



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:47 PM UTC

PDB ID : 9GDH / pdb_00009gdh
EMDB ID : EMD-51264
Title : RNAP-TopoI complex on long-overhang scaffold - orientation 2
Authors : Vidmar, V.; Weixlbaumer, A.; Lamour, V.
Deposited on : 2024-08-05
Resolution : 3.90 Å (reported)
Based on initial models : 6alh, 4rul, 3px7

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:

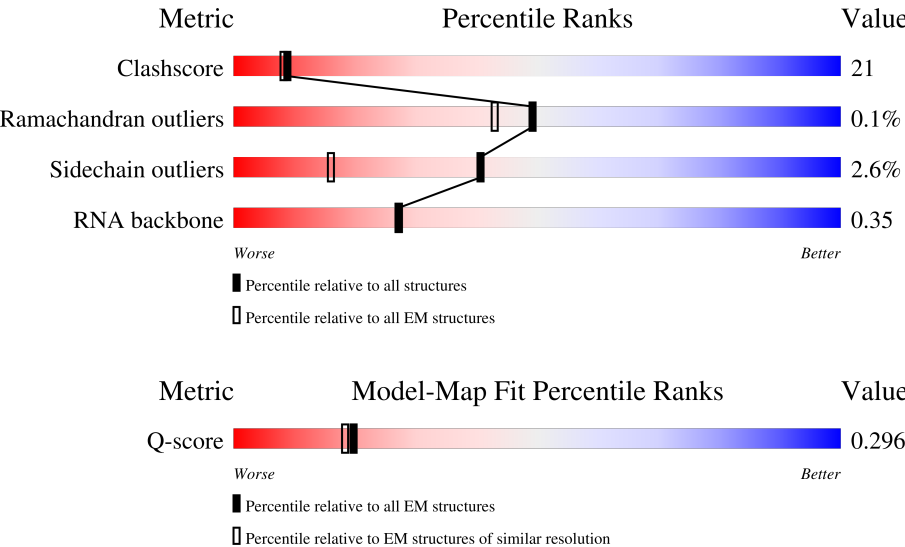
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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.






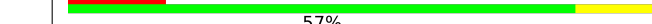
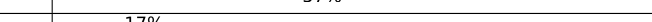

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	A	329	
1	B	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
3	D	1415	 60% 34% 5%
4	E	91	 11% 57% 42%
5	F	896	 17% 59% 31% 8%
6	N	50	 50% 26% 24%
7	R	14	 57% 21% 21%
8	T	50	 26% 34% 40%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 33258 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	233	Total	C	N	O	S	0	0
			1803	1122	320	355	6		
1	B	232	Total	C	N	O	S	0	0
			1799	1120	319	354	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0
			10577	6636	1842	2056	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1342	Total	C	N	O	S	0	0
			10433	6553	1861	1969	50		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	expression tag	UNP P0A8T7
D	1409	GLU	-	expression tag	UNP P0A8T7
D	1410	LEU	-	expression tag	UNP P0A8T7
D	1411	GLU	-	expression tag	UNP P0A8T7
D	1412	VAL	-	expression tag	UNP P0A8T7
D	1413	LEU	-	expression tag	UNP P0A8T7
D	1414	PHE	-	expression tag	UNP P0A8T7
D	1415	GLN	-	expression tag	UNP P0A8T7

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	90	Total	C	N	O	S	0	0
			709	430	136	142	1		

- Molecule 5 is a protein called DNA topoisomerase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	827	Total	C	N	O	S	0	0
			6558	4116	1167	1238	37		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-30	GLY	-	expression tag	UNP P06612
F	-29	PRO	-	expression tag	UNP P06612
F	-28	TRP	-	expression tag	UNP P06612
F	-27	SER	-	expression tag	UNP P06612
F	-26	HIS	-	expression tag	UNP P06612
F	-25	PRO	-	expression tag	UNP P06612
F	-24	GLN	-	expression tag	UNP P06612
F	-23	PHE	-	expression tag	UNP P06612
F	-22	GLU	-	expression tag	UNP P06612
F	-21	LYS	-	expression tag	UNP P06612
F	-20	GLY	-	expression tag	UNP P06612
F	-19	GLY	-	expression tag	UNP P06612
F	-18	GLY	-	expression tag	UNP P06612
F	-17	SER	-	expression tag	UNP P06612
F	-16	GLY	-	expression tag	UNP P06612
F	-15	GLY	-	expression tag	UNP P06612
F	-14	GLY	-	expression tag	UNP P06612
F	-13	SER	-	expression tag	UNP P06612
F	-12	GLY	-	expression tag	UNP P06612
F	-11	GLY	-	expression tag	UNP P06612
F	-10	SER	-	expression tag	UNP P06612
F	-9	ALA	-	expression tag	UNP P06612
F	-8	TRP	-	expression tag	UNP P06612
F	-7	SER	-	expression tag	UNP P06612
F	-6	HIS	-	expression tag	UNP P06612
F	-5	PRO	-	expression tag	UNP P06612
F	-4	GLN	-	expression tag	UNP P06612
F	-3	PHE	-	expression tag	UNP P06612
F	-2	GLU	-	expression tag	UNP P06612
F	-1	LYS	-	expression tag	UNP P06612
F	0	HIS	-	expression tag	UNP P06612

- Molecule 6 is a DNA chain called non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	38	Total	C	N	O	P	0	13
			530	247	95	150	38		

- Molecule 7 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	11	Total	C	N	O	P	0	0
			235	104	42	78	11		

- Molecule 8 is a DNA chain called template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	30	Total	C	N	O	P	0	0
			608	289	110	179	30		

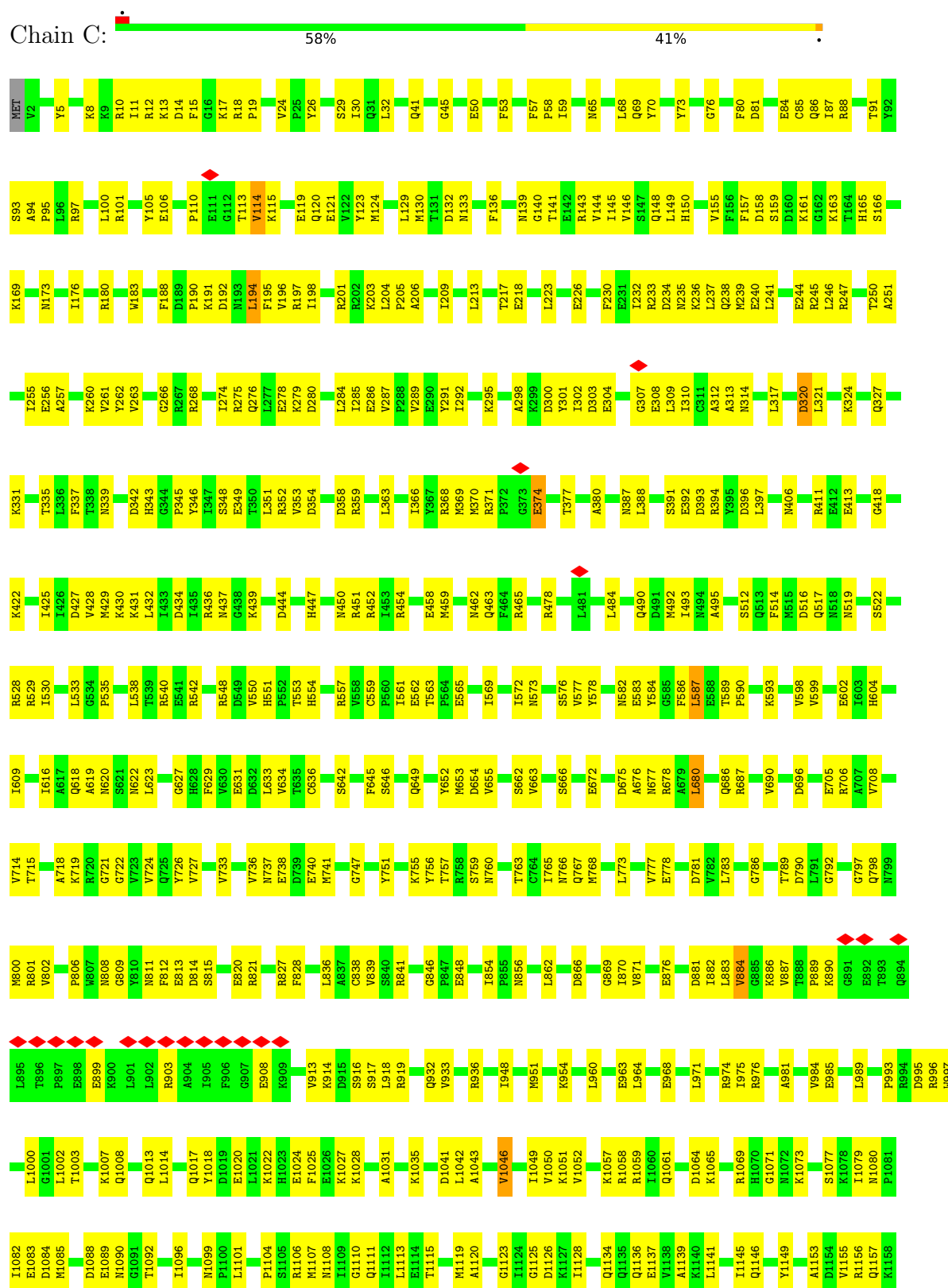
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

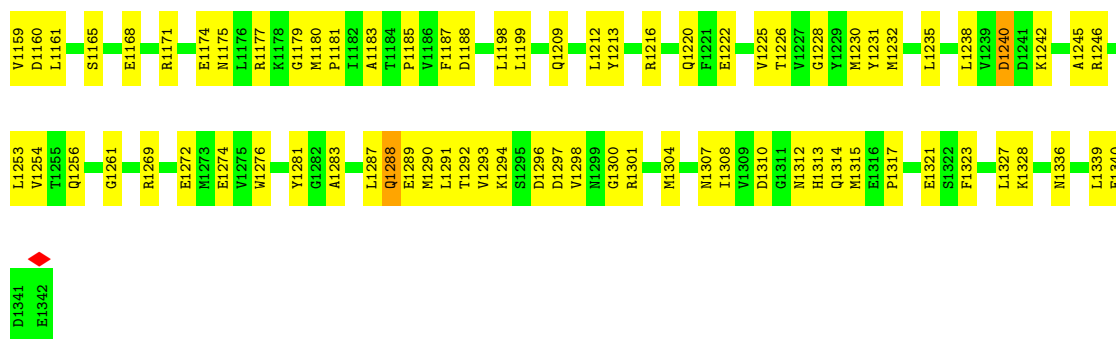
Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Mg	0
			1	1	

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

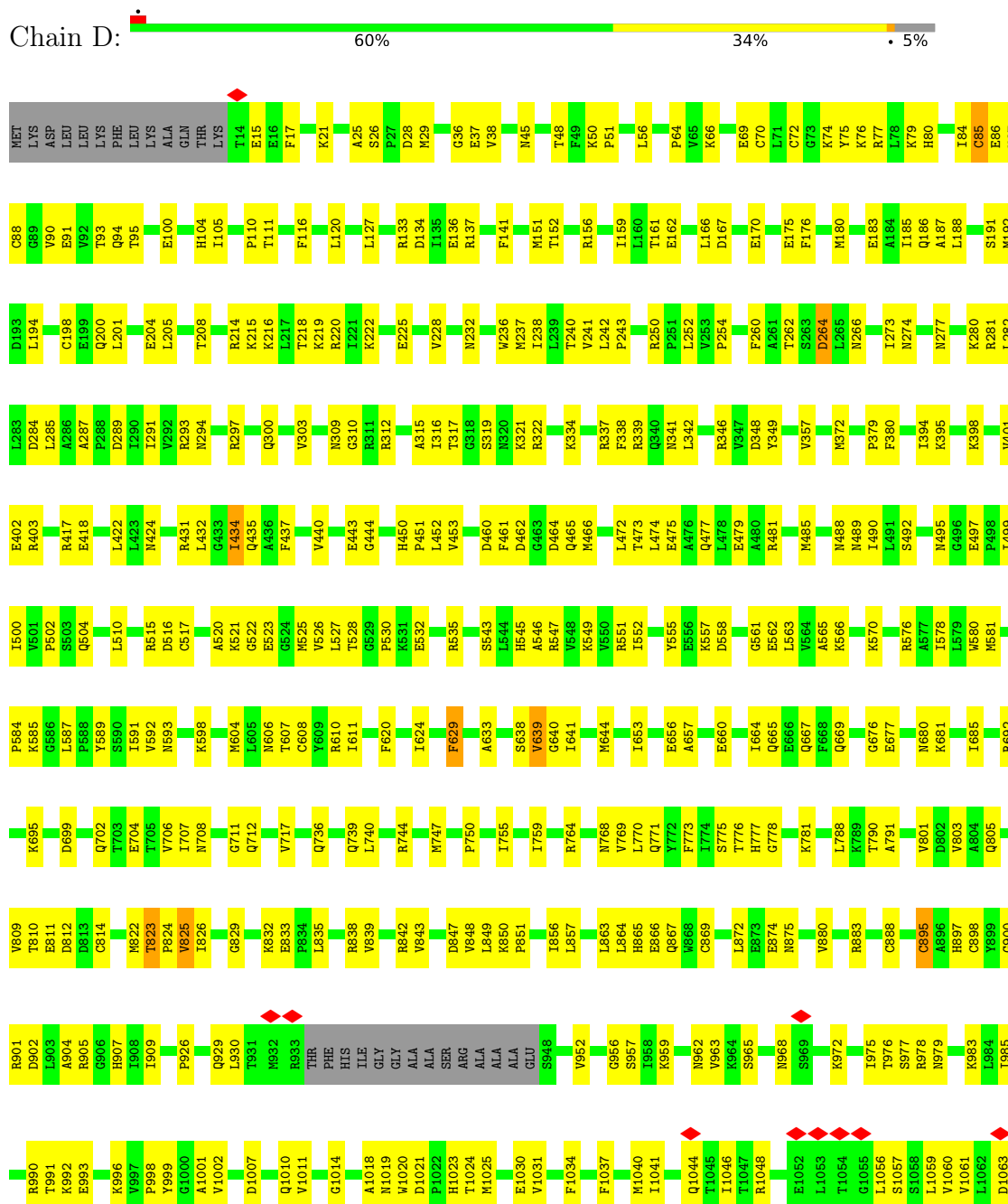
Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	
10	F	3	Total	Zn	0
			3	3	

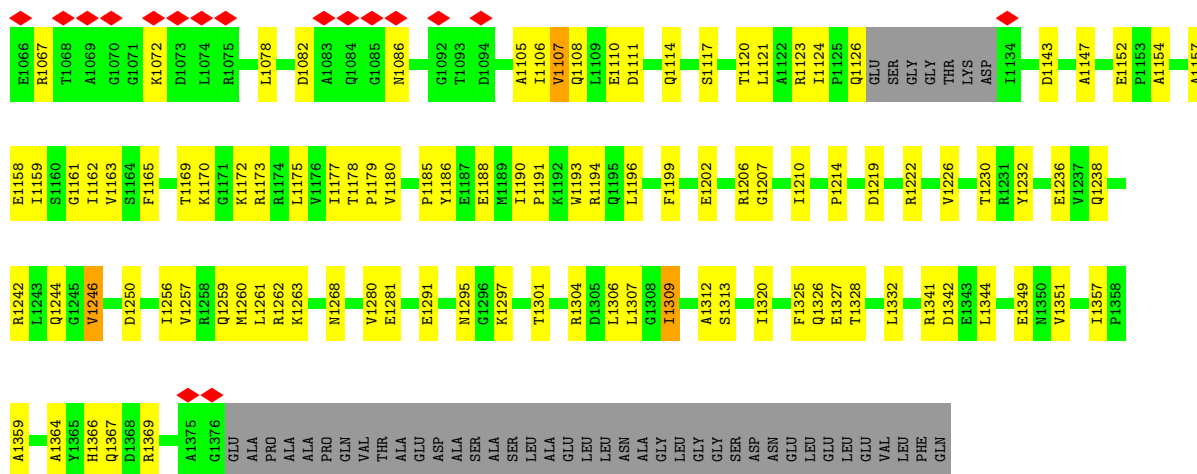
● Molecule 2: DNA-directed RNA polymerase subunit beta



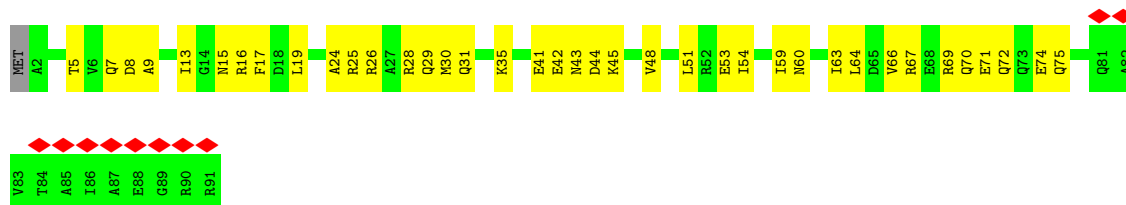


• Molecule 3: DNA-directed RNA polymerase subunit beta'

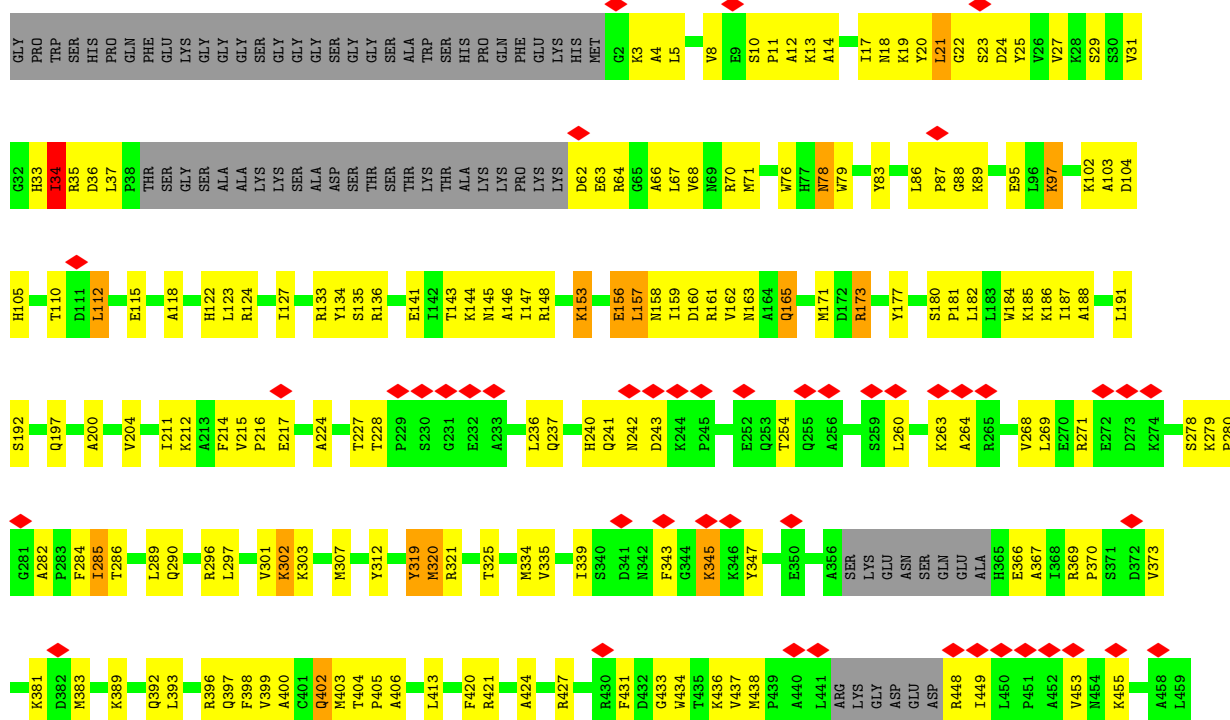




• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: DNA topoisomerase 1





G
A
G
U4
C5
C6
G7
C8
G9
G10
C11
G12
C13
G14

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10189	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.9	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.866	Depositor
Minimum map value	-0.324	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.174	Depositor
Map size (Å)	309.59998, 309.59998, 309.59998	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9987096, 0.9987096, 0.9987096	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/1825	0.31	0/2473
1	B	0.23	0/1821	0.32	0/2468
2	C	0.23	0/10746	0.30	0/14499
3	D	0.23	0/10590	0.31	0/14298
4	E	0.19	0/711	0.32	0/956
5	F	0.46	0/6688	0.81	9/9025 (0.1%)
6	N	0.29	0/580	0.56	0/891
7	R	0.36	0/261	0.58	0/405
8	T	0.38	0/680	0.59	0/1045
All	All	0.30	0/33902	0.47	9/46060 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	751	PRO	N-CA-C	6.79	122.01	111.21
5	F	750	PRO	N-CA-C	-6.65	102.59	110.70
5	F	560	TRP	N-CA-C	6.34	117.85	111.07
5	F	187	ILE	N-CA-C	6.25	117.35	111.48
5	F	285	ILE	N-CA-C	-5.86	103.66	110.05
5	F	402	GLN	CA-C-N	-5.35	113.16	122.64
5	F	402	GLN	C-N-CA	-5.35	113.16	122.64
5	F	200	ALA	N-CA-C	-5.19	105.52	111.07
5	F	589	PRO	N-CA-C	-5.14	103.75	111.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1803	0	1830	71	0
1	B	1799	0	1827	66	0
2	C	10577	0	10591	414	0
3	D	10433	0	10654	402	0
4	E	709	0	719	30	0
5	F	6558	0	6513	409	0
6	N	530	0	284	28	0
7	R	235	0	120	19	0
8	T	608	0	337	41	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
10	F	3	0	0	0	0
All	All	33258	0	32875	1378	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 (1378) 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)
5:F:521:LYS:CD	5:F:615:VAL:HG11	1.23	1.65
5:F:473:PRO:CD	5:F:653:THR:HA	1.12	1.58
5:F:473:PRO:HD2	5:F:653:THR:CA	1.18	1.58
5:F:521:LYS:HD2	5:F:615:VAL:CG1	1.39	1.53
5:F:472:LYS:CB	5:F:653:THR:HB	1.47	1.41
5:F:472:LYS:CA	5:F:653:THR:HB	1.56	1.35
5:F:521:LYS:HB2	5:F:615:VAL:CG2	1.61	1.31
5:F:404:THR:O	5:F:434:TRP:N	1.64	1.26
5:F:472:LYS:HA	5:F:653:THR:CB	1.69	1.22
5:F:280:PRO:HD3	5:F:434:TRP:CD1	1.73	1.22
5:F:212:LYS:O	5:F:668:ALA:CB	1.90	1.20
3:D:208:THR:CG2	3:D:214:ARG:HG2	1.73	1.18
5:F:473:PRO:HD3	5:F:653:THR:HA	1.20	1.17
5:F:212:LYS:O	5:F:668:ALA:HB2	1.42	1.16
5:F:97:LYS:HE2	5:F:127:ILE:HA	1.16	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:208:THR:HG23	3:D:214:ARG:HE	1.01	1.14
5:F:3:LYS:HD3	5:F:102:LYS:HE2	1.20	1.12
5:F:521:LYS:CB	5:F:615:VAL:HG21	1.82	1.10
5:F:521:LYS:HB2	5:F:615:VAL:HG21	1.10	1.09
5:F:211:ILE:O	5:F:656:LEU:HD13	1.53	1.07
5:F:473:PRO:HD2	5:F:653:THR:N	1.68	1.06
8:T:21:DG:H8	8:T:21:DG:H5"	1.23	1.03
5:F:522:MET:SD	5:F:612:SER:HA	1.99	1.02
5:F:70:ARG:NH1	6:N:14:DT:H71	1.76	1.01
2:C:70:TYR:HH	2:C:73:TYR:HD1	1.09	1.00
3:D:208:THR:HG23	3:D:214:ARG:NE	1.75	1.00
5:F:521:LYS:HE3	5:F:672:TYR:CZ	1.95	1.00
3:D:208:THR:HG21	3:D:214:ARG:HG2	1.01	0.99
5:F:97:LYS:NZ	5:F:127:ILE:HG12	1.77	0.99
5:F:312:TYR:CG	5:F:320:MET:HE2	1.98	0.98
5:F:475:ALA:HA	5:F:652:GLU:HG2	1.46	0.98
5:F:521:LYS:HE3	5:F:672:TYR:OH	1.61	0.98
5:F:339:ILE:HG12	5:F:403:MET:SD	2.03	0.98
5:F:472:LYS:CA	5:F:653:THR:CB	2.36	0.98
5:F:473:PRO:CD	5:F:653:THR:CA	1.97	0.97
5:F:216:PRO:HG2	5:F:657:ARG:HG3	1.46	0.97
5:F:472:LYS:CB	5:F:653:THR:CB	2.41	0.97
3:D:120:LEU:CD2	8:T:13:DT:H5"	1.95	0.97
3:D:1169:THR:HG23	6:N:48:DG:OP1	1.64	0.96
5:F:405:PRO:HA	5:F:434:TRP:HD1	1.29	0.96
2:C:255:ILE:HB	2:C:263:VAL:HG21	1.48	0.96
3:D:208:THR:HG21	3:D:214:ARG:CG	1.94	0.96
5:F:507:ARG:O	5:F:522:MET:HE1	1.63	0.96
5:F:472:LYS:HB2	5:F:653:THR:HB	1.48	0.96
5:F:521:LYS:HD3	5:F:615:VAL:HG11	1.47	0.95
5:F:650:ASP:O	5:F:653:THR:HG22	1.66	0.94
5:F:320:MET:H	5:F:320:MET:HE3	1.34	0.93
5:F:21:LEU:HD21	5:F:25:TYR:HB2	1.48	0.93
5:F:97:LYS:HE3	5:F:97:LYS:HA	1.50	0.93
5:F:472:LYS:HA	5:F:653:THR:HB	1.26	0.92
5:F:21:LEU:HD11	5:F:25:TYR:CG	2.05	0.91
5:F:473:PRO:HD2	5:F:653:THR:CB	2.00	0.91
1:B:19:VAL:HB	1:B:23:HIS:HB3	1.53	0.91
5:F:521:LYS:HD2	5:F:615:VAL:CB	2.02	0.90
5:F:78:ASN:ND2	5:F:561:LYS:HD3	1.85	0.90
3:D:208:THR:CG2	3:D:214:ARG:CG	2.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:302:LYS:HE2	5:F:302:LYS:H	1.35	0.90
5:F:263:LYS:C	5:F:263:LYS:HD2	1.97	0.90
5:F:472:LYS:HA	5:F:653:THR:OG1	1.70	0.89
5:F:3:LYS:HD3	5:F:102:LYS:CE	2.03	0.88
5:F:171:MET:HE2	5:F:546:MET:HE2	1.55	0.88
3:D:120:LEU:HD23	8:T:13:DT:H5"	1.53	0.88
5:F:118:ALA:HB2	5:F:165:GLN:HG2	1.54	0.88
5:F:521:LYS:HB2	5:F:615:VAL:HG22	1.54	0.87
5:F:70:ARG:NH1	6:N:14:DT:C7	2.37	0.87
5:F:70:ARG:HH12	6:N:14:DT:H71	1.35	0.87
3:D:134:ASP:OD1	3:D:159:ILE:HG21	1.76	0.86
5:F:37:LEU:CD1	5:F:173:ARG:HG3	2.06	0.86
5:F:339:ILE:HG23	5:F:403:MET:HE1	1.57	0.86
5:F:399:VAL:O	5:F:403:MET:HG2	1.76	0.86
5:F:335:VAL:HG11	5:F:402:GLN:HG3	1.58	0.85
5:F:79:TRP:CZ2	5:F:564:LEU:HB3	2.12	0.85
5:F:302:LYS:HE3	5:F:479:GLU:OE1	1.77	0.84
2:C:623:LEU:HD22	2:C:629:PHE:HA	1.59	0.84
5:F:280:PRO:HD3	5:F:434:TRP:CG	2.11	0.84
5:F:472:LYS:HB3	5:F:653:THR:HB	1.53	0.83
5:F:112:LEU:H	5:F:112:LEU:HD23	1.43	0.83
5:F:97:LYS:HZ3	5:F:127:ILE:HG12	1.44	0.83
3:D:208:THR:CG2	3:D:214:ARG:HE	1.90	0.82
5:F:260:LEU:O	5:F:263:LYS:HE3	1.78	0.82
5:F:521:LYS:CD	5:F:615:VAL:CG1	2.18	0.82
5:F:263:LYS:HD2	5:F:264:ALA:N	1.95	0.81
5:F:211:ILE:O	5:F:656:LEU:CD1	2.27	0.81
5:F:613:THR:OG1	5:F:722:MET:SD	2.39	0.80
3:D:198:CYS:SG	3:D:225:GLU:OE2	2.39	0.80
5:F:216:PRO:HG2	5:F:657:ARG:CG	2.12	0.80
5:F:3:LYS:CD	5:F:102:LYS:HE2	2.08	0.79
5:F:212:LYS:O	5:F:668:ALA:HB3	1.81	0.79
5:F:280:PRO:CD	5:F:434:TRP:CD1	2.61	0.79
5:F:405:PRO:HA	5:F:434:TRP:CD1	2.17	0.78
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.65	0.78
5:F:70:ARG:HH12	6:N:14:DT:C7	1.96	0.78
5:F:339:ILE:CG1	5:F:403:MET:SD	2.71	0.78
5:F:115:GLU:HG3	6:N:19:DT:OP1	1.82	0.77
8:T:21:DG:H5"	8:T:21:DG:C8	2.13	0.77
5:F:521:LYS:CG	5:F:615:VAL:HG21	2.14	0.77
2:C:45:GLY:HA2	2:C:50:GLU:HG2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:214:PHE:HB3	5:F:656:LEU:CD2	2.15	0.77
3:D:1327:GLU:N	8:T:15:DC:OP1	2.18	0.76
5:F:473:PRO:HG2	5:F:652:GLU:C	2.11	0.76
5:F:400:ALA:HB2	5:F:437:VAL:CG2	2.16	0.76
2:C:12:ARG:HD2	2:C:1183:ALA:HB2	1.67	0.75
3:D:1002:VAL:HB	3:D:1019:ASN:HB2	1.69	0.75
5:F:70:ARG:CZ	6:N:14:DT:C5	2.69	0.75
2:C:250:THR:HA	2:C:268:ARG:HA	1.69	0.75
5:F:473:PRO:CG	5:F:653:THR:HA	2.11	0.75
2:C:105:TYR:HA	2:C:114:VAL:HA	1.69	0.74
5:F:79:TRP:CE2	5:F:564:LEU:HB3	2.21	0.74
5:F:449:ILE:O	5:F:449:ILE:HG13	1.86	0.74
3:D:85:CYS:HB3	3:D:90:VAL:H	1.52	0.74
5:F:312:TYR:CD2	5:F:320:MET:HE2	2.22	0.74
5:F:533:ASN:HD21	5:F:587:MET:HA	1.53	0.73
3:D:1030:GLU:HG3	3:D:1031:VAL:HG13	1.69	0.73
3:D:111:THR:OG1	3:D:300:GLN:OE1	2.07	0.73
2:C:714:VAL:O	2:C:767:GLN:NE2	2.23	0.72
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.70	0.72
5:F:302:LYS:H	5:F:302:LYS:CE	2.01	0.72
3:D:895:CYS:SG	3:D:898:CYS:N	2.59	0.72
3:D:134:ASP:CG	3:D:159:ILE:HG21	2.14	0.72
5:F:334:MET:SD	5:F:373:VAL:HG23	2.30	0.72
3:D:127:LEU:O	3:D:220:ARG:NH2	2.23	0.72
5:F:280:PRO:HB3	5:F:434:TRP:CD2	2.25	0.71
3:D:422:LEU:HD23	3:D:434:ILE:HD11	1.72	0.71
3:D:530:PRO:HB2	3:D:581:MET:HE2	1.72	0.71
8:T:22:DC:H6	8:T:22:DC:C5'	2.02	0.71
1:A:192:VAL:HG12	1:A:193:GLU:HG2	1.73	0.71
5:F:171:MET:CE	5:F:546:MET:HE2	2.20	0.71
3:D:437:PHE:HZ	3:D:453:VAL:HG11	1.54	0.70
5:F:521:LYS:CE	5:F:615:VAL:HG11	2.19	0.70
2:C:932:GLN:HB2	2:C:1051:LYS:HB2	1.72	0.70
3:D:120:LEU:HD21	8:T:13:DT:H5''	1.71	0.70
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.30	0.70
2:C:1315:MET:HB2	3:D:473:THR:HG21	1.73	0.70
8:T:22:DC:H6	8:T:22:DC:H5''	1.56	0.70
5:F:472:LYS:HE2	5:F:649:GLU:HB3	1.73	0.70
8:T:22:DC:H5''	8:T:22:DC:C6	2.27	0.70
2:C:622:ASN:O	2:C:623:LEU:HD23	1.91	0.70
3:D:488:ASN:O	3:D:905:ARG:NH1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:791:ALA:HB2	8:T:17:DA:H8	1.57	0.70
2:C:76:GLY:HA3	2:C:95:PRO:HG2	1.75	0.69
2:C:444:ASP:O	2:C:450:ASN:ND2	2.25	0.69
2:C:1165:SER:OG	2:C:1168:GLU:HG3	1.91	0.69
5:F:751:PRO:HD2	5:F:775:GLY:CA	2.22	0.69
3:D:294:ASN:OD1	3:D:297:ARG:NH2	2.24	0.69
3:D:495:ASN:ND2	3:D:497:GLU:OE2	2.25	0.69
3:D:93:THR:HG22	3:D:94:GLN:H	1.57	0.69
5:F:191:LEU:CD1	5:F:612:SER:HB2	2.22	0.69
1:A:104:LYS:NZ	1:A:105:SER:O	2.26	0.69
1:A:164:ASP:O	1:A:166:ARG:NH2	2.24	0.69
5:F:320:MET:H	5:F:320:MET:CE	2.06	0.69
3:D:676:GLY:O	3:D:680:ASN:ND2	2.23	0.69
5:F:171:MET:HE2	5:F:546:MET:CE	2.23	0.69
2:C:314:ASN:O	2:C:352:ARG:NH1	2.26	0.69
2:C:821:ARG:HH21	2:C:1082:ILE:HD13	1.58	0.68
3:D:929:GLN:O	3:D:1244:GLN:NE2	2.27	0.68
5:F:472:LYS:HG3	5:F:649:GLU:O	1.93	0.68
5:F:473:PRO:CG	5:F:652:GLU:O	2.41	0.68
2:C:1340:GLU:HG2	3:D:1341:ARG:HH12	1.58	0.68
2:C:339:ASN:HB3	2:C:343:HIS:H	1.59	0.68
2:C:1272:GLU:N	2:C:1272:GLU:OE1	2.26	0.68
3:D:1238:GLN:HB3	3:D:1242:ARG:HH22	1.58	0.68
3:D:1291:GLU:O	3:D:1295:ASN:ND2	2.27	0.68
2:C:562:GLU:OE2	2:C:687:ARG:NH2	2.26	0.68
2:C:808:ASN:H	3:D:633:ALA:HB2	1.59	0.68
3:D:70:CYS:SG	3:D:90:VAL:HB	2.34	0.68
3:D:499:ILE:HG23	3:D:500:ILE:HD12	1.76	0.68
5:F:212:LYS:CA	5:F:668:ALA:HB3	2.24	0.68
1:A:106:GLY:HA2	1:A:136:GLU:HA	1.75	0.68
2:C:197:ARG:HG2	2:C:203:LYS:HA	1.74	0.68
5:F:3:LYS:HZ2	5:F:24:ASP:HA	1.59	0.68
3:D:338:PHE:HA	3:D:342:LEU:HD23	1.76	0.68
5:F:373:VAL:HG22	5:F:398:PHE:HE2	1.59	0.67
4:E:53:GLU:HB3	4:E:59:ILE:HD12	1.75	0.67
5:F:473:PRO:CG	5:F:652:GLU:C	2.67	0.67
2:C:1245:ALA:HB2	3:D:372:MET:HG3	1.76	0.67
3:D:502:PRO:O	3:D:598:LYS:NZ	2.28	0.67
3:D:791:ALA:HA	8:T:17:DA:C8	2.30	0.67
5:F:366:GLU:HG2	5:F:367:ALA:H	1.59	0.67
3:D:208:THR:CG2	3:D:214:ARG:NE	2.54	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:63:GLU:HB3	5:F:76:TRP:CD2	2.29	0.67
3:D:791:ALA:HA	8:T:17:DA:O4'	1.95	0.67
8:T:21:DG:H8	8:T:21:DG:C5'	2.04	0.67
3:D:488:ASN:HB3	3:D:905:ARG:HH12	1.60	0.67
5:F:212:LYS:HB3	5:F:668:ALA:HB3	1.75	0.66
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.77	0.66
5:F:78:ASN:CG	5:F:561:LYS:HD3	2.20	0.66
1:A:60:GLU:OE1	1:A:143:ARG:NH2	2.29	0.66
1:B:57:THR:HG21	1:B:147:GLN:HG2	1.75	0.66
1:A:68:TYR:OH	2:C:1057:LYS:NZ	2.29	0.66
2:C:755:LYS:NZ	2:C:768:MET:SD	2.69	0.66
3:D:558:ASP:OD1	3:D:562:GLU:N	2.29	0.66
5:F:214:PHE:HB3	5:F:656:LEU:HD22	1.77	0.66
5:F:521:LYS:CB	5:F:615:VAL:CG2	2.52	0.66
2:C:478:ARG:NH1	2:C:492:MET:O	2.29	0.66
2:C:100:LEU:HD12	2:C:493:ILE:HD11	1.78	0.66
2:C:933:VAL:HG12	2:C:1050:VAL:HG22	1.77	0.66
3:D:812:ASP:O	3:D:897:HIS:ND1	2.29	0.66
5:F:280:PRO:N	5:F:434:TRP:CE2	2.64	0.66
2:C:143:ARG:HH12	8:T:24:DG:H4'	1.60	0.66
3:D:485:MET:O	3:D:489:ASN:ND2	2.28	0.66
5:F:312:TYR:CD2	5:F:320:MET:CE	2.79	0.66
3:D:692:ARG:HA	3:D:695:LYS:HE3	1.77	0.65
3:D:803:VAL:HG22	3:D:1313:SER:HB3	1.78	0.65
5:F:147:ILE:HD12	5:F:148:ARG:N	2.11	0.65
5:F:521:LYS:CE	5:F:672:TYR:CZ	2.77	0.65
3:D:610:ARG:NH1	3:D:866:GLU:OE2	2.29	0.65
5:F:3:LYS:O	5:F:103:ALA:HA	1.95	0.65
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	1.78	0.65
3:D:957:SER:OG	3:D:959:LYS:NZ	2.29	0.65
1:A:59:VAL:HG22	1:A:144:ILE:HG23	1.79	0.65
3:D:208:THR:HG23	3:D:214:ARG:CG	2.25	0.65
3:D:952:VAL:O	3:D:1014:GLY:N	2.28	0.65
5:F:97:LYS:HE2	5:F:127:ILE:CA	2.10	0.65
5:F:339:ILE:CD1	5:F:403:MET:SD	2.84	0.65
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.79	0.65
5:F:345:LYS:HZ2	5:F:345:LYS:HB3	1.61	0.65
3:D:1018:ALA:HB1	3:D:1020:TRP:HZ3	1.62	0.65
3:D:1010:GLN:NE2	3:D:1011:VAL:O	2.29	0.64
5:F:37:LEU:HD12	5:F:173:ARG:HG3	1.77	0.64
3:D:110:PRO:HG2	3:D:186:GLN:HE22	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:751:PRO:HD2	5:F:775:GLY:HA3	1.79	0.64
3:D:75:TYR:HB3	3:D:80:HIS:CG	2.32	0.64
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.30	0.64
3:D:201:LEU:HD11	3:D:220:ARG:HH11	1.62	0.64
5:F:204:VAL:HG12	5:F:519:ALA:HB2	1.78	0.64
3:D:84:ILE:HA	3:D:91:GLU:HA	1.80	0.64
5:F:97:LYS:HZ1	5:F:127:ILE:HG12	1.59	0.64
5:F:508:GLY:C	5:F:522:MET:HE2	2.23	0.64
3:D:273:ILE:O	3:D:277:ASN:ND2	2.31	0.64
3:D:644:MET:N	3:D:644:MET:SD	2.70	0.64
5:F:67:LEU:HD13	5:F:71:MET:HE2	1.79	0.64
5:F:97:LYS:HE3	5:F:97:LYS:CA	2.27	0.64
5:F:676:PRO:HG3	5:F:701:ILE:HG22	1.78	0.64
2:C:17:LYS:NZ	2:C:1153:ALA:O	2.31	0.64
3:D:156:ARG:NH2	3:D:191:SER:O	2.31	0.63
5:F:35:ARG:NH1	5:F:83:TYR:HB2	2.14	0.63
2:C:890:LYS:HE2	2:C:914:LYS:HG3	1.79	0.63
2:C:1240:ASP:N	2:C:1240:ASP:OD1	2.31	0.63
5:F:347:TYR:HB3	5:F:403:MET:CE	2.28	0.63
5:F:347:TYR:HB3	5:F:403:MET:HE3	1.79	0.63
3:D:791:ALA:CA	8:T:17:DA:C8	2.81	0.63
5:F:347:TYR:O	5:F:404:THR:HG23	1.99	0.63
1:B:23:HIS:ND1	1:B:206:GLU:OE1	2.32	0.63
1:A:23:HIS:ND1	1:A:206:GLU:OE2	2.31	0.63
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.80	0.63
2:C:741:MET:HE3	2:C:974:ARG:HE	1.64	0.63
3:D:1143:ASP:O	3:D:1147:ALA:N	2.31	0.63
5:F:507:ARG:O	5:F:522:MET:CE	2.43	0.63
5:F:508:GLY:O	5:F:522:MET:HE2	1.98	0.63
2:C:251:ALA:O	2:C:266:GLY:N	2.31	0.63
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.80	0.63
2:C:636:CYS:O	2:C:642:SER:HA	1.97	0.63
2:C:678:ARG:NH2	2:C:1071:GLY:O	2.31	0.63
3:D:515:ARG:NH2	3:D:717:VAL:O	2.31	0.63
3:D:152:THR:HG21	3:D:176:PHE:HB3	1.82	0.62
3:D:587:LEU:HD21	3:D:608:CYS:HB2	1.80	0.62
5:F:400:ALA:C	5:F:403:MET:H	2.07	0.62
1:B:60:GLU:HG2	1:B:170:ARG:HA	1.80	0.62
2:C:148:GLN:OE1	2:C:454:ARG:NH2	2.32	0.62
2:C:201:ARG:NH2	2:C:369:MET:O	2.32	0.62
2:C:1253:LEU:O	2:C:1256:GLN:NE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:791:ALA:CB	8:T:17:DA:H8	2.12	0.62
1:A:191:ARG:HH22	1:A:196:THR:HG22	1.64	0.62
2:C:155:VAL:HG12	2:C:176:ILE:HG12	1.81	0.62
2:C:841:ARG:N	2:C:848:GLU:OE1	2.31	0.62
3:D:28:ASP:OD1	3:D:29:MET:N	2.33	0.62
1:A:182:ARG:NH2	2:C:1090:ASN:O	2.33	0.62
2:C:41:GLN:NE2	2:C:73:TYR:O	2.33	0.62
2:C:599:VAL:H	2:C:627:GLY:HA3	1.63	0.62
5:F:124:ARG:HE	5:F:157:LEU:HD21	1.64	0.62
5:F:212:LYS:CB	5:F:668:ALA:HB3	2.29	0.62
1:B:157:THR:O	1:B:160:HIS:NE2	2.32	0.62
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.32	0.62
5:F:580:LYS:O	5:F:586:GLY:HA3	1.98	0.62
2:C:14:ASP:OD1	2:C:15:PHE:N	2.32	0.62
2:C:198:ILE:CD1	2:C:388:LEU:HD21	2.29	0.62
5:F:339:ILE:HG23	5:F:403:MET:CE	2.28	0.62
2:C:12:ARG:O	2:C:1157:GLN:NE2	2.32	0.62
2:C:1165:SER:OG	2:C:1168:GLU:CG	2.47	0.62
3:D:829:GLY:HA2	3:D:993:GLU:HA	1.82	0.62
5:F:212:LYS:C	5:F:668:ALA:HB3	2.24	0.61
1:B:86:LYS:HE3	1:B:174:ASP:HB2	1.83	0.61
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	1.82	0.61
3:D:395:LYS:HD3	3:D:398:LYS:HZ3	1.64	0.61
5:F:19:LYS:C	5:F:21:LEU:H	2.07	0.61
5:F:66:ALA:O	5:F:70:ARG:HG2	2.00	0.61
5:F:661:ARG:NH1	5:F:666:GLY:O	2.30	0.61
1:B:61:ILE:HB	1:B:64:VAL:HB	1.80	0.61
1:B:75:GLN:HG3	1:B:134:THR:HG21	1.81	0.61
5:F:280:PRO:HB3	5:F:434:TRP:CG	2.36	0.61
1:B:73:GLY:O	1:B:134:THR:N	2.31	0.61
2:C:180:ARG:NH2	2:C:392:GLU:O	2.34	0.61
3:D:516:ASP:OD2	3:D:547:ARG:NH1	2.34	0.61
5:F:472:LYS:HD3	5:F:472:LYS:H	1.65	0.61
2:C:1171:ARG:O	2:C:1175:ASN:ND2	2.34	0.61
3:D:656:GLU:OE1	3:D:692:ARG:NH2	2.34	0.61
3:D:791:ALA:CA	8:T:17:DA:H8	2.13	0.61
5:F:404:THR:O	5:F:433:GLY:C	2.40	0.61
5:F:483:VAL:HG23	5:F:501:ILE:HD11	1.82	0.61
2:C:339:ASN:OD1	2:C:342:ASP:N	2.34	0.61
3:D:665:GLN:HE21	3:D:669:GLN:HG3	1.65	0.61
4:E:5:THR:HG22	4:E:7:GLN:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:HG23	1:A:134:THR:HA	1.83	0.60
7:R:12:G:C4	8:T:21:DG:N2	2.69	0.60
8:T:16:DG:H8	8:T:16:DG:H3'	1.66	0.60
3:D:576:ARG:NH1	3:D:593:ASN:OD1	2.34	0.60
5:F:320:MET:HE3	5:F:320:MET:N	2.11	0.60
3:D:105:ILE:HD11	3:D:242:LEU:HD23	1.84	0.60
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.82	0.60
1:B:155:ALA:N	1:B:174:ASP:OD1	2.32	0.60
3:D:282:LEU:HD12	5:F:104:ASP:CG	2.26	0.60
3:D:472:LEU:O	3:D:477:GLN:NE2	2.31	0.60
3:D:959:LYS:HB2	3:D:983:LYS:HG2	1.84	0.60
2:C:686:GLN:HE21	2:C:1069:ARG:HG2	1.67	0.60
5:F:191:LEU:HD13	5:F:612:SER:HB2	1.83	0.60
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.84	0.60
4:E:60:ASN:OD1	4:E:63:ILE:N	2.31	0.60
5:F:11:PRO:HG2	6:N:22:DT:P	2.42	0.60
3:D:888:CYS:SG	3:D:895:CYS:N	2.63	0.60
5:F:214:PHE:HB3	5:F:656:LEU:HD21	1.82	0.60
3:D:346:ARG:NH1	8:T:20:DC:OP1	2.35	0.59
1:B:59:VAL:HG22	1:B:144:ILE:HG22	1.84	0.59
2:C:195:PHE:HD2	2:C:203:LYS:HG2	1.67	0.59
3:D:978:ARG:HA	3:D:999:TYR:HB2	1.85	0.59
3:D:69:GLU:HG2	3:D:76:LYS:HG2	1.84	0.59
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.23	0.59
3:D:334:LYS:HA	3:D:339:ARG:HD3	1.83	0.59
3:D:1056:LEU:HB2	3:D:1108:GLN:HE21	1.66	0.59
2:C:1110:GLY:HA2	2:C:1113:LEU:HD12	1.84	0.59
5:F:112:LEU:H	5:F:112:LEU:CD2	2.14	0.59
5:F:595:THR:N	5:F:606:MET:O	2.36	0.59
5:F:343:PHE:HE1	5:F:436:LYS:HD2	1.68	0.59
2:C:582:ASN:HD21	2:C:584:TYR:HD2	1.51	0.59
5:F:339:ILE:HD13	5:F:403:MET:SD	2.43	0.59
1:B:180:VAL:O	3:D:535:ARG:NH1	2.36	0.58
5:F:473:PRO:HG3	5:F:652:GLU:O	2.04	0.58
5:F:521:LYS:HD2	5:F:615:VAL:HG11	0.61	0.58
2:C:759:SER:HB3	2:C:763:THR:H	1.67	0.58
2:C:675:ASP:OD1	2:C:676:ALA:N	2.37	0.58
2:C:813:GLU:OE1	3:D:504:GLN:NE2	2.36	0.58
5:F:400:ALA:O	5:F:403:MET:N	2.29	0.58
8:T:27:DA:H1'	8:T:28:DA:H5''	1.84	0.58
3:D:1082:ASP:OD1	3:D:1086:ASN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:115:GLU:HG3	6:N:19:DT:P	2.42	0.58
6:N:35:DC:O5'	6:N:35:DC:H6	1.86	0.58
2:C:120:GLN:OE1	2:C:490:GLN:N	2.36	0.58
3:D:79:LYS:HE3	3:D:80:HIS:CE1	2.39	0.58
3:D:319:SER:O	3:D:321:LYS:NZ	2.37	0.58
3:D:452:LEU:HB3	3:D:500:ILE:HG23	1.84	0.58
3:D:849:LEU:HA	3:D:856:ILE:HA	1.85	0.58
5:F:10:SER:HB2	5:F:319:TYR:OH	2.04	0.58
2:C:478:ARG:HD2	2:C:492:MET:HA	1.84	0.58
5:F:5:LEU:HB2	5:F:103:ALA:HB2	1.85	0.58
5:F:396:ARG:HB3	5:F:438:MET:HG3	1.85	0.58
5:F:403:MET:HB2	5:F:434:TRP:HA	1.84	0.58
2:C:755:LYS:NZ	2:C:767:GLN:O	2.36	0.58
3:D:69:GLU:OE2	3:D:76:LYS:NZ	2.36	0.58
5:F:70:ARG:NH1	6:N:14:DT:C5	2.72	0.58
5:F:312:TYR:CB	5:F:320:MET:HE2	2.34	0.58
2:C:84:GLU:OE2	2:C:88:ARG:NE	2.36	0.58
3:D:750:PRO:HA	3:D:781:LYS:HD3	1.86	0.58
1:A:9:LEU:O	1:B:227:GLN:NE2	2.34	0.58
2:C:309:LEU:HD21	2:C:312:ALA:HB2	1.86	0.57
3:D:492:SER:OG	3:D:495:ASN:O	2.22	0.57
2:C:582:ASN:OD1	2:C:583:GLU:N	2.36	0.57
2:C:886:LYS:HG2	2:C:916:SER:HB2	1.85	0.57
5:F:285:ILE:HG23	5:F:325:THR:HG22	1.87	0.57
2:C:13:LYS:HB2	2:C:1180:MET:HE2	1.86	0.57
3:D:497:GLU:OE1	3:D:497:GLU:N	2.37	0.57
1:B:93:GLN:NE2	1:B:120:ASP:O	2.38	0.57
2:C:19:PRO:HG3	2:C:1156:ARG:HD3	1.85	0.57
3:D:349:TYR:HE1	3:D:379:PRO:HG3	1.68	0.57
3:D:822:MET:SD	3:D:838:ARG:NH2	2.73	0.57
5:F:159:ILE:HG12	5:F:163:ASN:ND2	2.19	0.57
5:F:496:THR:HG22	5:F:500:ILE:HG12	1.87	0.57
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.86	0.57
2:C:620:ASN:ND2	3:D:768:ASN:OD1	2.38	0.57
2:C:846:GLY:HA3	2:C:889:PRO:HG2	1.85	0.57
3:D:86:GLU:N	3:D:86:GLU:OE1	2.36	0.57
5:F:677:LYS:HA	5:F:697:GLY:O	2.03	0.57
3:D:803:VAL:HG21	3:D:1309:ILE:HB	1.87	0.57
3:D:1170:LYS:HD2	6:N:47:DA:H5''	1.87	0.57
5:F:34:ILE:CD1	5:F:123:LEU:HD23	2.33	0.57
1:B:103:ASN:HA	1:B:140:ILE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:989:LEU:HB3	2:C:997:TRP:NE1	2.20	0.57
3:D:848:VAL:O	3:D:857:LEU:N	2.38	0.57
5:F:214:PHE:C	5:F:656:LEU:HD21	2.29	0.57
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.37	0.57
2:C:1290:MET:HA	2:C:1294:LYS:HD3	1.85	0.57
3:D:747:MET:HE2	3:D:775:SER:HA	1.87	0.57
3:D:1078:LEU:HD13	3:D:1121:LEU:HD11	1.87	0.57
8:T:22:DC:C5'	8:T:22:DC:C6	2.85	0.57
2:C:275:ARG:HH22	2:C:279:LYS:HB3	1.69	0.57
2:C:820:GLU:HG2	2:C:1079:ILE:HG22	1.86	0.57
5:F:156:GLU:OE1	5:F:156:GLU:N	2.36	0.57
5:F:486:LEU:HD22	5:F:491:ILE:HG21	1.85	0.57
2:C:1321:GLU:N	2:C:1321:GLU:OE1	2.38	0.56
1:A:9:LEU:N	1:A:32:GLU:OE2	2.36	0.56
5:F:144:LYS:HA	5:F:147:ILE:HG13	1.86	0.56
5:F:397:GLN:HA	5:F:438:MET:SD	2.45	0.56
2:C:1146:GLN:NE2	2:C:1159:VAL:O	2.38	0.56
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.86	0.56
3:D:337:ARG:NH1	3:D:341:ASN:OD1	2.39	0.56
3:D:998:PRO:HG2	3:D:1020:TRP:CE2	2.40	0.56
3:D:1295:ASN:HB2	3:D:1297:LYS:HG2	1.87	0.56
5:F:67:LEU:CD1	5:F:71:MET:HE2	2.34	0.56
5:F:97:LYS:HA	5:F:97:LYS:CE	2.30	0.56
5:F:493:ARG:HG3	6:N:18:DT:OP1	2.05	0.56
3:D:285:LEU:HD11	5:F:104:ASP:OD1	2.04	0.56
3:D:1060:VAL:HG13	3:D:1106:ILE:HG12	1.86	0.56
2:C:226:GLU:HB3	2:C:245:ARG:HH21	1.71	0.56
2:C:881:ASP:OD1	2:C:882:ILE:N	2.38	0.56
3:D:443:GLU:OE1	3:D:444:GLY:N	2.39	0.56
5:F:405:PRO:O	5:F:433:GLY:HA3	2.05	0.56
5:F:473:PRO:CD	5:F:653:THR:CB	2.73	0.56
2:C:320:ASP:OD1	2:C:320:ASP:N	2.34	0.56
2:C:1013:GLN:NE2	2:C:1017:GLN:OE1	2.37	0.56
2:C:262:TYR:O	2:C:263:VAL:HG23	2.06	0.56
2:C:540:ARG:HH12	7:R:10:G:P	2.29	0.56
2:C:602:GLU:OE2	2:C:604:HIS:NE2	2.37	0.56
3:D:77:ARG:H	3:D:80:HIS:HD2	1.52	0.56
4:E:70:GLN:NE2	4:E:74:GLU:OE1	2.36	0.56
8:T:21:DG:C8	8:T:21:DG:C5'	2.85	0.56
2:C:237:LEU:HD13	2:C:289:VAL:HG22	1.87	0.56
2:C:342:ASP:O	2:C:437:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:277:ASN:HA	3:D:280:LYS:HG2	1.87	0.56
4:E:67:ARG:O	4:E:71:GLU:HG2	2.06	0.56
3:D:1154:ALA:N	3:D:1214:PRO:O	2.36	0.56
2:C:223:LEU:O	2:C:430:LYS:NZ	2.30	0.56
2:C:1083:GLU:H	2:C:1083:GLU:CD	2.12	0.56
5:F:740:ARG:NH2	5:F:749:ALA:O	2.35	0.56
2:C:59:ILE:HG12	2:C:68:LEU:HB3	1.88	0.55
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.30	0.55
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.87	0.55
3:D:1169:THR:N	3:D:1172:LYS:O	2.40	0.55
5:F:796:LEU:HB2	5:F:799:GLU:HG3	1.89	0.55
1:A:7:GLU:O	1:B:150:ARG:NH2	2.34	0.55
2:C:517:GLN:OE1	2:C:760:ASN:N	2.40	0.55
3:D:1037:PHE:HD2	3:D:1040:MET:HE2	1.71	0.55
5:F:280:PRO:HB3	5:F:434:TRP:CE3	2.41	0.55
5:F:282:ALA:O	5:F:397:GLN:NE2	2.29	0.55
2:C:519:ASN:OD1	2:C:522:SER:N	2.38	0.55
2:C:550:VAL:HB	3:D:777:HIS:HD2	1.72	0.55
5:F:280:PRO:CD	5:F:434:TRP:CG	2.86	0.55
1:A:104:LYS:O	1:A:139:SER:OG	2.24	0.55
1:B:95:LYS:O	1:B:148:ARG:NH2	2.40	0.55
2:C:1137:GLU:HG2	2:C:1139:ALA:H	1.72	0.55
3:D:1046:ILE:HD13	3:D:1059:LEU:HD22	1.88	0.55
3:D:1261:LEU:O	3:D:1304:ARG:NH2	2.38	0.55
5:F:37:LEU:HD13	5:F:173:ARG:HG3	1.85	0.55
2:C:756:TYR:N	2:C:766:ASN:OD1	2.39	0.55
2:C:1336:ASN:HB2	3:D:25:ALA:HB2	1.87	0.55
5:F:147:ILE:HD12	5:F:148:ARG:HG3	1.89	0.55
1:B:13:LEU:HD11	1:B:16:ILE:HD11	1.88	0.55
2:C:964:LEU:HD21	2:C:1022:LYS:HD2	1.89	0.55
2:C:1289:GLU:OE2	3:D:472:LEU:N	2.26	0.55
3:D:77:ARG:HB3	3:D:79:LYS:HG2	1.89	0.54
3:D:490:ILE:HA	3:D:500:ILE:HD13	1.88	0.54
3:D:865:HIS:HE1	3:D:867:GLN:HB2	1.71	0.54
3:D:1169:THR:HB	3:D:1172:LYS:HB2	1.89	0.54
5:F:278:SER:O	5:F:405:PRO:HB3	2.07	0.54
5:F:509:TYR:CD1	5:F:522:MET:HE3	2.42	0.54
5:F:521:LYS:HD2	5:F:615:VAL:CG2	2.37	0.54
2:C:590:PRO:HB2	2:C:655:VAL:HG11	1.88	0.54
3:D:120:LEU:HD23	8:T:13:DT:C5'	2.33	0.54
3:D:398:LYS:HA	3:D:401:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:280:PRO:CA	5:F:434:TRP:CD2	2.90	0.54
5:F:704:TYR:CE1	5:F:719:HIS:HB3	2.42	0.54
1:B:97:GLU:OE2	1:B:145:LYS:NZ	2.39	0.54
3:D:1064:SER:HA	3:D:1067:ARG:HG2	1.89	0.54
5:F:161:ARG:HH11	5:F:161:ARG:HG3	1.72	0.54
1:A:100:LEU:HB3	1:A:115:ILE:HD11	1.89	0.54
2:C:81:ASP:OD1	2:C:84:GLU:N	2.31	0.54
2:C:976:ARG:CZ	2:C:976:ARG:HA	2.37	0.54
3:D:185:ILE:HD13	3:D:188:LEU:HD21	1.90	0.54
6:N:19:DT:H2''	6:N:20:DA:H5'	1.89	0.54
8:T:16:DG:C8	8:T:16:DG:C3'	2.90	0.54
1:A:234:LEU:HA	1:B:13:LEU:HD22	1.89	0.54
2:C:393:ASP:OD1	2:C:394:ARG:N	2.40	0.54
2:C:551:HIS:H	2:C:554:HIS:CE1	2.25	0.54
3:D:1157:ALA:O	3:D:1207:GLY:N	2.29	0.54
2:C:841:ARG:HG2	2:C:1046:VAL:HG12	1.89	0.54
3:D:527:LEU:HD23	3:D:532:GLU:HG2	1.90	0.54
3:D:1364:ALA:O	3:D:1367:GLN:HB2	2.08	0.54
5:F:78:ASN:HD21	5:F:561:LYS:HD3	1.71	0.54
2:C:201:ARG:HB3	2:C:369:MET:HE2	1.88	0.54
3:D:56:LEU:O	3:D:250:ARG:NH2	2.33	0.54
3:D:968:ASN:HD21	3:D:972:LYS:HB2	1.71	0.54
4:E:51:LEU:O	4:E:54:ILE:HG22	2.07	0.54
5:F:400:ALA:C	5:F:402:GLN:N	2.64	0.54
2:C:11:ILE:O	2:C:1149:TYR:OH	2.22	0.54
2:C:244:GLU:HA	2:C:247:ARG:HH11	1.73	0.54
5:F:36:ASP:CG	5:F:37:LEU:H	2.16	0.54
2:C:197:ARG:HD2	2:C:201:ARG:O	2.07	0.54
2:C:563:THR:HG22	2:C:573:ASN:HA	1.90	0.54
3:D:36:GLY:O	3:D:104:HIS:ND1	2.41	0.54
2:C:406:ASN:ND2	2:C:413:GLU:O	2.40	0.54
2:C:434:ASP:HB3	2:C:439:LYS:HB2	1.89	0.54
2:C:976:ARG:NH2	2:C:989:LEU:HD13	2.23	0.54
3:D:151:MET:N	3:D:175:GLU:OE2	2.41	0.54
3:D:1193:TRP:HD1	3:D:1194:ARG:HH21	1.55	0.54
5:F:555:ASN:O	5:F:557:GLU:HG3	2.09	0.54
5:F:582:PRO:HA	5:F:586:GLY:O	2.07	0.54
2:C:1293:VAL:HG21	2:C:1315:MET:HG3	1.90	0.53
8:T:14:DC:H2''	8:T:15:DC:H5'	1.90	0.53
4:E:42:GLU:O	4:E:43:ASN:ND2	2.41	0.53
5:F:143:THR:HG22	5:F:145:ASN:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:521:LYS:CE	5:F:672:TYR:OH	2.46	0.53
2:C:233:ARG:O	2:C:236:LYS:HB2	2.09	0.53
8:T:16:DG:H3'	8:T:16:DG:C8	2.43	0.53
2:C:899:GLU:O	2:C:903:ARG:HG2	2.09	0.53
2:C:971:LEU:HD12	2:C:1017:GLN:HE21	1.73	0.53
2:C:1134:GLN:OE1	2:C:1136:GLN:NE2	2.42	0.53
3:D:418:GLU:H	4:E:45:LYS:NZ	2.05	0.53
3:D:704:GLU:OE1	3:D:706:VAL:HG13	2.09	0.53
5:F:290:GLN:CD	5:F:301:VAL:HG13	2.33	0.53
2:C:1120:ALA:HB1	2:C:1198:LEU:HG	1.91	0.53
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.43	0.53
4:E:26:ARG:HE	4:E:30:MET:HG2	1.73	0.53
1:A:226:GLU:OE1	1:A:227:GLN:NE2	2.42	0.53
1:B:54:CYS:SG	1:B:148:ARG:NH1	2.82	0.53
1:B:158:ARG:HB2	1:B:172:LEU:HD21	1.90	0.53
2:C:1296:ASP:OD2	2:C:1321:GLU:N	2.42	0.53
2:C:1328:LYS:NZ	3:D:100:GLU:O	2.36	0.53
3:D:462:ASP:OD1	3:D:462:ASP:N	2.41	0.53
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.90	0.53
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.41	0.53
3:D:959:LYS:HG3	3:D:985:ILE:HD12	1.91	0.53
5:F:212:LYS:C	5:F:668:ALA:CB	2.75	0.53
5:F:319:TYR:HA	5:F:320:MET:HE3	1.90	0.53
5:F:527:THR:O	5:F:531:GLU:HG3	2.09	0.53
5:F:722:MET:HG2	5:F:727:LYS:HG2	1.91	0.53
2:C:948:ILE:O	2:C:951:MET:HG3	2.09	0.53
5:F:508:GLY:C	5:F:522:MET:CE	2.82	0.53
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.30	0.52
2:C:996:ARG:O	2:C:1000:LEU:HG	2.09	0.52
2:C:1024:GLU:HA	2:C:1027:LYS:HG2	1.90	0.52
2:C:1073:LYS:NZ	7:R:14:G:OP2	2.36	0.52
5:F:124:ARG:HH11	5:F:124:ARG:HG2	1.74	0.52
5:F:476:ARG:NE	5:F:518:TYR:CE2	2.77	0.52
5:F:507:ARG:NH2	6:N:16:DC:OP1	2.39	0.52
2:C:32:LEU:HA	2:C:130:MET:HE1	1.90	0.52
2:C:1113:LEU:HD23	3:D:641:ILE:HD12	1.90	0.52
2:C:577:VAL:HG12	2:C:663:VAL:HG13	1.91	0.52
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.82	0.52
3:D:1191:PRO:HB3	3:D:1193:TRP:CH2	2.44	0.52
5:F:744:ARG:HB2	5:F:790:ARG:HH11	1.73	0.52
1:B:212:ASP:OD1	1:B:215:GLU:N	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:838:CYS:SG	2:C:884:VAL:HG11	2.50	0.52
3:D:274:ASN:HA	3:D:277:ASN:HD21	1.74	0.52
5:F:597:ILE:HG23	5:F:678:ARG:HH22	1.74	0.52
7:R:8:C:H2'	7:R:9:G:C8	2.45	0.52
3:D:192:MET:HE1	3:D:194:LEU:HD23	1.91	0.52
5:F:404:THR:O	5:F:433:GLY:CA	2.57	0.52
5:F:617:LEU:HG	5:F:636:LEU:HD11	1.91	0.52
5:F:760:GLU:OE2	5:F:802:ARG:NH2	2.42	0.52
2:C:696:ASP:OD1	2:C:696:ASP:N	2.42	0.52
2:C:1041:ASP:OD1	2:C:1041:ASP:N	2.42	0.52
5:F:321:ARG:HH12	6:N:20:DA:H8	1.58	0.52
2:C:124:MET:HE1	2:C:495:ALA:HA	1.92	0.52
2:C:866:ASP:OD1	2:C:870:ILE:N	2.32	0.52
3:D:641:ILE:HA	3:D:644:MET:HE1	1.91	0.52
5:F:144:LYS:HA	5:F:147:ILE:CG1	2.40	0.52
5:F:518:TYR:OH	5:F:641:GLU:HB2	2.10	0.52
2:C:882:ILE:HG13	2:C:919:ARG:HG3	1.92	0.52
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.92	0.52
5:F:21:LEU:HD11	5:F:25:TYR:CD2	2.44	0.52
2:C:727:VAL:HG23	2:C:773:LEU:HD13	1.91	0.52
3:D:842:ARG:NH1	3:D:1250:ASP:OD2	2.43	0.52
3:D:1025:MET:HB3	3:D:1124:ILE:HB	1.92	0.52
5:F:158:ASN:O	5:F:162:VAL:HG23	2.10	0.52
7:R:6:C:H2'	7:R:7:G:C8	2.45	0.52
2:C:462:ASN:OD1	2:C:463:GLN:N	2.44	0.52
3:D:201:LEU:HD11	3:D:220:ARG:HD3	1.92	0.52
3:D:432:LEU:HD22	3:D:435:GLN:NE2	2.25	0.52
7:R:7:G:H2'	7:R:8:C:C6	2.45	0.52
7:R:11:C:H2'	7:R:12:G:C8	2.45	0.52
2:C:12:ARG:HG3	2:C:1181:PRO:HB2	1.91	0.51
2:C:951:MET:HA	2:C:954:LYS:HG2	1.91	0.51
3:D:736:GLN:O	3:D:740:LEU:HG	2.10	0.51
3:D:778:GLY:HA2	3:D:781:LYS:HE3	1.90	0.51
5:F:21:LEU:O	5:F:21:LEU:HG	2.10	0.51
5:F:595:THR:HG23	5:F:692:TYR:CD2	2.45	0.51
2:C:198:ILE:HD11	2:C:388:LEU:HD11	1.92	0.51
2:C:425:ILE:O	2:C:429:MET:HG2	2.09	0.51
2:C:677:ASN:OD1	2:C:678:ARG:N	2.43	0.51
3:D:77:ARG:H	3:D:80:HIS:CD2	2.28	0.51
5:F:472:LYS:HB3	5:F:653:THR:CB	2.25	0.51
1:B:208:ASN:OD1	1:B:210:THR:OG1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:444:ASP:OD2	2:C:551:HIS:NE2	2.43	0.51
2:C:883:LEU:HD13	2:C:1052:VAL:HG11	1.93	0.51
3:D:736:GLN:OE1	3:D:736:GLN:N	2.44	0.51
3:D:926:PRO:HB3	3:D:1246:VAL:HG11	1.93	0.51
1:A:4:SER:HB2	1:A:7:GLU:HB2	1.91	0.51
2:C:1125:GLY:HA2	2:C:1128:ILE:HD12	1.92	0.51
3:D:956:GLY:N	3:D:1010:GLN:HE22	2.09	0.51
5:F:280:PRO:CB	5:F:434:TRP:CD2	2.91	0.51
5:F:339:ILE:CG2	5:F:403:MET:SD	2.98	0.51
2:C:165:HIS:CE1	2:C:169:LYS:HB3	2.45	0.51
2:C:255:ILE:HB	2:C:263:VAL:CG2	2.31	0.51
2:C:317:LEU:HA	2:C:321:LEU:HD12	1.91	0.51
2:C:887:VAL:HB	2:C:913:VAL:HG12	1.93	0.51
3:D:116:PHE:HB3	3:D:237:MET:HE2	1.93	0.51
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.93	0.51
1:B:58:GLU:HB2	1:B:145:LYS:HD3	1.91	0.51
3:D:216:LYS:HA	3:D:219:LYS:HE2	1.92	0.51
3:D:739:GLN:OE1	3:D:744:ARG:NH2	2.44	0.51
3:D:1179:PRO:HD3	3:D:1185:PRO:HA	1.92	0.51
5:F:35:ARG:HG2	5:F:83:TYR:HB3	1.93	0.51
1:A:8:PHE:HD2	1:A:32:GLU:HG3	1.74	0.51
1:A:14:VAL:HG11	1:A:29:GLU:HB3	1.93	0.51
2:C:18:ARG:NH2	2:C:620:ASN:O	2.39	0.51
3:D:644:MET:O	3:D:764:ARG:NH1	2.42	0.51
5:F:296:ARG:O	5:F:297:LEU:HD23	2.11	0.51
5:F:302:LYS:H	5:F:302:LYS:CD	2.23	0.51
1:B:14:VAL:HG12	1:B:28:LEU:HA	1.93	0.51
2:C:238:GLN:HB3	2:C:284:LEU:HD21	1.93	0.51
3:D:357:VAL:HG12	3:D:461:PHE:CE2	2.46	0.51
2:C:1222:GLU:N	2:C:1222:GLU:OE1	2.43	0.51
2:C:1226:THR:OG1	3:D:639:VAL:O	2.26	0.51
2:C:1314:GLN:HB2	4:E:28:ARG:NH1	2.26	0.51
1:B:225:ALA:O	1:B:229:GLU:HG3	2.11	0.51
2:C:616:ILE:HG12	2:C:652:TYR:HB2	1.92	0.51
5:F:133:ARG:HG2	5:F:133:ARG:O	2.11	0.51
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.93	0.50
3:D:85:CYS:SG	3:D:88:CYS:N	2.77	0.50
3:D:790:THR:HG22	8:T:17:DA:C4	2.46	0.50
5:F:13:LYS:O	5:F:17:ILE:HG12	2.11	0.50
5:F:366:GLU:HG2	5:F:367:ALA:N	2.26	0.50
5:F:400:ALA:N	5:F:437:VAL:HG21	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:GLU:O	3:D:166:LEU:HG	2.12	0.50
3:D:1194:ARG:HA	3:D:1194:ARG:CZ	2.41	0.50
5:F:159:ILE:HG12	5:F:163:ASN:HD21	1.76	0.50
5:F:756:VAL:HG21	5:F:808:PRO:HD3	1.94	0.50
2:C:631:GLU:N	2:C:631:GLU:OE1	2.44	0.50
3:D:790:THR:CG2	8:T:17:DA:C5	2.95	0.50
5:F:241:GLN:HG3	5:F:420:PHE:CE2	2.46	0.50
5:F:404:THR:OG1	5:F:433:GLY:HA2	2.12	0.50
1:A:158:ARG:HH22	1:A:173:VAL:C	2.19	0.50
2:C:387:ASN:HA	2:C:391:SER:HB3	1.91	0.50
2:C:968:GLU:HG2	2:C:1018:TYR:HE1	1.77	0.50
3:D:809:VAL:HG21	3:D:909:ILE:HD13	1.92	0.50
5:F:279:LYS:C	5:F:434:TRP:CE2	2.89	0.50
5:F:284:PHE:CE2	5:F:393:LEU:HG	2.46	0.50
2:C:180:ARG:NH1	2:C:393:ASP:O	2.44	0.50
2:C:256:GLU:HB3	2:C:261:VAL:HG22	1.92	0.50
5:F:263:LYS:C	5:F:263:LYS:CD	2.76	0.50
5:F:268:VAL:HG21	5:F:453:VAL:HG11	1.94	0.50
5:F:676:PRO:HD3	5:F:701:ILE:HG21	1.92	0.50
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.75	0.50
3:D:26:SER:HB2	3:D:236:TRP:CE2	2.47	0.50
5:F:582:PRO:HG2	5:F:589:PRO:HD2	1.93	0.50
2:C:150:HIS:HE1	2:C:454:ARG:HB2	1.77	0.50
2:C:324:LYS:O	2:C:327:GLN:NE2	2.45	0.50
3:D:481:ARG:HA	3:D:485:MET:HG2	1.94	0.50
3:D:517:CYS:H	3:D:545:HIS:HB3	1.76	0.50
3:D:606:ASN:O	3:D:610:ARG:HG2	2.12	0.50
3:D:183:GLU:OE1	3:D:183:GLU:N	2.37	0.50
3:D:287:ALA:HB1	3:D:291:ILE:HD11	1.93	0.50
5:F:23:SER:C	5:F:25:TYR:H	2.20	0.50
5:F:242:ASN:O	5:F:243:ASP:HB2	2.12	0.50
5:F:737:LYS:O	5:F:739:THR:HG23	2.11	0.50
2:C:1185:PRO:HB2	2:C:1188:ASP:OD1	2.12	0.49
3:D:417:ARG:NH1	4:E:44:ASP:OD1	2.43	0.49
3:D:1040:MET:HG2	3:D:1046:ILE:HG12	1.93	0.49
5:F:214:PHE:CB	5:F:656:LEU:HD21	2.41	0.49
7:R:9:G:H2'	7:R:10:G:C8	2.46	0.49
2:C:70:TYR:OH	2:C:73:TYR:HD1	1.85	0.49
2:C:234:ASP:OD1	2:C:235:ASN:N	2.45	0.49
2:C:1120:ALA:HB2	2:C:1199:LEU:HD23	1.94	0.49
3:D:37:GLU:HB3	3:D:104:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:200:GLN:O	3:D:204:GLU:HG2	2.13	0.49
1:A:156:SER:HA	1:A:159:ILE:HG12	1.94	0.49
1:B:163:GLU:O	1:B:166:ARG:NE	2.45	0.49
2:C:459:MET:HA	2:C:462:ASN:ND2	2.28	0.49
2:C:528:ARG:NH2	2:C:576:SER:O	2.46	0.49
3:D:850:LYS:HB2	3:D:857:LEU:HD13	1.94	0.49
3:D:1044:GLN:O	3:D:1067:ARG:HB2	2.12	0.49
5:F:285:ILE:O	5:F:286:THR:C	2.54	0.49
5:F:472:LYS:HB2	5:F:653:THR:CB	2.28	0.49
8:T:11:DC:C6	8:T:12:DT:H72	2.46	0.49
1:B:23:HIS:CE1	1:B:206:GLU:HB2	2.47	0.49
2:C:165:HIS:CG	2:C:166:SER:H	2.30	0.49
2:C:932:GLN:O	2:C:1051:LYS:N	2.35	0.49
5:F:260:LEU:O	5:F:263:LYS:CE	2.54	0.49
5:F:472:LYS:HB3	5:F:653:THR:CG2	2.42	0.49
1:A:13:LEU:HD12	1:A:13:LEU:H	1.77	0.49
1:B:112:ALA:HA	1:B:130:ILE:HD11	1.94	0.49
2:C:287:VAL:HG23	2:C:292:ILE:HD11	1.94	0.49
3:D:526:VAL:HG22	3:D:549:LYS:HB2	1.94	0.49
1:A:92:VAL:HG22	1:A:121:VAL:HG12	1.95	0.49
2:C:447:HIS:CD2	2:C:553:THR:HG21	2.46	0.49
3:D:584:PRO:HD3	3:D:620:PHE:CD1	2.47	0.49
3:D:653:ILE:HG12	3:D:692:ARG:HH21	1.78	0.49
3:D:1344:LEU:HA	3:D:1349:GLU:CD	2.37	0.49
5:F:339:ILE:HG23	5:F:403:MET:SD	2.53	0.49
2:C:1276:TRP:CD2	3:D:801:VAL:HG11	2.48	0.49
3:D:660:GLU:HG3	3:D:685:ILE:HD12	1.94	0.49
3:D:1175:LEU:HB3	3:D:1190:ILE:HD13	1.94	0.49
4:E:25:ARG:HE	4:E:64:LEU:HD22	1.78	0.49
5:F:525:ILE:O	5:F:529:ARG:HG2	2.13	0.49
1:A:212:ASP:OD2	1:A:215:GLU:N	2.34	0.49
2:C:646:SER:N	2:C:649:GLN:OE1	2.35	0.49
3:D:1025:MET:N	3:D:1124:ILE:O	2.44	0.49
5:F:8:VAL:O	5:F:29:SER:HA	2.13	0.49
5:F:473:PRO:CD	5:F:653:THR:N	2.53	0.49
2:C:262:TYR:O	2:C:263:VAL:CG2	2.61	0.49
2:C:778:GLU:N	2:C:781:ASP:OD2	2.37	0.49
2:C:814:ASP:OD2	2:C:1106:ARG:NH2	2.44	0.49
3:D:826:ILE:HD13	3:D:992:LYS:HA	1.95	0.49
5:F:260:LEU:C	5:F:263:LYS:HE3	2.37	0.49
2:C:351:LEU:HA	2:C:354:ASP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1017:GLN:HA	2:C:1020:GLU:HG3	1.95	0.49
3:D:986:ASP:N	3:D:990:ARG:O	2.37	0.49
5:F:404:THR:O	5:F:433:GLY:HA3	2.13	0.49
1:B:52:PRO:HA	1:B:150:ARG:HA	1.94	0.48
2:C:158:ASP:OD2	2:C:173:ASN:ND2	2.37	0.48
2:C:165:HIS:CG	2:C:166:SER:N	2.81	0.48
3:D:208:THR:HG23	3:D:214:ARG:CD	2.42	0.48
5:F:186:LYS:NZ	5:F:580:LYS:O	2.43	0.48
1:A:185:TYR:HB2	1:A:201:LEU:HD11	1.95	0.48
3:D:847:ASP:OD1	3:D:847:ASP:O	2.31	0.48
5:F:5:LEU:HB2	5:F:103:ALA:CB	2.43	0.48
5:F:180:SER:HB2	5:F:181:PRO:HD3	1.95	0.48
5:F:343:PHE:CE1	5:F:436:LYS:HD2	2.46	0.48
5:F:704:TYR:CZ	5:F:719:HIS:HB3	2.48	0.48
1:A:71:LYS:HZ3	1:A:140:ILE:HA	1.78	0.48
2:C:97:ARG:NH1	2:C:123:TYR:HB2	2.28	0.48
2:C:1155:VAL:HG12	2:C:1157:GLN:H	1.78	0.48
3:D:1366:HIS:HA	3:D:1369:ARG:HB3	1.93	0.48
4:E:26:ARG:HH22	4:E:35:LYS:HB2	1.79	0.48
5:F:184:TRP:HA	5:F:188:ALA:O	2.13	0.48
2:C:797:GLY:O	2:C:798:GLN:NE2	2.47	0.48
2:C:1025:PHE:HA	2:C:1028:LYS:HG2	1.95	0.48
2:C:1292:THR:HG23	2:C:1293:VAL:HG23	1.95	0.48
3:D:664:ILE:O	3:D:667:GLN:HG2	2.13	0.48
3:D:708:ASN:OD1	3:D:712:GLN:N	2.37	0.48
3:D:978:ARG:O	3:D:996:LYS:NZ	2.28	0.48
5:F:268:VAL:HG21	5:F:453:VAL:CG1	2.43	0.48
5:F:397:GLN:OE1	5:F:438:MET:HE1	2.13	0.48
5:F:676:PRO:HG3	5:F:701:ILE:CG2	2.43	0.48
1:A:118:ASP:HB3	1:A:121:VAL:HG22	1.94	0.48
1:B:155:ALA:HA	1:B:158:ARG:HH21	1.79	0.48
2:C:561:ILE:O	2:C:680:LEU:HD13	2.14	0.48
3:D:1061:VAL:N	3:D:1105:ALA:O	2.38	0.48
1:A:11:PRO:HD3	1:B:227:GLN:NE2	2.29	0.48
2:C:257:ALA:HB2	2:C:285:ILE:HG22	1.94	0.48
3:D:85:CYS:SG	3:D:86:GLU:N	2.86	0.48
3:D:133:ARG:HB3	3:D:137:ARG:HH12	1.78	0.48
3:D:134:ASP:OD2	3:D:159:ILE:HG21	2.13	0.48
3:D:208:THR:O	3:D:214:ARG:NH2	2.32	0.48
5:F:224:ALA:HB2	5:F:464:LEU:HD23	1.94	0.48
5:F:254:THR:HG21	5:F:466:PRO:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:69:GLN:OE1	2:C:101:ARG:HD2	2.14	0.48
2:C:213:LEU:HD12	2:C:422:LYS:HG2	1.95	0.48
3:D:322:ARG:HH12	7:R:8:C:H4'	1.77	0.48
3:D:460:ASP:OD1	3:D:460:ASP:N	2.46	0.48
3:D:1186:TYR:CE2	3:D:1188:GLU:HB2	2.48	0.48
3:D:1307:LEU:HB2	3:D:1312:ALA:HB2	1.94	0.48
2:C:550:VAL:HB	3:D:777:HIS:CD2	2.48	0.48
4:E:41:GLU:OE1	4:E:41:GLU:N	2.46	0.48
5:F:86:LEU:C	5:F:88:GLY:H	2.21	0.48
5:F:269:LEU:O	5:F:455:LYS:HG3	2.14	0.48
5:F:521:LYS:O	5:F:525:ILE:HD13	2.13	0.48
1:B:27:THR:HG22	1:B:202:VAL:HG22	1.96	0.48
2:C:1058:ARG:NH1	2:C:1240:ASP:OD2	2.47	0.48
3:D:394:ILE:H	3:D:394:ILE:HD12	1.79	0.48
3:D:557:LYS:NZ	3:D:561:GLY:O	2.41	0.48
1:A:124:VAL:HG13	1:A:125:LYS:HG3	1.96	0.48
2:C:721:GLY:N	2:C:740:GLU:OE2	2.41	0.48
2:C:812:PHE:CE2	2:C:813:GLU:HG2	2.49	0.48
3:D:45:ASN:HB2	3:D:48:THR:O	2.13	0.48
3:D:495:ASN:OD1	3:D:495:ASN:N	2.46	0.48
3:D:1260:MET:HE2	3:D:1306:LEU:HD11	1.96	0.48
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.94	0.47
1:A:181:GLU:HG2	1:A:206:GLU:O	2.13	0.47
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.95	0.47
2:C:1269:ARG:HG2	8:T:19:DG:H5'	1.96	0.47
2:C:1283:ALA:HA	3:D:479:GLU:CD	2.39	0.47
2:C:1339:LEU:HD23	3:D:17:PHE:CD1	2.49	0.47
3:D:70:CYS:SG	3:D:85:CYS:HB2	2.54	0.47
3:D:1320:ILE:HG21	3:D:1349:GLU:HG3	1.96	0.47
5:F:97:LYS:CA	5:F:97:LYS:CE	2.89	0.47
5:F:182:LEU:HD21	5:F:578:ALA:HB1	1.96	0.47
5:F:191:LEU:CD1	5:F:612:SER:CB	2.91	0.47
5:F:392:GLN:CD	5:F:396:ARG:NH1	2.72	0.47
5:F:518:TYR:CE2	5:F:641:GLU:HB2	2.49	0.47
2:C:854:ILE:HG22	2:C:862:LEU:HD21	1.96	0.47
2:C:1188:ASP:OD1	2:C:1188:ASP:N	2.46	0.47
5:F:217:GLU:HB2	5:F:471:THR:CG2	2.44	0.47
1:A:71:LYS:NZ	1:A:140:ILE:HA	2.29	0.47
2:C:58:PRO:HB3	2:C:69:GLN:HB3	1.96	0.47
2:C:110:PRO:HG2	2:C:113:THR:HG23	1.95	0.47
2:C:387:ASN:O	2:C:391:SER:OG	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:619:ALA:HB2	2:C:654:ASP:HB2	1.95	0.47
3:D:1268:ASN:N	3:D:1301:THR:OG1	2.45	0.47
5:F:147:ILE:CD1	5:F:148:ARG:HG3	2.45	0.47
2:C:65:ASN:HB2	2:C:484:LEU:HD21	1.97	0.47
2:C:139:ASN:C	2:C:141:THR:H	2.20	0.47
2:C:300:ASP:OD1	2:C:313:ALA:N	2.38	0.47
2:C:1089:GLU:OE1	2:C:1089:GLU:N	2.46	0.47
3:D:161:THR:OG1	3:D:162:GLU:OE1	2.32	0.47
3:D:475:GLU:OE1	3:D:475:GLU:N	2.32	0.47
3:D:1152:GLU:HB3	3:D:1214:PRO:HD2	1.96	0.47
3:D:1165:PHE:HD2	3:D:1173:ARG:HD2	1.80	0.47
3:D:1342:ASP:OD1	3:D:1342:ASP:N	2.48	0.47
5:F:173:ARG:HH21	6:N:16:DC:N4	2.11	0.47
5:F:580:LYS:C	5:F:586:GLY:HA3	2.39	0.47
7:R:11:C:H2'	7:R:12:G:H8	1.79	0.47
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.96	0.47
1:B:57:THR:HG21	1:B:147:GLN:HE21	1.79	0.47
2:C:19:PRO:HA	2:C:1156:ARG:CZ	2.44	0.47
2:C:291:TYR:O	2:C:295:LYS:NZ	2.48	0.47
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.79	0.47
3:D:1059:LEU:HB2	3:D:1107:VAL:HG13	1.97	0.47
5:F:760:GLU:HB3	5:F:803:PHE:CE1	2.50	0.47
5:F:807:LEU:O	5:F:812:ARG:NH2	2.46	0.47
2:C:452:ARG:NH2	2:C:584:TYR:O	2.31	0.47
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.97	0.47
5:F:478:SER:H	5:F:481:SER:HB3	1.79	0.47
1:A:158:ARG:HH12	1:A:173:VAL:C	2.22	0.47
1:B:80:GLU:OE1	1:B:80:GLU:N	2.30	0.47
1:B:91:ARG:HG3	1:B:122:GLU:HB2	1.97	0.47
1:B:158:ARG:HH22	1:B:173:VAL:C	2.22	0.47
2:C:1080:ASN:ND2	2:C:1085:MET:SD	2.79	0.47
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.29	0.47
3:D:205:LEU:O	3:D:208:THR:HG22	2.15	0.47
3:D:1199:PHE:HB2	3:D:1202:GLU:HG2	1.96	0.47
3:D:1199:PHE:H	3:D:1202:GLU:HG3	1.79	0.47
3:D:1256:ILE:O	3:D:1260:MET:HG3	2.15	0.47
5:F:240:HIS:O	5:F:420:PHE:HA	2.14	0.47
5:F:302:LYS:HD2	5:F:303:LYS:H	1.79	0.47
2:C:968:GLU:HG2	2:C:1018:TYR:CE1	2.50	0.47
3:D:555:TYR:CD2	3:D:585:LYS:HE3	2.50	0.47
3:D:699:ASP:HA	3:D:702:GLN:HE21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:147:ILE:HD12	5:F:147:ILE:C	2.39	0.47
5:F:653:THR:HG23	5:F:654:ASN:N	2.30	0.47
1:A:5:VAL:O	1:B:150:ARG:NE	2.41	0.47
2:C:557:ARG:HG2	2:C:589:THR:OG1	2.15	0.47
3:D:72:CYS:SG	3:D:74:LYS:HB2	2.55	0.47
3:D:402:GLU:OE2	3:D:403:ARG:NE	2.35	0.47
3:D:790:THR:HG22	8:T:17:DA:C5	2.49	0.47
3:D:1194:ARG:HA	3:D:1194:ARG:NH1	2.30	0.47
5:F:21:LEU:HD11	5:F:25:TYR:CD1	2.46	0.47
5:F:284:PHE:HB3	5:F:289:LEU:CA	2.45	0.47
5:F:406:ALA:HA	5:F:431:PHE:O	2.15	0.47
5:F:476:ARG:NH2	5:F:641:GLU:OE2	2.42	0.47
1:A:29:GLU:OE1	1:A:30:PRO:HA	2.15	0.47
5:F:254:THR:CG2	5:F:466:PRO:HB3	2.45	0.47
3:D:240:THR:HG23	3:D:241:VAL:HG23	1.97	0.46
3:D:450:HIS:CD2	3:D:452:LEU:H	2.33	0.46
3:D:517:CYS:N	3:D:545:HIS:HB3	2.29	0.46
5:F:271:ARG:HG3	5:F:413:LEU:HD21	1.96	0.46
5:F:479:GLU:HB3	5:F:501:ILE:HD13	1.97	0.46
5:F:582:PRO:CG	5:F:589:PRO:CD	2.93	0.46
1:B:56:VAL:HA	1:B:146:VAL:HG22	1.96	0.46
1:B:192:VAL:O	1:B:193:GLU:HG2	2.15	0.46
3:D:309:ASN:ND2	3:D:316:ILE:O	2.47	0.46
3:D:755:ILE:HD12	3:D:755:ILE:H	1.79	0.46
5:F:62:ASP:OD1	5:F:63:GLU:N	2.49	0.46
5:F:302:LYS:CD	5:F:302:LYS:N	2.78	0.46
1:A:111:THR:HA	1:A:129:VAL:HA	1.96	0.46
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.98	0.46
2:C:377:THR:HB	2:C:380:ALA:HB3	1.97	0.46
2:C:557:ARG:HD3	2:C:587:LEU:HB3	1.97	0.46
3:D:424:ASN:O	3:D:466:MET:HG3	2.15	0.46
3:D:985:ILE:HA	3:D:991:THR:HA	1.97	0.46
3:D:1230:THR:HG22	3:D:1257:VAL:HG11	1.98	0.46
5:F:105:HIS:NE2	5:F:135:SER:HB2	2.30	0.46
5:F:505:GLN:NE2	5:F:512:VAL:HG23	2.29	0.46
3:D:152:THR:HG23	3:D:175:GLU:CD	2.41	0.46
3:D:1037:PHE:N	3:D:1111:ASP:OD1	2.38	0.46
5:F:12:ALA:HB3	5:F:312:TYR:CE2	2.51	0.46
5:F:635:ASN:ND2	5:F:704:TYR:HA	2.30	0.46
1:A:185:TYR:HB3	1:A:203:ILE:HD13	1.96	0.46
2:C:836:LEU:N	2:C:1052:VAL:O	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:264:ASP:OD1	3:D:264:ASP:N	2.49	0.46
5:F:3:LYS:NZ	5:F:24:ASP:HA	2.28	0.46
5:F:14:ALA:HB1	5:F:27:VAL:HG12	1.97	0.46
5:F:71:MET:HG2	5:F:177:TYR:CB	2.46	0.46
7:R:4:U:H1'	7:R:5:C:C2	2.51	0.46
1:A:160:HIS:O	1:A:162:GLU:HG2	2.16	0.46
1:A:186:ASN:OD1	1:A:187:VAL:N	2.48	0.46
2:C:722:GLY:N	2:C:777:VAL:O	2.44	0.46
2:C:887:VAL:HB	2:C:913:VAL:CG1	2.45	0.46
2:C:1238:LEU:O	2:C:1242:LYS:HG2	2.16	0.46
3:D:692:ARG:O	3:D:695:LYS:HG2	2.15	0.46
3:D:905:ARG:NH1	4:E:16:ARG:HH22	2.14	0.46
3:D:1048:ARG:HD2	3:D:1057:SER:HB2	1.98	0.46
3:D:1158:GLU:OE1	3:D:1158:GLU:N	2.47	0.46
5:F:31:VAL:HG12	5:F:31:VAL:O	2.15	0.46
5:F:403:MET:CB	5:F:434:TRP:HA	2.46	0.46
3:D:620:PHE:CZ	3:D:624:ILE:HD11	2.51	0.46
3:D:810:THR:OG1	3:D:811:GLU:OE1	2.24	0.46
4:E:26:ARG:NH2	4:E:29:GLN:HB3	2.31	0.46
5:F:751:PRO:HD2	5:F:775:GLY:HA2	1.97	0.46
1:A:118:ASP:OD1	1:A:119:GLY:N	2.47	0.46
1:A:155:ALA:O	1:A:158:ARG:HG2	2.16	0.46
1:B:215:GLU:OE2	1:B:219:ARG:NH2	2.48	0.46
2:C:262:TYR:C	2:C:263:VAL:HG23	2.41	0.46
2:C:538:LEU:HA	2:C:542:ARG:HH21	1.81	0.46
3:D:93:THR:HG22	3:D:94:GLN:N	2.29	0.46
5:F:3:LYS:CD	5:F:102:LYS:CE	2.81	0.46
2:C:358:ASP:OD1	2:C:359:ARG:N	2.49	0.46
3:D:141:PHE:CD1	3:D:180:MET:HB3	2.51	0.46
4:E:15:ASN:OD1	4:E:16:ARG:N	2.49	0.46
5:F:4:ALA:HB3	5:F:25:TYR:CD2	2.51	0.46
5:F:236:LEU:HD23	5:F:424:ALA:HB2	1.98	0.46
1:A:111:THR:OG1	1:A:112:ALA:N	2.48	0.46
2:C:149:LEU:HD21	2:C:451:ARG:HD3	1.98	0.46
2:C:1080:ASN:HD21	2:C:1084:ASP:HB2	1.81	0.46
2:C:1108:ASN:OD1	2:C:1108:ASN:N	2.45	0.46
5:F:64:ARG:O	5:F:68:VAL:HG23	2.16	0.46
5:F:227:THR:HG22	5:F:228:THR:O	2.16	0.46
2:C:159:SER:O	2:C:161:LYS:NZ	2.30	0.45
2:C:161:LYS:HB3	2:C:163:LYS:HE2	1.98	0.45
2:C:397:LEU:N	2:C:418:GLY:O	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:167:ASP:O	3:D:170:GLU:HG2	2.16	0.45
3:D:759:ILE:HD12	3:D:771:GLN:HB3	1.98	0.45
3:D:1357:ILE:HG13	3:D:1359:ALA:H	1.81	0.45
5:F:280:PRO:HA	5:F:434:TRP:CE3	2.51	0.45
5:F:809:GLU:HA	5:F:812:ARG:HH12	1.81	0.45
7:R:10:G:C2	8:T:23:DC:O2	2.69	0.45
1:A:154:PRO:O	1:A:157:THR:OG1	2.34	0.45
2:C:53:PHE:O	2:C:57:PHE:N	2.47	0.45
2:C:1187:PHE:CG	3:D:769:VAL:HG22	2.51	0.45
3:D:521:LYS:HD2	3:D:521:LYS:HA	1.82	0.45
4:E:60:ASN:H	4:E:63:ILE:HB	1.81	0.45
5:F:212:LYS:O	5:F:668:ALA:N	2.49	0.45
1:A:64:VAL:HG11	1:A:78:ILE:HD11	1.97	0.45
1:A:67:GLU:OE1	1:A:67:GLU:N	2.31	0.45
2:C:663:VAL:HA	2:C:666:SER:HB3	1.98	0.45
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.97	0.45
5:F:70:ARG:CZ	6:N:14:DT:C4	2.98	0.45
5:F:670:ASP:OD1	5:F:671:SER:N	2.46	0.45
1:B:86:LYS:HZ2	1:B:173:VAL:HG13	1.82	0.45
3:D:558:ASP:OD1	3:D:561:GLY:N	2.50	0.45
3:D:843:VAL:HG23	3:D:900:GLY:HA2	1.98	0.45
5:F:18:ASN:O	5:F:22:GLY:N	2.49	0.45
5:F:241:GLN:HG3	5:F:420:PHE:CZ	2.52	0.45
5:F:271:ARG:HG3	5:F:413:LEU:CD2	2.46	0.45
2:C:188:PHE:HE2	2:C:432:LEU:HG	1.82	0.45
2:C:797:GLY:HA3	2:C:1232:MET:O	2.17	0.45
2:C:971:LEU:O	2:C:975:ILE:HG12	2.17	0.45
2:C:989:LEU:HB3	2:C:997:TRP:HE1	1.82	0.45
3:D:281:ARG:HA	3:D:284:ASP:OD2	2.17	0.45
3:D:287:ALA:HB2	5:F:104:ASP:OD1	2.16	0.45
3:D:578:ILE:O	3:D:581:MET:HB3	2.16	0.45
3:D:850:LYS:NZ	3:D:851:PRO:O	2.49	0.45
5:F:19:LYS:C	5:F:21:LEU:N	2.73	0.45
5:F:369:ARG:HB2	5:F:370:PRO:HD2	1.98	0.45
8:T:14:DC:H6	8:T:14:DC:H5'	1.82	0.45
1:B:76:GLU:HB3	1:B:80:GLU:HB2	1.99	0.45
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.98	0.45
3:D:660:GLU:O	3:D:664:ILE:HG12	2.17	0.45
3:D:1193:TRP:CD1	3:D:1194:ARG:HE	2.34	0.45
5:F:507:ARG:NH1	5:F:507:ARG:HB2	2.31	0.45
5:F:582:PRO:HG2	5:F:589:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:MET:HB2	2:C:136:PHE:HE1	1.82	0.45
2:C:705:GLU:H	2:C:705:GLU:CD	2.22	0.45
2:C:719:LYS:HG2	2:C:751:TYR:OH	2.17	0.45
2:C:1209:GLN:HE21	3:D:640:GLY:HA3	1.81	0.45
3:D:432:LEU:CD1	3:D:499:ILE:HG12	2.47	0.45
3:D:791:ALA:HA	8:T:17:DA:C1'	2.47	0.45
3:D:901:ARG:HG3	3:D:907:HIS:C	2.42	0.45
3:D:968:ASN:OD1	3:D:972:LYS:N	2.49	0.45
3:D:1232:TYR:O	3:D:1236:GLU:HG2	2.17	0.45
5:F:19:LYS:O	5:F:21:LEU:N	2.49	0.45
5:F:105:HIS:CE1	5:F:135:SER:HB2	2.51	0.45
5:F:271:ARG:NH1	5:F:413:LEU:HD21	2.32	0.45
5:F:271:ARG:HH11	5:F:413:LEU:HD21	1.81	0.45
5:F:582:PRO:HG3	5:F:589:PRO:HD3	1.99	0.45
1:B:46:ILE:HD13	1:B:46:ILE:HA	1.82	0.45
1:B:191:ARG:HG2	1:B:196:THR:HA	1.98	0.45
2:C:436:ARG:O	2:C:436:ARG:NH1	2.36	0.45
2:C:1165:SER:OG	2:C:1168:GLU:CD	2.60	0.45
3:D:317:THR:OG1	3:D:322:ARG:N	2.50	0.45
3:D:464:ASP:CG	7:R:14:G:O2'	2.59	0.45
3:D:607:THR:O	3:D:611:ILE:HG12	2.17	0.45
3:D:791:ALA:HB2	8:T:17:DA:C8	2.46	0.45
3:D:866:GLU:OE1	3:D:866:GLU:N	2.42	0.45
3:D:1001:ALA:HA	3:D:1020:TRP:HB3	1.98	0.45
5:F:827:THR:HG22	5:F:842:SER:HB3	1.99	0.45
2:C:838:CYS:SG	2:C:1050:VAL:HB	2.57	0.45
5:F:35:ARG:NE	5:F:122:HIS:HD2	2.14	0.45
5:F:182:LEU:HD13	5:F:579:GLU:OE1	2.17	0.45
5:F:214:PHE:O	5:F:661:ARG:NH2	2.45	0.45
1:A:167:PRO:HG2	1:A:170:ARG:HE	1.81	0.45
2:C:198:ILE:HD11	2:C:388:LEU:HD21	1.98	0.45
2:C:439:LYS:HD2	2:C:439:LYS:N	2.32	0.45
2:C:590:PRO:HA	2:C:604:HIS:O	2.17	0.45
2:C:836:LEU:HD12	2:C:918:LEU:HD21	1.98	0.45
2:C:1061:GLN:HE22	2:C:1240:ASP:HB3	1.82	0.45
2:C:1242:LYS:HE2	3:D:465:GLN:NE2	2.32	0.45
2:C:1298:VAL:HA	2:C:1301:ARG:HG2	1.98	0.45
3:D:50:LYS:HG3	3:D:51:PRO:HD2	1.98	0.45
3:D:557:LYS:HD3	3:D:557:LYS:HA	1.78	0.45
4:E:44:ASP:HB3	4:E:48:VAL:HB	1.98	0.45
2:C:145:ILE:HD13	2:C:512:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:158:ASP:O	2:C:173:ASN:ND2	2.50	0.44
2:C:303:ASP:O	2:C:307:GLY:N	2.46	0.44
2:C:623:LEU:HD11	2:C:653:MET:HE1	1.99	0.44
3:D:522:GLY:O	3:D:525:MET:HG2	2.17	0.44
5:F:70:ARG:NH2	6:N:14:DT:C5	2.85	0.44
5:F:473:PRO:HG2	5:F:652:GLU:O	2.11	0.44
2:C:192:ASP:HB3	2:C:346:TYR:CD1	2.53	0.44
3:D:1163:VAL:HG13	3:D:1175:LEU:HD11	1.99	0.44
5:F:3:LYS:HZ2	5:F:24:ASP:CA	2.28	0.44
5:F:112:LEU:HD23	5:F:112:LEU:N	2.22	0.44
1:B:48:LEU:HD21	1:B:183:ILE:HG22	1.99	0.44
1:B:78:ILE:O	1:B:81:ILE:HG12	2.17	0.44
2:C:726:TYR:HB3	2:C:733:VAL:HB	1.98	0.44
2:C:738:GLU:O	2:C:741:MET:HG3	2.18	0.44
2:C:839:VAL:HG22	2:C:1049:ILE:HG23	1.98	0.44
2:C:1003:THR:O	2:C:1008:GLN:HB2	2.18	0.44
3:D:1021:ASP:HB3	3:D:1024:THR:HB	1.98	0.44
4:E:13:ILE:HG21	4:E:19:LEU:HB2	2.00	0.44
5:F:185:LYS:HE3	5:F:185:LYS:HB2	1.83	0.44
7:R:14:G:H4'	7:R:14:G:OP1	2.18	0.44
2:C:11:ILE:HG23	2:C:1149:TYR:OH	2.17	0.44
2:C:454:ARG:HG3	2:C:458:GLU:HB2	2.00	0.44
2:C:565:GLU:OE2	7:R:13:C:OP2	2.35	0.44
2:C:1288:GLN:O	2:C:1292:THR:HG22	2.17	0.44
3:D:1259:GLN:O	3:D:1262:ARG:NE	2.37	0.44
5:F:34:ILE:HG22	5:F:89:LYS:HZ1	1.81	0.44
5:F:78:ASN:HD22	5:F:78:ASN:HA	1.61	0.44
8:T:22:DC:C6	8:T:22:DC:C4'	3.01	0.44
1:B:91:ARG:CZ	1:B:124:VAL:HG22	2.48	0.44
2:C:757:THR:HG22	2:C:765:ILE:HB	2.00	0.44
2:C:960:LEU:HA	2:C:963:GLU:CD	2.42	0.44
3:D:349:TYR:CE1	3:D:379:PRO:HG3	2.50	0.44
1:A:231:PHE:HE1	1:B:28:LEU:HD22	1.83	0.44
2:C:985:GLU:H	2:C:989:LEU:HD11	1.83	0.44
2:C:1160:ASP:OD1	2:C:1161:LEU:N	2.51	0.44
3:D:474:LEU:H	3:D:474:LEU:HD23	1.82	0.44
3:D:869:CYS:O	3:D:872:LEU:HG	2.17	0.44
5:F:302:LYS:HD2	5:F:302:LYS:N	2.33	0.44
5:F:521:LYS:CD	5:F:615:VAL:HG21	2.46	0.44
8:T:15:DC:H1'	8:T:16:DG:H5'	2.00	0.44
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:194:LEU:HD13	2:C:194:LEU:HA	1.86	0.44
2:C:368:ARG:HH21	2:C:374:GLU:HG3	1.82	0.44
2:C:582:ASN:HB3	2:C:586:PHE:N	2.32	0.44
2:C:995:ASP:OD1	2:C:996:ARG:N	2.48	0.44
3:D:105:ILE:CG1	3:D:242:LEU:HB3	2.47	0.44
4:E:63:ILE:O	4:E:67:ARG:HG2	2.18	0.44
5:F:240:HIS:HB2	5:F:421:ARG:HG3	2.00	0.44
2:C:514:PHE:CZ	2:C:760:ASN:HB3	2.53	0.44
2:C:1313:HIS:CE1	3:D:380:PHE:HE1	2.36	0.44
3:D:111:THR:HG21	3:D:303:VAL:HG21	1.99	0.44
5:F:396:ARG:HD3	5:F:437:VAL:O	2.17	0.44
2:C:304:GLU:CD	2:C:304:GLU:H	2.26	0.44
2:C:828:PHE:HZ	2:C:1232:MET:HB2	1.82	0.44
2:C:1014:LEU:O	2:C:1017:GLN:HG2	2.18	0.44
2:C:1174:GLU:OE1	2:C:1177:ARG:NH2	2.43	0.44
2:C:1297:ASP:CG	2:C:1300:GLY:H	2.26	0.44
3:D:450:HIS:HD2	3:D:452:LEU:H	1.64	0.44
5:F:124:ARG:HG2	5:F:124:ARG:NH1	2.32	0.44
5:F:580:LYS:HE3	5:F:584:GLU:OE1	2.18	0.44
2:C:84:GLU:HA	2:C:87:ILE:HG22	2.00	0.43
2:C:230:PHE:CZ	2:C:239:MET:HG3	2.53	0.43
2:C:786:GLY:N	2:C:789:THR:OG1	2.50	0.43
3:D:219:LYS:HA	3:D:222:LYS:HG2	2.00	0.43
3:D:555:TYR:CE2	3:D:565:ALA:HB2	2.53	0.43
3:D:962:ASN:ND2	3:D:962:ASN:O	2.51	0.43
3:D:1309:ILE:H	3:D:1309:ILE:HG12	1.61	0.43
5:F:212:LYS:HE2	5:F:670:ASP:HB2	2.00	0.43
7:R:12:G:C2	8:T:21:DG:C2	3.06	0.43
2:C:157:PHE:CZ	2:C:431:LYS:HD3	2.53	0.43
2:C:706:ARG:NE	2:C:792:GLY:O	2.50	0.43
2:C:981:ALA:O	2:C:1007:LYS:NZ	2.50	0.43
2:C:1261:GLY:HA2	8:T:21:DG:OP1	2.19	0.43
3:D:180:MET:HE3	3:D:293:ARG:HD2	2.00	0.43
3:D:342:LEU:HD13	3:D:342:LEU:HA	1.86	0.43
1:A:17:GLU:OE2	1:A:25:LYS:HB3	2.18	0.43
1:A:66:HIS:HD2	1:A:68:TYR:H	1.66	0.43
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.83	0.43
2:C:276:GLN:HA	2:C:279:LYS:HE3	2.01	0.43
2:C:696:ASP:OD1	2:C:798:GLN:NE2	2.51	0.43
2:C:886:LYS:H	2:C:917:SER:HA	1.83	0.43
2:C:1123:GLY:O	2:C:1126:ASP:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1165:SER:N	2:C:1168:GLU:OE1	2.36	0.43
3:D:64:PRO:O	3:D:95:THR:HG23	2.17	0.43
5:F:124:ARG:HG3	5:F:134:TYR:CE2	2.53	0.43
5:F:280:PRO:CA	5:F:434:TRP:CE2	3.01	0.43
2:C:132:ASP:OD1	2:C:133:ASN:N	2.51	0.43
2:C:800:MET:SD	2:C:827:ARG:NH1	2.91	0.43
2:C:801:ARG:HH22	2:C:1119:MET:HE1	1.84	0.43
2:C:1031:ALA:O	2:C:1035:LYS:HG2	2.19	0.43
2:C:1141:LEU:O	2:C:1145:ILE:HG12	2.18	0.43
3:D:528:THR:N	3:D:532:GLU:OE1	2.30	0.43
3:D:591:ILE:HG13	3:D:592:VAL:HG13	2.01	0.43
3:D:1238:GLN:HB3	3:D:1242:ARG:NH2	2.30	0.43
5:F:192:SER:OG	5:F:197:GLN:NE2	2.49	0.43
5:F:214:PHE:CG	5:F:215:VAL:N	2.85	0.43
5:F:496:THR:O	5:F:500:ILE:HG12	2.18	0.43
5:F:582:PRO:CG	5:F:589:PRO:HD3	2.48	0.43
5:F:650:ASP:C	5:F:653:THR:HG22	2.37	0.43
1:A:199:ASP:OD1	1:A:200:LYS:N	2.51	0.43
2:C:26:TYR:HB3	2:C:29:SER:OG	2.19	0.43
2:C:370:MET:SD	2:C:371:ARG:NH2	2.90	0.43
2:C:1088:ASP:OD1	2:C:1092:THR:N	2.51	0.43
2:C:1296:ASP:CG	2:C:1321:GLU:H	2.27	0.43
4:E:54:ILE:HD12	4:E:54:ILE:HA	1.88	0.43
5:F:36:ASP:CG	5:F:37:LEU:N	2.75	0.43
5:F:307:MET:HE2	5:F:307:MET:HA	2.01	0.43
1:A:104:LYS:HD2	1:A:104:LYS:HA	1.76	0.43
2:C:183:TRP:CD1	2:C:183:TRP:N	2.85	0.43
2:C:1307:ASN:HA	2:C:1310:ASP:OD2	2.18	0.43
3:D:21:LYS:HZ2	3:D:1341:ARG:HD2	1.84	0.43
3:D:357:VAL:HG12	3:D:461:PHE:CZ	2.53	0.43
3:D:523:GLU:HA	3:D:546:ALA:HB1	2.00	0.43
3:D:657:ALA:O	3:D:660:GLU:HG2	2.19	0.43
5:F:11:PRO:HG3	5:F:31:VAL:HG22	2.01	0.43
5:F:486:LEU:HD22	5:F:491:ILE:CG2	2.49	0.43
5:F:709:VAL:O	5:F:718:MET:N	2.48	0.43
6:N:46:DC:H2"	6:N:47:DA:C8	2.53	0.43
1:A:136:GLU:CD	1:A:136:GLU:H	2.27	0.43
2:C:190:PRO:HB2	2:C:191:LYS:HZ2	1.83	0.43
2:C:714:VAL:HG23	2:C:715:THR:HG23	1.99	0.43
2:C:812:PHE:CD2	2:C:813:GLU:HG2	2.54	0.43
2:C:1281:TYR:OH	3:D:431:ARG:O	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1312:ASN:HA	4:E:31:GLN:HE21	1.83	0.43
3:D:79:LYS:HE3	3:D:80:HIS:NE2	2.34	0.43
3:D:555:TYR:HB3	3:D:563:LEU:HB3	2.01	0.43
3:D:975:ILE:HG12	3:D:977:SER:H	1.83	0.43
3:D:1063:ASP:O	3:D:1067:ARG:N	2.37	0.43
5:F:280:PRO:HA	5:F:434:TRP:CZ3	2.53	0.43
5:F:582:PRO:CG	5:F:589:PRO:HD2	2.49	0.43
1:A:93:GLN:HG2	1:A:120:ASP:O	2.19	0.43
1:A:133:LEU:HD23	1:A:133:LEU:HA	1.89	0.43
1:A:214:GLU:O	1:A:218:ARG:HG3	2.18	0.43
2:C:101:ARG:NE	2:C:119:GLU:OE2	2.39	0.43
2:C:587:LEU:HD13	2:C:587:LEU:HA	1.82	0.43
2:C:618:GLN:NE2	3:D:770:LEU:HB2	2.33	0.43
2:C:812:PHE:O	2:C:1099:ASN:ND2	2.51	0.43
2:C:985:GLU:O	2:C:989:LEU:HG	2.18	0.43
2:C:1225:VAL:HG13	3:D:638:SER:HB2	2.00	0.43
3:D:310:GLY:HA2	3:D:315:ALA:HB2	2.01	0.43
3:D:812:ASP:OD1	3:D:812:ASP:N	2.50	0.43
1:A:215:GLU:OE2	1:A:219:ARG:NH2	2.52	0.43
2:C:633:LEU:HA	2:C:645:PHE:O	2.18	0.43
2:C:809:GLY:HA3	3:D:629:PHE:CE2	2.53	0.43
2:C:1111:GLN:O	2:C:1115:THR:OG1	2.37	0.43
5:F:76:TRP:CZ2	5:F:568:PHE:HZ	2.37	0.43
2:C:5:TYR:HA	2:C:8:LYS:HE3	2.00	0.43
2:C:80:PHE:HB2	2:C:85:CYS:SG	2.58	0.43
2:C:209:ILE:O	2:C:213:LEU:N	2.51	0.43
3:D:187:ALA:O	3:D:191:SER:OG	2.29	0.43
3:D:277:ASN:HA	3:D:280:LYS:HZ3	1.84	0.43
3:D:1040:MET:HE3	3:D:1040:MET:HB3	1.95	0.43
5:F:70:ARG:CZ	6:N:14:DT:C7	2.92	0.43
5:F:161:ARG:HG3	5:F:161:ARG:NH1	2.33	0.43
5:F:312:TYR:CG	5:F:320:MET:CE	2.86	0.43
5:F:489:ARG:HB2	5:F:491:ILE:HG12	2.01	0.43
2:C:275:ARG:O	2:C:275:ARG:NH1	2.52	0.42
2:C:349:GLU:O	2:C:353:VAL:HG23	2.19	0.42
2:C:529:ARG:HD2	2:C:572:ILE:HG22	2.00	0.42
2:C:1235:LEU:HD23	2:C:1235:LEU:HA	1.86	0.42
3:D:289:ASP:OD2	3:D:293:ARG:NE	2.35	0.42
5:F:392:GLN:CG	5:F:396:ARG:NH1	2.81	0.42
1:A:85:LEU:HD12	1:A:85:LEU:HA	1.81	0.42
1:A:112:ALA:O	1:A:115:ILE:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:LYS:NZ	2:C:280:ASP:OD2	2.33	0.42
2:C:672:GLU:OE1	2:C:672:GLU:N	2.31	0.42
2:C:722:GLY:HA2	2:C:737:ASN:CG	2.45	0.42
2:C:839:VAL:HG13	2:C:1049:ILE:HG12	2.01	0.42
2:C:841:ARG:NH2	2:C:848:GLU:OE2	2.52	0.42
2:C:1018:TYR:O	2:C:1022:LYS:HG2	2.20	0.42
2:C:1213:TYR:HD1	2:C:1220:GLN:HA	1.84	0.42
2:C:1323:PHE:O	2:C:1327:LEU:HG	2.19	0.42
3:D:26:SER:HB3	3:D:28:ASP:OD1	2.19	0.42
5:F:10:SER:HA	5:F:11:PRO:HD3	1.94	0.42
1:B:25:LYS:NZ	1:B:204:GLU:HB2	2.34	0.42
2:C:718:ALA:HB2	2:C:783:LEU:HD11	2.01	0.42
2:C:963:GLU:OE1	2:C:1028:LYS:NZ	2.53	0.42
3:D:591:ILE:HD12	3:D:604:MET:HG3	2.00	0.42
5:F:153:LYS:HE3	5:F:153:LYS:O	2.19	0.42
5:F:472:LYS:CG	5:F:649:GLU:O	2.66	0.42
5:F:728:TYR:CE2	5:F:730:ALA:HB2	2.54	0.42
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.84	0.42
2:C:815:SER:OG	2:C:1077:SER:HB3	2.19	0.42
3:D:1121:LEU:HD23	3:D:1121:LEU:H	1.84	0.42
5:F:33:HIS:C	5:F:35:ARG:H	2.28	0.42
5:F:566:HIS:ND1	5:F:567:PHE:N	2.67	0.42
2:C:820:GLU:HG3	2:C:1080:ASN:O	2.18	0.42
2:C:866:ASP:OD1	2:C:869:GLY:N	2.52	0.42
3:D:322:ARG:NH1	7:R:8:C:H4'	2.34	0.42
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	2.00	0.42
5:F:70:ARG:NH2	6:N:14:DT:C6	2.88	0.42
5:F:160:ASP:HB3	5:F:554:ALA:HA	2.02	0.42
5:F:400:ALA:HB2	5:F:437:VAL:HG22	1.97	0.42
2:C:593:LYS:HA	2:C:652:TYR:CD1	2.55	0.42
2:C:757:THR:CG2	2:C:765:ILE:HB	2.50	0.42
2:C:856:ASN:N	2:C:908:GLU:OE1	2.40	0.42
2:C:1315:MET:HG2	2:C:1317:PRO:HD3	2.01	0.42
3:D:1120:THR:C	3:D:1123:ARG:HH12	2.28	0.42
5:F:312:TYR:CD2	5:F:320:MET:HE1	2.53	0.42
2:C:165:HIS:NE2	2:C:169:LYS:HB3	2.35	0.42
2:C:195:PHE:CD2	2:C:203:LYS:HG2	2.52	0.42
2:C:238:GLN:HG3	2:C:286:GLU:OE1	2.19	0.42
2:C:247:ARG:NH1	2:C:274:ILE:HG21	2.34	0.42
2:C:622:ASN:C	2:C:623:LEU:HD23	2.44	0.42
3:D:85:CYS:SG	3:D:87:LYS:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1280:VAL:HG12	3:D:1281:GLU:N	2.35	0.42
5:F:427:ARG:O	5:F:448:ARG:HB3	2.19	0.42
6:N:35:DC:H6	6:N:35:DC:C5'	2.33	0.42
1:B:65:LEU:HB3	1:B:66:HIS:CD2	2.54	0.42
1:B:104:LYS:HD2	1:B:114:ASP:OD2	2.18	0.42
1:B:185:TYR:HA	1:B:203:ILE:HD13	2.00	0.42
2:C:148:GLN:NE2	2:C:533:LEU:O	2.45	0.42
2:C:808:ASN:CG	2:C:1216:ARG:HH22	2.27	0.42
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.55	0.42
3:D:549:LYS:HE3	3:D:549:LYS:HB3	1.90	0.42
3:D:957:SER:HG	3:D:959:LYS:HZ1	1.67	0.42
5:F:271:ARG:HD2	5:F:453:VAL:O	2.19	0.42
5:F:479:GLU:HA	5:F:517:PHE:HE2	1.84	0.42
5:F:494:PRO:HA	5:F:497:TYR:CE2	2.55	0.42
5:F:521:LYS:HD2	5:F:615:VAL:HG21	2.00	0.42
6:N:45:DT:H2''	6:N:46:DC:C6	2.55	0.42
1:B:52:PRO:HB3	1:B:150:ARG:HG2	2.00	0.42
1:B:205:MET:HE3	1:B:205:MET:HB2	1.77	0.42
2:C:13:LYS:HG2	2:C:14:ASP:N	2.35	0.42
2:C:87:ILE:HD12	2:C:87:ILE:HA	1.89	0.42
2:C:298:ALA:HB2	2:C:335:THR:C	2.45	0.42
2:C:337:PHE:CE2	2:C:339:ASN:HB2	2.55	0.42
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.55	0.42
2:C:1101:LEU:C	2:C:1104:PRO:HD2	2.45	0.42
3:D:282:LEU:HD12	5:F:104:ASP:OD2	2.19	0.42
3:D:475:GLU:HG3	4:E:24:ALA:HB1	2.01	0.42
3:D:520:ALA:HB1	3:D:543:SER:HB3	2.01	0.42
3:D:825:VAL:HG13	3:D:833:GLU:H	1.85	0.42
3:D:965:SER:HA	3:D:976:THR:H	1.85	0.42
3:D:1325:PHE:CE2	3:D:1326:GLN:HB2	2.55	0.42
5:F:521:LYS:HD3	5:F:615:VAL:CG1	2.24	0.42
2:C:302:ILE:HA	2:C:309:LEU:HA	2.01	0.42
2:C:548:ARG:HD3	2:C:569:ILE:HG23	2.01	0.42
2:C:577:VAL:HG23	2:C:578:TYR:CD2	2.55	0.42
2:C:802:VAL:HG22	2:C:1096:ILE:HB	2.01	0.42
2:C:1291:LEU:HD12	2:C:1291:LEU:HA	1.80	0.42
3:D:863:LEU:HD11	3:D:901:ARG:HB2	2.01	0.42
4:E:8:ASP:OD1	4:E:9:ALA:N	2.53	0.42
5:F:241:GLN:HG2	5:F:242:ASN:ND2	2.35	0.42
8:T:5:DG:H2''	8:T:6:DA:C8	2.54	0.42
2:C:218:GLU:H	2:C:218:GLU:CD	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:275:ARG:NH1	2:C:278:GLU:HB2	2.35	0.41
2:C:736:VAL:HG12	2:C:747:GLY:O	2.20	0.41
2:C:936:ARG:HB2	2:C:1042:LEU:HD22	2.02	0.41
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.21	0.41
3:D:657:ALA:HA	3:D:660:GLU:HG2	2.02	0.41
5:F:399:VAL:HG12	5:F:437:VAL:HG11	2.02	0.41
1:A:86:LYS:NZ	1:A:174:ASP:O	2.34	0.41
1:B:83:LEU:HD13	1:B:83:LEU:HA	1.90	0.41
2:C:204:LEU:HD12	2:C:205:PRO:O	2.20	0.41
2:C:1314:GLN:HB2	4:E:28:ARG:HH12	1.85	0.41
3:D:26:SER:O	3:D:29:MET:HG2	2.20	0.41
3:D:664:ILE:HD12	3:D:681:LYS:HD3	2.01	0.41
3:D:874:GLU:OE1	3:D:875:ASN:ND2	2.53	0.41
3:D:930:LEU:HA	3:D:1244:GLN:HG2	2.01	0.41
3:D:962:ASN:HD21	3:D:979:ASN:C	2.29	0.41
3:D:1023:HIS:HA	3:D:1126:GLN:HB3	2.03	0.41
3:D:1219:ASP:HA	3:D:1222:ARG:NE	2.34	0.41
5:F:97:LYS:CE	5:F:127:ILE:HG12	2.48	0.41
5:F:110:THR:O	5:F:136:ARG:NH2	2.53	0.41
5:F:145:ASN:O	5:F:145:ASN:ND2	2.53	0.41
6:N:35:DC:H2'	6:N:36:DG:C8	2.55	0.41
7:R:9:G:H2'	7:R:10:G:H8	1.85	0.41
2:C:303:ASP:N	2:C:308:GLU:O	2.43	0.41
5:F:214:PHE:C	5:F:215:VAL:HG23	2.45	0.41
5:F:720:LEU:HD12	5:F:728:TYR:O	2.20	0.41
2:C:106:GLU:HG2	2:C:115:LYS:HB3	2.01	0.41
2:C:161:LYS:HB2	2:C:161:LYS:HE2	1.78	0.41
2:C:363:LEU:HD23	2:C:366:ILE:HD11	2.02	0.41
2:C:1230:MET:HE3	2:C:1231:TYR:H	1.85	0.41
3:D:215:LYS:HA	3:D:218:THR:HG22	2.01	0.41
3:D:825:VAL:HG13	3:D:832:LYS:HB2	2.03	0.41
5:F:63:GLU:HB3	5:F:76:TRP:CG	2.55	0.41
5:F:79:TRP:CE2	5:F:564:LEU:CB	2.99	0.41
6:N:35:DC:O5'	6:N:35:DC:C6	2.70	0.41
1:B:84:ASN:OD1	3:D:551:ARG:NH2	2.46	0.41
2:C:149:LEU:HB2	2:C:530:ILE:HD11	2.02	0.41
2:C:180:ARG:HH21	2:C:396:ASP:HB2	1.85	0.41
3:D:510:LEU:HD23	3:D:510:LEU:HA	1.84	0.41
3:D:1067:ARG:HD2	3:D:1072:LYS:HA	2.03	0.41
3:D:1159:ILE:HA	3:D:1159:ILE:HD12	1.88	0.41
3:D:1161:GLY:HA2	3:D:1180:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1162:ILE:HG22	3:D:1178:THR:HB	2.02	0.41
3:D:1169:THR:HG22	3:D:1170:LYS:N	2.35	0.41
3:D:1325:PHE:CD2	3:D:1326:GLN:HB2	2.56	0.41
5:F:473:PRO:HB3	5:F:656:LEU:HD22	2.00	0.41
1:A:58:GLU:OE1	1:A:170:ARG:NH1	2.53	0.41
3:D:677:GLU:O	3:D:681:LYS:HG2	2.20	0.41
3:D:978:ARG:HH21	3:D:1202:GLU:CD	2.29	0.41
1:A:67:GLU:O	1:A:78:ILE:HB	2.21	0.41
1:B:12:ARG:NH2	1:B:14:VAL:HA	2.36	0.41
2:C:301:TYR:O	2:C:310:ILE:N	2.53	0.41
3:D:823:THR:HA	3:D:835:LEU:HD12	2.03	0.41
3:D:979:ASN:OD1	3:D:979:ASN:N	2.53	0.41
3:D:998:PRO:HG2	3:D:1020:TRP:CZ2	2.55	0.41
4:E:15:ASN:HD21	4:E:17:PHE:HB2	1.86	0.41
5:F:472:LYS:HB2	5:F:653:THR:H	1.86	0.41
5:F:728:TYR:HE2	5:F:730:ALA:HB2	1.85	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.20	0.41
2:C:230:PHE:CD2	2:C:239:MET:HB2	2.55	0.41
2:C:811:ASN:OD1	2:C:811:ASN:N	2.53	0.41
2:C:247:ARG:HH12	2:C:274:ILE:HG21	1.86	0.41
2:C:301:TYR:O	2:C:309:LEU:HD12	2.20	0.41
2:C:629:PHE:CD2	2:C:634:VAL:HG21	2.56	0.41
3:D:208:THR:CG2	3:D:214:ARG:CD	2.98	0.41
3:D:552:ILE:HD11	3:D:570:LYS:HD2	2.03	0.41
3:D:644:MET:HB2	3:D:764:ARG:HD2	2.02	0.41
3:D:707:ILE:HG23	3:D:711:GLY:HA2	2.03	0.41
3:D:1048:ARG:HH12	3:D:1110:GLU:CD	2.28	0.41
4:E:26:ARG:O	4:E:30:MET:HG2	2.20	0.41
5:F:21:LEU:HD21	5:F:25:TYR:CB	2.35	0.41
5:F:280:PRO:N	5:F:434:TRP:NE1	2.69	0.41
5:F:594:LEU:HA	5:F:607:GLY:HA2	2.02	0.41
5:F:704:TYR:OH	5:F:707:PRO:HD2	2.20	0.41
5:F:760:GLU:HB3	5:F:803:PHE:HE1	1.85	0.41
1:B:46:ILE:O	1:B:50:SER:OG	2.26	0.41
1:B:67:GLU:HA	1:B:78:ILE:HG21	2.03	0.41
2:C:97:ARG:HB3	2:C:121:GLU:HG2	2.03	0.41
2:C:516:ASP:OD1	2:C:516:ASP:N	2.51	0.41
2:C:565:GLU:HA	2:C:569:ILE:HD13	2.02	0.41
2:C:705:GLU:HA	2:C:708:VAL:HG12	2.03	0.41
2:C:993:PRO:HG2	2:C:996:ARG:HB3	2.03	0.41
3:D:959:LYS:HD3	3:D:1007:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1263:LYS:HD3	3:D:1263:LYS:HA	1.76	0.41
5:F:86:LEU:O	5:F:88:GLY:N	2.54	0.41
1:A:98:VAL:HG11	1:A:121:VAL:HG11	2.02	0.40
2:C:91:THR:HG22	2:C:93:SER:HB3	2.02	0.40
2:C:148:GLN:NE2	2:C:535:PRO:O	2.49	0.40
2:C:345:PRO:O	2:C:348:SER:OG	2.34	0.40
2:C:550:VAL:O	3:D:777:HIS:NE2	2.54	0.40
2:C:1058:ARG:HD2	2:C:1238:LEU:HD22	2.02	0.40
3:D:66:LYS:HB3	3:D:69:GLU:HB3	2.03	0.40
3:D:110:PRO:HG2	3:D:186:GLN:NE2	2.32	0.40
3:D:192:MET:HE2	3:D:192:MET:HB2	1.82	0.40
3:D:495:ASN:O	3:D:497:GLU:N	2.54	0.40
3:D:580:TRP:CZ3	3:D:589:TYR:HA	2.56	0.40
5:F:582:PRO:HG3	5:F:589:PRO:CD	2.51	0.40
2:C:240:GLU:OE1	2:C:240:GLU:N	2.53	0.40
2:C:662:SER:O	2:C:666:SER:N	2.50	0.40
2:C:876:GLU:N	2:C:876:GLU:OE1	2.54	0.40
2:C:1035:LYS:HA	2:C:1035:LYS:HD2	1.91	0.40
2:C:1212:LEU:HA	2:C:1212:LEU:HD23	1.87	0.40
2:C:1287:LEU:HD21	3:D:1351:VAL:HG22	2.04	0.40
3:D:254:PRO:HA	3:D:260:PHE:CD1	2.55	0.40
3:D:629:PHE:HD1	3:D:629:PHE:HA	1.68	0.40
3:D:773:PHE:O	3:D:776:THR:HG22	2.21	0.40
3:D:902:ASP:CG	3:D:904:ALA:H	2.29	0.40
3:D:1034:PHE:CE2	3:D:1114:GLN:HB2	2.56	0.40
4:E:66:VAL:N	4:E:69:ARG:HH21	2.18	0.40
5:F:141:GLU:H	5:F:146:ALA:HB1	1.86	0.40
5:F:473:PRO:CG	5:F:653:THR:CA	2.88	0.40
5:F:704:TYR:CG	5:F:705:ASP:N	2.89	0.40
1:A:208:ASN:OD1	1:A:210:THR:HG22	2.21	0.40
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.95	0.40
2:C:232:ILE:HB	2:C:331:LYS:HA	2.03	0.40
3:D:136:GLU:HG3	3:D:312:ARG:HH22	1.86	0.40
3:D:232:ASN:OD1	3:D:232:ASN:N	2.54	0.40
5:F:763:CYS:HA	5:F:770:PHE:CE2	2.56	0.40
1:A:154:PRO:HB3	2:C:1059:ARG:NH1	2.36	0.40
2:C:951:MET:HE2	2:C:951:MET:HB2	1.94	0.40
3:D:464:ASP:CG	7:R:14:G:HO2'	2.29	0.40
3:D:968:ASN:HA	3:D:1117:SER:O	2.22	0.40
3:D:1344:LEU:HD13	3:D:1349:GLU:HG2	2.03	0.40
5:F:533:ASN:ND2	5:F:587:MET:HA	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:621:GLY:HA2	5:F:624:LEU:HD12	2.02	0.40
1:A:47:LEU:O	1:A:51:MET:HG2	2.21	0.40
1:B:37:HIS:CD2	1:B:187:VAL:HG21	2.57	0.40
3:D:566:LYS:HB2	3:D:566:LYS:HE3	1.87	0.40
3:D:1172:LYS:HA	3:D:1190:ILE:O	2.21	0.40
3:D:1328:THR:H	3:D:1328:THR:HG23	1.68	0.40
4:E:72:GLN:HA	4:E:75:GLN:HG3	2.04	0.40
5:F:173:ARG:HH21	6:N:16:DC:H42	1.68	0.40
5:F:177:TYR:OH	6:N:15:DT:C7	2.70	0.40
5:F:476:ARG:CZ	5:F:518:TYR:CD2	3.04	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	A	231/329 (70%)	226 (98%)	5 (2%)	0	100	100
1	B	230/329 (70%)	222 (96%)	8 (4%)	0	100	100
2	C	1339/1342 (100%)	1289 (96%)	50 (4%)	0	100	100
3	D	1336/1415 (94%)	1290 (97%)	46 (3%)	0	100	100
4	E	88/91 (97%)	86 (98%)	2 (2%)	0	100	100
5	F	819/896 (91%)	777 (95%)	39 (5%)	3 (0%)	30	64
All	All	4043/4402 (92%)	3890 (96%)	150 (4%)	3 (0%)	49	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	34	ILE
5	F	20	TYR
5	F	87	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	A	200/286 (70%)	195 (98%)	5 (2%)	42	62
1	B	200/286 (70%)	192 (96%)	8 (4%)	28	51
2	C	1156/1157 (100%)	1133 (98%)	23 (2%)	48	65
3	D	1124/1176 (96%)	1099 (98%)	25 (2%)	45	64
4	E	74/75 (99%)	74 (100%)	0	100	100
5	F	702/754 (93%)	672 (96%)	30 (4%)	26	49
All	All	3456/3734 (93%)	3365 (97%)	91 (3%)	41	60

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ILE
1	A	173	VAL
1	A	180	VAL
1	A	223	ILE
1	A	231	PHE
1	B	23	HIS
1	B	43	LEU
1	B	65	LEU
1	B	74	VAL
1	B	105	SER
1	B	153	VAL
1	B	193	GLU
1	B	211	ILE
2	C	24	VAL
2	C	30	ILE
2	C	114	VAL
2	C	144	VAL
2	C	146	VAL
2	C	194	LEU
2	C	320	ASP
2	C	374	GLU
2	C	465	ARG

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Mol	Chain	Res	Type
2	C	587	LEU
2	C	598	VAL
2	C	609	ILE
2	C	680	LEU
2	C	690	VAL
2	C	724	VAL
2	C	871	VAL
2	C	884	VAL
2	C	984	VAL
2	C	1046	VAL
2	C	1064	ASP
2	C	1240	ASP
2	C	1254	VAL
2	C	1288	GLN
3	D	15	GLU
3	D	38	VAL
3	D	85	CYS
3	D	238	ILE
3	D	252	LEU
3	D	264	ASP
3	D	434	ILE
3	D	440	VAL
3	D	629	PHE
3	D	639	VAL
3	D	788	LEU
3	D	805	GLN
3	D	823	THR
3	D	825	VAL
3	D	880	VAL
3	D	895	CYS
3	D	963	VAL
3	D	1041	ILE
3	D	1107	VAL
3	D	1177	ILE
3	D	1196	LEU
3	D	1226	VAL
3	D	1246	VAL
3	D	1309	ILE
3	D	1332	LEU
5	F	21	LEU
5	F	34	ILE
5	F	78	ASN

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Mol	Chain	Res	Type
5	F	95	GLU
5	F	97	LYS
5	F	112	LEU
5	F	153	LYS
5	F	156	GLU
5	F	157	LEU
5	F	165	GLN
5	F	173	ARG
5	F	237	GLN
5	F	302	LYS
5	F	319	TYR
5	F	320	MET
5	F	345	LYS
5	F	381	LYS
5	F	383	MET
5	F	389	LYS
5	F	472	LYS
5	F	487	GLU
5	F	493	ARG
5	F	507	ARG
5	F	537	LEU
5	F	539	ASN
5	F	556	HIS
5	F	566	HIS
5	F	590	ASN
5	F	595	THR
5	F	736	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	227	GLN
1	B	41	ASN
1	B	66	HIS
1	B	93	GLN
1	B	117	HIS
1	B	147	GLN
2	C	36	GLN
2	C	150	HIS
2	C	193	ASN
2	C	406	ASN

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Mol	Chain	Res	Type
2	C	437	ASN
2	C	510	GLN
2	C	513	GLN
2	C	628	HIS
2	C	658	GLN
2	C	686	GLN
2	C	688	GLN
2	C	808	ASN
2	C	832	HIS
2	C	955	GLN
2	C	1061	GLN
2	C	1136	GLN
2	C	1175	ASN
2	C	1209	GLN
2	C	1264	GLN
2	C	1288	GLN
3	D	80	HIS
3	D	186	GLN
3	D	266	ASN
3	D	365	GLN
3	D	419	HIS
3	D	450	HIS
3	D	465	GLN
3	D	560	ASN
3	D	665	GLN
3	D	702	GLN
3	D	777	HIS
3	D	951	GLN
3	D	1010	GLN
3	D	1108	GLN
3	D	1235	ASN
3	D	1295	ASN
3	D	1367	GLN
4	E	31	GLN
4	E	61	ASN
5	F	18	ASN
5	F	122	HIS
5	F	145	ASN
5	F	152	ASN
5	F	165	GLN
5	F	197	GLN
5	F	241	GLN

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Mol	Chain	Res	Type
5	F	242	ASN
5	F	253	GLN
5	F	291	GLN
5	F	342	ASN
5	F	353	ASN
5	F	469	HIS
5	F	505	GLN
5	F	533	ASN
5	F	548	ASN
5	F	590	ASN
5	F	681	HIS
5	F	738	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	R	10/14 (71%)	3 (30%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	R	5	C
7	R	6	C
7	R	14	G

There are no RNA pucker outliers to report.

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.

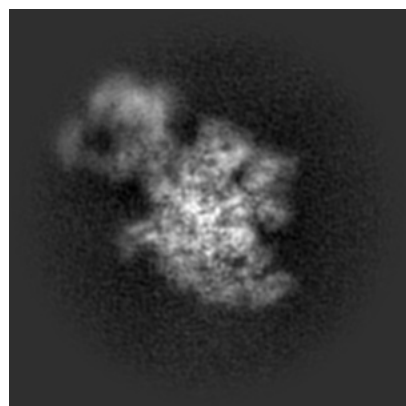
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51264. These allow visual inspection of the internal detail of the map and identification of artifacts.

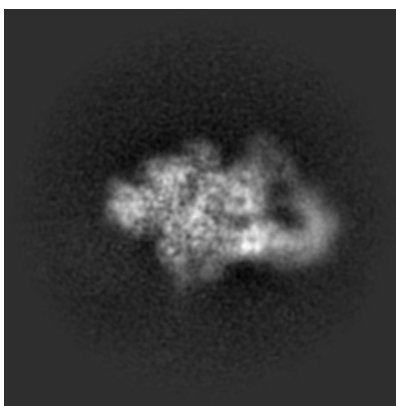
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

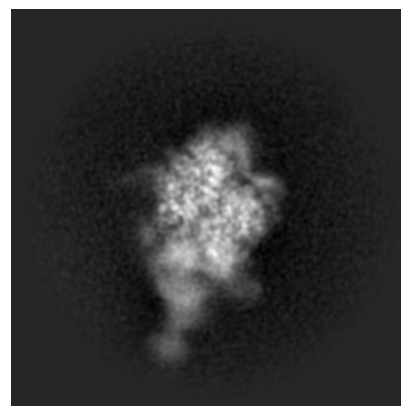
6.1.1 Primary map



X

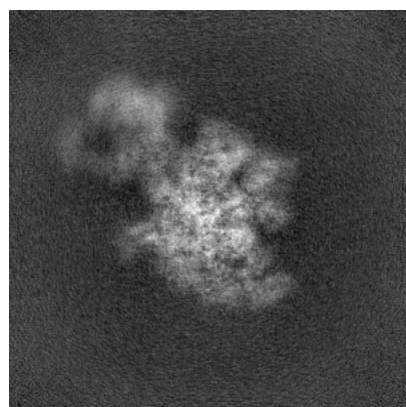


Y

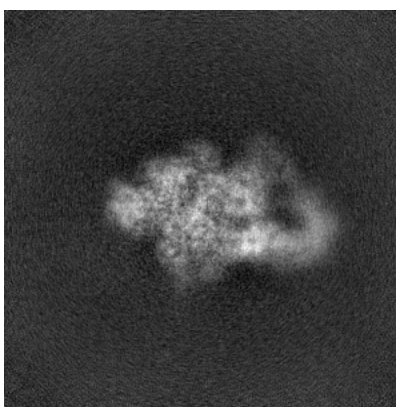


Z

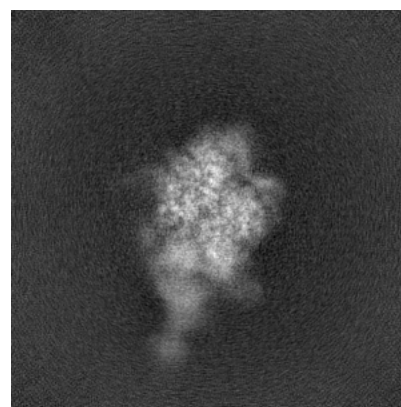
6.1.2 Raw map



X



Y

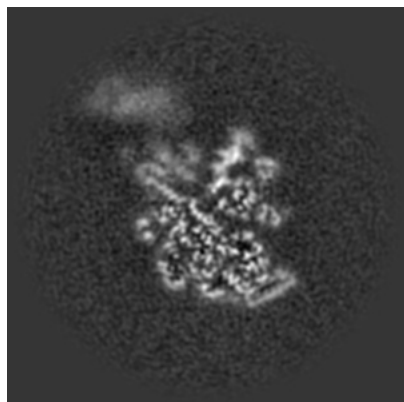


Z

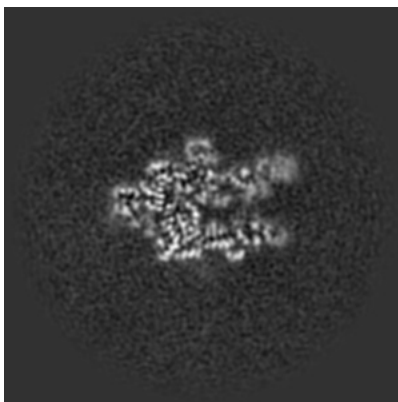
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

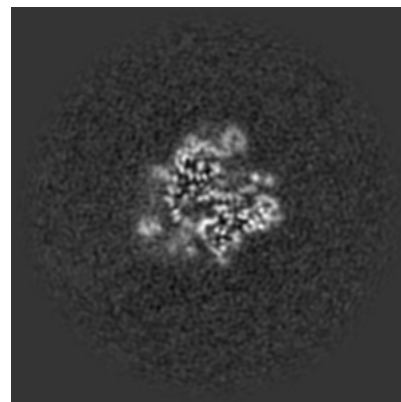
6.2.1 Primary map



X Index: 155

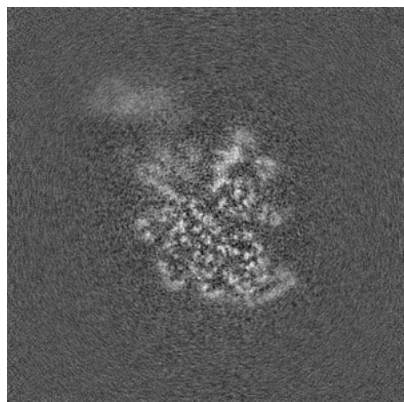


Y Index: 155

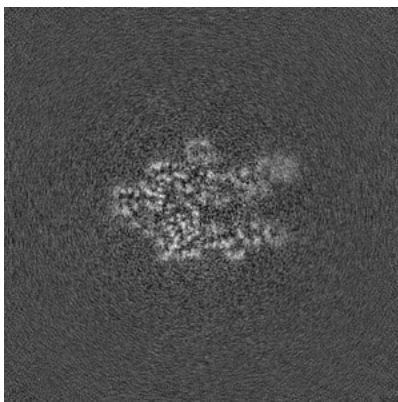


Z Index: 155

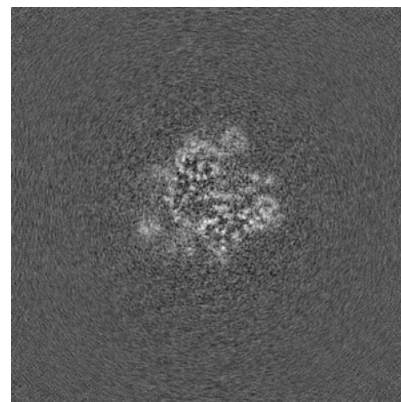
6.2.2 Raw map



X Index: 155



Y Index: 155

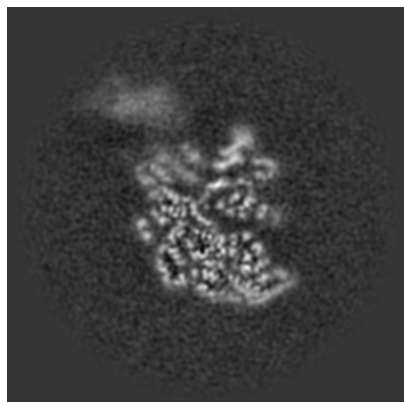


Z Index: 155

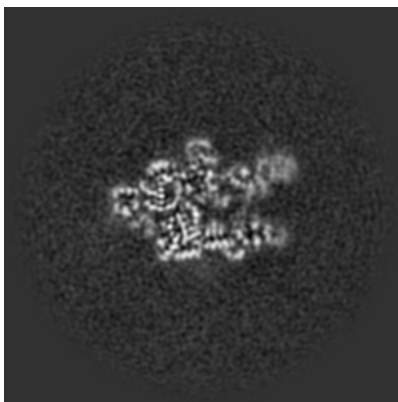
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

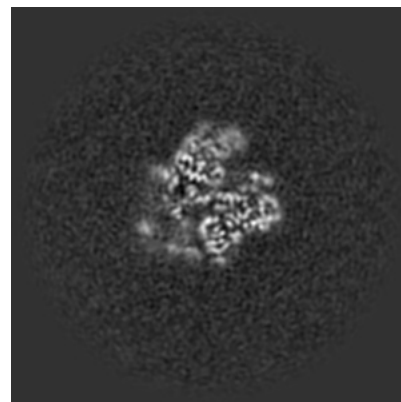
6.3.1 Primary map



X Index: 157

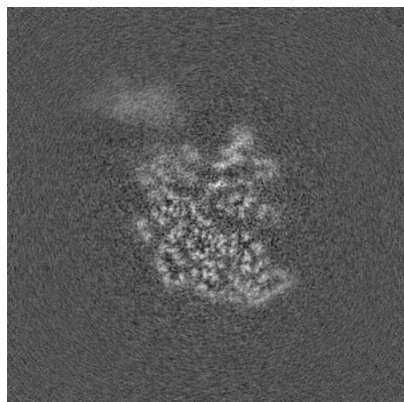


Y Index: 156

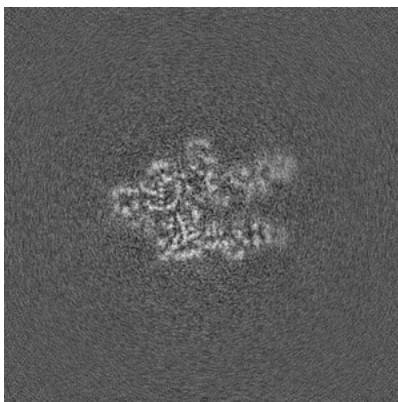


Z Index: 153

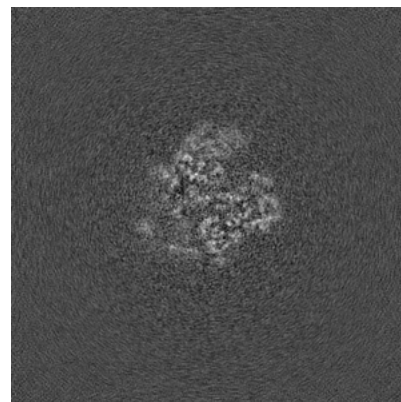
6.3.2 Raw map



X Index: 157



Y Index: 156

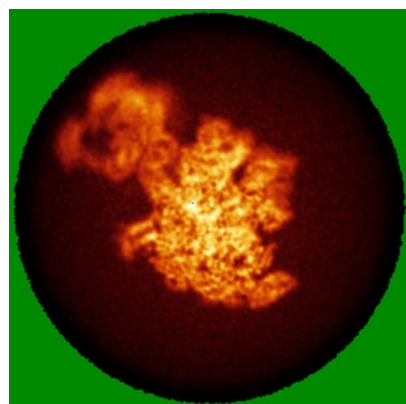


Z Index: 153

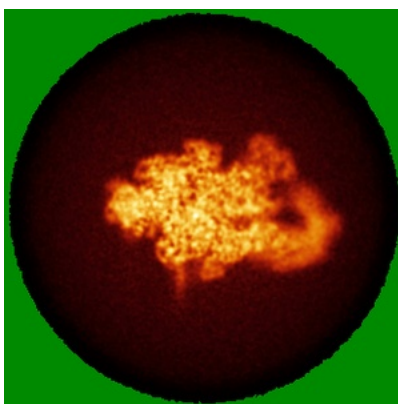
The images above show the largest variance slices of the map in three orthogonal directions.

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

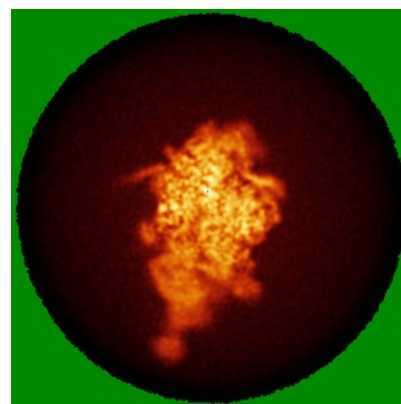
6.4.1 Primary map



X

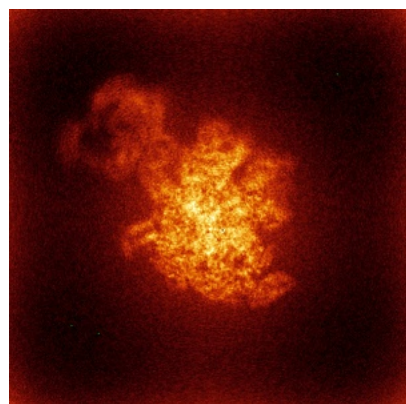


Y

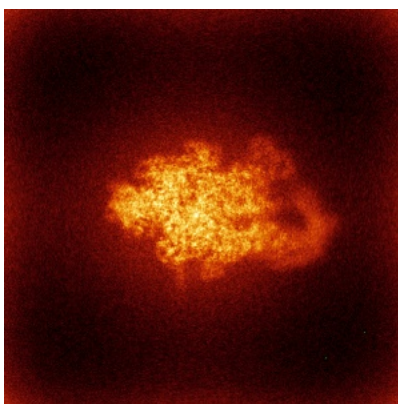


Z

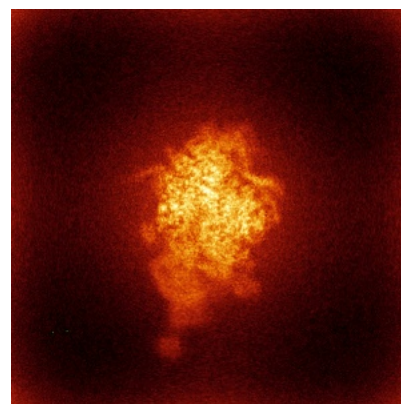
6.4.2 Raw map



X



Y



Z

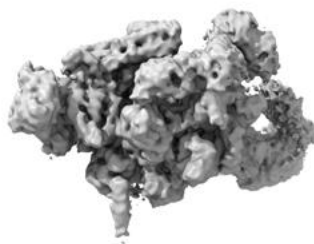
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



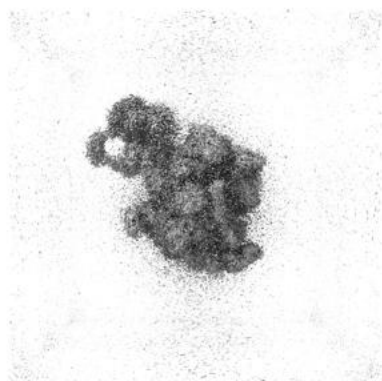
Y



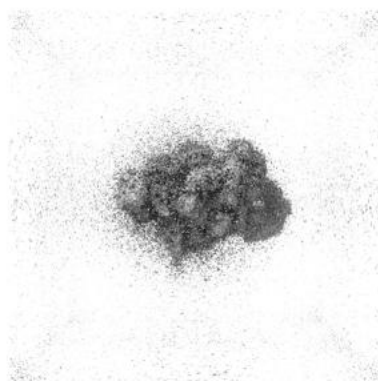
Z

The images above show the 3D surface view of the map at the recommended contour level 0.174. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

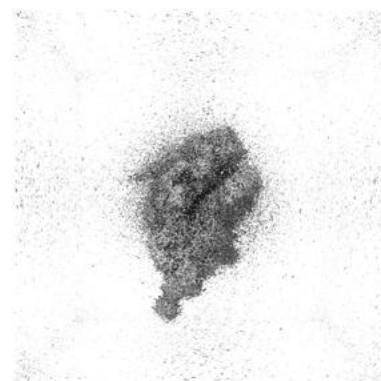
6.5.2 Raw map



X



Y



Z

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

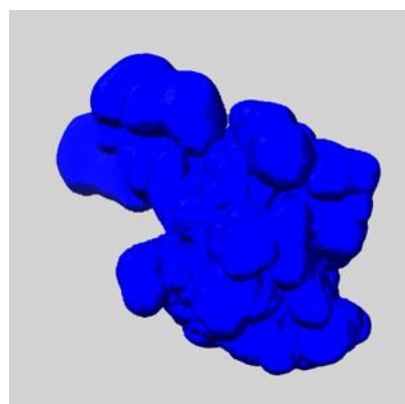
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

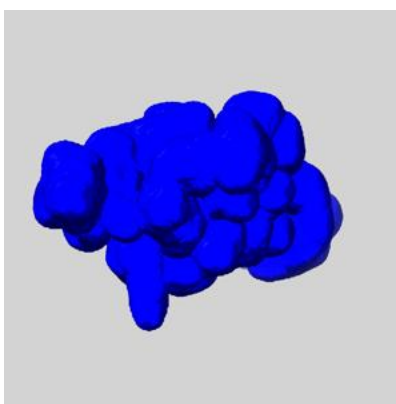
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

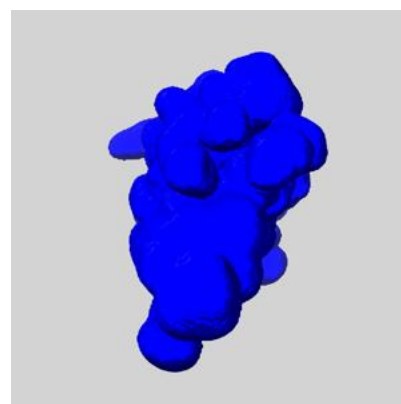
6.6.1 emd_51264_msk_1.map [i](#)



X

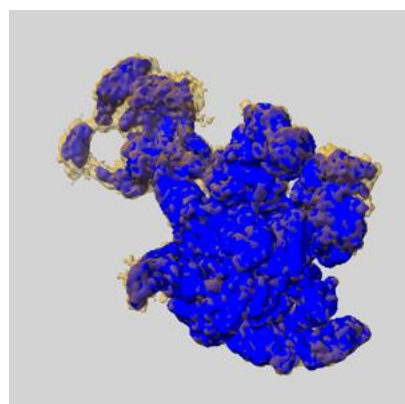


Y

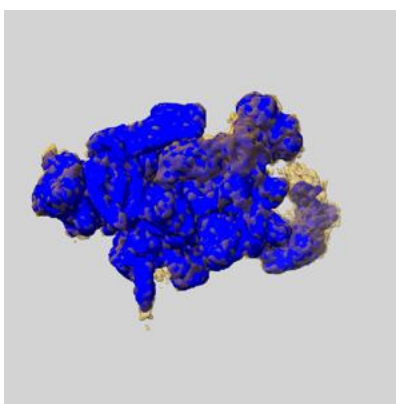


Z

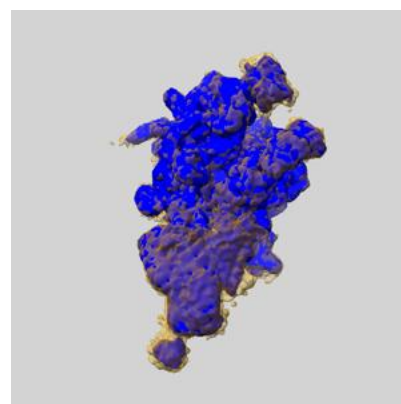
6.6.2 emd_51264_msk_2.map [i](#)



X



Y

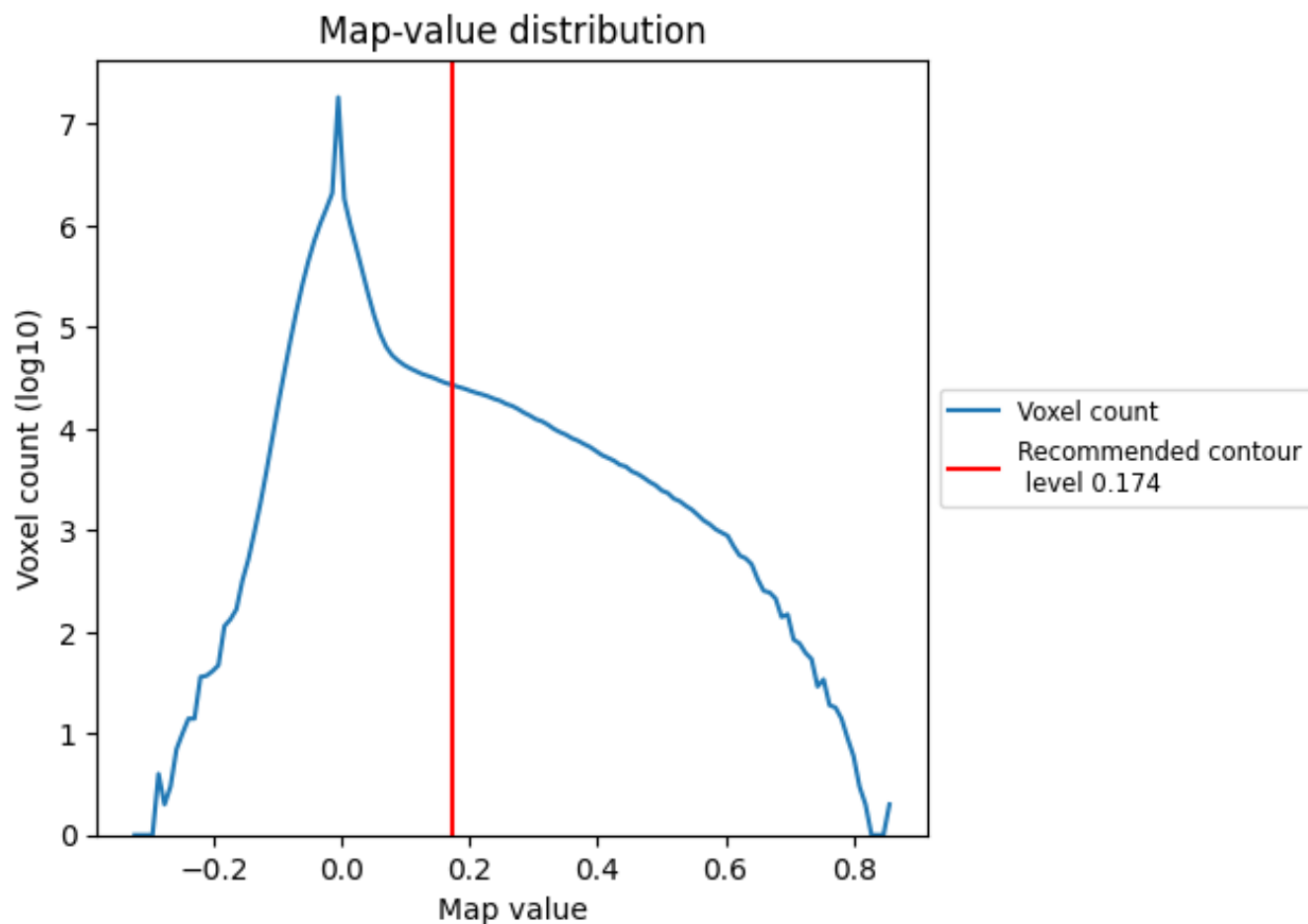


Z

7 Map analysis [i](#)

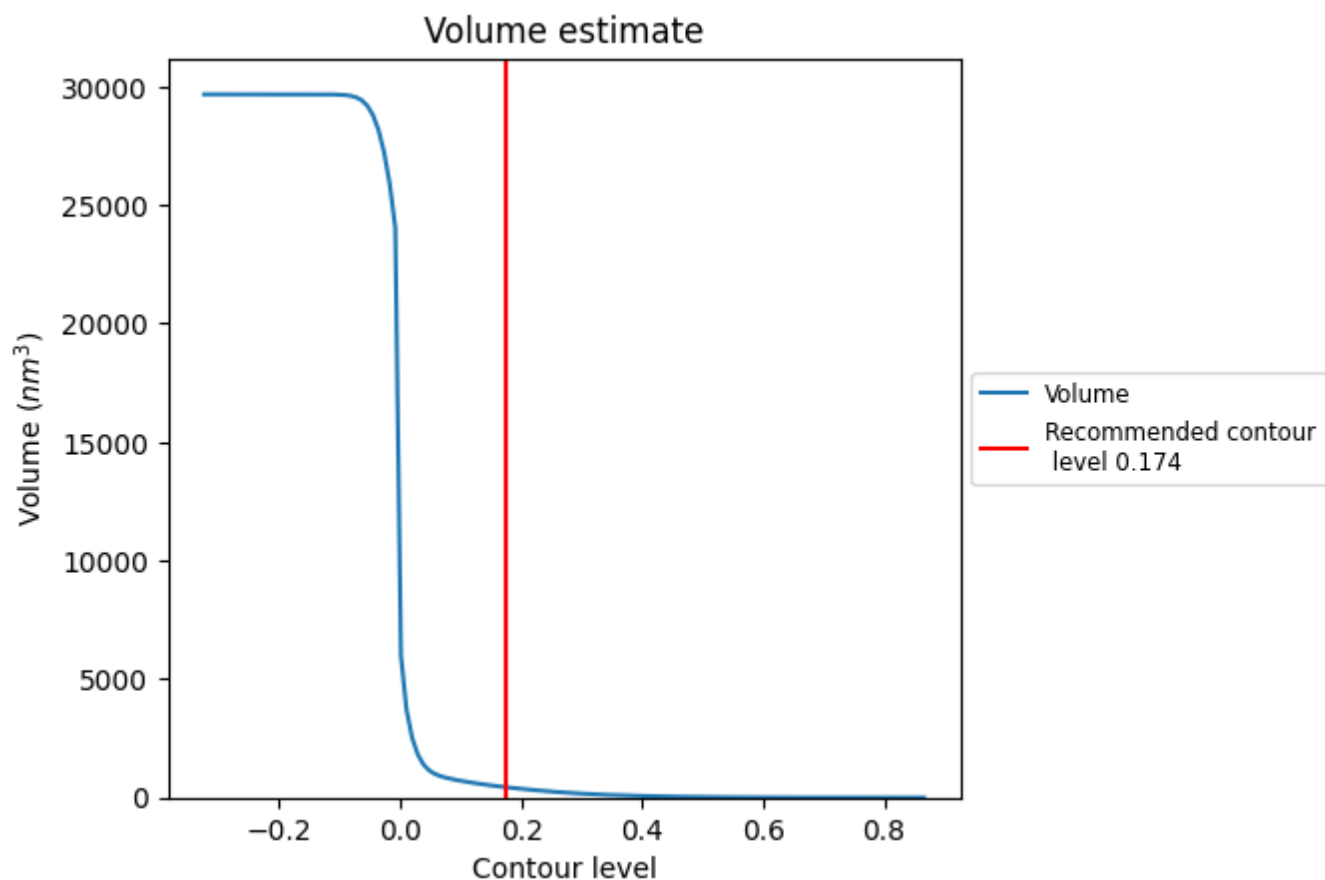
This section contains the results of statistical analysis of the map.

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.

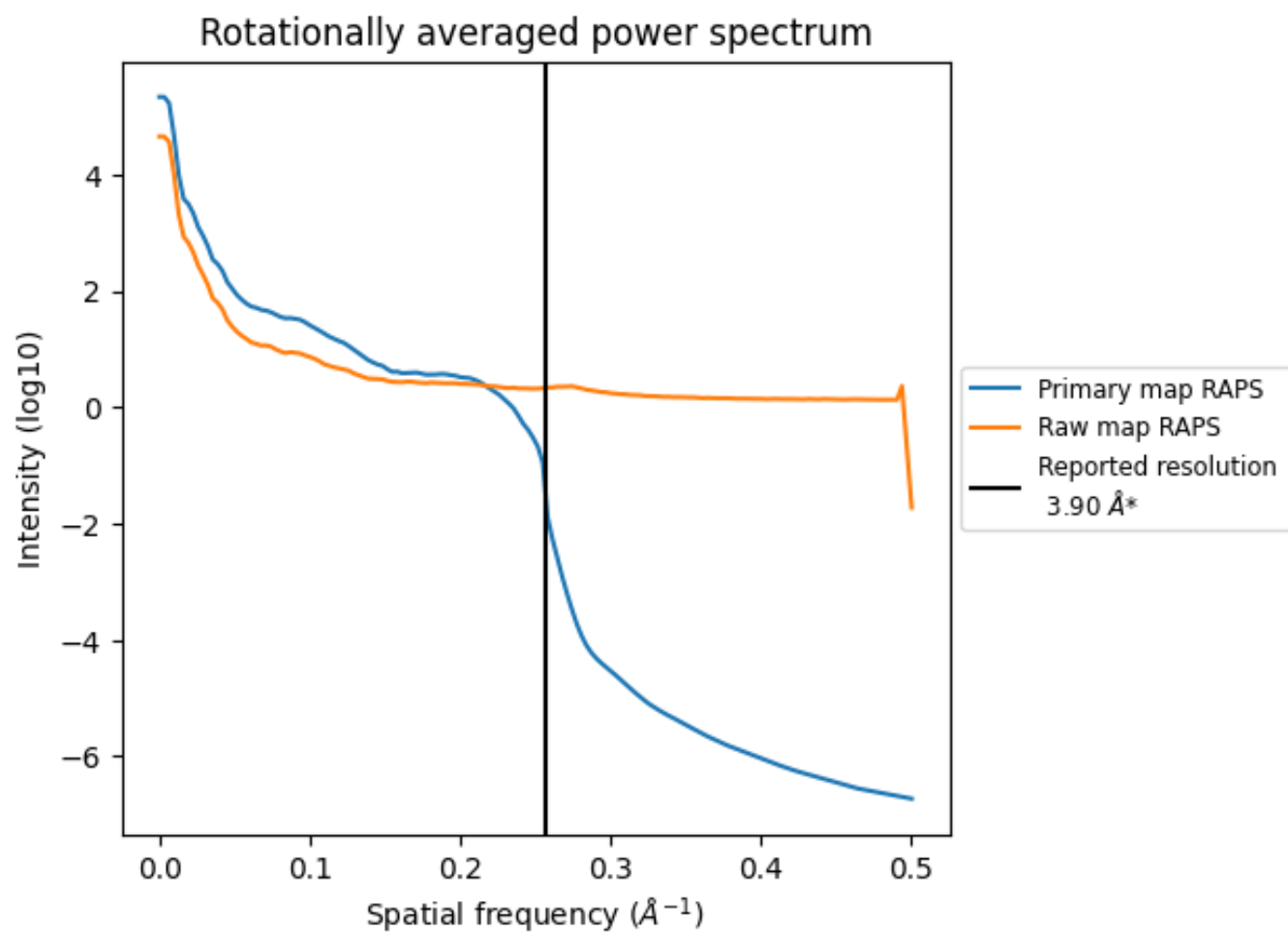
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 439 nm³; this corresponds to an approximate mass of 397 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 ⓘ

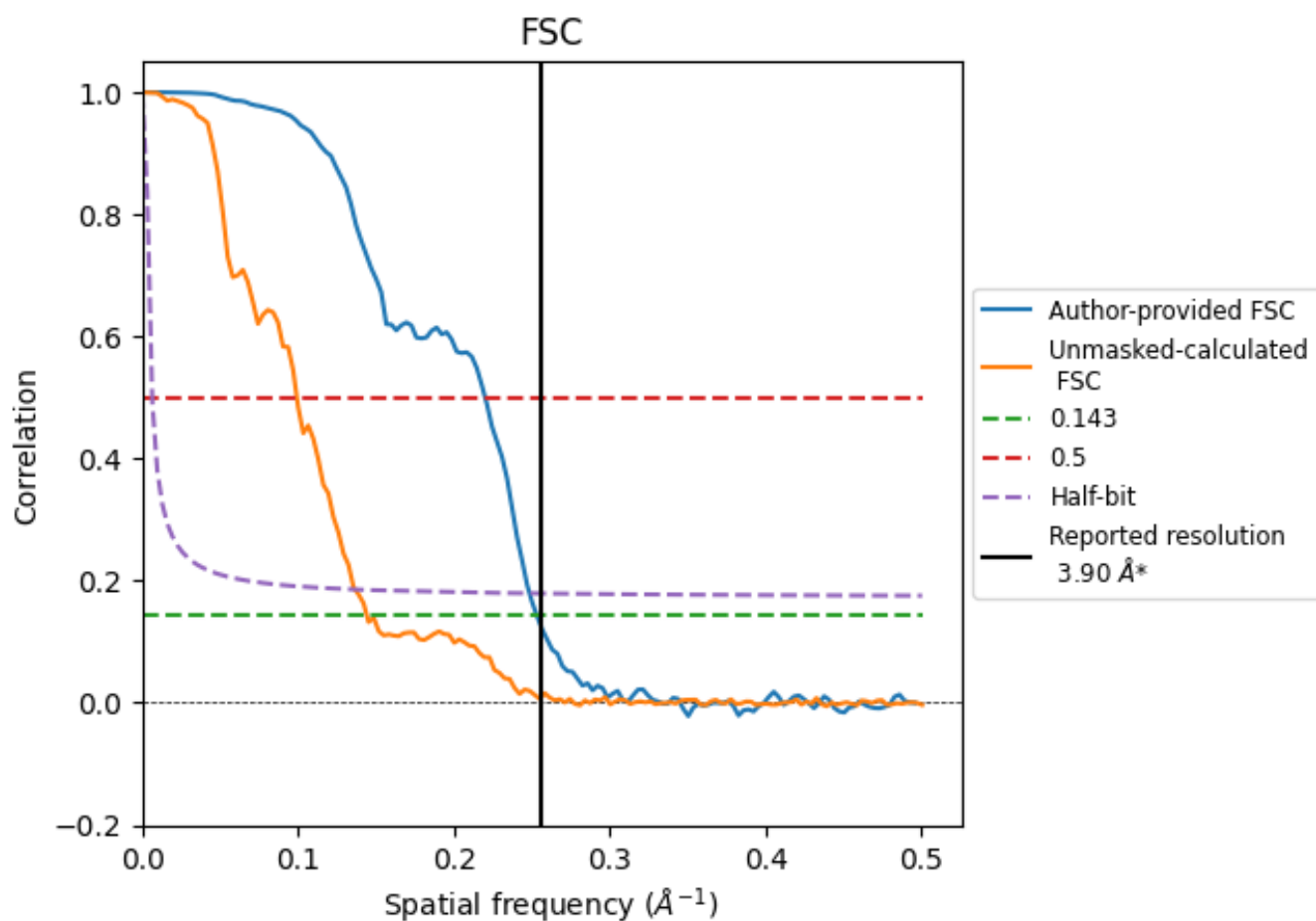


*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

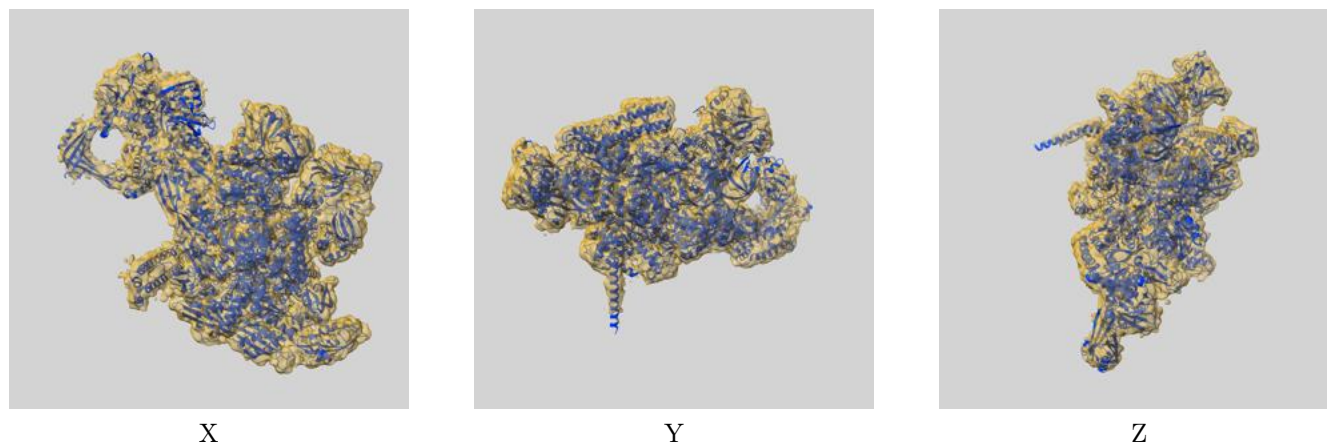
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.95	4.54	4.02
Unmasked-calculated*	6.93	10.07	7.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.93 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

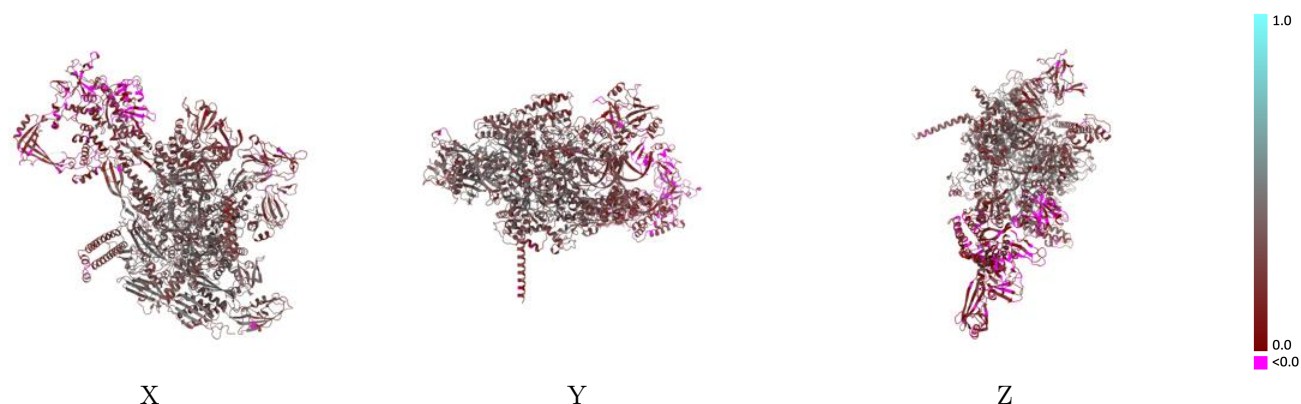
This section contains information regarding the fit between EMDB map EMD-51264 and PDB model 9GDH. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



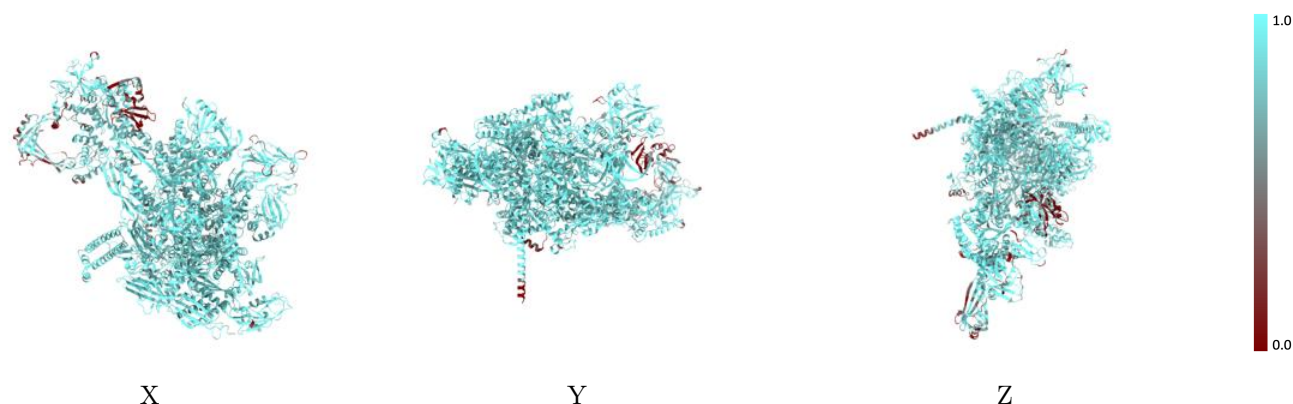
The images above show the 3D surface view of the map at the recommended contour level 0.174 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



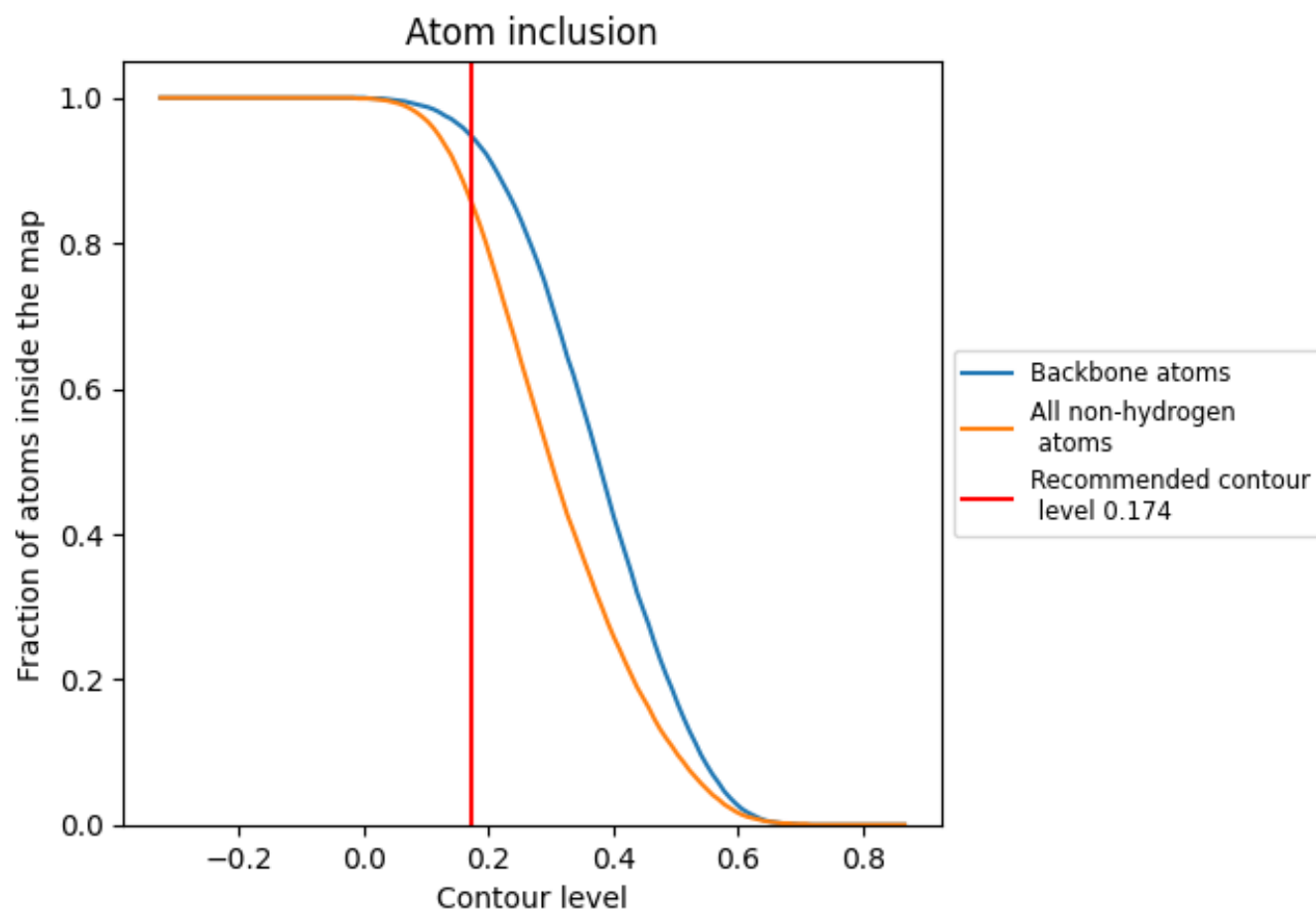
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.174).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.174) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8540	<div><div></div></div> 0.2960
A	<div><div></div></div> 0.9030	<div><div></div></div> 0.3760
B	<div><div></div></div> 0.9030	<div><div></div></div> 0.3470
C	<div><div></div></div> 0.8840	<div><div></div></div> 0.3460
D	<div><div></div></div> 0.8850	<div><div></div></div> 0.3420
E	<div><div></div></div> 0.7900	<div><div></div></div> 0.2880
F	<div><div></div></div> 0.7160	<div><div></div></div> 0.1090
N	<div><div></div></div> 0.9450	<div><div></div></div> 0.2390
R	<div><div></div></div> 0.9320	<div><div></div></div> 0.3300
T	<div><div></div></div> 0.9590	<div><div></div></div> 0.2990

1.0

0.0

<0.0