



Full wwPDB EM Validation Report ⓘ

Jul 15, 2026 – 03:34 AM JST

PDB ID : 9VW8 / pdb_00009vw8
EMDB ID : EMD-65391
Title : Cryo-EM structure of E.coli transcription initiation complex with Escherichia phage Mu late transcription activator C using the PI promoter DNA
Authors : Lin, W.
Deposited on : 2025-07-16
Resolution : 3.36 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

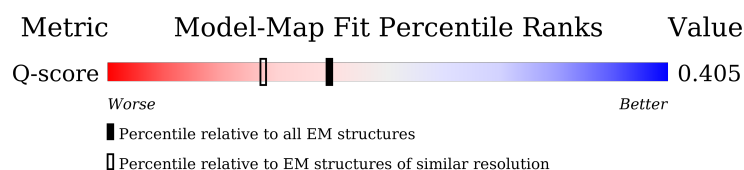
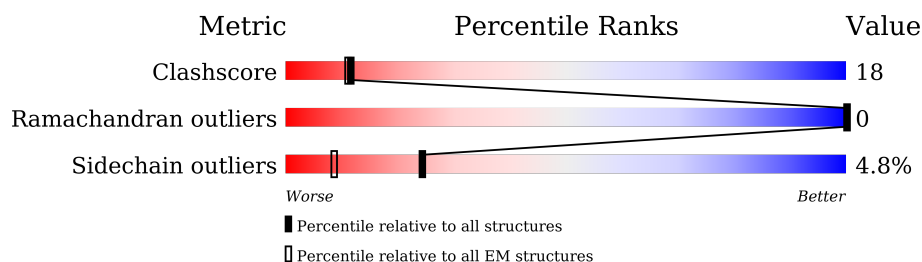
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 Å.

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



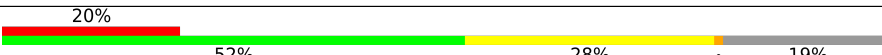
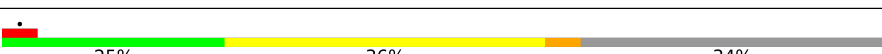
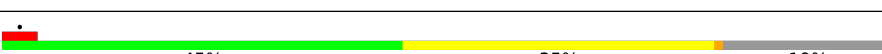
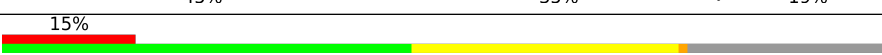
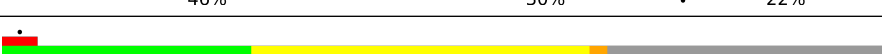
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14332 (2.86 - 3.86)

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

Mol	Chain	Length	Quality of chain
1	1	73	 21% 79%
2	2	73	 8% 33% 67%
3	A	329	 49% 20% 30%
3	B	329	 44% 24% 31%

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Mol	Chain	Length	Quality of chain
3	P	329	
4	C	1342	
5	D	1407	
6	E	91	
7	F	613	
8	I	160	
8	J	160	
8	K	160	
8	L	160	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 36500 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 DNA chain called DNA (73-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	73	Total	C	N	O	P	0	0
			1482	707	265	437	73		

- Molecule 2 is a DNA chain called DNA (73-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	73	Total	C	N	O	P	0	0
			1524	721	293	437	73		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		
3	B	228	Total	C	N	O	S	0	0
			1767	1100	312	349	6		
3	P	71	Total	C	N	O	S	0	0
			548	347	93	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1340	Total	C	N	O	S	0	0
			10560	6627	1840	2050	43		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	conflict	UNP P0A8V2

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	1333	Total	C	N	O	S	0	0
			10362	6509	1848	1955	50		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 7 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	496	Total	C	N	O	S	0	0
			3977	2484	707	764	22		

- Molecule 8 is a protein called Late transcription activator C.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	129	Total	C	N	O	S	0	0
			1074	671	208	190	5		
8	I	105	Total	C	N	O	S	0	0
			873	545	170	154	4		
8	K	124	Total	C	N	O	S	0	0
			1026	643	195	184	4		
8	L	108	Total	C	N	O	S	0	0
			894	558	173	159	4		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-19	MET	-	initiating methionine	UNP P06022
J	-18	GLY	-	expression tag	UNP P06022
J	-17	SER	-	expression tag	UNP P06022
J	-16	SER	-	expression tag	UNP P06022
J	-15	HIS	-	expression tag	UNP P06022
J	-14	HIS	-	expression tag	UNP P06022
J	-13	HIS	-	expression tag	UNP P06022
J	-12	HIS	-	expression tag	UNP P06022
J	-11	HIS	-	expression tag	UNP P06022
J	-10	HIS	-	expression tag	UNP P06022
J	-9	SER	-	expression tag	UNP P06022
J	-8	SER	-	expression tag	UNP P06022
J	-7	GLY	-	expression tag	UNP P06022

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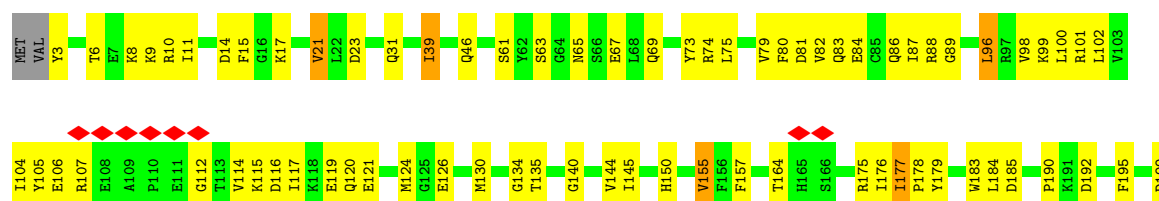
Chain	Residue	Modelled	Actual	Comment	Reference
J	-6	LEU	-	expression tag	UNP P06022
J	-5	VAL	-	expression tag	UNP P06022
J	-4	PRO	-	expression tag	UNP P06022
J	-3	ARG	-	expression tag	UNP P06022
J	-2	GLY	-	expression tag	UNP P06022
J	-1	SER	-	expression tag	UNP P06022
J	0	HIS	-	expression tag	UNP P06022
I	-19	MET	-	initiating methionine	UNP P06022
I	-18	GLY	-	expression tag	UNP P06022
I	-17	SER	-	expression tag	UNP P06022
I	-16	SER	-	expression tag	UNP P06022
I	-15	HIS	-	expression tag	UNP P06022
I	-14	HIS	-	expression tag	UNP P06022
I	-13	HIS	-	expression tag	UNP P06022
I	-12	HIS	-	expression tag	UNP P06022
I	-11	HIS	-	expression tag	UNP P06022
I	-10	HIS	-	expression tag	UNP P06022
I	-9	SER	-	expression tag	UNP P06022
I	-8	SER	-	expression tag	UNP P06022
I	-7	GLY	-	expression tag	UNP P06022
I	-6	LEU	-	expression tag	UNP P06022
I	-5	VAL	-	expression tag	UNP P06022
I	-4	PRO	-	expression tag	UNP P06022
I	-3	ARG	-	expression tag	UNP P06022
I	-2	GLY	-	expression tag	UNP P06022
I	-1	SER	-	expression tag	UNP P06022
I	0	HIS	-	expression tag	UNP P06022
K	-19	MET	-	initiating methionine	UNP P06022
K	-18	GLY	-	expression tag	UNP P06022
K	-17	SER	-	expression tag	UNP P06022
K	-16	SER	-	expression tag	UNP P06022
K	-15	HIS	-	expression tag	UNP P06022
K	-14	HIS	-	expression tag	UNP P06022
K	-13	HIS	-	expression tag	UNP P06022
K	-12	HIS	-	expression tag	UNP P06022
K	-11	HIS	-	expression tag	UNP P06022
K	-10	HIS	-	expression tag	UNP P06022
K	-9	SER	-	expression tag	UNP P06022
K	-8	SER	-	expression tag	UNP P06022
K	-7	GLY	-	expression tag	UNP P06022
K	-6	LEU	-	expression tag	UNP P06022
K	-5	VAL	-	expression tag	UNP P06022

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP P06022
K	-3	ARG	-	expression tag	UNP P06022
K	-2	GLY	-	expression tag	UNP P06022
K	-1	SER	-	expression tag	UNP P06022
K	0	HIS	-	expression tag	UNP P06022
L	-19	MET	-	initiating methionine	UNP P06022
L	-18	GLY	-	expression tag	UNP P06022
L	-17	SER	-	expression tag	UNP P06022
L	-16	SER	-	expression tag	UNP P06022
L	-15	HIS	-	expression tag	UNP P06022
L	-14	HIS	-	expression tag	UNP P06022
L	-13	HIS	-	expression tag	UNP P06022
L	-12	HIS	-	expression tag	UNP P06022
L	-11	HIS	-	expression tag	UNP P06022
L	-10	HIS	-	expression tag	UNP P06022
L	-9	SER	-	expression tag	UNP P06022
L	-8	SER	-	expression tag	UNP P06022
L	-7	GLY	-	expression tag	UNP P06022
L	-6	LEU	-	expression tag	UNP P06022
L	-5	VAL	-	expression tag	UNP P06022
L	-4	PRO	-	expression tag	UNP P06022
L	-3	ARG	-	expression tag	UNP P06022
L	-2	GLY	-	expression tag	UNP P06022
L	-1	SER	-	expression tag	UNP P06022
L	0	HIS	-	expression tag	UNP P06022

Chain B:

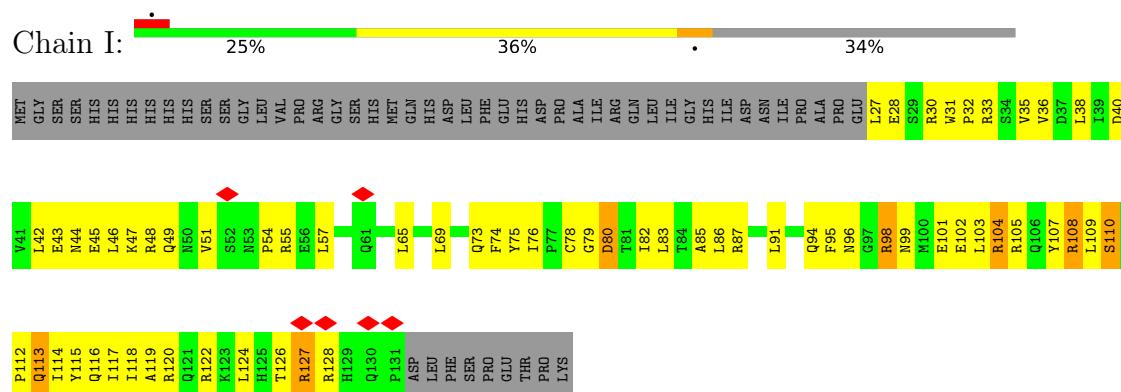




PHE
SER
PRO
GLU
THR
PRO
LYS

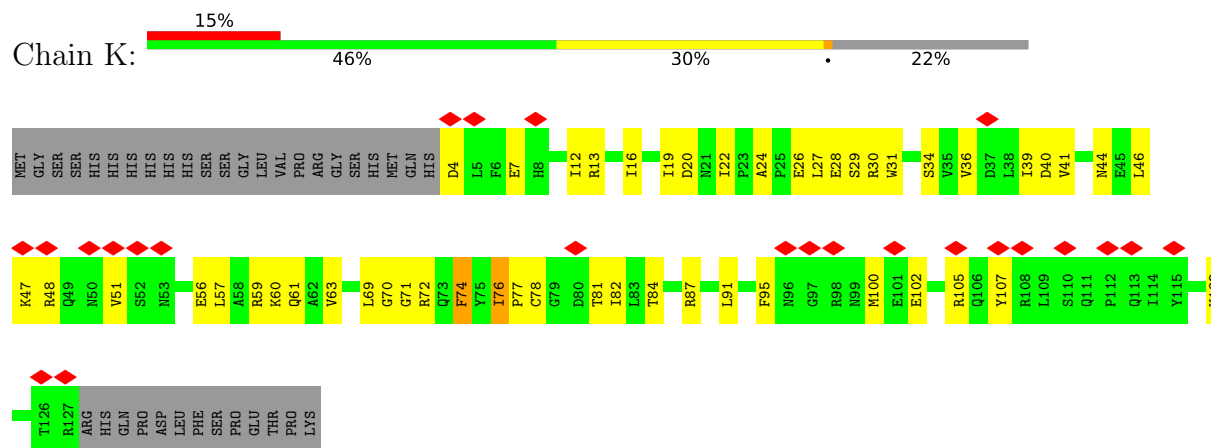
• Molecule 8: Late transcription activator C

Chain I:



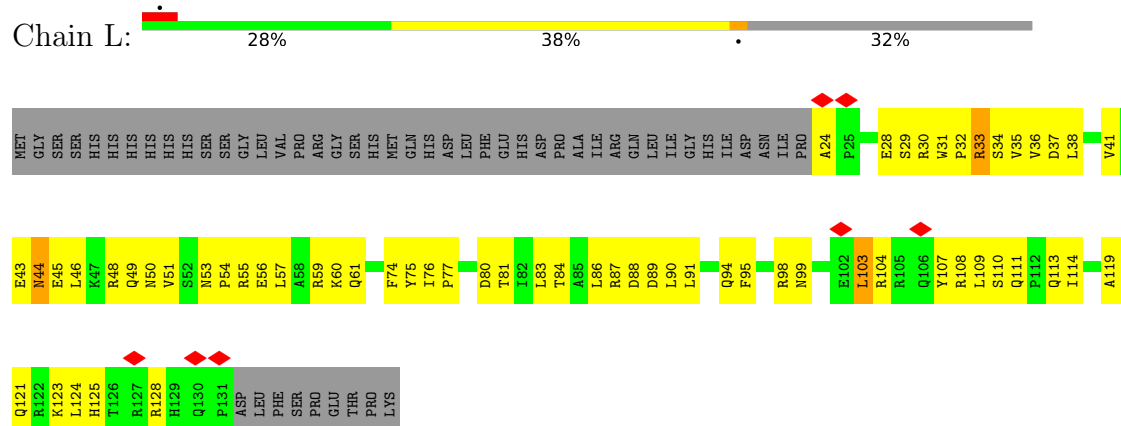
• Molecule 8: Late transcription activator C

Chain K:



• Molecule 8: Late transcription activator C

Chain L:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132241	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.489	Depositor
Minimum map value	-0.208	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	307.2, 307.2, 307.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.32	0/1659	0.46	0/2554
2	2	0.29	0/1715	0.45	0/2652
3	A	0.29	0/1808	0.38	0/2450
3	B	0.26	0/1789	0.39	0/2425
3	P	0.35	0/555	0.54	0/755
4	C	0.29	0/10728	0.39	0/14474
5	D	0.29	0/10513	0.39	0/14183
6	E	0.19	0/629	0.42	0/847
7	F	0.23	0/4028	0.38	0/5421
8	I	0.24	0/888	0.46	0/1197
8	J	0.27	0/1095	0.44	0/1478
8	K	0.21	0/1045	0.40	0/1412
8	L	0.27	0/910	0.50	0/1228
All	All	0.28	0/37362	0.41	0/51076

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1482	0	822	82	0
2	2	1524	0	822	59	0
3	A	1786	0	1813	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1767	0	1789	64	0
3	P	548	0	562	30	0
4	C	10560	0	10573	339	0
5	D	10362	0	10580	332	0
6	E	627	0	634	34	0
7	F	3977	0	4008	147	0
8	I	873	0	882	81	0
8	J	1074	0	1079	60	0
8	K	1026	0	1032	47	0
8	L	894	0	900	88	0
All	All	36500	0	35496	1272	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 18.

All (1272) 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)
8:L:31:TRP:CD1	8:L:33:ARG:HG3	1.70	1.27
8:L:31:TRP:HD1	8:L:33:ARG:CG	1.51	1.23
5:D:423:LEU:CD2	5:D:468:VAL:HG22	1.71	1.20
3:B:101:THR:HG22	3:B:143:ARG:HG2	1.28	1.16
5:D:807:LEU:HD11	5:D:1259:GLN:OE1	1.43	1.15
8:L:31:TRP:HD1	8:L:33:ARG:HG3	0.98	1.04
4:C:700:VAL:CG1	4:C:1117:LEU:HD23	1.88	1.03
4:C:700:VAL:HG13	4:C:1117:LEU:HD23	1.37	1.03
4:C:1209:GLN:HG2	4:C:1226:THR:HG22	1.42	1.00
4:C:1209:GLN:CG	4:C:1226:THR:HG22	1.94	0.98
5:D:803:VAL:HG12	5:D:1313:SER:OG	1.62	0.97
4:C:1209:GLN:HG2	4:C:1226:THR:CG2	1.94	0.96
8:L:31:TRP:CD1	8:L:33:ARG:CG	2.41	0.93
8:L:31:TRP:HD1	8:L:33:ARG:CB	1.79	0.93
5:D:423:LEU:HD22	5:D:468:VAL:HG22	1.51	0.93
4:C:1072:ASN:HD21	4:C:1230:MET:HE1	1.31	0.93
4:C:700:VAL:HG13	4:C:1117:LEU:CD2	1.99	0.92
5:D:807:LEU:CD1	5:D:1259:GLN:OE1	2.21	0.88
2:2:66:DC:H5"	3:P:294:ASN:HA	1.56	0.88
5:D:803:VAL:CG1	5:D:1313:SER:OG	2.22	0.86
8:L:31:TRP:CD1	8:L:33:ARG:H	1.93	0.85
5:D:201:LEU:HB2	5:D:221:ILE:HD11	1.59	0.84
6:E:19:LEU:CD1	6:E:54:ILE:HD12	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:31:TRP:CD1	8:L:33:ARG:CB	2.61	0.84
8:I:127:ARG:HE	8:I:128:ARG:HG3	1.43	0.84
6:E:19:LEU:HD11	6:E:54:ILE:CD1	2.07	0.83
4:C:80:PHE:CE2	4:C:88:ARG:HD2	2.15	0.82
8:J:101:GLU:HB3	8:J:104:ARG:HH21	1.43	0.82
8:L:31:TRP:CD1	8:L:33:ARG:N	2.49	0.81
2:2:3:DC:H2'	2:2:4:DA:C8	2.15	0.81
4:C:1024:GLU:HA	4:C:1027:LYS:HE2	1.63	0.80
7:F:111:LEU:CD1	7:F:116:GLU:HG3	2.11	0.80
5:D:789:LYS:HD2	5:D:931:THR:HG23	1.62	0.80
1:1:44:DT:H2'	7:F:455:HIS:CE1	2.19	0.78
4:C:80:PHE:HE2	4:C:88:ARG:NE	1.80	0.78
5:D:958:ILE:HG23	5:D:982:LEU:HD21	1.64	0.78
1:1:52:DA:H2'	7:F:429:THR:HG22	1.65	0.78
5:D:974:VAL:HG12	5:D:1002:VAL:HA	1.64	0.78
8:I:96:ASN:HD21	8:I:98:ARG:HH21	1.29	0.78
5:D:1266:ILE:HG22	5:D:1268:ASN:O	1.84	0.77
1:1:64:DC:H5'	4:C:542:ARG:HG3	1.64	0.77
4:C:375:PRO:HG3	7:F:87:VAL:HG11	1.64	0.77
4:C:232:ILE:H	4:C:331:LYS:HG3	1.50	0.76
5:D:876:SER:HA	5:D:990:ARG:HH21	1.50	0.76
2:2:35:DC:H2''	2:2:36:DG:C8	2.21	0.76
7:F:141:ILE:HD13	7:F:252:LEU:HD11	1.66	0.76
8:L:104:ARG:HH11	8:L:110:SER:HA	1.51	0.75
5:D:421:VAL:HG22	5:D:470:VAL:HG22	1.67	0.75
3:P:300:LEU:HD23	3:P:300:LEU:H	1.51	0.74
8:I:104:ARG:HH21	8:I:105:ARG:HA	1.51	0.74
4:C:80:PHE:HE2	4:C:88:ARG:CD	2.00	0.74
4:C:976:ARG:HG2	4:C:994:ARG:HE	1.52	0.74
5:D:601:ILE:HG23	5:D:604:MET:HE2	1.70	0.74
7:F:122:ARG:HE	7:F:371:LYS:HZ1	1.36	0.74
4:C:69:GLN:HB2	4:C:101:ARG:HB2	1.70	0.74
5:D:1173:ARG:HB2	5:D:1192:LYS:HE3	1.68	0.74
7:F:111:LEU:HD13	7:F:116:GLU:N	2.03	0.73
5:D:744:ARG:HH21	5:D:747:MET:HE1	1.53	0.73
7:F:91:ILE:HD12	7:F:93:ARG:HA	1.71	0.73
5:D:358:GLY:O	5:D:360:TYR:N	2.20	0.73
4:C:808:ASN:H	5:D:633:ALA:HB2	1.54	0.73
8:L:33:ARG:NH1	8:L:34:SER:OG	2.22	0.72
5:D:844:THR:OG1	5:D:858:VAL:HG21	1.88	0.72
4:C:302:ILE:HG22	4:C:309:LEU:HA	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:44:DT:H2'	7:F:455:HIS:HE1	1.52	0.72
7:F:152:GLU:OE2	7:F:218:ARG:NH2	2.23	0.72
5:D:285:LEU:HD21	7:F:413:MET:HE2	1.72	0.71
3:A:95:LYS:NZ	3:A:120:ASP:OD2	2.23	0.71
4:C:560:PRO:HB2	5:D:776:THR:HG21	1.73	0.71
8:J:46:LEU:HD22	8:J:54:PRO:HB3	1.70	0.71
5:D:812:ASP:O	5:D:897:HIS:ND1	2.20	0.71
5:D:965:SER:HB3	5:D:973:LEU:HD11	1.72	0.71
4:C:80:PHE:CE2	4:C:88:ARG:CD	2.73	0.71
6:E:19:LEU:HD11	6:E:54:ILE:HD11	1.71	0.71
3:B:91:ARG:HH21	3:B:210:THR:HA	1.55	0.71
4:C:135:THR:HG22	4:C:144:VAL:HG12	1.72	0.71
5:D:294:ASN:ND2	7:F:406:GLN:OE1	2.23	0.71
8:L:33:ARG:HD2	8:L:34:SER:H	1.54	0.71
4:C:611:GLU:OE2	4:C:637:ARG:NH1	2.23	0.71
3:P:283:GLN:HE22	3:P:317:ARG:HA	1.53	0.71
7:F:334:SER:HA	7:F:337:VAL:HG12	1.72	0.70
6:E:19:LEU:HD11	6:E:54:ILE:HD12	1.72	0.70
5:D:423:LEU:HD21	5:D:468:VAL:HG22	1.71	0.70
8:K:27:LEU:HG	8:K:31:TRP:HE1	1.57	0.70
4:C:275:ARG:NH1	4:C:278:GLU:OE1	2.25	0.69
5:D:1281:GLU:OE1	5:D:1281:GLU:N	2.23	0.69
8:I:43:GLU:HG3	8:I:54:PRO:HB2	1.73	0.69
8:J:4:ASP:HB3	8:L:44:ASN:HD22	1.58	0.69
8:K:4:ASP:HB3	8:K:7:GLU:HB2	1.74	0.69
4:C:803:ALA:HB2	4:C:1227:VAL:HG22	1.74	0.69
4:C:1072:ASN:ND2	4:C:1111:GLN:OE1	2.26	0.69
5:D:572:THR:HG21	5:D:589:TYR:CE2	2.28	0.69
5:D:1261:LEU:O	5:D:1304:ARG:NH2	2.25	0.69
4:C:452:ARG:NH2	4:C:458:GLU:OE2	2.24	0.69
7:F:597:LYS:O	7:F:603:ARG:NH1	2.26	0.69
5:D:1341:ARG:NH1	5:D:1343:GLU:OE2	2.26	0.69
2:2:28:DG:H2'	2:2:29:DG:C8	2.28	0.68
5:D:1069:ALA:HA	5:D:1072:LYS:HE2	1.75	0.68
2:2:44:DC:H2'	2:2:45:DT:C6	2.28	0.68
2:2:40:DA:H2''	2:2:41:DA:H5''	1.75	0.68
7:F:350:GLU:OE2	7:F:351:THR:CG2	2.41	0.68
8:I:78:CYS:SG	8:I:79:GLY:N	2.66	0.68
8:L:94:GLN:O	8:L:99:ASN:ND2	2.26	0.68
1:1:10:DA:H2''	1:1:11:DC:C5	2.29	0.68
6:E:3:ARG:NH1	6:E:44:ASP:OD1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:19:LEU:CD1	6:E:54:ILE:CD1	2.69	0.67
1:1:12:DT:H2'	1:1:13:DC:C6	2.29	0.67
4:C:74:ARG:NH1	4:C:121:GLU:OE2	2.24	0.67
5:D:968:ASN:ND2	5:D:970:SER:OG	2.28	0.67
7:F:460:ILE:HG22	7:F:497:VAL:HG13	1.76	0.67
4:C:562:GLU:O	4:C:563:THR:HG23	1.94	0.67
3:A:6:THR:HG23	3:A:8:PHE:H	1.60	0.67
3:B:101:THR:HG22	3:B:143:ARG:CG	2.17	0.67
5:D:367:GLY:HA3	5:D:448:GLN:HB2	1.77	0.67
5:D:799:ARG:NH1	5:D:1146:GLU:OE2	2.27	0.67
4:C:230:PHE:HB2	4:C:333:ILE:HB	1.76	0.67
4:C:1024:GLU:HG3	4:C:1025:PHE:CD2	2.30	0.67
7:F:111:LEU:HD11	7:F:116:GLU:CG	2.25	0.67
4:C:725:GLN:HB3	4:C:733:VAL:HG23	1.77	0.67
8:L:110:SER:N	8:L:113:GLN:OE1	2.27	0.67
5:D:846:GLU:HA	5:D:860:ARG:HG2	1.75	0.67
5:D:1219:ASP:OD1	5:D:1222:ARG:NH2	2.28	0.67
5:D:209:ASN:HA	5:D:214:ARG:HE	1.60	0.66
3:B:75:GLN:HG3	3:B:76:GLU:HG3	1.76	0.66
7:F:119:ILE:HG21	7:F:379:MET:HB2	1.78	0.66
4:C:700:VAL:HG11	4:C:1117:LEU:HD23	1.76	0.66
4:C:1205:PRO:HG2	4:C:1210:ILE:HG22	1.77	0.66
5:D:495:ASN:ND2	5:D:1247:LYS:O	2.28	0.66
2:2:52:DA:H2'	2:2:53:DT:O4'	1.95	0.66
4:C:1212:LEU:HD13	4:C:1225:VAL:HB	1.78	0.66
4:C:39:ILE:HD12	4:C:75:LEU:HD11	1.78	0.66
4:C:243:PRO:O	4:C:247:ARG:NH2	2.29	0.66
4:C:263:VAL:HA	4:C:267:ARG:HH21	1.61	0.66
5:D:1026:PRO:HB2	5:D:1028:ILE:HG23	1.78	0.66
5:D:285:LEU:HD21	7:F:413:MET:CE	2.26	0.66
5:D:926:PRO:HG2	5:D:1248:ILE:HD11	1.78	0.66
8:J:77:PRO:HG3	8:L:32:PRO:HG3	1.77	0.66
4:C:1321:GLU:OE2	5:D:99:ARG:NH1	2.29	0.66
4:C:1331:ARG:HB3	5:D:102:MET:HE1	1.77	0.65
8:J:46:LEU:HD11	8:J:57:LEU:HD23	1.78	0.65
8:L:32:PRO:O	8:L:35:VAL:HB	1.97	0.65
8:I:94:GLN:O	8:I:99:ASN:ND2	2.29	0.65
4:C:283:LYS:HG3	4:C:284:LEU:HG	1.79	0.65
5:D:309:ASN:N	5:D:326:SER:OG	2.30	0.65
1:1:23:DA:H2''	1:1:24:DA:C8	2.32	0.65
1:1:65:DA:H2''	1:1:66:DC:H5''	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:475:VAL:HG13	4:C:492:MET:HE1	1.79	0.65
2:2:55:DC:H2'	2:2:56:DT:H71	1.78	0.65
4:C:590:PRO:HG2	4:C:655:VAL:HG11	1.79	0.65
5:D:285:LEU:CD2	7:F:413:MET:CE	2.74	0.65
5:D:823:THR:HG22	5:D:879:ALA:HB2	1.79	0.65
5:D:702:GLN:HG3	5:D:703:THR:HG23	1.79	0.65
4:C:1024:GLU:O	4:C:1028:LYS:NZ	2.28	0.65
8:J:35:VAL:HG13	8:L:77:PRO:HG2	1.79	0.64
5:D:1327:GLU:OE1	5:D:1330:ARG:NE	2.30	0.64
7:F:142:THR:O	7:F:146:GLU:HG3	1.96	0.64
5:D:140:TYR:O	5:D:297:ARG:NH1	2.30	0.64
8:L:34:SER:O	8:L:38:LEU:N	2.30	0.64
4:C:120:GLN:OE1	4:C:490:GLN:N	2.28	0.64
6:E:60:ASN:O	6:E:64:LEU:N	2.29	0.64
3:A:92:VAL:O	3:A:148:ARG:NH2	2.31	0.64
4:C:870:ILE:HD13	4:C:884:VAL:HG13	1.80	0.64
5:D:1266:ILE:CG2	5:D:1268:ASN:O	2.46	0.64
4:C:528:ARG:NH2	4:C:576:SER:O	2.31	0.64
4:C:1209:GLN:HG3	4:C:1226:THR:HG22	1.78	0.64
6:E:41:GLU:HG3	6:E:43:ASN:H	1.63	0.64
1:1:30:DG:H2'	1:1:31:DA:C8	2.33	0.64
5:D:412:LEU:HD22	5:D:441:LEU:HD11	1.80	0.64
5:D:507:VAL:HG12	5:D:601:ILE:HD12	1.79	0.64
5:D:572:THR:HG21	5:D:589:TYR:HE2	1.61	0.64
4:C:632:ASP:OD1	4:C:647:ARG:NH2	2.29	0.63
4:C:1142:ARG:NH2	4:C:1166:ASP:OD1	2.31	0.63
4:C:1209:GLN:CG	4:C:1226:THR:CG2	2.65	0.63
3:P:280:ASP:OD1	3:P:280:ASP:N	2.29	0.63
5:D:709:ARG:NE	5:D:710:ASP:OD2	2.31	0.63
4:C:1328:LYS:HE3	5:D:102:MET:HE3	1.80	0.63
7:F:235:ILE:HD13	7:F:245:ALA:HB1	1.81	0.63
7:F:586:ARG:HD2	7:F:589:GLN:HE21	1.63	0.63
8:L:80:ASP:OD1	8:L:83:LEU:HD12	1.98	0.63
4:C:714:VAL:O	4:C:767:GLN:NE2	2.32	0.63
4:C:890:LYS:N	4:C:912:ASP:OD1	2.31	0.63
4:C:1246:ARG:NH2	4:C:1250:SER:O	2.32	0.63
5:D:970:SER:OG	5:D:972:LYS:NZ	2.32	0.63
7:F:350:GLU:OE2	7:F:351:THR:HG23	1.98	0.63
5:D:741:ALA:O	5:D:762:ASN:ND2	2.32	0.63
8:I:124:LEU:O	8:I:127:ARG:HG3	1.98	0.63
5:D:1346:GLY:O	5:D:1350:ASN:ND2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:31:TRP:CG	8:L:33:ARG:HG3	2.30	0.63
8:I:80:ASP:HB3	8:I:83:LEU:HB2	1.80	0.63
6:E:38:LEU:HD13	6:E:58:LEU:HD22	1.81	0.62
4:C:524:ILE:HD11	4:C:712:SER:HA	1.81	0.62
2:2:47:DG:H5"	8:L:30:ARG:HG2	1.80	0.62
1:1:58:DA:H2"	1:1:59:DG:H5"	1.80	0.62
3:B:77:ASP:OD1	3:B:78:ILE:N	2.33	0.62
4:C:1246:ARG:NH1	5:D:348:ASP:OD1	2.32	0.62
8:K:40:ASP:OD1	8:K:41:VAL:N	2.33	0.62
8:L:45:GLU:O	8:L:49:GLN:N	2.28	0.62
2:2:36:DG:H2"	2:2:37:DG:C8	2.34	0.62
4:C:297:VAL:HG12	4:C:315:MET:H	1.64	0.62
8:I:98:ARG:NH1	8:I:102:GLU:OE2	2.32	0.62
1:1:38:DC:H2"	1:1:39:DG:C8	2.35	0.62
4:C:411:ARG:NH2	4:C:427:ASP:OD2	2.32	0.62
5:D:885:VAL:HG13	5:D:894:VAL:HG11	1.82	0.62
1:1:21:DA:H2"	1:1:22:DT:H5"	1.82	0.62
5:D:259:ARG:NH2	7:F:503:GLU:O	2.31	0.62
7:F:109:GLU:N	7:F:109:GLU:OE1	2.32	0.62
8:K:102:GLU:OE2	8:K:105:ARG:NH2	2.32	0.62
7:F:111:LEU:HD11	7:F:116:GLU:HG2	1.82	0.62
8:J:72:ARG:CZ	8:I:105:ARG:HH22	2.12	0.62
8:I:28:GLU:HA	8:I:31:TRP:HB2	1.82	0.61
4:C:1020:GLU:HA	4:C:1023:HIS:CE1	2.36	0.61
4:C:393:ASP:OD1	4:C:393:ASP:N	2.32	0.61
4:C:942:ASP:OD1	4:C:943:LYS:N	2.33	0.61
5:D:54:ASP:N	5:D:58:CYS:SG	2.74	0.61
4:C:803:ALA:CB	4:C:1227:VAL:HG22	2.30	0.61
8:I:43:GLU:OE1	8:I:55:ARG:NH1	2.34	0.61
1:1:18:DA:H2"	1:1:19:DG:C8	2.36	0.61
6:E:61:ASN:HA	6:E:64:LEU:HB2	1.83	0.61
8:I:116:GLN:O	8:I:120:ARG:NH1	2.33	0.61
5:D:285:LEU:CD2	7:F:413:MET:HE1	2.31	0.61
8:J:19:ILE:HD11	8:J:60:LYS:HG2	1.82	0.61
4:C:276:GLN:NE2	4:C:280:ASP:OD2	2.33	0.60
3:A:97:GLU:OE2	3:A:145:LYS:NZ	2.30	0.60
5:D:325:LYS:HD2	7:F:508:GLU:HG2	1.82	0.60
5:D:1047:THR:HG23	5:D:1060:VAL:HB	1.83	0.60
7:F:227:GLN:HA	7:F:230:VAL:HG12	1.83	0.60
7:F:240:ARG:HE	7:F:357:GLN:HE22	1.49	0.60
7:F:347:ILE:O	7:F:351:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:12:ILE:O	8:J:16:ILE:HG12	2.01	0.60
5:D:1177:ILE:HB	5:D:1186:TYR:HB3	1.83	0.60
5:D:151:MET:HG3	5:D:153:ASN:H	1.64	0.60
7:F:88:GLU:HA	7:F:91:ILE:HG23	1.82	0.60
8:L:109:LEU:HD22	8:L:113:GLN:NE2	2.17	0.60
7:F:111:LEU:CD1	7:F:116:GLU:CG	2.79	0.60
1:1:64:DC:H2''	1:1:65:DA:C8	2.37	0.60
4:C:1271:GLY:O	4:C:1274:GLU:HG2	2.01	0.60
5:D:841:GLY:CA	5:D:901:ARG:HG2	2.32	0.60
5:D:841:GLY:HA2	5:D:901:ARG:HG2	1.82	0.60
4:C:607:SER:OG	4:C:608:ALA:N	2.35	0.60
4:C:1254:VAL:O	5:D:99:ARG:NH2	2.35	0.60
7:F:273:MET:HE2	7:F:273:MET:HA	1.82	0.60
4:C:562:GLU:O	4:C:563:THR:CG2	2.50	0.60
8:L:91:LEU:HD12	8:L:107:TYR:HD2	1.67	0.60
3:P:286:GLU:HG3	3:P:314:LEU:HD12	1.84	0.60
8:L:95:PHE:HA	8:L:99:ASN:HD21	1.66	0.60
2:2:59:DT:H2''	2:2:60:DT:H5'	1.84	0.59
5:D:1268:ASN:HD22	5:D:1301:THR:HG22	1.68	0.59
5:D:1321:SER:OG	5:D:1349:GLU:OE2	2.20	0.59
5:D:901:ARG:HH21	5:D:906:GLY:HA2	1.67	0.59
1:1:12:DT:OP1	3:P:268:ASN:ND2	2.34	0.59
4:C:96:LEU:HD22	4:C:98:VAL:HG23	1.84	0.59
5:D:421:VAL:CG1	5:D:468:VAL:HG13	2.31	0.59
8:K:4:ASP:OD2	8:K:13:ARG:NH2	2.32	0.59
5:D:423:LEU:HD23	5:D:468:VAL:HG22	1.76	0.59
5:D:572:THR:HG22	5:D:593:ASN:OD1	2.03	0.59
4:C:1243:MET:HE1	5:D:371:LYS:HB3	1.85	0.59
5:D:807:LEU:CG	5:D:1259:GLN:OE1	2.51	0.59
8:J:101:GLU:OE1	8:J:104:ARG:NE	2.36	0.59
5:D:966:VAL:HG13	5:D:974:VAL:HG23	1.84	0.59
8:L:56:GLU:OE1	8:L:56:GLU:N	2.25	0.59
8:L:80:ASP:CG	8:L:83:LEU:HD12	2.28	0.59
5:D:1271:SER:HB3	5:D:1290:ARG:HH12	1.68	0.59
6:E:67:ARG:O	6:E:70:GLN:NE2	2.35	0.58
8:L:31:TRP:CD1	8:L:33:ARG:HB3	2.38	0.58
1:1:29:DA:H2''	1:1:30:DG:C8	2.38	0.58
2:2:9:DT:H4'	5:D:1326:GLN:HE21	1.68	0.58
3:B:214:GLU:OE2	3:B:218:ARG:NE	2.33	0.58
7:F:336:GLU:HA	7:F:339:ARG:HG2	1.85	0.58
1:1:55:DG:H5'	1:1:55:DG:H8	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:555:GLU:N	7:F:555:GLU:OE1	2.37	0.58
1:1:29:DA:H2''	1:1:30:DG:H8	1.66	0.58
5:D:806:ASP:OD1	5:D:1346:GLY:CA	2.51	0.58
8:L:33:ARG:HD2	8:L:34:SER:N	2.19	0.58
4:C:894:GLN:HA	5:D:77:ARG:HH12	1.68	0.58
8:I:85:ALA:HB3	8:K:31:TRP:HH2	1.69	0.58
4:C:519:ASN:ND2	4:C:689:ALA:O	2.35	0.58
4:C:1250:SER:HB3	7:F:524:GLU:HG3	1.86	0.58
5:D:1021:ASP:OD2	5:D:1024:THR:N	2.27	0.58
7:F:315:TRP:H	7:F:315:TRP:CD1	2.22	0.58
7:F:598:LEU:O	7:F:604:SER:OG	2.22	0.58
4:C:1313:HIS:HB2	5:D:474:LEU:HD13	1.85	0.58
5:D:138:VAL:HG21	5:D:145:VAL:CG2	2.33	0.58
5:D:850:LYS:NZ	5:D:857:LEU:HB3	2.19	0.58
4:C:629:PHE:CD2	4:C:634:VAL:HG21	2.39	0.58
5:D:848:VAL:HG13	5:D:857:LEU:HD21	1.86	0.57
8:J:6:PHE:HD2	8:L:48:ARG:HD3	1.69	0.57
8:L:120:ARG:HA	8:L:123:LYS:HD2	1.85	0.57
1:1:18:DA:H2''	1:1:19:DG:H8	1.67	0.57
1:1:71:DG:H2''	1:1:72:DC:H5''	1.85	0.57
4:C:229:ILE:HB	4:C:240:GLU:HB3	1.86	0.57
5:D:1230:THR:HG22	5:D:1257:VAL:HG11	1.86	0.57
3:A:104:LYS:HG2	3:A:110:VAL:HG22	1.85	0.57
7:F:420:GLU:OE1	7:F:420:GLU:N	2.38	0.57
8:K:19:ILE:CD1	8:K:63:VAL:HG11	2.34	0.57
4:C:1219:GLU:N	4:C:1219:GLU:OE1	2.37	0.57
5:D:93:THR:OG1	5:D:94:GLN:N	2.36	0.57
5:D:901:ARG:HA	5:D:908:ILE:HA	1.85	0.57
4:C:838:CYS:HB2	4:C:918:LEU:HD12	1.84	0.57
5:D:495:ASN:ND2	5:D:1247:LYS:HG3	2.19	0.57
8:I:127:ARG:HH21	8:I:128:ARG:HE	1.52	0.57
1:1:15:DA:H2''	1:1:16:DA:C8	2.39	0.57
5:D:138:VAL:HG21	5:D:145:VAL:HG21	1.86	0.57
3:B:84:ASN:ND2	5:D:551:ARG:HH12	2.03	0.57
7:F:456:MET:HE1	7:F:497:VAL:HG22	1.86	0.57
8:K:28:GLU:HA	8:K:31:TRP:CD1	2.39	0.57
5:D:1271:SER:HB3	5:D:1290:ARG:NH1	2.20	0.57
7:F:111:LEU:HD13	7:F:116:GLU:H	1.68	0.57
7:F:137:TYR:CZ	7:F:139:GLU:HB2	2.40	0.57
7:F:238:LYS:HB3	7:F:242:HIS:CG	2.40	0.57
2:2:37:DG:H2''	2:2:38:DG:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:120:ASP:OD1	3:A:120:ASP:N	2.38	0.56
4:C:1209:GLN:HG2	4:C:1226:THR:HG23	1.82	0.56
8:I:127:ARG:HH22	8:K:30:ARG:HH21	1.54	0.56
1:1:32:DT:C6	1:1:33:DT:H72	2.40	0.56
3:B:51:MET:HB3	3:B:179:PRO:HD2	1.86	0.56
5:D:1058:SER:OG	5:D:1059:LEU:N	2.38	0.56
5:D:850:LYS:HB2	5:D:855:ASP:HB2	1.88	0.56
4:C:463:GLN:HG3	4:C:505:PHE:HB2	1.88	0.56
4:C:714:VAL:HB	4:C:787:PRO:HD2	1.88	0.56
8:J:12:ILE:HD12	8:L:83:LEU:HD13	1.88	0.56
8:K:46:LEU:HD21	8:K:61:GLN:HE22	1.69	0.56
8:I:96:ASN:OD1	8:I:99:ASN:N	2.39	0.56
8:I:102:GLU:OE1	8:I:102:GLU:N	2.29	0.56
8:I:104:ARG:HE	8:I:105:ARG:HD2	1.71	0.56
8:L:46:LEU:O	8:L:50:ASN:N	2.38	0.56
3:P:307:LEU:HA	3:P:310:ARG:HG2	1.87	0.56
4:C:73:TYR:HB2	4:C:98:VAL:HG22	1.87	0.56
4:C:821:ARG:HE	4:C:1082:ILE:HD12	1.71	0.56
5:D:1272:SER:OG	5:D:1286:LYS:NZ	2.22	0.56
3:P:305:ASP:OD1	3:P:306:VAL:N	2.36	0.56
3:B:47:LEU:CD1	3:B:183:ILE:HD13	2.36	0.56
4:C:67:GLU:OE2	4:C:69:GLN:NE2	2.39	0.56
4:C:593:LYS:HB2	4:C:602:GLU:CD	2.30	0.56
5:D:53:ARG:HH11	5:D:60:ARG:HH11	1.54	0.56
5:D:137:ARG:HD2	7:F:93:ARG:HH22	1.71	0.56
8:I:48:ARG:HE	8:K:13:ARG:HG3	1.71	0.56
3:B:9:LEU:HD23	3:B:9:LEU:H	1.71	0.55
3:B:61:ILE:HG12	3:B:142:MET:HB2	1.88	0.55
2:2:20:DT:H1'	2:2:21:DA:H5'	1.87	0.55
4:C:164:THR:HG21	4:C:190:PRO:HG3	1.87	0.55
4:C:1016:GLU:O	4:C:1020:GLU:HG3	2.06	0.55
4:C:629:PHE:HD2	4:C:634:VAL:HG21	1.69	0.55
5:D:1273:ASP:OD1	5:D:1274:PHE:N	2.34	0.55
5:D:495:ASN:OD1	5:D:495:ASN:N	2.40	0.55
7:F:148:TYR:HA	7:F:151:VAL:HG22	1.87	0.55
5:D:415:VAL:O	6:E:45:LYS:NZ	2.40	0.55
5:D:1368:ASP:HA	5:D:1371:ARG:HH11	1.69	0.55
8:J:46:LEU:HD21	8:J:51:VAL:HB	1.87	0.55
4:C:271:ALA:HA	4:C:274:ILE:HD12	1.88	0.55
4:C:1294:LYS:O	5:D:348:ASP:HB2	2.07	0.55
5:D:822:MET:O	5:D:879:ALA:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:866:GLU:OE1	5:D:866:GLU:N	2.40	0.55
5:D:601:ILE:O	5:D:604:MET:HG2	2.07	0.55
5:D:863:LEU:HD21	5:D:901:ARG:HB3	1.89	0.55
6:E:70:GLN:O	6:E:73:GLN:HG3	2.06	0.55
8:I:76:ILE:HG23	8:K:74:PHE:HZ	1.72	0.55
8:L:43:GLU:HG3	8:L:54:PRO:HB2	1.87	0.55
3:A:76:GLU:OE2	3:A:131:CYS:HA	2.07	0.55
8:K:27:LEU:HG	8:K:31:TRP:NE1	2.22	0.55
4:C:207:THR:HG21	4:C:351:LEU:HD23	1.88	0.55
4:C:533:LEU:HD21	4:C:571:LEU:HD13	1.89	0.55
5:D:285:LEU:HG	7:F:413:MET:HE1	1.89	0.55
5:D:930:LEU:HA	5:D:1244:GLN:HG2	1.88	0.55
7:F:233:ASP:OD1	7:F:233:ASP:N	2.39	0.55
3:B:54:CYS:SG	3:B:148:ARG:NE	2.64	0.55
8:L:31:TRP:CD1	8:L:33:ARG:CA	2.89	0.55
2:2:61:DG:H2''	2:2:62:DA:H5''	1.89	0.54
4:C:504:GLU:O	4:C:508:SER:HB3	2.07	0.54
3:P:290:LEU:HD21	3:P:300:LEU:HB3	1.90	0.54
8:I:96:ASN:HD21	8:I:98:ARG:NH2	2.03	0.54
1:1:19:DG:H1	2:2:55:DC:H42	1.54	0.54
3:A:33:ARG:HH21	3:A:197:ASP:HB2	1.72	0.54
4:C:1128:ILE:HD13	4:C:1176:LEU:HD13	1.89	0.54
5:D:806:ASP:OD1	5:D:1346:GLY:HA2	2.08	0.54
5:D:844:THR:HA	5:D:882:VAL:HA	1.89	0.54
5:D:1030:GLU:OE1	5:D:1099:TYR:OH	2.21	0.54
8:J:39:ILE:CG1	8:J:62:ALA:CB	2.85	0.54
8:I:113:GLN:H	8:I:113:GLN:CD	2.14	0.54
8:I:116:GLN:O	8:I:120:ARG:HG2	2.06	0.54
2:2:27:DG:H2'	2:2:28:DG:C8	2.41	0.54
3:A:131:CYS:SG	3:A:132:HIS:N	2.80	0.54
3:B:110:VAL:HG12	3:B:131:CYS:H	1.72	0.54
4:C:1280:ALA:HB1	5:D:918:ILE:HG22	1.89	0.54
7:F:605:GLU:N	7:F:605:GLU:OE1	2.36	0.54
8:J:68:PHE:HD2	8:L:41:VAL:HG22	1.72	0.54
8:K:36:VAL:HA	8:K:39:ILE:HG12	1.89	0.54
1:1:25:DC:P	7:F:586:ARG:HH22	2.31	0.54
1:1:60:DC:H3'	1:1:61:DT:H2'	1.88	0.54
4:C:99:LYS:HA	4:C:121:GLU:HA	1.90	0.54
4:C:884:VAL:HG21	4:C:1050:VAL:HG11	1.90	0.54
4:C:994:ARG:NH1	4:C:997:TRP:HB2	2.23	0.54
4:C:1245:ALA:HB2	5:D:372:MET:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:26:VAL:HG11	3:A:217:ILE:HD12	1.90	0.54
3:A:80:GLU:O	3:A:84:ASN:ND2	2.40	0.54
3:P:300:LEU:C	3:P:304:LYS:HZ1	2.16	0.54
3:A:186:ASN:N	3:A:186:ASN:OD1	2.39	0.54
4:C:21:VAL:HG11	4:C:592:ARG:HD2	1.89	0.54
5:D:517:CYS:HB2	5:D:520:ALA:HB2	1.89	0.54
5:D:697:MET:SD	5:D:741:ALA:HB3	2.48	0.54
8:L:34:SER:HA	8:L:37:ASP:HB2	1.90	0.54
4:C:892:GLU:OE1	4:C:893:THR:N	2.40	0.54
4:C:1191:LYS:N	4:C:1194:GLU:OE1	2.40	0.54
2:2:9:DT:H2'	2:2:10:DG:C8	2.43	0.54
4:C:666:SER:HA	4:C:1186:VAL:HG11	1.89	0.54
4:C:804:PHE:O	5:D:638:SER:OG	2.22	0.54
4:C:1341:ASP:N	4:C:1341:ASP:OD1	2.40	0.54
5:D:145:VAL:HG11	5:D:188:LEU:HD11	1.89	0.54
5:D:847:ASP:OD1	5:D:860:ARG:N	2.41	0.54
4:C:150:HIS:CE1	4:C:454:ARG:HH21	2.26	0.53
4:C:575:LEU:HD23	4:C:575:LEU:H	1.73	0.53
4:C:672:GLU:OE1	4:C:672:GLU:N	2.33	0.53
4:C:878:THR:OG1	4:C:879:GLY:N	2.41	0.53
7:F:117:ILE:O	7:F:121:LYS:HG2	2.08	0.53
4:C:17:LYS:N	4:C:1188:ASP:OD2	2.41	0.53
5:D:128:LEU:HD23	5:D:192:MET:HE3	1.90	0.53
5:D:1208:ASP:OD1	5:D:1209:VAL:N	2.41	0.53
8:J:114:ILE:HA	8:J:117:ILE:HD12	1.90	0.53
5:D:474:LEU:HB2	6:E:28:ARG:HH12	1.73	0.53
8:K:56:GLU:O	8:K:60:LYS:HG2	2.07	0.53
5:D:850:LYS:HZ2	5:D:857:LEU:HB3	1.73	0.53
1:1:58:DA:OP1	1:1:59:DG:N2	2.41	0.53
4:C:562:GLU:C	4:C:563:THR:HG23	2.32	0.53
3:P:275:ILE:HG21	3:P:281:LEU:HD13	1.91	0.53
3:A:184:ALA:HB2	4:C:1091:GLY:HA3	1.91	0.53
3:A:185:TYR:HB3	3:A:203:ILE:HG12	1.90	0.53
5:D:25:ALA:HA	5:D:29:MET:SD	2.49	0.53
1:1:57:DG:N2	4:C:374:GLU:OE1	2.31	0.53
2:2:43:DT:H2''	2:2:44:DC:O5'	2.07	0.53
2:2:59:DT:H2'	2:2:60:DT:H71	1.90	0.53
4:C:88:ARG:NH1	4:C:1040:ASP:OD1	2.41	0.53
5:D:202:ARG:HG3	5:D:203:GLU:N	2.23	0.53
6:E:29:GLN:HG3	6:E:35:LYS:HD2	1.90	0.53
7:F:364:ARG:O	7:F:367:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:453:PRO:HB2	7:F:455:HIS:NE2	2.24	0.53
2:2:34:DG:H4'	2:2:35:DC:OP1	2.09	0.53
2:2:43:DT:H4'	2:2:44:DC:OP1	2.09	0.53
5:D:355:ILE:HD13	5:D:447:ILE:HB	1.90	0.53
7:F:586:ARG:O	7:F:589:GLN:HG3	2.09	0.53
2:2:35:DC:H2''	2:2:36:DG:H8	1.73	0.53
4:C:258:ASN:OD1	4:C:259:GLY:N	2.42	0.53
5:D:1034:PHE:HD1	5:D:1036:ARG:HH22	1.56	0.53
7:F:291:CYS:O	7:F:295:CYS:N	2.42	0.53
3:P:285:THR:HG22	3:P:315:GLY:HA2	1.91	0.53
4:C:124:MET:HB2	4:C:498:ILE:HD13	1.92	0.52
4:C:777:VAL:HG21	4:C:783:LEU:HD21	1.90	0.52
4:C:1243:MET:HE3	5:D:372:MET:HG3	1.91	0.52
7:F:111:LEU:C	7:F:111:LEU:HD12	2.33	0.52
3:P:281:LEU:HD13	3:P:284:ARG:HH22	1.74	0.52
3:B:124:VAL:HG21	3:B:209:GLY:HA3	1.92	0.52
4:C:540:ARG:HH21	4:C:568:ASN:HD22	1.55	0.52
5:D:700:ASN:O	5:D:704:GLU:HB3	2.09	0.52
7:F:548:LEU:HD12	7:F:556:ALA:HA	1.91	0.52
1:1:55:DG:H5'	1:1:55:DG:C8	2.44	0.52
5:D:905:ARG:HH12	6:E:16:ARG:HD2	1.75	0.52
8:I:102:GLU:HA	8:I:105:ARG:HG2	1.90	0.52
2:2:15:DG:H2''	2:2:16:DA:N7	2.25	0.52
3:A:190:ALA:HB2	3:A:200:LYS:HB2	1.91	0.52
4:C:104:ILE:HD12	4:C:116:ASP:HB3	1.91	0.52
4:C:895:LEU:N	5:D:77:ARG:HH22	2.08	0.52
5:D:1109:LEU:HD13	5:D:1115:ILE:HG23	1.91	0.52
7:F:110:LEU:HD11	7:F:385:ARG:HD2	1.90	0.52
7:F:399:LEU:HB2	7:F:447:ALA:HB2	1.90	0.52
4:C:179:TYR:OH	4:C:462:ASN:ND2	2.28	0.52
4:C:658:GLN:HG3	4:C:1186:VAL:HG22	1.92	0.52
5:D:1144:LEU:HD21	5:D:1236:GLU:HG2	1.90	0.52
7:F:400:GLN:HG3	7:F:401:PHE:H	1.75	0.52
8:J:11:ALA:O	8:J:14:GLN:NE2	2.43	0.52
5:D:1215:GLU:OE2	5:D:1224:ARG:NH1	2.41	0.52
4:C:10:ARG:CZ	4:C:697:LYS:HD3	2.38	0.52
4:C:275:ARG:HA	4:C:275:ARG:HH11	1.75	0.52
8:K:78:CYS:HA	8:K:82:ILE:HD11	1.91	0.52
4:C:251:ALA:HB2	4:C:269:ILE:HD11	1.92	0.51
5:D:197:GLU:N	5:D:197:GLU:OE1	2.43	0.51
6:E:44:ASP:HB2	6:E:49:ILE:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:110:SER:O	8:I:114:ILE:HG13	2.10	0.51
2:2:18:DG:H1'	2:2:19:DG:C8	2.45	0.51
4:C:82:VAL:O	4:C:86:GLN:HG3	2.10	0.51
5:D:806:ASP:OD1	5:D:1346:GLY:HA3	2.10	0.51
1:1:21:DA:H2'	1:1:22:DT:H71	1.91	0.51
3:B:182:ARG:NH2	3:B:204:GLU:OE2	2.42	0.51
5:D:153:ASN:HD22	5:D:172:PHE:HZ	1.57	0.51
5:D:255:LEU:HD21	7:F:523:ILE:HD11	1.92	0.51
6:E:2:ALA:HA	6:E:55:GLU:HG3	1.93	0.51
6:E:45:LYS:O	6:E:49:ILE:HG12	2.10	0.51
8:J:117:ILE:O	8:J:121:GLN:HG2	2.09	0.51
8:I:74:PHE:HB3	8:K:74:PHE:HE1	1.75	0.51
3:B:84:ASN:HD21	5:D:551:ARG:HH12	1.56	0.51
4:C:528:ARG:NH2	4:C:575:LEU:O	2.42	0.51
4:C:1253:LEU:HA	7:F:525:ASP:HB2	1.92	0.51
5:D:77:ARG:HB2	5:D:79:LYS:HE3	1.92	0.51
5:D:673:VAL:HG23	5:D:677:GLU:HB2	1.92	0.51
8:I:76:ILE:HG13	8:K:70:GLY:HA2	1.93	0.51
8:L:33:ARG:HH11	8:L:34:SER:HG	1.57	0.51
1:1:33:DT:H2'	1:1:34:DT:C7	2.41	0.51
4:C:155:VAL:HA	4:C:175:ARG:O	2.10	0.51
4:C:1004:ASP:N	4:C:1004:ASP:OD1	2.43	0.51
5:D:348:ASP:HB3	5:D:349:TYR:CD1	2.46	0.51
7:F:444:ALA:HB1	7:F:454:VAL:HG12	1.93	0.51
8:J:39:ILE:HG12	8:J:62:ALA:HB2	1.93	0.51
3:P:294:ASN:O	3:P:299:SER:HB3	2.10	0.51
1:1:14:DA:C6	1:1:15:DA:N6	2.78	0.51
1:1:22:DT:H2''	1:1:23:DA:C8	2.46	0.51
4:C:483:ASP:OD1	4:C:485:ASP:N	2.42	0.51
5:D:1173:ARG:HH21	5:D:1192:LYS:HA	1.75	0.51
7:F:350:GLU:OE2	7:F:351:THR:HG22	2.11	0.51
4:C:1107:MET:HE2	5:D:739:GLN:HE21	1.76	0.51
5:D:1034:PHE:HA	5:D:1114:GLN:HB3	1.92	0.51
8:K:19:ILE:HD13	8:K:63:VAL:HG11	1.93	0.51
4:C:471:VAL:HG21	4:C:498:ILE:HD11	1.92	0.51
5:D:1079:LYS:HE2	5:D:1081:VAL:HG12	1.93	0.51
8:J:74:PHE:HD2	8:L:74:PHE:CZ	2.29	0.51
3:B:102:LEU:HB3	3:B:142:MET:SD	2.50	0.51
3:B:109:PRO:HB3	3:B:132:HIS:CD2	2.46	0.51
3:B:167:PRO:HD2	3:B:170:ARG:HE	1.76	0.51
4:C:23:ASP:N	4:C:23:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:256:GLU:N	4:C:256:GLU:OE1	2.44	0.51
4:C:1281:TYR:OH	5:D:489:ASN:ND2	2.44	0.51
3:P:285:THR:OG1	3:P:288:GLU:OE1	2.24	0.51
1:1:9:DT:H4'	1:1:10:DA:OP2	2.11	0.50
1:1:27:DC:H41	7:F:585:GLU:CD	2.19	0.50
1:1:57:DG:H5''	1:1:58:DA:N3	2.25	0.50
4:C:101:ARG:HD2	4:C:117:ILE:HD11	1.93	0.50
6:E:13:ILE:HG13	6:E:19:LEU:HD13	1.94	0.50
8:J:39:ILE:HG12	8:J:62:ALA:CB	2.41	0.50
8:I:104:ARG:O	8:I:108:ARG:N	2.37	0.50
4:C:11:ILE:O	4:C:1149:TYR:OH	2.26	0.50
4:C:106:GLU:HB2	4:C:115:LYS:HZ3	1.75	0.50
4:C:444:ASP:O	4:C:450:ASN:ND2	2.44	0.50
5:D:151:MET:HG3	5:D:153:ASN:N	2.26	0.50
8:J:127:ARG:HD3	8:J:128:ARG:HH21	1.75	0.50
1:1:22:DT:H3'	8:L:75:TYR:CE2	2.47	0.50
3:A:182:ARG:NH2	3:A:204:GLU:OE2	2.43	0.50
3:B:7:GLU:N	3:B:7:GLU:OE1	2.44	0.50
4:C:135:THR:HG21	4:C:515:MET:SD	2.51	0.50
4:C:631:GLU:N	4:C:631:GLU:OE1	2.43	0.50
6:E:67:ARG:NH1	6:E:68:GLU:HB3	2.27	0.50
7:F:456:MET:O	7:F:460:ILE:HG23	2.12	0.50
8:J:72:ARG:NE	8:I:105:ARG:HH22	2.08	0.50
2:2:65:DA:H2''	2:2:66:DC:H5'	1.93	0.50
8:J:39:ILE:CG1	8:J:62:ALA:HB2	2.42	0.50
8:L:120:ARG:O	8:L:124:LEU:HG	2.11	0.50
1:1:13:DC:H2''	1:1:14:DA:H8	1.76	0.50
3:B:129:VAL:HG21	3:B:132:HIS:HE1	1.77	0.50
7:F:133:SER:HA	7:F:364:ARG:NH2	2.27	0.50
1:1:24:DA:H2''	1:1:25:DC:C6	2.46	0.50
1:1:67:DG:H2'	1:1:68:DG:C8	2.46	0.50
3:A:34:GLY:O	3:B:45:ARG:NH2	2.45	0.50
4:C:947:GLU:HG2	4:C:948:ILE:N	2.25	0.50
4:C:976:ARG:HB3	4:C:997:TRP:HZ3	1.77	0.50
5:D:571:ASP:C	5:D:572:THR:HG23	2.37	0.50
6:E:38:LEU:HB3	6:E:58:LEU:HD13	1.93	0.50
8:J:18:HIS:NE2	8:L:89:ASP:OD2	2.45	0.50
8:I:104:ARG:NH2	8:I:105:ARG:HA	2.23	0.50
2:2:61:DG:C6	2:2:62:DA:C6	3.00	0.50
4:C:842:ASP:HA	4:C:847:PRO:HA	1.93	0.50
4:C:1109:ILE:HD12	5:D:644:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1024:THR:HG23	5:D:1123:ARG:HB3	1.93	0.50
7:F:326:TRP:CD1	7:F:326:TRP:H	2.29	0.50
8:L:103:LEU:HD23	8:L:104:ARG:N	2.26	0.50
1:1:17:DT:H3	2:2:57:DA:H2	1.59	0.50
1:1:36:DC:H2''	1:1:37:DC:H5'	1.93	0.50
3:B:56:VAL:HG12	3:B:146:VAL:HG22	1.93	0.50
4:C:895:LEU:H	5:D:77:ARG:HH22	1.58	0.50
5:D:807:LEU:HD21	5:D:1259:GLN:OE1	2.11	0.50
7:F:105:MET:HE1	7:F:385:ARG:HG2	1.93	0.50
7:F:395:THR:HA	7:F:397:ARG:HA	1.92	0.50
7:F:457:ILE:HA	7:F:460:ILE:HG12	1.94	0.50
8:J:4:ASP:HB3	8:L:44:ASN:ND2	2.26	0.50
8:I:119:ALA:HB3	8:I:120:ARG:NH1	2.27	0.50
8:K:22:ILE:HG21	8:K:27:LEU:HB2	1.94	0.50
4:C:229:ILE:HG23	4:C:332:ARG:NH1	2.27	0.50
4:C:1220:GLN:HG2	4:C:1221:PHE:O	2.12	0.50
7:F:562:ARG:HH21	7:F:573:LEU:HD13	1.77	0.50
8:L:124:LEU:O	8:L:128:ARG:HG3	2.11	0.50
4:C:112:GLY:HA3	4:C:115:LYS:HZ1	1.75	0.49
4:C:545:PHE:HZ	5:D:781:LYS:HG3	1.77	0.49
4:C:685:MET:SD	4:C:1073:LYS:HD3	2.52	0.49
6:E:44:ASP:OD2	6:E:52:ARG:NE	2.42	0.49
8:J:33:ARG:HH11	8:J:33:ARG:HA	1.77	0.49
5:D:298:MET:SD	7:F:402:LEU:HB3	2.52	0.49
5:D:1089:LEU:HG	5:D:1096:PRO:HA	1.94	0.49
6:E:19:LEU:HD12	6:E:54:ILE:HD12	1.90	0.49
7:F:360:ASP:HA	7:F:363:ARG:HG2	1.93	0.49
1:1:16:DA:H2''	1:1:17:DT:C7	2.42	0.49
2:2:9:DT:OP1	5:D:1327:GLU:N	2.30	0.49
3:B:100:LEU:HB3	3:B:115:ILE:HD11	1.93	0.49
4:C:1196:LYS:HD2	4:C:1206:THR:HG23	1.94	0.49
5:D:372:MET:HE1	5:D:447:ILE:HD11	1.94	0.49
7:F:122:ARG:HE	7:F:371:LYS:NZ	2.08	0.49
4:C:46:GLN:OE1	4:C:46:GLN:N	2.43	0.49
4:C:873:ILE:HD11	4:C:931:VAL:HG22	1.93	0.49
4:C:898:GLU:OE1	4:C:898:GLU:N	2.45	0.49
4:C:1008:GLN:HA	4:C:1011:LEU:HD12	1.95	0.49
5:D:875:ASN:O	5:D:990:ARG:NH2	2.46	0.49
7:F:147:GLN:HG2	7:F:150:ARG:HH12	1.76	0.49
7:F:214:PRO:O	7:F:218:ARG:HG2	2.12	0.49
8:J:55:ARG:HG2	8:J:59:ARG:HH21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:55:ARG:CG	8:L:59:ARG:HH21	2.24	0.49
2:2:53:DT:H2'	2:2:54:DG:N7	2.27	0.49
8:J:90:LEU:O	8:J:94:GLN:HG2	2.12	0.49
3:A:185:TYR:CB	3:A:203:ILE:HG12	2.43	0.49
3:A:219:ARG:O	3:A:223:ILE:HG22	2.12	0.49
4:C:14:ASP:HA	4:C:1183:ALA:HB3	1.94	0.49
5:D:960:LEU:HD13	5:D:963:VAL:HG21	1.94	0.49
5:D:1027:VAL:HG12	5:D:1122:ALA:H	1.77	0.49
3:P:275:ILE:HG21	3:P:281:LEU:CD1	2.42	0.49
3:P:307:LEU:HB3	3:P:312:LEU:O	2.12	0.49
3:B:113:ALA:HB2	3:B:126:PRO:HB2	1.95	0.49
4:C:661:VAL:HB	4:C:665:ALA:HB3	1.95	0.49
1:1:33:DT:H2'	1:1:34:DT:H72	1.94	0.49
5:D:80:HIS:HD2	5:D:83:VAL:HG11	1.77	0.49
5:D:147:ILE:O	5:D:156:ARG:HD3	2.12	0.49
5:D:800:LEU:HD23	5:D:1309:ILE:HD12	1.94	0.49
5:D:847:ASP:HA	5:D:858:VAL:HG13	1.93	0.49
1:1:66:DC:H2''	1:1:67:DG:O4'	2.12	0.49
3:B:166:ARG:HD3	3:B:170:ARG:HD2	1.94	0.49
4:C:1211:ARG:NH1	4:C:1220:GLN:OE1	2.46	0.49
4:C:1331:ARG:HG2	5:D:33:TRP:CH2	2.48	0.49
5:D:1023:HIS:HA	5:D:1126:GLN:HB3	1.95	0.49
8:I:108:ARG:HH22	8:I:109:LEU:HD13	1.77	0.49
2:2:17:DG:H4'	4:C:514:PHE:CZ	2.48	0.49
4:C:318:SER:OG	4:C:320:ASP:OD1	2.26	0.48
5:D:355:ILE:HG22	5:D:461:PHE:CD1	2.47	0.48
5:D:406:ALA:HA	5:D:409:TRP:HD1	1.77	0.48
5:D:986:ASP:OD1	5:D:989:GLY:N	2.42	0.48
4:C:230:PHE:CZ	4:C:292:ILE:HD12	2.48	0.48
4:C:866:ASP:OD2	4:C:944:ARG:NH1	2.42	0.48
4:C:937:ASP:OD1	4:C:937:ASP:N	2.44	0.48
8:L:29:SER:O	8:L:33:ARG:NH2	2.46	0.48
2:2:34:DG:H2'	2:2:35:DC:C5	2.49	0.48
3:B:214:GLU:OE1	3:B:218:ARG:NH2	2.46	0.48
5:D:34:SER:OG	5:D:36:GLY:O	2.30	0.48
3:B:43:LEU:O	3:B:47:LEU:HG	2.13	0.48
4:C:947:GLU:O	4:C:950:GLU:HG3	2.12	0.48
5:D:697:MET:HE1	5:D:738:ARG:HA	1.95	0.48
7:F:285:ARG:O	7:F:289:LYS:HG2	2.14	0.48
8:L:87:ARG:NH2	8:L:88:ASP:OD1	2.43	0.48
4:C:597:GLY:O	4:C:628:HIS:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:728:ASP:O	4:C:769:PRO:HG3	2.13	0.48
4:C:1125:GLY:HA3	4:C:1179:GLY:HA2	1.93	0.48
4:C:1321:GLU:O	4:C:1325:VAL:HG13	2.13	0.48
5:D:857:LEU:HG	5:D:858:VAL:HG12	1.95	0.48
5:D:923:ILE:HA	5:D:1248:ILE:HD13	1.95	0.48
7:F:338:HIS:HA	7:F:341:LEU:HD12	1.94	0.48
4:C:317:LEU:HA	4:C:321:LEU:HD22	1.95	0.48
4:C:630:VAL:C	4:C:647:ARG:HH12	2.21	0.48
5:D:963:VAL:HA	5:D:980:THR:OG1	2.13	0.48
3:P:288:GLU:OE1	3:P:288:GLU:N	2.46	0.48
8:I:80:ASP:HB3	8:I:83:LEU:HD12	1.95	0.48
2:2:33:DT:H2''	2:2:34:DG:C8	2.48	0.48
4:C:1150:ASP:N	4:C:1150:ASP:OD1	2.45	0.48
5:D:1346:GLY:N	5:D:1349:GLU:OE1	2.43	0.48
8:I:45:GLU:O	8:I:49:GLN:N	2.33	0.48
8:K:91:LEU:HD12	8:K:107:TYR:HD2	1.78	0.48
4:C:79:VAL:HG13	4:C:80:PHE:HD1	1.78	0.48
4:C:716:ALA:HB3	4:C:784:ALA:HB3	1.96	0.48
4:C:726:TYR:HB3	4:C:733:VAL:HG22	1.96	0.48
4:C:811:ASN:HA	4:C:815:SER:HB2	1.95	0.48
4:C:1128:ILE:HG12	4:C:1145:ILE:HD11	1.95	0.48
5:D:959:LYS:HB3	5:D:983:LYS:HB2	1.96	0.48
5:D:1175:LEU:HD12	5:D:1190:ILE:HD13	1.96	0.48
7:F:309:ASN:ND2	7:F:314:THR:OG1	2.46	0.48
8:J:95:PHE:CZ	8:J:97:GLY:HA2	2.49	0.48
3:P:285:THR:N	3:P:288:GLU:OE2	2.41	0.48
8:I:57:LEU:HD11	8:K:46:LEU:HD23	1.94	0.48
1:1:46:DC:H1'	1:1:47:DC:H5'	1.95	0.48
4:C:106:GLU:HB2	4:C:115:LYS:NZ	2.28	0.48
4:C:276:GLN:HA	4:C:279:LYS:HD3	1.94	0.48
4:C:397:LEU:O	4:C:398:SER:OG	2.26	0.48
4:C:1156:ARG:HG3	4:C:1157:GLN:N	2.29	0.48
5:D:211:GLU:HA	5:D:214:ARG:HB2	1.96	0.48
5:D:1194:ARG:HD2	5:D:1194:ARG:N	2.28	0.48
8:J:13:ARG:NH1	8:L:48:ARG:HG3	2.29	0.48
8:J:19:ILE:HG22	8:L:86:LEU:HG	1.96	0.48
8:J:43:GLU:CD	8:J:55:ARG:HA	2.39	0.48
3:P:253:LEU:HD12	3:P:254:LEU:HG	1.96	0.48
8:I:82:ILE:HG23	8:K:31:TRP:CZ2	2.49	0.48
4:C:231:GLU:HB3	4:C:331:LYS:HE2	1.95	0.48
4:C:1165:SER:N	4:C:1168:GLU:OE1	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:377:PHE:CE2	5:D:470:VAL:HG11	2.48	0.48
7:F:148:TYR:HB3	7:F:221:PHE:HE2	1.79	0.48
4:C:145:ILE:HG13	4:C:512:SER:HB3	1.96	0.47
4:C:239:MET:HE1	4:C:241:LEU:HD12	1.95	0.47
4:C:657:THR:OG1	4:C:1187:PHE:HB2	2.13	0.47
7:F:299:LYS:HA	7:F:302:PHE:HB3	1.96	0.47
1:1:63:DT:O4	4:C:175:ARG:NE	2.47	0.47
5:D:824:PRO:HD3	5:D:835:LEU:HB2	1.95	0.47
8:I:69:LEU:HD23	8:K:76:ILE:HG12	1.94	0.47
8:L:121:GLN:HA	8:L:124:LEU:HD12	1.96	0.47
1:1:12:DT:C2	2:2:63:DG:N2	2.82	0.47
1:1:23:DA:H2''	1:1:24:DA:H8	1.74	0.47
3:B:78:ILE:O	3:B:82:LEU:HG	2.15	0.47
3:B:92:VAL:O	3:B:148:ARG:NH2	2.48	0.47
5:D:615:LYS:HZ2	6:E:7:GLN:HG3	1.79	0.47
5:D:1024:THR:HG21	5:D:1123:ARG:NH2	2.30	0.47
3:B:88:LEU:HD23	3:B:88:LEU:HA	1.78	0.47
4:C:387:ASN:HB3	4:C:394:ARG:HD3	1.97	0.47
4:C:516:VAL:HG12	4:C:522:SER:HB2	1.95	0.47
5:D:825:VAL:HG11	5:D:833:GLU:HG3	1.96	0.47
8:I:47:LYS:HD2	8:I:48:ARG:N	2.29	0.47
3:B:19:VAL:HB	3:B:23:HIS:HB3	1.97	0.47
5:D:128:LEU:O	5:D:157:GLN:NE2	2.23	0.47
5:D:156:ARG:HD2	5:D:157:GLN:N	2.29	0.47
7:F:90:GLU:N	7:F:90:GLU:OE1	2.48	0.47
8:J:113:GLN:O	8:J:117:ILE:HG13	2.15	0.47
8:I:101:GLU:O	8:I:105:ARG:HG2	2.14	0.47
8:L:90:LEU:HD22	8:L:107:TYR:OH	2.15	0.47
3:A:6:THR:OG1	3:A:7:GLU:N	2.47	0.47
3:A:59:VAL:HG21	3:A:85:LEU:HD13	1.97	0.47
5:D:355:ILE:HG13	5:D:466:MET:HE2	1.96	0.47
8:L:104:ARG:NH1	8:L:110:SER:HA	2.26	0.47
1:1:56:DG:H2''	1:1:57:DG:O4'	2.15	0.47
2:2:63:DG:H2''	2:2:64:DT:C5	2.49	0.47
4:C:339:ASN:OD1	4:C:340:ASP:N	2.48	0.47
4:C:832:HIS:CE1	4:C:1058:ARG:HD2	2.50	0.47
4:C:902:LEU:HD11	7:F:607:LEU:HD12	1.95	0.47
5:D:825:VAL:CG1	5:D:833:GLU:H	2.27	0.47
8:J:42:LEU:O	8:J:45:GLU:HG3	2.14	0.47
8:K:81:THR:HA	8:K:84:THR:HB	1.96	0.47
4:C:241:LEU:HD11	4:C:246:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:557:ARG:NH2	4:C:607:SER:O	2.46	0.47
2:2:16:DA:C8	2:2:17:DG:C2	3.03	0.47
5:D:242:LEU:HD12	5:D:243:PRO:HD2	1.97	0.47
7:F:555:GLU:HA	7:F:558:VAL:HG12	1.96	0.47
8:K:20:ASP:N	8:K:20:ASP:OD1	2.45	0.47
8:K:24:ALA:HA	8:K:59:ARG:HH12	1.79	0.47
2:2:51:DT:H71	8:I:116:GLN:HE22	1.79	0.47
4:C:81:ASP:N	4:C:84:GLU:OE2	2.35	0.47
4:C:238:GLN:CD	4:C:284:LEU:HB3	2.40	0.47
4:C:1000:LEU:HD23	4:C:1000:LEU:H	1.79	0.47
4:C:1151:LEU:HA	4:C:1151:LEU:HD12	1.79	0.47
5:D:342:LEU:HD12	5:D:1352:ILE:HG23	1.97	0.47
5:D:809:VAL:HG23	5:D:911:LYS:HA	1.97	0.47
6:E:60:ASN:H	6:E:63:ILE:HG13	1.79	0.47
8:J:80:ASP:OD1	8:J:81:THR:N	2.48	0.47
4:C:1290:MET:SD	5:D:347:VAL:HG21	2.55	0.46
3:A:92:VAL:HG22	3:A:121:VAL:HG22	1.96	0.46
3:A:207:THR:OG1	3:A:208:ASN:N	2.48	0.46
4:C:39:ILE:O	4:C:73:TYR:OH	2.32	0.46
4:C:549:ASP:OD1	4:C:550:VAL:N	2.49	0.46
5:D:291:ILE:HG23	7:F:406:GLN:HE22	1.80	0.46
8:K:47:LYS:HD2	8:K:48:ARG:N	2.29	0.46
2:2:22:DA:H4'	4:C:497:PRO:HB3	1.96	0.46
3:A:222:THR:HG22	3:B:232:VAL:HA	1.96	0.46
4:C:192:ASP:HB3	4:C:346:TYR:CD1	2.50	0.46
5:D:516:ASP:OD1	5:D:516:ASP:N	2.45	0.46
5:D:1167:LYS:HB3	5:D:1170:LYS:HZ3	1.79	0.46
6:E:36:ASP:OD1	6:E:36:ASP:N	2.48	0.46
8:K:46:LEU:HD22	8:K:51:VAL:HG21	1.97	0.46
8:L:104:ARG:HD2	8:L:110:SER:C	2.40	0.46
5:D:1199:PHE:H	5:D:1202:GLU:HG3	1.80	0.46
1:I:21:DA:OP2	8:I:113:GLN:NE2	2.48	0.46
4:C:192:ASP:HB3	4:C:346:TYR:HD1	1.80	0.46
4:C:976:ARG:NH1	4:C:994:ARG:HD3	2.31	0.46
5:D:123:ARG:NH2	5:D:1334:GLU:OE2	2.45	0.46
7:F:452:ILE:CG2	7:F:457:ILE:HG13	2.45	0.46
8:J:71:GLY:HA2	8:I:110:SER:HB2	1.98	0.46
8:I:95:PHE:HA	8:I:103:LEU:HD11	1.97	0.46
8:K:19:ILE:HG23	8:K:27:LEU:HD22	1.97	0.46
4:C:549:ASP:OD2	5:D:750:PRO:HB3	2.16	0.46
4:C:1102:GLY:O	4:C:1106:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:288:PRO:HD2	5:D:291:ILE:HD12	1.98	0.46
5:D:822:MET:HG2	5:D:839:VAL:HG12	1.97	0.46
7:F:83:VAL:O	7:F:87:VAL:HG12	2.16	0.46
8:J:37:ASP:O	8:J:41:VAL:HG23	2.16	0.46
8:I:112:PRO:O	8:I:116:GLN:HG2	2.15	0.46
1:I:62:DG:H1	4:C:199:ASP:HA	1.81	0.46
3:A:211:ILE:HD13	3:A:211:ILE:HA	1.82	0.46
3:B:78:ILE:HA	3:B:81:ILE:HG12	1.97	0.46
3:B:155:ALA:N	3:B:174:ASP:OD1	2.47	0.46
3:B:209:GLY:O	3:B:210:THR:OG1	2.28	0.46
4:C:31:GLN:NE2	4:C:527:LYS:O	2.49	0.46
4:C:1117:LEU:HD11	4:C:1182:ILE:HD13	1.98	0.46
3:P:306:VAL:HB	3:P:310:ARG:NH2	2.31	0.46
4:C:675:ASP:OD1	4:C:676:ALA:N	2.49	0.46
5:D:865:HIS:CE1	5:D:867:GLN:HB2	2.51	0.46
5:D:1046:ILE:HG22	5:D:1061:VAL:HG22	1.97	0.46
7:F:111:LEU:HD12	7:F:116:GLU:HG3	1.97	0.46
7:F:532:LEU:O	7:F:536:THR:HG23	2.16	0.46
7:F:593:LYS:NZ	7:F:597:LYS:HD2	2.31	0.46
8:K:46:LEU:HD13	8:K:57:LEU:HB3	1.98	0.46
8:L:57:LEU:HD13	8:L:57:LEU:HA	1.73	0.46
4:C:237:LEU:HB2	4:C:287:VAL:HG23	1.97	0.46
4:C:704:MET:O	4:C:708:VAL:HG12	2.15	0.46
5:D:156:ARG:HE	5:D:157:GLN:HB2	1.81	0.46
5:D:198:CYS:O	5:D:202:ARG:HG2	2.16	0.46
5:D:503:SER:OG	5:D:504:GLN:N	2.49	0.46
5:D:1199:PHE:H	5:D:1202:GLU:CG	2.29	0.46
6:E:53:GLU:O	6:E:57:GLY:N	2.46	0.46
8:L:81:THR:O	8:L:84:THR:OG1	2.27	0.46
4:C:61:SER:HB3	4:C:479:LEU:HB3	1.98	0.46
4:C:425:ILE:O	4:C:429:MET:HG3	2.16	0.46
5:D:805:GLN:HE21	5:D:1348:LYS:HB2	1.81	0.46
5:D:901:ARG:NH2	5:D:906:GLY:HA2	2.31	0.46
5:D:1268:ASN:ND2	5:D:1301:THR:HG22	2.28	0.46
5:D:1330:ARG:O	5:D:1334:GLU:HG2	2.16	0.46
1:I:53:DA:OP2	7:F:428:SER:OG	2.29	0.45
5:D:1191:PRO:HB2	5:D:1194:ARG:HD3	1.97	0.45
7:F:88:GLU:O	7:F:91:ILE:HG12	2.15	0.45
7:F:159:SER:O	7:F:162:ILE:HG22	2.15	0.45
8:J:121:GLN:HA	8:J:124:LEU:HD12	1.98	0.45
1:I:39:DG:C8	1:I:39:DG:H5'	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:91:ARG:HE	3:A:210:THR:HA	1.80	0.45
3:A:192:VAL:HG21	3:A:198:LEU:HD12	1.98	0.45
3:B:47:LEU:HD13	3:B:205:MET:HE2	1.98	0.45
4:C:1121:ALA:HB2	4:C:1182:ILE:HD12	1.97	0.45
5:D:41:PRO:HA	5:D:273:ILE:HD11	1.96	0.45
5:D:58:CYS:SG	5:D:60:ARG:HG2	2.55	0.45
5:D:513:MET:HE3	5:D:579:LEU:HB2	1.98	0.45
5:D:953:LYS:HE2	5:D:953:LYS:HB2	1.78	0.45
8:I:87:ARG:NH1	8:I:109:LEU:HD21	2.32	0.45
8:L:103:LEU:HD23	8:L:104:ARG:H	1.82	0.45
3:A:118:ASP:OD1	3:A:119:GLY:N	2.46	0.45
3:B:104:LYS:NZ	3:B:105:SER:O	2.30	0.45
4:C:1026:GLU:N	4:C:1026:GLU:OE1	2.47	0.45
7:F:455:HIS:HD2	7:F:456:MET:HG2	1.81	0.45
7:F:552:THR:HB	7:F:555:GLU:OE1	2.17	0.45
2:2:34:DG:H2''	2:2:35:DC:O5'	2.15	0.45
2:2:51:DT:H2''	2:2:52:DA:N7	2.31	0.45
3:A:39:LEU:HA	3:A:39:LEU:HD23	1.84	0.45
3:A:163:GLU:CD	3:A:163:GLU:H	2.24	0.45
3:A:180:VAL:HG11	3:A:183:ILE:CD1	2.47	0.45
4:C:314:ASN:ND2	4:C:314:ASN:O	2.49	0.45
4:C:348:SER:O	4:C:352:ARG:HG2	2.15	0.45
5:D:770:LEU:O	5:D:774:ILE:HG12	2.17	0.45
5:D:1005:LYS:HE2	5:D:1005:LYS:HB3	1.85	0.45
8:L:125:HIS:HA	8:L:128:ARG:HD2	1.98	0.45
1:1:51:DT:H5'	1:1:51:DT:H6	1.81	0.45
1:1:63:DT:C5	4:C:183:TRP:HZ3	2.34	0.45
4:C:241:LEU:HD21	4:C:246:LEU:HD11	1.99	0.45
4:C:699:LEU:HG	4:C:799:ASN:ND2	2.31	0.45
7:F:479:THR:HB	7:F:482:GLU:HB2	1.98	0.45
8:L:56:GLU:O	8:L:60:LYS:HG2	2.17	0.45
3:B:127:GLN:OE1	3:B:127:GLN:N	2.46	0.45
4:C:176:ILE:HD12	4:C:405:PHE:HE1	1.81	0.45
4:C:177:ILE:HG22	4:C:183:TRP:CD2	2.51	0.45
5:D:72:CYS:SG	5:D:87:LYS:HD3	2.56	0.45
5:D:424:ASN:OD1	5:D:425:ARG:N	2.50	0.45
6:E:15:ASN:OD1	6:E:16:ARG:N	2.47	0.45
8:I:110:SER:OG	8:I:112:PRO:HD2	2.16	0.45
8:K:72:ARG:HD2	8:L:111:GLN:NE2	2.32	0.45
1:1:13:DC:H2''	1:1:14:DA:C8	2.52	0.45
1:1:20:DC:H2''	1:1:21:DA:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:194:GLN:OE1	3:B:194:GLN:N	2.39	0.45
8:K:84:THR:HG23	8:K:87:ARG:HH21	1.82	0.45
3:B:28:LEU:HD23	3:B:31:LEU:HD11	1.98	0.45
3:B:211:ILE:HD13	3:B:211:ILE:HA	1.82	0.45
4:C:877:VAL:HG23	4:C:881:ASP:HB2	1.99	0.45
5:D:393:THR:HG23	5:D:395:LYS:H	1.82	0.45
5:D:447:ILE:HD12	5:D:468:VAL:HG21	1.97	0.45
5:D:867:GLN:N	5:D:867:GLN:OE1	2.48	0.45
5:D:1261:LEU:HD21	5:D:1306:LEU:HD12	1.97	0.45
7:F:112:THR:C	7:F:114:GLU:H	2.23	0.45
8:J:42:LEU:HD13	8:J:42:LEU:HA	1.61	0.45
5:D:978:ARG:CZ	5:D:999:TYR:HB3	2.47	0.45
8:I:110:SER:HB3	8:I:113:GLN:HE22	1.81	0.45
1:I:20:DC:H2'	1:I:21:DA:H8	1.82	0.45
3:A:223:ILE:HD11	3:B:35:PHE:HZ	1.82	0.45
4:C:320:ASP:OD1	4:C:320:ASP:N	2.49	0.45
4:C:1250:SER:HB2	4:C:1259:LEU:HD13	1.97	0.45
5:D:264:ASP:HB3	5:D:324:LEU:HD22	1.99	0.45
5:D:678:ARG:O	5:D:682:VAL:HG12	2.17	0.45
5:D:901:ARG:HE	5:D:906:GLY:HA2	1.82	0.45
3:P:272:ALA:HA	8:L:98:ARG:HD2	1.98	0.45
4:C:260:LYS:HD2	4:C:262:TYR:CE2	2.51	0.44
4:C:633:LEU:HD13	4:C:633:LEU:HA	1.83	0.44
5:D:108:ALA:HB3	5:D:279:LEU:HD23	1.98	0.44
5:D:901:ARG:NH2	5:D:903:LEU:HA	2.32	0.44
8:J:45:GLU:CD	8:L:61:GLN:HG2	2.42	0.44
2:2:18:DG:H1'	2:2:19:DG:H8	1.82	0.44
3:B:84:ASN:O	3:B:128:HIS:HE1	2.00	0.44
4:C:616:ILE:HG13	4:C:652:TYR:HB2	1.98	0.44
4:C:1070:HIS:NE2	4:C:1114:GLU:OE1	2.46	0.44
5:D:200:GLN:O	5:D:203:GLU:HG2	2.17	0.44
5:D:309:ASN:ND2	5:D:324:LEU:O	2.29	0.44
5:D:475:GLU:OE2	6:E:28:ARG:NH2	2.49	0.44
7:F:402:LEU:HD23	7:F:402:LEU:HA	1.87	0.44
1:I:33:DT:H2'	1:I:34:DT:C6	2.53	0.44
2:2:26:DC:H2'	2:2:27:DG:C8	2.52	0.44
4:C:89:GLY:HA2	4:C:140:GLY:HA3	1.99	0.44
4:C:446:ASP:OD1	4:C:446:ASP:N	2.40	0.44
4:C:936:ARG:O	4:C:939:VAL:HG12	2.17	0.44
5:D:825:VAL:HG12	5:D:833:GLU:H	1.81	0.44
5:D:1036:ARG:NH2	5:D:1112:GLY:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:316:PHE:O	7:F:320:ILE:HG12	2.17	0.44
8:J:24:ALA:O	8:J:27:LEU:HG	2.18	0.44
3:P:307:LEU:HD23	3:P:310:ARG:HD2	1.99	0.44
8:I:33:ARG:O	8:I:36:VAL:HG12	2.17	0.44
8:K:123:LYS:HE2	8:K:123:LYS:HB2	1.65	0.44
4:C:1331:ARG:HD3	5:D:33:TRP:CE2	2.53	0.44
5:D:390:LEU:HD12	5:D:390:LEU:HA	1.79	0.44
5:D:826:ILE:HG22	5:D:831:VAL:HG12	2.00	0.44
5:D:1318:SER:OG	5:D:1342:ASP:OD2	2.30	0.44
6:E:62:GLN:N	6:E:62:GLN:OE1	2.46	0.44
7:F:470:MET:SD	7:F:486:ARG:HG3	2.58	0.44
7:F:551:LEU:HD11	7:F:598:LEU:HD23	2.00	0.44
2:2:51:DT:H2"	2:2:52:DA:C8	2.53	0.44
3:B:215:GLU:HG2	3:B:218:ARG:HH12	1.82	0.44
4:C:540:ARG:HH21	4:C:568:ASN:ND2	2.16	0.44
4:C:1101:LEU:HD23	5:D:731:ARG:HG3	2.00	0.44
7:F:292:VAL:HG11	7:F:299:LYS:HD3	2.00	0.44
8:I:107:TYR:HB3	8:I:109:LEU:HD23	2.00	0.44
8:K:12:ILE:O	8:K:16:ILE:HG13	2.17	0.44
1:1:22:DT:OP2	8:L:77:PRO:HA	2.17	0.44
4:C:814:ASP:OD2	4:C:1106:ARG:NH2	2.51	0.44
5:D:226:ALA:O	5:D:230:SER:OG	2.35	0.44
7:F:246:GLN:O	7:F:250:LEU:HG	2.18	0.44
8:J:89:ASP:OD1	8:L:36:VAL:HG22	2.18	0.44
8:I:27:LEU:HB3	8:I:31:TRP:CE2	2.53	0.44
8:I:76:ILE:HD11	8:K:69:LEU:C	2.43	0.44
8:K:72:ARG:HD3	8:L:104:ARG:NH2	2.33	0.44
1:1:47:DC:H2"	1:1:48:DG:C8	2.53	0.44
4:C:233:ARG:NH2	4:C:238:GLN:HG2	2.32	0.44
4:C:666:SER:O	4:C:702:THR:HG21	2.18	0.44
5:D:421:VAL:HG13	5:D:468:VAL:HG13	1.98	0.44
5:D:555:TYR:CE2	5:D:565:ALA:HB2	2.52	0.44
8:I:101:GLU:OE1	8:I:104:ARG:HD3	2.18	0.44
3:B:60:GLU:OE1	3:B:170:ARG:NH1	2.51	0.44
4:C:260:LYS:HD2	4:C:262:TYR:HE2	1.83	0.44
4:C:825:GLU:HG3	4:C:827:ARG:HG2	1.99	0.44
5:D:1332:LEU:HD23	5:D:1332:LEU:HA	1.75	0.44
7:F:309:ASN:OD1	7:F:310:GLU:N	2.51	0.44
8:I:48:ARG:NE	8:K:13:ARG:HG3	2.33	0.44
8:L:43:GLU:OE1	8:L:55:ARG:NH1	2.51	0.44
1:1:45:DC:C2	1:1:46:DC:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:81:ILE:HD12	3:B:131:CYS:HB3	1.99	0.44
5:D:37:GLU:HB2	5:D:104:HIS:CE1	2.53	0.44
5:D:138:VAL:CG2	5:D:145:VAL:HG23	2.48	0.44
5:D:1064:SER:HB2	5:D:1072:LYS:HD3	1.99	0.44
7:F:218:ARG:HH22	7:F:221:PHE:HD2	1.64	0.44
8:J:72:ARG:HD3	8:I:105:ARG:HH12	1.83	0.44
3:P:281:LEU:HD12	3:P:281:LEU:HA	1.80	0.44
8:L:57:LEU:O	8:L:61:GLN:HG3	2.17	0.44
1:I:20:DC:C4	1:I:21:DA:C6	3.06	0.43
4:C:175:ARG:HG2	4:C:185:ASP:OD1	2.18	0.43
4:C:235:ASN:OD1	4:C:236:LYS:HG2	2.18	0.43
4:C:1142:ARG:NH1	4:C:1161:LEU:O	2.51	0.43
4:C:1214:ASP:OD1	4:C:1215:GLY:N	2.51	0.43
5:D:1109:LEU:HD23	5:D:1109:LEU:H	1.83	0.43
8:I:32:PRO:HB3	8:K:77:PRO:HD3	2.00	0.43
8:I:55:ARG:HD2	8:I:55:ARG:HA	1.86	0.43
8:I:127:ARG:HE	8:I:128:ARG:CG	2.21	0.43
8:K:102:GLU:HG2	8:K:105:ARG:HH21	1.82	0.43
3:B:112:ALA:HB3	3:B:126:PRO:HA	1.99	0.43
4:C:270:THR:H	4:C:273:HIS:CE1	2.36	0.43
5:D:219:LYS:HB3	5:D:219:LYS:HE2	1.79	0.43
7:F:571:TYR:HB3	7:F:575:GLU:HB2	2.00	0.43
4:C:738:GLU:HA	4:C:741:MET:HG3	1.99	0.43
4:C:811:ASN:O	4:C:1099:ASN:ND2	2.48	0.43
8:I:122:ARG:O	8:I:126:THR:OG1	2.31	0.43
1:I:51:DT:H1'	1:I:52:DA:H5'	1.99	0.43
1:I:68:DG:H2''	1:I:69:DA:H5''	2.00	0.43
2:2:41:DA:H1'	2:2:42:DA:H5'	2.01	0.43
4:C:3:TYR:O	4:C:8:LYS:NZ	2.30	0.43
4:C:1124:ILE:HG21	4:C:1180:MET:SD	2.59	0.43
5:D:220:ARG:O	5:D:224:LEU:HD23	2.18	0.43
5:D:224:LEU:O	5:D:228:VAL:HG23	2.19	0.43
5:D:1004:ALA:N	5:D:1017:VAL:O	2.41	0.43
5:D:1198:VAL:HB	5:D:1202:GLU:HB2	2.00	0.43
7:F:91:ILE:HB	7:F:93:ARG:H	1.83	0.43
8:J:6:PHE:H	8:L:44:ASN:HD21	1.65	0.43
3:A:155:ALA:HA	3:A:158:ARG:HH11	1.83	0.43
4:C:733:VAL:HG12	4:C:750:ILE:HD13	2.01	0.43
4:C:1136:GLN:O	4:C:1137:GLU:HG2	2.18	0.43
5:D:549:LYS:HG2	5:D:571:ASP:OD1	2.17	0.43
5:D:1000:GLY:HA2	5:D:1028:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:47:LEU:HD12	3:B:183:ILE:HG12	1.99	0.43
4:C:448:LEU:HD23	4:C:448:LEU:HA	1.84	0.43
4:C:564:PRO:O	4:C:569:ILE:HA	2.18	0.43
4:C:971:LEU:O	4:C:975:ILE:HG12	2.19	0.43
4:C:1023:HIS:HA	4:C:1026:GLU:OE2	2.19	0.43
5:D:557:LYS:HB3	5:D:563:LEU:HD23	1.99	0.43
7:F:263:PRO:HD2	7:F:264:LYS:NZ	2.33	0.43
8:I:87:ARG:O	8:I:91:LEU:N	2.35	0.43
8:L:28:GLU:O	8:L:33:ARG:NH2	2.47	0.43
8:L:56:GLU:O	8:L:59:ARG:HG2	2.19	0.43
1:1:33:DT:N3	2:2:42:DA:C2	2.86	0.43
3:B:87:GLY:O	3:B:128:HIS:NE2	2.52	0.43
4:C:483:ASP:CG	4:C:486:THR:HG22	2.44	0.43
6:E:25:ARG:HH21	6:E:64:LEU:HD13	1.82	0.43
8:J:91:LEU:HD22	8:J:117:ILE:HG21	2.00	0.43
1:1:9:DT:H1'	1:1:10:DA:OP1	2.18	0.43
1:1:65:DA:H2	2:2:9:DT:H3	1.66	0.43
1:1:68:DG:H2''	1:1:69:DA:H8	1.83	0.43
4:C:39:ILE:HA	4:C:39:ILE:HD13	1.74	0.43
5:D:285:LEU:HG	7:F:413:MET:CE	2.49	0.43
5:D:1060:VAL:HG22	5:D:1106:ILE:HG13	2.00	0.43
5:D:1263:LYS:HE3	5:D:1263:LYS:HB3	1.81	0.43
7:F:256:PHE:HA	7:F:259:PHE:CE2	2.54	0.43
1:1:60:DC:H2'	1:1:61:DT:C6	2.54	0.43
4:C:210:LEU:HD13	4:C:210:LEU:HA	1.70	0.43
4:C:221:LEU:HD11	4:C:314:ASN:HB2	2.00	0.43
4:C:519:ASN:O	4:C:523:GLU:HG2	2.19	0.43
4:C:1274:GLU:CD	4:C:1274:GLU:H	2.26	0.43
5:D:1088:VAL:O	5:D:1097:ALA:HB3	2.18	0.43
5:D:1104:LYS:O	5:D:1125:PRO:HD2	2.18	0.43
7:F:253:SER:O	7:F:257:LYS:HG3	2.19	0.43
7:F:417:ASP:OD1	7:F:418:LYS:N	2.52	0.43
8:L:104:ARG:O	8:L:108:ARG:N	2.52	0.43
4:C:80:PHE:CD2	4:C:84:GLU:HG3	2.53	0.43
4:C:225:PHE:CE2	4:C:347:ILE:HB	2.54	0.43
4:C:257:ALA:HB2	4:C:262:TYR:HE1	1.83	0.43
5:D:712:GLN:N	5:D:712:GLN:OE1	2.52	0.43
5:D:1039:ASP:HB3	5:D:1077:ALA:O	2.19	0.43
5:D:1203:ARG:NH1	5:D:1205:GLU:OE2	2.52	0.43
5:D:1221:LEU:HD11	5:D:1226:VAL:HG12	2.00	0.43
8:J:26:GLU:H	8:J:26:GLU:CD	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:40:ASP:OD1	8:I:40:ASP:N	2.51	0.43
3:A:232:VAL:HG13	3:B:222:THR:HG22	2.00	0.42
5:D:285:LEU:CG	7:F:413:MET:HE1	2.48	0.42
5:D:355:ILE:HD13	5:D:355:ILE:HA	1.83	0.42
5:D:1167:LYS:HB3	5:D:1170:LYS:HD2	2.01	0.42
7:F:97:PRO:HA	7:F:100:MET:SD	2.59	0.42
7:F:426:LYS:HE3	7:F:426:LYS:HB3	1.89	0.42
8:J:74:PHE:HD2	8:L:74:PHE:HZ	1.67	0.42
8:J:75:TYR:HA	8:L:74:PHE:CE1	2.54	0.42
8:K:81:THR:O	8:K:84:THR:HB	2.19	0.42
8:K:95:PHE:HE1	8:K:100:MET:HB2	1.84	0.42
4:C:14:ASP:H	4:C:1157:GLN:NE2	2.17	0.42
4:C:253:PHE:CZ	4:C:287:VAL:HG12	2.54	0.42
4:C:519:ASN:HD21	4:C:689:ALA:C	2.26	0.42
4:C:842:ASP:OD1	4:C:842:ASP:N	2.52	0.42
4:C:1243:MET:SD	5:D:445:LYS:HD2	2.59	0.42
5:D:251:PRO:HG2	7:F:507:MET:HE3	2.01	0.42
5:D:507:VAL:HG11	5:D:598:LYS:HD3	1.99	0.42
5:D:1231:ARG:O	5:D:1235:ASN:ND2	2.52	0.42
7:F:225:ARG:HA	7:F:225:ARG:NH1	2.33	0.42
7:F:394:TYR:OH	7:F:436:ARG:NH1	2.46	0.42
8:I:91:LEU:HD13	8:I:107:TYR:CD2	2.54	0.42
1:I:57:DG:H2'	1:I:59:DG:O6	2.19	0.42
4:C:6:THR:O	4:C:9:LYS:HG2	2.19	0.42
4:C:453:ILE:HG13	4:C:587:LEU:HD21	2.01	0.42
4:C:700:VAL:HG13	4:C:1117:LEU:HD21	1.93	0.42
4:C:1021:LEU:HA	4:C:1024:GLU:CD	2.44	0.42
5:D:113:HIS:CE1	5:D:115:TRP:HB2	2.55	0.42
5:D:497:GLU:OE1	5:D:497:GLU:N	2.50	0.42
5:D:1063:ASP:OD1	5:D:1063:ASP:N	2.51	0.42
5:D:1290:ARG:HA	5:D:1295:ASN:HB3	2.01	0.42
7:F:562:ARG:HG2	7:F:563:PHE:CE1	2.55	0.42
8:I:42:LEU:O	8:I:46:LEU:HG	2.19	0.42
8:L:31:TRP:HB3	8:L:33:ARG:HG3	1.99	0.42
3:B:19:VAL:HB	3:B:23:HIS:CG	2.53	0.42
4:C:207:THR:HG23	4:C:350:THR:HG22	2.02	0.42
4:C:447:HIS:CD2	4:C:553:THR:HG21	2.54	0.42
4:C:1212:LEU:HD21	4:C:1227:VAL:HG21	2.01	0.42
4:C:1295:SER:O	4:C:1301:ARG:NH1	2.53	0.42
5:D:474:LEU:HD12	5:D:474:LEU:HA	1.79	0.42
5:D:981:GLU:OE1	5:D:996:LYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1084:GLN:H	5:D:1084:GLN:CD	2.27	0.42
3:P:256:PRO:HA	3:P:277:TYR:HA	2.00	0.42
4:C:388:LEU:HD23	4:C:388:LEU:HA	1.89	0.42
4:C:879:GLY:HA2	4:C:920:VAL:HG12	2.02	0.42
4:C:960:LEU:HD12	4:C:960:LEU:HA	1.88	0.42
5:D:1169:THR:HG22	5:D:1192:LYS:HE2	2.02	0.42
1:I:15:DA:C5	1:I:16:DA:C6	3.08	0.42
5:D:1207:GLY:O	5:D:1224:ARG:NH2	2.53	0.42
7:F:88:GLU:OE1	7:F:91:ILE:HD13	2.19	0.42
7:F:276:MET:HE1	7:F:279:ARG:NH2	2.35	0.42
7:F:332:ASP:N	7:F:332:ASP:OD1	2.51	0.42
8:J:8:HIS:ND1	8:J:9:ASP:HB2	2.35	0.42
1:I:5:DC:H2''	1:I:6:DC:H5'	2.01	0.42
4:C:452:ARG:HH22	4:C:458:GLU:CD	2.20	0.42
5:D:955:LYS:HD2	5:D:1011:VAL:O	2.19	0.42
5:D:1323:ALA:HA	5:D:1331:VAL:HG21	2.02	0.42
8:I:127:ARG:HD2	8:I:127:ARG:C	2.44	0.42
1:I:51:DT:H2''	1:I:52:DA:C8	2.55	0.42
3:B:79:LEU:HD13	3:B:79:LEU:HA	1.88	0.42
3:B:93:GLN:OE1	3:B:93:GLN:N	2.53	0.42
4:C:63:SER:O	4:C:107:ARG:NH2	2.53	0.42
4:C:112:GLY:HA3	4:C:115:LYS:NZ	2.34	0.42
4:C:979:LEU:HD22	4:C:1000:LEU:HD21	2.01	0.42
7:F:272:SER:O	7:F:276:MET:HG2	2.20	0.42
7:F:339:ARG:NH1	7:F:339:ARG:HA	2.34	0.42
3:A:224:LEU:HD23	3:B:228:LEU:HD11	2.01	0.42
4:C:207:THR:CG2	4:C:351:LEU:HD23	2.49	0.42
4:C:234:ASP:OD1	4:C:234:ASP:N	2.50	0.42
4:C:1069:ARG:NH2	4:C:1114:GLU:OE2	2.42	0.42
4:C:1192:GLU:O	4:C:1196:LYS:HG2	2.19	0.42
5:D:919:ALA:O	5:D:923:ILE:HG23	2.19	0.42
7:F:455:HIS:CD2	7:F:456:MET:N	2.88	0.42
8:L:31:TRP:CD2	8:L:32:PRO:HD2	2.55	0.42
3:B:11:PRO:HG3	3:B:31:LEU:HD21	2.02	0.42
3:B:53:GLY:O	3:B:148:ARG:HD3	2.20	0.42
4:C:484:LEU:HD23	4:C:484:LEU:H	1.84	0.42
5:D:26:SER:HB3	5:D:236:TRP:CE2	2.55	0.42
5:D:163:GLU:OE1	5:D:163:GLU:N	2.46	0.42
5:D:807:LEU:HD13	5:D:1255:VAL:HG23	2.02	0.42
5:D:859:PRO:C	5:D:861:ASN:H	2.28	0.42
8:J:46:LEU:CD2	8:J:51:VAL:HB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:70:DT:H2''	1:1:71:DG:C8	2.55	0.41
4:C:499:SER:HA	4:C:502:VAL:HG12	2.01	0.41
5:D:26:SER:O	5:D:30:ILE:HG13	2.20	0.41
5:D:732:GLY:HA2	5:D:736:GLN:HG3	2.02	0.41
5:D:848:VAL:HG12	5:D:858:VAL:HG11	2.02	0.41
3:P:277:TYR:O	3:P:281:LEU:HD22	2.19	0.41
8:L:53:ASN:HB3	8:L:56:GLU:CD	2.45	0.41
1:1:12:DT:H2'	1:1:13:DC:H6	1.82	0.41
5:D:138:VAL:CG2	5:D:145:VAL:CG2	2.98	0.41
5:D:674:THR:HG22	5:D:677:GLU:CD	2.45	0.41
5:D:1158:GLU:OE2	5:D:1186:TYR:OH	2.29	0.41
5:D:1251:LYS:O	5:D:1255:VAL:HG12	2.21	0.41
6:E:67:ARG:HH11	6:E:68:GLU:HB3	1.84	0.41
7:F:288:MET:O	7:F:293:GLU:HG2	2.20	0.41
8:J:68:PHE:CD2	8:L:41:VAL:HG22	2.55	0.41
8:K:84:THR:HG23	8:K:87:ARG:NH2	2.35	0.41
1:1:58:DA:H1'	1:1:59:DG:C8	2.55	0.41
2:2:36:DG:H2''	2:2:37:DG:H8	1.82	0.41
3:B:104:LYS:HE3	3:B:104:LYS:HB3	1.87	0.41
4:C:101:ARG:HG2	4:C:119:GLU:HG2	2.01	0.41
4:C:489:PRO:O	4:C:492:MET:HG3	2.20	0.41
5:D:1011:VAL:HG21	5:D:1015:GLU:OE1	2.20	0.41
5:D:1057:SER:O	5:D:1110:GLU:HG2	2.20	0.41
5:D:1175:LEU:HB2	5:D:1190:ILE:HD13	2.02	0.41
7:F:543:ALA:HA	7:F:546:ASP:OD2	2.21	0.41
8:I:110:SER:CB	8:I:113:GLN:HE22	2.33	0.41
2:2:49:DG:OP2	8:I:115:TYR:OH	2.33	0.41
4:C:802:VAL:HA	4:C:1096:ILE:O	2.20	0.41
4:C:1101:LEU:HB3	5:D:731:ARG:HG3	2.01	0.41
4:C:1324:ASN:O	4:C:1328:LYS:HG2	2.20	0.41
5:D:283:LEU:HD13	5:D:283:LEU:HA	1.91	0.41
5:D:416:ILE:HG13	5:D:417:ARG:N	2.35	0.41
5:D:523:GLU:OE1	5:D:709:ARG:NH1	2.54	0.41
5:D:742:GLY:O	5:D:762:ASN:HB3	2.21	0.41
5:D:1079:LYS:HB2	5:D:1079:LYS:HE3	1.87	0.41
7:F:462:LYS:O	7:F:466:ILE:HG12	2.20	0.41
8:J:74:PHE:HB3	8:L:74:PHE:CE2	2.56	0.41
8:I:45:GLU:HA	8:I:48:ARG:HB3	2.02	0.41
8:I:75:TYR:CZ	8:K:71:GLY:HA2	2.56	0.41
8:L:24:ALA:O	8:L:28:GLU:HG3	2.20	0.41
1:1:26:DC:H2''	1:1:27:DC:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:69:DA:H2'	1:1:70:DT:H71	2.02	0.41
3:A:96:ASP:OD1	3:A:148:ARG:HD2	2.21	0.41
3:A:158:ARG:HH22	3:A:175:ALA:HB2	1.85	0.41
3:B:66:HIS:CE1	3:B:68:TYR:HB2	2.55	0.41
4:C:994:ARG:HD2	4:C:994:ARG:HA	1.83	0.41
7:F:452:ILE:HG22	7:F:457:ILE:HG13	2.03	0.41
8:I:74:PHE:HB3	8:K:74:PHE:CE1	2.55	0.41
8:I:98:ARG:HE	8:I:98:ARG:HB3	1.40	0.41
8:L:91:LEU:HG	8:L:103:LEU:HD12	2.02	0.41
2:2:49:DG:H2''	2:2:50:DT:H71	2.01	0.41
3:A:95:LYS:HD2	3:A:98:VAL:HG22	2.02	0.41
3:B:51:MET:HE2	3:B:51:MET:HA	2.01	0.41
4:C:238:GLN:OE1	4:C:285:ILE:N	2.54	0.41
4:C:246:LEU:H	4:C:247:ARG:HH21	1.68	0.41
4:C:1107:MET:HE3	4:C:1107:MET:HB3	1.87	0.41
5:D:886:VAL:HG21	5:D:1230:THR:HG21	2.02	0.41
7:F:98:VAL:HG22	7:F:402:LEU:HG	2.02	0.41
7:F:312:SER:OG	7:F:313:ASP:N	2.53	0.41
7:F:463:LEU:HD11	7:F:483:LEU:HD13	2.03	0.41
8:I:44:ASN:OD1	8:I:45:GLU:N	2.54	0.41
8:I:74:PHE:CZ	8:K:34:SER:HB2	2.56	0.41
8:I:113:GLN:HA	8:I:116:GLN:HG2	2.03	0.41
2:2:44:DC:OP2	7:F:573:LEU:HB2	2.20	0.41
4:C:229:ILE:HG12	4:C:332:ARG:HH22	1.86	0.41
5:D:71:LEU:HD12	5:D:71:LEU:HA	1.87	0.41
5:D:215:LYS:HD2	5:D:215:LYS:HA	1.88	0.41
5:D:421:VAL:CG2	5:D:470:VAL:HG22	2.45	0.41
5:D:664:ILE:HD12	5:D:681:LYS:HD3	2.03	0.41
8:J:39:ILE:HG13	8:J:62:ALA:CB	2.51	0.41
3:P:267:ALA:O	3:P:270:LEU:HG	2.21	0.41
8:I:38:LEU:HD13	8:I:65:LEU:HD13	2.02	0.41
8:I:78:CYS:SG	8:L:110:SER:HB3	2.61	0.41
8:L:46:LEU:HD22	8:L:51:VAL:HG11	2.02	0.41
1:1:44:DT:OP2	7:F:455:HIS:NE2	2.53	0.41
1:1:48:DG:H2''	1:1:49:DT:H71	2.01	0.41
2:2:53:DT:H2'	2:2:54:DG:C5	2.55	0.41
3:A:194:GLN:CD	3:A:195:ARG:HG3	2.46	0.41
3:B:33:ARG:HG3	3:B:197:ASP:OD1	2.20	0.41
4:C:65:ASN:HA	4:C:105:TYR:HB2	2.03	0.41
4:C:677:ASN:O	4:C:681:MET:HG3	2.21	0.41
4:C:930:ASP:OD1	4:C:931:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:154:LEU:HD23	5:D:154:LEU:HA	1.86	0.41
5:D:521:LYS:HG3	5:D:542:ALA:HA	2.02	0.41
5:D:695:LYS:HE2	5:D:695:LYS:HB3	1.91	0.41
5:D:1111:ASP:OD1	5:D:1112:GLY:N	2.53	0.41
6:E:64:LEU:HD23	6:E:64:LEU:HA	1.87	0.41
2:2:34:DG:H2'	2:2:35:DC:C6	2.56	0.41
3:B:98:VAL:HG11	3:B:121:VAL:HG21	2.03	0.41
4:C:83:GLN:O	4:C:87:ILE:HG12	2.21	0.41
4:C:134:GLY:C	4:C:135:THR:HG23	2.46	0.41
4:C:815:SER:HB3	4:C:1077:SER:HB3	2.03	0.41
4:C:819:SER:OG	4:C:820:GLU:N	2.53	0.41
4:C:887:VAL:HG13	4:C:913:VAL:HG23	2.03	0.41
4:C:935:THR:HG21	4:C:941:LYS:HG2	2.03	0.41
4:C:942:ASP:OD1	4:C:943:LYS:HG2	2.21	0.41
5:D:118:LYS:HE3	5:D:118:LYS:HB3	1.92	0.41
5:D:749:LYS:H	5:D:749:LYS:HG2	1.66	0.41
5:D:1049:GLN:HB2	5:D:1060:VAL:HG21	2.03	0.41
7:F:313:ASP:HB3	7:F:316:PHE:HB2	2.03	0.41
7:F:414:LYS:HE3	7:F:434:TRP:CZ3	2.56	0.41
7:F:473:GLU:HG3	7:F:474:MET:H	1.86	0.41
3:P:268:ASN:N	3:P:268:ASN:OD1	2.52	0.41
8:I:46:LEU:HB3	8:I:51:VAL:HB	2.03	0.41
8:K:26:GLU:O	8:K:29:SER:OG	2.24	0.41
8:L:31:TRP:CB	8:L:33:ARG:HG3	2.51	0.41
2:2:42:DA:H4'	2:2:43:DT:OP1	2.21	0.41
3:A:218:ARG:O	3:A:222:THR:HG23	2.20	0.41
3:B:85:LEU:HD23	3:B:85:LEU:HA	1.88	0.41
4:C:15:PHE:CG	4:C:1190:ALA:HB2	2.56	0.41
4:C:69:GLN:HG3	4:C:101:ARG:NH1	2.36	0.41
4:C:157:PHE:O	4:C:442:VAL:HG23	2.21	0.41
4:C:206:ALA:O	4:C:209:ILE:HG22	2.21	0.41
4:C:994:ARG:HD2	4:C:997:TRP:CG	2.56	0.41
4:C:1095:ASP:OD1	4:C:1095:ASP:N	2.49	0.41
5:D:647:PRO:HG3	5:D:697:MET:HA	2.02	0.41
5:D:682:VAL:HA	5:D:685:ILE:HG12	2.02	0.41
5:D:1060:VAL:HG13	5:D:1106:ILE:HB	2.02	0.41
7:F:290:LEU:HD11	7:F:337:VAL:HG23	2.02	0.41
7:F:455:HIS:CD2	7:F:456:MET:HG2	2.55	0.41
8:J:46:LEU:HD22	8:J:54:PRO:CB	2.45	0.41
2:2:62:DA:H62	8:I:73:GLN:NE2	2.19	0.40
3:B:95:LYS:HG2	3:B:120:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:176:ILE:HD11	4:C:428:VAL:HG21	2.03	0.40
4:C:230:PHE:CE2	4:C:292:ILE:HG23	2.56	0.40
4:C:1084:ASP:OD1	4:C:1216:ARG:HG2	2.20	0.40
7:F:133:SER:HB3	7:F:365:MET:HB2	2.02	0.40
7:F:137:TYR:CE2	7:F:139:GLU:HB2	2.56	0.40
7:F:466:ILE:O	7:F:470:MET:HG2	2.21	0.40
3:P:257:VAL:HG11	3:P:270:LEU:HD13	2.02	0.40
8:I:27:LEU:O	8:I:31:TRP:N	2.54	0.40
8:L:86:LEU:HD13	8:L:86:LEU:HA	1.86	0.40
1:1:13:DC:C2	1:1:14:DA:N7	2.89	0.40
2:2:25:DA:H1'	2:2:26:DC:O4'	2.21	0.40
2:2:52:DA:O5'	2:2:52:DA:H8	2.05	0.40
3:A:201:LEU:HD21	3:A:203:ILE:HD11	2.03	0.40
4:C:130:MET:SD	4:C:134:GLY:HA2	2.62	0.40
4:C:277:LEU:HA	4:C:277:LEU:HD13	1.85	0.40
4:C:746:ALA:HB1	4:C:970:GLY:HA3	2.04	0.40
4:C:788:SER:OG	4:C:795:ALA:O	2.39	0.40
4:C:1122:LYS:HE3	4:C:1229:TYR:CZ	2.55	0.40
5:D:492:SER:HB2	5:D:499:ILE:HD12	2.02	0.40
5:D:583:VAL:HG13	5:D:587:LEU:HD12	2.02	0.40
2:2:1:DT:H2''	2:2:2:DG:C8	2.56	0.40
3:A:10:LYS:HD3	3:A:10:LYS:HA	1.87	0.40
4:C:195:PHE:HB3	4:C:203:LYS:HB2	2.04	0.40
4:C:404:LYS:HE3	4:C:404:LYS:HB3	1.88	0.40
4:C:615:VAL:HA	4:C:638:SER:HB3	2.03	0.40
4:C:835:GLU:HB2	4:C:1053:TYR:HE1	1.85	0.40
5:D:226:ALA:O	5:D:230:SER:CB	2.69	0.40
5:D:473:THR:OG1	5:D:475:GLU:OE1	2.38	0.40
5:D:803:VAL:HG13	5:D:1313:SER:OG	2.13	0.40
5:D:1029:THR:HG22	5:D:1031:VAL:H	1.85	0.40
7:F:511:ILE:HA	7:F:511:ILE:HD13	1.88	0.40
8:J:19:ILE:HA	8:L:86:LEU:HD11	2.03	0.40
3:P:307:LEU:HD23	3:P:310:ARG:HH11	1.86	0.40
2:2:55:DC:H1'	2:2:56:DT:H5'	2.03	0.40
3:A:133:LEU:HD11	3:A:140:ILE:HG22	2.02	0.40
4:C:236:LYS:HE2	4:C:286:GLU:CD	2.47	0.40
4:C:696:ASP:O	4:C:795:ALA:HB1	2.21	0.40
5:D:221:ILE:HD13	5:D:221:ILE:HA	1.90	0.40
8:J:6:PHE:CD2	8:L:48:ARG:HD3	2.52	0.40
8:J:43:GLU:OE1	8:J:55:ARG:HD2	2.21	0.40
8:J:72:ARG:CD	8:I:105:ARG:HH12	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:120:ARG:HA	8:J:123:LYS:HZ2	1.85	0.40
8:I:27:LEU:O	8:I:30:ARG:HG2	2.22	0.40
2:2:44:DC:H2'	2:2:45:DT:H6	1.82	0.40
3:A:180:VAL:HG11	3:A:183:ILE:HD11	2.02	0.40
4:C:178:PRO:HD2	4:C:183:TRP:CD1	2.57	0.40
4:C:303:ASP:OD1	4:C:308:GLU:HG3	2.22	0.40
4:C:805:MET:HE3	4:C:805:MET:HB2	1.92	0.40
4:C:821:ARG:O	4:C:825:GLU:HG2	2.21	0.40
4:C:1117:LEU:HD11	4:C:1182:ILE:HG21	2.03	0.40
5:D:127:LEU:O	5:D:192:MET:HE1	2.21	0.40
5:D:510:LEU:HD23	5:D:510:LEU:HA	1.91	0.40
5:D:514:THR:OG1	5:D:595:ALA:O	2.39	0.40
5:D:747:MET:HE2	5:D:747:MET:HB3	1.61	0.40
5:D:950:ILE:HD13	5:D:950:ILE:HA	1.89	0.40
7:F:136:GLU:CD	7:F:364:ARG:HH21	2.29	0.40
7:F:525:ASP:OD1	7:F:527:THR:HG22	2.22	0.40
8:I:117:ILE:HD12	8:I:117:ILE:HA	1.99	0.40
8:L:110:SER:O	8:L:114:ILE:HG12	2.22	0.40
8:L:119:ALA:O	8:L:123:LYS:HG3	2.21	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	
3	A	228/329 (69%)	219 (96%)	9 (4%)	0	100	100
3	B	226/329 (69%)	217 (96%)	9 (4%)	0	100	100
3	P	67/329 (20%)	64 (96%)	3 (4%)	0	100	100
4	C	1338/1342 (100%)	1281 (96%)	57 (4%)	0	100	100
5	D	1319/1407 (94%)	1251 (95%)	68 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E	77/91 (85%)	71 (92%)	6 (8%)	0	100	100
7	F	490/613 (80%)	465 (95%)	25 (5%)	0	100	100
8	I	103/160 (64%)	98 (95%)	5 (5%)	0	100	100
8	J	127/160 (79%)	124 (98%)	3 (2%)	0	100	100
8	K	122/160 (76%)	119 (98%)	3 (2%)	0	100	100
8	L	106/160 (66%)	96 (91%)	10 (9%)	0	100	100
All	All	4203/5080 (83%)	4005 (95%)	198 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	
3	A	198/286 (69%)	189 (96%)	9 (4%)	24	51
3	B	196/286 (68%)	188 (96%)	8 (4%)	27	53
3	P	62/286 (22%)	58 (94%)	4 (6%)	15	42
4	C	1152/1157 (100%)	1095 (95%)	57 (5%)	22	49
5	D	1114/1168 (95%)	1053 (94%)	61 (6%)	19	47
6	E	67/75 (89%)	65 (97%)	2 (3%)	36	60
7	F	430/540 (80%)	416 (97%)	14 (3%)	33	58
8	I	95/145 (66%)	85 (90%)	10 (10%)	6	24
8	J	117/145 (81%)	114 (97%)	3 (3%)	40	61
8	K	112/145 (77%)	109 (97%)	3 (3%)	39	60
8	L	97/145 (67%)	93 (96%)	4 (4%)	27	53
All	All	3640/4378 (83%)	3465 (95%)	175 (5%)	24	49

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	22	THR
3	A	31	LEU
3	A	90	VAL
3	A	130	ILE
3	A	159	ILE
3	A	186	ASN
3	A	205	MET
3	A	211	ILE
3	A	223	ILE
3	B	59	VAL
3	B	110	VAL
3	B	129	VAL
3	B	153	VAL
3	B	183	ILE
3	B	201	LEU
3	B	202	VAL
3	B	211	ILE
4	C	21	VAL
4	C	39	ILE
4	C	96	LEU
4	C	100	LEU
4	C	102	LEU
4	C	114	VAL
4	C	126	GLU
4	C	155	VAL
4	C	177	ILE
4	C	184	LEU
4	C	210	LEU
4	C	219	GLN
4	C	234	ASP
4	C	277	LEU
4	C	317	LEU
4	C	371	ARG
4	C	400	VAL
4	C	442	VAL
4	C	471	VAL
4	C	479	LEU
4	C	523	GLU
4	C	527	LYS
4	C	538	LEU
4	C	542	ARG
4	C	558	VAL
4	C	576	SER

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Mol	Chain	Res	Type
4	C	602	GLU
4	C	633	LEU
4	C	655	VAL
4	C	658	GLN
4	C	723	VAL
4	C	741	MET
4	C	750	ILE
4	C	777	VAL
4	C	822	VAL
4	C	843	THR
4	C	877	VAL
4	C	887	VAL
4	C	893	THR
4	C	935	THR
4	C	947	GLU
4	C	960	LEU
4	C	971	LEU
4	C	1034	ARG
4	C	1046	VAL
4	C	1082	ILE
4	C	1113	LEU
4	C	1132	LEU
4	C	1135	GLN
4	C	1149	TYR
4	C	1159	VAL
4	C	1222	GLU
4	C	1232	MET
4	C	1274	GLU
4	C	1325	VAL
4	C	1333	LEU
4	C	1341	ASP
5	D	70	CYS
5	D	78	LEU
5	D	90	VAL
5	D	93	THR
5	D	97	VAL
5	D	100	GLU
5	D	164	GLN
5	D	198	CYS
5	D	205	LEU
5	D	235	GLU
5	D	241	VAL

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Mol	Chain	Res	Type
5	D	244	VAL
5	D	264	ASP
5	D	283	LEU
5	D	312	ARG
5	D	330	MET
5	D	347	VAL
5	D	348	ASP
5	D	354	VAL
5	D	361	LEU
5	D	395	LYS
5	D	408	VAL
5	D	421	VAL
5	D	432	LEU
5	D	434	ILE
5	D	440	VAL
5	D	447	ILE
5	D	474	LEU
5	D	495	ASN
5	D	506	VAL
5	D	545	HIS
5	D	592	VAL
5	D	605	LEU
5	D	622	ASP
5	D	641	ILE
5	D	666	GLU
5	D	672	LEU
5	D	673	VAL
5	D	713	GLU
5	D	714	GLU
5	D	747	MET
5	D	801	VAL
5	D	822	MET
5	D	826	ILE
5	D	849	LEU
5	D	857	LEU
5	D	858	VAL
5	D	880	VAL
5	D	910	ASN
5	D	975	ILE
5	D	982	LEU
5	D	997	VAL
5	D	1046	ILE

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Mol	Chain	Res	Type
5	D	1074	LEU
5	D	1141	VAL
5	D	1158	GLU
5	D	1163	VAL
5	D	1224	ARG
5	D	1255	VAL
5	D	1292	LEU
5	D	1309	ILE
6	E	49	ILE
6	E	63	ILE
7	F	162	ILE
7	F	230	VAL
7	F	244	THR
7	F	277	MET
7	F	286	LEU
7	F	291	CYS
7	F	297	MET
7	F	323	ASN
7	F	471	LEU
7	F	505	ILE
7	F	506	SER
7	F	541	ARG
7	F	552	THR
7	F	598	LEU
8	J	42	LEU
8	J	67	CYS
8	J	69	LEU
3	P	257	VAL
3	P	268	ASN
3	P	281	LEU
3	P	290	LEU
8	I	35	VAL
8	I	80	ASP
8	I	86	LEU
8	I	98	ARG
8	I	104	ARG
8	I	108	ARG
8	I	110	SER
8	I	113	GLN
8	I	118	ILE
8	I	127	ARG
8	K	44	ASN

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Mol	Chain	Res	Type
8	K	74	PHE
8	K	76	ILE
8	L	33	ARG
8	L	44	ASN
8	L	76	ILE
8	L	103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	18	GLN
3	A	160	HIS
3	B	84	ASN
4	C	36	GLN
4	C	69	GLN
4	C	86	GLN
4	C	150	HIS
4	C	314	ASN
4	C	613	ASN
4	C	932	GLN
4	C	1023	HIS
4	C	1157	GLN
4	C	1268	GLN
5	D	80	HIS
5	D	206	ASN
5	D	266	ASN
5	D	294	ASN
5	D	364	HIS
5	D	488	ASN
5	D	489	ASN
5	D	651	HIS
5	D	739	GLN
5	D	771	GLN
5	D	792	ASN
5	D	805	GLN
5	D	1023	HIS
5	D	1044	GLN
5	D	1195	GLN
5	D	1197	ASN
5	D	1235	ASN
5	D	1326	GLN
6	E	7	GLN

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Mol	Chain	Res	Type
7	F	406	GLN
7	F	409	ASN
7	F	455	HIS
7	F	579	GLN
7	F	589	GLN
8	J	61	GLN
8	J	73	GLN
8	J	111	GLN
8	J	125	HIS
3	P	283	GLN
3	P	294	ASN
8	I	125	HIS
8	K	61	GLN
8	L	44	ASN
8	L	129	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

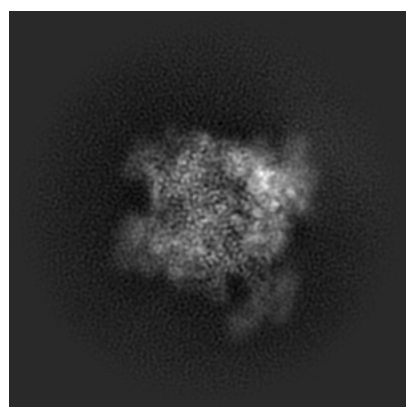
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65391. These allow visual inspection of the internal detail of the map and identification of artifacts.

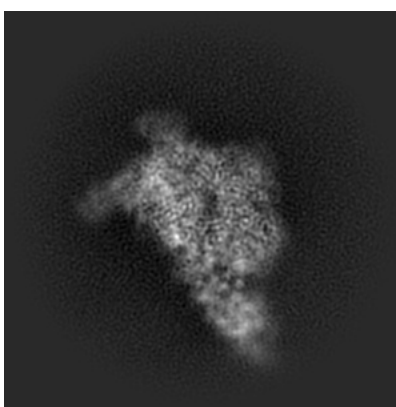
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

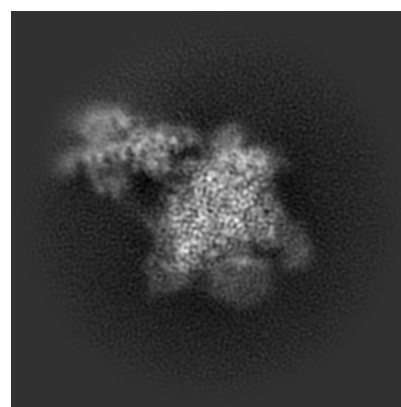
6.1.1 Primary map



X



Y

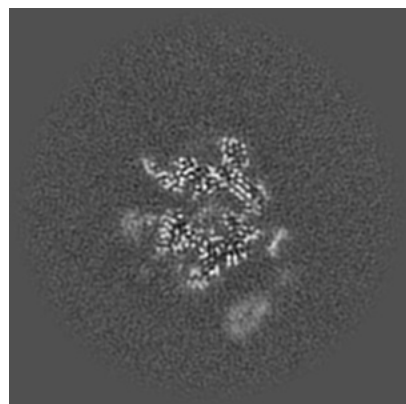


Z

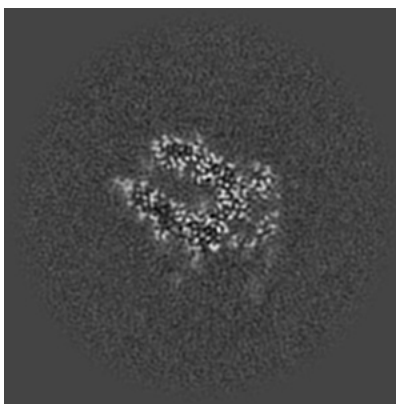
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

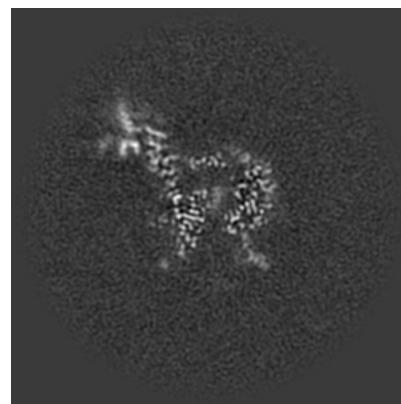
6.2.1 Primary map



X Index: 128



Y Index: 128

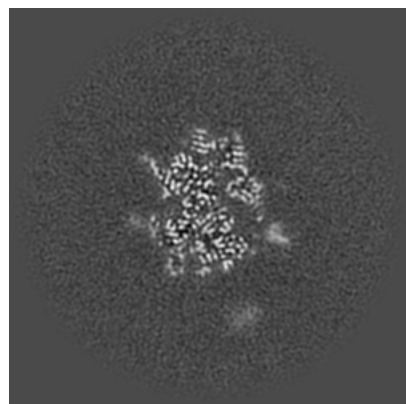


Z Index: 128

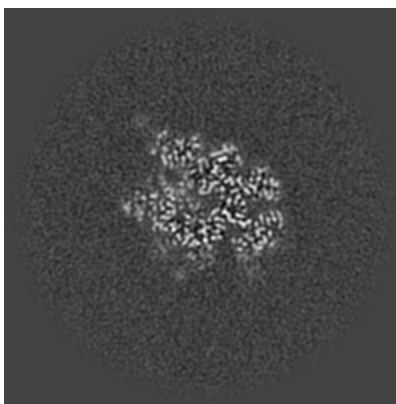
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

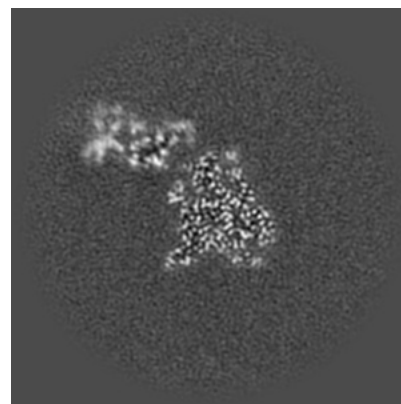
6.3.1 Primary map



X Index: 121



Y Index: 122

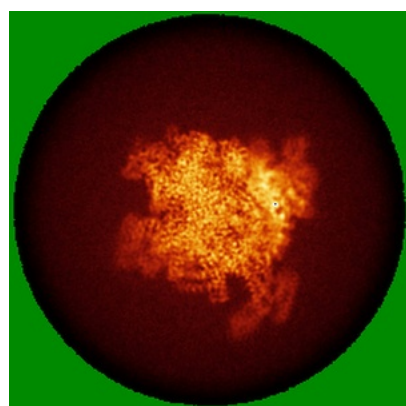


Z Index: 139

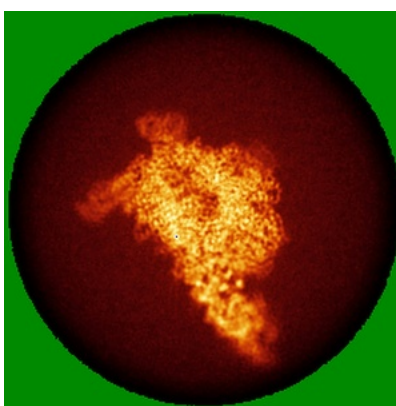
The images above show the largest variance slices of the map in three orthogonal directions.

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

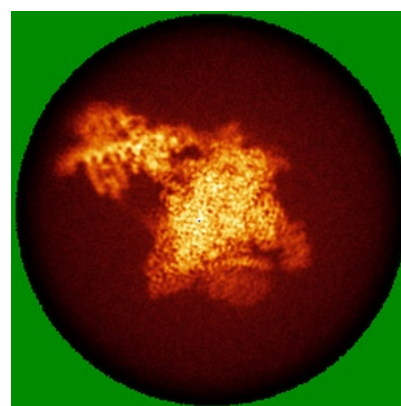
6.4.1 Primary map



X



Y



Z

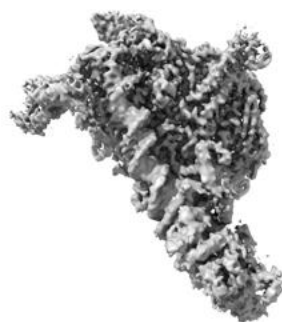
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

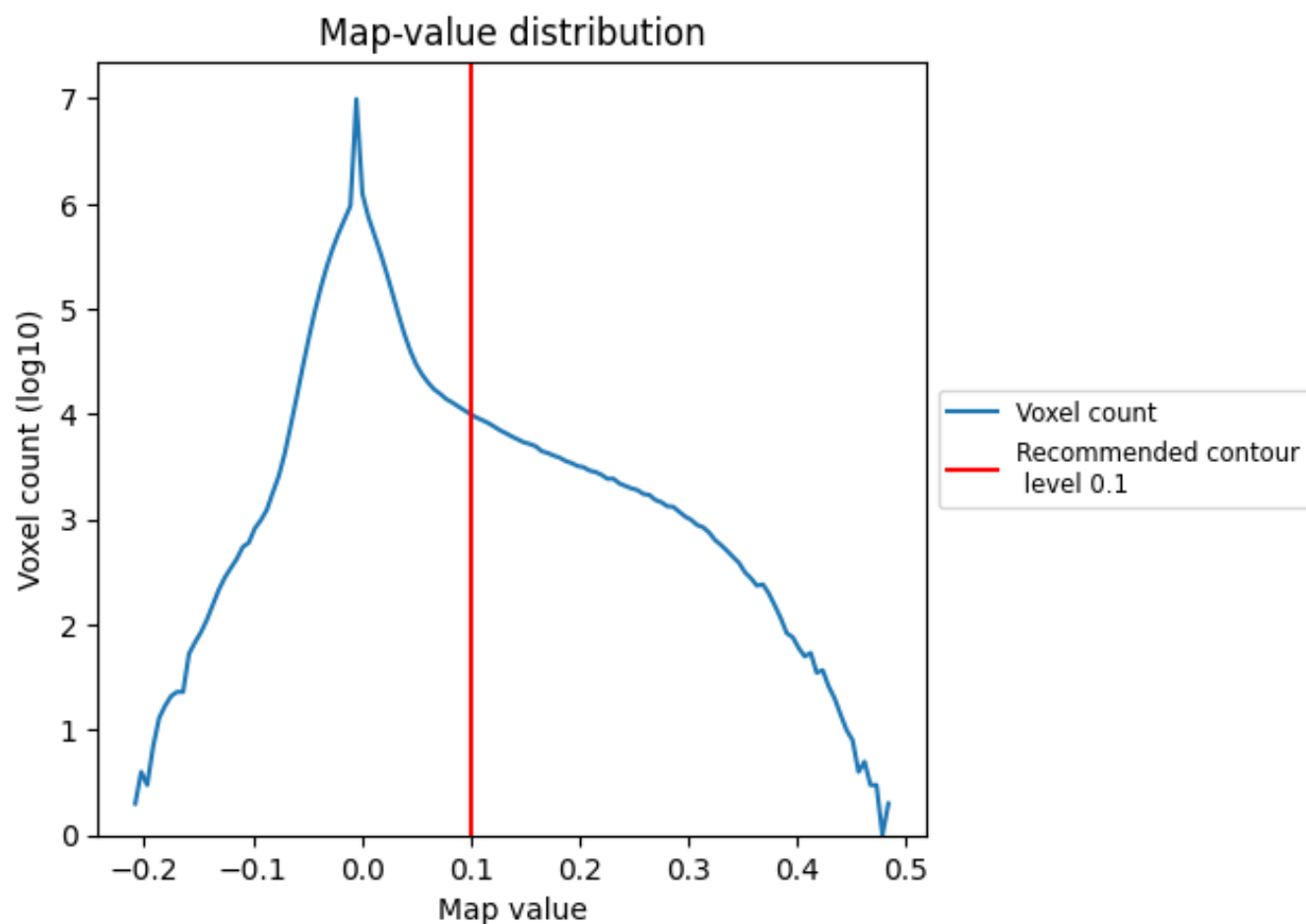
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

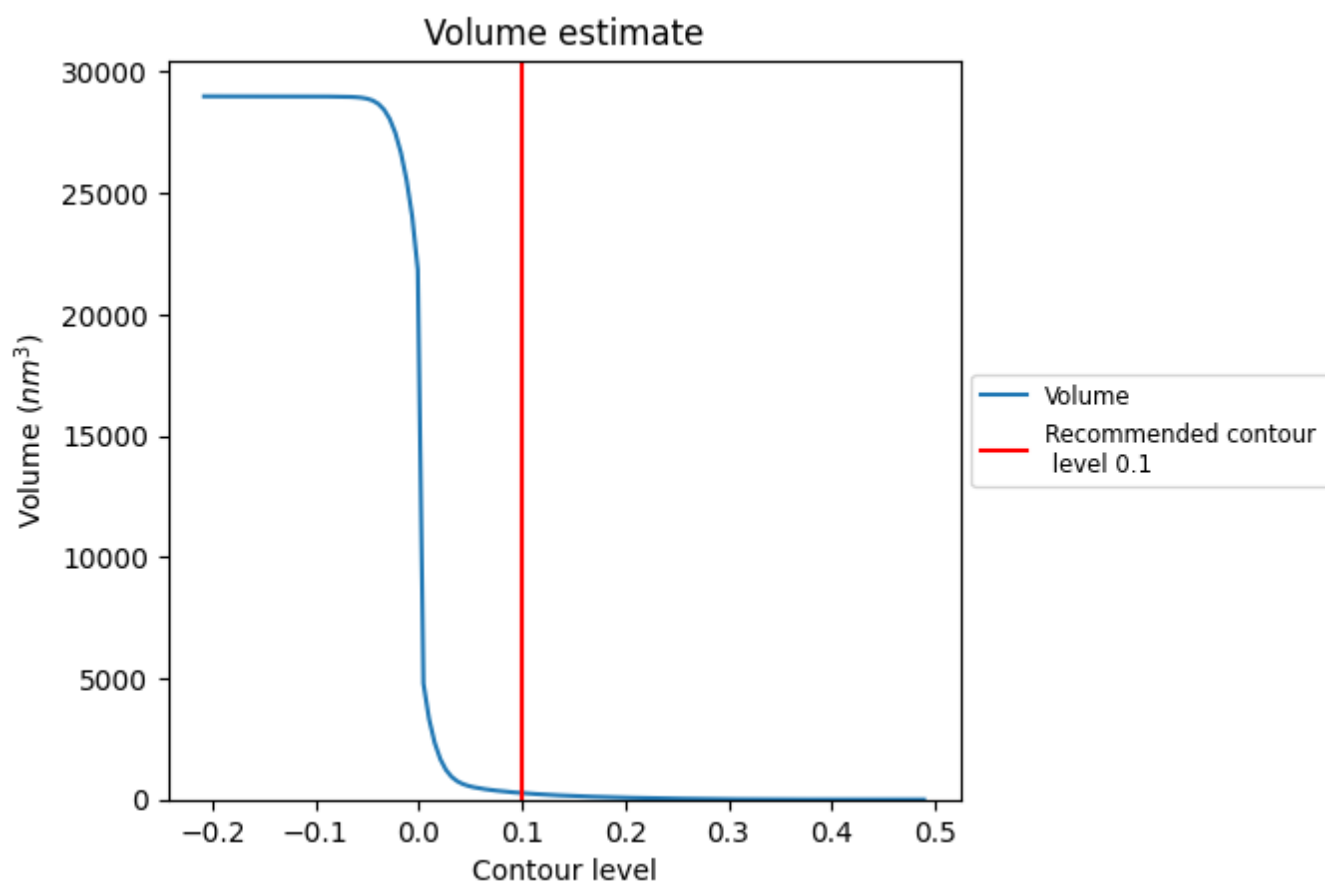
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

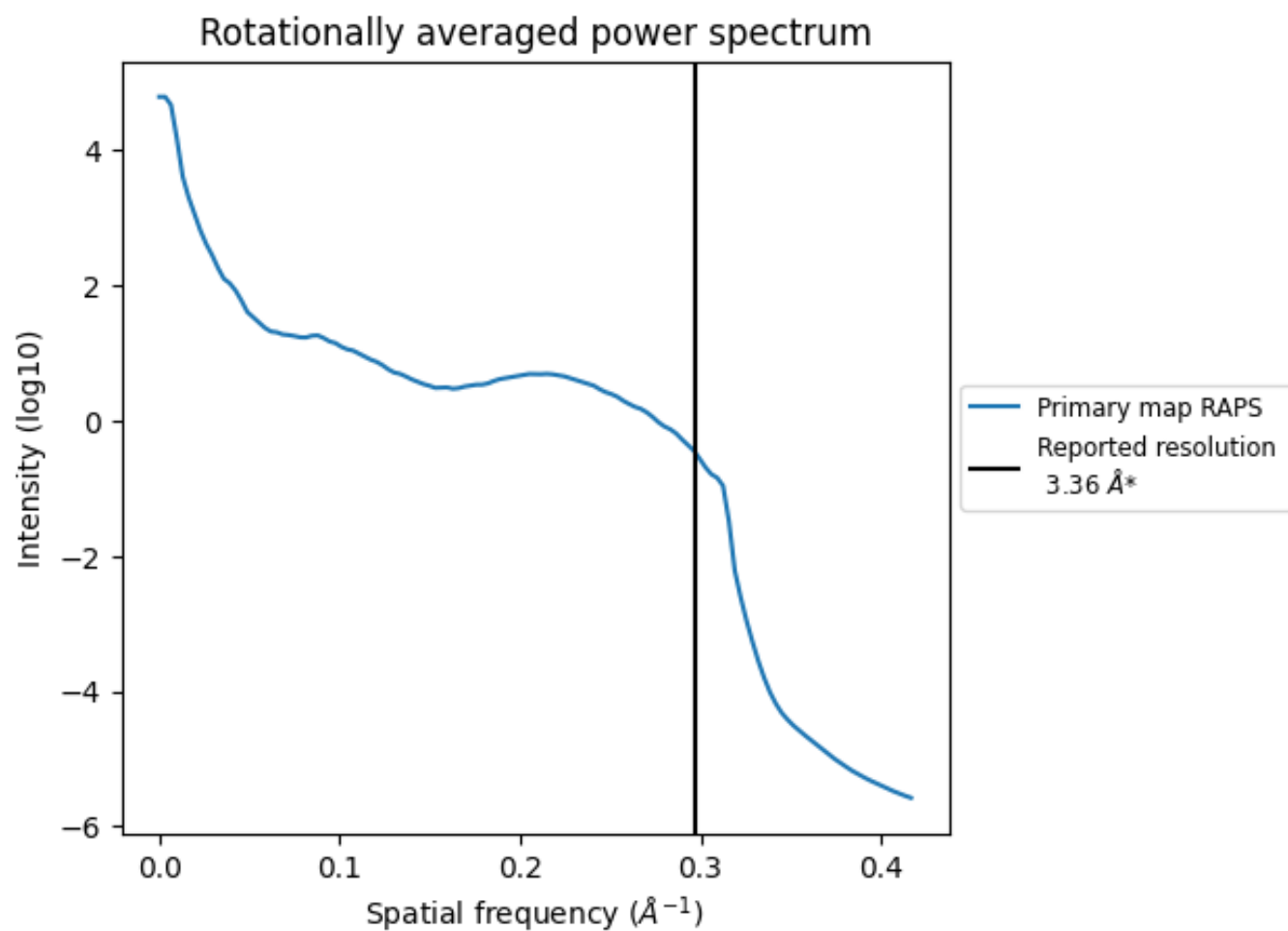
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm³; this corresponds to an approximate mass of 243 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 0.298 Å⁻¹

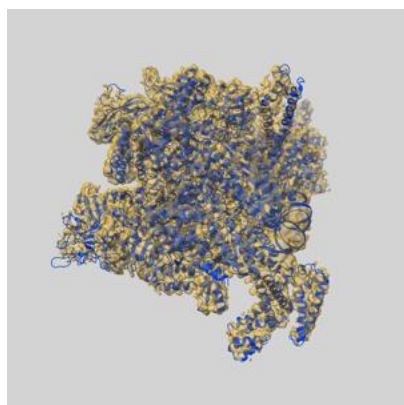
8 Fourier-Shell correlation

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

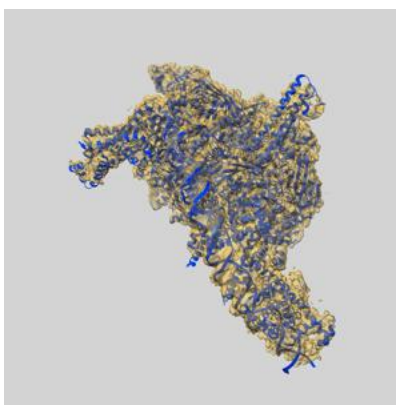
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65391 and PDB model 9VW8. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

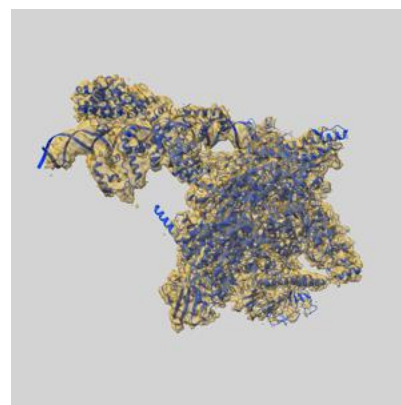
9.1 Map-model overlay [i](#)



X



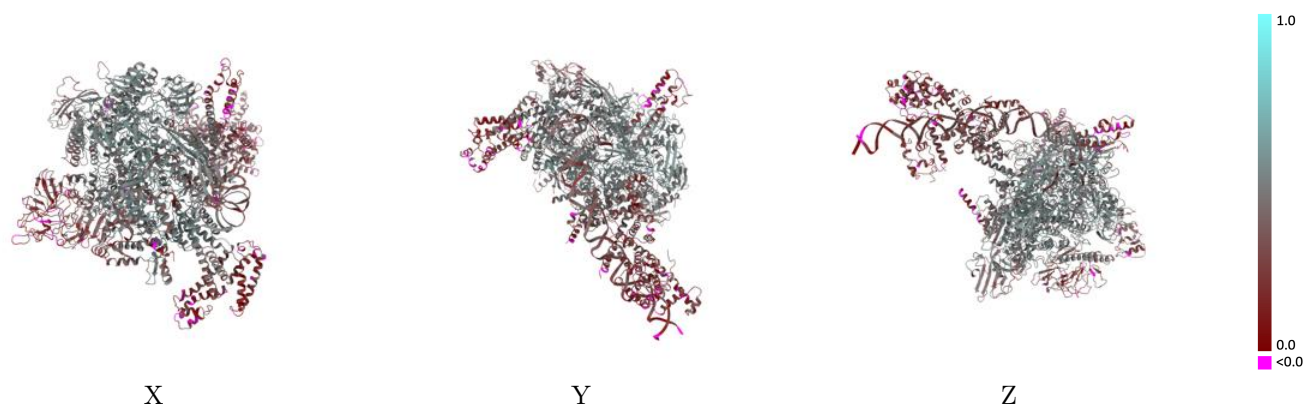
Y



Z

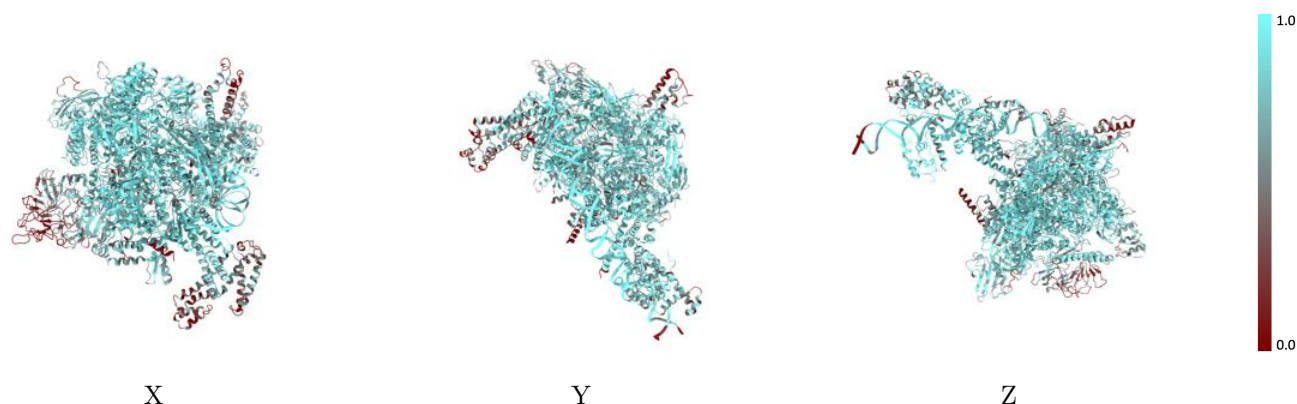
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



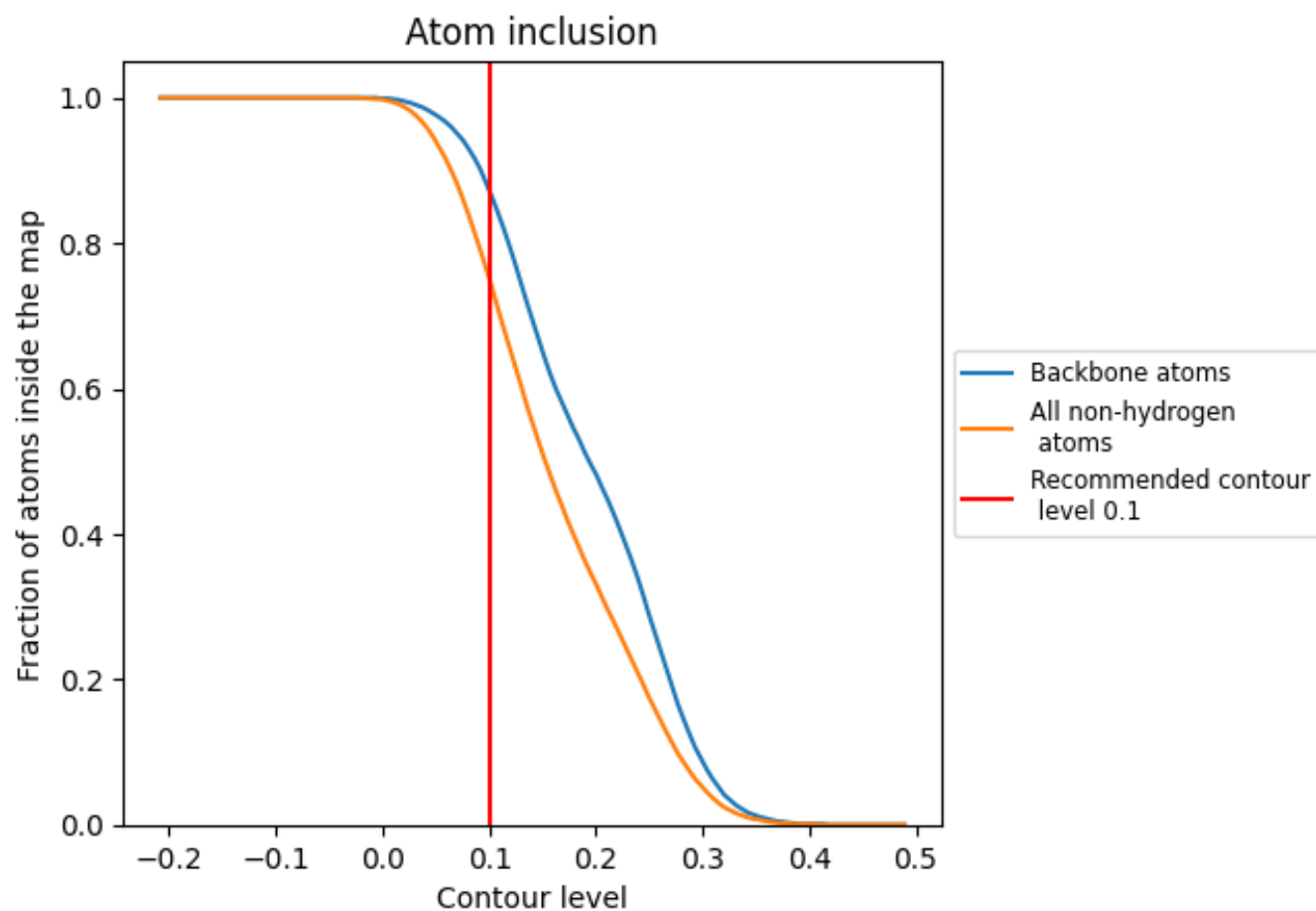
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 75% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.4050
1	0.8620	0.3390
2	0.8080	0.3000
A	0.8130	0.4910
B	0.7440	0.4370
C	0.7970	0.4690
D	0.7420	0.4430
E	0.3040	0.3020
F	0.6200	0.3380
I	0.7700	0.2150
J	0.7830	0.2990
K	0.6660	0.2000
L	0.7870	0.2730
P	0.8880	0.2480

