



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 01:32 AM EST

PDB ID : 6VOY
EMDB ID : EMD-21301
Title : Cryo-EM structure of HTLV-1 instasome
Authors : Bhatt, V.; Shi, K.; Sundborger, A.; Aihara, H.
Deposited on : 2020-02-01
Resolution : 3.70 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:

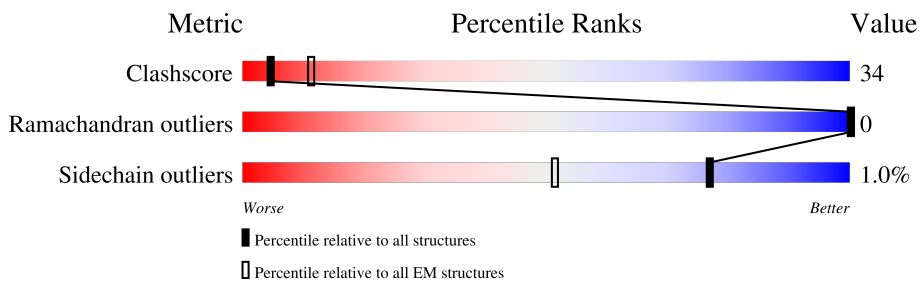
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.





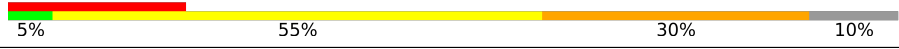

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	390	
1	B	390	
1	C	390	
1	D	390	
2	E	343	
2	F	343	
3	I	49	
3	L	49	

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Mol	Chain	Length	Quality of chain
4	J	25	 16% 76% 8%
4	M	25	 28% 64% 8%
5	K	20	 20% 5% 55% 30% 10%
5	N	20	 20% 30% 50% 10% 10%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 17556 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-binding protein 7d.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	276	Total	C	N	O	S	0	0
			2200	1394	405	393	8		
1	B	259	Total	C	N	O	S	0	0
			2058	1309	370	372	7		
1	C	276	Total	C	N	O	S	0	0
			2200	1394	405	393	8		
1	D	259	Total	C	N	O	S	0	0
			2058	1309	370	372	7		

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-94	MET	-	expression tag	UNP P39476
A	-93	GLY	-	expression tag	UNP P39476
A	-92	SER	-	expression tag	UNP P39476
A	-91	SER	-	expression tag	UNP P39476
A	-90	HIS	-	expression tag	UNP P39476
A	-89	HIS	-	expression tag	UNP P39476
A	-88	HIS	-	expression tag	UNP P39476
A	-87	HIS	-	expression tag	UNP P39476
A	-86	HIS	-	expression tag	UNP P39476
A	-85	HIS	-	expression tag	UNP P39476
A	-84	SER	-	expression tag	UNP P39476
A	-83	SER	-	expression tag	UNP P39476
A	-82	GLY	-	expression tag	UNP P39476
A	-81	LEU	-	expression tag	UNP P39476
A	-80	VAL	-	expression tag	UNP P39476
A	-79	PRO	-	expression tag	UNP P39476
A	-78	ARG	-	expression tag	UNP P39476
A	-77	GLY	-	expression tag	UNP P39476
A	-76	SER	-	expression tag	UNP P39476
A	-75	HIS	-	expression tag	UNP P39476
A	-51	ALA	TRP	engineered mutation	UNP P39476
A	-32	GLU	ARG	conflict	UNP P39476

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	linker	UNP P39476
A	-9	GLY	-	linker	UNP P39476
A	-8	SER	-	linker	UNP P39476
A	-7	LEU	-	linker	UNP P39476
A	-6	GLU	-	linker	UNP P39476
A	-5	VAL	-	linker	UNP P39476
A	-4	LEU	-	linker	UNP P39476
A	-3	PHE	-	linker	UNP P39476
A	-2	GLN	-	linker	UNP P39476
A	-1	GLY	-	linker	UNP P39476
A	0	PRO	-	linker	UNP P39476
A	156	GLN	GLU	conflict	UNP A0A1Y1CAW1
B	-94	MET	-	expression tag	UNP P39476
B	-93	GLY	-	expression tag	UNP P39476
B	-92	SER	-	expression tag	UNP P39476
B	-91	SER	-	expression tag	UNP P39476
B	-90	HIS	-	expression tag	UNP P39476
B	-89	HIS	-	expression tag	UNP P39476
B	-88	HIS	-	expression tag	UNP P39476
B	-87	HIS	-	expression tag	UNP P39476
B	-86	HIS	-	expression tag	UNP P39476
B	-85	HIS	-	expression tag	UNP P39476
B	-84	SER	-	expression tag	UNP P39476
B	-83	SER	-	expression tag	UNP P39476
B	-82	GLY	-	expression tag	UNP P39476
B	-81	LEU	-	expression tag	UNP P39476
B	-80	VAL	-	expression tag	UNP P39476
B	-79	PRO	-	expression tag	UNP P39476
B	-78	ARG	-	expression tag	UNP P39476
B	-77	GLY	-	expression tag	UNP P39476
B	-76	SER	-	expression tag	UNP P39476
B	-75	HIS	-	expression tag	UNP P39476
B	-51	ALA	TRP	engineered mutation	UNP P39476
B	-32	GLU	ARG	conflict	UNP P39476
B	-10	GLY	-	linker	UNP P39476
B	-9	GLY	-	linker	UNP P39476
B	-8	SER	-	linker	UNP P39476
B	-7	LEU	-	linker	UNP P39476
B	-6	GLU	-	linker	UNP P39476
B	-5	VAL	-	linker	UNP P39476
B	-4	LEU	-	linker	UNP P39476
B	-3	PHE	-	linker	UNP P39476

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	linker	UNP P39476
B	-1	GLY	-	linker	UNP P39476
B	0	PRO	-	linker	UNP P39476
B	156	GLN	GLU	conflict	UNP A0A1Y1CAW1
C	-94	MET	-	expression tag	UNP P39476
C	-93	GLY	-	expression tag	UNP P39476
C	-92	SER	-	expression tag	UNP P39476
C	-91	SER	-	expression tag	UNP P39476
C	-90	HIS	-	expression tag	UNP P39476
C	-89	HIS	-	expression tag	UNP P39476
C	-88	HIS	-	expression tag	UNP P39476
C	-87	HIS	-	expression tag	UNP P39476
C	-86	HIS	-	expression tag	UNP P39476
C	-85	HIS	-	expression tag	UNP P39476
C	-84	SER	-	expression tag	UNP P39476
C	-83	SER	-	expression tag	UNP P39476
C	-82	GLY	-	expression tag	UNP P39476
C	-81	LEU	-	expression tag	UNP P39476
C	-80	VAL	-	expression tag	UNP P39476
C	-79	PRO	-	expression tag	UNP P39476
C	-78	ARG	-	expression tag	UNP P39476
C	-77	GLY	-	expression tag	UNP P39476
C	-76	SER	-	expression tag	UNP P39476
C	-75	HIS	-	expression tag	UNP P39476
C	-51	ALA	TRP	engineered mutation	UNP P39476
C	-32	GLU	ARG	conflict	UNP P39476
C	-10	GLY	-	linker	UNP P39476
C	-9	GLY	-	linker	UNP P39476
C	-8	SER	-	linker	UNP P39476
C	-7	LEU	-	linker	UNP P39476
C	-6	GLU	-	linker	UNP P39476
C	-5	VAL	-	linker	UNP P39476
C	-4	LEU	-	linker	UNP P39476
C	-3	PHE	-	linker	UNP P39476
C	-2	GLN	-	linker	UNP P39476
C	-1	GLY	-	linker	UNP P39476
C	0	PRO	-	linker	UNP P39476
C	156	GLN	GLU	conflict	UNP A0A1Y1CAW1
D	-94	MET	-	expression tag	UNP P39476
D	-93	GLY	-	expression tag	UNP P39476
D	-92	SER	-	expression tag	UNP P39476
D	-91	SER	-	expression tag	UNP P39476

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-90	HIS	-	expression tag	UNP P39476
D	-89	HIS	-	expression tag	UNP P39476
D	-88	HIS	-	expression tag	UNP P39476
D	-87	HIS	-	expression tag	UNP P39476
D	-86	HIS	-	expression tag	UNP P39476
D	-85	HIS	-	expression tag	UNP P39476
D	-84	SER	-	expression tag	UNP P39476
D	-83	SER	-	expression tag	UNP P39476
D	-82	GLY	-	expression tag	UNP P39476
D	-81	LEU	-	expression tag	UNP P39476
D	-80	VAL	-	expression tag	UNP P39476
D	-79	PRO	-	expression tag	UNP P39476
D	-78	ARG	-	expression tag	UNP P39476
D	-77	GLY	-	expression tag	UNP P39476
D	-76	SER	-	expression tag	UNP P39476
D	-75	HIS	-	expression tag	UNP P39476
D	-51	ALA	TRP	engineered mutation	UNP P39476
D	-32	GLU	ARG	conflict	UNP P39476
D	-10	GLY	-	linker	UNP P39476
D	-9	GLY	-	linker	UNP P39476
D	-8	SER	-	linker	UNP P39476
D	-7	LEU	-	linker	UNP P39476
D	-6	GLU	-	linker	UNP P39476
D	-5	VAL	-	linker	UNP P39476
D	-4	LEU	-	linker	UNP P39476
D	-3	PHE	-	linker	UNP P39476
D	-2	GLN	-	linker	UNP P39476
D	-1	GLY	-	linker	UNP P39476
D	0	PRO	-	linker	UNP P39476
D	156	GLN	GLU	conflict	UNP A0A1Y1CAW1

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	327	Total	C	N	O	S	0	0
			2676	1770	426	468	12		
2	F	327	Total	C	N	O	S	0	0
			2676	1770	426	468	12		

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*CP*AP*CP*AP*CP*TP*TP*GP*AP*CP*TP*AP*GP*GP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	47	Total	C	N	O	P	0	0
			966	460	182	277	47		
3	L	47	Total	C	N	O	P	0	0
			966	460	182	277	47		

- Molecule 4 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	25	Total	C	N	O	P	0	0
			504	244	83	153	24		
4	M	25	Total	C	N	O	P	0	0
			504	244	83	153	24		

- Molecule 5 is a DNA chain called DNA (5'-D(P*AP*CP*AP*CP*AP*CP*TP*TP*GP*AP*CP*TP*AP*GP*GP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	18	Total	C	N	O	P	0	0
			371	176	70	107	18		
5	N	18	Total	C	N	O	P	0	0
			371	176	70	107	18		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	
6	B	1	Total	Zn	0
			1	1	
6	C	1	Total	Zn	0
			1	1	
6	D	1	Total	Zn	0
			1	1	

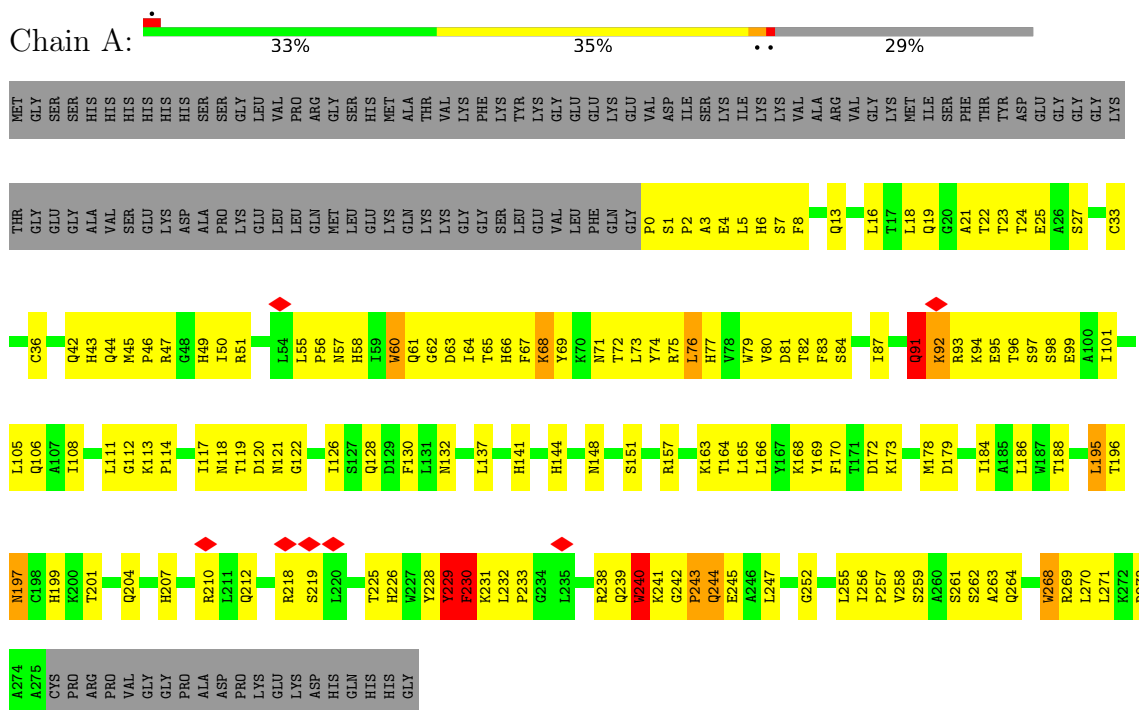
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	C	1	Total	Mg	0
			1	1	

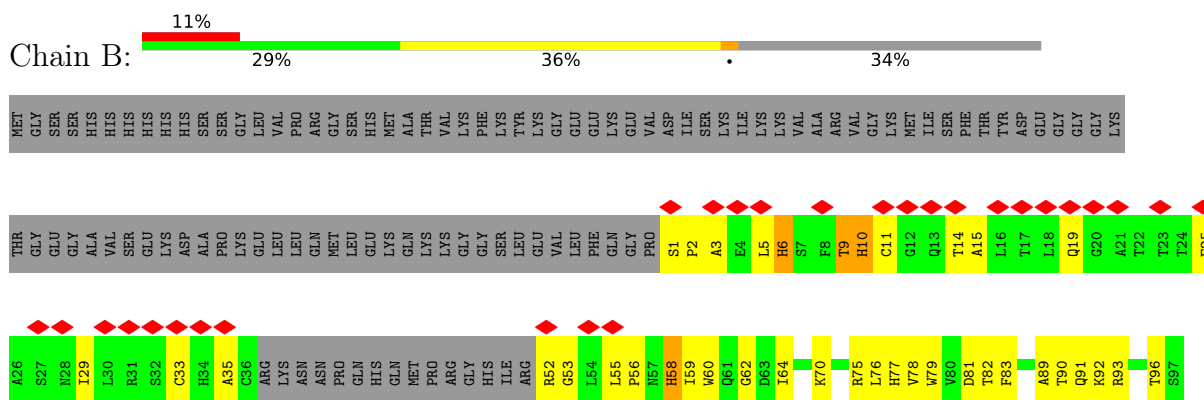
3 Residue-property plots

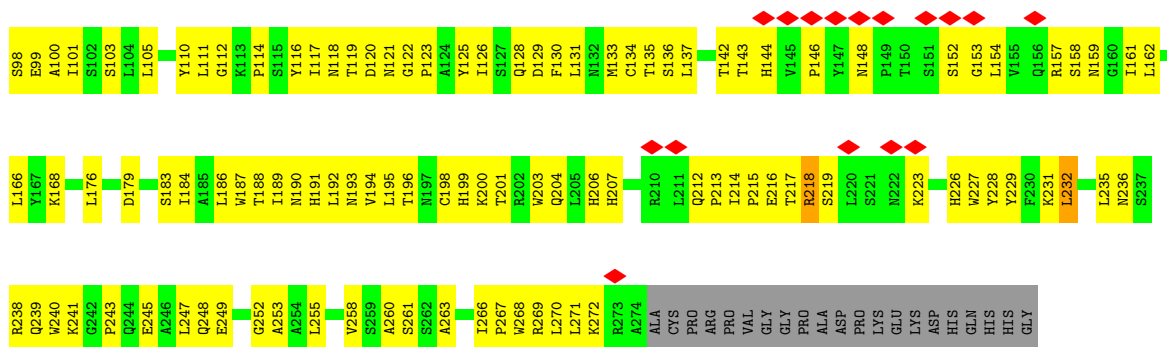
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-binding protein 7d



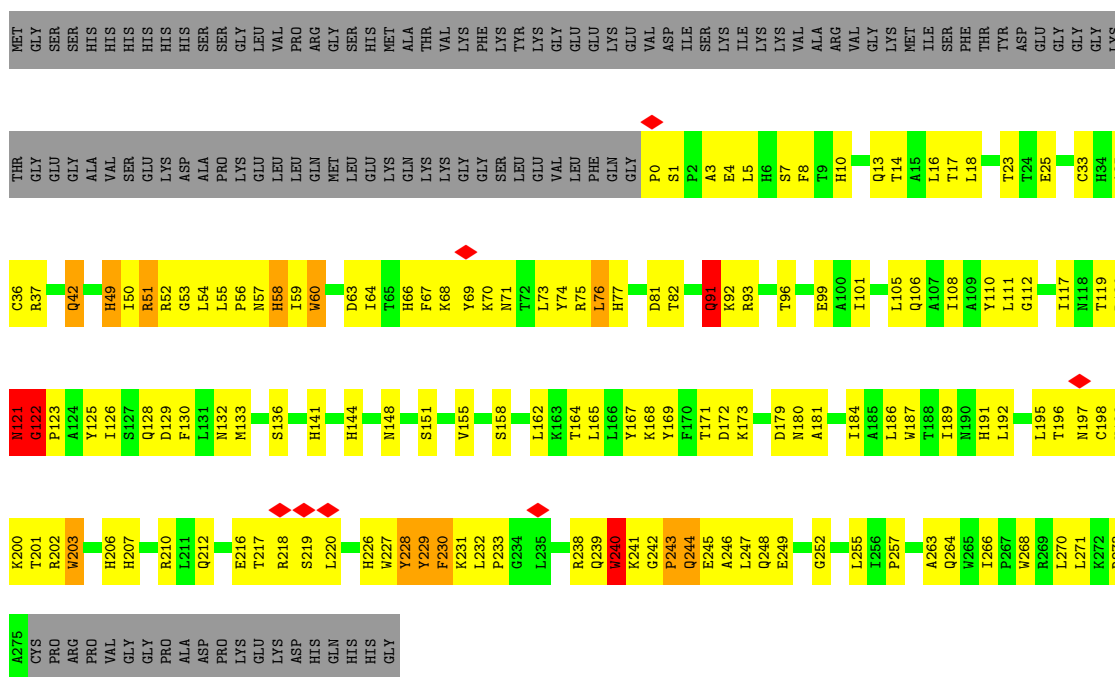
• Molecule 1: DNA-binding protein 7d





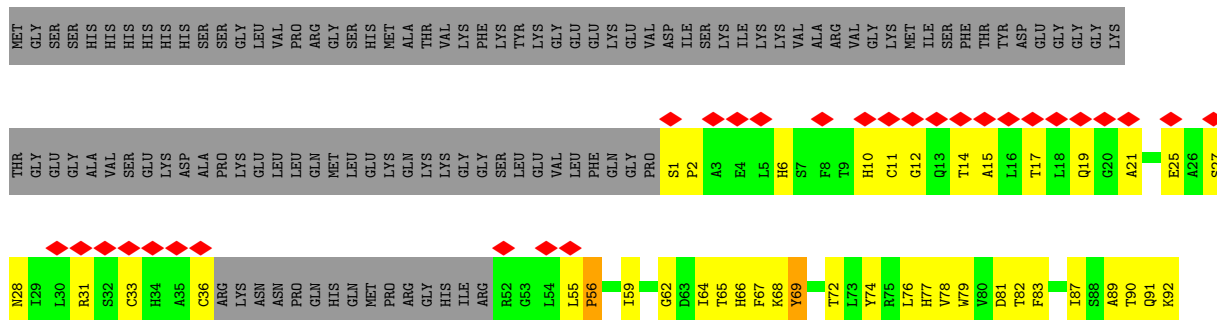
● Molecule 1: DNA-binding protein 7d

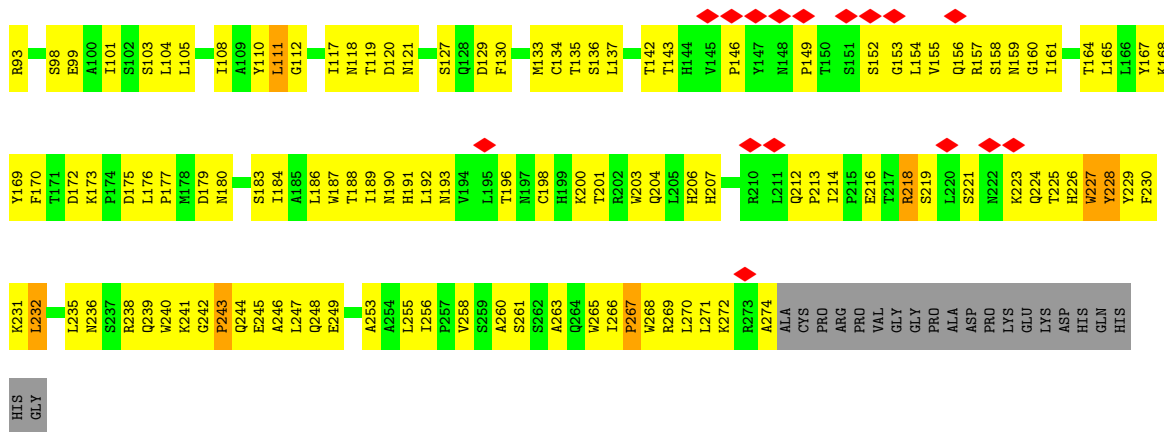
Chain C: 34% 33% 29%



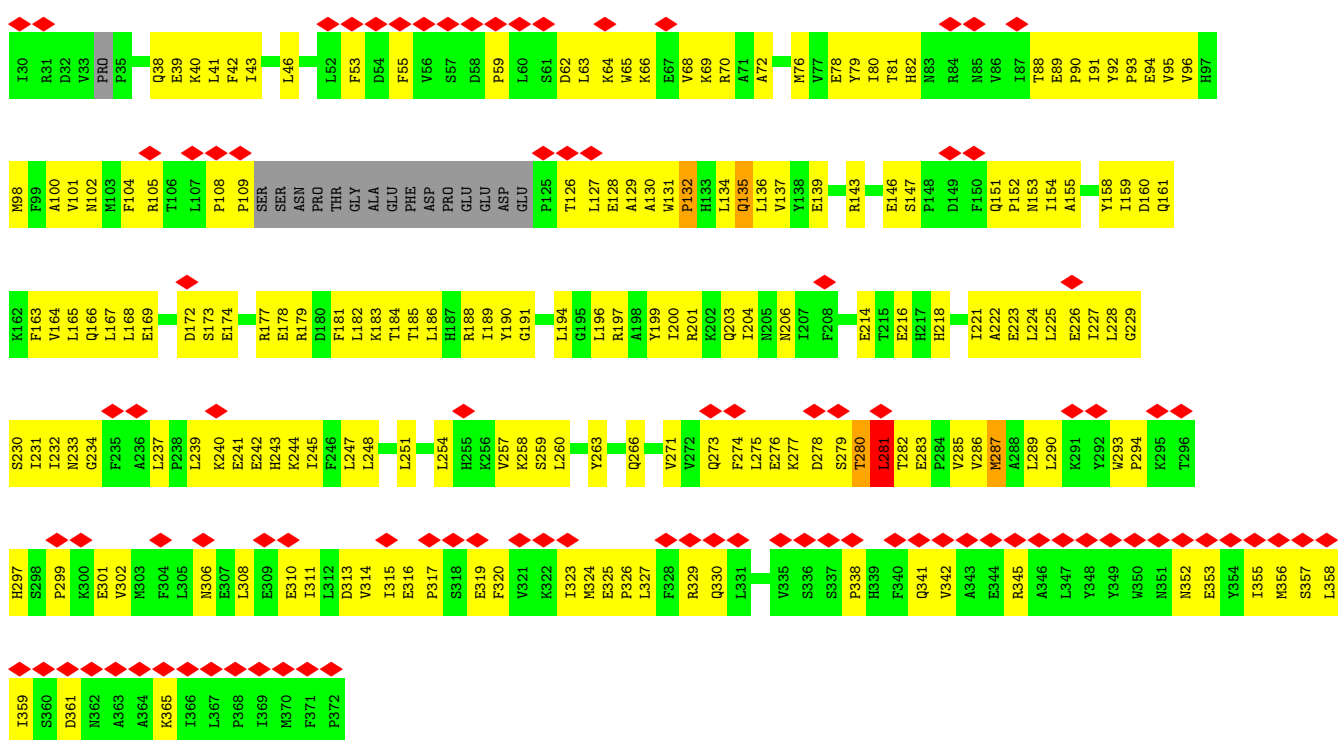
● Molecule 1: DNA-binding protein 7d

Chain D: 12% 26% 38% 34%

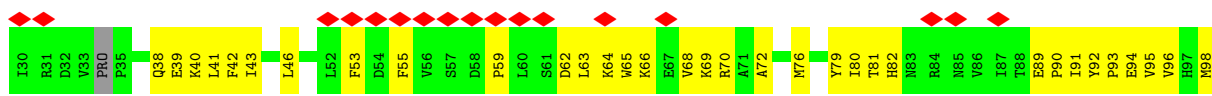


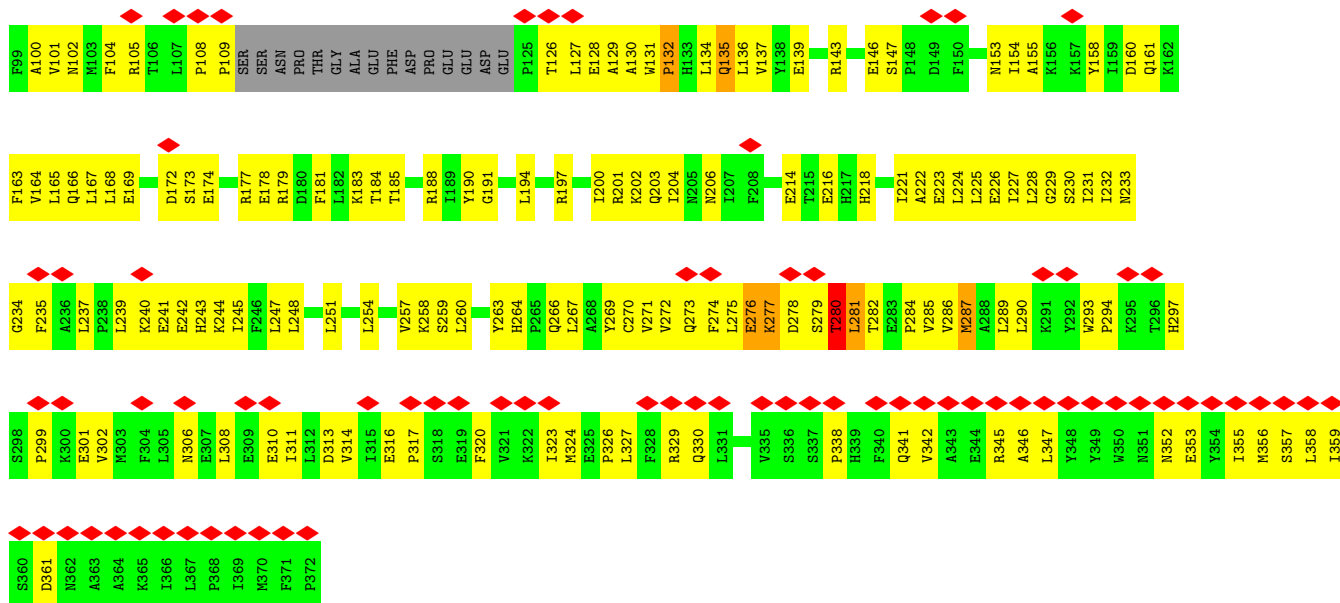


• Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

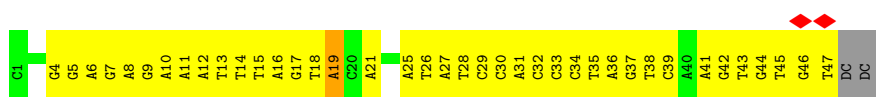


• Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

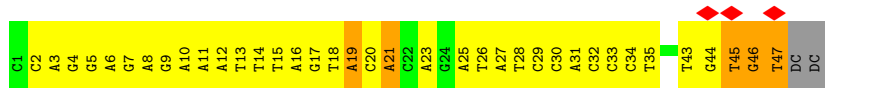




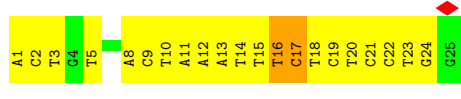
• Molecule 3: DNA (5'-D(P*AP*CP*AP*CP*AP*CP*TP*TP*GP*AP*CP*TP*AP*GP*GP*G P*TP*G)-3')



• Molecule 3: DNA (5'-D(P*AP*CP*AP*CP*AP*CP*TP*TP*GP*AP*CP*TP*AP*GP*GP*G P*TP*G)-3')



• Molecule 4: DNA (25-MER)



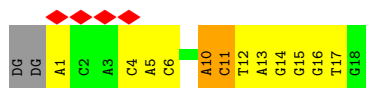
• Molecule 4: DNA (25-MER)



- Molecule 5: DNA (5'-D(P*AP*CP*AP*CP*AP*CP*TP*TP*GP*AP*CP*TP*AP*GP*GP*G P*TP*G)-3')



- Molecule 5: DNA (5'-D(P*AP*CP*AP*CP*AP*CP*TP*TP*GP*AP*CP*TP*AP*GP*GP*G P*TP*G)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	30434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00782	Depositor
Map size (Å)	235.83119, 235.83119, 235.83119	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8933, 0.8933, 0.8933	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.81	3/2264 (0.1%)	0.98	9/3085 (0.3%)
1	B	0.59	0/2116	0.76	1/2885 (0.0%)
1	C	0.79	3/2264 (0.1%)	0.96	7/3085 (0.2%)
1	D	0.59	0/2116	0.82	5/2885 (0.2%)
2	E	0.42	0/2750	0.71	3/3737 (0.1%)
2	F	0.42	0/2750	0.70	3/3737 (0.1%)
3	I	1.28	1/1085 (0.1%)	1.10	1/1672 (0.1%)
3	L	1.32	1/1085 (0.1%)	1.15	4/1672 (0.2%)
4	J	1.47	0/562	1.25	2/865 (0.2%)
4	M	1.48	0/562	1.27	2/865 (0.2%)
5	K	1.39	0/416	1.50	8/640 (1.2%)
5	N	1.23	0/416	1.19	3/640 (0.5%)
All	All	0.84	8/18386 (0.0%)	0.93	48/25768 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	12
1	D	0	8
2	E	0	5
2	F	0	5
All	All	0	44

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	TRP	CB-CG	-7.58	1.36	1.50
1	C	60	TRP	CB-CG	-7.23	1.37	1.50
1	C	240	TRP	CB-CG	-6.10	1.39	1.50
1	A	268	TRP	CB-CG	-6.07	1.39	1.50
1	A	60	TRP	CB-CG	-6.04	1.39	1.50
3	I	21	DA	N3-C4	-5.43	1.31	1.34
3	L	21	DA	N3-C4	-5.38	1.31	1.34
1	C	203	TRP	CB-CG	-5.29	1.40	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	PHE	N-CA-CB	-17.63	78.86	110.60
1	C	230	PHE	N-CA-CB	-15.12	83.38	110.60
5	K	11	DC	O4'-C1'-N1	14.11	117.88	108.00
1	D	227	TRP	C-N-CA	11.57	150.62	121.70
3	L	46	DG	O4'-C1'-N9	-9.36	101.45	108.00
1	D	228	TYR	N-CA-C	9.08	135.51	111.00
3	L	47	DT	O4'-C1'-N1	-8.04	102.37	108.00
5	K	10	DA	O4'-C1'-N9	8.00	113.60	108.00
1	C	230	PHE	N-CA-C	7.81	132.09	111.00
1	A	230	PHE	N-CA-C	7.68	131.72	111.00
1	A	76	LEU	CA-CB-CG	7.54	132.63	115.30
4	J	17	DC	O4'-C1'-N1	7.22	113.06	108.00
1	C	243	PRO	N-CA-C	7.13	130.65	112.10
1	D	232	LEU	CA-CB-CG	7.10	131.63	115.30
5	K	3	DA	O4'-C1'-N9	7.09	112.96	108.00
1	A	243	PRO	N-CA-C	6.98	130.24	112.10
5	N	11	DC	O4'-C1'-N1	6.95	112.86	108.00
1	A	91	GLN	C-N-CA	-6.93	104.37	121.70
1	C	91	GLN	C-N-CA	-6.89	104.47	121.70
1	B	232	LEU	CA-CB-CG	6.83	131.01	115.30
4	M	17	DC	O4'-C1'-N1	6.82	112.78	108.00
4	J	16	DT	O4'-C4'-C3'	-6.81	101.78	104.50
4	M	16	DT	O4'-C4'-C3'	-6.76	101.80	104.50
1	C	76	LEU	CA-CB-CG	6.73	130.77	115.30
5	K	8	DT	O4'-C1'-N1	-6.48	103.46	108.00
1	A	229	TYR	C-N-CA	-6.26	106.04	121.70
5	K	1	DA	O4'-C1'-N9	6.24	112.37	108.00
1	D	111	LEU	CA-CB-CG	-6.18	101.08	115.30
2	E	287	MET	CB-CG-SD	6.11	130.74	112.40
2	F	287	MET	CB-CG-SD	6.09	130.66	112.40
5	K	11	DC	C1'-O4'-C4'	-6.03	104.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	GLY	N-CA-C	6.00	128.10	113.10
3	L	19	DA	O4'-C4'-C3'	-5.97	102.11	104.50
1	A	195	LEU	CA-CB-CG	5.95	129.00	115.30
2	E	287	MET	CA-CB-CG	5.95	123.42	113.30
3	I	19	DA	O4'-C4'-C3'	-5.88	102.15	104.50
5	K	12	DT	O4'-C4'-C3'	-5.87	102.15	104.50
2	F	287	MET	CA-CB-CG	5.85	123.25	113.30
5	K	9	DG	O4'-C1'-N9	5.81	112.07	108.00
1	A	55	LEU	CA-CB-CG	5.56	128.09	115.30
1	D	227	TRP	CB-CA-C	-5.42	99.57	110.40
2	F	280	THR	C-N-CA	5.35	135.08	121.70
1	C	121	ASN	C-N-CA	-5.33	111.12	122.30
5	N	6	DC	O4'-C1'-N1	5.30	111.71	108.00
1	A	92	LYS	N-CA-C	5.25	125.17	111.00
2	E	281	LEU	CB-CG-CD1	5.13	119.72	111.00
5	N	10	DA	O4'-C4'-C3'	-5.11	102.46	104.50
3	L	45	DT	N3-C4-O4	5.10	122.96	119.90

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	THR	Mainchain
1	A	229	TYR	Mainchain
1	A	230	PHE	Mainchain
1	A	240	TRP	Peptide
1	A	244	GLN	Peptide
1	A	61	GLN	Mainchain
1	A	91	GLN	Peptide
1	B	11	CYS	Peptide
1	B	153	GLY	Mainchain
1	B	267	PRO	Peptide
1	B	56	PRO	Peptide
1	B	58	HIS	Peptide
1	B	70	LYS	Peptide
1	B	9	THR	Peptide
1	C	121	ASN	Peptide
1	C	122	GLY	Peptide
1	C	164	THR	Mainchain
1	C	181	ALA	Mainchain
1	C	229	TYR	Peptide,Mainchain
1	C	240	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	C	244	GLN	Peptide
1	C	42	GLN	Peptide
1	C	49	HIS	Peptide
1	C	58	HIS	Peptide
1	C	91	GLN	Peptide
1	D	153	GLY	Mainchain
1	D	224	GLN	Peptide
1	D	243	PRO	Peptide,Mainchain
1	D	25	GLU	Mainchain
1	D	267	PRO	Peptide
1	D	56	PRO	Peptide
1	D	69	TYR	Peptide
2	E	132	PRO	Mainchain
2	E	135	GLN	Mainchain
2	E	179	ARG	Mainchain
2	E	276	GLU	Peptide
2	E	280	THR	Mainchain
2	F	132	PRO	Mainchain
2	F	135	GLN	Mainchain
2	F	179	ARG	Mainchain
2	F	276	GLU	Peptide
2	F	280	THR	Mainchain

5.2 Too-close contacts [i](#)

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	2200	0	2184	170	0
1	B	2058	0	2040	147	0
1	C	2200	0	2184	164	0
1	D	2058	0	2039	152	0
2	E	2676	0	2650	182	0
2	F	2676	0	2650	168	0
3	I	966	0	529	48	0
3	L	966	0	529	49	0
4	J	504	0	287	29	0
4	M	504	0	287	22	0
5	K	371	0	203	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	371	0	203	14	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
All	All	17556	0	15785	1126	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 34.

All (1126) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:TRP:O	1:A:80:VAL:O	1.58	1.21
1:B:6:HIS:HD2	1:B:10:HIS:CD2	1.30	1.16
1:D:229:TYR:HA	1:D:243:PRO:HG3	1.33	1.10
2:F:278:ASP:O	2:F:281:LEU:HB2	1.51	1.08
1:D:227:TRP:HA	1:D:243:PRO:O	1.55	1.05
1:A:6:HIS:CD2	1:A:33:CYS:SG	2.47	1.05
1:A:44:GLN:HG3	4:J:10:DT:H5'	1.38	1.03
1:A:49:HIS:H	1:A:50:ILE:HD12	1.27	0.98
1:C:122:GLY:O	1:C:125:TYR:N	1.97	0.98
1:A:44:GLN:NE2	4:J:10:DT:OP1	2.01	0.92
3:I:37:DG:N1	5:K:11:DC:N3	2.16	0.92
1:B:6:HIS:O	1:B:10:HIS:HB2	1.71	0.91
1:D:229:TYR:CA	1:D:243:PRO:HG3	2.00	0.90
2:E:275:LEU:O	2:E:279:SER:N	2.05	0.90
2:E:299:PRO:HA	2:E:302:VAL:HG22	1.54	0.90
1:A:231:LYS:HA	1:A:241:LYS:HB2	1.56	0.88
1:C:231:LYS:HA	1:C:241:LYS:HB3	1.56	0.87
2:F:299:PRO:HA	2:F:302:VAL:HG22	1.56	0.87
2:F:275:LEU:O	2:F:279:SER:N	2.08	0.87
1:B:10:HIS:C	1:B:10:HIS:HD1	1.78	0.86
2:E:297:HIS:HB3	2:E:338:PRO:HG2	1.59	0.85
1:C:248:GLN:NE2	1:C:249:GLU:O	2.08	0.85
3:I:9:DG:H2''	3:I:10:DA:H2'	1.60	0.84
3:L:9:DG:H2''	3:L:10:DA:H2'	1.58	0.84
1:D:261:SER:O	2:E:82:HIS:NE2	2.11	0.83
1:A:226:HIS:O	1:A:245:GLU:HB2	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ASN:ND2	1:C:151:SER:OG	2.13	0.82
1:A:118:ASN:OD1	1:A:144:HIS:NE2	2.14	0.81
1:A:148:ASN:ND2	1:A:151:SER:OG	2.13	0.81
1:D:33:CYS:SG	1:D:36:CYS:HB3	2.21	0.80
1:D:227:TRP:CA	1:D:243:PRO:O	2.29	0.80
1:B:261:SER:O	2:F:82:HIS:NE2	2.14	0.80
1:A:230:PHE:CG	1:A:231:LYS:N	2.48	0.80
1:C:10:HIS:HE1	1:C:33:CYS:SG	1.91	0.79
2:E:317:PRO:HA	2:E:320:PHE:HB3	1.65	0.79
1:D:239:GLN:NE2	4:M:13:DA:OP1	2.16	0.79
1:C:120:ASP:OD1	1:C:121:ASN:N	2.14	0.79
1:D:216:GLU:O	1:D:218:ARG:NH2	2.16	0.79
2:F:317:PRO:HA	2:F:320:PHE:HB3	1.65	0.79
1:B:6:HIS:HD2	1:B:10:HIS:CG	1.97	0.79
1:B:118:ASN:OD1	1:B:144:HIS:N	2.16	0.78
1:C:230:PHE:HD1	1:C:230:PHE:H	1.31	0.78
1:D:236:ASN:ND2	4:M:12:DA:OP1	2.17	0.78
1:A:230:PHE:HD1	1:A:230:PHE:H	1.28	0.78
3:I:37:DG:N2	5:K:11:DC:O2	2.16	0.77
2:E:342:VAL:HA	2:E:345:ARG:HB2	1.66	0.77
2:F:297:HIS:HB3	2:F:338:PRO:HG2	1.65	0.77
2:E:194:LEU:O	2:E:197:ARG:HB3	1.84	0.77
1:C:42:GLN:HB2	4:M:9:DC:H5"	1.66	0.77
1:A:57:ASN:O	1:A:58:HIS:ND1	2.19	0.76
2:F:342:VAL:HA	2:F:345:ARG:HB2	1.65	0.76
2:F:194:LEU:O	2:F:197:ARG:HB3	1.85	0.76
1:C:230:PHE:CG	1:C:231:LYS:N	2.49	0.76
1:D:227:TRP:CD1	1:D:244:GLN:HA	2.21	0.76
1:C:248:GLN:HB3	1:C:255:LEU:HD23	1.67	0.75
1:A:63:ASP:OD1	1:A:64:ILE:N	2.20	0.75
1:D:227:TRP:CE3	1:D:243:PRO:HD2	2.21	0.75
2:E:260:LEU:HD13	2:E:263:TYR:HE1	1.51	0.75
1:D:213:PRO:HB2	2:E:233:ASN:HD22	1.50	0.75
1:A:230:PHE:HB2	1:A:270:LEU:O	1.87	0.74
2:E:132:PRO:O	2:E:136:LEU:HG	1.86	0.74
1:B:212:GLN:NE2	1:B:213:PRO:O	2.21	0.74
2:F:132:PRO:O	2:F:136:LEU:HG	1.86	0.74
1:B:216:GLU:O	1:B:218:ARG:NH2	2.21	0.74
2:F:260:LEU:HD13	2:F:263:TYR:HE1	1.53	0.73
1:B:200:LYS:HA	1:B:204:GLN:HE21	1.53	0.73
1:B:226:HIS:HB3	1:B:272:LYS:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLN:NE2	4:J:13:DA:OP1	2.20	0.73
1:B:110:TYR:HD1	1:B:111:LEU:H	1.36	0.73
3:L:26:DT:H2''	3:L:27:DA:H5''	1.70	0.73
1:A:57:ASN:HA	1:A:83:PHE:HB3	1.71	0.73
1:B:213:PRO:HB2	2:F:233:ASN:HD22	1.53	0.73
1:C:75:ARG:NH2	1:C:93:ARG:O	2.20	0.73
4:J:20:DT:H1'	4:J:21:DC:H5'	1.71	0.73
1:C:230:PHE:CD2	1:C:231:LYS:N	2.57	0.73
1:D:110:TYR:HD1	1:D:111:LEU:H	1.37	0.73
1:C:247:LEU:HG	1:C:257:PRO:HD3	1.71	0.73
2:E:233:ASN:HB2	2:E:273:GLN:HE22	1.52	0.72
2:F:233:ASN:HB2	2:F:273:GLN:HE22	1.51	0.72
1:B:6:HIS:O	1:B:10:HIS:CB	2.37	0.72
1:A:60:TRP:NE1	1:A:114:PRO:HB3	2.04	0.72
2:E:260:LEU:HD13	2:E:263:TYR:CE1	2.24	0.72
1:D:157:ARG:O	1:D:161:ILE:HG13	1.89	0.72
1:D:28:ASN:HA	1:D:31:ARG:HG3	1.70	0.72
1:B:10:HIS:C	1:B:10:HIS:ND1	2.40	0.72
1:B:228:TYR:HB2	1:B:270:LEU:HB3	1.72	0.72
1:B:240:TRP:NE1	1:B:269:ARG:HD3	2.05	0.72
1:D:228:TYR:HA	1:D:270:LEU:HB3	1.70	0.72
1:C:226:HIS:O	1:C:245:GLU:HB2	1.90	0.71
1:C:67:PHE:O	1:C:73:LEU:O	2.09	0.71
1:B:78:VAL:HG23	1:B:89:ALA:HB2	1.73	0.71
1:B:81:ASP:OD1	1:B:82:THR:N	2.24	0.70
2:E:279:SER:O	2:E:282:THR:HB	1.91	0.70
1:A:81:ASP:OD1	1:A:82:THR:N	2.23	0.70
1:D:212:GLN:NE2	1:D:213:PRO:O	2.25	0.70
2:F:53:PHE:HZ	2:F:65:TRP:HB2	1.57	0.70
2:F:245:ILE:HD13	2:F:248:LEU:HD21	1.74	0.70
1:C:92:LYS:HG3	1:C:93:ARG:H	1.57	0.70
2:E:53:PHE:HZ	2:E:65:TRP:HB2	1.56	0.70
1:A:230:PHE:O	1:A:240:TRP:HA	1.91	0.70
1:D:81:ASP:OD1	1:D:82:THR:N	2.25	0.70
1:C:268:TRP:HD1	1:C:271:LEU:HD12	1.56	0.70
2:E:263:TYR:HA	2:E:266:GLN:HE22	1.56	0.69
4:J:18:DT:H2''	4:J:19:DC:C5	2.27	0.69
2:F:221:ILE:O	2:F:224:LEU:HG	1.92	0.69
4:M:18:DT:H2''	4:M:19:DC:C5	2.27	0.69
1:A:76:LEU:HD23	1:A:91:GLN:HG3	1.74	0.69
3:L:6:DA:H1'	3:L:7:DG:H5'	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:245:ILE:HD13	2:E:248:LEU:HD21	1.73	0.69
1:D:200:LYS:HZ1	1:D:204:GLN:HB3	1.56	0.69
2:E:221:ILE:O	2:E:224:LEU:HG	1.92	0.69
5:K:6:DC:C4	5:K:7:DT:H73	2.28	0.69
1:A:22:THR:HG21	1:A:25:GLU:HB2	1.75	0.68
5:K:14:DG:C2	5:K:15:DG:C5	2.81	0.68
1:D:33:CYS:SG	1:D:36:CYS:CB	2.79	0.68
3:I:46:DG:H2''	3:I:47:DT:H5''	1.75	0.68
1:A:230:PHE:CD1	1:A:230:PHE:N	2.58	0.68
1:D:78:VAL:HG23	1:D:89:ALA:HB2	1.75	0.68
1:B:247:LEU:HD23	1:B:247:LEU:H	1.59	0.68
1:C:68:LYS:HE3	1:C:70:LYS:HE2	1.76	0.68
3:L:25:DA:H2''	3:L:26:DT:H5''	1.74	0.68
1:B:60:TRP:HZ2	1:B:112:GLY:H	1.40	0.68
1:D:190:ASN:O	1:D:191:HIS:ND1	2.27	0.68
2:F:260:LEU:HD13	2:F:263:TYR:CE1	2.29	0.68
3:I:6:DA:H1'	3:I:7:DG:H5'	1.75	0.68
4:M:14:DT:H2''	4:M:15:DT:H71	1.76	0.68
1:A:42:GLN:OE1	1:A:44:GLN:N	2.28	0.68
1:C:4:GLU:HA	1:C:7:SER:HB3	1.75	0.67
1:A:49:HIS:N	1:A:50:ILE:HD12	2.07	0.67
1:A:60:TRP:C	1:A:80:VAL:O	2.32	0.67
1:B:75:ARG:NH2	1:B:93:ARG:O	2.26	0.67
2:F:136:LEU:HA	2:F:139:GLU:HG3	1.77	0.67
4:J:15:DT:H2''	4:J:16:DT:H71	1.76	0.67
1:C:63:ASP:OD1	1:C:64:ILE:N	2.26	0.67
1:A:16:LEU:O	1:A:19:GLN:HG3	1.95	0.67
1:A:43:HIS:CE1	1:A:240:TRP:HH2	2.12	0.67
1:A:74:TYR:HE1	1:A:93:ARG:HE	1.42	0.67
1:A:92:LYS:HG3	1:A:93:ARG:H	1.59	0.67
1:C:180:ASN:HB2	1:D:105:LEU:HD23	1.75	0.67
3:I:26:DT:H2''	3:I:27:DA:H5''	1.76	0.67
4:J:19:DC:C6	4:J:20:DT:H72	2.29	0.67
4:M:15:DT:H2''	4:M:16:DT:H71	1.76	0.67
2:F:91:ILE:HG13	2:F:95:VAL:HG13	1.76	0.67
1:D:120:ASP:OD1	1:D:121:ASN:N	2.28	0.66
1:C:117:ILE:HG22	1:C:141:HIS:HA	1.77	0.66
2:E:136:LEU:HA	2:E:139:GLU:HG3	1.77	0.66
1:A:44:GLN:N	1:A:44:GLN:OE1	2.29	0.66
4:J:14:DT:H2''	4:J:15:DT:H71	1.77	0.66
1:A:111:LEU:HD21	1:B:203:TRP:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:ILE:HG13	2:E:95:VAL:HG13	1.77	0.66
2:F:279:SER:O	2:F:282:THR:HB	1.96	0.66
1:A:247:LEU:HB2	1:A:255:LEU:HD23	1.78	0.65
1:C:128:GLN:NE2	1:C:132:ASN:OD1	2.28	0.65
2:F:233:ASN:HB2	2:F:273:GLN:NE2	2.11	0.65
2:E:165:LEU:HA	2:E:168:LEU:CD2	2.27	0.65
1:C:229:TYR:HD1	1:C:242:GLY:C	2.00	0.65
4:M:20:DT:H1'	4:M:21:DC:H5'	1.79	0.65
1:C:230:PHE:O	1:C:240:TRP:HA	1.97	0.65
2:E:233:ASN:HB2	2:E:273:GLN:NE2	2.12	0.65
2:F:91:ILE:HD12	2:F:94:GLU:HB2	1.79	0.65
1:D:230:PHE:HD1	1:D:243:PRO:HB3	1.61	0.65
2:E:225:LEU:HD22	2:E:266:GLN:HG2	1.79	0.64
2:F:43:ILE:HG13	2:F:91:ILE:HD13	1.79	0.64
1:A:43:HIS:HE1	1:A:240:TRP:HH2	1.45	0.64
2:E:223:GLU:OE2	2:E:223:GLU:N	2.28	0.64
1:D:67:PHE:HD2	1:D:74:TYR:HB2	1.62	0.64
1:B:248:GLN:HB3	1:B:255:LEU:HB3	1.80	0.64
3:L:46:DG:H2''	3:L:47:DT:H5''	1.77	0.64
5:N:11:DC:H2''	5:N:12:DT:H71	1.80	0.64
2:E:172:ASP:OD1	2:E:218:HIS:NE2	2.30	0.64
2:F:165:LEU:HA	2:F:168:LEU:CD2	2.28	0.64
1:A:111:LEU:HD11	1:B:203:TRP:HE1	1.62	0.64
1:C:230:PHE:CD1	1:C:230:PHE:N	2.61	0.64
1:D:192:LEU:O	1:D:193:ASN:ND2	2.31	0.64
2:F:172:ASP:OD1	2:F:218:HIS:NE2	2.31	0.64
1:C:13:GLN:HA	1:C:16:LEU:HD13	1.79	0.64
1:A:105:LEU:O	1:B:183:SER:OG	2.13	0.63
2:E:43:ILE:HG13	2:E:91:ILE:HD13	1.79	0.63
2:F:223:GLU:OE1	2:F:223:GLU:N	2.29	0.63
1:A:65:THR:OG1	1:A:66:HIS:N	2.31	0.63
1:C:196:THR:O	1:C:199:HIS:ND1	2.31	0.63
1:D:118:ASN:OD1	1:D:119:THR:N	2.31	0.63
1:D:267:PRO:HA	1:D:268:TRP:HE3	1.63	0.63
2:E:91:ILE:HD12	2:E:94:GLU:HB2	1.81	0.63
2:E:227:ILE:O	2:E:230:SER:OG	2.16	0.63
3:L:43:DT:O4	5:N:4:DC:N4	2.32	0.63
2:E:131:TRP:NE1	2:E:135:GLN:OE1	2.32	0.63
1:C:241:LYS:HZ3	1:C:243:PRO:HG3	1.64	0.63
1:B:190:ASN:O	1:B:191:HIS:ND1	2.31	0.63
1:A:201:THR:OG1	1:A:204:GLN:NE2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:LYS:O	1:D:243:PRO:HD3	1.99	0.62
5:K:7:DT:H2'	5:K:8:DT:C6	2.34	0.62
1:A:128:GLN:NE2	1:A:132:ASN:OD1	2.32	0.62
1:A:230:PHE:O	1:A:240:TRP:CA	2.47	0.62
2:F:131:TRP:NE1	2:F:135:GLN:OE1	2.33	0.62
5:K:12:DT:C4	5:K:13:DA:N7	2.67	0.62
1:A:57:ASN:HB2	1:A:210:ARG:NH1	2.14	0.62
1:C:49:HIS:N	1:C:50:ILE:HG12	2.15	0.62
2:F:72:ALA:O	2:F:76:MET:HG2	2.00	0.62
3:I:25:DA:H2''	3:I:26:DT:H5''	1.80	0.62
2:E:221:ILE:HD12	2:E:221:ILE:H	1.65	0.62
2:E:275:LEU:HB3	2:E:279:SER:HB3	1.81	0.62
2:E:355:ILE:O	2:E:359:ILE:HG13	2.00	0.62
5:K:7:DT:H2'	5:K:8:DT:C5	2.35	0.62
2:E:263:TYR:HA	2:E:266:GLN:NE2	2.15	0.62
2:F:221:ILE:HD12	2:F:221:ILE:H	1.65	0.62
1:A:229:TYR:HD1	1:A:242:GLY:C	2.03	0.61
1:C:81:ASP:OD1	1:C:82:THR:N	2.32	0.61
2:F:227:ILE:O	2:F:230:SER:OG	2.17	0.61
1:D:103:SER:OG	1:D:104:LEU:N	2.31	0.61
2:E:72:ALA:O	2:E:76:MET:HG2	2.00	0.61
2:E:237:LEU:O	2:E:277:LYS:NZ	2.30	0.61
3:I:34:DC:H2'	3:I:35:DT:H71	1.81	0.61
1:B:144:HIS:CE1	1:B:148:ASN:HB3	2.35	0.61
1:D:227:TRP:HB3	1:D:243:PRO:HG2	1.81	0.61
1:D:154:LEU:HD22	1:D:157:ARG:CZ	2.30	0.61
2:E:243:HIS:O	2:E:247:LEU:HG	2.00	0.61
1:C:231:LYS:CA	1:C:241:LYS:HB3	2.28	0.61
2:E:228:LEU:HA	2:E:231:ILE:HD12	1.82	0.61
1:A:62:GLY:HA3	1:A:79:TRP:HA	1.82	0.61
2:F:237:LEU:HD23	2:F:239:LEU:N	2.15	0.61
1:A:76:LEU:HD23	1:A:91:GLN:HB2	1.82	0.61
2:F:243:HIS:O	2:F:247:LEU:HG	2.01	0.61
2:F:355:ILE:O	2:F:359:ILE:HG13	2.00	0.61
1:C:96:THR:OG1	1:C:99:GLU:N	2.33	0.60
3:L:32:DC:H2'	3:L:33:DC:C6	2.36	0.60
1:C:230:PHE:O	1:C:240:TRP:CA	2.49	0.60
1:D:160:GLY:O	1:D:164:THR:HG23	2.02	0.60
5:K:15:DG:C2	5:K:16:DG:C5	2.90	0.60
1:A:207:HIS:HE1	1:B:207:HIS:CD2	2.20	0.60
1:B:10:HIS:ND1	1:B:10:HIS:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:324:MET:HA	2:E:327:LEU:HD12	1.84	0.60
1:A:68:LYS:HD2	1:A:69:TYR:C	2.22	0.60
1:A:255:LEU:HD11	1:A:263:ALA:HB1	1.84	0.60
2:F:70:ARG:HH22	2:F:132:PRO:HB2	1.65	0.60
2:F:324:MET:HA	2:F:327:LEU:HD12	1.82	0.60
1:C:53:GLY:C	1:C:54:LEU:HD22	2.22	0.60
3:L:31:DA:C8	3:L:31:DA:H5'	2.37	0.60
1:C:197:ASN:HA	1:C:199:HIS:CE1	2.37	0.60
2:F:38:GLN:O	2:F:41:LEU:HG	2.02	0.60
2:F:163:PHE:CE1	2:F:167:LEU:HD11	2.36	0.60
1:C:13:GLN:O	1:C:17:THR:HG23	2.01	0.60
2:E:237:LEU:HD23	2:E:239:LEU:N	2.17	0.60
5:N:11:DC:H1'	5:N:12:DT:C6	2.36	0.60
1:C:76:LEU:HA	1:C:91:GLN:HB3	1.82	0.59
1:D:270:LEU:HG	1:D:271:LEU:H	1.67	0.59
2:E:70:ARG:HH22	2:E:132:PRO:HB2	1.65	0.59
1:D:256:ILE:HD11	1:D:266:ILE:HD13	1.84	0.59
2:E:274:PHE:O	2:E:278:ASP:HB2	2.02	0.59
1:A:13:GLN:HA	1:A:16:LEU:HD13	1.84	0.59
1:D:155:VAL:HG23	1:D:156:GLN:HE21	1.66	0.59
2:E:165:LEU:HA	2:E:168:LEU:HD23	1.83	0.59
1:B:186:LEU:O	1:B:189:ILE:N	2.35	0.59
1:C:212:GLN:OE1	1:D:248:GLN:NE2	2.34	0.59
1:A:101:ILE:HD11	1:A:130:PHE:HA	1.84	0.59
1:B:118:ASN:OD1	1:B:144:HIS:HB2	2.03	0.59
1:B:100:ALA:O	1:B:103:SER:OG	2.20	0.59
1:B:214:ILE:O	2:F:234:GLY:HA3	2.03	0.59
1:B:269:ARG:CZ	1:B:270:LEU:HB2	2.32	0.59
1:C:91:GLN:OE1	1:C:92:LYS:HA	2.03	0.59
1:B:101:ILE:HD11	1:B:130:PHE:HA	1.85	0.59
1:B:269:ARG:HH12	1:B:270:LEU:HD13	1.66	0.59
2:E:143:ARG:O	2:E:147:SER:OG	2.20	0.59
2:F:228:LEU:HA	2:F:231:ILE:HD12	1.83	0.59
1:D:81:ASP:OD1	1:D:83:PHE:N	2.34	0.59
2:E:38:GLN:O	2:E:41:LEU:HG	2.02	0.59
2:E:163:PHE:CE1	2:E:167:LEU:HD11	2.37	0.59
2:E:271:VAL:O	2:E:274:PHE:HB3	2.03	0.59
1:B:154:LEU:HG	1:B:157:ARG:NH2	2.17	0.58
1:D:221:SER:OG	1:D:223:LYS:NZ	2.36	0.58
1:A:36:CYS:HA	1:C:168:LYS:HE2	1.85	0.58
2:E:200:ILE:HD12	2:E:203:GLN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PRO:HA	1:A:262:SER:O	2.04	0.58
1:C:51:ARG:HD2	4:J:5:DT:OP1	2.03	0.58
1:D:196:THR:OG1	1:D:198:CYS:SG	2.48	0.58
2:E:214:GLU:N	2:E:214:GLU:OE1	2.36	0.58
1:B:58:HIS:HE2	1:B:112:GLY:HA3	1.68	0.58
2:F:128:GLU:OE1	2:F:130:ALA:N	2.29	0.58
5:K:16:DG:H2''	5:K:17:DT:H71	1.84	0.58
1:C:241:LYS:NZ	1:C:243:PRO:HG3	2.18	0.58
1:B:196:THR:OG1	1:B:198:CYS:SG	2.55	0.58
1:C:76:LEU:HD23	1:C:91:GLN:HB3	1.85	0.58
1:C:167:TYR:O	1:C:171:THR:HG23	2.04	0.58
1:C:207:HIS:HE1	1:D:207:HIS:CD2	2.22	0.58
2:F:214:GLU:N	2:F:214:GLU:OE1	2.37	0.58
1:D:170:PHE:HB3	1:D:176:LEU:HD21	1.86	0.58
1:C:228:TYR:HB3	1:C:273:ARG:HA	1.84	0.58
3:L:4:DG:H1'	3:L:5:DG:H5'	1.84	0.58
2:E:275:LEU:O	2:E:278:ASP:N	2.37	0.58
1:D:229:TYR:HA	1:D:243:PRO:CG	2.21	0.57
2:F:240:LYS:HG3	2:F:242:GLU:H	1.69	0.57
5:K:12:DT:N3	5:K:13:DA:N7	2.52	0.57
1:A:95:GLU:N	1:A:95:GLU:OE1	2.37	0.57
1:C:54:LEU:HD11	1:C:82:THR:HG23	1.86	0.57
1:B:214:ILE:HD11	2:F:197:ARG:NH2	2.19	0.57
1:C:64:ILE:HD13	1:C:77:HIS:CD2	2.38	0.57
2:E:64:LYS:O	2:E:68:VAL:HG22	2.05	0.57
2:F:200:ILE:HD12	2:F:203:GLN:HB2	1.86	0.57
5:K:16:DG:C2'	5:K:17:DT:H71	2.34	0.57
2:E:282:THR:O	2:E:285:VAL:HG22	2.04	0.57
1:C:172:ASP:OD1	1:C:173:LYS:N	2.36	0.57
3:I:13:DT:H1'	3:I:14:DT:H5''	1.87	0.57
2:E:128:GLU:OE1	2:E:130:ALA:N	2.29	0.57
2:F:282:THR:O	2:F:285:VAL:HG22	2.04	0.57
1:C:231:LYS:HA	1:C:241:LYS:CB	2.33	0.57
2:F:165:LEU:HA	2:F:168:LEU:HD23	1.86	0.57
2:F:190:TYR:CE1	2:F:197:ARG:HG3	2.40	0.57
4:J:19:DC:N1	4:J:20:DT:H72	2.20	0.57
1:D:228:TYR:C	1:D:243:PRO:HG3	2.25	0.57
2:F:222:ALA:HA	2:F:225:LEU:HD13	1.87	0.57
2:F:286:VAL:HB	2:F:323:ILE:HD13	1.87	0.57
1:C:218:ARG:HG3	1:C:219:SER:H	1.69	0.56
2:E:323:ILE:HG13	2:E:327:LEU:HG	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:143:ARG:O	2:F:147:SER:OG	2.22	0.56
2:F:197:ARG:HG2	2:F:201:ARG:HH21	1.70	0.56
2:F:323:ILE:HD12	2:F:326:PRO:HG2	1.86	0.56
4:M:19:DC:C6	4:M:20:DT:H72	2.40	0.56
1:B:19:GLN:N	1:B:19:GLN:OE1	2.39	0.56
2:E:240:LYS:HG3	2:E:242:GLU:H	1.70	0.56
2:F:46:LEU:HD22	2:F:91:ILE:HD11	1.87	0.56
2:F:64:LYS:O	2:F:68:VAL:HG22	2.05	0.56
1:A:196:THR:O	1:A:199:HIS:N	2.38	0.56
1:A:218:ARG:NH1	1:A:219:SER:HB2	2.20	0.56
1:B:81:ASP:OD1	1:B:83:PHE:N	2.37	0.56
1:B:134:CYS:SG	1:B:135:THR:N	2.78	0.56
1:D:65:THR:HG22	1:D:66:HIS:O	2.05	0.56
1:D:249:GLU:N	1:D:249:GLU:OE1	2.38	0.56
2:E:323:ILE:HD12	2:E:326:PRO:HG2	1.87	0.56
3:I:32:DC:H2'	3:I:33:DC:C6	2.41	0.56
1:A:179:ASP:OD1	1:A:179:ASP:N	2.31	0.56
1:D:149:PRO:O	1:D:152:SER:OG	2.18	0.56
2:E:40:LYS:HA	2:E:43:ILE:HG22	1.88	0.56
1:A:60:TRP:HZ2	1:A:112:GLY:O	1.89	0.56
1:C:0:PRO:O	1:C:3:ALA:N	2.38	0.56
1:D:62:GLY:HA3	1:D:79:TRP:CE3	2.39	0.56
1:D:214:ILE:O	2:E:234:GLY:HA3	2.05	0.56
1:D:227:TRP:NE1	1:D:244:GLN:HA	2.21	0.56
1:A:172:ASP:OD1	1:A:173:LYS:N	2.39	0.56
1:A:238:ARG:HE	1:A:239:GLN:H	1.52	0.56
2:F:224:LEU:O	2:F:228:LEU:HD23	2.06	0.56
1:C:232:LEU:HD12	1:C:233:PRO:HD2	1.88	0.56
2:E:93:PRO:HA	2:E:96:VAL:HG12	1.88	0.56
1:B:157:ARG:O	1:B:161:ILE:HG13	2.05	0.56
2:E:46:LEU:HD22	2:E:91:ILE:HD11	1.87	0.56
1:C:14:THR:O	1:C:17:THR:OG1	2.19	0.55
1:C:56:PRO:HA	1:C:210:ARG:HH12	1.72	0.55
2:F:40:LYS:HA	2:F:43:ILE:HG22	1.88	0.55
2:F:93:PRO:HA	2:F:96:VAL:HG12	1.88	0.55
4:M:17:DC:H2''	4:M:18:DT:H71	1.87	0.55
1:A:80:VAL:HG23	1:A:87:ILE:HD13	1.88	0.55
1:A:121:ASN:ND2	5:K:18:DG:OP1	2.39	0.55
1:B:229:TYR:HB3	1:B:240:TRP:HB3	1.88	0.55
2:F:323:ILE:HG13	2:F:327:LEU:HG	1.89	0.55
1:A:231:LYS:CA	1:A:241:LYS:HB2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:SER:OG	1:D:129:ASP:OD1	2.13	0.55
1:D:186:LEU:O	1:D:189:ILE:N	2.39	0.55
1:D:214:ILE:HD12	2:E:191:GLY:HA2	1.87	0.55
2:E:306:ASN:O	2:E:310:GLU:HG2	2.06	0.55
3:L:13:DT:H1'	3:L:14:DT:H5''	1.87	0.55
1:C:196:THR:O	1:C:199:HIS:N	2.40	0.55
1:C:244:GLN:H	1:C:244:GLN:CD	2.10	0.55
2:F:306:ASN:O	2:F:310:GLU:HG2	2.06	0.55
1:A:57:ASN:HB2	1:A:210:ARG:HH12	1.71	0.55
1:B:219:SER:OG	2:F:197:ARG:NH2	2.39	0.55
1:D:77:HIS:O	1:D:89:ALA:HB1	2.06	0.55
2:E:160:ASP:O	2:E:163:PHE:HB3	2.07	0.55
1:B:53:GLY:C	1:B:55:LEU:HG	2.27	0.55
1:B:111:LEU:HD13	1:B:112:GLY:HA2	1.88	0.55
1:B:122:GLY:O	1:B:126:ILE:HG12	2.05	0.55
1:C:230:PHE:HB3	1:C:271:LEU:HA	1.87	0.55
1:D:228:TYR:C	1:D:243:PRO:CG	2.75	0.55
1:D:240:TRP:NE1	1:D:269:ARG:HD3	2.21	0.55
2:F:203:GLN:HA	2:F:206:ASN:ND2	2.22	0.55
1:C:59:ILE:O	1:C:82:THR:HG22	2.07	0.55
1:C:206:HIS:HD2	1:C:207:HIS:HD2	1.54	0.55
1:A:69:TYR:CD2	1:A:71:ASN:HA	2.42	0.55
1:A:118:ASN:OD1	1:A:119:THR:N	2.40	0.55
1:A:196:THR:OG1	1:A:197:ASN:N	2.40	0.55
1:B:137:LEU:HD21	1:C:8:PHE:CE2	2.42	0.55
1:C:67:PHE:O	1:C:74:TYR:HB2	2.06	0.55
1:C:171:THR:OG1	1:C:172:ASP:N	2.40	0.55
2:E:329:ARG:O	2:E:330:GLN:NE2	2.40	0.55
3:I:34:DC:H2'	3:I:35:DT:C6	2.42	0.55
3:L:43:DT:H2''	3:L:44:DG:N7	2.21	0.55
1:C:1:SER:O	1:C:5:LEU:HB2	2.07	0.55
2:E:203:GLN:HA	2:E:206:ASN:ND2	2.22	0.55
2:F:155:ALA:HA	2:F:158:TYR:HD2	1.72	0.55
1:B:255:LEU:HD11	1:B:263:ALA:HB1	1.88	0.54
2:F:160:ASP:O	2:F:163:PHE:HB3	2.06	0.54
1:C:111:LEU:CD1	1:C:112:GLY:HA2	2.37	0.54
2:F:81:THR:HA	2:F:143:ARG:NH2	2.22	0.54
2:F:329:ARG:O	2:F:330:GLN:NE2	2.40	0.54
1:A:45:MET:SD	1:A:268:TRP:HB2	2.47	0.54
1:D:79:TRP:CH2	1:D:117:ILE:HD11	2.42	0.54
2:E:224:LEU:O	2:E:228:LEU:HD23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:HIS:O	1:D:207:HIS:ND1	2.41	0.54
3:I:43:DT:H2''	3:I:44:DG:N7	2.21	0.54
1:C:227:TRP:CG	1:C:245:GLU:HB3	2.42	0.54
1:D:19:GLN:N	1:D:19:GLN:OE1	2.40	0.54
2:E:197:ARG:HG2	2:E:201:ARG:HH21	1.72	0.54
3:I:31:DA:H5'	3:I:31:DA:C8	2.43	0.54
1:B:128:GLN:N	1:B:128:GLN:OE1	2.41	0.54
2:F:275:LEU:O	2:F:278:ASP:N	2.41	0.54
5:K:15:DG:C2	5:K:16:DG:C6	2.96	0.54
1:A:188:THR:O	1:A:188:THR:OG1	2.26	0.54
1:B:62:GLY:HA3	1:B:79:TRP:CE3	2.43	0.54
2:E:357:SER:O	2:E:361:ASP:N	2.41	0.54
3:I:35:DT:C2	3:I:36:DA:N7	2.76	0.54
5:K:6:DC:C5	5:K:7:DT:H73	2.42	0.54
1:B:55:LEU:O	1:B:83:PHE:HB2	2.07	0.54
1:C:119:THR:O	1:C:144:HIS:ND1	2.36	0.54
2:F:357:SER:O	2:F:361:ASP:N	2.40	0.54
1:B:128:GLN:HA	1:B:131:LEU:HG	1.89	0.54
2:E:81:THR:HA	2:E:143:ARG:NH2	2.22	0.54
2:F:271:VAL:O	2:F:274:PHE:HB3	2.08	0.54
1:A:22:THR:OG1	1:A:23:THR:N	2.41	0.54
1:B:214:ILE:HD12	2:F:191:GLY:HA2	1.90	0.54
1:A:75:ARG:O	1:A:91:GLN:HA	2.08	0.53
1:A:165:LEU:HG	1:A:169:TYR:HE1	1.73	0.53
2:F:341:GLN:O	2:F:345:ARG:HG2	2.09	0.53
1:A:97:SER:OG	1:A:98:SER:N	2.40	0.53
1:B:3:ALA:O	1:B:6:HIS:HB3	2.08	0.53
1:B:249:GLU:N	1:B:249:GLU:OE1	2.41	0.53
1:B:253:ALA:HB1	1:B:266:ILE:N	2.24	0.53
1:D:172:ASP:OD1	1:D:173:LYS:N	2.42	0.53
1:D:242:GLY:O	1:D:244:GLN:NE2	2.40	0.53
4:J:23:DT:H2''	4:J:24:DG:N9	2.23	0.53
5:K:5:DA:C5	5:K:6:DC:C4	2.95	0.53
1:A:57:ASN:ND2	1:A:84:SER:OG	2.41	0.53
2:F:166:GLN:HA	2:F:169:GLU:OE2	2.09	0.53
1:A:244:GLN:OE1	1:A:244:GLN:N	2.30	0.53
1:B:25:GLU:O	1:B:29:ILE:HG12	2.08	0.53
1:D:214:ILE:HD11	2:E:197:ARG:NH2	2.24	0.53
2:E:313:ASP:OD1	2:E:314:VAL:HG23	2.09	0.53
1:A:50:ILE:HG22	1:A:51:ARG:O	2.09	0.53
1:B:206:HIS:O	1:B:207:HIS:ND1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ASN:HD21	4:J:12:DA:P	2.32	0.53
1:C:165:LEU:HG	1:C:169:TYR:HE1	1.74	0.53
2:E:166:GLN:HA	2:E:169:GLU:OE2	2.09	0.53
2:F:63:LEU:HA	2:F:66:LYS:NZ	2.24	0.53
1:C:66:HIS:CE1	1:C:75:ARG:HE	2.27	0.53
1:C:148:ASN:ND2	1:C:151:SER:HG	2.07	0.53
2:E:155:ALA:HA	2:E:158:TYR:HD2	1.72	0.53
3:I:4:DG:H1'	3:I:5:DG:H5'	1.89	0.53
3:L:31:DA:H5'	3:L:31:DA:H8	1.73	0.53
1:B:231:LYS:HZ2	1:B:232:LEU:HB3	1.73	0.53
2:E:341:GLN:O	2:E:345:ARG:HG2	2.09	0.53
2:F:313:ASP:OD1	2:F:314:VAL:HG23	2.08	0.53
5:K:13:DA:C2	5:K:14:DG:C4	2.97	0.53
1:A:2:PRO:HG3	1:A:19:GLN:HE22	1.74	0.52
1:B:131:LEU:O	1:B:135:THR:HG22	2.09	0.52
1:D:226:HIS:HD2	1:D:245:GLU:OE2	1.92	0.52
2:E:164:VAL:HA	2:E:167:LEU:HD13	1.91	0.52
2:F:164:VAL:HA	2:F:167:LEU:HD13	1.91	0.52
1:A:43:HIS:HE1	1:A:240:TRP:CH2	2.25	0.52
1:B:213:PRO:CB	2:F:233:ASN:HD22	2.22	0.52
1:D:90:THR:OG1	1:D:91:GLN:N	2.42	0.52
1:D:238:ARG:HG3	1:D:239:GLN:O	2.09	0.52
2:E:190:TYR:CE1	2:E:197:ARG:HG3	2.43	0.52
5:K:14:DG:H2''	5:K:15:DG:H8	1.74	0.52
4:M:8:DA:H1'	4:M:9:DC:H5'	1.90	0.52
2:E:63:LEU:HA	2:E:66:LYS:NZ	2.24	0.52
1:A:24:THR:O	1:A:27:SER:N	2.42	0.52
1:A:238:ARG:HA	1:A:238:ARG:NE	2.25	0.52
1:B:119:THR:HG23	1:B:120:ASP:H	1.73	0.52
1:C:54:LEU:HG	1:C:82:THR:O	2.09	0.52
2:E:254:LEU:O	2:E:257:VAL:HG12	2.09	0.52
2:E:278:ASP:O	2:E:281:LEU:HD13	2.10	0.52
1:B:59:ILE:HG23	1:B:116:TYR:HB2	1.91	0.52
1:C:238:ARG:HG3	1:C:239:GLN:H	1.73	0.52
5:K:12:DT:O4	5:K:13:DA:N6	2.42	0.52
3:L:30:DC:H2''	3:L:31:DA:C8	2.45	0.52
1:A:56:PRO:HB2	1:A:210:ARG:HE	1.74	0.52
1:C:56:PRO:HA	1:C:210:ARG:HH22	1.75	0.52
1:C:229:TYR:HB3	1:C:242:GLY:HA2	1.92	0.52
1:D:225:THR:HA	1:D:274:ALA:HB3	1.91	0.52
1:D:227:TRP:CD2	1:D:243:PRO:HD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2:DC:H2''	3:L:3:DA:N7	2.25	0.52
1:A:119:THR:OG1	1:A:120:ASP:N	2.43	0.52
1:D:152:SER:HA	1:D:155:VAL:HG22	1.91	0.52
1:D:231:LYS:HZ2	1:D:232:LEU:HB3	1.74	0.52
5:N:16:DG:H2''	5:N:17:DT:H71	1.91	0.52
1:A:212:GLN:OE1	1:B:248:GLN:NE2	2.43	0.52
1:A:230:PHE:CD2	1:A:231:LYS:N	2.70	0.52
1:D:253:ALA:HB1	1:D:266:ILE:N	2.24	0.52
2:F:254:LEU:O	2:F:257:VAL:HG12	2.09	0.52
2:F:276:GLU:HA	2:F:276:GLU:OE2	2.10	0.52
5:K:9:DG:O3'	5:K:10:DA:H2'	2.09	0.52
3:L:44:DG:H2'	3:L:45:DT:H71	1.91	0.52
1:A:0:PRO:O	1:A:3:ALA:N	2.43	0.52
1:B:137:LEU:HD21	1:C:8:PHE:HE2	1.75	0.52
1:C:105:LEU:O	1:D:183:SER:OG	2.22	0.52
1:A:7:SER:OG	1:A:7:SER:O	2.28	0.51
4:J:17:DC:H2''	4:J:18:DT:H71	1.92	0.51
1:A:45:MET:HG2	1:A:46:PRO:HD2	1.92	0.51
1:B:157:ARG:HD2	1:B:161:ILE:HD11	1.91	0.51
1:C:229:TYR:HD1	1:C:242:GLY:CA	2.23	0.51
1:C:241:LYS:O	1:C:241:LYS:HD3	2.10	0.51
2:E:153:ASN:OD1	2:E:154:ILE:HD12	2.10	0.51
2:F:277:LYS:C	2:F:279:SER:H	2.13	0.51
2:F:352:ASN:HB2	2:F:355:ILE:HB	1.92	0.51
1:C:230:PHE:CZ	1:C:266:ILE:HG13	2.45	0.51
1:C:238:ARG:HE	1:C:239:GLN:H	1.59	0.51
3:I:37:DG:N2	5:K:11:DC:C2	2.73	0.51
3:L:8:DA:H1'	3:L:9:DG:C8	2.45	0.51
1:C:238:ARG:HA	1:C:238:ARG:NE	2.24	0.51
1:D:175:ASP:N	1:D:175:ASP:OD1	2.43	0.51
1:D:226:HIS:CE1	1:D:227:TRP:CD1	2.99	0.51
2:E:186:LEU:HA	2:E:189:ILE:HG22	1.92	0.51
1:A:243:PRO:HG2	1:A:256:ILE:HD11	1.91	0.51
1:C:227:TRP:NE1	1:C:245:GLU:HG2	2.26	0.51
1:D:134:CYS:SG	1:D:135:THR:N	2.84	0.51
2:F:251:LEU:O	2:F:254:LEU:HB3	2.10	0.51
4:J:8:DA:H1'	4:J:9:DC:H5'	1.92	0.51
1:B:6:HIS:CE1	1:B:33:CYS:HB3	2.45	0.51
1:B:123:PRO:HA	1:B:126:ILE:HG12	1.93	0.51
5:N:12:DT:H2''	5:N:13:DA:H5'	1.92	0.51
1:C:64:ILE:HD12	1:C:76:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:THR:OG1	1:D:21:ALA:O	2.13	0.51
2:F:128:GLU:HG3	2:F:131:TRP:N	2.26	0.51
1:B:269:ARG:NH2	1:B:270:LEU:HB2	2.26	0.51
1:D:219:SER:OG	2:E:197:ARG:NH1	2.44	0.51
1:D:87:ILE:HD11	1:D:158:SER:HB2	1.93	0.51
3:I:27:DA:H2'	3:I:28:DT:H71	1.92	0.51
5:K:10:DA:H1'	5:K:11:DC:C1'	2.41	0.51
1:A:80:VAL:HG22	1:A:81:ASP:N	2.26	0.50
1:B:96:THR:HG1	1:B:98:SER:HG	1.58	0.50
1:C:25:GLU:OE1	1:C:25:GLU:N	2.27	0.50
2:E:251:LEU:O	2:E:254:LEU:HB3	2.10	0.50
2:F:153:ASN:OD1	2:F:154:ILE:HD12	2.10	0.50
1:A:92:LYS:HG3	1:A:93:ARG:N	2.24	0.50
1:D:129:ASP:OD1	1:D:130:PHE:N	2.43	0.50
3:I:45:DT:H2'	3:I:46:DG:C8	2.45	0.50
2:E:178:GLU:HA	2:E:181:PHE:HD1	1.76	0.50
2:E:277:LYS:C	2:E:279:SER:H	2.15	0.50
3:I:42:DG:H2'	3:I:43:DT:H71	1.93	0.50
1:B:227:TRP:HB3	1:B:243:PRO:HB2	1.92	0.50
1:D:11:CYS:SG	1:D:12:GLY:N	2.83	0.50
2:E:223:GLU:N	2:E:223:GLU:CD	2.65	0.50
2:E:286:VAL:HB	2:E:323:ILE:HD13	1.93	0.50
1:C:255:LEU:HA	1:C:264:GLN:O	2.10	0.50
1:A:49:HIS:CE1	1:A:50:ILE:HG13	2.47	0.50
1:A:230:PHE:HA	1:A:240:TRP:HE3	1.77	0.50
1:C:203:TRP:HH2	1:D:207:HIS:CE1	2.29	0.50
2:E:260:LEU:HA	2:E:263:TYR:CZ	2.46	0.50
2:F:173:SER:OG	2:F:174:GLU:N	2.44	0.50
3:I:8:DA:H1'	3:I:9:DG:C8	2.46	0.50
1:B:229:TYR:HB2	1:B:269:ARG:HH11	1.75	0.50
2:E:128:GLU:HG3	2:E:131:TRP:N	2.26	0.50
2:F:134:LEU:HA	2:F:137:VAL:HG12	1.92	0.50
5:N:12:DT:H2'	5:N:13:DA:C8	2.47	0.50
1:A:122:GLY:O	1:A:126:ILE:HG12	2.10	0.50
1:D:55:LEU:HB3	1:D:59:ILE:HB	1.94	0.50
1:D:240:TRP:CE2	1:D:269:ARG:HD3	2.47	0.50
2:E:98:MET:O	2:E:102:ASN:ND2	2.45	0.50
2:E:341:GLN:HB3	2:E:345:ARG:HE	1.77	0.50
2:E:355:ILE:HA	2:E:358:LEU:HD12	1.94	0.50
2:F:223:GLU:N	2:F:223:GLU:CD	2.65	0.50
1:B:184:ILE:O	1:B:188:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:VAL:HG13	1:B:260:ALA:H	1.77	0.50
2:F:227:ILE:O	2:F:231:ILE:HG13	2.12	0.50
2:F:270:CYS:SG	2:F:271:VAL:N	2.85	0.50
3:I:44:DG:H2'	3:I:45:DT:H71	1.94	0.50
1:A:76:LEU:HD23	1:A:91:GLN:CG	2.42	0.49
1:A:94:LYS:HG3	1:A:96:THR:H	1.77	0.49
1:C:230:PHE:HB2	1:C:270:LEU:O	2.12	0.49
1:C:230:PHE:CB	1:C:271:LEU:HA	2.42	0.49
1:D:142:THR:OG1	1:D:143:THR:N	2.45	0.49
2:E:221:ILE:HG22	2:E:225:LEU:CD1	2.41	0.49
5:K:14:DG:C4	5:K:15:DG:N7	2.80	0.49
1:A:69:TYR:HD2	1:A:71:ASN:HA	1.77	0.49
1:A:238:ARG:HE	1:A:239:GLN:N	2.09	0.49
1:B:118:ASN:HA	1:B:143:THR:HA	1.94	0.49
2:E:231:ILE:O	2:E:234:GLY:N	2.45	0.49
2:F:128:GLU:HB3	2:F:131:TRP:HB2	1.94	0.49
2:F:183:LYS:HE2	2:F:223:GLU:HB3	1.93	0.49
3:I:17:DG:C8	3:I:18:DT:H72	2.47	0.49
1:B:121:ASN:ND2	1:B:146:PRO:HG3	2.26	0.49
2:E:173:SER:OG	2:E:174:GLU:N	2.43	0.49
2:E:227:ILE:O	2:E:231:ILE:HG13	2.13	0.49
3:I:30:DC:H2''	3:I:31:DA:H5'	1.94	0.49
1:D:213:PRO:CB	2:E:233:ASN:HD22	2.24	0.49
1:D:225:THR:O	1:D:228:TYR:OH	2.06	0.49
1:D:247:LEU:HD12	1:D:247:LEU:H	1.77	0.49
2:E:128:GLU:HG2	2:E:134:LEU:HD13	1.93	0.49
2:F:341:GLN:HB3	2:F:345:ARG:HE	1.78	0.49
3:L:4:DG:C6	3:L:5:DG:C6	3.00	0.49
1:A:45:MET:HG2	1:A:46:PRO:CD	2.43	0.49
1:B:144:HIS:NE2	1:B:148:ASN:HB3	2.26	0.49
1:B:227:TRP:N	1:B:227:TRP:CD1	2.81	0.49
1:B:240:TRP:CE2	1:B:269:ARG:HD3	2.48	0.49
1:C:60:TRP:HZ2	1:C:112:GLY:H	1.58	0.49
2:E:128:GLU:HB3	2:E:131:TRP:HB2	1.95	0.49
2:E:287:MET:HA	2:E:290:LEU:HD23	1.95	0.49
2:F:98:MET:O	2:F:102:ASN:ND2	2.45	0.49
1:A:8:PHE:CE2	1:D:137:LEU:HD21	2.47	0.49
1:A:47:ARG:HA	1:A:268:TRP:CH2	2.48	0.49
1:C:155:VAL:O	1:C:158:SER:N	2.46	0.49
1:D:184:ILE:O	1:D:188:THR:HG22	2.12	0.49
2:E:134:LEU:HA	2:E:137:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:184:THR:O	2:E:188:ARG:HG2	2.13	0.49
2:F:241:GLU:O	2:F:244:LYS:HG2	2.12	0.49
3:L:13:DT:H3'	3:L:13:DT:OP2	2.13	0.49
3:L:44:DG:C2'	3:L:45:DT:H71	2.43	0.49
3:I:42:DG:N1	5:K:7:DT:O4	2.46	0.49
1:C:51:ARG:HH12	1:C:54:LEU:HD23	1.78	0.49
1:A:168:LYS:HE2	1:C:36:CYS:HA	1.94	0.49
1:B:188:THR:O	1:B:193:ASN:ND2	2.44	0.49
1:C:57:ASN:HB2	1:C:58:HIS:CD2	2.48	0.49
1:D:229:TYR:HD2	1:D:269:ARG:NH1	2.10	0.49
1:D:229:TYR:O	1:D:269:ARG:HB3	2.12	0.49
2:F:225:LEU:HB3	2:F:266:GLN:HG3	1.95	0.49
2:F:280:THR:C	2:F:282:THR:H	2.14	0.49
1:A:111:LEU:HD21	1:B:203:TRP:NE1	2.28	0.49
1:B:238:ARG:HG3	1:B:239:GLN:O	2.12	0.49
1:C:111:LEU:HD13	1:C:112:GLY:HA2	1.95	0.49
1:C:197:ASN:HA	1:C:199:HIS:CD2	2.48	0.49
1:D:64:ILE:HG12	1:D:77:HIS:HD2	1.77	0.49
1:D:229:TYR:N	1:D:243:PRO:HG3	2.28	0.49
2:E:222:ALA:HA	2:E:225:LEU:HD13	1.94	0.49
2:E:277:LYS:O	2:E:279:SER:N	2.46	0.49
2:F:355:ILE:HA	2:F:358:LEU:HD12	1.95	0.49
1:A:108:ILE:HD11	1:A:113:LYS:HG2	1.95	0.48
1:B:195:LEU:HD12	1:B:195:LEU:H	1.78	0.48
1:D:206:HIS:CD2	1:D:207:HIS:CE1	3.01	0.48
2:E:241:GLU:HA	2:E:244:LYS:NZ	2.27	0.48
2:E:241:GLU:O	2:E:244:LYS:HG2	2.13	0.48
2:F:231:ILE:O	2:F:234:GLY:N	2.46	0.48
2:F:241:GLU:HA	2:F:244:LYS:NZ	2.27	0.48
1:C:218:ARG:HH11	1:C:220:LEU:HD22	1.78	0.48
1:A:75:ARG:HD2	1:A:95:GLU:OE1	2.13	0.48
1:B:152:SER:O	1:B:154:LEU:N	2.46	0.48
1:D:158:SER:OG	1:D:159:ASN:N	2.47	0.48
2:E:183:LYS:HE2	2:E:223:GLU:HA	1.94	0.48
2:E:247:LEU:HA	2:E:251:LEU:HD23	1.96	0.48
2:F:274:PHE:O	2:F:278:ASP:HB2	2.13	0.48
1:A:1:SER:O	1:A:5:LEU:HB2	2.13	0.48
1:C:68:LYS:O	1:C:68:LYS:HG3	2.14	0.48
2:E:280:THR:C	2:E:282:THR:H	2.17	0.48
2:E:325:GLU:OE1	2:E:365:LYS:NZ	2.37	0.48
2:F:128:GLU:OE1	2:F:129:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:221:ILE:HG22	2:F:225:LEU:CD1	2.43	0.48
2:F:287:MET:HA	2:F:290:LEU:HD23	1.94	0.48
3:I:13:DT:OP2	3:I:13:DT:H3'	2.13	0.48
2:E:221:ILE:HG22	2:E:225:LEU:HD11	1.95	0.48
2:F:241:GLU:OE1	2:F:241:GLU:N	2.40	0.48
2:F:260:LEU:HA	2:F:263:TYR:CZ	2.48	0.48
1:C:70:LYS:HE3	1:C:71:ASN:OD1	2.14	0.48
2:E:70:ARG:HH12	2:E:132:PRO:HB2	1.77	0.48
5:K:15:DG:C4	5:K:16:DG:N7	2.81	0.48
1:A:60:TRP:CD1	1:A:114:PRO:HB3	2.48	0.48
1:A:232:LEU:HD12	1:A:233:PRO:HD2	1.96	0.48
2:F:39:GLU:HA	2:F:42:PHE:HD2	1.78	0.48
5:N:1:DA:O5'	5:N:1:DA:H8	1.96	0.48
1:A:148:ASN:ND2	1:A:151:SER:HG	2.10	0.48
2:E:241:GLU:OE1	2:E:241:GLU:N	2.40	0.48
2:F:70:ARG:HH12	2:F:132:PRO:HB2	1.78	0.48
3:L:15:DT:H4'	3:L:16:DA:OP1	2.14	0.48
2:E:128:GLU:OE1	2:E:129:ALA:N	2.46	0.48
3:L:17:DG:C8	3:L:18:DT:H72	2.49	0.48
1:B:111:LEU:HA	1:B:112:GLY:HA2	1.68	0.48
1:D:228:TYR:OH	1:D:246:ALA:N	2.47	0.48
3:I:15:DT:H4'	3:I:16:DA:OP1	2.14	0.48
2:E:352:ASN:HB2	2:E:355:ILE:HB	1.94	0.47
2:F:247:LEU:HA	2:F:251:LEU:HD23	1.96	0.47
3:I:30:DC:H2''	3:I:31:DA:C8	2.49	0.47
1:A:117:ILE:HG22	1:A:141:HIS:HA	1.95	0.47
1:C:227:TRP:CD2	1:C:245:GLU:HB3	2.49	0.47
1:D:91:GLN:O	1:D:92:LYS:HD2	2.14	0.47
2:E:127:LEU:HD12	2:E:177:ARG:CZ	2.44	0.47
1:B:168:LYS:HD3	1:B:168:LYS:HA	1.71	0.47
1:C:198:CYS:O	1:C:200:LYS:HG2	2.14	0.47
1:C:226:HIS:CE1	1:C:273:ARG:HH11	2.33	0.47
1:C:245:GLU:OE1	1:C:246:ALA:N	2.48	0.47
1:D:129:ASP:OD1	1:D:129:ASP:N	2.46	0.47
2:E:53:PHE:CZ	2:E:65:TRP:HB2	2.44	0.47
2:F:128:GLU:HG2	2:F:134:LEU:HD13	1.95	0.47
3:I:41:DA:H2''	3:I:42:DG:H5''	1.95	0.47
5:K:10:DA:H1'	5:K:11:DC:H2'	1.94	0.47
1:B:179:ASP:OD1	1:B:179:ASP:N	2.36	0.47
1:C:54:LEU:HD13	1:C:54:LEU:HA	1.46	0.47
1:D:227:TRP:CB	1:D:243:PRO:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:TYR:HB3	1:D:240:TRP:CB	2.44	0.47
2:F:277:LYS:C	2:F:279:SER:N	2.68	0.47
1:A:69:TYR:O	1:A:69:TYR:CG	2.67	0.47
1:A:184:ILE:HG12	1:B:105:LEU:HD21	1.97	0.47
1:A:230:PHE:CB	1:A:271:LEU:HA	2.44	0.47
1:B:6:HIS:O	1:B:10:HIS:CA	2.62	0.47
1:B:216:GLU:O	1:B:217:THR:OG1	2.32	0.47
1:C:57:ASN:H	1:C:210:ARG:CZ	2.28	0.47
1:D:133:MET:O	1:D:136:SER:OG	2.31	0.47
1:D:255:LEU:CD2	1:D:263:ALA:HB1	2.44	0.47
2:E:63:LEU:HA	2:E:66:LYS:HZ2	1.78	0.47
2:E:79:TYR:O	2:E:82:HIS:HB3	2.15	0.47
2:E:200:ILE:O	2:E:204:ILE:HG22	2.15	0.47
2:F:127:LEU:HD12	2:F:177:ARG:CZ	2.45	0.47
2:F:134:LEU:HD12	2:F:134:LEU:H	1.80	0.47
2:F:200:ILE:O	2:F:204:ILE:HG22	2.14	0.47
2:F:277:LYS:O	2:F:279:SER:N	2.47	0.47
3:I:37:DG:H1'	3:I:38:DT:OP2	2.14	0.47
4:M:16:DT:C4	4:M:17:DC:N4	2.83	0.47
1:D:69:TYR:HB2	1:D:72:THR:N	2.30	0.47
1:D:111:LEU:HA	1:D:112:GLY:HA2	1.67	0.47
2:F:223:GLU:HA	2:F:226:GLU:OE1	2.14	0.47
4:J:23:DT:H2''	4:J:24:DG:C4	2.49	0.47
5:K:5:DA:C6	5:K:6:DC:N4	2.82	0.47
1:B:5:LEU:O	1:B:9:THR:HG23	2.15	0.47
1:C:216:GLU:OE2	1:C:217:THR:N	2.48	0.47
2:E:237:LEU:HB2	2:E:277:LYS:HE3	1.97	0.47
2:F:62:ASP:OD2	2:F:65:TRP:NE1	2.48	0.47
2:F:229:GLY:HA2	2:F:232:ILE:HG12	1.97	0.47
3:I:12:DA:H4'	3:I:13:DT:OP1	2.14	0.47
1:A:56:PRO:HB2	1:A:210:ARG:NE	2.29	0.47
1:B:119:THR:HG21	1:B:125:TYR:CE1	2.50	0.47
1:B:229:TYR:HB2	1:B:269:ARG:HE	1.79	0.47
1:C:238:ARG:HE	1:C:239:GLN:N	2.13	0.47
2:E:277:LYS:C	2:E:279:SER:N	2.68	0.47
2:E:286:VAL:O	2:E:287:MET:SD	2.73	0.47
2:E:320:PHE:HA	2:E:323:ILE:HG22	1.97	0.47
2:E:341:GLN:C	2:E:345:ARG:HG2	2.35	0.47
2:F:178:GLU:HA	2:F:181:PHE:HD1	1.80	0.47
1:A:42:GLN:CD	1:A:43:HIS:N	2.69	0.46
1:C:110:TYR:C	1:C:111:LEU:HD22	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PHE:CA	1:C:240:TRP:HE3	2.28	0.46
2:E:130:ALA:O	2:E:134:LEU:HD12	2.15	0.46
3:I:38:DT:H2'	3:I:38:DT:OP1	2.14	0.46
3:I:41:DA:C4	3:I:42:DG:C8	3.03	0.46
4:J:1:DA:H2'	4:J:2:DC:C6	2.49	0.46
3:L:45:DT:H2'	3:L:46:DG:C8	2.49	0.46
1:A:238:ARG:HG3	1:A:239:GLN:H	1.80	0.46
1:D:76:LEU:HB2	1:D:90:THR:O	2.16	0.46
2:E:266:GLN:OE1	2:E:266:GLN:N	2.38	0.46
2:E:323:ILE:O	2:E:327:LEU:HG	2.16	0.46
2:F:98:MET:HA	2:F:101:VAL:HG12	1.97	0.46
2:F:286:VAL:O	2:F:287:MET:SD	2.73	0.46
1:A:0:PRO:H2	1:A:2:PRO:HD2	1.80	0.46
1:B:6:HIS:HE1	1:B:33:CYS:HB3	1.80	0.46
1:C:220:LEU:HD11	4:J:1:DA:N1	2.30	0.46
2:F:341:GLN:C	2:F:345:ARG:HG2	2.35	0.46
3:I:11:DA:H4'	3:I:12:DA:OP1	2.15	0.46
5:K:5:DA:C4	5:K:6:DC:C5	3.04	0.46
1:C:108:ILE:HG22	1:D:187:TRP:CD1	2.51	0.46
2:F:53:PHE:CZ	2:F:65:TRP:HB2	2.44	0.46
1:A:247:LEU:HG	1:A:257:PRO:HD3	1.97	0.46
1:C:122:GLY:O	1:C:123:PRO:C	2.53	0.46
1:D:179:ASP:OD1	1:D:180:ASN:N	2.45	0.46
1:D:201:THR:HG23	1:D:204:GLN:OE1	2.15	0.46
2:E:98:MET:HA	2:E:101:VAL:HG12	1.97	0.46
2:E:134:LEU:HD12	2:E:134:LEU:H	1.81	0.46
2:F:130:ALA:O	2:F:134:LEU:HD12	2.16	0.46
5:K:13:DA:C4	5:K:14:DG:C8	3.04	0.46
3:L:30:DC:H2''	3:L:31:DA:H8	1.81	0.46
1:A:241:LYS:O	1:A:243:PRO:HD2	2.16	0.46
1:C:197:ASN:HA	1:C:199:HIS:NE2	2.30	0.46
2:F:323:ILE:O	2:F:327:LEU:HG	2.15	0.46
3:I:13:DT:H2''	3:I:14:DT:H71	1.98	0.46
4:M:23:DT:H2''	4:M:24:DG:C4	2.51	0.46
2:E:190:TYR:CZ	2:E:197:ARG:HG3	2.50	0.46
2:F:259:SER:O	2:F:259:SER:OG	2.31	0.46
5:K:5:DA:C5	5:K:6:DC:N4	2.84	0.46
1:C:129:ASP:OD1	1:C:130:PHE:N	2.48	0.46
3:L:34:DC:H2'	3:L:35:DT:C6	2.50	0.46
1:A:172:ASP:CG	1:A:173:LYS:HG3	2.37	0.46
1:C:241:LYS:O	1:C:243:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:GLY:HA3	4:J:3:DT:O2	2.16	0.46
1:D:253:ALA:HB3	1:D:265:TRP:HE3	1.81	0.46
2:E:203:GLN:HA	2:E:206:ASN:HD22	1.81	0.46
2:E:308:LEU:O	2:E:311:ILE:HG22	2.16	0.46
3:L:12:DA:H4'	3:L:13:DT:OP1	2.15	0.46
3:L:30:DC:H2''	3:L:31:DA:H5'	1.98	0.46
1:A:106:GLN:HA	1:B:183:SER:OG	2.15	0.46
1:B:158:SER:HA	1:B:161:ILE:HD12	1.98	0.46
1:C:7:SER:O	1:C:7:SER:OG	2.32	0.46
1:C:92:LYS:HG3	1:C:93:ARG:N	2.29	0.46
1:D:155:VAL:HG23	1:D:156:GLN:NE2	2.30	0.46
3:L:6:DA:H2''	3:L:7:DG:H2'	1.98	0.46
1:A:229:TYR:HD1	1:A:242:GLY:CA	2.29	0.45
1:B:90:THR:OG1	1:B:91:GLN:N	2.48	0.45
2:F:203:GLN:HA	2:F:206:ASN:HD22	1.81	0.45
4:M:15:DT:C2	4:M:16:DT:C4	3.04	0.45
5:N:14:DG:H2''	5:N:15:DG:H8	1.81	0.45
2:E:78:GLU:OE1	2:E:81:THR:HB	2.16	0.45
1:A:218:ARG:HG2	1:A:219:SER:H	1.81	0.45
1:C:133:MET:O	1:C:136:SER:OG	2.27	0.45
1:D:101:ILE:HD11	1:D:130:PHE:HA	1.99	0.45
2:F:146:GLU:HA	2:F:146:GLU:OE2	2.15	0.45
3:L:13:DT:H2''	3:L:14:DT:H71	1.98	0.45
1:D:229:TYR:HB2	1:D:269:ARG:HH11	1.82	0.45
4:J:16:DT:C4	4:J:17:DC:N4	2.85	0.45
4:J:21:DC:N3	4:J:22:DC:N4	2.64	0.45
3:L:28:DT:C2	3:L:29:DC:C6	3.05	0.45
1:B:119:THR:HG23	1:B:120:ASP:N	2.30	0.45
1:C:122:GLY:HA3	1:C:126:ILE:HG12	1.99	0.45
1:C:230:PHE:CG	1:C:271:LEU:HD23	2.52	0.45
1:C:230:PHE:HA	1:C:240:TRP:HE3	1.81	0.45
1:D:229:TYR:HD2	1:D:269:ARG:HH11	1.62	0.45
2:F:184:THR:O	2:F:188:ARG:HG2	2.16	0.45
5:N:14:DG:C2	5:N:15:DG:C5	3.05	0.45
1:D:56:PRO:HA	1:D:83:PHE:HB2	1.98	0.45
2:E:146:GLU:OE2	2:E:146:GLU:HA	2.16	0.45
1:B:60:TRP:CD2	1:B:114:PRO:HB3	2.50	0.45
2:E:242:GLU:HG3	2:E:243:HIS:N	2.32	0.45
2:E:257:VAL:HG22	2:E:258:LYS:H	1.82	0.45
2:F:308:LEU:O	2:F:311:ILE:HG22	2.16	0.45
3:I:18:DT:H2''	3:I:19:DA:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3:DA:C2	3:L:4:DG:C6	3.04	0.45
2:E:89:GLU:O	2:E:91:ILE:N	2.49	0.45
2:E:229:GLY:HA2	2:E:232:ILE:HG12	1.98	0.45
2:E:239:LEU:HG	2:E:240:LYS:H	1.82	0.45
4:J:15:DT:C2	4:J:16:DT:C4	3.05	0.45
3:L:46:DG:OP2	3:L:46:DG:H8	2.00	0.45
1:A:157:ARG:NH2	4:M:6:DG:H21	2.15	0.45
1:B:6:HIS:HD2	1:B:10:HIS:CE1	2.32	0.45
1:B:14:THR:OG1	1:B:15:ALA:N	2.50	0.45
1:C:101:ILE:HD11	1:C:130:PHE:HA	1.98	0.45
2:E:279:SER:O	2:E:282:THR:CB	2.63	0.45
2:F:89:GLU:O	2:F:91:ILE:N	2.50	0.45
3:I:38:DT:H2''	3:I:39:DC:C6	2.52	0.45
1:A:101:ILE:HG13	1:A:130:PHE:HD1	1.81	0.45
1:C:69:TYR:HB3	1:C:73:LEU:HD12	1.99	0.45
1:C:191:HIS:O	1:C:192:LEU:HD23	2.17	0.45
2:E:89:GLU:HG3	2:E:154:ILE:HG21	1.98	0.45
3:L:11:DA:H4'	3:L:12:DA:OP1	2.15	0.45
3:L:44:DG:H2'	3:L:45:DT:C6	2.51	0.45
1:A:57:ASN:HD21	1:A:84:SER:CB	2.30	0.44
1:B:206:HIS:CD2	1:B:207:HIS:CE1	3.05	0.44
1:C:55:LEU:HB2	1:C:56:PRO:HD3	1.98	0.44
1:D:158:SER:HA	1:D:161:ILE:HD12	1.97	0.44
3:L:18:DT:H2''	3:L:19:DA:C8	2.52	0.44
1:B:229:TYR:HB3	1:B:240:TRP:CB	2.46	0.44
2:E:63:LEU:HA	2:E:66:LYS:HD2	2.00	0.44
2:F:181:PHE:O	2:F:185:THR:HG22	2.16	0.44
2:F:257:VAL:HG22	2:F:258:LYS:H	1.83	0.44
1:D:235:LEU:HD23	1:D:235:LEU:H	1.83	0.44
1:D:258:VAL:HG12	1:D:260:ALA:H	1.83	0.44
2:E:62:ASP:OD2	2:E:65:TRP:NE1	2.48	0.44
2:E:161:GLN:O	2:E:165:LEU:HG	2.17	0.44
2:F:214:GLU:HG2	2:F:216:GLU:OE1	2.18	0.44
2:F:239:LEU:HG	2:F:240:LYS:H	1.80	0.44
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.72	0.44
1:B:227:TRP:NE1	1:B:245:GLU:HG2	2.32	0.44
1:D:56:PRO:HA	1:D:83:PHE:CG	2.52	0.44
2:F:63:LEU:HA	2:F:66:LYS:HZ2	1.83	0.44
1:A:76:LEU:HD23	1:A:91:GLN:CB	2.46	0.44
1:A:105:LEU:HA	1:A:105:LEU:HD13	1.81	0.44
1:B:252:GLY:O	1:B:268:TRP:HZ3	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:55:PHE:CE1	2:E:59:PRO:HB3	2.52	0.44
2:E:163:PHE:O	2:E:166:GLN:N	2.50	0.44
2:E:259:SER:O	2:E:259:SER:OG	2.31	0.44
4:M:14:DT:C2	4:M:15:DT:C4	3.05	0.44
1:A:64:ILE:HD12	1:A:77:HIS:CE1	2.53	0.44
1:A:268:TRP:CE3	1:A:269:ARG:HA	2.53	0.44
1:C:184:ILE:HG13	1:D:105:LEU:HD21	2.00	0.44
1:C:227:TRP:CE2	1:C:245:GLU:HG2	2.52	0.44
2:E:92:TYR:O	2:E:95:VAL:HG22	2.18	0.44
1:A:0:PRO:HB2	1:A:1:SER:H	1.59	0.44
1:A:219:SER:O	1:A:219:SER:OG	2.36	0.44
1:A:228:TYR:HD1	1:A:273:ARG:HA	1.83	0.44
1:C:111:LEU:HD22	1:C:111:LEU:N	2.32	0.44
1:D:14:THR:OG1	1:D:15:ALA:N	2.49	0.44
1:D:238:ARG:NH1	1:D:239:GLN:OE1	2.51	0.44
2:F:163:PHE:O	2:F:166:GLN:N	2.51	0.44
2:F:242:GLU:HG3	2:F:243:HIS:N	2.32	0.44
5:K:14:DG:N1	5:K:15:DG:C6	2.85	0.44
5:K:15:DG:N3	5:K:16:DG:C5	2.86	0.44
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.70	0.44
1:B:189:ILE:HG23	1:B:190:ASN:OD1	2.18	0.44
1:C:106:GLN:HA	1:D:183:SER:OG	2.17	0.44
2:F:161:GLN:O	2:F:165:LEU:HG	2.18	0.44
5:K:10:DA:H1'	5:K:11:DC:O4'	2.18	0.44
5:N:16:DG:C2'	5:N:17:DT:H71	2.48	0.44
1:C:18:LEU:HD13	1:C:18:LEU:HA	1.84	0.44
2:F:55:PHE:CE1	2:F:59:PRO:HB3	2.53	0.44
2:F:79:TYR:O	2:F:82:HIS:HB3	2.18	0.44
2:F:289:LEU:O	2:F:293:TRP:N	2.51	0.44
3:L:28:DT:C2	3:L:29:DC:C5	3.06	0.44
4:M:21:DC:N3	4:M:22:DC:N4	2.65	0.44
5:N:10:DA:H1'	5:N:11:DC:C6	2.53	0.44
1:A:128:GLN:OE1	1:A:132:ASN:ND2	2.50	0.43
1:B:158:SER:OG	1:B:159:ASN:N	2.51	0.43
1:B:241:LYS:HE2	1:B:241:LYS:HB2	1.75	0.43
1:C:229:TYR:CD1	1:C:242:GLY:CA	3.01	0.43
2:E:169:GLU:OE1	2:E:169:GLU:N	2.51	0.43
2:E:223:GLU:HA	2:E:226:GLU:OE1	2.18	0.43
2:F:63:LEU:HA	2:F:66:LYS:HD2	2.00	0.43
2:F:320:PHE:HA	2:F:323:ILE:HG22	1.99	0.43
4:J:14:DT:C2	4:J:15:DT:C4	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:14:DG:N3	5:K:15:DG:C8	2.86	0.43
1:A:57:ASN:HB2	1:A:210:ARG:CZ	2.48	0.43
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.62	0.43
1:B:128:GLN:O	1:B:129:ASP:C	2.55	0.43
1:C:203:TRP:HH2	1:D:207:HIS:NE2	2.15	0.43
1:D:271:LEU:HD23	1:D:272:LYS:O	2.18	0.43
1:A:57:ASN:OD1	1:A:84:SER:N	2.51	0.43
1:A:184:ILE:HD11	1:B:105:LEU:HD11	1.99	0.43
1:A:230:PHE:HE1	1:A:243:PRO:CG	2.31	0.43
1:A:252:GLY:O	1:A:268:TRP:HB3	2.18	0.43
1:B:235:LEU:H	1:B:235:LEU:HD23	1.83	0.43
1:C:91:GLN:H	1:C:91:GLN:HG3	1.60	0.43
1:D:227:TRP:O	1:D:272:LYS:HB2	2.18	0.43
1:D:231:LYS:NZ	1:D:232:LEU:HB3	2.34	0.43
2:E:65:TRP:O	2:E:69:LYS:HG3	2.18	0.43
2:F:222:ALA:O	2:F:226:GLU:OE1	2.35	0.43
3:L:30:DC:C2	3:L:31:DA:N7	2.86	0.43
1:A:207:HIS:CE1	1:B:207:HIS:CD2	3.03	0.43
1:A:229:TYR:HB3	1:A:242:GLY:CA	2.48	0.43
1:A:230:PHE:CD1	1:A:243:PRO:HD2	2.53	0.43
1:B:35:ALA:O	1:B:168:LYS:NZ	2.37	0.43
1:C:162:LEU:HD12	1:C:162:LEU:HA	1.74	0.43
1:D:105:LEU:O	1:D:108:ILE:HG22	2.18	0.43
1:D:154:LEU:HD22	1:D:157:ARG:NH2	2.33	0.43
2:E:100:ALA:O	2:E:104:PHE:HB2	2.19	0.43
4:J:10:DT:H2''	4:J:11:DA:C8	2.53	0.43
1:A:80:VAL:HG22	1:A:81:ASP:O	2.19	0.43
1:A:256:ILE:HG13	1:A:257:PRO:HD2	2.00	0.43
1:C:122:GLY:HA3	1:C:126:ILE:HD11	2.00	0.43
1:D:76:LEU:HD23	1:D:76:LEU:H	1.83	0.43
1:A:75:ARG:O	1:A:91:GLN:HG2	2.18	0.43
2:E:39:GLU:HA	2:E:42:PHE:HD2	1.84	0.43
2:E:151:GLN:HA	2:E:152:PRO:HD3	1.86	0.43
3:I:4:DG:C4	3:I:5:DG:C8	3.07	0.43
3:I:39:DC:N3	5:K:9:DG:N2	2.66	0.43
3:L:44:DG:H3'	3:L:45:DT:H71	2.01	0.43
1:A:232:LEU:H	1:A:241:LYS:HG3	1.83	0.43
1:B:117:ILE:O	1:B:142:THR:O	2.37	0.43
1:C:56:PRO:HA	1:C:210:ARG:NH1	2.33	0.43
1:C:76:LEU:HD23	1:C:91:GLN:CB	2.48	0.43
1:D:206:HIS:HD2	1:D:207:HIS:CE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:183:LYS:HB2	2:E:183:LYS:HE3	1.74	0.43
2:E:214:GLU:HG2	2:E:216:GLU:OE1	2.19	0.43
2:E:245:ILE:HD13	2:E:245:ILE:HA	1.88	0.43
2:F:92:TYR:O	2:F:95:VAL:HG22	2.18	0.43
2:F:264:HIS:O	2:F:267:LEU:HG	2.19	0.43
3:L:44:DG:H2'	3:L:45:DT:H6	1.84	0.43
1:A:230:PHE:HB2	1:A:271:LEU:HA	1.99	0.43
1:B:271:LEU:HD12	1:B:271:LEU:O	2.19	0.43
2:E:89:GLU:N	2:E:90:PRO:HD2	2.34	0.43
2:F:65:TRP:O	2:F:69:LYS:HG3	2.18	0.43
5:K:16:DG:C2	5:K:17:DT:C4	3.07	0.43
1:A:18:LEU:HD13	1:A:18:LEU:HA	1.82	0.43
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.89	0.43
1:A:94:LYS:HG3	1:A:96:THR:HG22	2.01	0.43
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.71	0.43
1:A:230:PHE:C	1:A:240:TRP:HE3	2.22	0.43
1:D:200:LYS:HB3	1:D:200:LYS:HE3	1.68	0.43
2:E:283:GLU:O	2:E:286:VAL:HG13	2.19	0.43
2:E:289:LEU:O	2:E:293:TRP:N	2.51	0.43
2:F:80:ILE:O	2:F:143:ARG:NH1	2.52	0.43
2:F:279:SER:C	2:F:281:LEU:N	2.72	0.43
3:I:7:DG:C4	3:I:8:DA:C6	3.07	0.43
1:B:255:LEU:CD1	1:B:263:ALA:HB1	2.48	0.43
2:F:294:PRO:HG2	2:F:301:GLU:HG2	2.00	0.43
2:F:353:GLU:O	2:F:356:MET:HG3	2.19	0.43
3:I:9:DG:H2''	3:I:10:DA:C2'	2.42	0.42
4:J:21:DC:C2	4:J:22:DC:C4	3.07	0.42
3:L:8:DA:C4	3:L:9:DG:C5	3.07	0.42
3:L:9:DG:C4	3:L:10:DA:C8	3.07	0.42
5:N:10:DA:O4'	5:N:11:DC:H5'	2.19	0.42
1:B:111:LEU:HD13	1:B:111:LEU:HA	1.72	0.42
1:B:200:LYS:HB3	1:B:200:LYS:HE3	1.70	0.42
1:B:226:HIS:O	1:B:228:TYR:HD1	2.02	0.42
2:E:294:PRO:HG2	2:E:301:GLU:HG2	2.01	0.42
2:F:169:GLU:OE1	2:F:169:GLU:N	2.51	0.42
3:L:8:DA:C6	3:L:9:DG:C6	3.08	0.42
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.70	0.42
1:B:216:GLU:CD	2:F:235:PHE:HA	2.40	0.42
1:C:201:THR:O	1:C:202:ARG:C	2.57	0.42
1:C:218:ARG:NH1	1:C:220:LEU:HD22	2.33	0.42
1:C:252:GLY:HA2	1:C:268:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:SER:OG	1:D:99:GLU:OE2	2.22	0.42
5:K:2:DC:O2	5:K:3:DA:C8	2.72	0.42
5:K:10:DA:H1'	5:K:11:DC:C2'	2.48	0.42
5:K:14:DG:C2	5:K:15:DG:C4	3.07	0.42
1:C:172:ASP:CG	1:C:173:LYS:HG3	2.39	0.42
1:D:242:GLY:HA2	1:D:243:PRO:HD3	1.38	0.42
2:F:89:GLU:N	2:F:90:PRO:HD2	2.34	0.42
2:F:190:TYR:CZ	2:F:197:ARG:HG3	2.55	0.42
1:A:77:HIS:NE2	1:A:99:GLU:OE1	2.52	0.42
1:A:137:LEU:HA	1:A:137:LEU:HD12	1.79	0.42
1:C:241:LYS:O	1:C:243:PRO:CD	2.68	0.42
1:D:165:LEU:HD12	1:D:168:LYS:HE2	2.01	0.42
2:E:88:THR:HG23	2:E:90:PRO:HD2	2.00	0.42
2:F:183:LYS:HE2	2:F:223:GLU:CB	2.49	0.42
3:L:9:DG:H1'	3:L:10:DA:H5'	2.00	0.42
1:D:104:LEU:HD23	1:D:105:LEU:N	2.34	0.42
1:D:248:GLN:HB3	1:D:255:LEU:HB2	2.02	0.42
2:E:353:GLU:O	2:E:356:MET:HG3	2.20	0.42
2:F:100:ALA:O	2:F:104:PHE:HB2	2.18	0.42
3:I:9:DG:C4	3:I:10:DA:C8	3.07	0.42
1:A:2:PRO:HB3	1:A:21:ALA:HB2	2.02	0.42
1:A:69:TYR:HB2	1:A:72:THR:N	2.34	0.42
1:B:176:LEU:HD13	1:B:176:LEU:HA	1.91	0.42
1:C:70:LYS:HE3	1:C:71:ASN:CG	2.39	0.42
1:D:226:HIS:O	1:D:228:TYR:CE2	2.73	0.42
2:E:126:THR:C	2:E:127:LEU:HD22	2.39	0.42
2:E:190:TYR:O	2:E:197:ARG:NH2	2.44	0.42
2:E:228:LEU:O	2:E:231:ILE:N	2.51	0.42
2:E:365:LYS:HA	2:E:365:LYS:HD2	1.88	0.42
2:F:108:PRO:HA	2:F:109:PRO:HD3	1.91	0.42
1:A:170:PHE:HZ	1:A:178:MET:HA	1.85	0.42
1:B:133:MET:O	1:B:136:SER:OG	2.35	0.42
1:D:189:ILE:HG23	1:D:190:ASN:OD1	2.19	0.42
2:E:196:LEU:HA	2:E:199:TYR:HB3	2.01	0.42
2:E:315:ILE:HD11	2:E:320:PHE:CD1	2.55	0.42
2:F:70:ARG:NH2	2:F:132:PRO:HB2	2.34	0.42
2:F:289:LEU:O	2:F:289:LEU:HD23	2.20	0.42
4:J:14:DT:H1'	4:J:15:DT:C6	2.55	0.42
1:B:238:ARG:NH1	1:B:239:GLN:OE1	2.52	0.42
1:B:269:ARG:NH1	1:B:270:LEU:HB2	2.35	0.42
1:C:144:HIS:HD1	1:C:144:HIS:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LEU:O	1:C:187:TRP:C	2.58	0.42
1:D:67:PHE:HB3	1:D:74:TYR:O	2.20	0.42
2:F:81:THR:HA	2:F:143:ARG:CZ	2.50	0.42
2:F:126:THR:C	2:F:127:LEU:HD22	2.39	0.42
3:I:8:DA:C4	3:I:9:DG:C5	3.08	0.42
3:I:38:DT:H2'	3:I:38:DT:P	2.60	0.42
1:A:225:THR:O	1:A:226:HIS:ND1	2.52	0.42
1:B:1:SER:OG	1:B:2:PRO:HD3	2.20	0.42
1:C:252:GLY:HA2	1:C:268:TRP:CZ3	2.55	0.42
1:D:169:TYR:HD1	1:D:169:TYR:HA	1.66	0.42
2:E:181:PHE:O	2:E:185:THR:HG22	2.20	0.42
2:E:283:GLU:HG3	2:E:319:GLU:HG3	2.01	0.42
2:E:289:LEU:O	2:E:289:LEU:HD23	2.20	0.42
2:F:221:ILE:HG22	2:F:225:LEU:HD11	2.01	0.42
1:A:67:PHE:CD1	1:A:68:LYS:N	2.87	0.41
1:B:248:GLN:HB2	1:B:255:LEU:HD23	2.02	0.41
2:F:281:LEU:O	2:F:284:PRO:HD2	2.20	0.41
2:F:316:GLU:HA	2:F:317:PRO:HD3	1.92	0.41
5:K:6:DC:H2'	5:K:7:DT:C6	2.56	0.41
1:B:64:ILE:HD12	1:B:76:LEU:O	2.20	0.41
1:C:255:LEU:HD11	1:C:263:ALA:HB1	2.02	0.41
1:D:270:LEU:HG	1:D:271:LEU:N	2.34	0.41
2:F:346:ALA:O	2:F:347:LEU:HD23	2.20	0.41
4:J:1:DA:C8	4:J:2:DC:H5	2.38	0.41
1:A:42:GLN:CD	1:A:43:HIS:H	2.24	0.41
1:A:51:ARG:HG2	1:A:51:ARG:HH21	1.85	0.41
1:A:258:VAL:HG11	1:A:264:GLN:HE22	1.85	0.41
1:B:6:HIS:O	1:B:10:HIS:HA	2.20	0.41
1:B:194:VAL:HG11	1:B:199:HIS:HA	2.01	0.41
3:I:37:DG:N2	5:K:12:DT:O2	2.54	0.41
1:A:163:LYS:NZ	3:L:23:DA:OP1	2.40	0.41
1:B:187:TRP:CH2	1:B:192:LEU:HD11	2.55	0.41
1:C:111:LEU:HG	1:D:203:TRP:CZ2	2.56	0.41
2:E:182:LEU:HA	2:E:185:THR:HG22	2.02	0.41
1:A:22:THR:CG2	1:A:25:GLU:HB2	2.49	0.41
2:E:91:ILE:HG13	2:E:95:VAL:CG1	2.50	0.41
2:E:341:GLN:HB3	2:E:345:ARG:HG2	2.02	0.41
3:I:28:DT:C2	3:I:29:DC:C5	3.09	0.41
1:B:226:HIS:CB	1:B:272:LYS:HB3	2.47	0.41
1:D:120:ASP:OD1	1:D:146:PRO:HB3	2.20	0.41
2:F:279:SER:O	2:F:282:THR:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:10:DA:O4'	5:K:11:DC:H5'	2.21	0.41
1:B:10:HIS:CG	1:B:10:HIS:O	2.72	0.41
1:B:162:LEU:O	1:B:166:LEU:HG	2.20	0.41
1:B:206:HIS:HD2	1:B:207:HIS:CE1	2.38	0.41
1:D:6:HIS:CE1	1:D:10:HIS:HA	2.55	0.41
2:E:80:ILE:HG22	2:E:143:ARG:HH11	1.86	0.41
4:M:7:DT:H2''	4:M:8:DA:C8	2.56	0.41
4:M:21:DC:H1'	4:M:22:DC:C5	2.56	0.41
1:C:56:PRO:HA	1:C:210:ARG:NH2	2.35	0.41
1:C:111:LEU:HG	1:D:203:TRP:CH2	2.55	0.41
1:C:122:GLY:HA3	1:C:126:ILE:CD1	2.51	0.41
3:I:8:DA:C6	3:I:9:DG:C6	3.08	0.41
3:I:33:DC:H2'	3:I:34:DC:C6	2.56	0.41
3:L:20:DC:H2''	3:L:21:DA:C8	2.56	0.41
3:L:29:DC:C2	3:L:30:DC:C5	3.08	0.41
1:A:4:GLU:O	1:A:7:SER:N	2.52	0.41
1:A:50:ILE:O	1:A:51:ARG:NH1	2.54	0.41
1:A:69:TYR:HD2	1:A:71:ASN:CA	2.33	0.41
1:A:268:TRP:CD1	1:A:268:TRP:N	2.88	0.41
1:B:92:LYS:HZ2	1:B:99:GLU:HG3	1.86	0.41
1:C:50:ILE:HB	4:J:3:DT:C2	2.56	0.41
1:C:50:ILE:O	1:C:51:ARG:C	2.59	0.41
1:C:195:LEU:HD12	1:C:195:LEU:N	2.36	0.41
2:E:108:PRO:HA	2:E:109:PRO:HD3	1.92	0.41
2:F:341:GLN:HB3	2:F:345:ARG:HG2	2.03	0.41
4:M:13:DA:H2''	4:M:14:DT:C6	2.56	0.41
4:M:23:DT:H2''	4:M:24:DG:N9	2.36	0.41
5:N:10:DA:C4	5:N:11:DC:C2	3.09	0.41
1:B:77:HIS:CE1	1:B:100:ALA:HA	2.56	0.41
1:B:201:THR:HG23	1:B:204:GLN:CD	2.42	0.41
1:B:227:TRP:CD1	1:B:245:GLU:OE2	2.74	0.41
1:C:229:TYR:HB3	1:C:242:GLY:CA	2.51	0.41
1:D:1:SER:OG	1:D:2:PRO:HD3	2.20	0.41
1:D:74:TYR:CG	1:D:93:ARG:NH1	2.89	0.41
2:E:316:GLU:HA	2:E:317:PRO:HD3	1.89	0.41
5:K:12:DT:C2	5:K:13:DA:C8	3.08	0.41
5:K:14:DG:N2	5:K:15:DG:C4	2.89	0.41
3:L:9:DG:C6	3:L:10:DA:C6	3.09	0.41
4:M:15:DT:H1'	4:M:16:DT:C6	2.56	0.41
1:C:179:ASP:N	1:C:179:ASP:OD1	2.54	0.40
1:C:231:LYS:N	1:C:241:LYS:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:SER:O	1:D:31:ARG:HG3	2.21	0.40
4:J:15:DT:H1'	4:J:16:DT:C6	2.55	0.40
1:A:252:GLY:HA3	4:M:3:DT:O2	2.22	0.40
1:A:259:SER:C	1:A:261:SER:H	2.23	0.40
1:C:35:ALA:C	1:C:37:ARG:H	2.25	0.40
1:C:51:ARG:O	1:C:52:ARG:HB2	2.20	0.40
1:D:228:TYR:O	1:D:229:TYR:C	2.60	0.40
1:A:64:ILE:HD13	1:A:64:ILE:HG21	1.85	0.40
1:A:268:TRP:CD2	1:A:269:ARG:N	2.90	0.40
1:D:68:LYS:HB3	1:D:167:TYR:OH	2.21	0.40
2:E:81:THR:HA	2:E:143:ARG:CZ	2.52	0.40
2:E:159:ILE:HD12	2:E:159:ILE:HA	1.86	0.40
2:E:241:GLU:HA	2:E:244:LYS:HZ3	1.87	0.40
5:K:10:DA:C8	5:K:11:DC:C6	3.09	0.40
3:L:27:DA:H2'	3:L:28:DT:H71	2.03	0.40
3:L:47:DT:H6	3:L:47:DT:H2'	1.54	0.40
1:B:52:ARG:HB3	2:F:306:ASN:HD21	1.86	0.40
1:C:23:THR:H	1:C:23:THR:HG23	1.63	0.40
1:C:111:LEU:HD13	1:C:111:LEU:HA	1.67	0.40
1:C:230:PHE:CE2	1:C:266:ILE:HG21	2.56	0.40
2:E:320:PHE:HD1	2:E:323:ILE:HG23	1.86	0.40
2:F:202:LYS:HE3	2:F:202:LYS:HB3	1.88	0.40
2:F:269:TYR:HA	2:F:272:VAL:HG12	2.03	0.40
4:J:21:DC:H1'	4:J:22:DC:C5	2.57	0.40
3:L:11:DA:C6	3:L:12:DA:C6	3.09	0.40
5:N:4:DC:H2''	5:N:5:DA:C8	2.57	0.40
1:A:56:PRO:C	1:A:210:ARG:NH1	2.75	0.40
1:B:214:ILE:HA	1:B:215:PRO:HD3	1.98	0.40
1:C:189:ILE:HG23	1:C:189:ILE:HD12	1.73	0.40
1:D:177:PRO:HB2	1:D:179:ASP:OD1	2.22	0.40
1:D:226:HIS:CG	1:D:227:TRP:H	2.40	0.40
2:E:80:ILE:HG22	2:E:143:ARG:NH1	2.37	0.40
3:I:4:DG:C6	3:I:5:DG:C6	3.09	0.40
5:K:15:DG:H2''	5:K:16:DG:H8	1.85	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	274/390 (70%)	260 (95%)	14 (5%)	0	100	100
1	B	255/390 (65%)	245 (96%)	10 (4%)	0	100	100
1	C	274/390 (70%)	265 (97%)	9 (3%)	0	100	100
1	D	255/390 (65%)	251 (98%)	4 (2%)	0	100	100
2	E	321/343 (94%)	319 (99%)	2 (1%)	0	100	100
2	F	321/343 (94%)	319 (99%)	2 (1%)	0	100	100
All	All	1700/2246 (76%)	1659 (98%)	41 (2%)	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	
1	A	240/333 (72%)	237 (99%)	3 (1%)	69	83
1	B	225/333 (68%)	221 (98%)	4 (2%)	59	77
1	C	240/333 (72%)	238 (99%)	2 (1%)	81	89
1	D	225/333 (68%)	224 (100%)	1 (0%)	91	95
2	E	288/319 (90%)	286 (99%)	2 (1%)	84	91
2	F	288/319 (90%)	285 (99%)	3 (1%)	76	86
All	All	1506/1970 (76%)	1491 (99%)	15 (1%)	77	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	195	LEU
1	A	197	ASN
1	B	6	HIS
1	B	10	HIS
1	B	218	ARG
1	B	223	LYS
1	C	51	ARG
1	C	228	TYR
1	D	218	ARG
2	E	105	ARG
2	E	281	LEU
2	F	105	ARG
2	F	277	LYS
2	F	281	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	39	ASN
1	A	43	HIS
1	A	128	GLN
1	A	132	ASN
1	A	141	HIS
1	A	148	ASN
1	A	199	HIS
1	A	204	GLN
1	A	207	HIS
1	A	224	GLN
1	B	34	HIS
1	B	57	ASN
1	B	66	HIS
1	B	193	ASN
1	B	204	GLN
1	B	207	HIS
1	B	224	GLN
1	B	248	GLN
1	C	6	HIS
1	C	58	HIS
1	C	128	GLN

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Mol	Chain	Res	Type
1	C	132	ASN
1	C	141	HIS
1	C	148	ASN
1	C	204	GLN
1	C	207	HIS
1	C	226	HIS
1	D	61	GLN
1	D	77	HIS
1	D	141	HIS
1	D	148	ASN
1	D	156	GLN
1	D	206	HIS
1	D	224	GLN
1	D	226	HIS
2	E	38	GLN
2	E	205	ASN
2	E	206	ASN
2	E	233	ASN
2	E	273	GLN
2	E	306	ASN
2	E	330	GLN
2	F	38	GLN
2	F	85	ASN
2	F	205	ASN
2	F	206	ASN
2	F	233	ASN
2	F	273	GLN
2	F	306	ASN
2	F	330	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

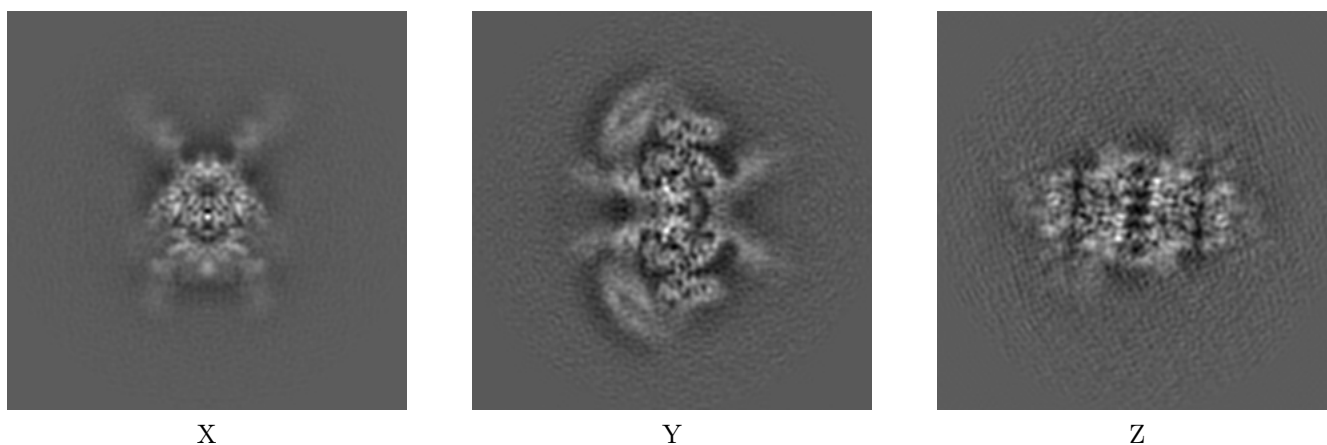
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21301. 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](#)

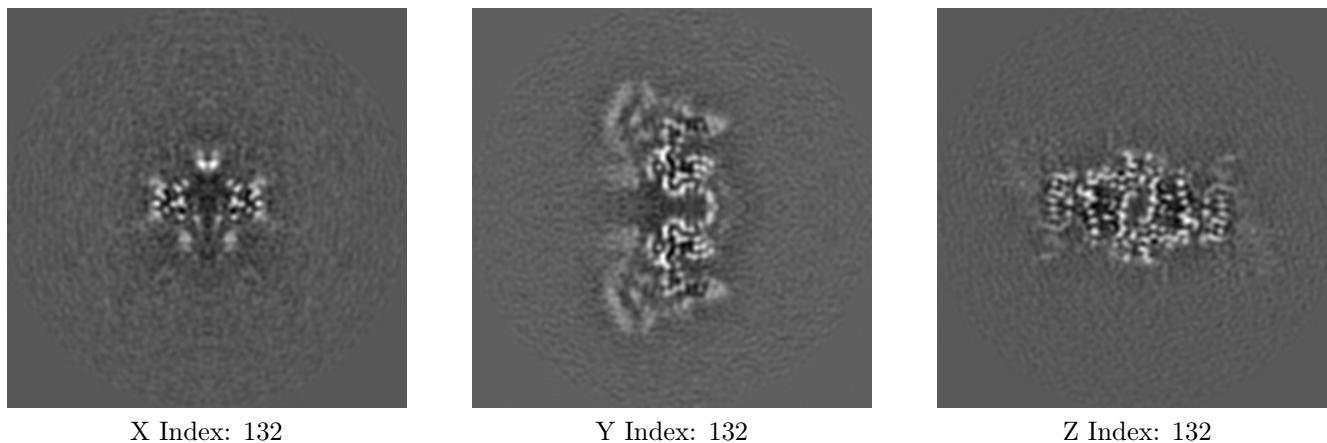
6.1.1 Primary map



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

6.2 Central slices [i](#)

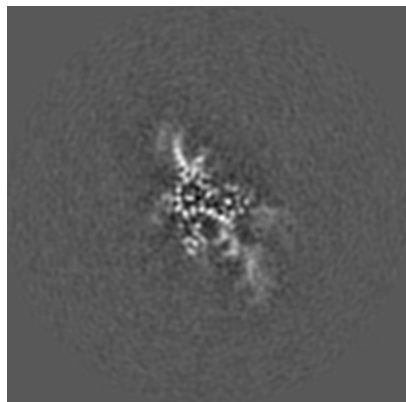
6.2.1 Primary map



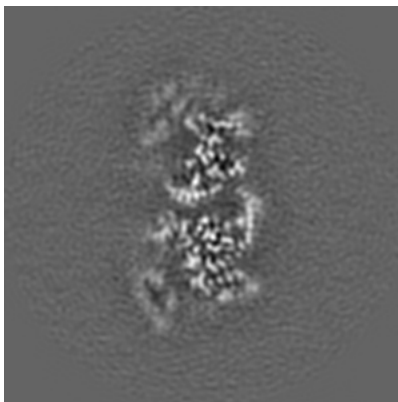
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

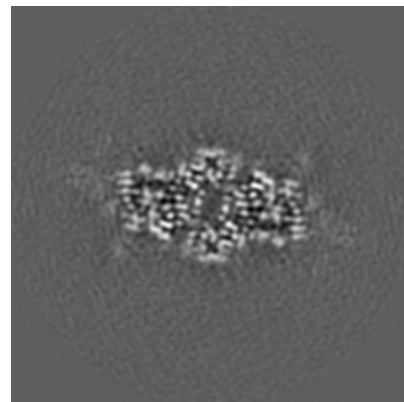
6.3.1 Primary map



X Index: 119



Y Index: 126



Z Index: 135

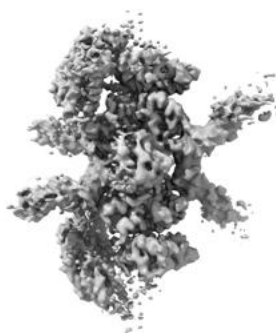
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00782. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

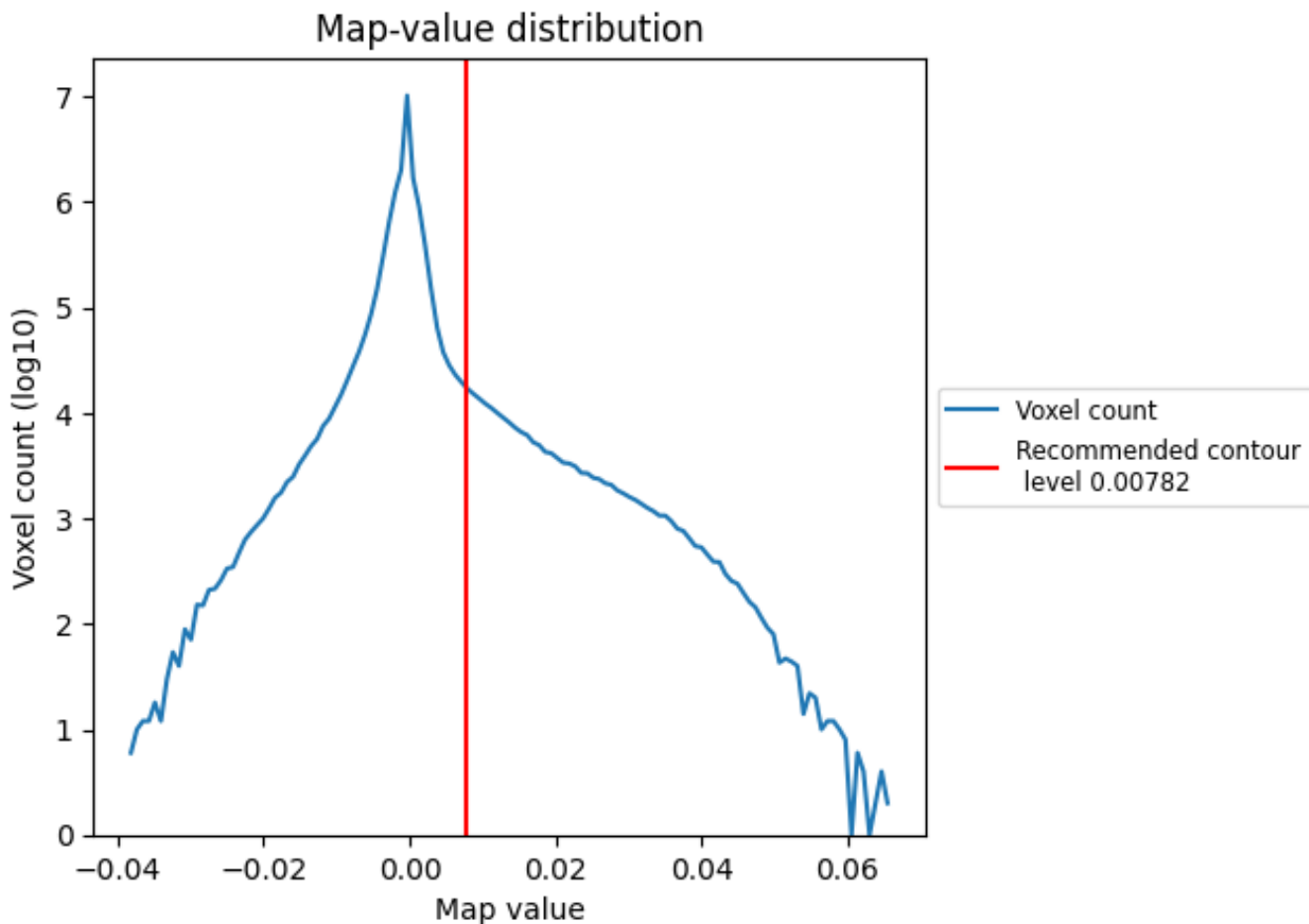
6.5 Mask visualisation

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

7 Map analysis [i](#)

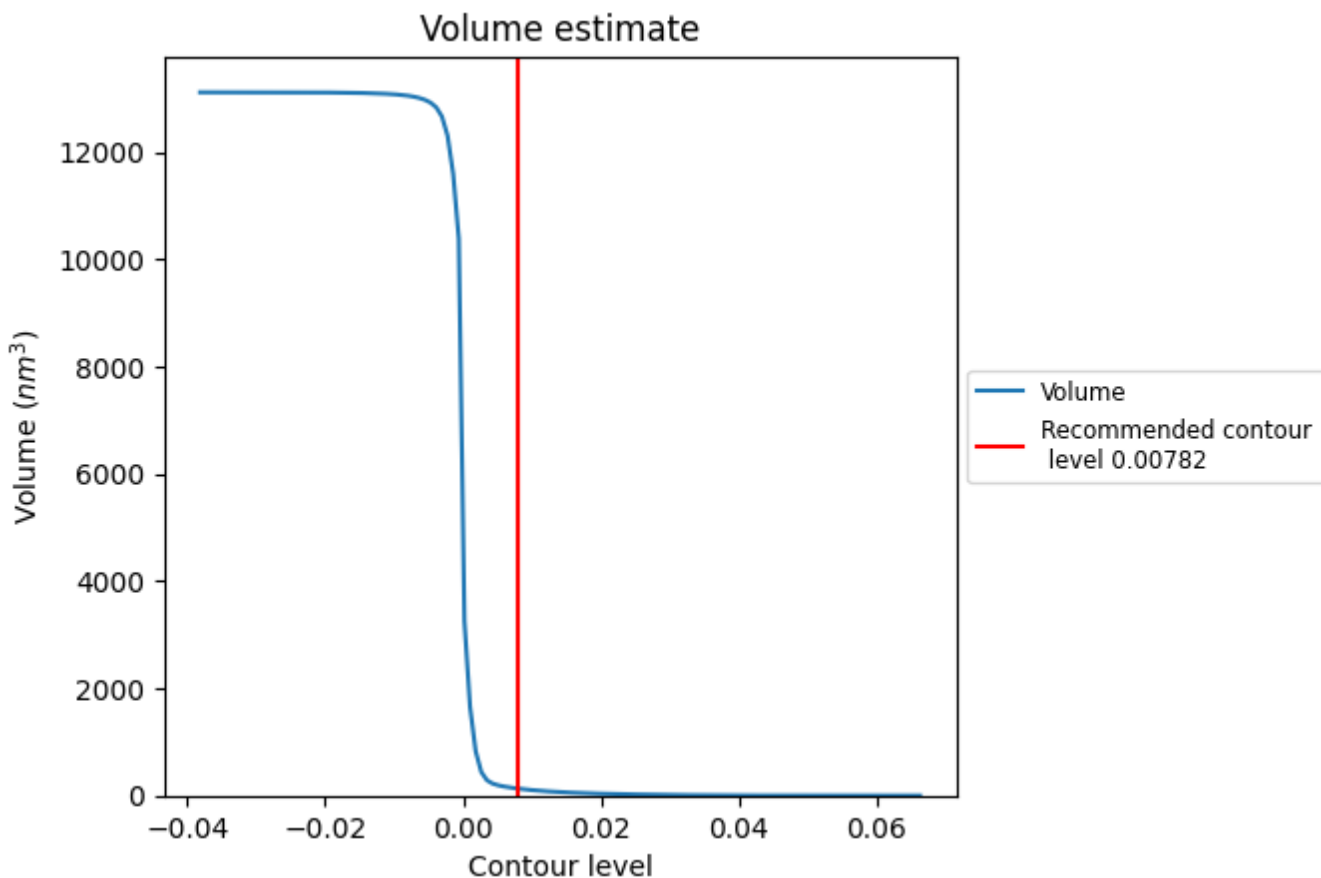
This section contains the results of statistical analysis of the map.

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.

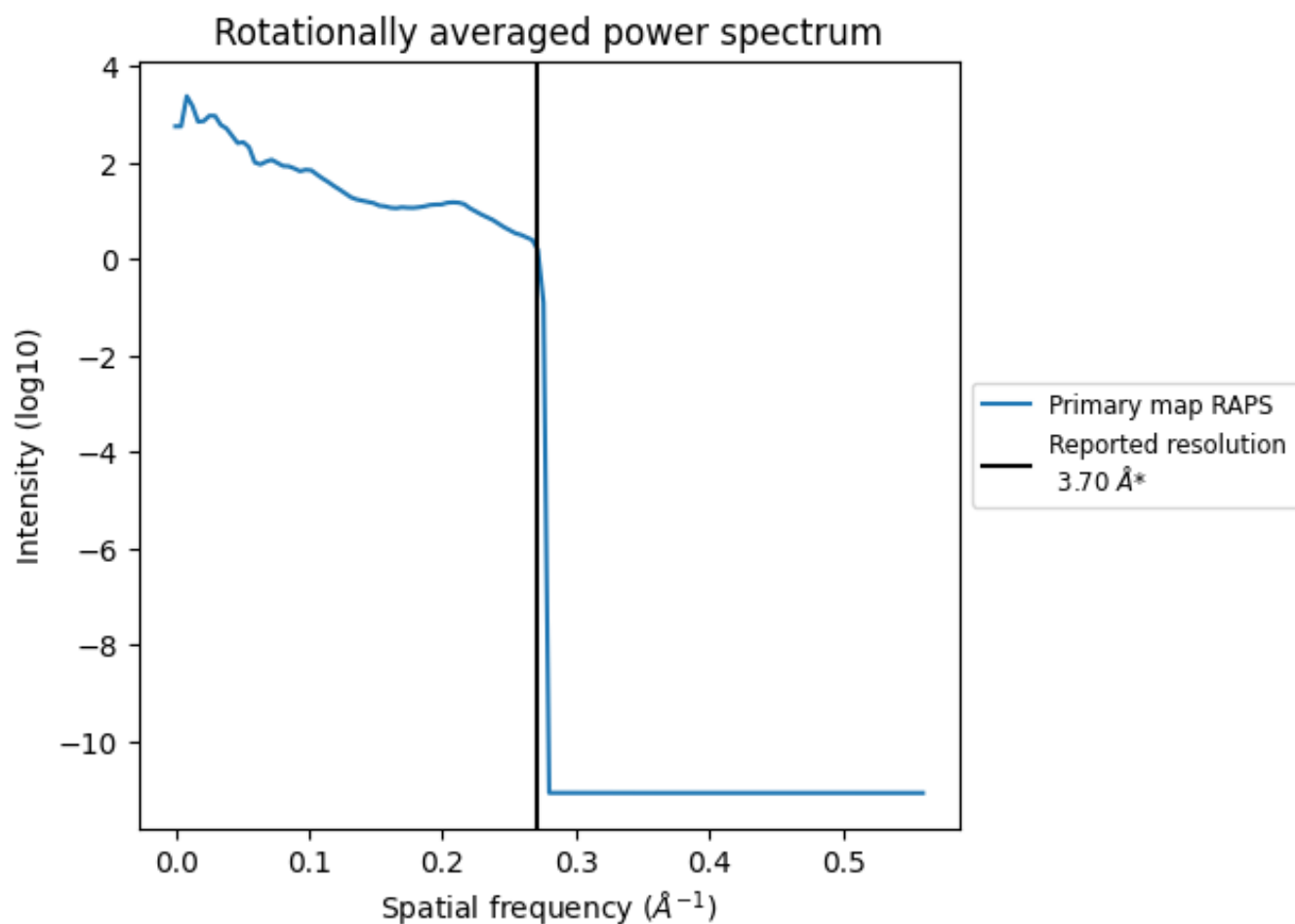
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; this corresponds to an approximate mass of 119 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 [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

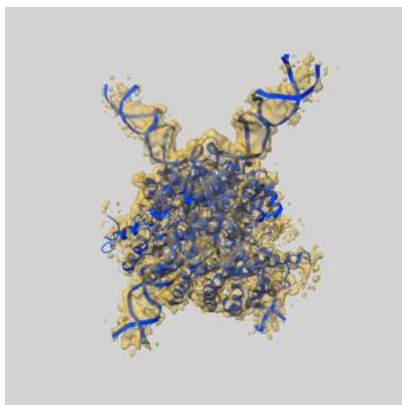
8 Fourier-Shell correlation

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

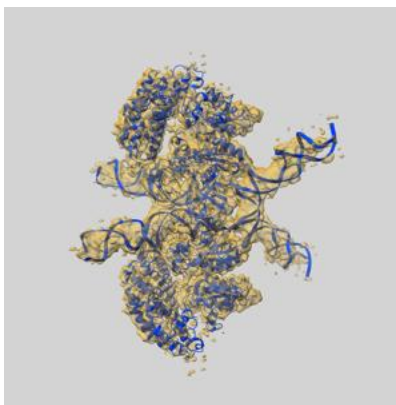
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21301 and PDB model 6VOY. Per-residue inclusion information can be found in section 3 on page 9.

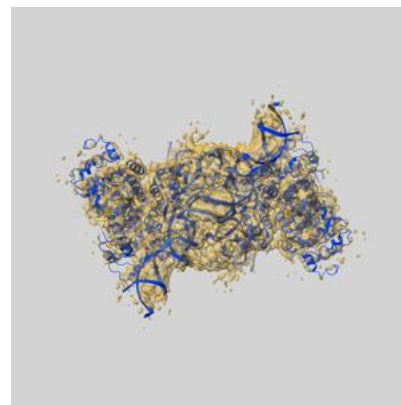
9.1 Map-model overlay [i](#)



X



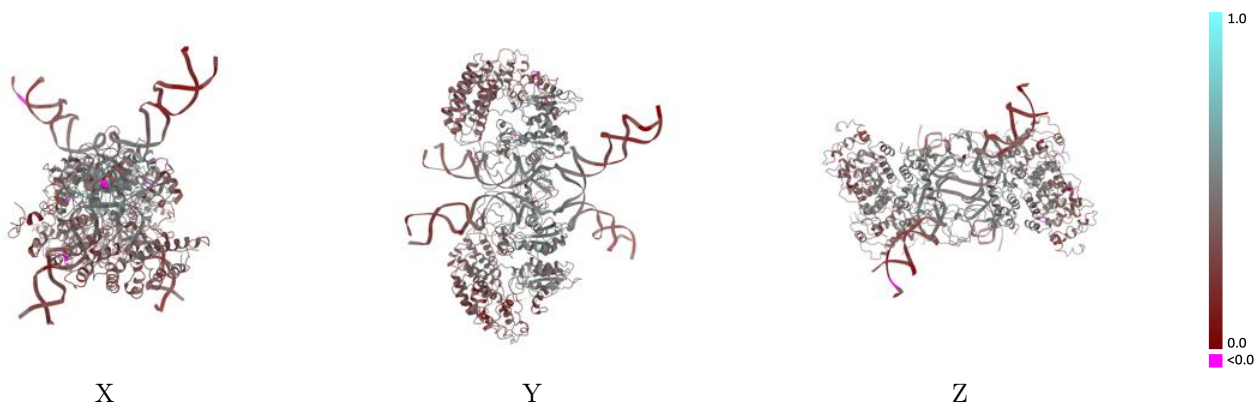
Y



Z

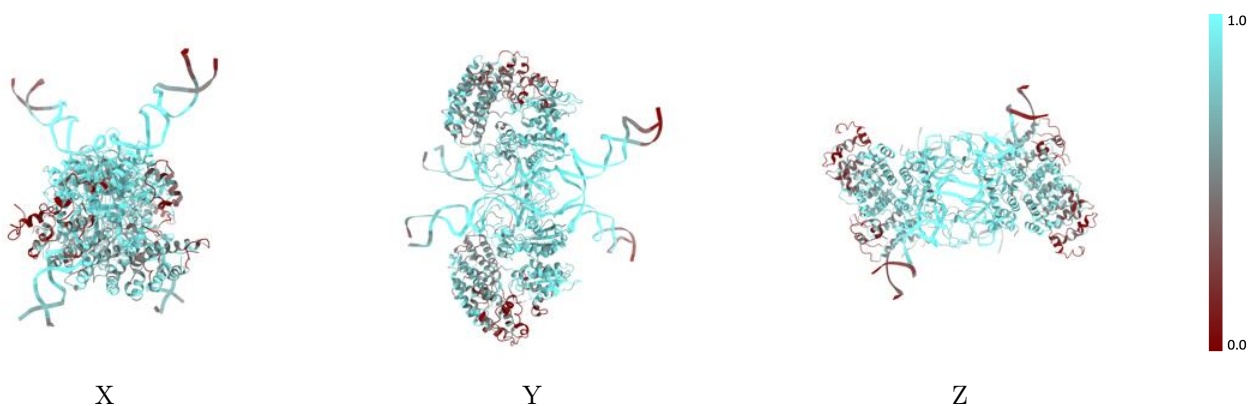
The images above show the 3D surface view of the map at the recommended contour level 0.00782 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



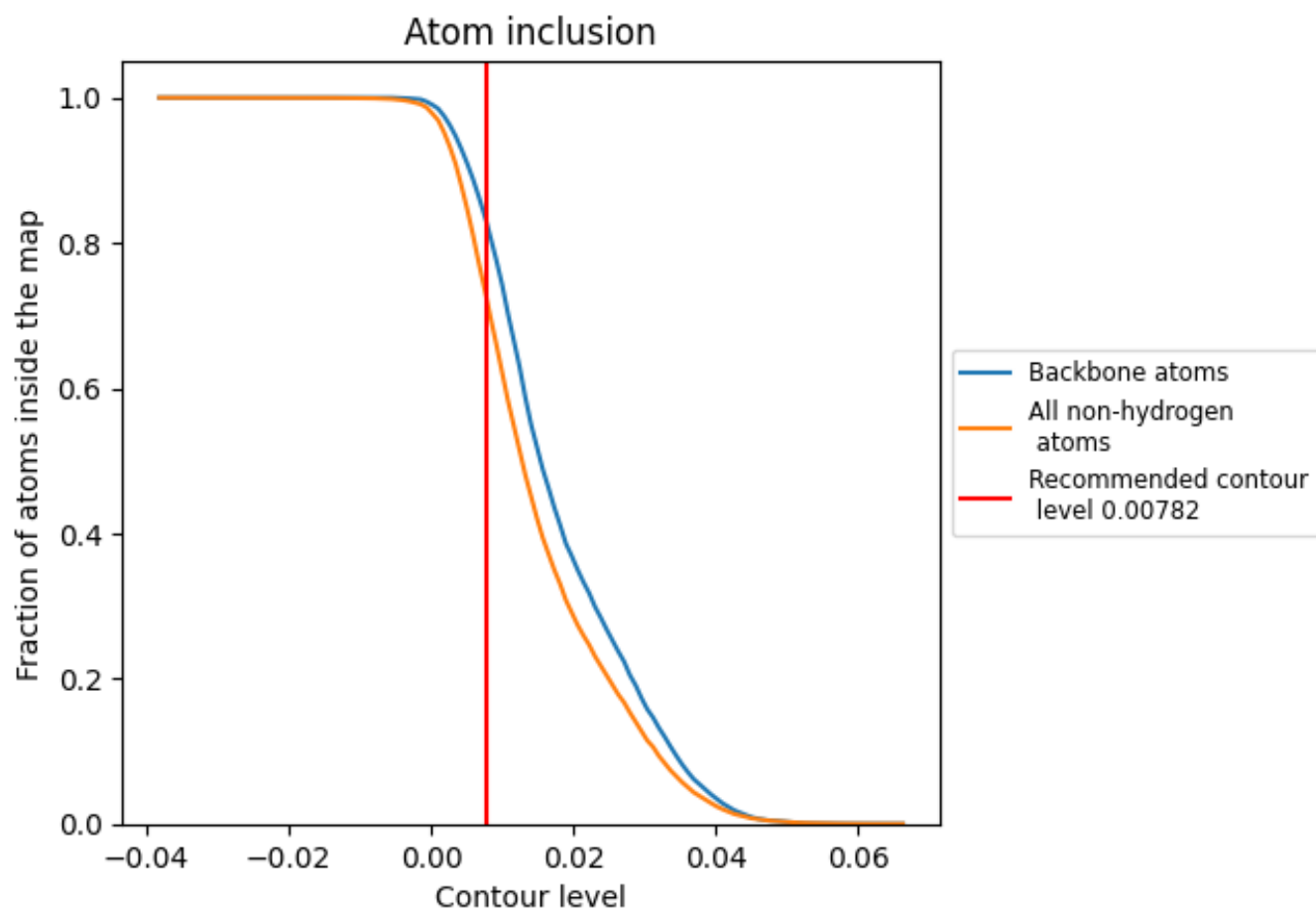
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00782).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00782) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7231	 0.3890
A	 0.8593	 0.4600
B	 0.7268	 0.4110
C	 0.8682	 0.4660
D	 0.7353	 0.4140
E	 0.5163	 0.3420
F	 0.5175	 0.3440
I	 0.8540	 0.3510
J	 0.8968	 0.3800
K	 0.7385	 0.2730
L	 0.8520	 0.3510
M	 0.9127	 0.3790
N	 0.7439	 0.2800

