



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 11:46 PM UTC

PDB ID : 3JBW / pdb_00003jbw
EMDB ID : EMD-6489
Title : Cryo-electron microscopy structure of RAG Paired Complex (with NBD, no symmetry)
Authors : Ru, H.; Chambers, M.G.; Fu, T.-M.; Tong, A.B.; Liao, M.; Wu, H.
Deposited on : 2015-10-21
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

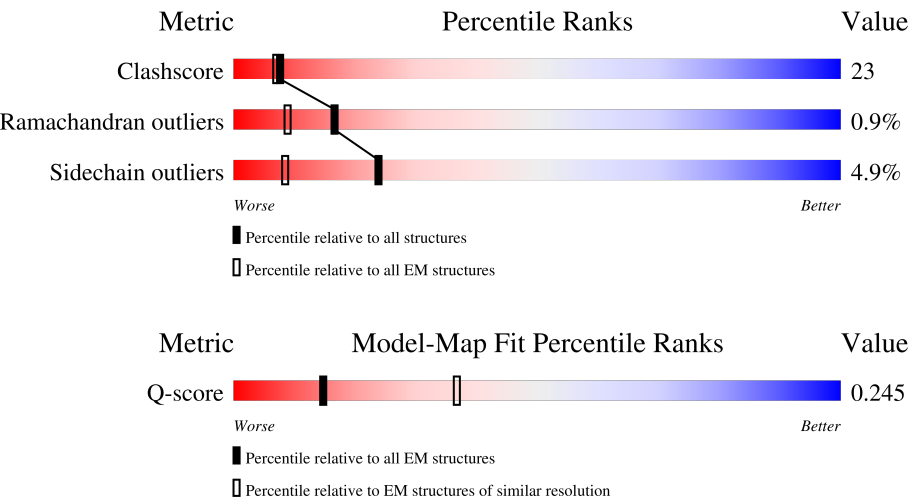
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.60 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	2407 (4.10 - 5.10)

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	764	12% 48% 28% • • 19%
1	C	764	12% 46% 31% • • 19%
2	B	533	14% 37% 27% • 34%
2	D	533	14% 38% 26% • 34%

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Mol	Chain	Length	Quality of chain
3	E	34	 26% 26% 74%
4	F	50	 22% 38% 62%
5	G	61	 30% 30% 64% 7%
6	H	45	 42% 40% 49% 11%
7	I	16	 12% 19% 81%
7	J	16	 12% 100%



2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19997 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 V(D)J recombination-activating protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	622	Total	C	N	O	S	0	0
			5008	3134	901	936	37		
1	C	622	Total	C	N	O	S	0	0
			5008	3134	901	936	37		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	GLY	-	expression tag	UNP O13033
A	269	GLY	-	expression tag	UNP O13033
A	270	SER	-	expression tag	UNP O13033
C	268	GLY	-	expression tag	UNP O13033
C	269	GLY	-	expression tag	UNP O13033
C	270	SER	-	expression tag	UNP O13033

- Molecule 2 is a protein called V(D)J recombination-activating protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		
2	D	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q1RLW7
B	-1	GLY	-	expression tag	UNP Q1RLW7
B	0	SER	-	expression tag	UNP Q1RLW7
D	-2	GLY	-	expression tag	UNP Q1RLW7
D	-1	GLY	-	expression tag	UNP Q1RLW7
D	0	SER	-	expression tag	UNP Q1RLW7

- Molecule 3 is a DNA chain called 12-RSS signal end forward strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	34	Total	C	N	O	P	0	0
			697	330	138	195	34		

- Molecule 4 is a DNA chain called Nicked 12-RSS intermediate reverse strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	50	Total	C	N	O	P	0	0
			1027	489	183	305	50		

- Molecule 5 is a DNA chain called Nicked 23-RSS intermediate reverse strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	61	Total	C	N	O	P	0	0
			1256	596	235	364	61		

- Molecule 6 is a DNA chain called Nicked 23-RSS intermediate forward strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	45	Total	C	N	O	P	0	0
			919	437	169	268	45		

- Molecule 7 is a DNA chain called 5'-D(P*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	16	Total	C	N	O	P	0	0
			326	156	54	100	16		
7	J	16	Total	C	N	O	P	0	0
			326	156	54	100	16		

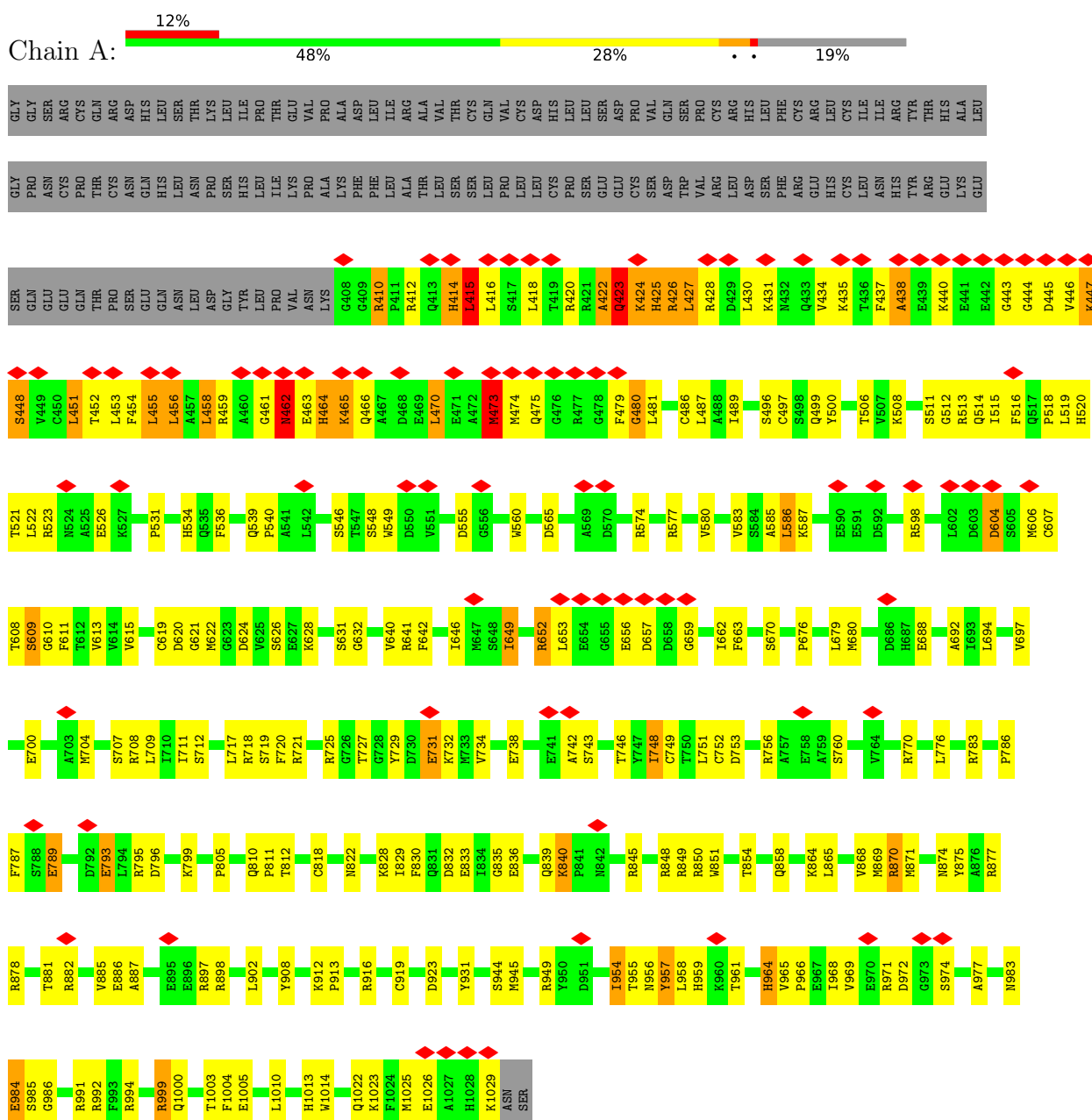
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Zn	0
			1	1	
8	C	1	Total	Zn	0
			1	1	

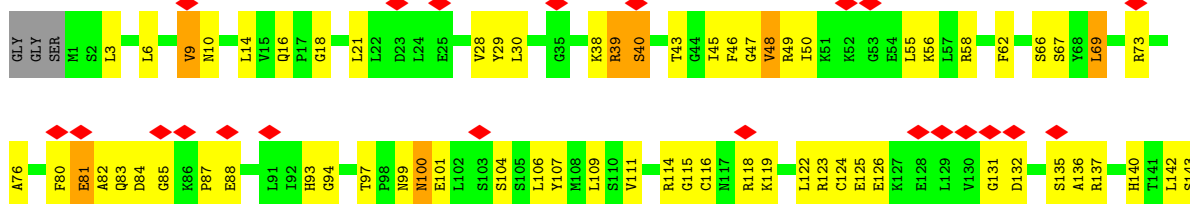
3 Residue-property plots

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.

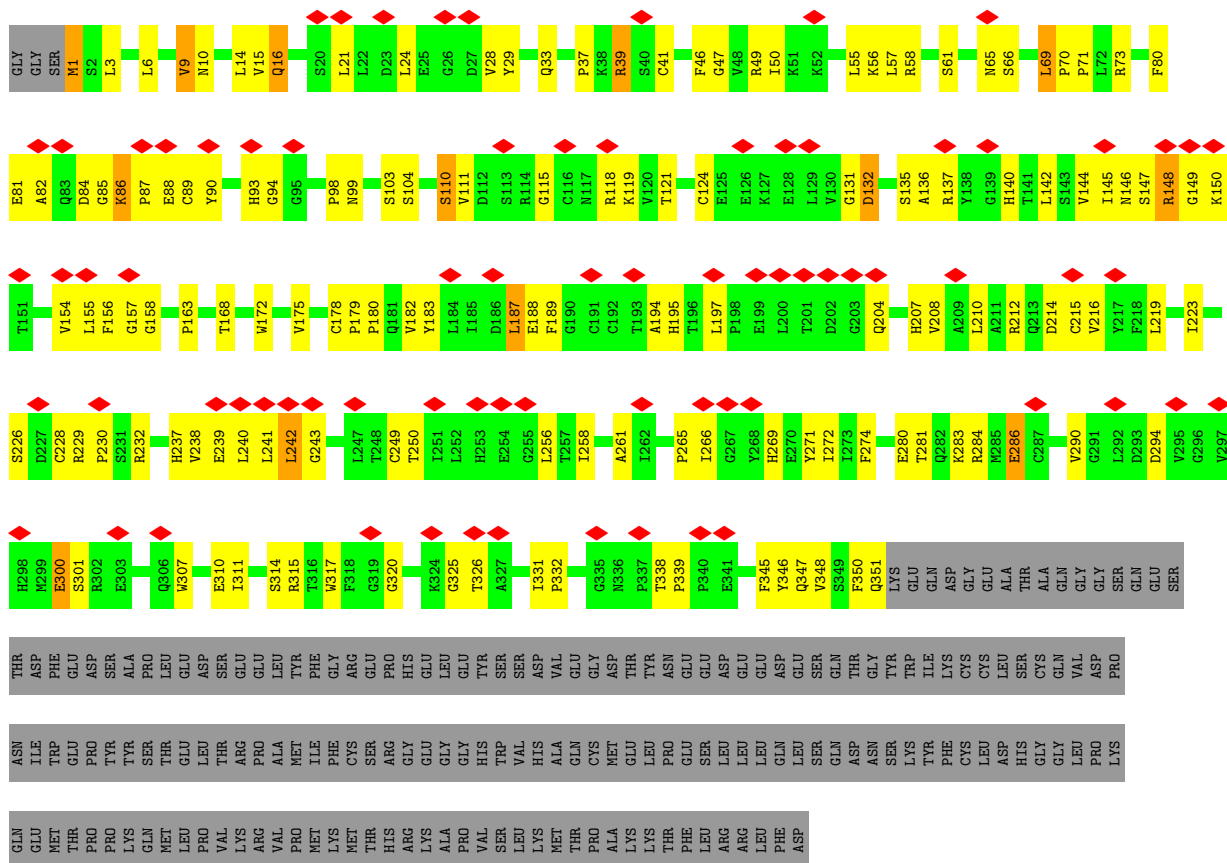
- Molecule 1: V(D)J recombination-activating protein 1



Chain C:



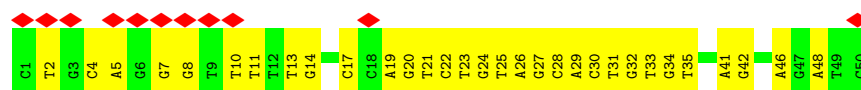
- Molecule 2: V(D)J recombination-activating protein 2



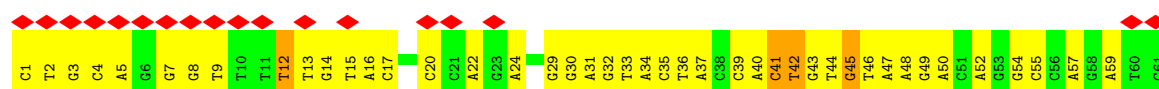
- Molecule 3: 12-RSS signal end forward strand



- Molecule 4: Nicked 12-RSS intermediate reverse strand



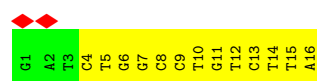
- Molecule 5: Nicked 23-RSS intermediate reverse strand



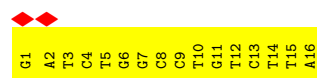
- Molecule 6: Nicked 23-RSS intermediate forward strand



- Molecule 7: 5'-D(P*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3',



- Molecule 7: 5'-D(P*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3',



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14129	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	40607	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.049	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	236.16, 236.16, 236.16	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.23, 1.23, 1.23	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.60	0/5106	1.15	38/6867 (0.6%)
1	C	0.62	1/5106 (0.0%)	1.19	39/6867 (0.6%)
2	B	0.53	1/2784 (0.0%)	0.98	8/3784 (0.2%)
2	D	0.54	0/2784	0.99	11/3784 (0.3%)
3	E	0.77	0/784	0.83	0/1206
4	F	0.70	0/1150	0.79	0/1774
5	G	0.87	5/1410 (0.4%)	0.85	3/2175 (0.1%)
6	H	1.09	8/1030 (0.8%)	0.97	4/1586 (0.3%)
7	I	1.00	0/363	0.96	0/558
7	J	0.72	0/363	0.78	0/558
All	All	0.66	15/20880 (0.1%)	1.05	103/29159 (0.4%)

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	1
1	C	0	2
All	All	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	2	DA	O3'-P	10.65	1.77	1.61
5	G	42	DT	P-O5'	-10.23	1.40	1.60
5	G	41	DC	O3'-P	8.99	1.74	1.61
6	H	2	DA	C3'-O3'	8.74	1.68	1.42
5	G	45	DG	C3'-O3'	7.90	1.66	1.42
6	H	5	DG	C3'-O3'	7.89	1.66	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	6	DT	P-O5'	6.83	1.74	1.60
6	H	4	DA	C3'-O3'	6.15	1.61	1.42
6	H	6	DT	P-OP2	5.77	1.59	1.48
6	H	3	DC	N3-C4	5.52	1.44	1.33
1	C	983	ASN	CA-C	-5.32	1.45	1.52
2	B	266	ILE	CA-CB	5.17	1.61	1.54
6	H	3	DC	P-OP2	-5.14	1.38	1.48
5	G	42	DT	P-OP1	-5.13	1.38	1.48
5	G	42	DT	O5'-C5'	-5.04	1.27	1.42

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	420	ARG	N-CA-C	16.67	131.50	111.33
1	C	422	ALA	N-CA-C	-16.30	92.89	113.43
1	C	999	ARG	N-CA-C	12.44	124.38	111.07
1	C	468	ASP	N-CA-C	11.18	123.22	111.14
1	A	426	ARG	N-CA-C	10.17	124.20	111.69
1	A	454	PHE	N-CA-C	10.16	121.94	111.07
1	C	418	LEU	N-CA-C	10.04	125.71	109.85
1	A	999	ARG	N-CA-C	9.78	121.53	111.07
6	H	6	DT	O5'-P-OP2	9.77	137.32	108.00
1	C	454	PHE	N-CA-C	9.14	121.24	111.28
1	C	421	ARG	N-CA-C	9.09	124.62	112.25
5	G	42	DT	P-O5'-C5'	-9.09	106.36	120.00
1	A	446	VAL	N-CA-C	8.83	118.90	110.42
1	A	957	TYR	N-CA-C	8.77	120.92	111.36
1	A	984	GLU	N-CA-C	8.77	121.63	111.11
1	A	659	GLY	N-CA-C	-8.60	98.14	110.96
1	A	447	LYS	N-CA-C	8.15	120.96	111.02
1	C	426	ARG	N-CA-C	-8.10	102.42	111.82
2	B	40	SER	N-CA-C	-8.02	102.49	111.07
1	A	462	ASN	N-CA-C	7.99	121.55	108.52
1	A	415	LEU	N-CA-C	7.88	120.86	111.33
1	A	985	SER	N-CA-C	-7.73	102.55	110.97
2	D	339	PRO	N-CA-C	7.59	119.97	110.70
6	H	3	DC	OP1-P-OP2	-7.59	97.24	120.00
1	A	448	SER	N-CA-C	7.44	119.39	111.28
5	G	12	DT	OP2-P-O3'	-7.44	85.67	108.00
1	C	424	LYS	N-CA-C	7.44	119.39	111.28
1	A	414	HIS	CA-C-N	7.43	130.56	120.38
1	A	414	HIS	C-N-CA	7.43	130.56	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	HIS	N-CA-C	7.42	119.45	111.36
2	D	338	THR	CA-C-N	7.22	127.82	120.38
2	D	338	THR	C-N-CA	7.22	127.82	120.38
5	G	41	DC	OP2-P-O3'	7.18	129.54	108.00
1	C	478	GLY	N-CA-C	-7.11	96.33	113.18
1	C	420	ARG	CB-CA-C	-7.11	98.59	110.68
6	H	4	DA	N9-C1'-C2'	7.08	124.12	113.50
1	A	451	LEU	N-CA-C	7.06	118.98	111.28
1	C	415	LEU	CB-CA-C	-7.02	108.47	116.54
1	A	475	GLN	N-CA-C	6.95	121.51	112.89
1	A	461	GLY	N-CA-C	-6.92	96.78	113.18
1	C	420	ARG	CA-C-N	-6.87	111.55	122.95
1	C	420	ARG	C-N-CA	-6.87	111.55	122.95
2	D	148	ARG	N-CA-C	6.87	120.87	111.39
1	C	462	ASN	N-CA-C	6.85	125.39	110.80
1	C	658	ASP	CB-CA-C	-6.85	108.67	116.54
1	A	840	LYS	CA-C-N	6.74	126.36	119.56
1	A	840	LYS	C-N-CA	6.74	126.36	119.56
1	C	655	GLY	N-CA-C	-6.53	101.94	110.29
1	A	423	GLN	N-CA-C	6.44	119.12	111.33
1	A	427	LEU	N-CA-C	6.41	121.10	113.28
1	C	425	HIS	N-CA-C	-6.41	105.04	112.92
1	A	919	CYS	CA-C-N	6.39	126.08	119.56
1	A	919	CYS	C-N-CA	6.39	126.08	119.56
2	B	339	PRO	N-CA-C	6.37	118.47	110.70
1	C	870	ARG	N-CA-C	-6.34	99.38	109.59
1	A	868	VAL	N-CA-C	6.34	118.62	108.85
1	A	881	THR	N-CA-C	-6.32	99.11	108.79
1	A	464	HIS	N-CA-C	6.21	118.12	111.36
1	C	420	ARG	CB-CG-CD	-6.12	97.23	111.30
1	C	464	HIS	N-CA-C	-6.11	97.79	110.80
1	A	868	VAL	CA-C-N	6.06	128.68	120.44
1	A	868	VAL	C-N-CA	6.06	128.68	120.44
1	C	421	ARG	CG-CD-NE	-6.00	98.81	112.00
1	A	473	MET	N-CA-C	5.98	123.53	110.80
2	D	110	SER	N-CA-C	5.95	116.42	108.38
1	C	453	LEU	N-CA-C	5.90	117.71	111.28
1	A	470	LEU	N-CA-C	5.69	117.56	111.36
1	C	984	GLU	N-CA-C	5.68	122.90	110.80
6	H	3	DC	O4'-C1'-N1	5.64	116.86	108.40
1	C	412	ARG	CA-CB-CG	-5.59	102.92	114.10
1	C	463	GLU	N-CA-CB	-5.59	101.05	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	481	LEU	N-CA-C	-5.57	102.15	110.23
2	D	99	ASN	N-CA-C	-5.57	101.67	109.96
2	D	163	PRO	CA-C-N	5.49	125.16	119.56
2	D	163	PRO	C-N-CA	5.49	125.16	119.56
2	B	99	ASN	N-CA-C	-5.45	102.46	110.52
2	B	99	ASN	CA-C-N	-5.43	114.43	122.41
2	B	99	ASN	C-N-CA	-5.43	114.43	122.41
1	C	455	LEU	N-CA-C	5.38	117.57	111.11
1	C	463	GLU	N-CA-C	5.38	122.26	110.80
1	C	468	ASP	CB-CA-C	-5.34	102.46	110.90
1	C	659	GLY	N-CA-C	-5.34	102.73	110.90
1	A	964	HIS	N-CA-C	5.30	119.74	113.16
1	C	984	GLU	CA-CB-CG	-5.30	103.49	114.10
1	C	919	CYS	CA-C-N	5.28	124.89	119.56
1	C	919	CYS	C-N-CA	5.28	124.89	119.56
1	A	438	ALA	N-CA-C	5.26	117.69	111.33
1	C	465	LYS	N-CA-C	-5.24	105.57	111.28
2	D	290	VAL	CB-CA-C	-5.22	104.52	110.73
1	C	637	GLU	N-CA-C	5.21	117.04	111.36
2	D	86	LYS	CA-C-N	5.18	125.63	120.14
2	D	86	LYS	C-N-CA	5.18	125.63	120.14
1	A	870	ARG	N-CA-C	-5.16	100.19	108.55
2	B	258	ILE	N-CA-C	5.14	116.69	108.87
1	A	410	ARG	CB-CG-CD	-5.13	99.50	111.30
2	B	81	GLU	CA-CB-CG	5.13	124.36	114.10
1	A	461	GLY	CA-C-N	-5.11	115.89	123.05
1	A	461	GLY	C-N-CA	-5.11	115.89	123.05
1	C	417	SER	N-CA-C	5.11	119.57	113.23
1	C	461	GLY	N-CA-C	-5.10	101.09	113.18
2	B	100	ASN	N-CA-C	5.10	116.96	107.99
1	C	416	LEU	N-CA-C	5.08	121.62	110.80
1	A	609	SER	N-CA-C	5.06	119.55	113.17

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	ASN	Peptide
1	C	477	ARG	Peptide
1	C	742	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5008	0	4968	226	0
1	C	5008	0	4968	244	0
2	B	2714	0	2665	127	0
2	D	2714	0	2665	115	0
3	E	697	0	379	36	0
4	F	1027	0	566	57	0
5	G	1256	0	686	81	0
6	H	919	0	506	59	0
7	I	326	0	183	32	0
7	J	326	0	183	36	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
All	All	19997	0	17769	841	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 23.

All (841) 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)
6:H:5:DG:C3'	6:H:5:DG:O3'	1.66	1.44
5:G:45:DG:O3'	5:G:45:DG:C3'	1.66	1.44
6:H:2:DA:C3'	6:H:2:DA:O3'	1.68	1.38
2:D:58:ARG:HH12	7:I:6:DG:H5''	1.20	1.02
5:G:12:DT:H2''	5:G:13:DT:H5'	1.41	1.01
1:A:456:LEU:HG	1:C:420:ARG:HE	1.27	0.97
2:B:119:LYS:NZ	7:J:6:DG:OP1	1.98	0.97
5:G:57:DA:H61	7:J:4:DC:H42	1.11	0.96
2:B:58:ARG:HH22	7:J:6:DG:H5''	1.30	0.93
2:D:140:HIS:HD2	2:D:155:LEU:HD11	1.36	0.89
3:E:15:DC:O2	4:F:20:DG:N2	2.07	0.88
1:A:513:ARG:HH11	1:C:513:ARG:HE	1.20	0.88
2:B:140:HIS:HD2	2:B:155:LEU:HD11	1.39	0.87
5:G:47:DA:H2	7:J:15:DT:H3	1.17	0.86
1:C:866:LYS:HD2	1:C:867:PRO:HD2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:GLN:NE2	1:A:887:ALA:O	2.10	0.84
1:C:415:LEU:O	1:C:417:SER:N	2.11	0.83
5:G:47:DA:H2	7:J:15:DT:N3	1.77	0.83
4:F:34:DG:H3'	4:F:35:DT:H5''	1.61	0.82
5:G:31:DA:H61	6:H:15:DT:H3	1.28	0.81
1:A:770:ARG:NH2	1:A:799:LYS:O	2.14	0.81
2:D:58:ARG:NH1	7:I:6:DG:H5''	1.94	0.81
1:C:466:GLN:HG3	1:C:467:ALA:N	1.95	0.81
1:A:415:LEU:HD21	1:C:452:THR:HG21	1.61	0.79
1:A:463:GLU:HG3	1:A:465:LYS:HE2	1.64	0.79
1:A:877:ARG:HH21	1:A:916:ARG:HH21	1.30	0.78
1:A:481:LEU:HD11	1:A:486:CYS:HB2	1.65	0.78
2:B:82:ALA:HA	2:B:87:PRO:HB3	1.64	0.78
1:C:738:GLU:HA	1:C:805:PRO:HB3	1.65	0.78
1:A:513:ARG:HE	1:C:513:ARG:HH11	1.30	0.77
2:B:266:ILE:HG22	2:B:325:GLY:HA2	1.67	0.77
5:G:36:DT:O2	6:H:11:DG:N2	2.18	0.77
2:D:1:MET:SD	2:D:1:MET:N	2.57	0.77
1:C:468:ASP:HA	1:C:471:GLU:HG2	1.65	0.76
1:C:426:ARG:NH2	5:G:12:DT:OP1	2.16	0.76
4:F:26:DA:H2''	4:F:27:DG:C8	2.20	0.76
1:A:738:GLU:HA	1:A:805:PRO:HB3	1.68	0.76
1:C:814:ASP:OD2	1:C:817:HIS:ND1	2.18	0.76
1:A:479:PHE:N	1:A:480:GLY:O	2.20	0.75
5:G:54:DG:O6	7:J:7:DG:N1	2.18	0.75
2:D:58:ARG:HH12	7:I:6:DG:C5'	2.00	0.75
2:D:283:LYS:HD2	2:D:317:TRP:CD1	2.22	0.75
1:A:656:GLU:HG2	1:A:657:ASP:H	1.52	0.74
1:C:424:LYS:O	1:C:428:ARG:HG3	1.88	0.74
1:C:486:CYS:SG	1:C:500:TYR:OH	2.45	0.74
1:A:456:LEU:HD21	1:C:420:ARG:HG2	1.69	0.74
1:A:463:GLU:HA	5:G:22:DA:H4'	1.69	0.73
2:B:278:GLN:HG3	2:B:284:ARG:HB2	1.71	0.73
1:C:1000:GLN:HE21	5:G:42:DT:H4'	1.54	0.73
1:A:513:ARG:NH1	1:C:513:ARG:HE	1.87	0.73
5:G:7:DG:H2'	5:G:8:DG:H8	1.53	0.73
4:F:46:DA:H61	7:I:4:DC:H42	1.37	0.72
1:A:613:VAL:HG22	1:A:649:ILE:HD13	1.69	0.72
3:E:10:DA:N6	4:F:24:DG:O6	2.19	0.72
4:F:7:DG:H2'	4:F:8:DG:H8	1.54	0.72
1:C:436:THR:HG22	1:C:440:LYS:HE2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:57:DA:H61	7:J:4:DC:N4	1.87	0.72
2:B:208:VAL:HG21	2:B:261:ALA:HB3	1.72	0.72
1:C:788:SER:HB2	2:D:65:ASN:HA	1.72	0.71
1:C:669:ASN:HD22	3:E:2:DA:H4'	1.55	0.71
5:G:54:DG:H2''	5:G:55:DC:H5'	1.73	0.71
2:B:49:ARG:HH22	2:B:58:ARG:HH11	1.37	0.70
5:G:55:DC:N3	7:J:7:DG:N2	2.39	0.70
1:A:913:PRO:HB3	6:H:1:DC:C2	2.27	0.70
2:B:58:ARG:NH2	7:J:6:DG:H5''	2.03	0.70
7:J:13:DC:H2''	7:J:14:DT:H5'	1.73	0.70
1:C:523:ARG:NH1	6:H:8:DG:OP2	2.24	0.70
4:F:29:DA:H1'	4:F:30:DC:H5'	1.72	0.70
1:C:610:GLY:HA3	1:C:653:LEU:HG	1.72	0.70
1:A:486:CYS:SG	1:A:500:TYR:OH	2.49	0.69
2:B:3:LEU:HD23	2:B:305:PRO:HB2	1.74	0.69
3:E:4:DA:H2''	3:E:5:DG:H5''	1.74	0.69
1:A:486:CYS:HG	1:A:500:TYR:HH	1.39	0.69
1:A:727:THR:HG22	1:A:812:THR:HG21	1.73	0.69
1:C:472:ALA:O	1:C:477:ARG:NH1	2.26	0.69
1:A:548:SER:O	1:A:577:ARG:NH1	2.26	0.69
2:B:6:LEU:HD11	2:B:347:GLN:HB2	1.75	0.69
1:A:608:THR:HB	1:A:718:ARG:HG2	1.73	0.69
1:A:688:GLU:OE1	2:B:73:ARG:NH1	2.21	0.69
6:H:15:DT:H2''	6:H:16:DC:OP2	1.91	0.69
7:I:15:DT:H2'	7:I:16:DA:H8	1.58	0.68
1:A:546:SER:O	1:A:577:ARG:NH2	2.26	0.68
1:C:497:CYS:HB2	6:H:7:DG:P	2.33	0.68
1:C:413:GLN:HE21	1:C:426:ARG:HH22	1.41	0.68
1:C:708:ARG:NH2	1:C:719:SER:OG	2.27	0.68
1:A:760:SER:HB2	1:A:954:ILE:HD11	1.75	0.68
1:C:490:ARG:NH2	1:C:497:CYS:SG	2.66	0.68
1:A:479:PHE:HE1	1:C:469:GLU:HB2	1.59	0.68
5:G:33:DT:O4	5:G:34:DA:N6	2.27	0.68
1:C:420:ARG:HD3	1:C:421:ARG:NH2	2.10	0.67
2:B:168:THR:O	2:B:172:TRP:N	2.28	0.67
5:G:47:DA:C2	7:J:15:DT:N3	2.60	0.67
2:B:39:ARG:N	5:G:50:DA:OP1	2.27	0.67
1:C:984:GLU:OE1	4:F:34:DG:H1'	1.93	0.67
1:C:897:ARG:HH11	1:C:945:MET:HE2	1.60	0.67
1:A:708:ARG:HG2	1:A:721:ARG:HG2	1.76	0.67
2:D:258:ILE:HD13	2:D:284:ARG:HD2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:LYS:NZ	2:B:314:SER:O	2.28	0.67
2:D:187:LEU:HD12	2:D:188:GLU:H	1.60	0.67
2:D:148:ARG:NH2	2:D:240:LEU:O	2.28	0.67
2:B:154:VAL:HG11	2:B:216:VAL:HG21	1.76	0.67
2:B:135:SER:OG	2:B:137:ARG:NH2	2.27	0.66
5:G:20:DC:N3	6:H:26:DG:N2	2.43	0.66
1:C:415:LEU:HB2	1:C:416:LEU:HD13	1.77	0.66
1:C:822:ASN:HD21	1:C:961:THR:HG21	1.60	0.66
1:A:955:THR:HG23	1:A:958:LEU:H	1.59	0.66
3:E:9:DT:O4	3:E:10:DA:N6	2.29	0.66
5:G:45:DG:H3'	5:G:46:DT:H5''	1.76	0.66
1:A:489:ILE:HD11	1:C:503:MET:HA	1.78	0.66
2:D:110:SER:OG	2:D:111:VAL:N	2.28	0.66
1:A:587:LYS:NZ	1:A:712:SER:O	2.28	0.66
2:D:154:VAL:HG11	2:D:216:VAL:HG21	1.76	0.66
1:C:735:ARG:NH1	1:C:741:GLU:O	2.29	0.65
2:B:140:HIS:CD2	2:B:155:LEU:HD11	2.28	0.65
1:A:513:ARG:N	1:C:471:GLU:OE2	2.30	0.65
1:A:822:ASN:HD21	1:A:961:THR:HG21	1.61	0.65
1:C:418:LEU:HD12	1:C:426:ARG:HH22	1.61	0.65
2:B:49:ARG:NH2	2:B:58:ARG:HD2	2.12	0.65
1:C:760:SER:OG	1:C:951:ASP:O	2.11	0.65
1:C:764:VAL:HG11	1:C:936:GLN:HA	1.76	0.65
1:C:465:LYS:O	1:C:469:GLU:HG2	1.97	0.65
2:D:15:VAL:HG21	2:D:345:PHE:HZ	1.62	0.65
1:A:511:SER:O	1:A:511:SER:OG	2.14	0.65
1:C:462:ASN:HD22	1:C:466:GLN:NE2	1.94	0.65
7:J:1:DG:H2''	7:J:2:DA:H5'	1.78	0.65
1:C:810:GLN:NE2	1:C:972:ASP:OD1	2.29	0.65
2:D:229:ARG:HH22	2:D:280:GLU:HG2	1.62	0.64
1:A:410:ARG:HH11	4:F:11:DT:H4'	1.61	0.64
1:C:459:ARG:NH1	3:E:16:DT:OP1	2.29	0.64
1:A:410:ARG:NH1	4:F:11:DT:H4'	2.12	0.64
2:D:208:VAL:HG21	2:D:261:ALA:HB3	1.79	0.64
4:F:34:DG:C3'	4:F:35:DT:H5''	2.27	0.64
7:I:15:DT:H2'	7:I:16:DA:C8	2.32	0.64
1:A:452:THR:HG23	1:C:427:LEU:HD21	1.80	0.64
1:C:488:ALA:HA	1:C:1021:LEU:HD23	1.78	0.64
2:D:66:SER:HB2	2:D:124:CYS:H	1.62	0.64
1:A:465:LYS:HG3	1:A:466:GLN:HG3	1.80	0.64
1:A:512:GLY:HA2	1:A:513:ARG:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:31:DA:N6	6:H:15:DT:H3	1.94	0.63
7:I:9:DC:C4	7:I:10:DT:C4	2.87	0.63
1:A:451:LEU:HD23	1:C:454:PHE:HE2	1.61	0.63
1:A:456:LEU:HG	1:C:420:ARG:NE	2.09	0.63
1:A:620:ASP:OD1	1:A:621:GLY:N	2.32	0.63
2:B:204:GLN:HB2	2:B:207:HIS:HD2	1.63	0.63
2:D:80:PHE:HB2	2:D:144:VAL:HG21	1.80	0.63
5:G:30:DG:H1	6:H:16:DC:H42	1.47	0.63
6:H:32:DC:H2''	6:H:33:DA:H5''	1.80	0.63
1:C:420:ARG:O	1:C:423:GLN:HB2	1.99	0.63
5:G:37:DA:N6	6:H:8:DG:O6	2.32	0.63
1:A:540:PRO:HD2	1:A:707:SER:HA	1.81	0.62
2:D:104:SER:HB2	2:D:136:ALA:HB2	1.81	0.62
5:G:44:DT:C4	5:G:45:DG:N1	2.67	0.62
1:A:822:ASN:HD22	1:A:908:TYR:HE1	1.46	0.62
5:G:43:DG:N2	6:H:4:DA:C2	2.66	0.62
1:C:731:GLU:OE2	1:C:960:LYS:NZ	2.27	0.62
3:E:28:DC:H4'	3:E:29:DC:OP1	1.98	0.62
1:A:410:ARG:HD2	4:F:10:DT:O2	1.99	0.62
1:A:828:LYS:HD3	1:A:949:ARG:HH22	1.65	0.62
1:A:984:GLU:OE1	5:G:45:DG:H1'	1.99	0.62
1:A:1025:MET:HG3	1:A:1026:GLU:N	2.14	0.62
2:B:118:ARG:HH21	5:G:59:DA:H5''	1.64	0.62
2:B:274:PHE:CE2	2:B:348:VAL:HG21	2.34	0.62
2:D:58:ARG:NH2	7:I:7:DG:OP1	2.32	0.62
2:B:43:THR:HG22	2:B:45:ILE:H	1.65	0.62
1:A:414:HIS:HD2	1:A:415:LEU:N	1.98	0.62
1:C:425:HIS:O	1:C:425:HIS:ND1	2.30	0.62
2:B:278:GLN:NE2	2:B:282:GLN:HE22	1.98	0.62
1:A:447:LYS:O	1:A:451:LEU:HG	1.99	0.61
5:G:30:DG:H1	6:H:16:DC:N4	1.98	0.61
1:A:473:MET:HA	1:A:479:PHE:CG	2.35	0.61
1:A:427:LEU:HD12	1:C:456:LEU:HD12	1.83	0.61
7:I:4:DC:H2''	7:I:5:DT:H5'	1.83	0.61
1:A:508:LYS:NZ	4:F:24:DG:OP1	2.33	0.61
2:B:50:ILE:HG12	2:B:55:LEU:HD12	1.83	0.61
1:C:865:LEU:HB3	1:C:875:TYR:HE1	1.66	0.61
2:D:94:GLY:O	2:D:103:SER:OG	2.19	0.61
2:D:140:HIS:CD2	2:D:155:LEU:HD11	2.28	0.61
1:A:692:ALA:HA	2:B:100:ASN:ND2	2.15	0.61
1:A:854:THR:HB	2:D:310:GLU:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:TYR:HD2	1:A:966:PRO:HG3	1.64	0.61
1:A:423:GLN:O	1:A:425:HIS:N	2.34	0.60
1:A:931:TYR:OH	1:A:961:THR:O	2.17	0.60
2:B:274:PHE:HE2	2:B:348:VAL:HG21	1.65	0.60
1:C:459:ARG:CB	1:C:466:GLN:HE22	2.15	0.60
1:A:583:VAL:HB	1:A:711:ILE:HD11	1.83	0.60
1:C:1011:LYS:NZ	6:H:8:DG:OP1	2.22	0.60
1:A:513:ARG:NH2	1:C:478:GLY:O	2.34	0.60
1:C:860:ARG:HH21	1:C:866:LYS:CG	2.14	0.60
2:B:28:VAL:HG13	2:B:48:VAL:HG13	1.84	0.60
2:B:169:THR:HA	2:B:172:TRP:HB2	1.84	0.60
1:A:414:HIS:CD2	1:A:415:LEU:N	2.69	0.59
1:C:611:PHE:HB2	1:C:720:PHE:HD1	1.67	0.59
2:B:233:LEU:HB2	2:B:255:GLY:HA3	1.84	0.59
7:J:7:DG:H2'	7:J:8:DC:C6	2.37	0.59
1:A:508:LYS:HG3	1:A:514:GLN:HB3	1.83	0.59
2:B:256:LEU:HD21	2:B:284:ARG:HH12	1.67	0.59
1:C:592:ASP:OD1	1:C:1023:LYS:NZ	2.31	0.59
1:A:830:PHE:HZ	1:A:885:VAL:HG22	1.66	0.59
1:A:473:MET:HG3	1:A:474:MET:HG2	1.84	0.59
2:B:256:LEU:CD2	2:B:284:ARG:HH12	2.16	0.59
2:D:24:LEU:HB3	2:D:90:TYR:HE2	1.68	0.59
2:D:16:GLN:NE2	2:D:73:ARG:HG3	2.16	0.59
5:G:14:DG:N2	6:H:32:DC:O2	2.28	0.58
1:A:999:ARG:HH12	3:E:8:DC:H4'	1.68	0.58
4:F:25:DT:H2''	4:F:26:DA:C8	2.38	0.58
1:A:418:LEU:HD22	1:A:426:ARG:HH12	1.68	0.58
2:B:266:ILE:HG13	2:B:267:GLY:H	1.68	0.58
4:F:41:DA:H61	7:I:9:DC:H42	1.51	0.58
1:A:459:ARG:CZ	6:H:27:DC:OP1	2.51	0.58
2:D:16:GLN:HE21	2:D:73:ARG:HG3	1.68	0.58
1:C:721:ARG:HH21	1:C:723:PHE:HE1	1.51	0.58
1:C:913:PRO:HB3	3:E:1:DC:C2	2.39	0.58
3:E:27:DC:H2''	3:E:28:DC:H5'	1.86	0.58
2:B:28:VAL:HG11	2:B:322:LEU:HD22	1.84	0.58
2:B:204:GLN:HB2	2:B:207:HIS:CD2	2.39	0.58
1:C:451:LEU:HD12	1:C:452:THR:HG23	1.85	0.58
1:C:675:ARG:NH2	1:C:1018:SER:HA	2.18	0.58
4:F:13:DT:H4'	4:F:14:DG:OP1	2.03	0.58
2:D:80:PHE:HD1	2:D:144:VAL:HG11	1.69	0.58
1:C:628:LYS:HE3	1:C:1000:GLN:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:LEU:HD13	1:C:1010:LEU:HD13	1.85	0.58
1:C:911:MET:HB2	1:C:931:TYR:CE1	2.39	0.58
1:C:866:LYS:CD	1:C:867:PRO:HD2	2.33	0.57
1:A:810:GLN:NE2	1:A:972:ASP:OD2	2.36	0.57
1:A:931:TYR:CD2	1:A:966:PRO:HG3	2.39	0.57
1:C:420:ARG:CZ	6:H:27:DC:H5''	2.33	0.57
1:C:529:LEU:HD13	1:C:1021:LEU:HD11	1.85	0.57
1:C:466:GLN:HG3	1:C:467:ALA:H	1.67	0.57
3:E:8:DC:N4	4:F:26:DA:N6	2.52	0.57
3:E:18:DG:H1	4:F:17:DC:H42	1.52	0.57
5:G:32:DG:H2''	5:G:33:DT:OP2	2.03	0.57
1:A:624:ASP:OD1	1:A:991:ARG:NH1	2.37	0.57
1:C:628:LYS:HB2	1:C:1002:LYS:HG2	1.86	0.57
1:C:771:SER:O	1:C:775:ASN:ND2	2.33	0.57
7:J:9:DC:C4	7:J:10:DT:C4	2.92	0.57
1:C:583:VAL:HG12	1:C:709:LEU:HD21	1.85	0.57
2:D:69:LEU:HD12	2:D:70:PRO:HD2	1.87	0.57
1:C:651:ILE:O	1:C:660:ILE:N	2.36	0.57
1:A:445:ASP:OD2	1:C:415:LEU:HD11	2.04	0.56
1:A:676:PRO:HG3	1:A:1013:HIS:HB3	1.87	0.56
1:C:421:ARG:CA	1:C:421:ARG:HE	2.17	0.56
1:A:619:CYS:HB2	1:A:642:PHE:CD2	2.41	0.56
2:D:135:SER:OG	2:D:137:ARG:NH2	2.38	0.56
1:A:830:PHE:CZ	1:A:885:VAL:HG22	2.40	0.56
1:C:999:ARG:O	6:H:6:DT:H1'	2.05	0.56
5:G:52:DA:N1	7:J:11:DG:C2	2.73	0.56
1:A:520:HIS:CE1	4:F:23:DT:OP2	2.59	0.56
2:B:344:HIS:HB3	1:C:850:ARG:HH12	1.71	0.56
2:D:284:ARG:HG3	2:D:286:GLU:HG3	1.88	0.56
5:G:54:DG:C6	7:J:7:DG:N1	2.69	0.56
1:A:877:ARG:CZ	6:H:2:DA:N7	2.68	0.56
2:B:115:GLY:O	2:B:119:LYS:HB3	2.06	0.56
1:C:697:VAL:O	1:C:700:GLU:HG2	2.06	0.56
1:C:999:ARG:HH22	6:H:8:DG:H5'	1.71	0.56
1:A:506:THR:OG1	1:C:1025:MET:SD	2.63	0.56
1:C:424:LYS:HD2	1:C:431:LYS:HE3	1.88	0.56
1:C:709:LEU:HD21	1:C:711:ILE:HD11	1.88	0.56
1:A:415:LEU:HD13	1:A:426:ARG:HH21	1.69	0.56
1:A:513:ARG:NE	1:C:513:ARG:HH11	2.00	0.56
1:C:818:CYS:HA	1:C:957:TYR:CD1	2.41	0.56
1:C:823:ALA:HA	1:C:880:MET:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:999:ARG:HE	1:C:1004:PHE:HB3	1.70	0.56
2:D:212:ARG:HH21	2:D:294:ASP:N	2.03	0.56
1:A:458:LEU:O	1:C:447:LYS:NZ	2.28	0.56
2:D:9:VAL:HG13	2:D:10:ASN:H	1.71	0.56
2:D:229:ARG:HH12	2:D:280:GLU:HG3	1.71	0.56
1:A:850:ARG:NE	2:D:346:TYR:OH	2.38	0.55
2:B:123:ARG:NH1	2:B:125:GLU:OE2	2.40	0.55
5:G:57:DA:N6	7:J:4:DC:H42	1.93	0.55
1:A:869:MET:HG3	1:A:870:ARG:HB3	1.89	0.55
2:D:137:ARG:NH1	2:D:178:CYS:SG	2.79	0.55
2:B:131:GLY:HA3	2:B:132:ASP:C	2.31	0.55
2:B:84:ASP:CG	2:B:85:GLY:HA2	2.32	0.55
2:B:107:TYR:CE1	2:B:126:GLU:HB2	2.42	0.55
1:C:638:LYS:HD2	1:C:683:ASP:OD1	2.07	0.55
2:D:39:ARG:HG3	2:D:39:ARG:HH11	1.71	0.55
4:F:7:DG:H2'	4:F:8:DG:C8	2.37	0.55
2:B:97:THR:HG21	2:B:101:GLU:OE2	2.06	0.55
1:C:458:LEU:HB3	1:C:462:ASN:HD21	1.71	0.55
1:C:517:GLN:HB3	1:C:521:THR:HG21	1.88	0.55
7:I:10:DT:H2''	7:I:11:DG:H8	1.72	0.54
2:D:93:HIS:O	2:D:140:HIS:NE2	2.39	0.54
2:B:30:LEU:HD22	2:B:46:PHE:HD2	1.73	0.54
1:C:476:GLY:HA3	1:C:477:ARG:HD2	1.89	0.54
1:C:418:LEU:HD12	1:C:426:ARG:NH2	2.22	0.54
1:C:429:ASP:OD1	1:C:430:LEU:HD12	2.07	0.54
1:A:428:ARG:N	1:A:431:LYS:HZ2	2.05	0.54
1:C:897:ARG:NH1	1:C:945:MET:HB3	2.22	0.54
5:G:45:DG:C3'	5:G:46:DT:P	2.95	0.54
1:A:836:GLU:HB3	1:A:839:GLN:OE1	2.08	0.54
5:G:15:DT:H2''	5:G:16:DA:H5''	1.90	0.54
1:A:451:LEU:HA	1:C:454:PHE:HZ	1.72	0.53
2:D:265:PRO:HA	2:D:271:TYR:HD1	1.72	0.53
1:A:465:LYS:HE3	1:A:466:GLN:OE1	2.08	0.53
1:A:473:MET:HA	1:A:479:PHE:CD2	2.43	0.53
1:A:513:ARG:HG3	1:C:477:ARG:NH2	2.23	0.53
2:D:6:LEU:HD11	2:D:347:GLN:HB2	1.89	0.53
2:D:145:ILE:HD13	2:D:238:VAL:HG21	1.89	0.53
2:D:212:ARG:HG3	2:D:269:HIS:CE1	2.43	0.53
1:A:748:ILE:HG22	1:A:956:ASN:OD1	2.09	0.53
5:G:42:DT:H2''	5:G:43:DG:H5'	1.90	0.53
2:D:50:ILE:HG12	2:D:55:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:3:DT:H2'	7:J:4:DC:C6	2.43	0.53
2:D:168:THR:O	2:D:172:TRP:N	2.42	0.53
5:G:36:DT:H3	6:H:10:DA:H61	1.57	0.53
1:A:531:PRO:HB2	1:A:580:VAL:HG12	1.90	0.53
2:B:249:CYS:SG	2:B:250:THR:N	2.81	0.53
1:C:968:ILE:HG22	1:C:971:ARG:HH11	1.74	0.53
2:D:86:LYS:NZ	2:D:110:SER:OG	2.20	0.53
2:D:230:PRO:HB2	2:D:232:ARG:HG2	1.89	0.53
2:D:307:TRP:HB3	2:D:311:ILE:HG23	1.91	0.53
5:G:40:DA:C5	5:G:41:DC:C4	2.97	0.53
1:A:437:PHE:HA	1:A:440:LYS:HE3	1.90	0.53
1:A:481:LEU:HD12	1:A:481:LEU:C	2.33	0.53
1:A:586:LEU:HD21	1:A:720:PHE:CE2	2.44	0.53
1:C:832:ASP:HB3	1:C:837:VAL:HG21	1.91	0.53
1:C:467:ALA:O	1:C:471:GLU:HB3	2.09	0.53
2:D:80:PHE:CD1	2:D:144:VAL:HG11	2.44	0.53
5:G:17:DC:H6	5:G:17:DC:H5''	1.74	0.53
5:G:59:DA:N6	7:J:2:DA:C6	2.77	0.53
6:H:5:DG:C3'	6:H:6:DT:P	2.96	0.53
2:D:14:LEU:HD13	2:D:46:PHE:CE2	2.43	0.53
2:B:306:GLN:H	2:B:306:GLN:CD	2.17	0.52
5:G:48:DA:N1	5:G:49:DG:C6	2.78	0.52
7:I:12:DT:H2''	7:I:13:DC:H5'	1.91	0.52
1:A:610:GLY:HA3	1:A:653:LEU:HG	1.90	0.52
1:C:465:LYS:H	1:C:465:LYS:HD2	1.74	0.52
2:D:146:ASN:O	2:D:214:ASP:HB3	2.09	0.52
5:G:55:DC:C2	7:J:7:DG:N2	2.77	0.52
1:A:456:LEU:CG	1:C:420:ARG:HE	2.12	0.52
1:A:458:LEU:HD11	1:A:466:GLN:HE21	1.75	0.52
2:D:49:ARG:NH1	7:I:7:DG:OP1	2.43	0.52
2:D:115:GLY:O	2:D:119:LYS:HB3	2.10	0.52
2:B:29:TYR:HD1	2:B:47:GLY:HA2	1.74	0.52
1:A:688:GLU:OE1	2:B:73:ARG:HD3	2.10	0.52
2:B:93:HIS:HB2	2:B:106:LEU:HA	1.92	0.52
1:C:603:ASP:OD2	1:C:606:MET:HG2	2.10	0.52
5:G:7:DG:H2'	5:G:8:DG:C8	2.39	0.52
1:A:640:VAL:HB	1:A:680:MET:HE3	1.92	0.52
2:B:282:GLN:NE2	2:B:283:LYS:O	2.43	0.52
3:E:23:DA:H2''	3:E:24:DA:OP2	2.09	0.52
1:A:864:LYS:HD2	1:C:631:SER:HA	1.91	0.52
2:B:307:TRP:HB3	2:B:311:ILE:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:7:DG:C5	7:J:8:DC:N4	2.78	0.52
1:A:420:ARG:NH1	1:C:459:ARG:HE	2.08	0.51
2:B:66:SER:HB3	2:B:123:ARG:HA	1.91	0.51
2:B:290:VAL:HG22	2:B:299:MET:SD	2.50	0.51
1:A:451:LEU:HD23	1:C:454:PHE:CE2	2.44	0.51
1:C:999:ARG:HE	1:C:1004:PHE:CB	2.24	0.51
4:F:46:DA:N6	7:I:4:DC:H42	2.08	0.51
1:A:626:SER:O	1:A:994:ARG:NH2	2.42	0.51
1:A:828:LYS:HD3	1:A:949:ARG:NH2	2.25	0.51
1:C:727:THR:HG22	1:C:812:THR:HG21	1.92	0.51
2:D:284:ARG:NH2	2:D:286:GLU:OE2	2.44	0.51
5:G:34:DA:N6	6:H:11:DG:H1	2.09	0.51
1:A:729:TYR:HB2	1:A:734:VAL:HG23	1.92	0.51
1:A:818:CYS:HA	1:A:957:TYR:CD1	2.45	0.51
3:E:13:DG:N2	4:F:22:DC:N3	2.57	0.51
7:J:12:DT:C4	7:J:13:DC:N4	2.79	0.51
1:A:465:LYS:HG3	1:A:466:GLN:H	1.75	0.51
1:A:679:LEU:HD13	1:A:1010:LEU:HD13	1.92	0.51
1:C:520:HIS:HA	1:C:523:ARG:HD2	1.93	0.51
1:C:620:ASP:OD2	1:C:984:GLU:OE2	2.28	0.51
2:D:148:ARG:NH2	2:D:241:LEU:HG	2.25	0.51
2:D:283:LYS:HD2	2:D:317:TRP:NE1	2.25	0.51
4:F:23:DT:H2"	4:F:24:DG:C8	2.45	0.51
2:D:274:PHE:CZ	2:D:348:VAL:HG21	2.44	0.51
1:A:832:ASP:OD2	1:A:949:ARG:NH1	2.44	0.51
2:D:148:ARG:HH22	2:D:241:LEU:HG	1.76	0.51
2:D:226:SER:HG	2:D:228:CYS:HG	1.58	0.51
6:H:16:DC:OP2	6:H:16:DC:H6	1.93	0.51
1:A:632:GLY:HA2	1:C:860:ARG:HH12	1.76	0.51
1:C:512:GLY:HA2	1:C:513:ARG:C	2.35	0.51
1:C:913:PRO:HB3	3:E:1:DC:N3	2.26	0.51
1:A:430:LEU:O	1:A:434:VAL:HG12	2.11	0.50
1:A:453:LEU:HB2	1:C:427:LEU:HD23	1.93	0.50
1:A:496:SER:HB3	1:A:499:GLN:HG2	1.92	0.50
1:A:692:ALA:HA	2:B:100:ASN:HD22	1.76	0.50
2:B:281:THR:OG1	2:B:282:GLN:N	2.44	0.50
1:C:619:CYS:HB2	1:C:642:PHE:CD2	2.46	0.50
5:G:40:DA:C2	5:G:41:DC:C2	2.99	0.50
2:D:9:VAL:HG13	2:D:10:ASN:N	2.26	0.50
2:D:24:LEU:HB3	2:D:90:TYR:CE2	2.45	0.50
2:D:156:PHE:HB2	2:D:182:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:VAL:HG13	2:D:197:LEU:HD11	1.93	0.50
1:A:465:LYS:HG3	1:A:466:GLN:N	2.27	0.50
5:G:20:DC:C2	6:H:26:DG:N2	2.80	0.50
2:B:269:HIS:HB3	2:B:292:LEU:HD11	1.93	0.50
2:B:181:GLN:HG3	2:B:196:THR:HB	1.93	0.50
1:A:1026:GLU:HG2	1:A:1029:LYS:N	2.27	0.50
1:C:458:LEU:HB3	1:C:462:ASN:ND2	2.26	0.50
1:C:975:ILE:HG12	1:C:976:GLY:N	2.27	0.50
1:A:611:PHE:HB2	1:A:720:PHE:HD1	1.76	0.50
1:A:965:VAL:O	1:A:969:VAL:HG22	2.12	0.50
2:B:202:ASP:OD1	2:B:203:GLY:N	2.44	0.50
1:A:420:ARG:O	1:A:423:GLN:HB3	2.12	0.50
2:B:157:GLY:HA3	2:B:207:HIS:NE2	2.26	0.50
7:I:11:DG:H2'	7:I:12:DT:C5	2.47	0.50
2:B:151:THR:HG22	2:B:187:LEU:HD11	1.94	0.50
1:C:411:PRO:HD2	6:H:37:DA:H4'	1.94	0.50
2:D:142:LEU:HB2	2:D:155:LEU:HD13	1.93	0.50
5:G:44:DT:C4	5:G:45:DG:C6	3.00	0.50
1:A:448:SER:O	1:A:452:THR:HG22	2.12	0.49
1:A:622:MET:SD	1:A:991:ARG:NH2	2.85	0.49
1:C:459:ARG:O	3:E:16:DT:H5'	2.12	0.49
1:C:635:VAL:HG21	1:C:681:PHE:HB2	1.94	0.49
2:D:207:HIS:O	2:D:207:HIS:ND1	2.45	0.49
5:G:40:DA:H1'	5:G:41:DC:H5'	1.94	0.49
1:A:458:LEU:HD21	1:A:466:GLN:HB2	1.93	0.49
1:C:421:ARG:NH1	1:C:424:LYS:HD3	2.27	0.49
4:F:33:DT:C4	4:F:34:DG:N1	2.80	0.49
7:J:12:DT:N3	7:J:13:DC:C4	2.80	0.49
2:B:38:LYS:O	2:B:40:SER:N	2.45	0.49
1:C:754:SER:OG	1:C:759:ALA:HB2	2.13	0.49
2:D:182:VAL:HG23	2:D:195:HIS:HB2	1.93	0.49
2:D:350:PHE:HD1	2:D:351:GLN:HG3	1.75	0.49
4:F:19:DA:C8	4:F:20:DG:C8	3.00	0.49
7:I:4:DC:H2''	7:I:5:DT:C5'	2.41	0.49
1:A:437:PHE:CE1	1:C:430:LEU:HD11	2.46	0.49
1:A:869:MET:HG3	1:A:870:ARG:N	2.27	0.49
2:B:283:LYS:HE3	2:B:311:ILE:O	2.13	0.49
1:C:420:ARG:NH1	6:H:28:DT:OP2	2.46	0.49
1:C:897:ARG:NH1	1:C:945:MET:HE2	2.26	0.49
5:G:29:DG:H1'	5:G:30:DG:O4'	2.12	0.49
1:A:431:LYS:HE3	1:C:456:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LEU:HD23	1:A:515:ILE:HG22	1.94	0.49
2:B:14:LEU:HD13	2:B:46:PHE:CE2	2.48	0.49
1:C:676:PRO:HG3	1:C:1013:HIS:HB3	1.95	0.49
1:C:871:MET:HG3	1:C:875:TYR:HD2	1.78	0.49
1:C:877:ARG:NH2	3:E:2:DA:N7	2.60	0.49
1:C:423:GLN:HA	1:C:426:ARG:HD2	1.94	0.49
5:G:46:DT:P	7:J:16:DA:O3'	2.71	0.49
1:A:877:ARG:NH2	6:H:2:DA:N7	2.60	0.49
1:A:882:ARG:O	1:A:886:GLU:HG3	2.13	0.49
2:B:83:GLN:O	2:B:87:PRO:HG3	2.12	0.49
2:B:217:TYR:CE1	2:B:235:ARG:HG3	2.48	0.49
1:C:846:GLU:OE2	1:C:850:ARG:NE	2.44	0.49
1:A:518:PRO:O	1:A:521:THR:HG22	2.12	0.49
2:B:66:SER:HB2	2:B:124:CYS:H	1.78	0.49
2:D:266:ILE:HD12	2:D:272:ILE:HG23	1.94	0.49
3:E:11:DC:H1'	3:E:12:DA:C8	2.47	0.49
2:B:283:LYS:HB2	2:B:317:TRP:HE1	1.78	0.48
2:D:80:PHE:HB3	2:D:89:CYS:HB2	1.95	0.48
2:D:283:LYS:NZ	2:D:311:ILE:O	2.27	0.48
1:A:709:LEU:O	1:A:719:SER:HA	2.13	0.48
6:H:11:DG:C6	6:H:12:DT:C4	3.02	0.48
1:A:418:LEU:HD23	1:A:422:ALA:HB1	1.95	0.48
1:A:458:LEU:HD11	1:A:466:GLN:NE2	2.28	0.48
1:C:748:ILE:HG23	1:C:756:ARG:HE	1.78	0.48
1:C:760:SER:HA	1:C:954:ILE:CD1	2.43	0.48
1:C:796:ASP:O	1:C:799:LYS:HD2	2.13	0.48
7:I:6:DG:H2''	7:I:7:DG:C8	2.49	0.48
1:A:464:HIS:O	1:A:466:GLN:N	2.46	0.48
1:A:598:ARG:NH1	1:A:604:ASP:OD1	2.47	0.48
2:D:29:TYR:HD1	2:D:47:GLY:HA2	1.79	0.48
2:D:56:LYS:HD2	2:D:57:LEU:H	1.78	0.48
5:G:59:DA:N6	7:J:2:DA:N6	2.61	0.48
1:A:641:ARG:NH1	1:A:983:ASN:O	2.46	0.48
2:B:16:GLN:HG3	2:B:18:GLY:O	2.14	0.48
1:C:486:CYS:HG	1:C:500:TYR:HH	1.57	0.48
1:A:534:HIS:CG	1:A:587:LYS:HD2	2.49	0.48
1:C:413:GLN:HG3	1:C:415:LEU:H	1.78	0.48
1:C:669:ASN:ND2	3:E:2:DA:H4'	2.26	0.48
1:A:455:LEU:HD11	1:A:470:LEU:HB3	1.96	0.48
1:A:760:SER:CB	1:A:954:ILE:HD11	2.42	0.48
2:B:104:SER:HB2	2:B:136:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:PHE:CD1	1:C:583:VAL:HG21	2.48	0.48
1:C:770:ARG:NH2	1:C:799:LYS:O	2.47	0.48
2:D:33:GLN:NE2	2:D:37:PRO:HA	2.29	0.48
1:C:968:ILE:HD11	1:C:975:ILE:HD12	1.95	0.48
6:H:12:DT:H2''	6:H:13:DA:O4'	2.14	0.48
1:A:999:ARG:HG3	1:A:1004:PHE:HB3	1.96	0.47
2:B:226:SER:OG	2:B:228:CYS:SG	2.67	0.47
1:C:511:SER:O	1:C:513:ARG:HB3	2.14	0.47
1:C:564:VAL:HG22	2:D:315:ARG:HH12	1.78	0.47
1:C:760:SER:HA	1:C:954:ILE:HD13	1.95	0.47
4:F:33:DT:H71	4:F:34:DG:C6	2.49	0.47
1:C:451:LEU:HD12	1:C:452:THR:N	2.29	0.47
1:C:918:THR:O	1:C:974:SER:HB3	2.15	0.47
2:D:188:GLU:HG3	2:D:189:PHE:HA	1.96	0.47
4:F:46:DA:H61	7:I:4:DC:N4	2.07	0.47
7:J:12:DT:H2''	7:J:13:DC:H5'	1.95	0.47
1:A:725:ARG:HD2	1:A:810:GLN:OE1	2.14	0.47
1:A:756:ARG:HH11	7:J:14:DT:H5''	1.80	0.47
1:C:523:ARG:HH12	6:H:8:DG:P	2.35	0.47
2:D:242:LEU:HA	2:D:243:GLY:HA2	1.61	0.47
1:A:435:LYS:HD3	1:A:435:LYS:HA	1.76	0.47
1:A:523:ARG:O	1:A:526:GLU:HB2	2.14	0.47
2:B:226:SER:HG	2:B:228:CYS:HG	1.57	0.47
1:C:860:ARG:HH21	1:C:866:LYS:HG2	1.77	0.47
1:C:984:GLU:O	1:C:987:ASN:HB2	2.14	0.47
1:C:798:VAL:HG23	1:C:801:VAL:H	1.79	0.47
1:A:497:CYS:SG	3:E:7:DG:H5''	2.54	0.47
1:A:536:PHE:CD2	1:A:583:VAL:HG21	2.49	0.47
1:A:712:SER:HA	1:A:717:LEU:HA	1.96	0.47
1:A:742:ALA:HA	1:A:743:SER:HA	1.72	0.47
1:A:746:THR:HB	1:A:795:ARG:HH12	1.80	0.47
1:A:897:ARG:NH1	1:A:945:MET:HG2	2.29	0.47
2:B:49:ARG:HH21	2:B:58:ARG:HD2	1.78	0.47
2:B:156:PHE:HB2	2:B:182:VAL:HG12	1.97	0.47
2:B:311:ILE:HG13	2:B:331:ILE:HD11	1.97	0.47
1:C:462:ASN:HD22	1:C:466:GLN:CD	2.22	0.47
1:C:810:GLN:HE21	1:C:971:ARG:HH22	1.63	0.47
2:B:21:LEU:HD23	2:B:30:LEU:HA	1.96	0.47
1:C:518:PRO:O	1:C:521:THR:HG22	2.15	0.47
1:C:752:CYS:SG	1:C:753:ASP:N	2.88	0.47
1:C:926:ASP:OD1	1:C:926:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:19:DA:H2'	4:F:20:DG:O4'	2.14	0.47
5:G:34:DA:H61	6:H:11:DG:H1	1.61	0.47
2:B:256:LEU:HD12	2:B:256:LEU:HA	1.71	0.47
1:C:776:LEU:HD23	1:C:805:PRO:HD2	1.95	0.47
5:G:13:DT:H2''	5:G:14:DG:OP2	2.14	0.47
1:A:459:ARG:C	1:A:462:ASN:HB3	2.40	0.47
1:A:752:CYS:SG	1:A:753:ASP:N	2.88	0.47
2:B:69:LEU:HD12	2:B:69:LEU:HA	1.53	0.47
1:C:931:TYR:HD2	1:C:966:PRO:HG3	1.78	0.47
6:H:2:DA:C8	6:H:2:DA:H5''	2.50	0.47
1:A:964:HIS:O	1:A:968:ILE:HG13	2.16	0.46
1:C:865:LEU:HD21	1:C:878:ARG:HE	1.80	0.46
4:F:41:DA:H61	7:I:9:DC:N4	2.13	0.46
1:A:835:GLY:HA3	1:A:851:TRP:CE2	2.50	0.46
2:D:131:GLY:HA3	2:D:132:ASP:C	2.41	0.46
6:H:2:DA:C2	6:H:3:DC:O2	2.68	0.46
1:A:473:MET:HA	1:A:479:PHE:CD1	2.50	0.46
1:A:609:SER:OG	1:A:719:SER:HB3	2.15	0.46
1:C:651:ILE:HG13	1:C:652:ARG:N	2.31	0.46
1:C:741:GLU:HG2	2:D:39:ARG:HD3	1.96	0.46
1:C:877:ARG:CZ	3:E:2:DA:N7	2.78	0.46
6:H:28:DT:OP2	6:H:28:DT:H73	2.16	0.46
2:B:43:THR:HG23	2:B:62:PHE:CE2	2.50	0.46
2:B:266:ILE:HG13	2:B:267:GLY:N	2.29	0.46
4:F:42:DG:N2	7:I:10:DT:O2	2.48	0.46
7:I:11:DG:H2'	7:I:12:DT:H71	1.97	0.46
1:A:513:ARG:HG3	1:C:477:ARG:HH21	1.81	0.46
4:F:13:DT:C5	4:F:14:DG:C5	3.04	0.46
2:B:93:HIS:HA	2:B:94:GLY:HA2	1.65	0.46
2:B:118:ARG:HE	5:G:59:DA:H4'	1.81	0.46
1:C:453:LEU:HD23	1:C:453:LEU:HA	1.68	0.46
1:C:420:ARG:NH2	6:H:27:DC:H5''	2.30	0.46
1:C:626:SER:O	1:C:994:ARG:NH2	2.47	0.46
1:C:725:ARG:HB3	1:C:810:GLN:OE1	2.16	0.46
2:D:157:GLY:HA3	2:D:207:HIS:NE2	2.31	0.46
2:D:311:ILE:HG13	2:D:331:ILE:HD11	1.98	0.46
5:G:39:DC:H2''	5:G:40:DA:H5''	1.96	0.46
1:A:479:PHE:HE1	1:C:469:GLU:CB	2.28	0.46
1:A:486:CYS:SG	1:A:522:LEU:HD21	2.56	0.46
1:A:652:ARG:HG3	1:A:653:LEU:N	2.31	0.46
1:A:731:GLU:N	7:J:16:DA:OP1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ARG:HH22	5:G:12:DT:C5'	2.29	0.46
1:A:628:LYS:HE3	1:A:1000:GLN:HB2	1.98	0.46
1:C:826:PHE:CD2	1:C:905:MET:HE1	2.51	0.46
2:D:283:LYS:NZ	2:D:314:SER:HB3	2.31	0.46
5:G:35:DC:H2''	5:G:36:DT:OP2	2.16	0.46
2:B:268:TYR:HD1	2:B:269:HIS:ND1	2.14	0.45
1:C:430:LEU:O	1:C:434:VAL:HG23	2.16	0.45
1:C:983:ASN:HB3	1:C:984:GLU:H	1.52	0.45
2:D:249:CYS:SG	2:D:250:THR:N	2.89	0.45
2:D:266:ILE:HG12	2:D:325:GLY:CA	2.46	0.45
5:G:7:DG:H22	6:H:39:DC:H42	1.62	0.45
5:G:46:DT:OP1	7:J:16:DA:C3'	2.64	0.45
6:H:2:DA:C3'	6:H:3:DC:P	3.03	0.45
6:H:39:DC:H4'	6:H:40:DC:OP1	2.16	0.45
1:A:410:ARG:CD	4:F:10:DT:O2	2.63	0.45
3:E:6:DT:O4	4:F:28:DC:N4	2.49	0.45
4:F:29:DA:C6	4:F:30:DC:N3	2.84	0.45
5:G:31:DA:C6	5:G:32:DG:C2	3.04	0.45
1:C:709:LEU:O	1:C:719:SER:HA	2.16	0.45
5:G:13:DT:H3	6:H:33:DA:H2	1.61	0.45
6:H:11:DG:C2	6:H:12:DT:C2	3.05	0.45
7:I:13:DC:H2''	7:I:14:DT:H5'	1.98	0.45
1:A:776:LEU:HD23	1:A:805:PRO:HD2	1.98	0.45
1:A:1026:GLU:HG2	1:A:1029:LYS:H	1.80	0.45
2:B:256:LEU:HD22	2:B:299:MET:CE	2.46	0.45
1:C:464:HIS:ND1	1:C:465:LYS:HD2	2.32	0.45
1:C:670:SER:HA	3:E:3:DC:H4'	1.98	0.45
1:A:585:ALA:HB2	1:A:1014:TRP:CH2	2.52	0.45
2:B:232:ARG:HG3	2:B:234:ILE:HD11	1.98	0.45
2:B:242:LEU:HA	2:B:243:GLY:HA2	1.65	0.45
1:C:615:VAL:HG22	1:C:646:ILE:HG12	1.98	0.45
1:C:747:TYR:CE1	1:C:755:THR:HG22	2.52	0.45
7:I:12:DT:O2	7:I:13:DC:C2	2.70	0.45
1:C:416:LEU:HD13	1:C:416:LEU:H	1.82	0.45
1:C:424:LYS:HD2	1:C:431:LYS:CE	2.47	0.45
1:C:915:TRP:HA	1:C:975:ILE:HG23	1.99	0.45
5:G:40:DA:C6	5:G:41:DC:N3	2.84	0.45
7:J:5:DT:C4	7:J:6:DG:C6	3.04	0.45
1:C:676:PRO:HG3	1:C:1013:HIS:CG	2.51	0.45
1:C:885:VAL:CG2	1:C:905:MET:HE3	2.46	0.45
3:E:21:DC:H2''	3:E:22:DA:H5''	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:SER:OG	1:A:945:MET:N	2.50	0.45
2:B:107:TYR:CD1	2:B:126:GLU:HB2	2.52	0.45
2:B:150:LYS:HG2	2:B:240:LEU:HD22	1.99	0.45
1:C:497:CYS:HB2	6:H:7:DG:OP2	2.16	0.45
3:E:33:DA:H2	4:F:2:DT:H3	1.64	0.45
1:C:548:SER:O	1:C:577:ARG:NH1	2.49	0.45
1:C:865:LEU:HB3	1:C:875:TYR:CE1	2.51	0.45
5:G:32:DG:H1	6:H:14:DC:H42	1.63	0.45
1:A:1000:GLN:HE21	4:F:31:DT:H1'	1.82	0.44
2:B:142:LEU:HD11	2:B:153:CYS:HB3	1.99	0.44
2:B:207:HIS:ND1	2:B:207:HIS:O	2.50	0.44
1:C:931:TYR:OH	1:C:961:THR:O	2.35	0.44
3:E:12:DA:N6	4:F:22:DC:N4	2.65	0.44
1:A:955:THR:CG2	1:A:958:LEU:HB2	2.47	0.44
1:C:530:LEU:HD11	1:C:1011:LYS:HD2	1.98	0.44
3:E:9:DT:C4	3:E:10:DA:N7	2.86	0.44
4:F:7:DG:N3	4:F:8:DG:C8	2.85	0.44
5:G:8:DG:H3'	5:G:9:DT:H71	2.00	0.44
1:A:874:ASN:HA	1:A:877:ARG:HH11	1.82	0.44
2:B:3:LEU:HB3	2:B:348:VAL:HG12	2.00	0.44
2:B:212:ARG:HD3	2:B:269:HIS:CG	2.51	0.44
1:C:476:GLY:HA3	1:C:477:ARG:CD	2.45	0.44
1:C:768:ILE:HD11	1:C:964:HIS:HB3	1.98	0.44
7:I:11:DG:H2'	7:I:12:DT:C7	2.46	0.44
1:A:748:ILE:H	1:A:748:ILE:HG13	1.51	0.44
2:B:315:ARG:HG2	2:B:316:THR:HG23	1.99	0.44
1:C:653:LEU:HB3	1:C:654:GLU:HA	1.98	0.44
2:D:84:ASP:HA	2:D:85:GLY:HA2	1.55	0.44
1:A:423:GLN:NE2	1:C:456:LEU:HD11	2.33	0.44
1:A:1022:GLN:O	1:A:1025:MET:HG2	2.17	0.44
1:C:838:TYR:OH	1:C:897:ARG:HG3	2.18	0.44
4:F:35:DT:P	7:I:16:DA:O3'	2.76	0.44
5:G:29:DG:C6	5:G:30:DG:C2	3.05	0.44
1:A:704:MET:HE3	1:A:704:MET:HB2	1.83	0.44
2:B:258:ILE:HG21	2:B:284:ARG:HD2	1.98	0.44
2:B:326:THR:CG2	2:B:347:GLN:HE21	2.30	0.44
1:C:999:ARG:HH22	6:H:8:DG:C5'	2.31	0.44
1:A:786:PRO:HG2	1:A:787:PHE:CD2	2.53	0.44
2:B:9:VAL:HG12	2:B:55:LEU:O	2.18	0.44
2:B:292:LEU:HA	2:B:297:VAL:HA	1.99	0.44
1:C:622:MET:HE1	1:C:990:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:789:GLU:OE2	1:C:797:ARG:NH2	2.48	0.44
1:C:999:ARG:HH22	6:H:8:DG:C4'	2.30	0.44
3:E:23:DA:H2''	3:E:24:DA:H8	1.83	0.44
2:B:266:ILE:HG22	2:B:325:GLY:CA	2.44	0.44
1:C:449:VAL:O	1:C:452:THR:OG1	2.33	0.44
1:C:828:LYS:HD3	1:C:949:ARG:HH22	1.83	0.44
4:F:32:DG:H5'	4:F:32:DG:C8	2.53	0.44
7:J:7:DG:C6	7:J:8:DC:N4	2.86	0.44
2:B:87:PRO:HA	2:B:88:GLU:HA	1.68	0.44
2:B:147:SER:OG	2:B:239:GLU:HA	2.17	0.44
1:C:942:LEU:HD22	1:C:950:TYR:HE2	1.83	0.44
5:G:4:DC:H2''	5:G:5:DA:H8	1.82	0.44
5:G:44:DT:C5	5:G:45:DG:C6	3.05	0.44
5:G:47:DA:C2	7:J:15:DT:C4	3.06	0.44
1:A:598:ARG:N	1:A:598:ARG:HD3	2.33	0.43
1:C:482:HIS:CG	1:C:483:PRO:HD2	2.53	0.43
1:C:587:LYS:HE3	1:C:712:SER:O	2.18	0.43
2:D:71:PRO:O	2:D:98:PRO:HD3	2.18	0.43
3:E:28:DC:O2	4:F:8:DG:C2	2.71	0.43
4:F:41:DA:N6	7:I:9:DC:H42	2.15	0.43
5:G:46:DT:H2''	5:G:47:DA:O5'	2.18	0.43
1:A:463:GLU:CG	1:A:465:LYS:HE2	2.43	0.43
1:A:717:LEU:O	1:A:717:LEU:HD12	2.18	0.43
1:A:1025:MET:CG	1:A:1026:GLU:N	2.82	0.43
1:C:555:ASP:N	1:C:555:ASP:OD1	2.51	0.43
2:D:3:LEU:HA	2:D:347:GLN:O	2.18	0.43
2:D:274:PHE:CE1	2:D:348:VAL:HG21	2.53	0.43
4:F:4:DC:H2''	4:F:5:DA:H8	1.83	0.43
1:A:697:VAL:O	1:A:700:GLU:HB2	2.18	0.43
2:B:104:SER:HB2	2:B:136:ALA:CB	2.48	0.43
1:C:517:GLN:HB3	1:C:521:THR:CG2	2.48	0.43
2:D:150:LYS:NZ	2:D:240:LEU:HB3	2.33	0.43
1:C:955:THR:HG23	1:C:958:LEU:H	1.83	0.43
2:D:179:PRO:HA	2:D:180:PRO:HD3	1.72	0.43
5:G:24:DA:H61	6:H:22:DT:H3	1.67	0.43
6:H:11:DG:H2'	6:H:12:DT:O4'	2.18	0.43
1:A:871:MET:HE2	1:A:871:MET:HB2	1.89	0.43
2:B:187:LEU:HD12	2:B:187:LEU:H	1.83	0.43
2:D:61:SER:O	2:D:121:THR:HA	2.18	0.43
1:A:632:GLY:HA2	1:C:860:ARG:NH1	2.33	0.43
2:B:137:ARG:NH1	2:B:178:CYS:SG	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:GLN:HE21	1:C:426:ARG:NH2	2.11	0.43
1:C:424:LYS:O	1:C:431:LYS:NZ	2.51	0.43
2:D:148:ARG:N	2:D:149:GLY:HA2	2.33	0.43
2:D:204:GLN:HB3	2:D:223:ILE:HG12	2.01	0.43
4:F:28:DC:C4	4:F:29:DA:N6	2.87	0.43
4:F:33:DT:C5	4:F:34:DG:C2	3.07	0.43
1:A:423:GLN:O	1:A:424:LYS:C	2.61	0.43
1:A:423:GLN:CD	1:C:456:LEU:HD11	2.43	0.43
1:A:615:VAL:HG22	1:A:646:ILE:HG12	2.00	0.43
2:B:80:PHE:HB2	2:B:144:VAL:HG21	2.00	0.43
2:D:300:GLU:HG3	2:D:301:SER:O	2.18	0.43
2:D:350:PHE:CD1	2:D:351:GLN:HG3	2.53	0.43
1:A:999:ARG:O	3:E:6:DT:H2''	2.18	0.43
1:A:999:ARG:NH1	3:E:8:DC:H4'	2.32	0.43
2:B:10:ASN:HD21	2:B:56:LYS:NZ	2.16	0.43
1:C:546:SER:HB3	2:D:168:THR:HG21	2.00	0.43
1:C:953:LYS:NZ	7:I:13:DC:H5''	2.34	0.43
2:D:93:HIS:HA	2:D:94:GLY:HA2	1.66	0.43
1:A:415:LEU:HA	1:A:418:LEU:HD13	1.99	0.43
1:A:749:CYS:HB2	1:A:959:HIS:NE2	2.34	0.43
1:A:897:ARG:HD2	1:A:945:MET:HE2	2.00	0.43
2:B:62:PHE:HB3	2:B:66:SER:OG	2.19	0.43
2:B:143:SER:HB2	2:B:154:VAL:HG13	2.01	0.43
1:C:423:GLN:NE2	1:C:426:ARG:HH11	2.17	0.43
1:C:496:SER:HB3	1:C:499:GLN:HG2	2.00	0.43
7:J:11:DG:H2''	7:J:12:DT:C7	2.49	0.43
1:A:649:ILE:CG2	1:A:663:PHE:HB3	2.49	0.43
1:C:426:ARG:C	1:C:427:LEU:HD12	2.44	0.43
4:F:29:DA:C5	4:F:30:DC:C5	3.06	0.43
5:G:1:DC:H2'	5:G:2:DT:C6	2.53	0.43
5:G:30:DG:N2	6:H:16:DC:N3	2.62	0.43
1:A:520:HIS:NE2	4:F:23:DT:OP2	2.52	0.42
1:A:670:SER:HA	6:H:3:DC:H4'	2.00	0.42
2:B:163:PRO:HD2	2:B:166:GLU:OE2	2.19	0.42
2:D:283:LYS:HD2	2:D:317:TRP:HD1	1.80	0.42
5:G:7:DG:H22	6:H:39:DC:N4	2.17	0.42
1:A:426:ARG:O	1:C:437:PHE:HZ	2.02	0.42
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.82	0.42
1:A:500:TYR:OH	1:A:516:PHE:HB3	2.19	0.42
1:A:574:ARG:NH2	1:A:1003:THR:O	2.48	0.42
1:C:519:LEU:O	1:C:523:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:ASP:OD2	1:C:660:ILE:HD11	2.19	0.42
1:C:748:ILE:CG2	1:C:756:ARG:HE	2.32	0.42
1:C:772:HIS:HB2	1:C:808:GLU:HG2	2.01	0.42
1:C:1006:LEU:HD23	1:C:1006:LEU:HA	1.85	0.42
2:D:21:LEU:HD12	2:D:320:GLY:HA3	2.01	0.42
2:D:118:ARG:NH1	4:F:48:DA:O3'	2.52	0.42
4:F:19:DA:H2'	4:F:20:DG:C1'	2.48	0.42
1:A:912:LYS:N	1:A:913:PRO:HD2	2.35	0.42
2:B:115:GLY:HA3	2:B:116:CYS:C	2.44	0.42
1:A:555:ASP:OD1	1:A:555:ASP:N	2.52	0.42
2:B:38:LYS:C	2:B:40:SER:H	2.27	0.42
1:A:420:ARG:NH1	1:C:459:ARG:NE	2.68	0.42
1:A:877:ARG:HH21	1:A:916:ARG:NH2	2.06	0.42
1:C:573:SER:HB3	1:C:680:MET:HG2	2.00	0.42
2:D:93:HIS:C	2:D:140:HIS:HE2	2.27	0.42
2:D:210:LEU:HD22	2:D:271:TYR:CD2	2.54	0.42
5:G:15:DT:C4	5:G:16:DA:C6	3.07	0.42
1:A:536:PHE:CE2	1:A:549:TRP:HB2	2.55	0.42
1:C:459:ARG:HB2	1:C:466:GLN:HE22	1.84	0.42
1:C:460:ALA:O	3:E:16:DT:H4'	2.20	0.42
2:D:69:LEU:HD12	2:D:69:LEU:HA	1.61	0.42
4:F:29:DA:N7	4:F:30:DC:C5	2.88	0.42
5:G:29:DG:H2''	5:G:30:DG:OP2	2.19	0.42
1:A:487:LEU:HD21	1:A:526:GLU:OE2	2.19	0.42
1:A:611:PHE:CD1	1:A:649:ILE:HD11	2.55	0.42
2:B:69:LEU:HD11	2:B:107:TYR:CZ	2.55	0.42
1:C:428:ARG:HA	1:C:431:LYS:NZ	2.34	0.42
1:C:493:THR:HG23	1:C:495:LEU:HG	2.02	0.42
1:C:680:MET:HB3	1:C:682:VAL:HG23	2.02	0.42
2:D:41:CYS:HB3	2:D:46:PHE:HE1	1.85	0.42
2:D:150:LYS:HZ3	2:D:240:LEU:HB3	1.85	0.42
7:I:12:DT:C2	7:I:13:DC:C4	3.08	0.42
1:C:742:ALA:HA	1:C:743:SER:HA	1.69	0.42
5:G:33:DT:C4	5:G:34:DA:C6	3.08	0.42
6:H:35:DA:H2''	6:H:36:DA:OP2	2.20	0.42
1:A:414:HIS:CD2	1:A:416:LEU:H	2.38	0.42
1:A:833:GLU:OE2	1:A:897:ARG:NE	2.44	0.42
2:B:84:ASP:OD1	2:B:85:GLY:HA2	2.20	0.42
1:C:470:LEU:O	1:C:473:MET:HG3	2.20	0.42
1:C:573:SER:O	1:C:574:ARG:NH1	2.51	0.42
3:E:12:DA:H61	4:F:22:DC:N4	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLU:O	1:A:732:LYS:C	2.63	0.42
2:B:222:HIS:HB2	2:B:259:THR:HG21	2.02	0.42
1:C:710:ILE:HG23	1:C:717:LEU:HG	2.01	0.42
1:C:733:MET:HE3	1:C:733:MET:HB2	1.85	0.42
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.83	0.41
1:A:793:GLU:O	1:A:796:ASP:HB3	2.20	0.41
1:C:999:ARG:NH2	6:H:8:DG:H5'	2.35	0.41
2:D:94:GLY:H	2:D:140:HIS:CE1	2.38	0.41
6:H:2:DA:H5''	6:H:2:DA:H8	1.84	0.41
7:I:7:DG:H2''	7:I:8:DC:O4'	2.20	0.41
1:A:865:LEU:HB3	1:A:875:TYR:CE1	2.55	0.41
2:B:179:PRO:HB2	2:B:181:GLN:OE1	2.20	0.41
2:B:324:LYS:HD2	2:B:324:LYS:HA	1.76	0.41
1:C:885:VAL:HG21	1:C:905:MET:HE3	2.01	0.41
7:J:12:DT:N3	7:J:13:DC:N4	2.68	0.41
1:A:519:LEU:HA	1:A:519:LEU:HD23	1.84	0.41
1:A:620:ASP:OD2	1:A:984:GLU:OE2	2.39	0.41
1:A:631:SER:HA	1:C:864:LYS:HD2	2.01	0.41
1:C:539:GLN:HA	1:C:540:PRO:C	2.45	0.41
1:C:1004:PHE:O	1:C:1007:GLU:HB3	2.21	0.41
3:E:18:DG:C5	3:E:19:DA:C6	3.08	0.41
1:A:586:LEU:HD21	1:A:720:PHE:CD2	2.56	0.41
1:A:606:MET:HG2	1:A:607:CYS:N	2.35	0.41
1:A:738:GLU:CA	1:A:805:PRO:HB3	2.45	0.41
2:B:76:ALA:HB3	2:B:93:HIS:O	2.20	0.41
2:B:148:ARG:HH12	2:B:241:LEU:HB2	1.85	0.41
2:D:147:SER:OG	2:D:240:LEU:HB2	2.21	0.41
1:A:974:SER:OG	1:A:977:ALA:HB3	2.20	0.41
4:F:29:DA:C6	4:F:30:DC:C4	3.09	0.41
6:H:6:DT:H6	6:H:6:DT:H2'	1.38	0.41
1:A:515:ILE:HG12	1:C:515:ILE:HG12	2.01	0.41
2:B:111:VAL:HG21	2:B:114:ARG:HH11	1.86	0.41
2:B:233:LEU:HD22	2:B:252:LEU:HD22	2.03	0.41
2:D:150:LYS:HE2	2:D:240:LEU:HB3	2.03	0.41
7:I:13:DC:C4	7:I:14:DT:O4	2.74	0.41
1:A:787:PHE:HB2	1:A:789:GLU:HG2	2.02	0.41
1:A:845:ARG:NH2	7:J:12:DT:OP2	2.53	0.41
1:A:878:ARG:HH22	5:G:41:DC:H2'	1.85	0.41
2:B:43:THR:HG23	2:B:62:PHE:CD2	2.56	0.41
2:B:167:ARG:NH2	2:B:172:TRP:O	2.54	0.41
1:C:413:GLN:OE1	1:C:417:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:29:DA:C5	4:F:30:DC:C4	3.09	0.41
1:A:783:ARG:O	2:B:67:SER:HB2	2.21	0.41
2:B:93:HIS:O	2:B:140:HIS:NE2	2.54	0.41
2:B:109:LEU:HD21	2:B:122:LEU:HD13	2.02	0.41
2:B:237:HIS:O	2:B:248:THR:HG22	2.20	0.41
1:C:475:GLN:H	1:C:475:GLN:CD	2.29	0.41
1:C:628:LYS:HZ3	1:C:628:LYS:HG2	1.52	0.41
1:C:640:VAL:HB	1:C:680:MET:HE3	2.02	0.41
2:D:215:CYS:HG	2:D:237:HIS:CE1	2.30	0.41
5:G:47:DA:N1	7:J:15:DT:O4	2.53	0.41
1:A:676:PRO:HG3	1:A:1013:HIS:CG	2.56	0.41
2:B:38:LYS:C	2:B:40:SER:N	2.79	0.41
2:B:184:LEU:HB2	2:B:193:THR:OG1	2.20	0.41
2:D:88:GLU:OE1	2:D:88:GLU:HA	2.20	0.41
2:D:219:LEU:HD11	2:D:256:LEU:HB3	2.02	0.41
2:D:237:HIS:HD2	2:D:239:GLU:OE2	2.03	0.41
3:E:28:DC:H42	4:F:7:DG:H1	1.68	0.41
5:G:2:DT:H2'	5:G:3:DG:C8	2.55	0.41
1:A:539:GLN:HA	1:A:540:PRO:HA	1.93	0.41
1:A:829:ILE:O	1:A:833:GLU:HB2	2.21	0.41
1:A:898:ARG:O	1:A:902:LEU:HB2	2.21	0.41
1:C:669:ASN:HD22	3:E:2:DA:C4'	2.31	0.41
2:D:283:LYS:HB2	2:D:317:TRP:HE1	1.86	0.41
2:D:81:GLU:HA	2:D:88:GLU:OE2	2.20	0.40
2:D:183:TYR:CE1	2:D:194:ALA:HB2	2.57	0.40
1:A:489:ILE:HD12	1:A:489:ILE:HA	1.82	0.40
1:C:421:ARG:CZ	1:C:424:LYS:HD3	2.51	0.40
4:F:21:DT:H6	4:F:21:DT:H2'	1.65	0.40
4:F:35:DT:OP2	7:I:16:DA:O3'	2.39	0.40
5:G:34:DA:C2	6:H:13:DA:C2	3.09	0.40
1:A:438:ALA:O	1:A:443:GLY:N	2.53	0.40
1:C:562:VAL:HG23	1:C:569:ALA:HB3	2.02	0.40
1:C:846:GLU:OE2	1:C:850:ARG:NH2	2.53	0.40
2:D:82:ALA:HA	2:D:87:PRO:HB3	2.02	0.40
2:D:158:GLY:N	2:D:204:GLN:O	2.54	0.40
2:D:326:THR:CG2	2:D:347:GLN:HE21	2.35	0.40
5:G:14:DG:C5	5:G:15:DT:C4	3.09	0.40
1:A:412:ARG:HD3	4:F:11:DT:H5''	2.04	0.40
6:H:38:DC:H2'	6:H:39:DC:C6	2.56	0.40
7:I:15:DT:H2''	7:I:16:DA:H5'	2.04	0.40
2:B:69:LEU:HD11	2:B:107:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:LEU:HB2	2:B:255:GLY:CA	2.48	0.40
1:C:430:LEU:HD12	1:C:430:LEU:H	1.86	0.40
1:C:538:TRP:CZ3	1:C:709:LEU:HB2	2.56	0.40
1:C:577:ARG:NH2	1:C:579:ASP:OD2	2.52	0.40
2:D:331:ILE:HA	2:D:332:PRO:HD2	1.95	0.40
6:H:38:DC:H2''	6:H:39:DC:H5'	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	620/764 (81%)	574 (93%)	38 (6%)	8 (1%)	9	41
1	C	620/764 (81%)	572 (92%)	42 (7%)	6 (1%)	12	47
2	B	349/533 (66%)	332 (95%)	15 (4%)	2 (1%)	21	58
2	D	349/533 (66%)	335 (96%)	13 (4%)	1 (0%)	36	71
All	All	1938/2594 (75%)	1813 (94%)	108 (6%)	17 (1%)	16	49

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	LYS
1	A	465	LYS
1	A	473	MET
1	C	416	LEU
1	C	464	HIS
1	C	473	MET
1	A	480	GLY
1	C	475	GLN
1	C	986	GLY

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Mol	Chain	Res	Type
1	A	444	GLY
2	B	9	VAL
2	B	39	ARG
1	C	443	GLY
2	D	9	VAL
1	A	422	ALA
1	A	986	GLY
1	A	811	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	548/681 (80%)	521 (95%)	27 (5%)	22	44
1	C	548/681 (80%)	517 (94%)	31 (6%)	18	40
2	B	303/465 (65%)	290 (96%)	13 (4%)	26	47
2	D	303/465 (65%)	291 (96%)	12 (4%)	28	49
All	All	1702/2292 (74%)	1619 (95%)	83 (5%)	24	44

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	415	LEU
1	A	423	GLN
1	A	455	LEU
1	A	456	LEU
1	A	458	LEU
1	A	560	TRP
1	A	565	ASP
1	A	586	LEU
1	A	604	ASP
1	A	649	ILE
1	A	652	ARG
1	A	662	ILE
1	A	694	LEU

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Mol	Chain	Res	Type
1	A	731	GLU
1	A	748	ILE
1	A	751	LEU
1	A	789	GLU
1	A	793	GLU
1	A	840	LYS
1	A	848	ARG
1	A	849	ARG
1	A	923	ASP
1	A	954	ILE
1	A	971	ARG
1	A	992	ARG
1	A	1005	GLU
1	A	1023	LYS
2	B	48	VAL
2	B	69	LEU
2	B	81	GLU
2	B	154	VAL
2	B	166	GLU
2	B	256	LEU
2	B	266	ILE
2	B	292	LEU
2	B	297	VAL
2	B	298	HIS
2	B	300	GLU
2	B	302	ARG
2	B	334	GLU
1	C	415	LEU
1	C	416	LEU
1	C	421	ARG
1	C	430	LEU
1	C	441	GLU
1	C	446	VAL
1	C	464	HIS
1	C	466	GLN
1	C	470	LEU
1	C	474	MET
1	C	477	ARG
1	C	491	VAL
1	C	560	TRP
1	C	565	ASP
1	C	567	VAL

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Mol	Chain	Res	Type
1	C	586	LEU
1	C	595	GLU
1	C	649	ILE
1	C	694	LEU
1	C	700	GLU
1	C	702	LYS
1	C	707	SER
1	C	710	ILE
1	C	736	GLU
1	C	778	ARG
1	C	831	GLN
1	C	848	ARG
1	C	849	ARG
1	C	885	VAL
1	C	975	ILE
1	C	992	ARG
2	D	1	MET
2	D	16	GLN
2	D	28	VAL
2	D	39	ARG
2	D	69	LEU
2	D	132	ASP
2	D	175	VAL
2	D	187	LEU
2	D	242	LEU
2	D	281	THR
2	D	286	GLU
2	D	300	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	HIS
1	A	501	HIS
1	A	766	HIS
1	A	772	HIS
1	A	822	ASN
1	A	964	HIS
2	B	100	ASN
2	B	173	ASN
2	B	278	GLN
2	B	282	GLN

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Mol	Chain	Res	Type
2	B	347	GLN
1	C	462	ASN
1	C	466	GLN
1	C	492	ASN
1	C	669	ASN
1	C	772	HIS
1	C	822	ASN
1	C	1000	GLN
2	D	347	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	2:DA	O3'	3:DC	P	1.77

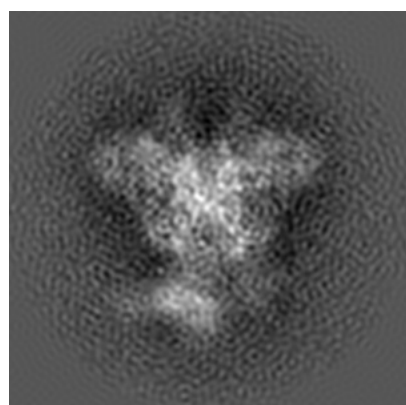
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6489. These allow visual inspection of the internal detail of the map and identification of artifacts.

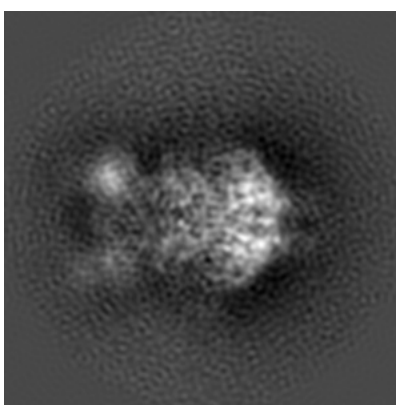
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

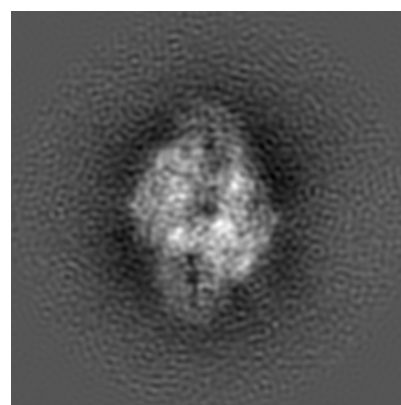
6.1.1 Primary map



X



Y

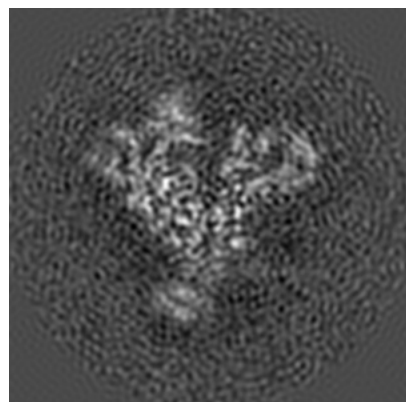


Z

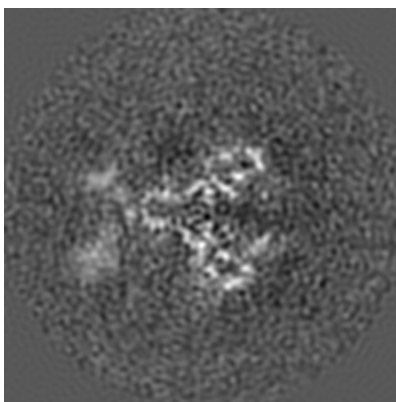
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

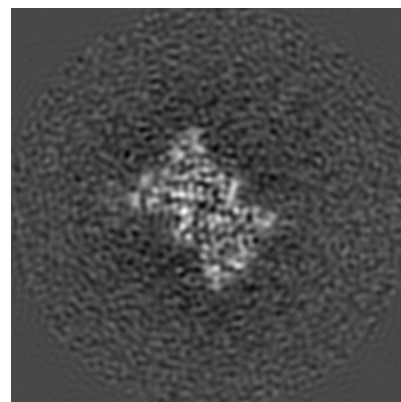
6.2.1 Primary map



X Index: 96



Y Index: 96

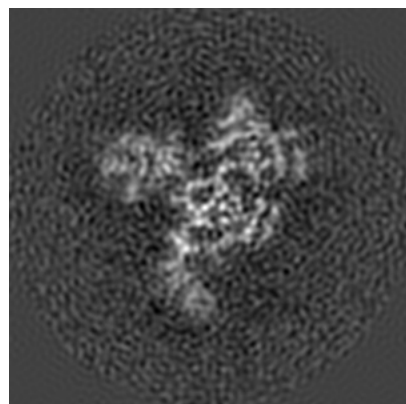


Z Index: 96

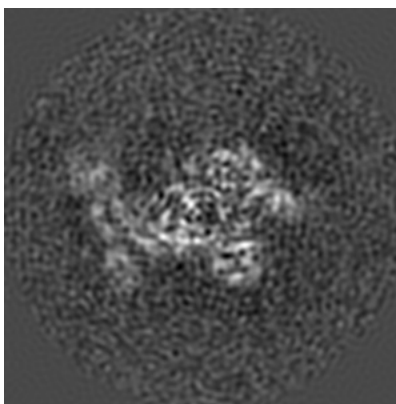
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

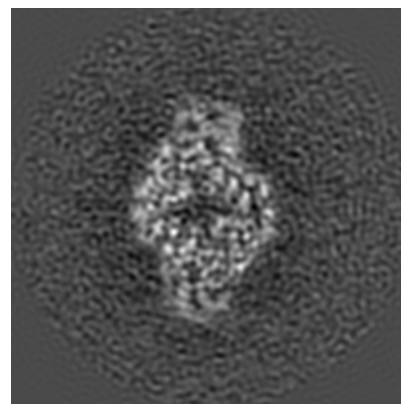
6.3.1 Primary map



X Index: 82



Y Index: 84

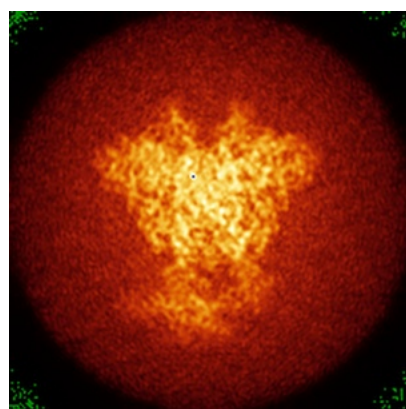


Z Index: 115

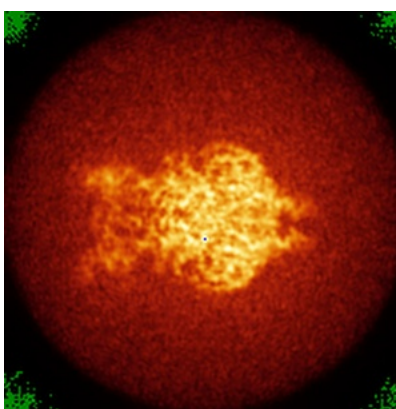
The images above show the largest variance slices of the map in three orthogonal directions.

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

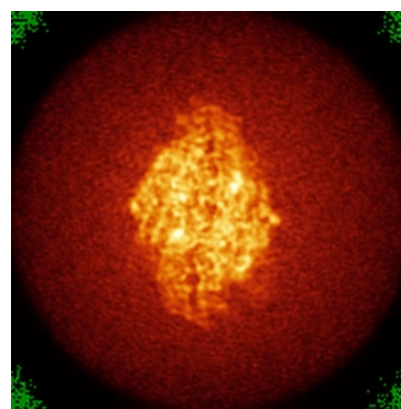
6.4.1 Primary map



X



Y

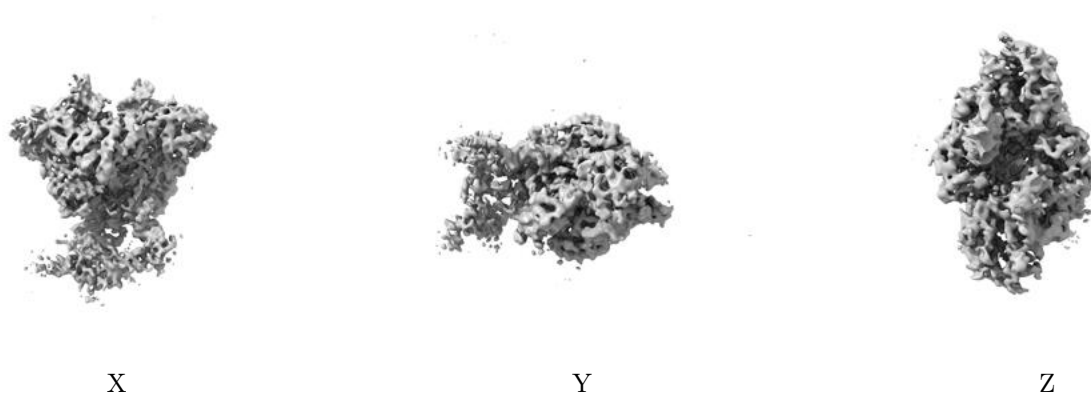


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

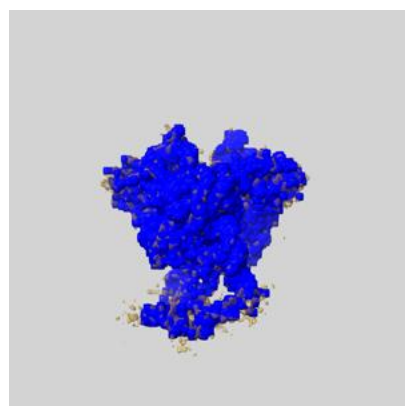
6.6 Mask visualisation [i](#)

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

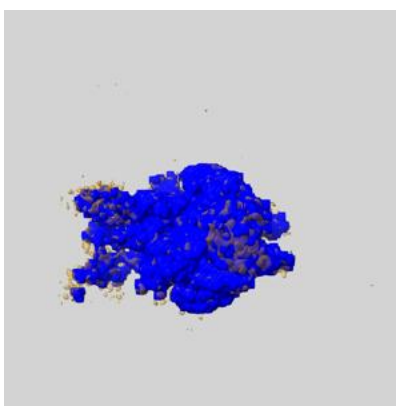
A mask typically either:

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

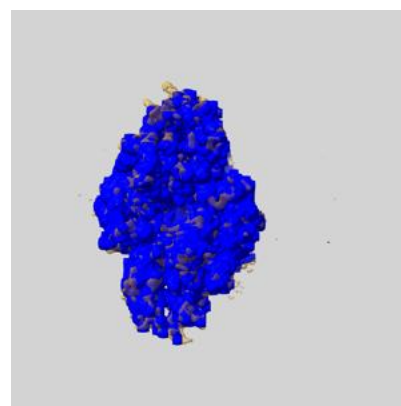
6.6.1 emd_6489_msk_1.map [i](#)



X



Y

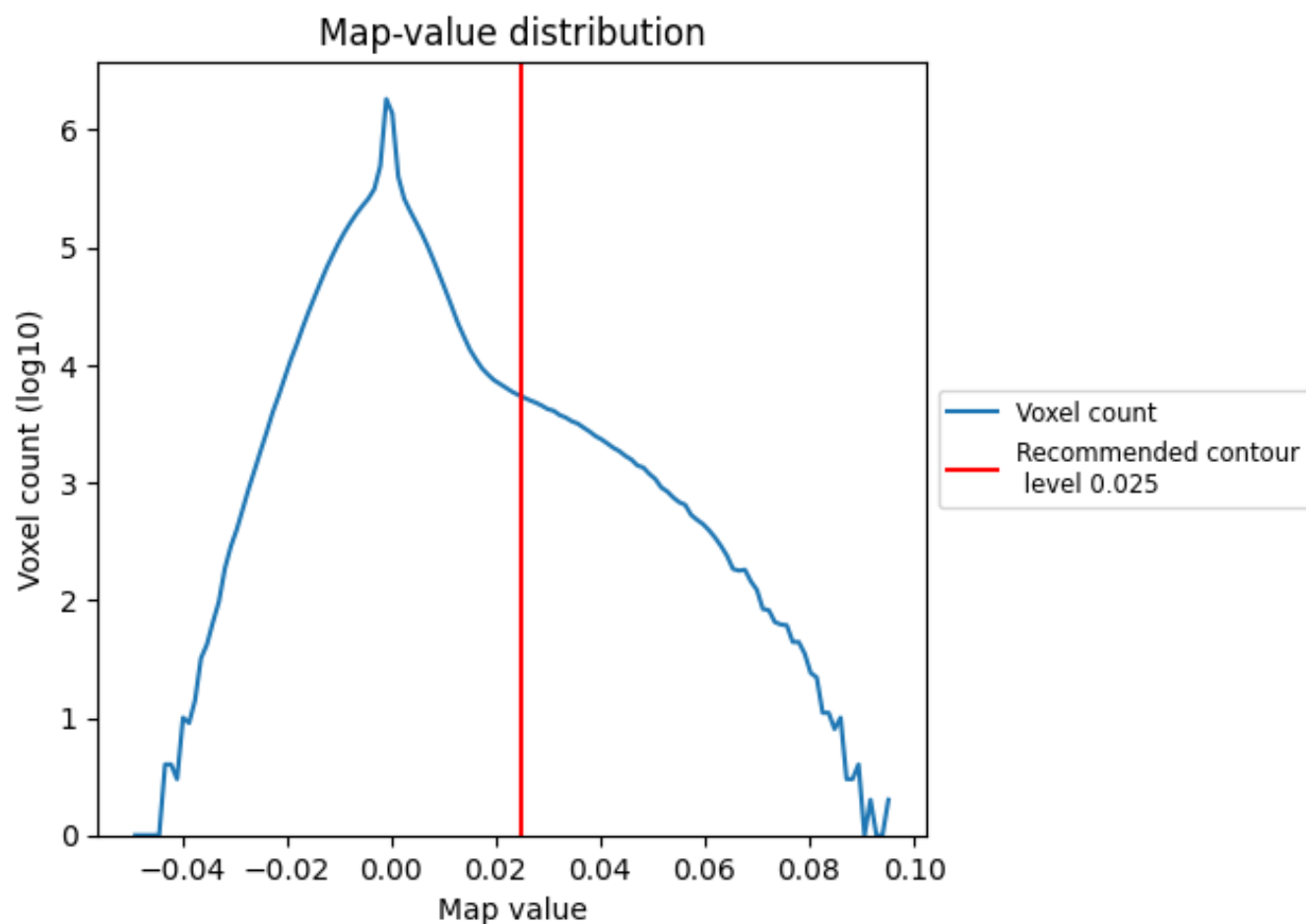


Z

7 Map analysis [i](#)

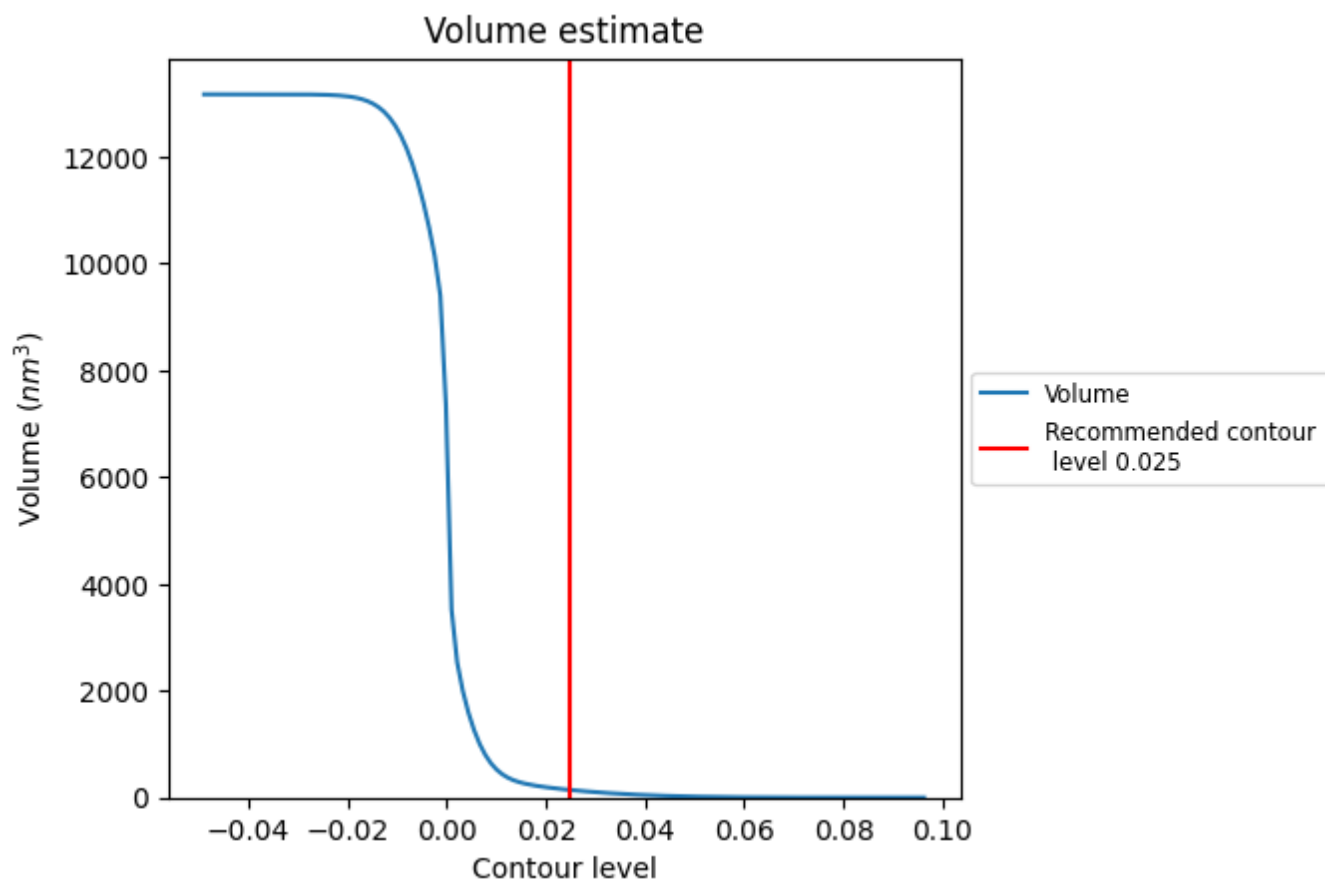
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

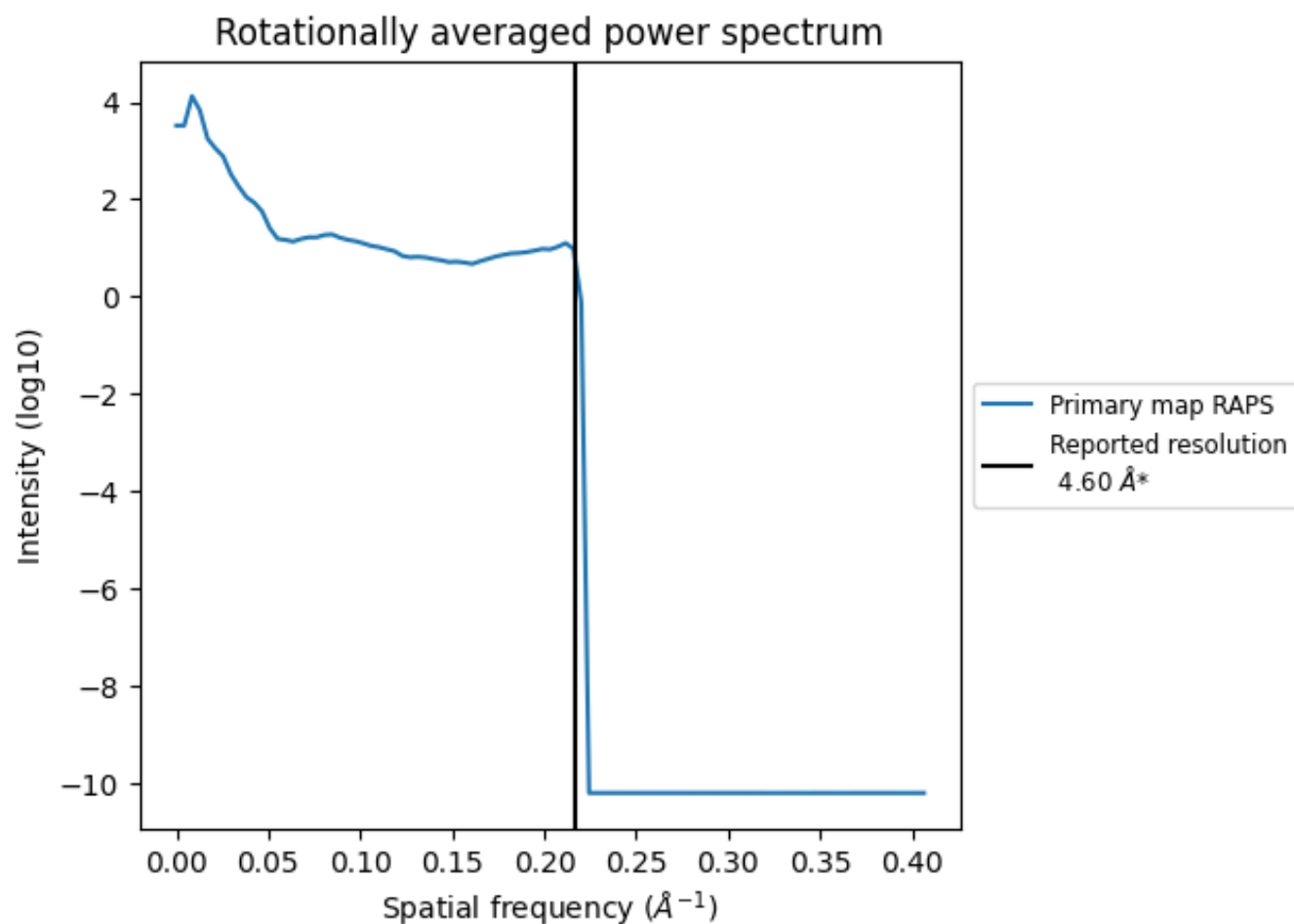
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm³; this corresponds to an approximate mass of 128 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 ⓘ

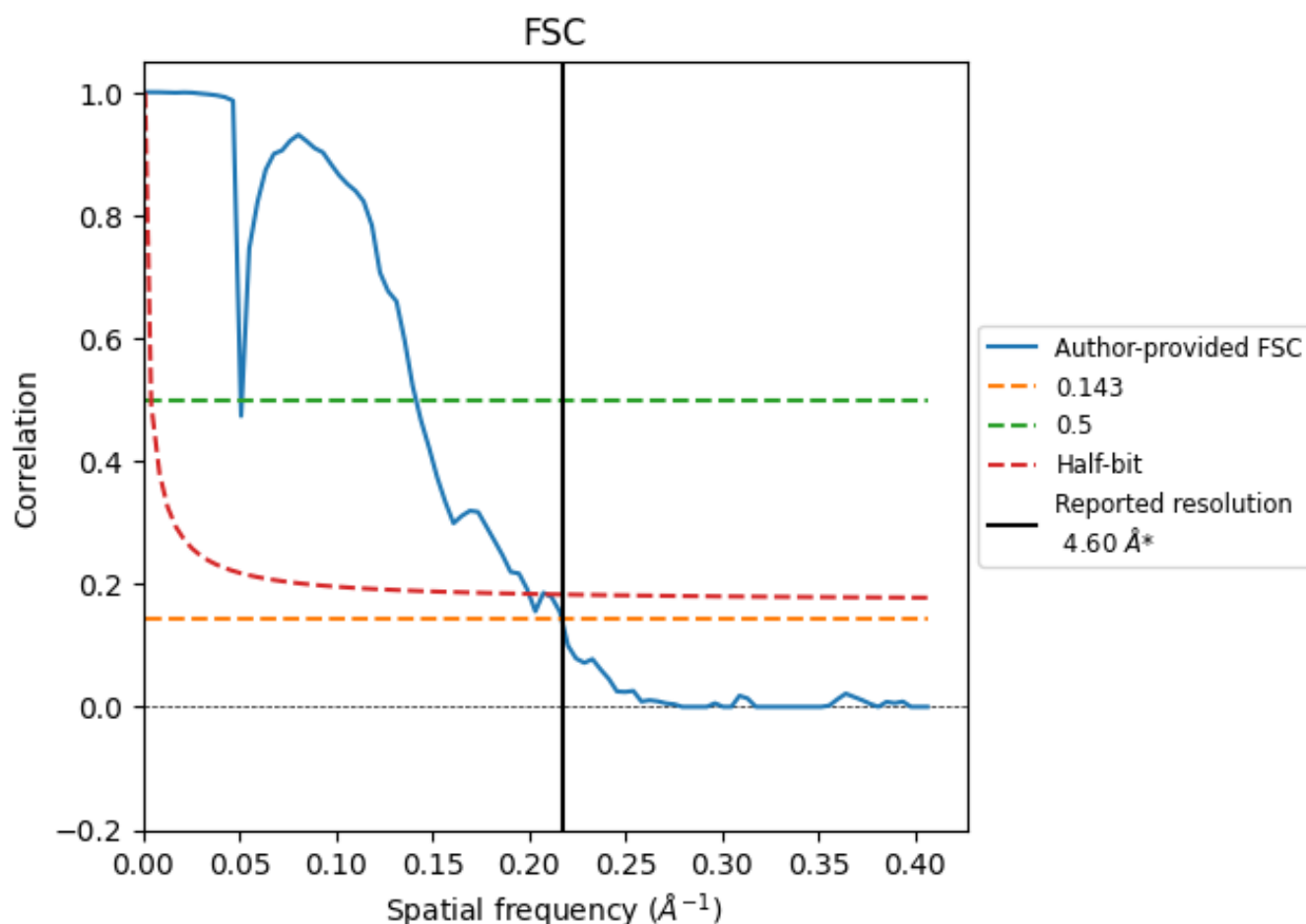


*Reported resolution corresponds to spatial frequency of 0.217 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

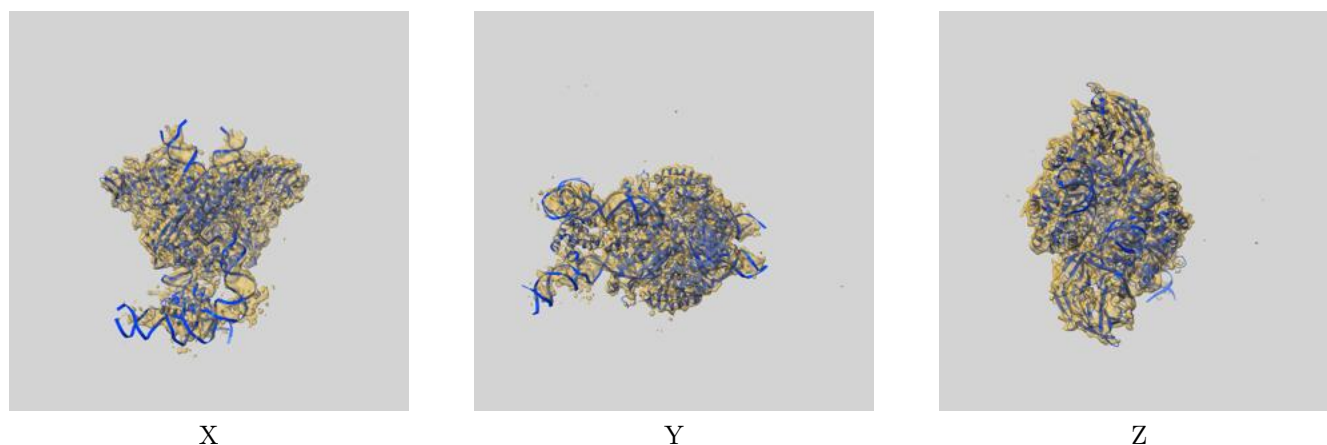
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.61	19.76	5.00
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

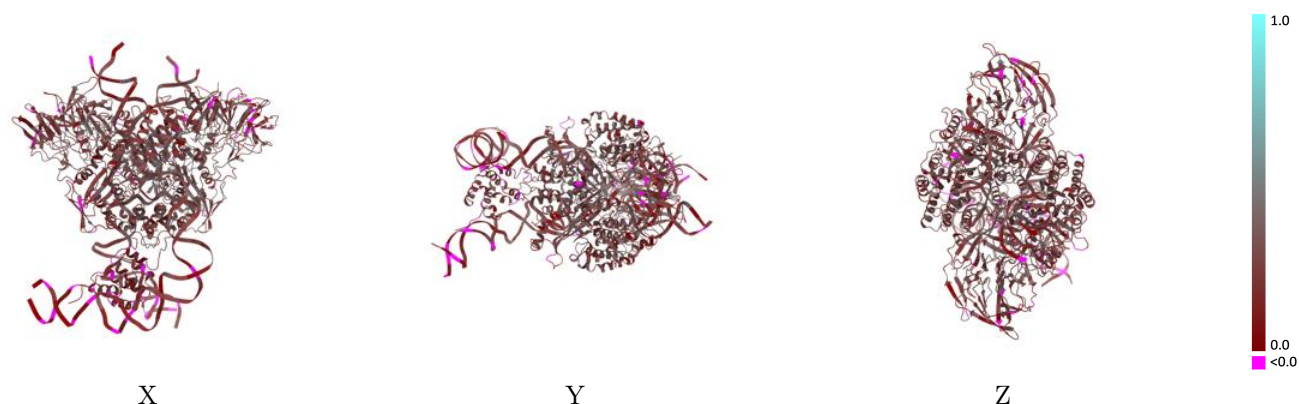
This section contains information regarding the fit between EMDB map EMD-6489 and PDB model 3JBW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



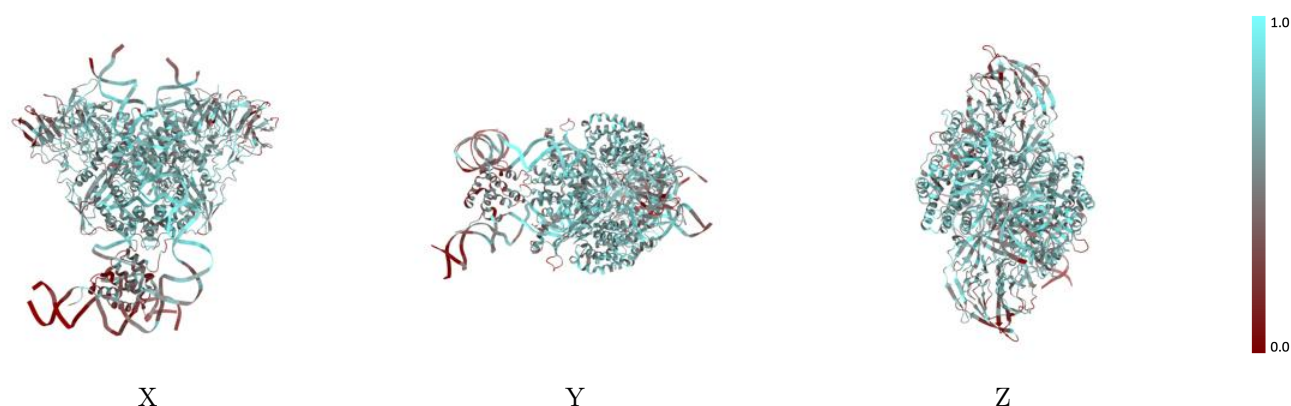
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



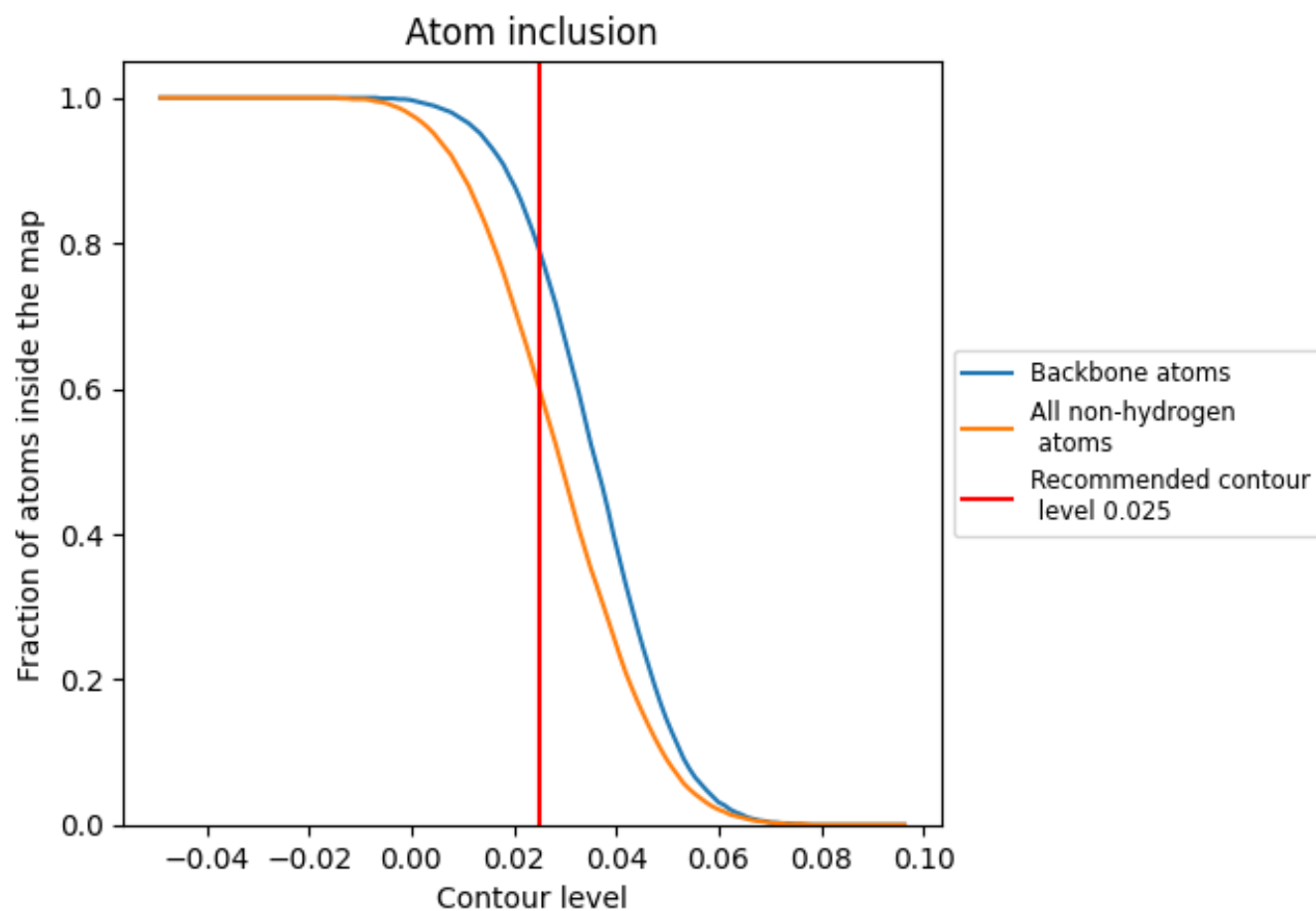
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 60% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6000	0.2450
A	0.6130	0.2600
B	0.5740	0.2600
C	0.6150	0.2610
D	0.5720	0.2500
E	0.5710	0.1780
F	0.6450	0.2320
G	0.5820	0.1920
H	0.5160	0.1720
I	0.7060	0.2410
J	0.7240	0.2150

1.0

0.0

<0.0