:513:LEU:HD22	2.01	0.41
1:7:544:SER:O	1:7:549:ILE:HD11	2.20	0.41
5:0:97:LEU:HD23	5:0:97:LEU:HA	1.75	0.41
7:4:175:ARG:HA	7:4:208:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:254:ILE:HD12	7:4:254:ILE:O	2.19	0.41
7:4:293:LEU:HD13	7:4:293:LEU:HA	1.82	0.41
5:0:76:MET:HB3	6:1:346:ASP:OD2	2.21	0.41
5:0:143:ARG:O	5:0:147:GLU:HG2	2.20	0.41
6:1:274:VAL:N	6:1:275:PRO:HD2	2.35	0.41
7:4:33:ALA:HB3	7:4:36:LEU:CB	2.50	0.41
8:6:224:VAL:O	8:6:230:ARG:NH2	2.53	0.41
8:6:246:ASP:OD1	8:6:248:HIS:N	2.53	0.41
9:A:652:LEU:CD2	10:E:137:ILE:HD11	2.49	0.41
10:E:101:LEU:HD23	10:E:101:LEU:HA	1.66	0.41
1:7:693:ALA:HA	1:7:695:ARG:NH2	2.36	0.41
1:7:768:GLU:CG	10:E:107:ARG:HH22	2.31	0.41
5:0:20:GLU:H	5:0:20:GLU:CD	2.24	0.41
5:0:294:HIS:NE2	5:0:297:ASP:HB3	2.35	0.41
5:0:505:ALA:HB1	5:0:684:ARG:HB3	2.02	0.41
6:1:253:ARG:HA	6:1:256:ILE:HG12	2.01	0.41
6:1:562:LYS:HA	6:1:562:LYS:HD2	1.80	0.41
8:6:107:LYS:HE3	8:6:107:LYS:HB3	1.92	0.41
10:E:125:LEU:CD2	10:E:149:ILE:CD1	2.89	0.41
1:7:510:LYS:HB2	1:7:531:ILE:HG23	2.01	0.41
5:0:27:ASP:N	5:0:27:ASP:OD1	2.53	0.41
6:1:270:TYR:HE2	6:1:284:TRP:NE1	2.19	0.41
6:1:321:PHE:O	6:1:324:LYS:HG2	2.19	0.41
7:4:126:VAL:O	7:4:129:ILE:HG22	2.20	0.41
7:4:273:ARG:CG	7:4:273:ARG:HH21	2.33	0.41
1:7:219:SER:O	1:7:336:PRO:HG2	2.21	0.41
1:7:372:LYS:HD3	1:7:535:LEU:O	2.20	0.41
5:0:127:THR:CA	6:1:348:VAL:HG11	2.47	0.41
5:0:312:LEU:HB3	5:0:315:ASP:OD1	2.20	0.41
5:0:629:TYR:OH	5:0:636:LYS:HE2	2.21	0.41
5:0:685:ARG:HB3	5:0:689:LYS:NZ	2.34	0.41
9:A:585:PHE:HZ	9:A:659:ARG:HH11	1.66	0.41
1:7:415:VAL:HB	1:7:419:GLN:NE2	2.35	0.41
1:7:421:ARG:NH1	1:7:437:VAL:HG11	2.36	0.41
5:0:280:GLN:CD	5:0:280:GLN:H	2.29	0.41
5:0:309:THR:O	5:0:309:THR:OG1	2.33	0.41
5:0:393:VAL:O	5:0:396:PHE:N	2.43	0.41
7:4:90:SER:HB3	8:6:407:GLN:HE22	1.84	0.41
5:0:341:TYR:CE1	5:0:366:LEU:HD12	2.55	0.41
5:0:577:GLN:OE1	6:1:340:ASP:OD2	2.39	0.41
5:0:709:SER:OG	5:0:710:THR:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:62:ASN:OD1	7:4:118:PHE:HB3	2.20	0.41
8:6:449:HIS:ND1	8:6:449:HIS:N	2.69	0.41
1:7:330:CYS:HA	1:7:335:TYR:HB2	2.03	0.41
1:7:349:ASN:HA	1:7:350:PRO:HD2	1.92	0.41
1:7:362:ILE:HD11	1:7:367:GLU:HB3	2.03	0.41
3:W:25:DA:C2'	3:W:26:DG:H5'	2.50	0.41
4:5:27:MET:HE2	4:5:27:MET:HB2	1.78	0.41
5:0:113:ASN:O	5:0:114:LEU:HD23	2.21	0.41
5:0:117:HIS:HD2	5:0:156:CYS:HA	1.86	0.41
5:0:158:TYR:HB3	5:0:190:LEU:C	2.45	0.41
5:0:486:THR:O	5:0:486:THR:OG1	2.32	0.41
5:0:654:LEU:HD13	5:0:654:LEU:HA	1.90	0.41
5:0:710:THR:O	5:0:714:ILE:HG12	2.21	0.41
5:0:741:TYR:O	5:0:743:ASP:N	2.54	0.41
6:1:257:LEU:HA	6:1:260:PHE:CD2	2.56	0.41
6:1:259:ILE:HG23	6:1:263:TYR:CD2	2.56	0.41
7:4:118:PHE:N	7:4:118:PHE:CD1	2.89	0.41
8:6:132:CYS:O	8:6:175:ARG:HG2	2.21	0.41
8:6:287:PHE:N	8:6:287:PHE:CD1	2.89	0.41
8:6:308:LEU:HD23	8:6:308:LEU:H	1.86	0.41
10:E:102:TRP:O	10:E:102:TRP:CE3	2.74	0.41
11:2:20:GLN:O	11:2:24:ARG:HG2	2.20	0.41
11:2:347:ILE:HD11	11:2:378:ILE:HB	2.02	0.41
11:2:431:GLN:HE21	11:2:431:GLN:HB2	1.54	0.41
1:7:519:ARG:NE	1:7:521:ASP:HB2	2.35	0.41
5:0:471:ARG:HH22	5:0:647:ARG:H	1.69	0.41
5:0:588:LYS:HE3	5:0:588:LYS:HB2	1.88	0.41
5:0:746:LYS:HE3	5:0:746:LYS:HB2	1.85	0.41
6:1:204:LEU:HD21	6:1:208:GLU:HG2	2.03	0.41
1:7:633:GLN:OE1	1:7:636:ARG:NH1	2.54	0.40
5:0:119:GLU:HA	5:0:122:LYS:HZ3	1.86	0.40
7:4:66:ALA:HB2	7:4:118:PHE:HZ	1.85	0.40
7:4:137:LYS:HG3	7:4:139:GLN:HG3	2.01	0.40
7:4:228:THR:O	7:4:233:GLY:N	2.51	0.40
8:6:145:ARG:O	8:6:149:ILE:HG12	2.21	0.40
1:7:265:PRO:O	1:7:269:LEU:HG	2.21	0.40
1:7:376:ASN:H	1:7:380:ARG:NH2	2.19	0.40
1:7:581:TYR:CZ	1:7:715:GLU:HB2	2.56	0.40
1:7:696:ARG:HG2	1:7:701:PHE:CZ	2.56	0.40
5:0:133:CYS:HB2	12:0:801:SF4:S4	2.61	0.40
5:0:689:LYS:O	5:0:692:GLN:N	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:233:GLY:O	7:4:263:VAL:HG11	2.21	0.40
7:4:271:ASP:HB3	7:4:273:ARG:NH2	2.36	0.40
8:6:141:LEU:HD23	8:6:145:ARG:HG2	2.02	0.40
8:6:222:LEU:HD22	8:6:222:LEU:HA	1.75	0.40
8:6:237:GLY:HA2	8:6:266:LEU:HG	2.03	0.40
8:6:322:MET:HE2	8:6:322:MET:HB3	1.82	0.40
11:2:403:HIS:C	11:2:405:HIS:H	2.30	0.40
1:7:415:VAL:HG22	2:Y:3:DC:OP1	2.22	0.40
4:5:17:LYS:NZ	4:5:37:ASP:HA	2.37	0.40
5:0:213:LEU:HD12	5:0:213:LEU:HA	1.79	0.40
5:0:267:LEU:HD11	5:0:399:LEU:HD13	2.03	0.40
5:0:379:GLU:H	5:0:379:GLU:HG3	1.54	0.40
5:0:481:LYS:HA	5:0:481:LYS:HD3	1.73	0.40
6:1:339:LEU:HD12	6:1:342:ASN:HD22	1.85	0.40
7:4:87:TYR:HE1	7:4:121:VAL:HG22	1.87	0.40
7:4:297:SER:C	7:4:299:ILE:H	2.29	0.40
7:4:298:ILE:C	7:4:300:PRO:HD3	2.47	0.40
11:2:86:LEU:HD12	11:2:87:LEU:N	2.36	0.40
1:7:354:ILE:HD11	1:7:405:LYS:O	2.22	0.40
1:7:408:ILE:HG23	1:7:482:TRP:CE3	2.56	0.40
1:7:613:TYR:C	1:7:615:LEU:N	2.79	0.40
2:Y:-3:DA:N1	3:W:28:DT:O2	2.54	0.40
5:0:227:SER:HA	5:0:230:SER:OG	2.21	0.40
5:0:545:LEU:HA	5:0:545:LEU:HD13	1.79	0.40
6:1:385:MET:HE3	6:1:385:MET:HB2	1.72	0.40
8:6:182:VAL:HG21	8:6:199:ILE:HD11	2.04	0.40
8:6:227:HIS:CD2	8:6:320:VAL:HG11	2.57	0.40
8:6:332:THR:C	8:6:334:THR:H	2.29	0.40
9:A:662:LEU:HD12	9:A:662:LEU:HA	1.95	0.40
11:2:19:GLN:O	11:2:22:GLN:HB2	2.21	0.40
11:2:338:SER:H	11:2:351:SER:C	2.29	0.40
11:2:394:ASP:OD1	11:2:395:GLN:N	2.49	0.40
11:2:478:ILE:HD13	11:2:500:GLN:HE22	1.86	0.40
5:0:37:ASN:HA	5:0:456:VAL:O	2.21	0.40
5:0:131:GLU:OE1	5:0:132:LYS:N	2.55	0.40
5:0:158:TYR:HB2	5:0:191:CYS:HB3	2.04	0.40
5:0:210:TYR:O	5:0:211:HIS:C	2.65	0.40
5:0:493:LEU:HD11	5:0:720:PHE:HB2	2.04	0.40
5:0:509:ARG:HB2	5:0:685:ARG:CZ	2.52	0.40
5:0:754:GLN:H	5:0:754:GLN:HG3	1.64	0.40
6:1:343:ILE:C	6:1:345:ASP:N	2.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:157:LEU:HA	7:4:157:LEU:HD23	1.86	0.40
7:4:192:GLN:O	7:4:195:PRO:HD2	2.22	0.40
8:6:161:PHE:CG	8:6:189:PRO:HG3	2.56	0.40
11:2:361:SER:HA	11:2:364:VAL:HG12	2.03	0.40
11:2:380:ARG:HG2	11:2:384:ARG:NH2	2.37	0.40
11:2:410:ARG:H	11:2:410:ARG:NE	2.18	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	7	634/843 (75%)	562 (89%)	65 (10%)	7 (1%)	11	46
4	5	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
5	0	752/778 (97%)	632 (84%)	118 (16%)	2 (0%)	36	72
6	1	357/642 (56%)	280 (78%)	40 (11%)	37 (10%)	0	6
7	4	280/338 (83%)	210 (75%)	65 (23%)	5 (2%)	6	34
8	6	349/461 (76%)	284 (81%)	59 (17%)	6 (2%)	7	36
9	A	101/754 (13%)	93 (92%)	7 (7%)	1 (1%)	12	49
10	E	58/177 (33%)	47 (81%)	9 (16%)	2 (3%)	3	21
11	2	456/513 (89%)	380 (83%)	71 (16%)	5 (1%)	11	46
All	All	3051/4572 (67%)	2547 (84%)	439 (14%)	65 (2%)	8	30

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1	230	PRO
6	1	236	THR

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Mol	Chain	Res	Type
6	1	239	PRO
6	1	338	ASP
6	1	344	GLN
6	1	354	PRO
6	1	518	ASN
7	4	255	ASP
8	6	411	PRO
8	6	425	SER
11	2	335	PRO
1	7	625	PRO
6	1	225	SER
6	1	240	VAL
6	1	241	ALA
6	1	247	VAL
6	1	277	ASN
6	1	301	ILE
6	1	307	GLY
6	1	352	ASN
6	1	389	LEU
6	1	492	ASN
6	1	516	HIS
7	4	115	TYR
11	2	331	ASN
11	2	341	VAL
1	7	576	LYS
6	1	235	SER
6	1	244	GLU
6	1	246	LYS
6	1	281	PRO
6	1	493	ASN
6	1	494	GLU
6	1	517	ASN
8	6	417	LYS
8	6	422	LEU
9	A	603	SER
10	E	147	GLU
1	7	655	SER
1	7	696	ARG
1	7	741	GLY
5	0	228	LYS
6	1	243	SER
6	1	309	VAL

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Mol	Chain	Res	Type
6	1	353	ARG
6	1	467	GLN
6	1	495	VAL
7	4	114	MET
8	6	412	ILE
8	6	415	ASN
10	E	106	ILE
11	2	70	GLY
1	7	667	ALA
5	0	172	PRO
6	1	487	ASN
1	7	551	ASN
6	1	232	ASN
6	1	238	LYS
6	1	249	VAL
6	1	484	LEU
7	4	290	SER
6	1	280	GLU
11	2	337	GLY
7	4	256	PRO
6	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	7	417/737 (57%)	388 (93%)	29 (7%)	14	35
4	5	53/60 (88%)	52 (98%)	1 (2%)	50	67
5	0	686/707 (97%)	587 (86%)	99 (14%)	3	13
6	1	169/589 (29%)	144 (85%)	25 (15%)	3	13
7	4	198/300 (66%)	163 (82%)	35 (18%)	2	9
8	6	247/418 (59%)	204 (83%)	43 (17%)	2	9
9	A	87/678 (13%)	86 (99%)	1 (1%)	65	76
10	E	56/165 (34%)	50 (89%)	6 (11%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	2	258/468 (55%)	228 (88%)	30 (12%)	5	18
All	All	2171/4122 (53%)	1902 (88%)	269 (12%)	7	17

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	7	342	ASP
1	7	343	PHE
1	7	349	ASN
1	7	356	LEU
1	7	357	LYS
1	7	378	ARG
1	7	385	VAL
1	7	393	THR
1	7	440	SER
1	7	444	GLU
1	7	445	MET
1	7	449	GLU
1	7	477	LEU
1	7	485	ILE
1	7	490	VAL
1	7	514	THR
1	7	518	VAL
1	7	530	LEU
1	7	549	ILE
1	7	575	ARG
1	7	576	LYS
1	7	586	THR
1	7	607	VAL
1	7	657	VAL
1	7	662	ILE
1	7	701	PHE
1	7	709	VAL
1	7	735	VAL
1	7	737	THR
4	5	54	LEU
5	0	6	ASP
5	0	11	LEU
5	0	17	ILE
5	0	28	ILE
5	0	32	LEU
5	0	34	VAL

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Mol	Chain	Res	Type
5	0	39	ILE
5	0	46	THR
5	0	48	LYS
5	0	66	HIS
5	0	72	CYS
5	0	80	GLU
5	0	109	THR
5	0	110	SER
5	0	124	ARG
5	0	127	THR
5	0	130	ASP
5	0	131	GLU
5	0	148	ASP
5	0	155	LEU
5	0	157	GLU
5	0	162	LEU
5	0	170	TYR
5	0	173	LYS
5	0	190	LEU
5	0	196	VAL
5	0	198	ARG
5	0	206	ILE
5	0	207	ILE
5	0	208	TYR
5	0	218	ILE
5	0	221	ARG
5	0	222	VAL
5	0	227	SER
5	0	231	ILE
5	0	239	ASN
5	0	248	LEU
5	0	249	SER
5	0	254	THR
5	0	255	ASP
5	0	273	GLU
5	0	280	GLN
5	0	284	ASP
5	0	290	VAL
5	0	298	ILE
5	0	312	LEU
5	0	318	THR
5	0	329	GLU

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Mol	Chain	Res	Type
5	0	338	LEU
5	0	350	HIS
5	0	355	THR
5	0	379	GLU
5	0	382	SER
5	0	383	LEU
5	0	413	GLU
5	0	417	LEU
5	0	438	THR
5	0	462	THR
5	0	477	THR
5	0	486	THR
5	0	487	LEU
5	0	498	THR
5	0	506	ILE
5	0	512	ILE
5	0	515	ASP
5	0	533	THR
5	0	537	MET
5	0	538	VAL
5	0	539	VAL
5	0	545	LEU
5	0	556	THR
5	0	560	LEU
5	0	563	VAL
5	0	568	LEU
5	0	573	THR
5	0	597	ILE
5	0	598	LEU
5	0	599	LEU
5	0	614	HIS
5	0	620	VAL
5	0	625	ILE
5	0	639	LEU
5	0	649	ARG
5	0	651	ASN
5	0	654	LEU
5	0	657	ASP
5	0	659	MET
5	0	674	ASP
5	0	680	VAL
5	0	683	ASP

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Mol	Chain	Res	Type
5	0	705	ASP
5	0	710	THR
5	0	711	ASP
5	0	715	SER
5	0	721	LEU
5	0	729	ASP
5	0	741	TYR
5	0	745	ILE
5	0	747	HIS
6	1	185	LEU
6	1	198	THR
6	1	201	ASN
6	1	214	ILE
6	1	216	LEU
6	1	263	TYR
6	1	266	VAL
6	1	276	LYS
6	1	279	LYS
6	1	280	GLU
6	1	282	GLU
6	1	287	PHE
6	1	315	LEU
6	1	329	LEU
6	1	339	LEU
6	1	346	ASP
6	1	372	VAL
6	1	378	MET
6	1	382	SER
6	1	389	LEU
6	1	516	HIS
6	1	551	ARG
6	1	553	LEU
6	1	558	CYS
6	1	597	PHE
7	4	26	LEU
7	4	27	THR
7	4	30	ILE
7	4	86	LEU
7	4	134	GLU
7	4	136	GLU
7	4	137	LYS
7	4	149	LEU

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Mol	Chain	Res	Type
7	4	162	ARG
7	4	163	ILE
7	4	176	LEU
7	4	180	THR
7	4	197	MET
7	4	204	THR
7	4	210	ILE
7	4	211	ASP
7	4	212	VAL
7	4	228	THR
7	4	234	VAL
7	4	236	LEU
7	4	244	LEU
7	4	248	LEU
7	4	252	MET
7	4	254	ILE
7	4	258	LEU
7	4	260	PRO
7	4	261	ILE
7	4	263	VAL
7	4	264	LYS
7	4	272	PHE
7	4	273	ARG
7	4	274	THR
7	4	288	ILE
7	4	293	LEU
7	4	297	SER
8	6	116	THR
8	6	118	TYR
8	6	119	GLN
8	6	125	SER
8	6	136	MET
8	6	150	ILE
8	6	158	HIS
8	6	161	PHE
8	6	164	ASN
8	6	166	ILE
8	6	185	VAL
8	6	191	ASP
8	6	194	ASP
8	6	202	GLN
8	6	214	LEU

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Mol	Chain	Res	Type
8	6	222	LEU
8	6	243	ASP
8	6	254	LEU
8	6	263	VAL
8	6	267	SER
8	6	274	LYS
8	6	280	THR
8	6	290	ILE
8	6	292	LEU
8	6	293	ASP
8	6	297	LEU
8	6	306	THR
8	6	310	VAL
8	6	311	ASN
8	6	326	THR
8	6	336	CYS
8	6	352	CYS
8	6	353	HIS
8	6	356	VAL
8	6	363	CYS
8	6	372	LEU
8	6	381	HIS
8	6	382	HIS
8	6	384	MET
8	6	406	CYS
8	6	429	CYS
8	6	444	ILE
8	6	448	LEU
9	A	662	LEU
10	E	103	SER
10	E	104	MET
10	E	107	ARG
10	E	147	GLU
10	E	148	MET
10	E	149	ILE
11	2	8	HIS
11	2	11	THR
11	2	14	LEU
11	2	16	GLU
11	2	17	ILE
11	2	27	THR
11	2	28	SER

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Mol	Chain	Res	Type
11	2	61	ASP
11	2	67	ASN
11	2	72	LEU
11	2	84	LEU
11	2	88	ILE
11	2	95	THR
11	2	100	LEU
11	2	112	LEU
11	2	208	LEU
11	2	286	ARG
11	2	346	LYS
11	2	347	ILE
11	2	348	TYR
11	2	356	GLN
11	2	383	ILE
11	2	387	LEU
11	2	413	GLU
11	2	416	LEU
11	2	431	GLN
11	2	432	VAL
11	2	433	LEU
11	2	450	ARG
11	2	486	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	7	347	HIS
1	7	366	GLN
1	7	442	ASN
1	7	539	ASN
1	7	584	ASN
1	7	641	GLN
1	7	740	HIS
4	5	11	GLN
5	0	21	GLN
5	0	239	ASN
6	1	226	GLN
6	1	258	ASN
6	1	262	ASN
6	1	342	ASN
7	4	161	ASN

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Mol	Chain	Res	Type
8	6	151	GLN
8	6	190	GLN
8	6	375	HIS
9	A	558	ASN
10	E	141	GLN
11	2	67	ASN
11	2	69	ASN
11	2	90	ASN
11	2	395	GLN
11	2	431	GLN
11	2	500	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 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	$\# Z > 2$
12	SF4	0	801	5	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
12	SF4	0	801	5	-	-	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	0	801	SF4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

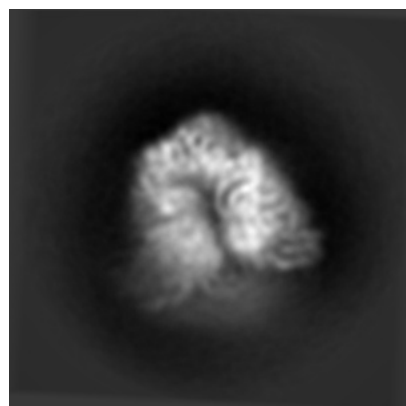
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22576. These allow visual inspection of the internal detail of the map and identification of artifacts.

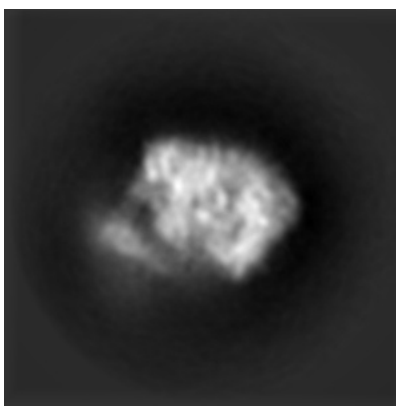
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

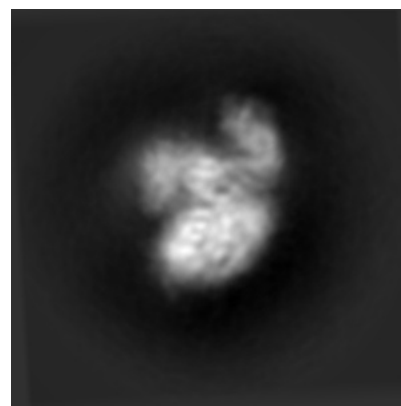
6.1.1 Primary map



X

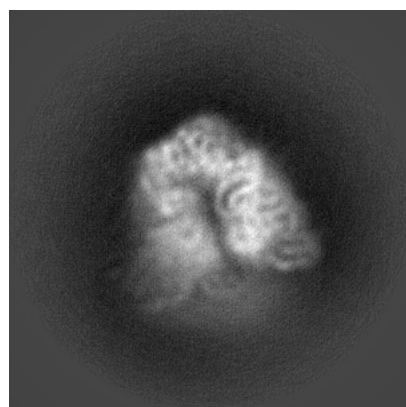


Y

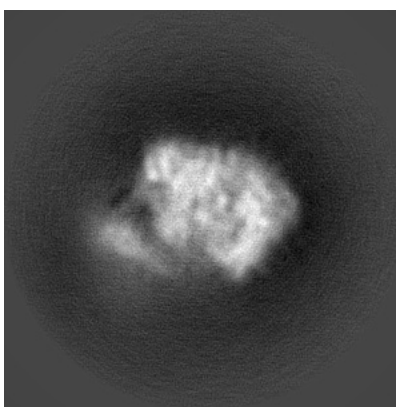


Z

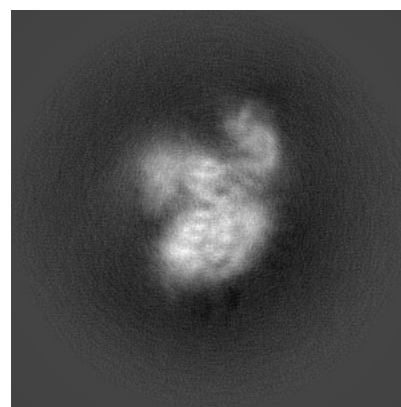
6.1.2 Raw map



X



Y

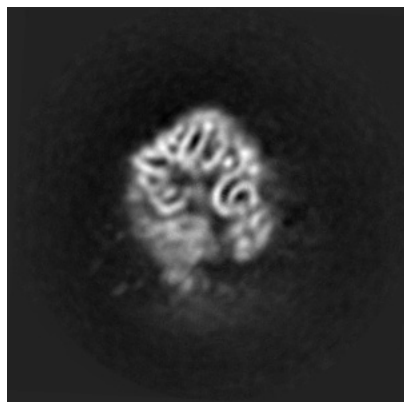


Z

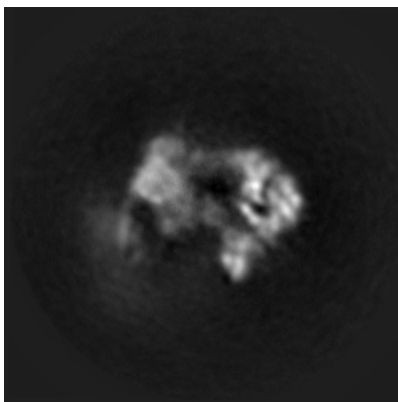
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

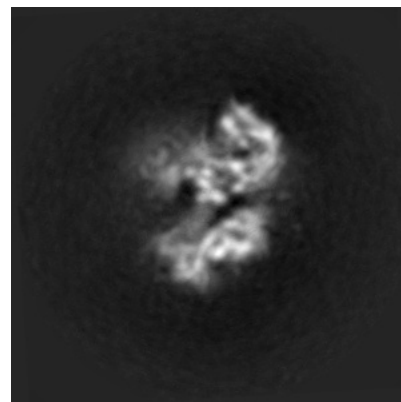
6.2.1 Primary map



X Index: 150

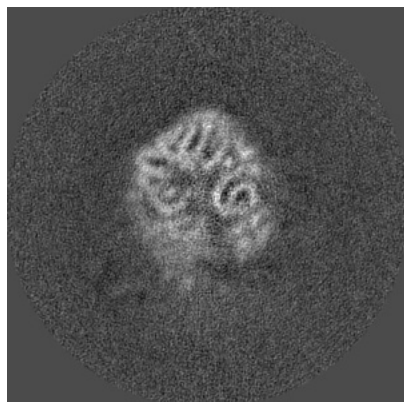


Y Index: 150

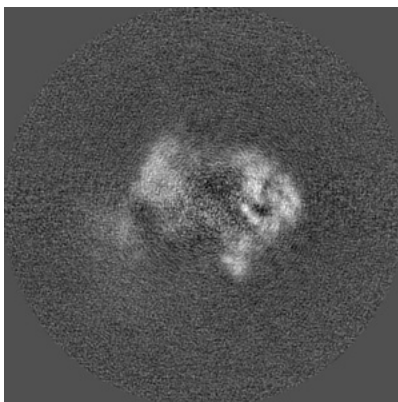


Z Index: 150

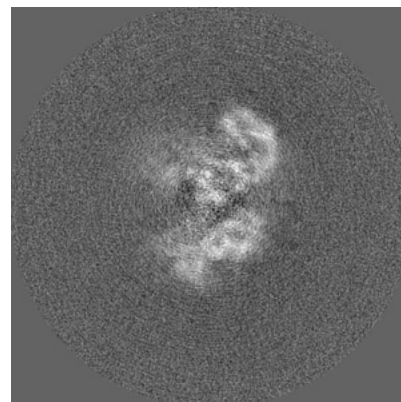
6.2.2 Raw map



X Index: 150



Y Index: 150

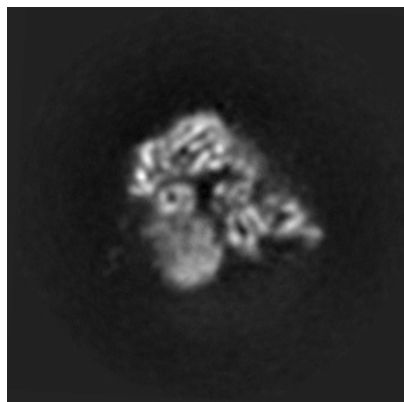


Z Index: 150

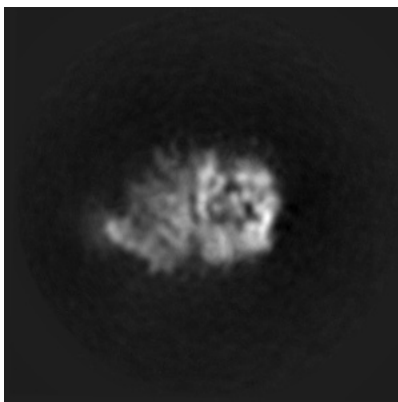
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

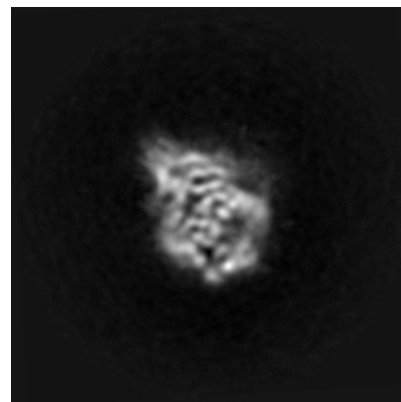
6.3.1 Primary map



X Index: 161

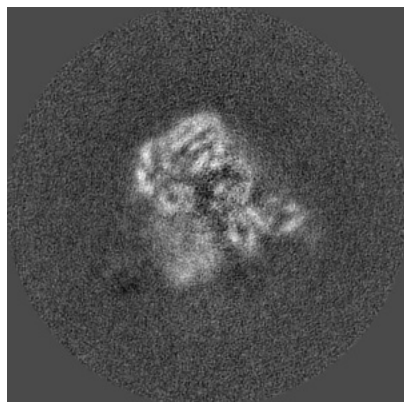


Y Index: 118

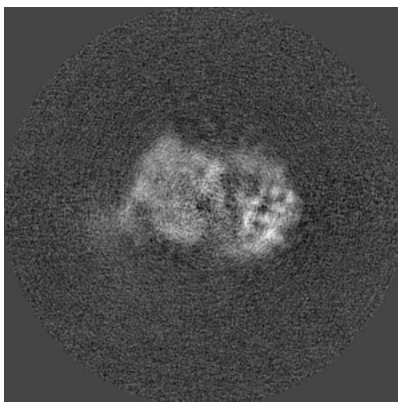


Z Index: 184

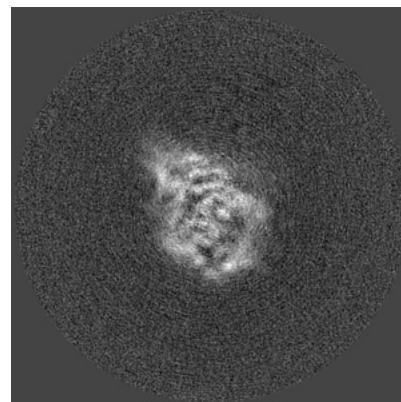
6.3.2 Raw map



X Index: 160



Y Index: 137



Z Index: 184

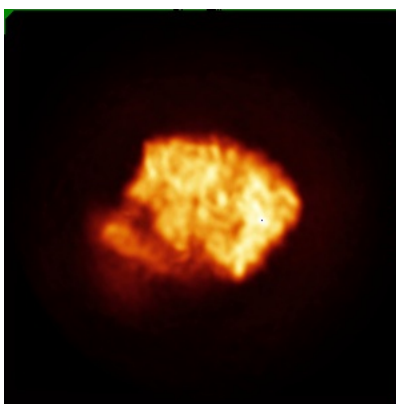
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

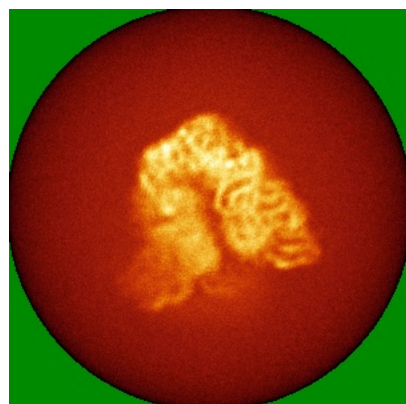


Y

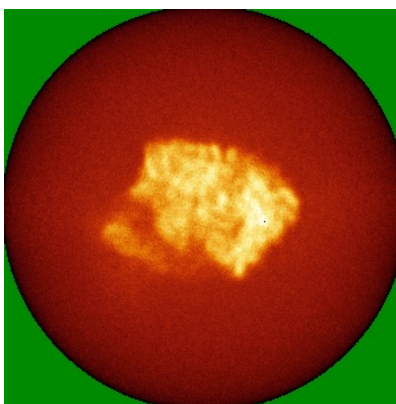


Z

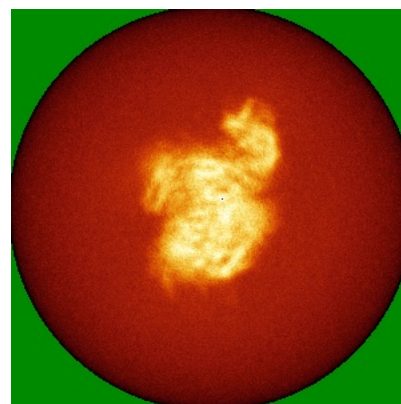
6.4.2 Raw map



X



Y

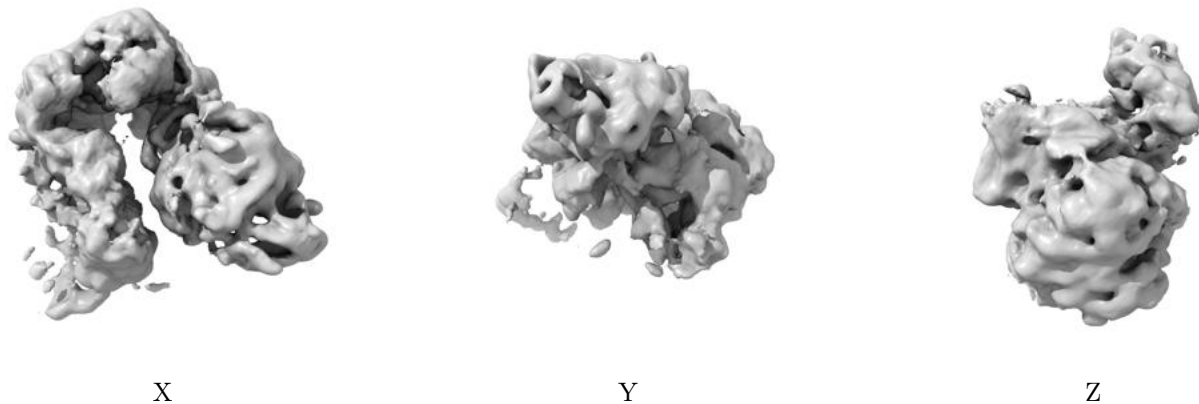


Z

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.

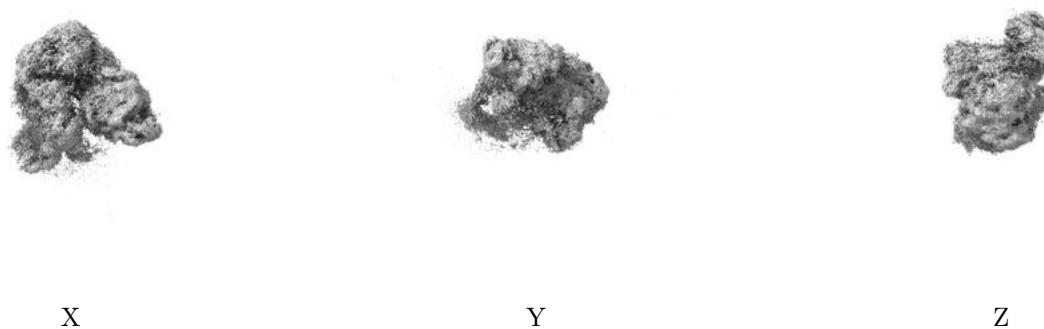
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00239. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

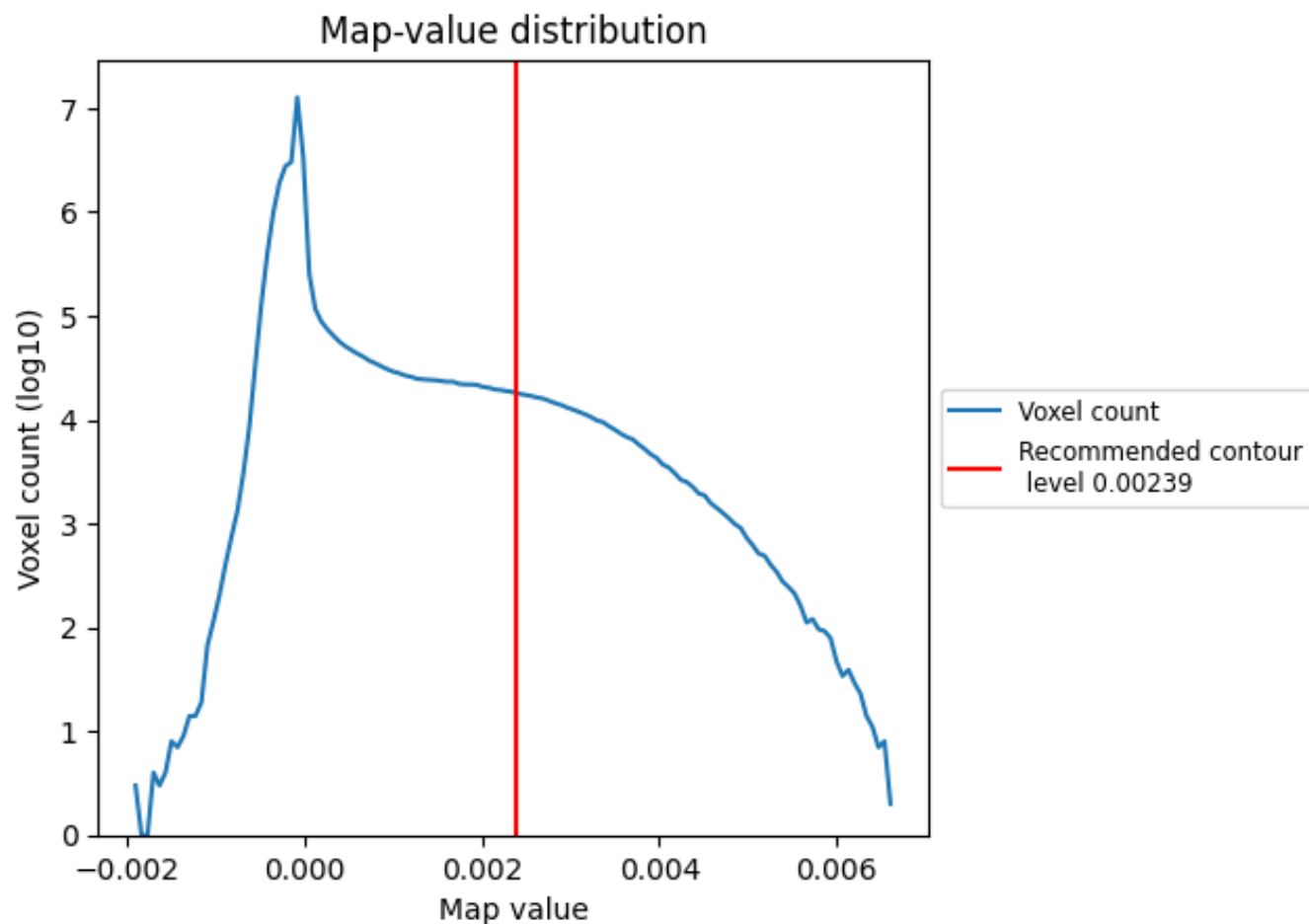
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

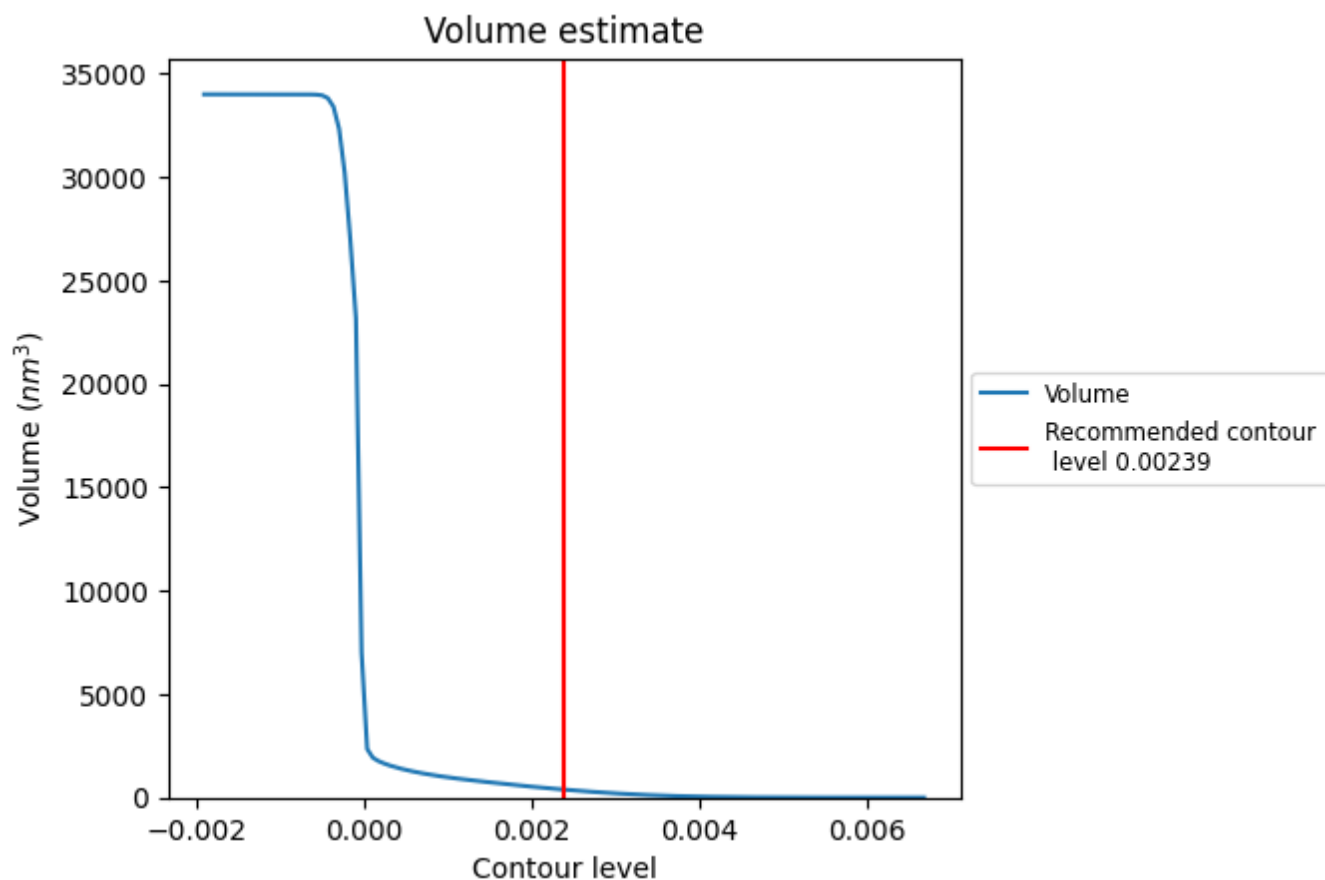
This section contains the results of statistical analysis of the map.

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.

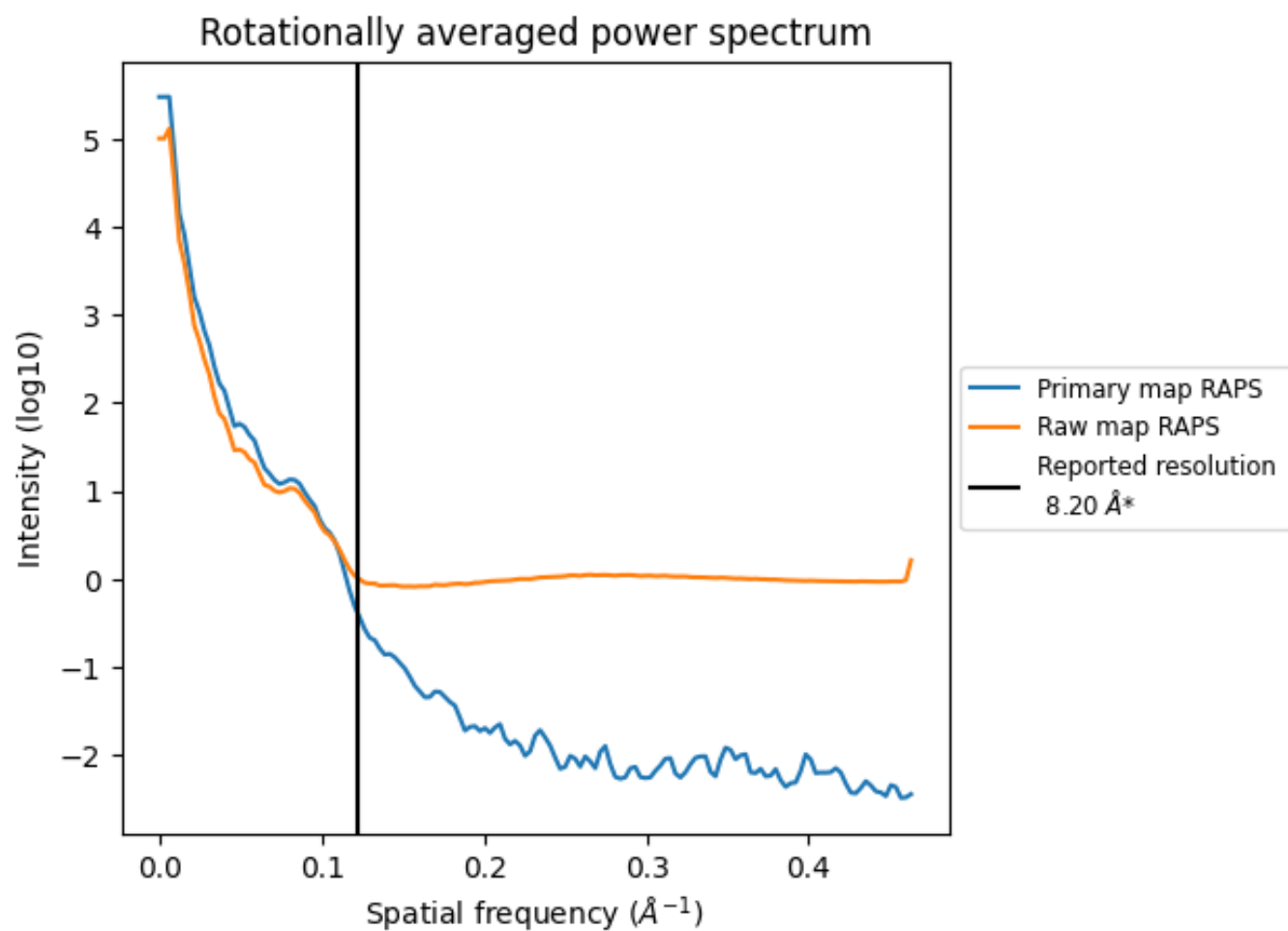
7.2 Volume estimate [i](#)



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 ⓘ

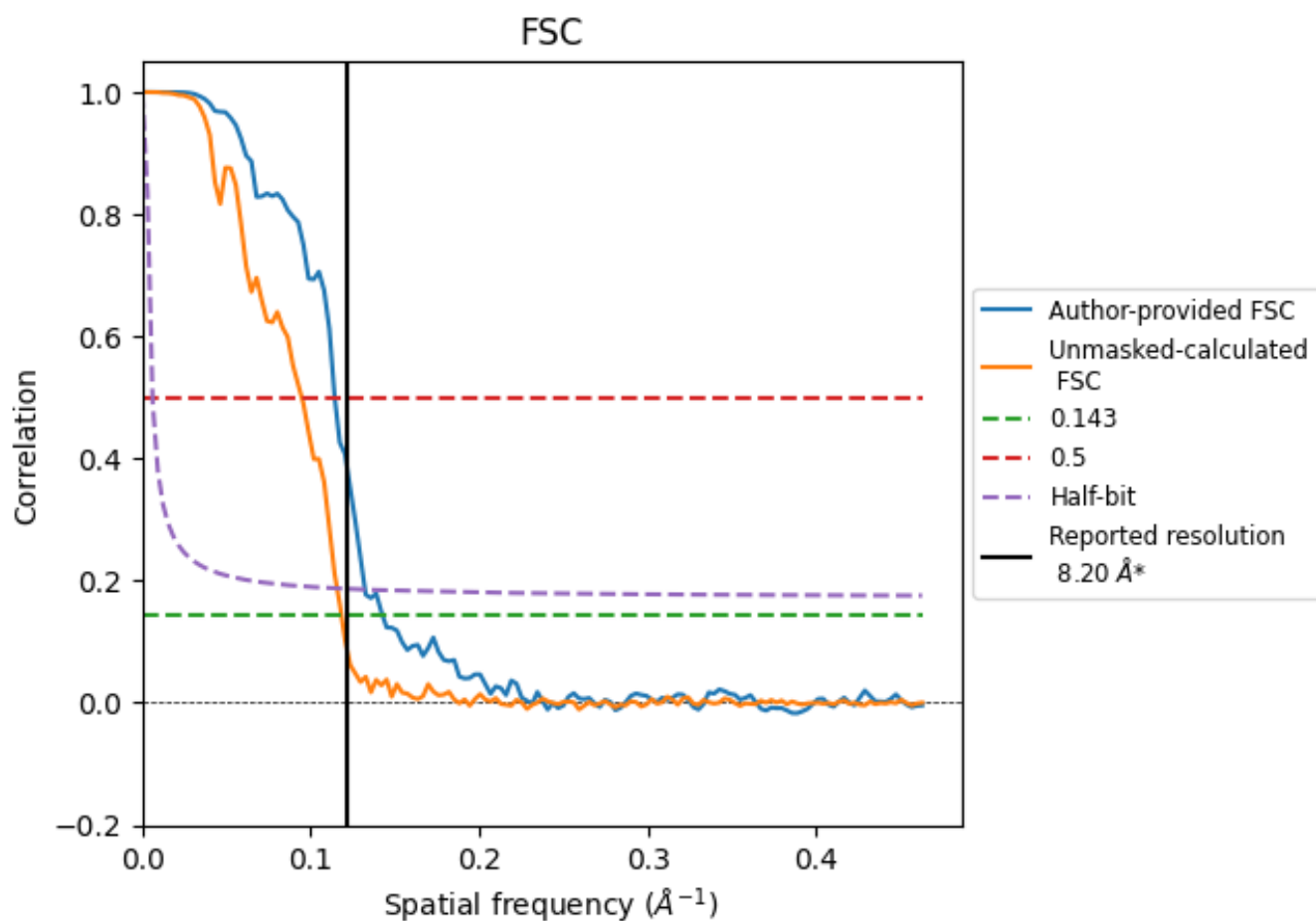


*Reported resolution corresponds to spatial frequency of 0.122 Å⁻¹

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 $0.122 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

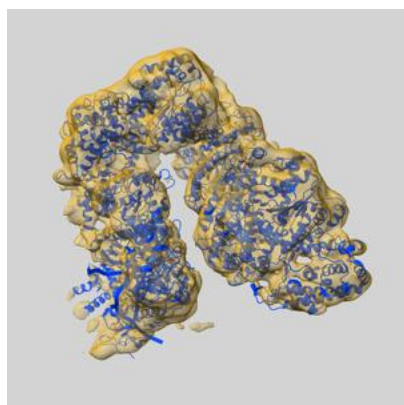
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.20	-	-
Author-provided FSC curve	7.01	8.75	7.56
Unmasked-calculated*	8.46	10.56	8.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.01 differs from the reported value 8.2 by more than 10 %

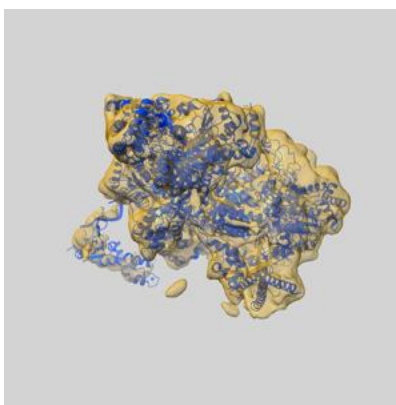
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22576 and PDB model 7M2U. Per-residue inclusion information can be found in section [3](#) on page [7](#).

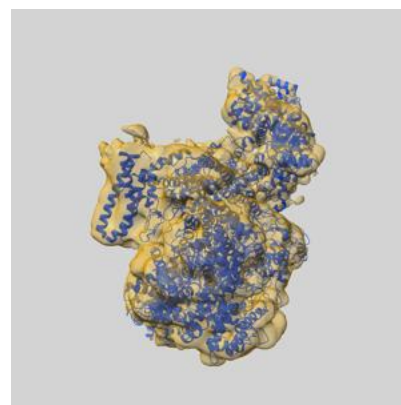
9.1 Map-model overlay [i](#)



X



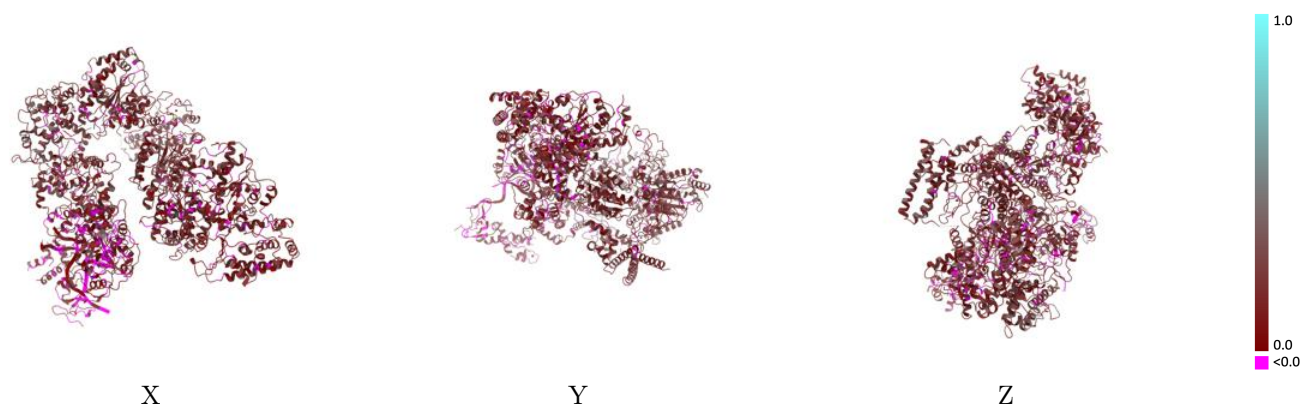
Y



Z

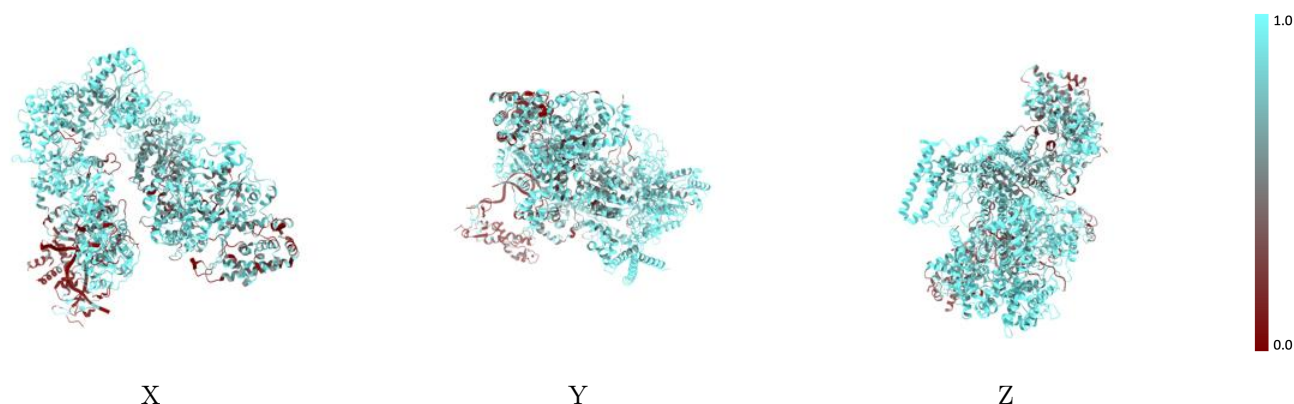
The images above show the 3D surface view of the map at the recommended contour level 0.00239 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



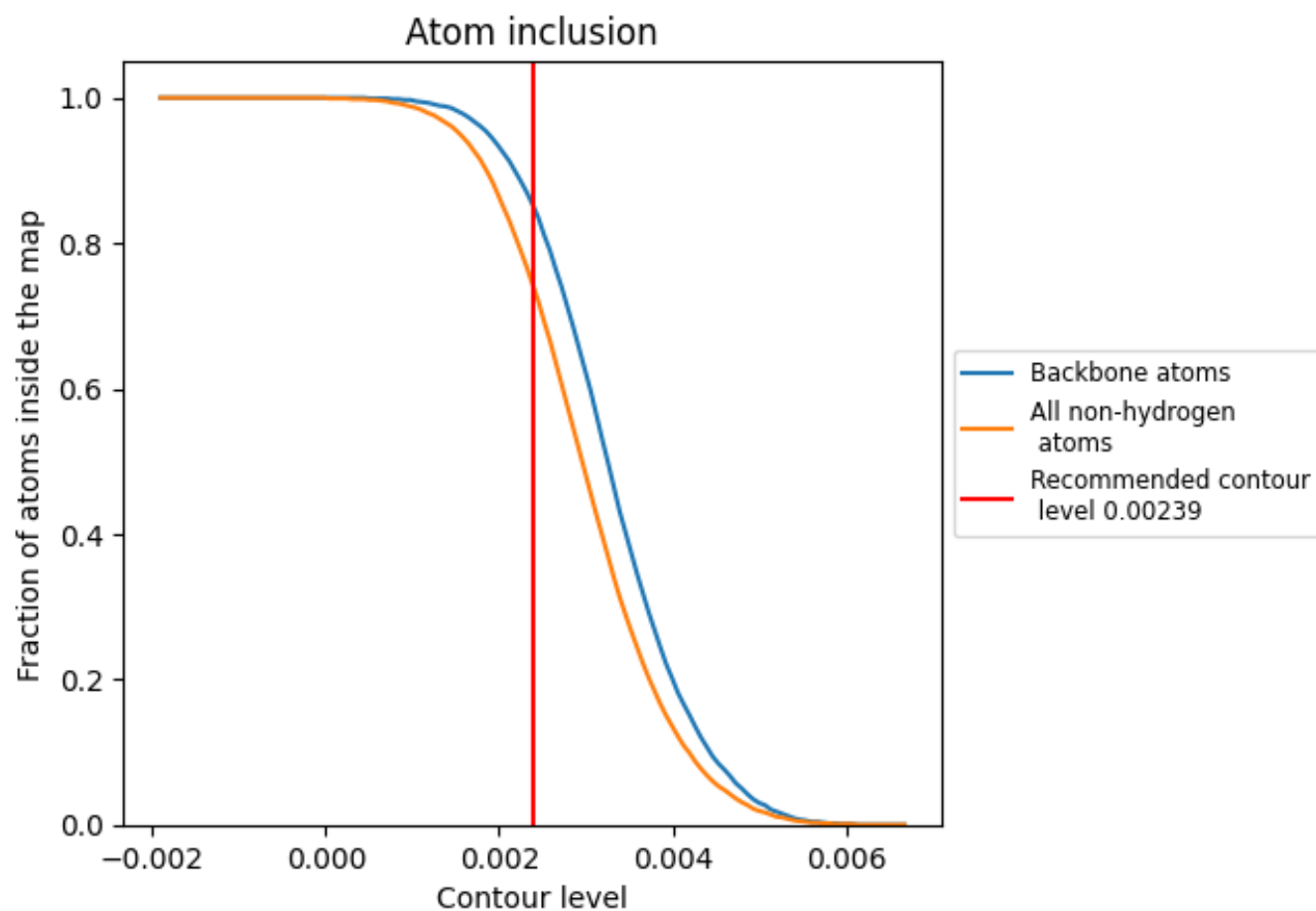
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.00239).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% 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 (0.00239) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7420	0.1460
0	0.7310	0.1490
1	0.8310	0.1980
2	0.8410	0.1740
4	0.8720	0.1750
5	0.9020	0.1370
6	0.7970	0.1710
7	0.7540	0.1010
A	0.2800	0.0620
E	0.1060	0.0650
W	0.1900	0.0530
Y	0.0640	0.0450

1.0

0.0

<0.0