



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:41 AM UTC

PDB ID : 5X6O / pdb_00005x6o
EMDB ID : EMD-6708
Title : Intact ATR/Mec1-ATRIP/Ddc2 complex
Authors : Wang, X.; Ran, T.; Cai, G.
Deposited on : 2017-02-22
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

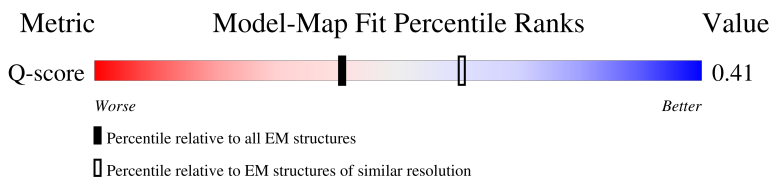
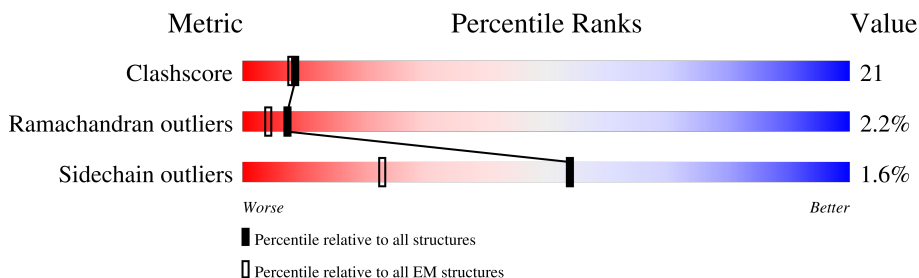
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	C	2368	
2	G	747	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19309 atoms, of which 0 are hydrogens and 0 are deuteriums.

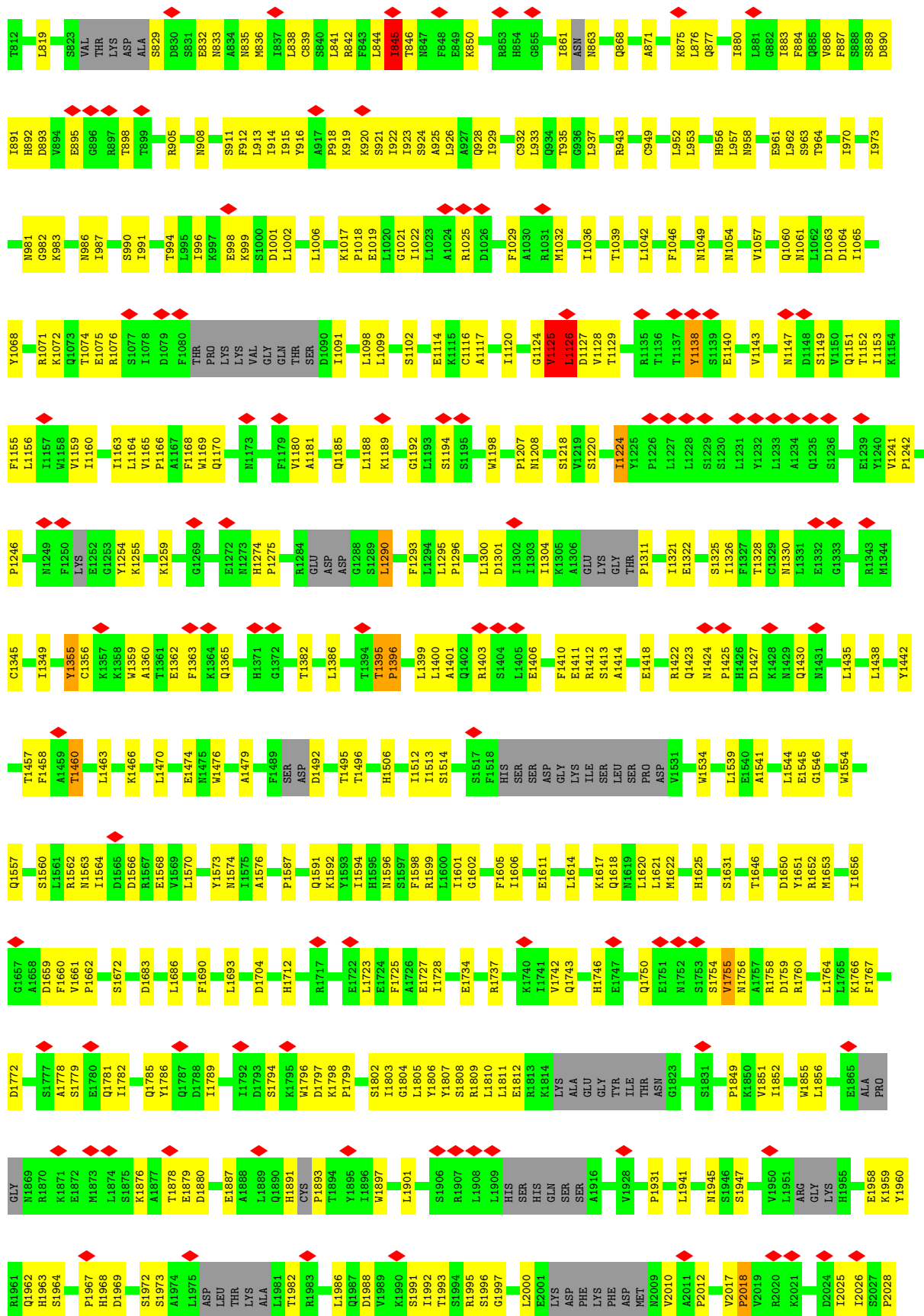
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

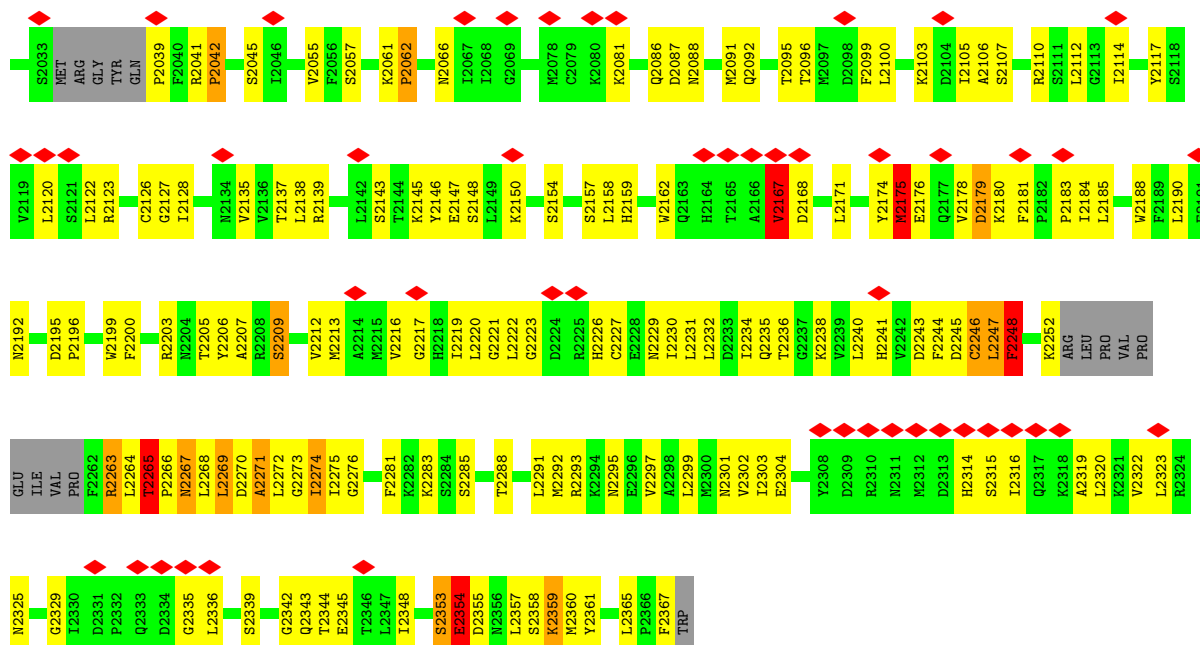
- Molecule 1 is a protein called Serine/threonine-protein kinase MEC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1997	Total	C	N	O	S	0	0
			14240	8995	2502	2692	51		

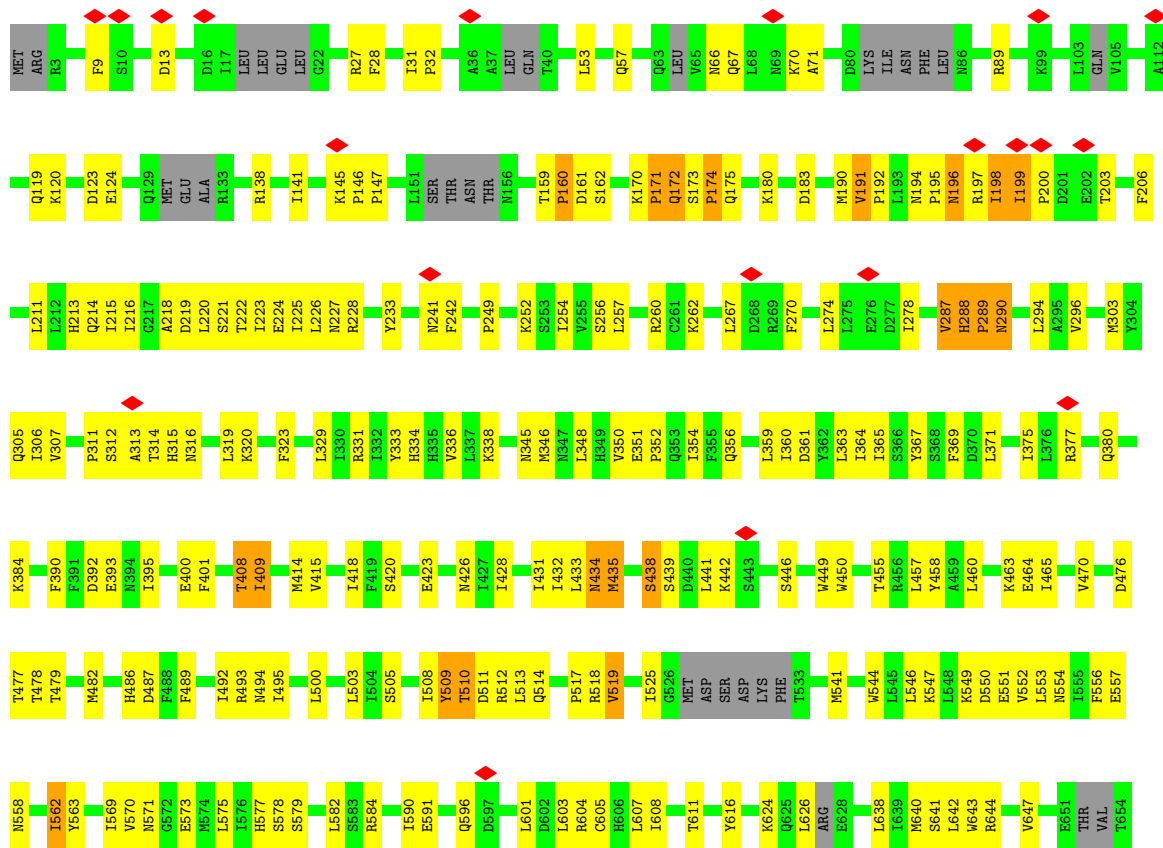
- Molecule 2 is a protein called DNA damage checkpoint protein LCD1.

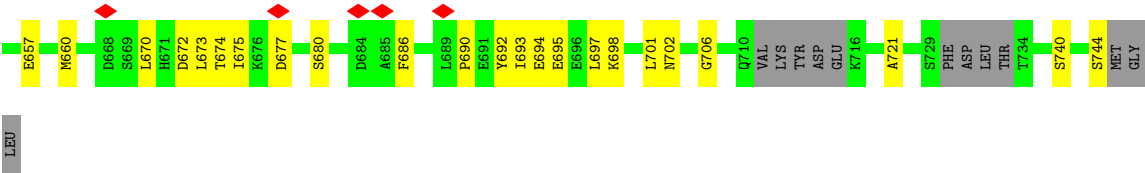
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	704	Total	C	N	O	S	0	0
			5069	3234	875	941	19		





• Molecule 2: DNA damage checkpoint protein LCD1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63132	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.244	Depositor
Minimum map value	-0.151	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0518	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	C	0.34	2/14428 (0.0%)	0.64	36/19608 (0.2%)
2	G	0.37	0/5140	0.65	10/6985 (0.1%)
All	All	0.35	2/19568 (0.0%)	0.64	46/26593 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1355	TYR	C-O	-5.67	1.17	1.24
1	C	1254	TYR	C-O	-5.48	1.17	1.24

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	385	PRO	N-CA-CB	9.73	110.00	101.83
1	C	2018	PRO	N-CA-CB	7.88	111.52	103.25
2	G	146	PRO	N-CA-CB	7.81	110.66	103.08
2	G	160	PRO	N-CA-CB	7.70	111.34	103.25
1	C	356	PRO	N-CA-CB	7.55	111.18	103.25
2	G	171	PRO	N-CA-CB	7.18	110.79	103.25
1	C	1849	PRO	N-CA-CB	7.06	110.67	103.25
2	G	192	PRO	N-CA-CB	7.02	110.62	103.25
1	C	808	PRO	N-CA-CB	6.99	109.97	103.41
1	C	844	LEU	N-CA-C	6.88	119.95	110.24
1	C	2039	PRO	N-CA-CB	6.85	110.53	103.00
1	C	1931	PRO	N-CA-CB	6.77	110.47	103.23
1	C	1893	PRO	N-CA-CB	6.77	110.44	103.00
1	C	1311	PRO	N-CA-CB	6.76	110.44	103.00
1	C	375	PRO	N-CA-CB	6.70	110.37	103.00
1	C	1401	ALA	N-CA-C	-6.67	103.93	111.07
1	C	1967	PRO	N-CA-CB	6.56	110.14	103.25
1	C	1275	PRO	N-CA-CB	6.54	110.02	103.48
2	G	147	PRO	N-CA-CB	6.51	110.09	103.25
1	C	1396	PRO	N-CA-CB	6.50	109.98	103.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2062	PRO	N-CA-CB	6.47	110.04	103.25
1	C	1207	PRO	N-CA-CB	6.46	110.19	103.15
1	C	2028	PRO	N-CA-CB	6.46	110.03	103.25
1	C	2042	PRO	N-CA-CB	6.43	110.12	102.60
2	G	408	THR	CA-C-N	6.42	133.52	121.97
2	G	408	THR	C-N-CA	6.42	133.52	121.97
2	G	174	PRO	N-CA-CB	6.38	109.95	103.25
1	C	2012	PRO	N-CA-CB	6.29	110.19	103.39
1	C	1246	PRO	N-CA-CB	6.27	110.17	103.52
1	C	1126	LEU	N-CA-C	6.21	120.64	113.38
1	C	1242	PRO	N-CA-CB	6.18	109.74	103.25
1	C	685	SER	CA-C-N	6.13	127.51	119.84
1	C	685	SER	C-N-CA	6.13	127.51	119.84
1	C	1460	THR	CB-CA-C	-6.03	109.64	116.63
1	C	2353	SER	CB-CA-C	-5.94	108.72	115.79
1	C	1878	THR	N-CA-C	-5.54	106.18	113.17
1	C	2248	PHE	CB-CA-C	-5.49	109.26	115.79
1	C	1254	TYR	CA-C-N	5.44	127.51	120.44
1	C	1254	TYR	C-N-CA	5.44	127.51	120.44
2	G	288	HIS	CA-C-N	5.37	126.55	119.84
2	G	288	HIS	C-N-CA	5.37	126.55	119.84
1	C	845	ILE	N-CA-C	5.28	120.32	109.34
1	C	1125	VAL	N-CA-C	5.12	120.00	109.34
1	C	1395	THR	CA-C-N	5.10	124.76	119.56
1	C	1395	THR	C-N-CA	5.10	124.76	119.56
1	C	2175	MET	N-CA-C	-5.10	105.37	112.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	14240	0	12588	580	0
2	G	5069	0	4486	201	0
All	All	19309	0	17074	771	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 21.

All (771) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:SER:HB3	1:C:686:PRO:CD	1.30	1.44
1:C:2167:VAL:CG1	1:C:2168:ASP:H	1.32	1.38
2:G:191:VAL:CB	2:G:195:PRO:HD2	1.54	1.37
1:C:2265:THR:HB	1:C:2266:PRO:CD	1.57	1.29
1:C:1124:GLY:O	1:C:1125:VAL:HG22	1.35	1.24
1:C:1124:GLY:O	1:C:1125:VAL:CG2	1.86	1.24
1:C:2265:THR:CB	1:C:2266:PRO:HD2	1.64	1.23
1:C:2167:VAL:HG13	1:C:2168:ASP:N	1.42	1.20
1:C:685:SER:CB	1:C:686:PRO:CD	2.18	1.18
1:C:685:SER:CB	1:C:686:PRO:HD2	1.74	1.17
2:G:191:VAL:CB	2:G:195:PRO:CD	2.32	1.08
1:C:685:SER:HB3	1:C:686:PRO:HD3	1.38	1.03
1:C:648:LEU:HA	1:C:687:ILE:CD1	1.91	1.01
1:C:648:LEU:CA	1:C:687:ILE:HD11	1.90	0.99
1:C:1124:GLY:C	1:C:1125:VAL:HG22	1.89	0.95
2:G:233:TYR:HD2	2:G:290:ASN:O	1.49	0.94
2:G:233:TYR:CD2	2:G:290:ASN:O	2.20	0.94
2:G:198:ILE:CG2	2:G:199:ILE:N	2.31	0.93
1:C:1852:ILE:O	1:C:1856:LEU:CB	2.16	0.93
1:C:518:ILE:HD13	1:C:518:ILE:H	1.34	0.91
1:C:1876:LYS:O	1:C:1880:ASP:N	2.03	0.91
1:C:1125:VAL:HG21	1:C:1656:ILE:HG22	1.53	0.90
1:C:2252:LYS:HD3	1:C:2360:MET:HG2	1.56	0.88
2:G:198:ILE:HG22	2:G:199:ILE:H	1.39	0.88
1:C:586:LEU:HD13	2:G:590:ILE:HD11	1.54	0.87
1:C:2167:VAL:CG1	1:C:2168:ASP:N	2.03	0.87
1:C:558:LYS:HB3	1:C:601:HIS:CD2	2.10	0.87
1:C:1570:LEU:O	1:C:1574:ASN:ND2	2.08	0.87
2:G:233:TYR:CD2	2:G:290:ASN:HB3	2.10	0.86
1:C:1124:GLY:O	1:C:1125:VAL:HG23	1.74	0.84
1:C:318:HIS:O	1:C:320:PRO:HD3	1.78	0.84
1:C:648:LEU:CA	1:C:687:ILE:CD1	2.54	0.84
1:C:585:ARG:HB3	1:C:626:ASN:HD21	1.44	0.83
1:C:2145:LYS:HB3	1:C:2184:ILE:HD13	1.61	0.82
1:C:2185:LEU:HD23	1:C:2185:LEU:O	1.78	0.82
1:C:686:PRO:O	1:C:689:PRO:HD2	1.79	0.82
1:C:846:THR:O	1:C:850:LYS:CB	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2112:LEU:HD22	1:C:2212:VAL:HG11	1.62	0.82
2:G:400:GLU:HB2	2:G:449:TRP:HE1	1.44	0.82
1:C:685:SER:HB3	1:C:686:PRO:HD2	0.84	0.82
1:C:2252:LYS:CD	1:C:2360:MET:HG2	2.09	0.81
1:C:2263:ARG:HG2	1:C:2263:ARG:HH11	1.46	0.80
2:G:233:TYR:HD2	2:G:290:ASN:C	1.89	0.80
1:C:557:PRO:HG2	1:C:566:ILE:CG2	2.12	0.80
1:C:2196:PRO:HA	1:C:2199:TRP:HB3	1.63	0.80
1:C:558:LYS:CB	1:C:601:HIS:CD2	2.65	0.79
2:G:198:ILE:CG2	2:G:199:ILE:H	1.93	0.79
2:G:435:MET:HA	2:G:435:MET:HE2	1.65	0.79
1:C:2171:LEU:HD23	1:C:2359:LYS:HB2	1.61	0.79
2:G:198:ILE:HG23	2:G:199:ILE:N	1.96	0.79
2:G:172:GLN:O	2:G:175:GLN:N	2.15	0.78
1:C:961:GLU:CD	1:C:962:LEU:H	1.91	0.78
1:C:525:ASN:O	1:C:529:HIS:NE2	2.18	0.77
1:C:1290:LEU:HD12	1:C:1290:LEU:O	1.84	0.77
1:C:2285:SER:O	1:C:2288:THR:OG1	2.04	0.76
2:G:638:LEU:O	2:G:641:SER:OG	2.03	0.75
1:C:2295:ASN:HD21	1:C:2299:LEU:HD23	1.52	0.75
1:C:1887:GLU:O	1:C:1891:HIS:N	2.19	0.75
1:C:2265:THR:HB	1:C:2266:PRO:HD2	0.78	0.74
1:C:440:SER:HB2	1:C:521:ILE:HD12	1.69	0.74
1:C:2167:VAL:HG13	1:C:2168:ASP:H	0.58	0.73
1:C:493:CYS:SG	1:C:553:HIS:NE2	2.62	0.73
2:G:384:LYS:O	2:G:435:MET:CG	2.37	0.73
2:G:218:ALA:HB1	2:G:505:SER:HB2	1.70	0.73
1:C:2293:ARG:NH1	1:C:2343:GLN:OE1	2.22	0.72
1:C:648:LEU:N	1:C:687:ILE:HD11	2.03	0.72
1:C:1124:GLY:C	1:C:1125:VAL:CG2	2.55	0.71
1:C:1598:PHE:HA	1:C:1601:ILE:HG22	1.73	0.71
2:G:222:THR:HA	2:G:225:ILE:HG22	1.72	0.71
1:C:648:LEU:CB	1:C:687:ILE:HD11	2.20	0.71
2:G:463:LYS:HE2	2:G:477:THR:HA	1.73	0.71
2:G:509:TYR:HD2	2:G:511:ASP:H	1.39	0.71
1:C:1125:VAL:CG2	1:C:1656:ILE:HG22	2.20	0.71
1:C:2205:THR:O	1:C:2209:SER:HB3	1.91	0.71
2:G:435:MET:HA	2:G:435:MET:CE	2.11	0.71
1:C:465:LEU:O	1:C:469:GLU:N	2.23	0.71
1:C:2167:VAL:HG13	1:C:2168:ASP:OD1	1.90	0.70
2:G:198:ILE:HG23	2:G:199:ILE:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:ASN:ND2	1:C:508:ASN:O	2.24	0.70
1:C:2196:PRO:O	1:C:2200:PHE:N	2.22	0.70
2:G:348:LEU:HD13	2:G:350:VAL:HG12	1.72	0.70
1:C:1002:LEU:HD12	1:C:1006:LEU:HB2	1.74	0.69
1:C:1564:ILE:HD12	2:G:352:PRO:HD3	1.74	0.69
1:C:237:ALA:HB1	1:C:289:LEU:HD21	1.73	0.69
1:C:1958:GLU:O	1:C:1962:GLN:N	2.24	0.69
2:G:363:LEU:HD22	2:G:367:TYR:HE2	1.58	0.69
1:C:845:ILE:HG12	1:C:875:LYS:HZ3	1.58	0.69
1:C:1099:LEU:HD22	1:C:1606:ILE:HD11	1.75	0.69
1:C:845:ILE:CG1	1:C:875:LYS:HZ3	2.05	0.69
2:G:433:LEU:O	2:G:434:ASN:O	2.10	0.69
1:C:317:ASP:OD1	1:C:318:HIS:ND1	2.26	0.68
1:C:518:ILE:HD13	1:C:518:ILE:N	2.07	0.68
2:G:211:LEU:HD12	2:G:223:ILE:HG21	1.74	0.68
2:G:435:MET:HE2	2:G:435:MET:CA	2.22	0.68
1:C:443:ILE:O	1:C:447:PHE:N	2.25	0.68
1:C:919:LYS:HD2	1:C:922:ILE:HD12	1.76	0.68
1:C:1876:LYS:O	1:C:1879:GLU:N	2.25	0.68
1:C:593:PRO:HG3	1:C:633:GLN:HB3	1.73	0.68
1:C:648:LEU:HB2	1:C:687:ILE:HD11	1.75	0.68
2:G:384:LYS:O	2:G:435:MET:HG3	1.93	0.68
1:C:579:ASN:OD1	1:C:580:SER:N	2.27	0.67
1:C:2175:MET:HE3	1:C:2358:SER:OG	1.94	0.67
1:C:309:ASN:OD1	1:C:310:ASP:N	2.27	0.67
1:C:518:ILE:H	1:C:518:ILE:CD1	1.99	0.67
1:C:2265:THR:CB	1:C:2266:PRO:CD	2.35	0.67
2:G:67:GLN:O	2:G:71:ALA:N	2.26	0.67
1:C:628:VAL:HG11	1:C:664:MET:HG2	1.76	0.67
1:C:1470:LEU:HB2	1:C:1479:ALA:HB2	1.75	0.67
1:C:685:SER:CB	1:C:686:PRO:HD3	2.07	0.67
1:C:2110:ARG:HH22	1:C:2283:LYS:HE2	1.60	0.67
1:C:1127:ASP:OD1	1:C:1129:THR:OG1	2.12	0.67
1:C:1185:GLN:NE2	1:C:1220:SER:O	2.27	0.67
2:G:582:LEU:HD12	2:G:608:ILE:HD11	1.77	0.67
1:C:1185:GLN:HE21	1:C:1224:ILE:H	1.41	0.67
1:C:835:ASN:O	1:C:839:CYS:N	2.24	0.66
1:C:1021:GLY:O	1:C:1025:ARG:N	2.27	0.66
1:C:1072:LYS:O	1:C:1076:ARG:N	2.28	0.66
1:C:415:TYR:OH	1:C:484:MET:O	2.10	0.65
1:C:920:LYS:NZ	1:C:1218:SER:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:MET:SD	1:C:618:GLN:NE2	2.69	0.65
1:C:1897:TRP:O	1:C:1901:LEU:N	2.24	0.65
1:C:543:ILE:O	1:C:547:LEU:N	2.28	0.65
1:C:632:THR:O	1:C:635:THR:OG1	2.15	0.65
1:C:2167:VAL:CG1	1:C:2168:ASP:OD1	2.44	0.65
1:C:2265:THR:CG2	1:C:2266:PRO:HD2	2.27	0.65
2:G:27:ARG:O	2:G:31:ILE:N	2.21	0.65
2:G:241:ASN:O	2:G:260:ARG:NH2	2.30	0.65
2:G:369:PHE:O	2:G:420:SER:OG	2.10	0.65
2:G:392:ASP:H	2:G:395:ILE:HG22	1.61	0.65
1:C:2123:ARG:HB2	1:C:2126:CYS:H	1.61	0.64
1:C:2216:VAL:HA	1:C:2219:ILE:HD12	1.78	0.64
1:C:2223:GLY:HA2	1:C:2245:ASP:OD2	1.95	0.64
1:C:1102:SER:OG	1:C:1116:CYS:SG	2.51	0.64
1:C:2243:ASP:CG	1:C:2244:PHE:H	2.06	0.64
1:C:297:LYS:O	1:C:301:ARG:N	2.29	0.64
1:C:509:ARG:HB2	1:C:510:PRO:HD2	1.78	0.64
1:C:1779:SER:HA	1:C:1782:ILE:HD12	1.79	0.64
1:C:322:ASP:HA	1:C:325:ALA:HB2	1.78	0.64
1:C:648:LEU:HA	1:C:687:ILE:HD12	1.76	0.64
1:C:440:SER:HB2	1:C:521:ILE:CD1	2.28	0.64
1:C:1544:LEU:O	1:C:1672:SER:OG	2.16	0.64
1:C:1742:VAL:HG12	1:C:1767:PHE:HD1	1.61	0.64
1:C:1594:ILE:HG21	1:C:1631:SER:HB2	1.80	0.64
2:G:28:PHE:O	2:G:32:PRO:N	2.30	0.64
1:C:929:ILE:O	1:C:933:LEU:N	2.26	0.63
1:C:1049:ASN:ND2	1:C:1061:ASN:OD1	2.29	0.63
2:G:434:ASN:O	2:G:435:MET:C	2.39	0.63
1:C:2139:ARG:O	1:C:2143:SER:OG	2.10	0.63
1:C:452:ILE:HG13	1:C:453:THR:HG23	1.80	0.63
1:C:925:ALA:O	1:C:928:GLN:N	2.32	0.63
1:C:1054:ASN:HB3	1:C:1057:VAL:HG12	1.80	0.63
1:C:290:ASP:CG	1:C:291:ASN:H	2.07	0.63
1:C:663:ILE:O	1:C:666:THR:OG1	2.17	0.62
1:C:1017:LYS:HE3	1:C:1019:GLU:HB3	1.79	0.62
1:C:845:ILE:HG12	1:C:875:LYS:NZ	2.15	0.62
1:C:2088:ASN:O	1:C:2092:GLN:N	2.25	0.62
1:C:2117:TYR:CE1	1:C:2240:LEU:HD21	2.35	0.62
1:C:517:GLU:OE2	1:C:521:ILE:CG1	2.48	0.62
1:C:895:GLU:HB3	1:C:898:THR:HG22	1.80	0.62
2:G:446:SER:O	2:G:450:TRP:N	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:702:ASN:O	2:G:706:GLY:N	2.31	0.62
1:C:1185:GLN:O	1:C:1189:LYS:N	2.33	0.62
1:C:2359:LYS:O	1:C:2359:LYS:HG3	2.00	0.62
2:G:249:PRO:HG2	2:G:252:LYS:HB2	1.82	0.62
2:G:438:SER:O	2:G:441:LEU:N	2.33	0.62
1:C:991:ILE:O	1:C:994:THR:OG1	2.17	0.62
2:G:287:VAL:HG12	2:G:287:VAL:O	2.00	0.62
1:C:912:PHE:HA	1:C:915:ILE:HD12	1.82	0.62
1:C:1412:ARG:HA	1:C:2196:PRO:HG2	1.82	0.62
1:C:521:ILE:O	1:C:525:ASN:ND2	2.32	0.62
1:C:1355:TYR:HD1	1:C:1355:TYR:O	1.83	0.61
1:C:1756:ASN:HB2	1:C:1759:ASP:H	1.64	0.61
1:C:775:ALA:O	1:C:779:HIS:N	2.30	0.61
1:C:2167:VAL:HG12	1:C:2168:ASP:N	2.11	0.61
1:C:2213:MET:HG2	1:C:2241:HIS:HD2	1.65	0.61
1:C:2243:ASP:OD1	1:C:2244:PHE:N	2.33	0.61
1:C:1435:LEU:HD13	1:C:1458:PHE:HD2	1.66	0.61
1:C:1778:ALA:O	1:C:1782:ILE:N	2.33	0.61
1:C:2185:LEU:HD23	1:C:2185:LEU:C	2.25	0.61
1:C:558:LYS:HB2	1:C:601:HIS:CD2	2.36	0.61
1:C:628:VAL:HG21	1:C:664:MET:HE3	1.83	0.61
1:C:2270:ASP:C	1:C:2272:LEU:H	2.08	0.61
2:G:334:HIS:HB3	2:G:338:LYS:HD3	1.83	0.61
2:G:384:LYS:O	2:G:435:MET:HG2	1.99	0.61
1:C:2263:ARG:C	1:C:2263:ARG:HD2	2.26	0.61
2:G:476:ASP:C	2:G:478:THR:H	2.08	0.61
2:G:345:ASN:OD1	2:G:346:MET:N	2.33	0.61
1:C:953:LEU:HD22	1:C:957:LEU:HD12	1.83	0.60
1:C:2217:GLY:O	1:C:2221:GLY:N	2.34	0.60
2:G:408:THR:O	2:G:409:ILE:HG12	2.01	0.60
1:C:2145:LYS:O	1:C:2148:SER:OG	2.15	0.60
1:C:512:ALA:O	1:C:516:SER:OG	2.18	0.60
1:C:540:LEU:HD11	1:C:572:LEU:HD11	1.83	0.60
1:C:1969:ASP:O	1:C:1973:SER:N	2.27	0.60
1:C:1424:ASN:HB2	1:C:1425:PRO:HD3	1.82	0.60
1:C:2365:LEU:HD23	1:C:2365:LEU:O	2.01	0.60
1:C:516:SER:OG	1:C:519:PHE:HB3	2.02	0.60
2:G:89:ARG:H	2:G:686:PHE:HZ	1.50	0.60
2:G:331:ARG:HG3	2:G:401:PHE:HE2	1.67	0.60
1:C:1941:LEU:O	1:C:1945:ASN:N	2.32	0.60
1:C:2175:MET:HE3	1:C:2358:SER:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2175:MET:CE	1:C:2358:SER:OG	2.48	0.60
2:G:313:ALA:O	2:G:316:ASN:ND2	2.35	0.60
1:C:2263:ARG:HH11	1:C:2263:ARG:CG	2.15	0.59
1:C:318:HIS:C	1:C:320:PRO:HD3	2.27	0.59
1:C:839:CYS:HA	1:C:842:ARG:HD3	1.85	0.59
1:C:880:ILE:HD12	1:C:883:ILE:HD11	1.84	0.59
1:C:926:LEU:HA	1:C:929:ILE:HG22	1.83	0.59
2:G:233:TYR:CE2	2:G:290:ASN:O	2.56	0.59
1:C:1057:VAL:O	1:C:1061:ASN:ND2	2.35	0.59
1:C:1438:LEU:HD22	1:C:1442:TYR:HE2	1.68	0.59
1:C:2252:LYS:HB3	1:C:2360:MET:HA	1.83	0.59
1:C:928:GLN:HE21	1:C:932:CYS:HB2	1.68	0.59
1:C:386:PHE:O	1:C:389:ARG:N	2.36	0.59
1:C:741:LEU:O	1:C:745:ALA:N	2.32	0.59
1:C:1960:TYR:O	1:C:1964:SER:N	2.29	0.59
1:C:266:VAL:HG23	1:C:267:CYS:H	1.66	0.59
2:G:120:LYS:O	2:G:124:GLU:N	2.27	0.59
2:G:690:PRO:O	2:G:694:GLU:N	2.28	0.59
1:C:886:VAL:O	1:C:889:SER:OG	2.18	0.58
2:G:514:GLN:N	2:G:514:GLN:OE1	2.33	0.58
1:C:487:TRP:HZ2	1:C:490:CYS:HB2	1.68	0.58
2:G:172:GLN:O	2:G:174:PRO:N	2.36	0.58
1:C:2171:LEU:HA	1:C:2174:TYR:HE1	1.68	0.58
1:C:919:LYS:HA	1:C:922:ILE:HD12	1.86	0.58
1:C:1568:GLU:HA	1:C:1605:PHE:HZ	1.68	0.58
1:C:301:ARG:O	1:C:304:SER:OG	2.13	0.58
1:C:770:GLN:O	1:C:774:VAL:N	2.29	0.58
1:C:1982:THR:O	1:C:1986:LEU:N	2.37	0.58
1:C:1114:GLU:HB2	1:C:1599:ARG:HG2	1.84	0.58
1:C:512:ALA:O	1:C:519:PHE:HD2	1.87	0.58
1:C:541:SER:HA	1:C:544:LEU:HD12	1.86	0.58
1:C:585:ARG:HH21	1:C:626:ASN:ND2	2.01	0.58
1:C:1356:CYS:HA	1:C:1359:TRP:HB3	1.86	0.58
1:C:1704:ASP:OD1	1:C:1704:ASP:N	2.32	0.57
1:C:648:LEU:HB2	1:C:687:ILE:CD1	2.34	0.57
1:C:2354:GLU:OE1	1:C:2354:GLU:HA	2.03	0.57
1:C:1140:GLU:N	1:C:1140:GLU:OE1	2.37	0.57
1:C:1993:THR:O	1:C:1997:GLY:N	2.37	0.57
1:C:2086:GLN:NE2	1:C:2243:ASP:O	2.36	0.57
1:C:2092:GLN:O	1:C:2095:THR:OG1	2.13	0.57
2:G:351:GLU:HB3	2:G:352:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:670:LEU:O	2:G:673:LEU:N	2.38	0.57
1:C:443:ILE:HA	1:C:446:CYS:HB2	1.86	0.57
1:C:729:ILE:HG13	1:C:730:PRO:HD3	1.87	0.57
2:G:482:MET:HG2	2:G:541:MET:HE3	1.85	0.57
2:G:489:PHE:HB3	2:G:494:ASN:HD22	1.69	0.57
2:G:119:GLN:O	2:G:123:ASP:N	2.37	0.57
2:G:390:PHE:CZ	2:G:395:ILE:HG12	2.40	0.57
1:C:609:ALA:HA	1:C:612:ILE:HD12	1.87	0.57
1:C:994:THR:O	1:C:998:GLU:N	2.35	0.56
1:C:585:ARG:HB3	1:C:626:ASN:ND2	2.17	0.56
1:C:1160:ILE:HA	1:C:1164:LEU:HD12	1.86	0.56
1:C:1322:GLU:O	1:C:1326:ILE:N	2.31	0.56
1:C:1564:ILE:HG22	1:C:1566:ASP:H	1.70	0.56
1:C:2220:LEU:HB3	1:C:2222:LEU:HD13	1.87	0.56
1:C:659:TYR:HA	1:C:662:ARG:HG2	1.87	0.56
1:C:1064:ASP:O	1:C:1068:TYR:N	2.37	0.56
2:G:380:GLN:HG3	2:G:431:ILE:HD13	1.88	0.56
1:C:317:ASP:OD1	1:C:318:HIS:N	2.38	0.56
2:G:214:GLN:NE2	2:G:218:ALA:O	2.39	0.56
1:C:590:ARG:NH2	2:G:591:GLU:O	2.38	0.56
1:C:2185:LEU:HB3	1:C:2271:ALA:HB2	1.86	0.56
1:C:868:GLN:HA	1:C:871:ALA:HB3	1.87	0.56
1:C:1412:ARG:CA	1:C:2196:PRO:HG2	2.36	0.55
1:C:2319:ALA:O	1:C:2323:LEU:HB2	2.06	0.55
1:C:416:ARG:O	1:C:420:LEU:N	2.40	0.55
1:C:1772:ASP:OD1	1:C:1782:ILE:HG12	2.07	0.55
1:C:2135:VAL:HG21	1:C:2231:LEU:HD11	1.88	0.55
1:C:2227:CYS:O	1:C:2230:ILE:HG22	2.07	0.55
1:C:1194:SER:O	1:C:1198:TRP:N	2.39	0.55
1:C:2360:MET:O	1:C:2361:TYR:C	2.48	0.55
1:C:987:ILE:O	1:C:990:SER:OG	2.18	0.55
1:C:2302:VAL:HG13	1:C:2303:ILE:H	1.70	0.55
2:G:334:HIS:HE1	2:G:401:PHE:CZ	2.24	0.55
1:C:648:LEU:CB	1:C:687:ILE:CD1	2.84	0.55
1:C:2087:ASP:O	1:C:2091:MET:N	2.31	0.55
2:G:392:ASP:OD1	2:G:393:GLU:N	2.39	0.55
1:C:1560:SER:HB3	2:G:519:VAL:HG22	1.89	0.55
2:G:438:SER:O	2:G:442:LYS:N	2.30	0.55
2:G:303:MET:HA	2:G:306:ILE:HD12	1.88	0.55
2:G:482:MET:HE3	2:G:487:ASP:HB3	1.89	0.55
2:G:509:TYR:CE2	2:G:512:ARG:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1804:GLY:HA2	1:C:1807:TYR:HB3	1.89	0.54
1:C:447:PHE:HA	1:C:455:LEU:HD12	1.89	0.54
1:C:2190:LEU:HA	1:C:2199:TRP:CD1	2.42	0.54
2:G:608:ILE:O	2:G:611:THR:OG1	2.23	0.54
1:C:1764:LEU:HD23	1:C:1789:ILE:HG12	1.89	0.54
2:G:66:ASN:O	2:G:70:LYS:N	2.35	0.54
2:G:428:ILE:O	2:G:432:ILE:HG12	2.07	0.54
1:C:662:ARG:NH1	1:C:708:ASN:OD1	2.41	0.54
1:C:1614:LEU:HD12	1:C:1617:LYS:HD2	1.89	0.54
1:C:921:SER:HA	1:C:924:SER:HB2	1.90	0.54
1:C:2213:MET:HG2	1:C:2241:HIS:CD2	2.42	0.54
2:G:578:SER:OG	2:G:579:SER:N	2.40	0.54
1:C:2273:GLY:C	1:C:2275:ILE:H	2.16	0.54
1:C:458:TRP:O	1:C:462:LEU:HG	2.07	0.54
1:C:558:LYS:HB3	1:C:601:HIS:NE2	2.23	0.54
1:C:2234:ILE:C	1:C:2236:THR:H	2.16	0.54
1:C:2320:LEU:O	1:C:2323:LEU:HB3	2.08	0.54
1:C:845:ILE:CD1	1:C:875:LYS:HZ3	2.21	0.54
1:C:1756:ASN:HD22	1:C:1759:ASP:HB2	1.71	0.54
2:G:53:LEU:O	2:G:57:GLN:N	2.41	0.54
1:C:442:SER:O	1:C:445:THR:OG1	2.23	0.54
1:C:506:ASN:O	1:C:509:ARG:NH1	2.40	0.54
1:C:880:ILE:HD11	1:C:913:LEU:HD21	1.89	0.54
1:C:557:PRO:HG2	1:C:566:ILE:HG23	1.88	0.53
1:C:2110:ARG:NH2	1:C:2283:LYS:HE2	2.22	0.53
1:C:2263:ARG:HG3	1:C:2263:ARG:O	2.08	0.53
2:G:557:GLU:OE1	2:G:557:GLU:N	2.37	0.53
1:C:664:MET:HB2	2:G:640:MET:HE3	1.90	0.53
1:C:1165:VAL:HB	1:C:1166:PRO:HD3	1.89	0.53
1:C:1734:GLU:HG2	1:C:1737:ARG:HD2	1.91	0.53
2:G:305:GLN:O	2:G:305:GLN:NE2	2.41	0.53
1:C:961:GLU:OE1	1:C:962:LEU:N	2.36	0.53
1:C:2273:GLY:O	1:C:2275:ILE:HG12	2.08	0.53
2:G:350:VAL:O	2:G:351:GLU:HG3	2.08	0.53
1:C:1300:LEU:HB3	1:C:1304:ILE:HD11	1.91	0.53
1:C:1810:LEU:HD22	1:C:1811:LEU:HD12	1.91	0.53
1:C:786:ILE:O	1:C:790:LEU:N	2.41	0.53
1:C:1001:ASP:OD1	1:C:1002:LEU:N	2.41	0.53
1:C:2247:LEU:N	1:C:2247:LEU:HD22	2.24	0.53
2:G:334:HIS:HE1	2:G:401:PHE:HZ	1.56	0.53
1:C:1804:GLY:O	1:C:1808:SER:N	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ASP:OD1	1:C:291:ASN:N	2.40	0.53
2:G:191:VAL:CB	2:G:195:PRO:HD3	2.33	0.53
1:C:884:PHE:HA	1:C:887:PHE:HB2	1.90	0.53
1:C:803:ILE:O	1:C:807:LEU:N	2.40	0.52
1:C:1138:TYR:H	1:C:1138:TYR:HD1	1.53	0.52
1:C:1355:TYR:CD1	1:C:1355:TYR:C	2.86	0.52
1:C:1659:ASP:OD1	1:C:1660:PHE:N	2.40	0.52
2:G:203:THR:HB	2:G:267:LEU:HD13	1.91	0.52
2:G:352:PRO:HB2	2:G:354:ILE:HG23	1.90	0.52
1:C:1140:GLU:CD	1:C:1140:GLU:H	2.16	0.52
1:C:510:PRO:HG2	1:C:554:PHE:HD1	1.73	0.52
1:C:1147:ASN:O	1:C:1152:THR:OG1	2.27	0.52
1:C:2143:SER:HA	1:C:2146:TYR:CE2	2.44	0.52
1:C:1690:PHE:O	1:C:1693:LEU:N	2.43	0.52
1:C:1988:ASP:O	1:C:1992:ILE:N	2.35	0.52
2:G:161:ASP:O	2:G:162:SER:C	2.49	0.52
1:C:842:ARG:HH12	1:C:916:TYR:HB2	1.74	0.52
1:C:2137:THR:HG22	1:C:2138:LEU:N	2.25	0.52
2:G:312:SER:HB2	2:G:314:THR:HG23	1.92	0.52
1:C:891:ILE:HD12	1:C:932:CYS:SG	2.50	0.52
1:C:1181:ALA:O	1:C:1185:GLN:HG2	2.10	0.52
1:C:2273:GLY:O	1:C:2274:ILE:HG22	2.09	0.52
1:C:2185:LEU:HD22	1:C:2271:ALA:HB1	1.91	0.52
1:C:2234:ILE:HG22	1:C:2235:GLN:H	1.73	0.52
2:G:194:ASN:N	2:G:195:PRO:HD3	2.24	0.52
1:C:582:ARG:HE	1:C:586:LEU:HD11	1.75	0.52
1:C:2325:ASN:O	1:C:2329:GLY:N	2.42	0.52
1:C:519:PHE:CD1	1:C:519:PHE:C	2.85	0.51
1:C:2268:LEU:C	1:C:2268:LEU:HD23	2.35	0.51
2:G:294:LEU:HD12	2:G:517:PRO:HG3	1.92	0.51
1:C:923:ILE:HD11	1:C:958:ASN:ND2	2.26	0.51
1:C:981:ASN:OD1	1:C:982:GLY:N	2.43	0.51
1:C:1541:ALA:O	1:C:1544:LEU:N	2.43	0.51
1:C:2154:SER:O	1:C:2157:SER:OG	2.26	0.51
1:C:500:ASN:O	1:C:503:VAL:HG12	2.10	0.51
1:C:557:PRO:O	1:C:566:ILE:HG12	2.10	0.51
1:C:1149:SER:O	1:C:1153:ILE:HG12	2.10	0.51
1:C:2137:THR:HG22	1:C:2138:LEU:H	1.76	0.51
2:G:323:PHE:CD1	2:G:395:ILE:HD11	2.45	0.51
1:C:647:LEU:HD22	1:C:687:ILE:HG13	1.92	0.51
2:G:435:MET:HE2	2:G:435:MET:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:889:SER:O	1:C:893:ASP:N	2.44	0.51
1:C:1328:THR:C	1:C:1330:ASN:H	2.18	0.51
2:G:371:LEU:O	2:G:375:ILE:HG12	2.11	0.51
1:C:455:LEU:HD21	1:C:526:PHE:HE1	1.76	0.51
1:C:517:GLU:OE2	1:C:521:ILE:HG12	2.10	0.51
1:C:1746:HIS:NE2	1:C:1764:LEU:HD13	2.26	0.51
1:C:557:PRO:O	1:C:566:ILE:HG23	2.09	0.51
1:C:2042:PRO:O	1:C:2045:SER:N	2.43	0.51
2:G:503:LEU:HD11	2:G:525:ILE:HD13	1.93	0.51
2:G:509:TYR:O	2:G:510:THR:OG1	2.22	0.51
2:G:569:ILE:HG13	2:G:570:VAL:N	2.26	0.51
1:C:742:SER:O	1:C:746:LYS:N	2.39	0.51
1:C:829:SER:N	1:C:832:GLU:HB2	2.26	0.51
1:C:1091:ILE:HG23	1:C:1126:LEU:HD21	1.92	0.51
1:C:1188:LEU:O	1:C:1192:GLY:N	2.44	0.51
1:C:1427:ASP:HB2	1:C:1430:GLN:HG2	1.93	0.51
1:C:1356:CYS:O	1:C:1360:ALA:N	2.32	0.50
1:C:1802:SER:HA	1:C:1805:LEU:HB3	1.91	0.50
2:G:392:ASP:O	2:G:395:ILE:HG22	2.10	0.50
2:G:455:THR:HA	2:G:458:TYR:HD2	1.76	0.50
1:C:247:VAL:HA	1:C:250:TYR:HB3	1.91	0.50
1:C:1301:ASP:HA	1:C:1304:ILE:HD12	1.93	0.50
1:C:2175:MET:SD	1:C:2176:GLU:N	2.85	0.50
1:C:436:LEU:HD13	1:C:517:GLU:HG2	1.93	0.50
1:C:1042:LEU:HB3	1:C:1046:PHE:CE2	2.47	0.50
1:C:1796:TRP:C	1:C:1798:LYS:H	2.19	0.50
2:G:206:PHE:CE2	2:G:270:PHE:HE2	2.30	0.50
2:G:438:SER:O	2:G:439:SER:C	2.54	0.50
1:C:996:ILE:HD11	1:C:1022:ILE:HD11	1.93	0.50
1:C:1422:ARG:NH2	1:C:1423:GLN:HE21	2.09	0.50
2:G:553:LEU:O	2:G:556:PHE:N	2.38	0.50
2:G:180:LYS:O	2:G:183:ASP:N	2.45	0.50
2:G:605:CYS:O	2:G:608:ILE:HG22	2.11	0.50
1:C:585:ARG:HD2	1:C:626:ASN:HD21	1.75	0.50
1:C:2314:HIS:CG	1:C:2315:SER:H	2.29	0.50
1:C:1382:THR:O	1:C:1386:LEU:N	2.40	0.50
2:G:198:ILE:O	2:G:199:ILE:HG22	2.11	0.50
2:G:224:GLU:HA	2:G:227:ASN:HB2	1.94	0.50
2:G:672:ASP:HA	2:G:675:ILE:HG22	1.94	0.50
1:C:2223:GLY:HA3	1:C:2245:ASP:HB3	1.94	0.50
1:C:2222:LEU:HD11	1:C:2246:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2316:ILE:HG22	1:C:2319:ALA:H	1.77	0.49
1:C:1029:PHE:O	1:C:1032:MET:N	2.39	0.49
1:C:1438:LEU:HD22	1:C:1442:TYR:CE2	2.46	0.49
1:C:1617:LYS:O	1:C:1620:LEU:N	2.40	0.49
1:C:1851:VAL:O	1:C:1855:TRP:N	2.45	0.49
1:C:2096:THR:HA	1:C:2099:PHE:HB3	1.93	0.49
1:C:510:PRO:HG2	1:C:554:PHE:CD1	2.47	0.49
1:C:1321:ILE:O	1:C:1325:SER:N	2.45	0.49
1:C:2110:ARG:HH12	1:C:2283:LYS:C	2.20	0.49
1:C:585:ARG:HD2	1:C:626:ASN:ND2	2.28	0.49
1:C:1756:ASN:C	1:C:1758:ARG:H	2.20	0.49
1:C:2252:LYS:HD2	1:C:2360:MET:HG2	1.89	0.49
1:C:571:LYS:O	1:C:574:GLN:HB2	2.11	0.49
1:C:1422:ARG:HA	1:C:2274:ILE:HD12	1.94	0.49
2:G:296:VAL:HG12	2:G:364:ILE:HD13	1.94	0.49
1:C:558:LYS:C	1:C:558:LYS:CD	2.86	0.49
1:C:625:GLU:O	1:C:629:ILE:HG12	2.13	0.49
1:C:1071:ARG:O	1:C:1074:THR:OG1	2.31	0.49
2:G:356:GLN:HG3	2:G:517:PRO:HB2	1.94	0.49
1:C:321:ILE:O	1:C:323:GLN:N	2.45	0.49
1:C:1959:LYS:O	1:C:1963:HIS:N	2.37	0.49
1:C:2057:SER:CB	1:C:2066:ASN:H	2.26	0.49
2:G:206:PHE:HE2	2:G:270:PHE:HE2	1.61	0.49
1:C:1755:VAL:HG12	1:C:1756:ASN:H	1.78	0.48
1:C:1778:ALA:O	1:C:1781:GLN:N	2.45	0.48
1:C:2268:LEU:HD23	1:C:2268:LEU:O	2.12	0.48
2:G:9:PHE:O	2:G:13:ASP:N	2.44	0.48
1:C:937:LEU:O	1:C:943:ARG:HG2	2.12	0.48
2:G:569:ILE:HG13	2:G:570:VAL:HG23	1.95	0.48
1:C:868:GLN:O	1:C:871:ALA:N	2.43	0.48
1:C:1076:ARG:HB2	1:C:1651:TYR:CZ	2.49	0.48
1:C:582:ARG:HH12	2:G:644:ARG:HG3	1.78	0.48
1:C:964:THR:HB	1:C:1169:TRP:CZ2	2.48	0.48
1:C:1185:GLN:HE21	1:C:1224:ILE:N	2.09	0.48
1:C:1345:CYS:O	1:C:1349:ILE:HG13	2.13	0.48
1:C:1562:ARG:O	1:C:1562:ARG:HG2	2.13	0.48
1:C:2143:SER:HA	1:C:2146:TYR:CZ	2.48	0.48
1:C:1799:PRO:O	1:C:1802:SER:N	2.47	0.48
1:C:2319:ALA:HA	1:C:2322:VAL:HG22	1.94	0.48
1:C:1290:LEU:HD12	1:C:1290:LEU:C	2.38	0.48
1:C:343:LEU:O	1:C:346:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:911:SER:O	1:C:915:ILE:HG13	2.13	0.48
1:C:1513:ILE:HG13	1:C:1514:SER:N	2.28	0.48
1:C:2342:GLY:O	1:C:2345:GLU:N	2.46	0.48
1:C:1042:LEU:HB3	1:C:1046:PHE:HE2	1.78	0.48
1:C:1153:ILE:O	1:C:1156:LEU:N	2.47	0.48
1:C:1355:TYR:HD1	1:C:1355:TYR:C	2.21	0.48
2:G:465:ILE:HA	2:G:479:THR:OG1	2.14	0.48
2:G:607:LEU:O	2:G:611:THR:HG23	2.13	0.48
2:G:426:ASN:ND2	2:G:551:GLU:OE2	2.47	0.48
1:C:606:GLU:O	1:C:609:ALA:N	2.43	0.48
1:C:845:ILE:HD11	1:C:875:LYS:HZ3	1.78	0.48
1:C:876:LEU:O	1:C:880:ILE:N	2.47	0.48
1:C:1300:LEU:HD11	1:C:1355:TYR:CE2	2.48	0.48
1:C:1406:GLU:OE1	1:C:1413:SER:OG	2.31	0.48
1:C:2263:ARG:HG2	1:C:2263:ARG:NH1	2.22	0.48
1:C:2302:VAL:HG13	1:C:2303:ILE:N	2.29	0.48
2:G:558:ASN:O	2:G:562:ILE:HG22	2.14	0.48
1:C:1794:SER:O	1:C:1797:ASP:N	2.45	0.47
1:C:1621:LEU:O	1:C:1625:HIS:N	2.45	0.47
2:G:400:GLU:HB2	2:G:449:TRP:NE1	2.22	0.47
2:G:509:TYR:HE2	2:G:511:ASP:HB2	1.78	0.47
1:C:570:PHE:O	1:C:574:GLN:HG2	2.14	0.47
1:C:1185:GLN:NE2	1:C:1224:ILE:H	2.11	0.47
1:C:2120:LEU:O	1:C:2128:ILE:N	2.47	0.47
1:C:2314:HIS:CD2	1:C:2315:SER:H	2.33	0.47
2:G:199:ILE:CG1	2:G:200:PRO:HD2	2.45	0.47
2:G:225:ILE:CG1	2:G:508:ILE:HG12	2.44	0.47
1:C:321:ILE:C	1:C:323:GLN:N	2.72	0.47
1:C:456:THR:O	1:C:459:THR:OG1	2.22	0.47
1:C:1781:GLN:O	1:C:1785:GLN:HG2	2.15	0.47
2:G:486:HIS:O	2:G:486:HIS:ND1	2.47	0.47
1:C:728:ILE:HG13	1:C:729:ILE:N	2.30	0.47
1:C:949:CYS:O	1:C:952:LEU:HB2	2.15	0.47
1:C:2273:GLY:O	1:C:2275:ILE:N	2.48	0.47
1:C:2304:GLU:HG3	1:C:2323:LEU:HD11	1.96	0.47
2:G:172:GLN:C	2:G:174:PRO:N	2.70	0.47
2:G:377:ARG:NH1	2:G:423:GLU:OE2	2.48	0.47
2:G:624:LYS:HE2	2:G:626:LEU:HA	1.97	0.47
2:G:677:ASP:O	2:G:680:SER:OG	2.30	0.47
2:G:692:TYR:CE2	2:G:693:ILE:HG12	2.50	0.47
1:C:459:THR:O	1:C:546:SER:OG	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:PHE:CZ	1:C:587:LEU:HD11	2.49	0.47
1:C:596:ASN:ND2	1:C:637:THR:OG1	2.48	0.47
1:C:1743:GLN:HA	1:C:1767:PHE:HE1	1.79	0.47
1:C:2179:ASP:C	1:C:2181:PHE:N	2.73	0.47
1:C:2231:LEU:HD22	1:C:2240:LEU:HB3	1.97	0.47
1:C:545:PHE:CE2	1:C:587:LEU:HD11	2.50	0.47
1:C:653:ILE:HG23	1:C:654:PHE:CD1	2.50	0.47
1:C:290:ASP:C	1:C:292:ASP:H	2.23	0.47
1:C:686:PRO:O	1:C:689:PRO:CD	2.56	0.47
1:C:861:ILE:HA	1:C:863:ASN:HA	1.97	0.47
2:G:199:ILE:HG23	2:G:200:PRO:O	2.15	0.47
2:G:288:HIS:HA	2:G:289:PRO:HD3	1.73	0.47
2:G:495:ILE:HA	2:G:544:TRP:NE1	2.29	0.47
1:C:684:LEU:N	1:C:684:LEU:HD23	2.30	0.46
1:C:1727:GLU:OE1	1:C:1766:LYS:NZ	2.47	0.46
1:C:1755:VAL:HG12	1:C:1756:ASN:N	2.30	0.46
2:G:199:ILE:HG12	2:G:200:PRO:HD2	1.98	0.46
1:C:321:ILE:O	1:C:322:ASP:C	2.58	0.46
1:C:412:LEU:HD11	1:C:487:TRP:O	2.16	0.46
2:G:138:ARG:O	2:G:141:ILE:N	2.47	0.46
2:G:476:ASP:C	2:G:478:THR:N	2.73	0.46
1:C:494:ASP:OD1	2:G:596:GLN:HB2	2.16	0.46
1:C:679:THR:O	1:C:683:LEU:N	2.48	0.46
1:C:845:ILE:CG1	1:C:875:LYS:NZ	2.75	0.46
1:C:1300:LEU:O	1:C:1304:ILE:HG13	2.15	0.46
1:C:1458:PHE:O	1:C:1460:THR:HG23	2.14	0.46
1:C:2137:THR:HG21	1:C:2230:ILE:O	2.15	0.46
1:C:1786:TYR:CE2	1:C:1803:ILE:HA	2.50	0.46
1:C:1968:HIS:O	1:C:1972:SER:N	2.41	0.46
2:G:190:MET:O	2:G:194:ASN:HA	2.15	0.46
2:G:740:SER:O	2:G:744:SER:N	2.49	0.46
1:C:628:VAL:CG2	1:C:664:MET:HE3	2.46	0.46
1:C:2223:GLY:CA	1:C:2245:ASP:HB3	2.46	0.46
1:C:877:GLN:HG2	1:C:921:SER:HB2	1.98	0.46
1:C:1400:LEU:HA	1:C:1403:ARG:CB	2.45	0.46
1:C:1653:MET:O	1:C:1656:ILE:HG12	2.16	0.46
1:C:2270:ASP:C	1:C:2272:LEU:N	2.71	0.46
1:C:321:ILE:CD1	1:C:347:TYR:HB2	2.46	0.46
1:C:455:LEU:HD21	1:C:526:PHE:CE1	2.51	0.46
1:C:1345:CYS:O	1:C:1349:ILE:N	2.35	0.46
1:C:2122:LEU:H	1:C:2127:GLY:HA2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2207:ALA:HB2	1:C:2272:LEU:HD11	1.98	0.46
1:C:2247:LEU:N	1:C:2247:LEU:CD2	2.79	0.46
2:G:457:LEU:O	2:G:460:LEU:N	2.48	0.46
2:G:692:TYR:CD2	2:G:693:ILE:HG12	2.51	0.46
1:C:2243:ASP:CG	1:C:2244:PHE:N	2.73	0.46
1:C:918:PRO:HG2	1:C:921:SER:HB3	1.98	0.46
1:C:540:LEU:O	1:C:543:ILE:HG22	2.16	0.46
1:C:631:TRP:CD1	1:C:654:PHE:HE2	2.34	0.45
1:C:1065:ILE:HA	1:C:1068:TYR:HB3	1.98	0.45
1:C:1422:ARG:HH21	1:C:1423:GLN:HE21	1.63	0.45
1:C:2263:ARG:C	1:C:2263:ARG:CD	2.85	0.45
1:C:1513:ILE:HD13	1:C:1545:GLU:HG3	1.98	0.45
1:C:1746:HIS:O	1:C:1750:GLN:HG2	2.15	0.45
1:C:2272:LEU:HD13	1:C:2281:PHE:HE2	1.80	0.45
1:C:557:PRO:HG2	1:C:566:ILE:HG21	1.94	0.45
1:C:892:HIS:NE2	1:C:935:THR:HG21	2.31	0.45
1:C:1155:PHE:O	1:C:1159:VAL:HG23	2.15	0.45
1:C:1545:GLU:OE1	1:C:1546:GLY:N	2.48	0.45
1:C:453:THR:HA	1:C:456:THR:HG22	1.98	0.45
1:C:1098:LEU:HD13	1:C:1120:ILE:HG22	1.97	0.45
1:C:2147:GLU:C	1:C:2150:LYS:H	2.24	0.45
2:G:348:LEU:H	2:G:348:LEU:HG	1.62	0.45
1:C:983:LYS:O	1:C:986:ASN:N	2.50	0.45
1:C:1622:MET:SD	1:C:1662:PRO:HA	2.57	0.45
2:G:196:ASN:ND2	2:G:196:ASN:C	2.74	0.45
1:C:923:ILE:HD11	1:C:958:ASN:HD21	1.82	0.45
1:C:1625:HIS:HE1	1:C:1652:ARG:NE	2.14	0.45
1:C:606:GLU:OE1	1:C:606:GLU:N	2.48	0.45
1:C:1255:LYS:O	1:C:1259:LYS:N	2.39	0.45
1:C:1362:GLU:HA	1:C:1365:GLN:HB3	1.99	0.45
2:G:465:ILE:HG13	2:G:465:ILE:O	2.16	0.45
2:G:546:LEU:HD23	2:G:603:LEU:HD23	1.98	0.45
1:C:259:ALA:HB2	2:G:674:THR:HB	1.98	0.45
1:C:518:ILE:O	1:C:519:PHE:C	2.60	0.45
1:C:1160:ILE:HA	1:C:1164:LEU:HB2	1.99	0.45
1:C:2107:SER:HB3	1:C:2291:LEU:HD11	1.99	0.45
1:C:2264:LEU:CD2	1:C:2268:LEU:HD13	2.47	0.45
2:G:203:THR:HG23	2:G:262:LYS:HE2	1.98	0.45
2:G:219:ASP:O	2:G:220:LEU:HB2	2.17	0.45
1:C:345:ILE:O	1:C:348:PHE:HB3	2.17	0.45
1:C:1017:LYS:HD2	1:C:1018:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:215:ILE:CG2	2:G:218:ALA:HB3	2.47	0.45
2:G:641:SER:OG	2:G:642:LEU:N	2.50	0.45
1:C:512:ALA:O	1:C:519:PHE:CD2	2.69	0.44
1:C:653:ILE:O	1:C:656:SER:OG	2.19	0.44
1:C:1410:PHE:O	1:C:1414:ALA:N	2.48	0.44
1:C:2203:ARG:O	1:C:2206:TYR:HB3	2.17	0.44
2:G:432:ILE:HG21	2:G:562:ILE:HD12	1.99	0.44
2:G:435:MET:CE	2:G:435:MET:CA	2.86	0.44
1:C:1683:ASP:O	1:C:1686:LEU:N	2.51	0.44
1:C:274:VAL:O	1:C:277:THR:N	2.50	0.44
1:C:1163:ILE:HG13	1:C:1293:PHE:CZ	2.53	0.44
1:C:1411:GLU:HB3	1:C:2196:PRO:HB2	1.99	0.44
2:G:196:ASN:ND2	2:G:196:ASN:O	2.50	0.44
1:C:517:GLU:OE1	1:C:517:GLU:HA	2.16	0.44
1:C:2103:LYS:O	1:C:2107:SER:OG	2.35	0.44
2:G:434:ASN:HB3	2:G:435:MET:H	1.58	0.44
2:G:508:ILE:HG13	2:G:508:ILE:O	2.17	0.44
1:C:729:ILE:CG1	1:C:730:PRO:HD3	2.48	0.44
1:C:2263:ARG:CG	1:C:2263:ARG:NH1	2.73	0.44
1:C:839:CYS:HA	1:C:842:ARG:CD	2.48	0.44
1:C:877:GLN:O	1:C:880:ILE:HG22	2.18	0.44
1:C:1060:GLN:O	1:C:1063:ASP:N	2.49	0.44
1:C:1587:PRO:O	1:C:1591:GLN:HG2	2.18	0.44
1:C:1754:SER:H	1:C:1760:ARG:NH2	2.15	0.44
2:G:223:ILE:HD11	2:G:254:ILE:HG21	1.99	0.44
2:G:575:LEU:HA	2:G:578:SER:OG	2.18	0.44
1:C:2229:ASN:HD21	1:C:2243:ASP:HB3	1.82	0.44
1:C:2288:THR:O	1:C:2292:MET:HG2	2.18	0.44
2:G:359:LEU:O	2:G:363:LEU:HG	2.18	0.44
2:G:500:LEU:HB3	2:G:525:ILE:HD11	1.99	0.44
2:G:551:GLU:O	2:G:554:ASN:N	2.50	0.44
1:C:274:VAL:HG13	1:C:275:LEU:N	2.33	0.44
1:C:648:LEU:HD13	1:C:687:ILE:HD13	1.99	0.44
1:C:819:LEU:HA	1:C:838:LEU:HD21	2.00	0.44
1:C:1160:ILE:HD11	1:C:1208:ASN:O	2.18	0.44
1:C:2264:LEU:HD13	1:C:2269:LEU:CD1	2.47	0.44
1:C:1725:PHE:O	1:C:1728:ILE:HG13	2.18	0.43
1:C:2265:THR:HG21	1:C:2367:PHE:H	1.81	0.43
2:G:222:THR:O	2:G:226:LEU:N	2.39	0.43
2:G:464:GLU:OE2	2:G:584:ARG:NH1	2.47	0.43
1:C:512:ALA:HB2	1:C:554:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:509:TYR:HA	2:G:518:ARG:HD3	2.01	0.43
1:C:544:LEU:HD13	1:C:587:LEU:HD22	2.00	0.43
1:C:1127:ASP:O	1:C:1128:VAL:C	2.62	0.43
1:C:1425:PRO:C	1:C:1427:ASP:H	2.26	0.43
1:C:1661:VAL:CG1	1:C:1662:PRO:HD3	2.48	0.43
2:G:274:LEU:O	2:G:278:ILE:HD12	2.18	0.43
2:G:697:LEU:O	2:G:701:LEU:HD13	2.18	0.43
1:C:721:LEU:O	1:C:725:GLN:N	2.52	0.43
1:C:1117:ALA:HB2	1:C:1602:GLY:HA3	2.00	0.43
1:C:1170:GLN:OE1	1:C:1170:GLN:N	2.51	0.43
1:C:2110:ARG:HH22	1:C:2283:LYS:HB3	1.83	0.43
1:C:2212:VAL:HA	1:C:2288:THR:HG21	1.99	0.43
1:C:1457:THR:OG1	1:C:1458:PHE:N	2.52	0.43
2:G:219:ASP:N	2:G:219:ASP:OD1	2.50	0.43
2:G:643:TRP:O	2:G:647:VAL:HG23	2.18	0.43
1:C:2185:LEU:HB3	1:C:2271:ALA:CB	2.49	0.43
2:G:415:VAL:HA	2:G:418:ILE:HD12	2.01	0.43
1:C:517:GLU:CD	1:C:517:GLU:C	2.85	0.43
1:C:602:ASN:HA	1:C:605:ASP:HB2	1.99	0.43
1:C:846:THR:O	1:C:850:LYS:N	2.50	0.43
1:C:970:ILE:O	1:C:973:ILE:HG13	2.19	0.43
1:C:1474:GLU:HG3	1:C:1474:GLU:O	2.19	0.43
1:C:2206:TYR:OH	1:C:2268:LEU:HD21	2.17	0.43
2:G:571:ASN:O	2:G:573:GLU:HG2	2.19	0.43
1:C:2247:LEU:HB3	1:C:2248:PHE:H	1.56	0.43
2:G:197:ARG:O	2:G:198:ILE:C	2.59	0.43
2:G:315:HIS:HB3	2:G:319:LEU:HG	2.00	0.43
1:C:620:LEU:HB2	1:C:623:VAL:HG23	2.00	0.43
1:C:710:ILE:HD12	1:C:720:ILE:HG21	2.01	0.42
1:C:1143:VAL:O	1:C:1151:GLN:NE2	2.52	0.42
1:C:2138:LEU:HA	1:C:2227:CYS:HB2	2.01	0.42
1:C:2158:LEU:HD12	1:C:2159:HIS:N	2.34	0.42
1:C:2188:TRP:O	1:C:2192:ASN:HB2	2.18	0.42
2:G:254:ILE:O	2:G:257:LEU:N	2.52	0.42
1:C:1554:TRP:O	1:C:1557:GLN:N	2.50	0.42
2:G:329:LEU:HD11	2:G:333:TYR:HE2	1.84	0.42
2:G:242:PHE:CD1	2:G:257:LEU:HD22	2.54	0.42
1:C:633:GLN:NE2	2:G:591:GLU:OE2	2.50	0.42
1:C:1492:ASP:HB3	1:C:1495:THR:OG1	2.20	0.42
1:C:1806:TYR:O	1:C:1809:ARG:N	2.53	0.42
1:C:2335:GLY:C	1:C:2336:LEU:HD12	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:360:ILE:O	2:G:364:ILE:HG22	2.20	0.42
2:G:390:PHE:CE2	2:G:395:ILE:HG12	2.54	0.42
2:G:549:LYS:HA	2:G:552:VAL:HG22	2.01	0.42
2:G:562:ILE:HG23	2:G:563:TYR:H	1.84	0.42
1:C:512:ALA:HB1	1:C:519:PHE:CD2	2.54	0.42
1:C:1418:GLU:O	1:C:1422:ARG:N	2.52	0.42
1:C:1646:THR:O	1:C:1650:ASP:N	2.44	0.42
1:C:274:VAL:O	1:C:275:LEU:C	2.62	0.42
1:C:558:LYS:HB2	1:C:601:HIS:HD2	1.79	0.42
1:C:623:VAL:HG13	1:C:626:ASN:HB2	2.00	0.42
1:C:1074:THR:OG1	1:C:1075:GLU:OE1	2.26	0.42
1:C:1496:THR:HB	1:C:1534:TRP:CZ2	2.55	0.42
1:C:1512:ILE:HD11	1:C:1541:ALA:HB2	2.02	0.42
1:C:1712:HIS:O	1:C:1712:HIS:ND1	2.52	0.42
1:C:2209:SER:OG	1:C:2238:LYS:HA	2.19	0.42
2:G:303:MET:O	2:G:307:VAL:HG23	2.19	0.42
2:G:455:THR:HA	2:G:458:TYR:CD2	2.53	0.42
2:G:657:GLU:O	2:G:660:MET:N	2.53	0.42
1:C:2154:SER:C	1:C:2157:SER:HG	2.24	0.42
1:C:2223:GLY:CA	1:C:2245:ASP:OD2	2.64	0.42
1:C:2339:SER:O	1:C:2342:GLY:N	2.52	0.42
2:G:465:ILE:HD11	2:G:546:LEU:HD13	2.02	0.42
1:C:576:CYS:SG	1:C:588:SER:HB3	2.60	0.42
1:C:690:VAL:O	1:C:693:ARG:HG2	2.20	0.42
1:C:842:ARG:HH12	1:C:916:TYR:CB	2.32	0.42
1:C:890:ASP:HA	1:C:893:ASP:OD2	2.20	0.42
1:C:1573:TYR:O	1:C:1576:ALA:N	2.52	0.42
2:G:414:MET:O	2:G:418:ILE:HG13	2.20	0.42
2:G:458:TYR:CD1	2:G:577:HIS:CG	3.07	0.42
1:C:283:ASP:HA	1:C:324:TRP:HZ2	1.84	0.42
1:C:1991:SER:O	1:C:1995:ARG:N	2.35	0.42
1:C:2178:VAL:O	1:C:2178:VAL:HG12	2.20	0.42
1:C:2183:PRO:HB3	1:C:2267:ASN:HA	2.01	0.42
2:G:334:HIS:O	2:G:336:VAL:N	2.53	0.42
1:C:1947:SER:CB	1:C:2122:LEU:HA	2.50	0.42
1:C:2105:ILE:HG23	1:C:2106:ALA:N	2.35	0.42
1:C:838:LEU:HD12	1:C:841:LEU:HB2	2.02	0.41
1:C:1125:VAL:HG21	1:C:1656:ILE:CG2	2.39	0.41
1:C:1996:SER:O	1:C:2000:LEU:N	2.47	0.41
1:C:2188:TRP:HZ2	1:C:2234:ILE:HD12	1.85	0.41
2:G:311:PRO:O	2:G:314:THR:OG1	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:547:LYS:O	2:G:550:ASP:N	2.49	0.41
2:G:601:LEU:O	2:G:604:ARG:N	2.53	0.41
2:G:356:GLN:CD	2:G:519:VAL:HA	2.45	0.41
1:C:877:GLN:CG	1:C:921:SER:HB2	2.50	0.41
1:C:2135:VAL:HG23	1:C:2232:LEU:O	2.20	0.41
2:G:518:ARG:HG2	2:G:518:ARG:O	2.21	0.41
1:C:279:HIS:CE1	1:C:320:PRO:HD2	2.55	0.41
1:C:905:ARG:O	1:C:908:ASN:HB2	2.21	0.41
1:C:1128:VAL:HG23	1:C:1618:GLN:HE21	1.85	0.41
1:C:1396:PRO:HA	1:C:1399:LEU:CB	2.50	0.41
1:C:1562:ARG:O	1:C:1563:ASN:HB2	2.20	0.41
1:C:274:VAL:HG13	1:C:275:LEU:H	1.85	0.41
1:C:528:SER:OG	1:C:529:HIS:N	2.54	0.41
1:C:605:ASP:HB3	1:C:606:GLU:OE1	2.20	0.41
1:C:688:LEU:HB2	1:C:689:PRO:HD3	2.02	0.41
1:C:833:ASN:HA	1:C:836:MET:HB2	2.02	0.41
1:C:956:HIS:O	1:C:956:HIS:CG	2.74	0.41
1:C:2081:LYS:HA	1:C:2126:CYS:O	2.21	0.41
2:G:616:TYR:CE1	2:G:721:ALA:HB1	2.56	0.41
2:G:695:GLU:O	2:G:698:LYS:HB2	2.21	0.41
1:C:963:SER:OG	1:C:964:THR:N	2.54	0.41
1:C:1476:TRP:CD1	1:C:1506:HIS:HD1	2.38	0.41
1:C:2162:TRP:CD1	1:C:2174:TYR:CZ	3.09	0.41
1:C:2185:LEU:C	1:C:2185:LEU:CD2	2.93	0.41
2:G:350:VAL:O	2:G:350:VAL:HG13	2.21	0.41
1:C:548:HIS:ND1	1:C:594:LEU:HD11	2.35	0.41
1:C:599:ASP:CG	1:C:600:SER:H	2.28	0.41
1:C:962:LEU:HD12	1:C:999:LYS:NZ	2.35	0.41
1:C:2265:THR:CG2	1:C:2266:PRO:CD	2.92	0.41
1:C:2344:THR:O	1:C:2348:ILE:HG22	2.20	0.41
1:C:547:LEU:HD11	1:C:551:PHE:CZ	2.56	0.41
1:C:1168:PHE:CB	1:C:1180:VAL:HG11	2.51	0.41
1:C:2226:HIS:CE1	1:C:2229:ASN:HB2	2.55	0.41
2:G:213:HIS:O	2:G:221:SER:HB2	2.21	0.41
2:G:224:GLU:C	2:G:227:ASN:H	2.28	0.41
1:C:241:LEU:HD23	1:C:241:LEU:O	2.20	0.41
1:C:539:LEU:O	1:C:542:GLY:N	2.54	0.41
1:C:1156:LEU:O	1:C:1160:ILE:HG23	2.21	0.41
1:C:1295:LEU:HB3	1:C:1296:PRO:HD3	2.02	0.41
1:C:1495:THR:OG1	1:C:1496:THR:N	2.54	0.41
1:C:1611:GLU:O	1:C:1611:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2179:ASP:C	1:C:2181:PHE:H	2.29	0.41
2:G:294:LEU:O	2:G:294:LEU:HD23	2.20	0.41
2:G:320:LYS:HA	2:G:390:PHE:HE1	1.86	0.41
2:G:579:SER:HA	2:G:582:LEU:HB3	2.03	0.41
1:C:557:PRO:O	1:C:566:ILE:CG2	2.69	0.41
1:C:1463:LEU:HD12	1:C:1466:LYS:HB2	2.01	0.41
1:C:1596:ASN:OD1	2:G:350:VAL:HB	2.21	0.41
1:C:1789:ILE:HD12	1:C:1789:ILE:HG23	1.79	0.41
1:C:2297:VAL:O	1:C:2301:ASN:N	2.53	0.41
2:G:361:ASP:O	2:G:365:ILE:HG12	2.21	0.41
1:C:1163:ILE:HG13	1:C:1293:PHE:CE1	2.56	0.40
1:C:1789:ILE:HG22	1:C:1789:ILE:O	2.21	0.40
1:C:2171:LEU:HB3	1:C:2359:LYS:CB	2.51	0.40
1:C:2179:ASP:O	1:C:2181:PHE:N	2.54	0.40
1:C:290:ASP:O	1:C:293:PRO:HD3	2.21	0.40
1:C:1036:ILE:O	1:C:1039:THR:OG1	2.37	0.40
1:C:1778:ALA:O	1:C:1782:ILE:HG13	2.21	0.40
1:C:272:LYS:HE3	1:C:314:CYS:SG	2.61	0.40
1:C:915:ILE:HG22	1:C:916:TYR:CE1	2.56	0.40
1:C:1360:ALA:HA	1:C:1363:PHE:HB3	2.04	0.40
1:C:1592:LYS:O	1:C:1596:ASN:HB2	2.21	0.40
1:C:2100:LEU:HD21	1:C:2112:LEU:HB2	2.04	0.40
1:C:1539:LEU:HD13	1:C:1554:TRP:HB3	2.02	0.40
1:C:1723:LEU:HD21	1:C:1766:LYS:HE3	2.04	0.40
1:C:1764:LEU:HA	1:C:1767:PHE:HB3	2.04	0.40
1:C:2223:GLY:HA2	1:C:2245:ASP:CG	2.46	0.40
2:G:228:ARG:HB2	2:G:513:LEU:HA	2.02	0.40
1:C:283:ASP:HA	1:C:324:TRP:CZ2	2.55	0.40
1:C:1661:VAL:HG13	1:C:1662:PRO:HD3	2.03	0.40
1:C:1786:TYR:OH	1:C:1802:SER:O	2.33	0.40
1:C:1809:ARG:HA	1:C:1812:GLU:HB3	2.03	0.40
1:C:2269:LEU:O	1:C:2276:GLY:HA2	2.22	0.40
2:G:256:SER:OG	2:G:260:ARG:NE	2.52	0.40
2:G:314:THR:OG1	2:G:315:HIS:N	2.54	0.40
2:G:487:ASP:N	2:G:487:ASP:OD1	2.53	0.40
2:G:492:ILE:HD13	2:G:493:ARG:NH2	2.36	0.40
2:G:670:LEU:HD23	2:G:670:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1943/2368 (82%)	1595 (82%)	311 (16%)	37 (2%)	6	33
2	G	678/747 (91%)	556 (82%)	102 (15%)	20 (3%)	3	26
All	All	2621/3115 (84%)	2151 (82%)	413 (16%)	57 (2%)	7	31

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	356	PRO
1	C	685	SER
1	C	845	ILE
1	C	1241	VAL
1	C	1395	THR
1	C	2017	VAL
1	C	2018	PRO
1	C	2061	LYS
1	C	2062	PRO
1	C	2274	ILE
2	G	159	THR
2	G	160	PRO
2	G	170	LYS
2	G	171	PRO
2	G	289	PRO
2	G	409	ILE
2	G	434	ASN
1	C	1755	VAL
1	C	2055	VAL
2	G	510	THR
1	C	687	ILE
1	C	2114	ILE
1	C	2180	LYS
1	C	2271	ALA
2	G	172	GLN

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Mol	Chain	Res	Type
2	G	173	SER
2	G	191	VAL
2	G	290	ASN
1	C	307	ILE
1	C	322	ASP
1	C	357	VAL
1	C	2010	VAL
1	C	2167	VAL
1	C	2265	THR
2	G	199	ILE
2	G	438	SER
2	G	509	TYR
1	C	2248	PHE
1	C	2354	GLU
1	C	603	SER
1	C	623	VAL
1	C	652	ASP
1	C	2041	ARG
1	C	2195	ASP
2	G	145	LYS
1	C	489	VAL
2	G	216	ILE
2	G	470	VAL
2	G	519	VAL
1	C	780	GLY
2	G	562	ILE
1	C	1125	VAL
1	C	1224	ILE
1	C	2025	ILE
1	C	2026	ILE
1	C	529	HIS
1	C	1274	HIS

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	C	1257/2174 (58%)	1233 (98%)	24 (2%)	50	66
2	G	447/698 (64%)	443 (99%)	4 (1%)	70	75
All	All	1704/2872 (59%)	1676 (98%)	28 (2%)	54	69

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	518	ILE
1	C	558	LYS
1	C	684	LEU
1	C	685	SER
1	C	687	ILE
1	C	914	ILE
1	C	1126	LEU
1	C	1138	TYR
1	C	1290	LEU
1	C	2167	VAL
1	C	2175	MET
1	C	2179	ASP
1	C	2209	SER
1	C	2246	CYS
1	C	2247	LEU
1	C	2263	ARG
1	C	2265	THR
1	C	2267	ASN
1	C	2269	LEU
1	C	2353	SER
1	C	2354	GLU
1	C	2355	ASP
1	C	2357	LEU
1	C	2359	LYS
2	G	196	ASN
2	G	198	ILE
2	G	287	VAL
2	G	435	MET

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

Mol	Chain	Res	Type
1	C	279	HIS
1	C	444	GLN

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Mol	Chain	Res	Type
1	C	565	GLN
1	C	574	GLN
1	C	601	HIS
1	C	626	ASN
1	C	877	GLN
1	C	928	GLN
1	C	1185	GLN
1	C	1423	GLN
1	C	1543	ASN
1	C	1572	GLN
1	C	1618	GLN
1	C	1625	HIS
1	C	1743	GLN
1	C	1756	ASN
1	C	2089	GLN
1	C	2198	ASN
1	C	2229	ASN
1	C	2314	HIS
2	G	196	ASN
2	G	305	GLN
2	G	334	HIS
2	G	353	GLN
2	G	494	ASN
2	G	600	ASN
2	G	649	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

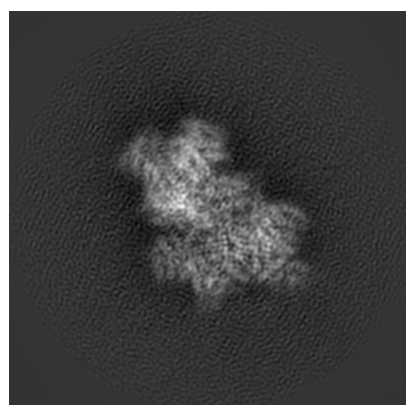
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6708. These allow visual inspection of the internal detail of the map and identification of artifacts.

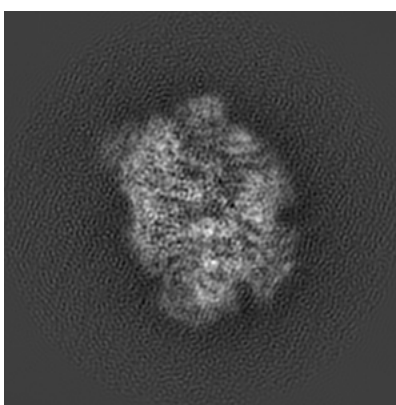
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

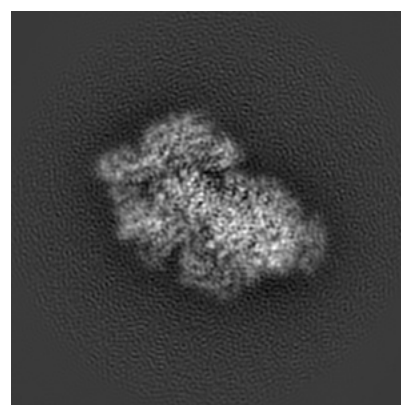
6.1.1 Primary map



X



Y

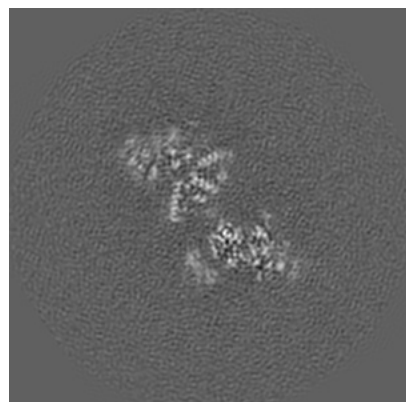


Z

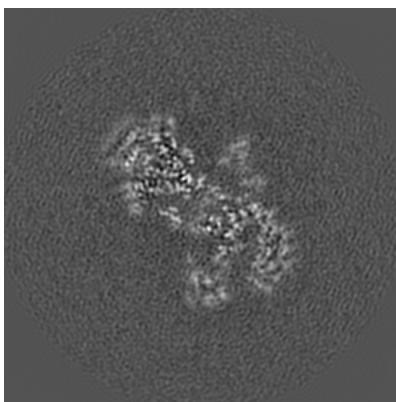
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

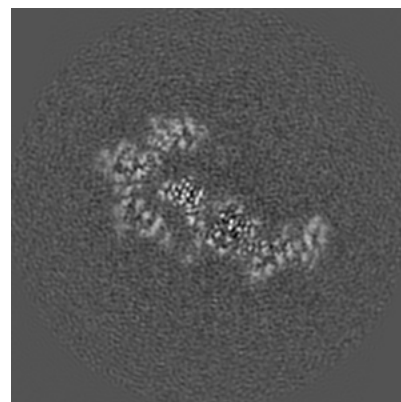
6.2.1 Primary map



X Index: 128



Y Index: 128

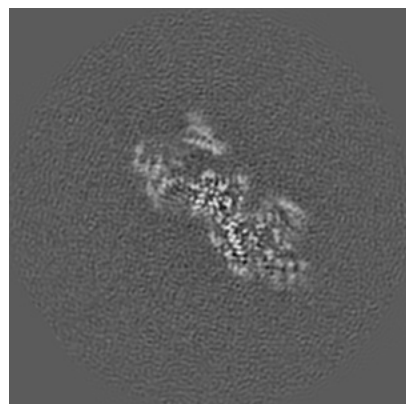


Z Index: 128

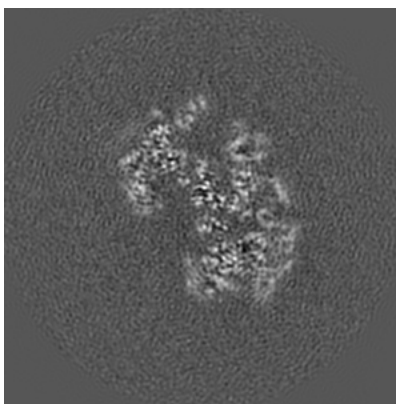
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

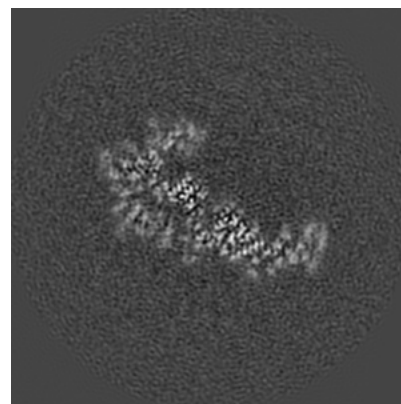
6.3.1 Primary map



X Index: 115



Y Index: 119

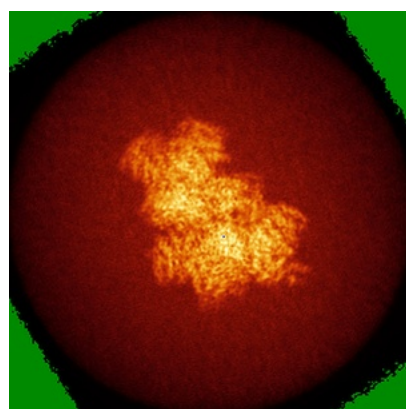


Z Index: 130

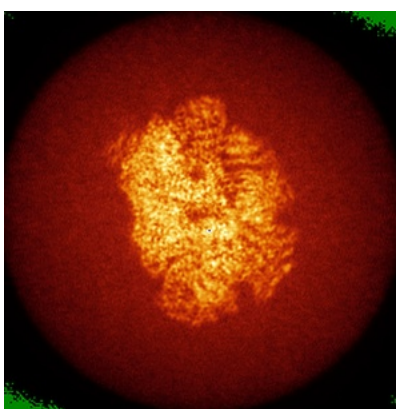
The images above show the largest variance slices of the map in three orthogonal directions.

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

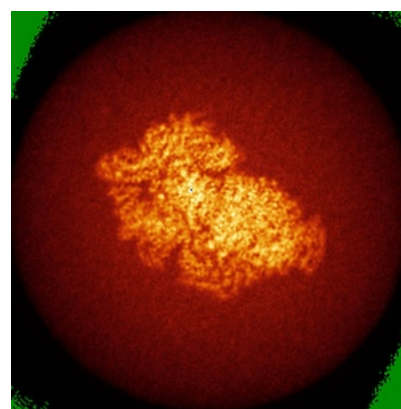
6.4.1 Primary map



X



Y



Z

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 0.0518. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

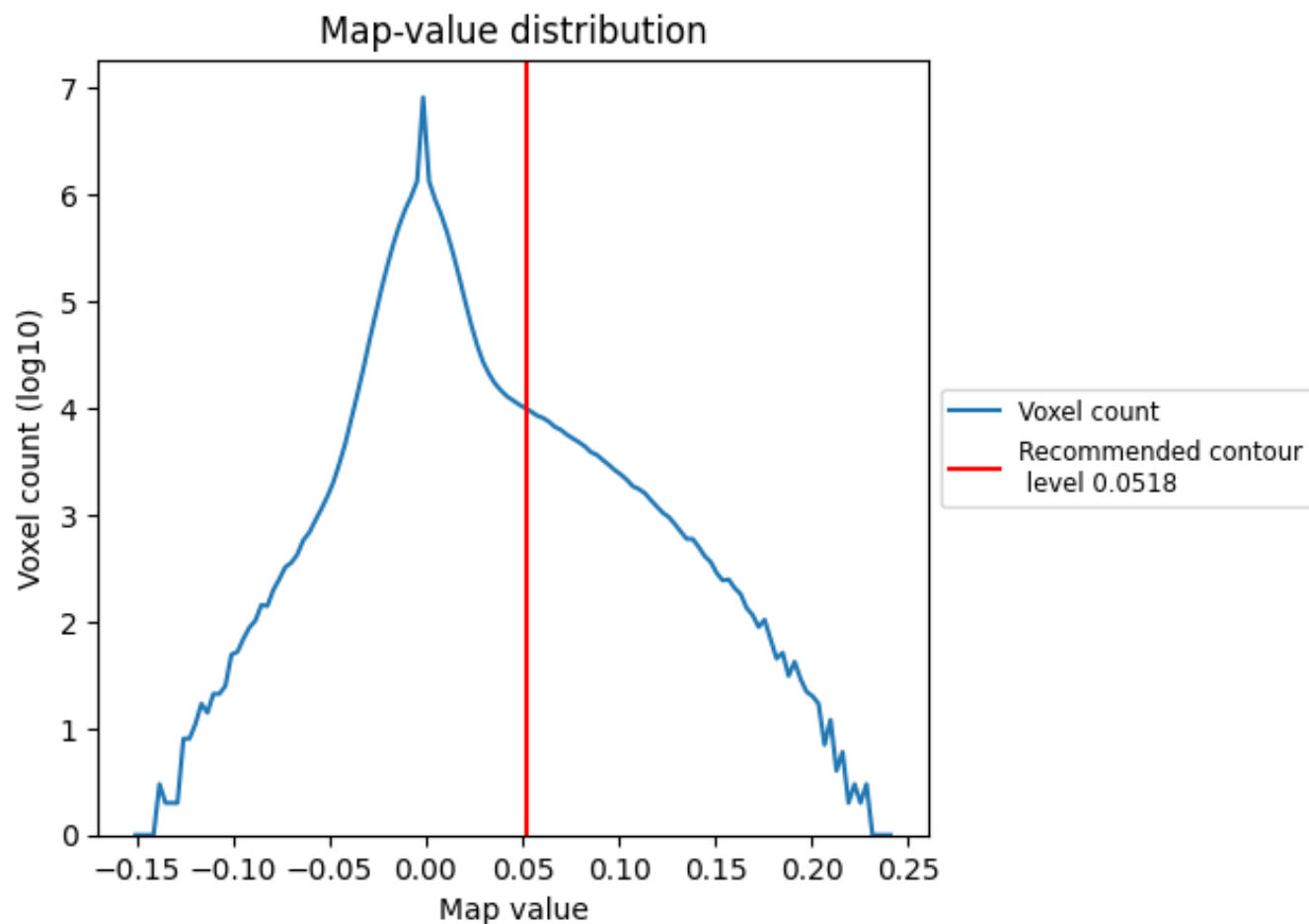
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

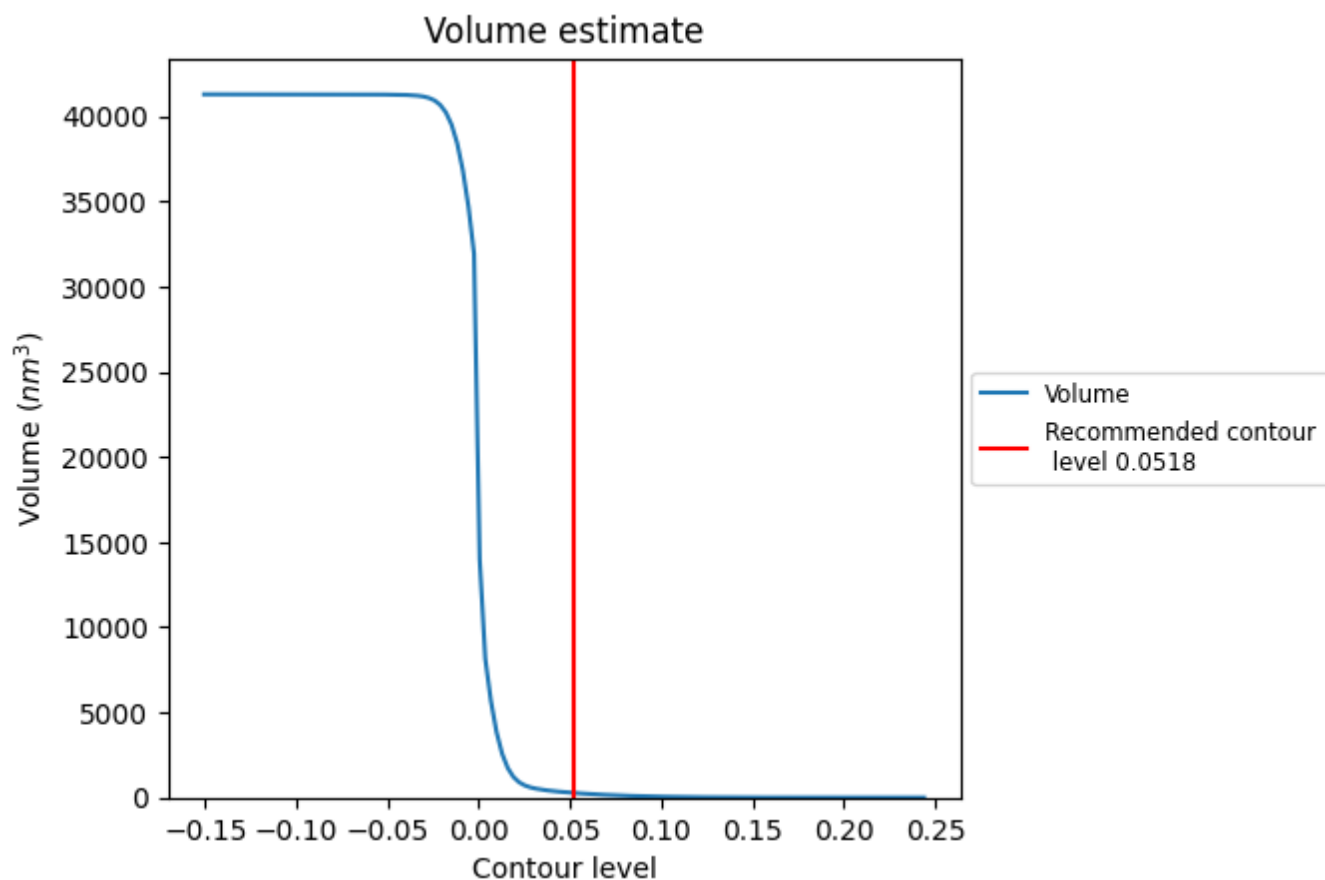
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

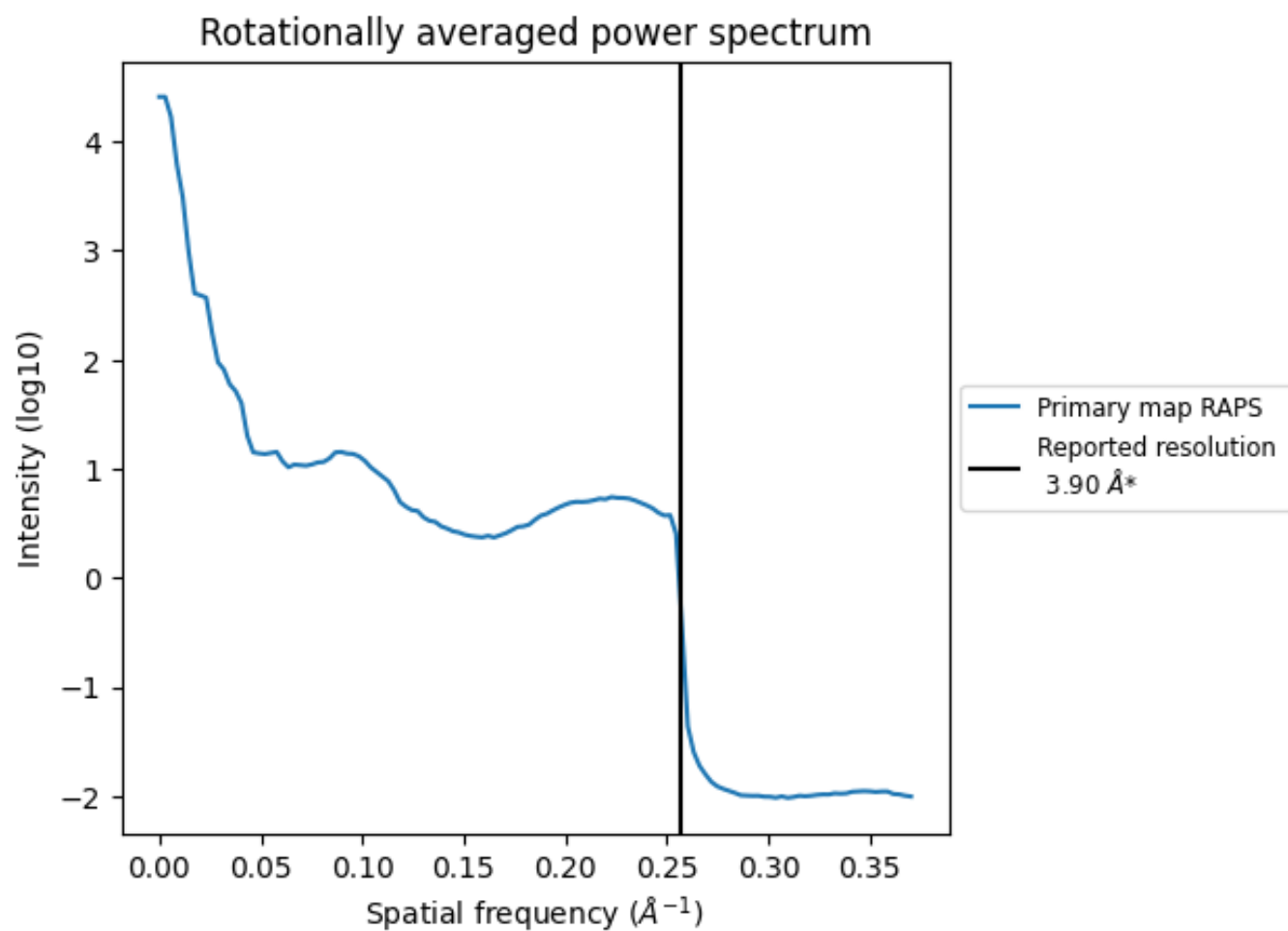
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 274 nm³; this corresponds to an approximate mass of 248 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

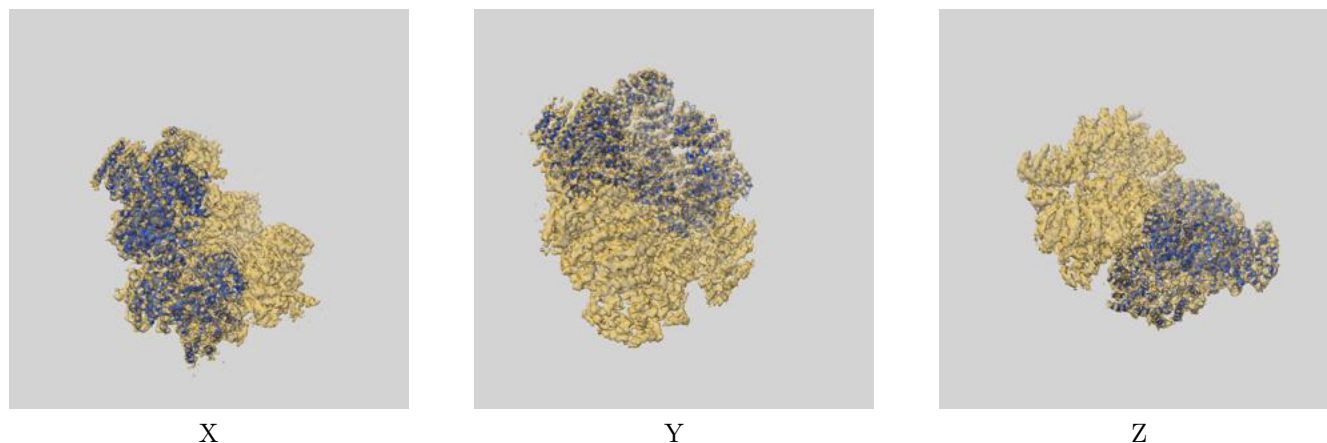
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

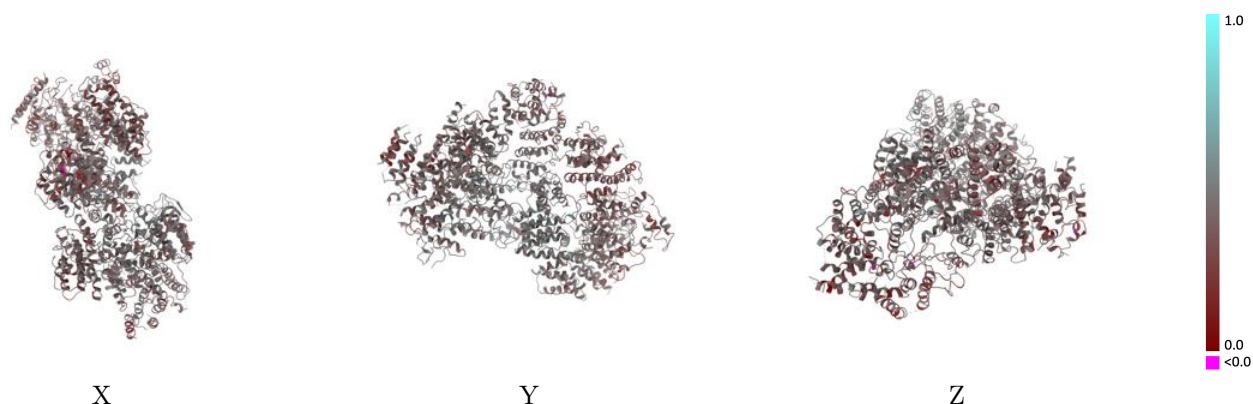
This section contains information regarding the fit between EMDB map EMD-6708 and PDB model 5X6O. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



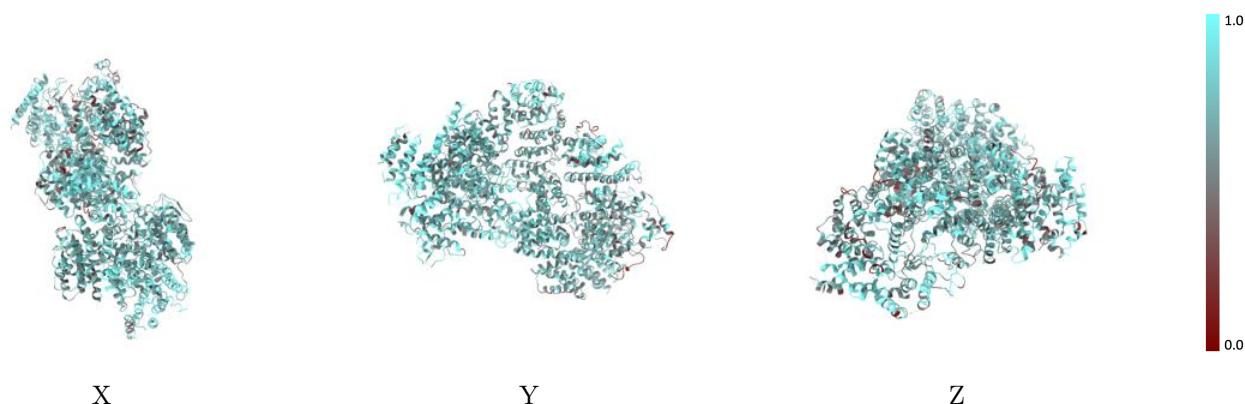
The images above show the 3D surface view of the map at the recommended contour level 0.0518 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



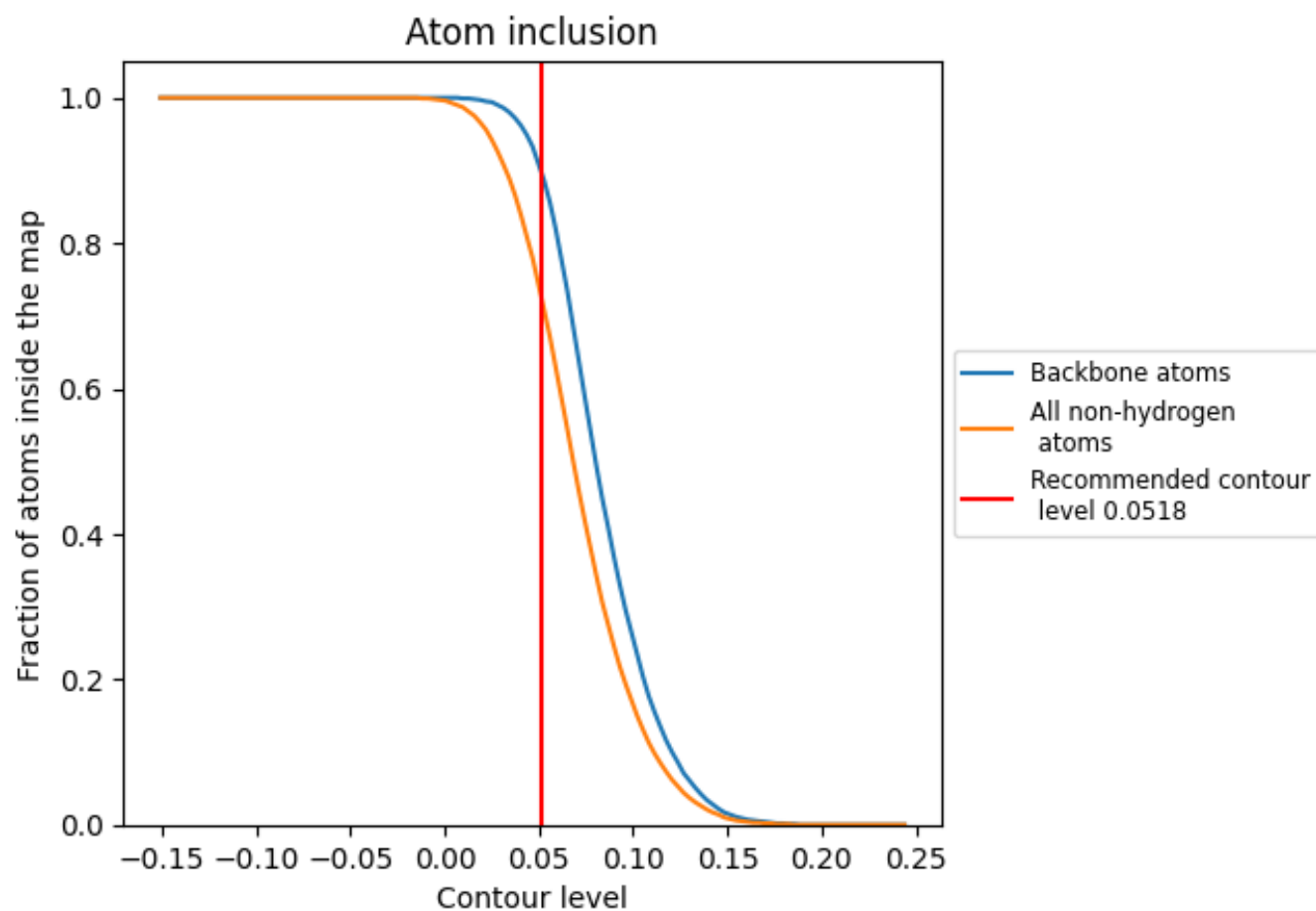
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0518).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 72% 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 (0.0518) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.4100
C	0.7060	0.4020
G	0.7640	0.4310

