



## Full wwPDB EM Validation Report ⓘ

Mar 4, 2024 – 09:21 PM EST

PDB ID : 6DBW  
EMDB ID : EMD-7852  
Title : Cryo-EM structure of RAG in complex with 12-RSS substrate DNA  
Authors : Wu, H.; Liao, M.; Ru, H.; Mi, W.  
Deposited on : 2018-05-03  
Resolution : 4.70 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

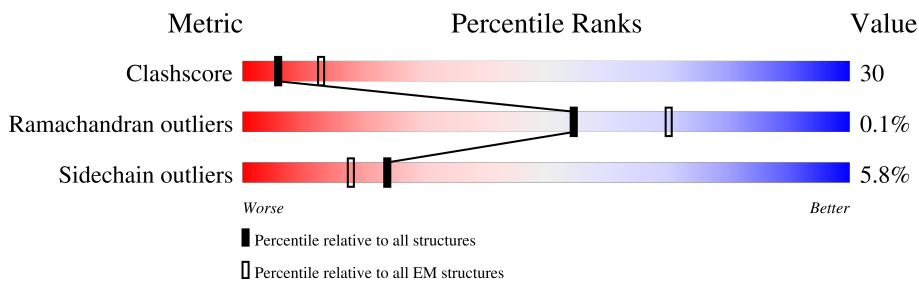
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.70 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  $\geq 3$ , 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	1159	
1	C	1159	
2	B	533	
2	D	533	
3	E	50	
4	F	50	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 17418 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 Recombination activating gene 1 - MBP chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	614	4954	3102	890	925	37	0	0
1	C	615	4980	3116	898	929	37	2	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-127	MET	-	initiating methionine	UNP P0AEX9
A	-126	GLY	-	expression tag	UNP P0AEX9
A	-125	SER	-	expression tag	UNP P0AEX9
A	-124	SER	-	expression tag	UNP P0AEX9
A	-123	HIS	-	expression tag	UNP P0AEX9
A	-122	HIS	-	expression tag	UNP P0AEX9
A	-121	HIS	-	expression tag	UNP P0AEX9
A	-120	HIS	-	expression tag	UNP P0AEX9
A	-119	HIS	-	expression tag	UNP P0AEX9
A	-118	HIS	-	expression tag	UNP P0AEX9
A	-117	GLY	-	expression tag	UNP P0AEX9
A	-116	THR	-	expression tag	UNP P0AEX9
A	-115	LYS	-	expression tag	UNP P0AEX9
A	-114	THR	-	expression tag	UNP P0AEX9
A	251	GLY	-	linker	UNP P0AEX9
A	252	THR	-	linker	UNP P0AEX9
A	253	ASP	-	linker	UNP P0AEX9
A	254	TYR	-	linker	UNP P0AEX9
A	255	ASP	-	linker	UNP P0AEX9
A	256	ILE	-	linker	UNP P0AEX9
A	257	PRO	-	linker	UNP P0AEX9
A	258	THR	-	linker	UNP P0AEX9
A	259	THR	-	linker	UNP P0AEX9
A	260	LEU	-	linker	UNP P0AEX9
A	261	GLU	-	linker	UNP P0AEX9
A	262	VAL	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LEU	-	linker	UNP P0AEX9
A	264	PHE	-	linker	UNP P0AEX9
A	265	GLN	-	linker	UNP P0AEX9
A	266	GLY	-	linker	UNP P0AEX9
A	267	PRO	-	linker	UNP P0AEX9
A	268	LEU	-	linker	UNP P0AEX9
A	269	GLY	-	linker	UNP P0AEX9
A	270	SER	-	linker	UNP P0AEX9
C	-127	MET	-	initiating methionine	UNP P0AEX9
C	-126	GLY	-	expression tag	UNP P0AEX9
C	-125	SER	-	expression tag	UNP P0AEX9
C	-124	SER	-	expression tag	UNP P0AEX9
C	-123	HIS	-	expression tag	UNP P0AEX9
C	-122	HIS	-	expression tag	UNP P0AEX9
C	-121	HIS	-	expression tag	UNP P0AEX9
C	-120	HIS	-	expression tag	UNP P0AEX9
C	-119	HIS	-	expression tag	UNP P0AEX9
C	-118	HIS	-	expression tag	UNP P0AEX9
C	-117	GLY	-	expression tag	UNP P0AEX9
C	-116	THR	-	expression tag	UNP P0AEX9
C	-115	LYS	-	expression tag	UNP P0AEX9
C	-114	THR	-	expression tag	UNP P0AEX9
C	251	GLY	-	linker	UNP P0AEX9
C	252	THR	-	linker	UNP P0AEX9
C	253	ASP	-	linker	UNP P0AEX9
C	254	TYR	-	linker	UNP P0AEX9
C	255	ASP	-	linker	UNP P0AEX9
C	256	ILE	-	linker	UNP P0AEX9
C	257	PRO	-	linker	UNP P0AEX9
C	258	THR	-	linker	UNP P0AEX9
C	259	THR	-	linker	UNP P0AEX9
C	260	LEU	-	linker	UNP P0AEX9
C	261	GLU	-	linker	UNP P0AEX9
C	262	VAL	-	linker	UNP P0AEX9
C	263	LEU	-	linker	UNP P0AEX9
C	264	PHE	-	linker	UNP P0AEX9
C	265	GLN	-	linker	UNP P0AEX9
C	266	GLY	-	linker	UNP P0AEX9
C	267	PRO	-	linker	UNP P0AEX9
C	268	LEU	-	linker	UNP P0AEX9
C	269	GLY	-	linker	UNP P0AEX9
C	270	SER	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Recombination activating gene 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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 Forward strand of 12-RSS substrate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	E	50	Total	C	N	O	P	0	0
			1023	486	192	295	50		

- Molecule 4 is a DNA chain called Reverse strand of 12-RSS substrate DNA.

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
6	A	2	Total	Ca	0
			2	2	

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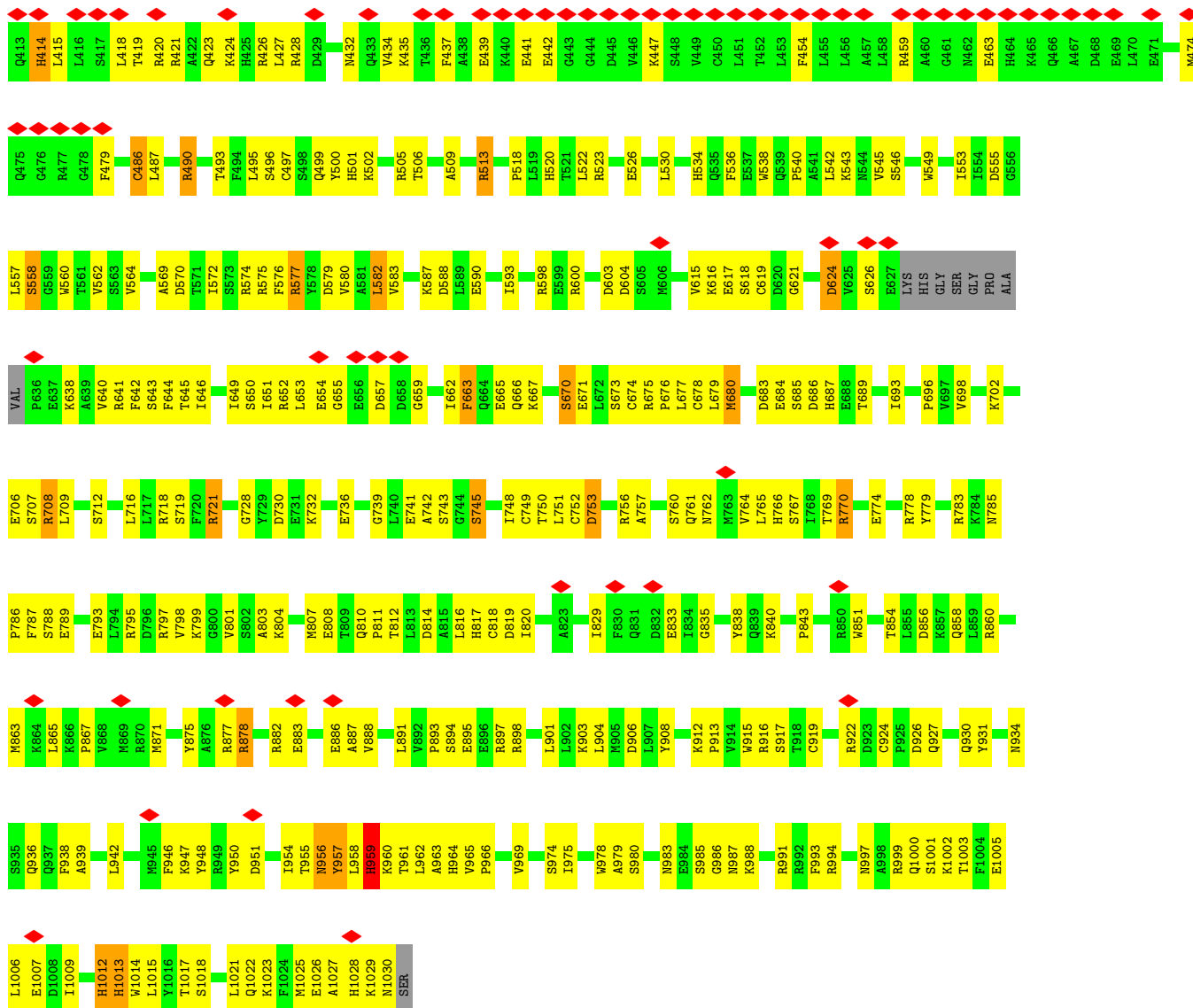
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
6	C	2	Total 2	Ca 2	0

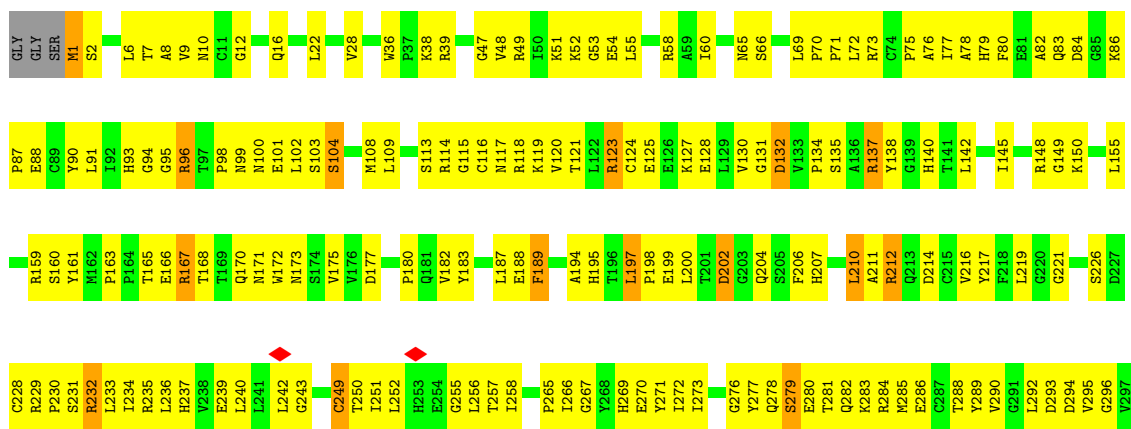
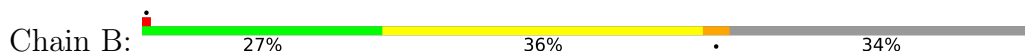




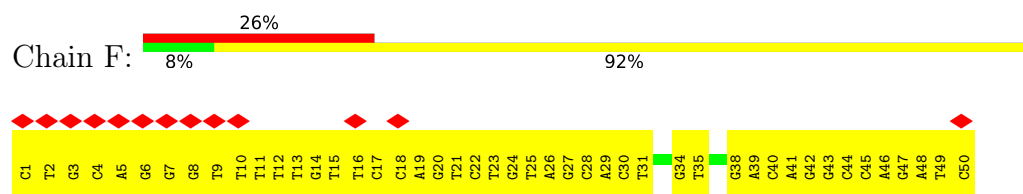




• Molecule 2: Recombination activating gene 2







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48851	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 ( $e^-/\text{\AA}^2$ )	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.053	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.39	3/5049 (0.1%)	0.71	11/6789 (0.2%)
1	C	0.34	1/5081 (0.0%)	0.75	18/6829 (0.3%)
2	B	0.32	0/2784	0.53	1/3784 (0.0%)
2	D	0.30	0/2784	0.69	6/3784 (0.2%)
3	E	0.65	0/1148	0.91	0/1768
4	F	0.68	0/1150	1.01	0/1774
All	All	0.40	4/17996 (0.0%)	0.74	36/24728 (0.1%)

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	2
1	C	0	4
2	D	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	517	GLN	CD-NE2	10.41	1.58	1.32
1	A	517	GLN	CD-OE1	-9.68	1.02	1.24
1	A	517	GLN	CB-CG	-7.15	1.33	1.52
1	C	1012	HIS	CG-CD2	5.34	1.44	1.35

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	GLN	CG-CD-OE1	29.00	179.59	121.60
1	C	1012	HIS	CB-CG-ND1	18.21	168.72	123.20
2	D	237	HIS	CB-CG-ND1	15.46	161.84	123.20
1	C	414	HIS	CB-CA-C	14.50	139.41	110.40
1	C	1012	HIS	ND1-CG-CD2	-14.13	86.22	106.00
1	A	517	GLN	CG-CD-NE2	-13.94	83.23	116.70
1	A	1028	HIS	CB-CG-ND1	13.14	156.05	123.20
1	C	1012	HIS	CB-CG-CD2	-13.01	90.48	130.80
1	C	959	HIS	CB-CA-C	-12.81	84.77	110.40
1	A	517	GLN	CA-CB-CG	12.64	141.21	113.40
2	D	237	HIS	CB-CG-CD2	-12.60	91.75	130.80
1	C	959	HIS	CB-CG-CD2	-12.28	92.73	130.80
1	A	1028	HIS	CB-CG-CD2	-11.79	94.25	130.80
1	C	959	HIS	CB-CG-ND1	11.65	152.32	123.20
1	A	517	GLN	OE1-CD-NE2	-11.01	96.59	121.90
1	C	1012	HIS	N-CA-CB	10.66	129.79	110.60
2	D	237	HIS	ND1-CG-CD2	-10.32	91.56	106.00
1	C	1012	HIS	CG-ND1-CE1	10.31	122.63	108.20
1	C	414	HIS	ND1-CG-CD2	-10.23	91.68	106.00
1	A	1028	HIS	ND1-CG-CD2	-9.86	92.20	106.00
2	B	200	LEU	CB-CG-CD2	-8.79	96.06	111.00
1	C	959	HIS	ND1-CG-CD2	-8.77	93.72	106.00
1	C	1012	HIS	CA-CB-CG	-8.44	99.25	113.60
1	C	414	HIS	N-CA-CB	-8.13	95.96	110.60
2	D	214	ASP	CB-CG-OD1	7.88	125.39	118.30
1	A	1028	HIS	CB-CA-C	7.72	125.85	110.40
2	D	237	HIS	CG-ND1-CE1	7.65	118.91	108.20
1	C	414	HIS	CA-C-N	-6.48	102.95	117.20
2	D	237	HIS	N-CA-CB	6.38	122.08	110.60
1	A	516	PHE	C-N-CA	-6.21	106.17	121.70
1	A	1028	HIS	CG-ND1-CE1	5.82	116.35	108.20
1	C	959	HIS	N-CA-CB	5.54	120.56	110.60
1	C	414	HIS	ND1-CE1-NE2	-5.50	97.80	109.90
1	C	959	HIS	N-CA-C	-5.32	96.64	111.00
1	A	1028	HIS	CA-C-N	-5.16	105.86	117.20
1	C	959	HIS	CG-ND1-CE1	5.14	115.39	108.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1028	HIS	Sidechain,Mainchain
1	C	1012	HIS	Sidechain

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Mol	Chain	Res	Type	Group
1	C	414	HIS	Sidechain,Mainchain
1	C	959	HIS	Sidechain
2	D	237	HIS	Sidechain

## 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	4954	0	4918	298	0
1	C	4980	0	4948	288	0
2	B	2714	0	2665	204	0
2	D	2714	0	2665	147	0
3	E	1023	0	561	73	0
4	F	1027	0	566	80	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
All	All	17418	0	16323	1003	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 30.

All (1003) 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)
2:D:86:LYS:NZ	2:D:125:GLU:OE2	1.79	1.13
1:C:435:LYS:NZ	1:C:439:GLU:OE2	1.81	1.12
1:A:638:LYS:NZ	1:A:683:ASP:OD2	1.85	1.10
2:B:76:ALA:HB3	2:B:93:HIS:O	1.53	1.07
2:D:159:ARG:NH1	2:D:205:SER:OG	1.87	1.07
1:C:1023:LYS:O	1:C:1027:ALA:N	1.88	1.05
1:A:641:ARG:NH1	1:A:983:ASN:O	1.91	1.04
1:C:410:ARG:NH1	3:E:41:DA:N3	2.07	1.02
2:D:338:THR:HG22	2:D:340:PRO:HA	1.43	1.01
1:A:860:ARG:O	1:A:860:ARG:NH1	1.95	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:GLU:OE2	2:B:344:HIS:ND1	1.97	0.97
2:B:86:LYS:NZ	2:B:87:PRO:O	1.96	0.97
1:C:641:ARG:NH1	1:C:987:ASN:OD1	1.97	0.97
1:C:778:ARG:NH1	1:C:798:VAL:O	1.98	0.97
2:B:1:MET:HA	2:B:349:SER:O	1.63	0.96
2:D:1:MET:HA	2:D:349:SER:O	1.65	0.96
1:A:412:ARG:NH1	1:C:441:GLU:O	1.99	0.95
1:C:675:ARG:NH1	1:C:1014:TRP:O	1.99	0.94
2:D:167:ARG:NH1	2:D:172:TRP:O	1.99	0.94
1:C:745:SER:O	1:C:756:ARG:NH1	2.00	0.94
1:C:575:ARG:NH1	1:C:576:PHE:O	2.01	0.93
1:A:435:LYS:NZ	1:A:439:GLU:OE2	2.02	0.93
1:A:573:SER:O	1:A:574:ARG:NH1	2.01	0.92
1:A:846:GLU:OE2	1:A:850:ARG:NH2	2.03	0.92
1:A:840:LYS:NZ	1:A:842:ASN:O	2.03	0.92
1:A:575:ARG:NH1	1:A:576:PHE:O	2.03	0.92
2:B:226:SER:HG	2:B:228:CYS:HG	1.07	0.90
3:E:9:DC:N3	4:F:42:DG:N1	2.20	0.90
1:C:814:ASP:OD2	1:C:817:HIS:ND1	2.04	0.90
1:C:882:ARG:NH1	1:C:886:GLU:OE2	2.03	0.90
1:C:665:GLU:OE2	1:C:667:LYS:N	2.07	0.88
1:A:626:SER:O	1:A:994:ARG:NH1	2.07	0.88
1:A:789:GLU:OE2	1:A:797:ARG:NH2	2.06	0.87
1:A:756:ARG:NH1	1:A:954:ILE:O	2.07	0.87
1:C:778:ARG:NH1	1:C:799:LYS:HB2	1.89	0.87
1:A:577:ARG:NH1	2:B:170:GLN:OE1	2.06	0.87
1:C:424:LYS:NZ	3:E:33:DG:OP1	2.07	0.87
1:A:479:PHE:HA	1:A:513:ARG:HH11	1.40	0.86
1:A:738:GLU:OE2	1:A:775:ASN:ND2	2.09	0.86
2:B:39:ARG:NH1	4:F:40:DC:OP2	2.09	0.86
2:B:339:PRO:HB2	2:B:341:GLU:OE1	1.76	0.86
3:E:37:DC:O2	4:F:14:DG:N2	2.09	0.86
2:B:128:GLU:OE2	2:B:130:VAL:HG23	1.76	0.85
1:C:877:ARG:HE	1:C:916:ARG:HH12	1.20	0.85
1:C:749:CYS:HA	1:C:960:LYS:HZ3	1.42	0.84
1:A:566:ASP:OD2	2:B:138:TYR:OH	1.96	0.83
1:C:774:GLU:OE2	1:C:778:ARG:NE	2.09	0.83
1:C:671:GLU:OE2	1:C:985:SER:OG	1.95	0.83
2:B:123:ARG:NH2	2:B:125:GLU:OE2	2.12	0.83
1:C:783:ARG:O	2:D:67:SER:OG	1.96	0.83
1:A:727:THR:HG21	1:A:978:TRP:HB3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:LYS:NZ	4:F:38:DG:OP1	2.12	0.82
1:A:713:VAL:HG13	1:A:718:ARG:HD2	1.61	0.82
1:A:882:ARG:HH12	1:A:906:ASP:CG	1.83	0.82
1:C:598:ARG:NH2	1:C:604:ASP:OD2	2.12	0.82
1:C:956:ASN:O	1:C:960:LYS:HG2	1.79	0.81
2:B:284:ARG:NE	2:B:286:GLU:OE2	2.12	0.81
1:C:520:HIS:NE2	4:F:23:DT:OP2	2.14	0.81
1:C:778:ARG:HH12	1:C:799:LYS:HB2	1.41	0.80
1:C:789:GLU:OE2	1:C:797:ARG:NH2	2.13	0.80
3:E:9:DC:O2	4:F:42:DG:N2	2.13	0.80
2:B:165:THR:OG1	2:B:166:GLU:OE2	1.98	0.80
1:C:575:ARG:HH12	1:C:577:ARG:HA	1.44	0.80
2:B:277:TYR:OH	2:B:317:TRP:N	2.15	0.79
1:C:931:TYR:OH	1:C:961:THR:O	2.00	0.79
1:C:770:ARG:NH2	1:C:799:LYS:O	2.15	0.79
2:B:258:ILE:HD13	2:B:284:ARG:HH11	1.45	0.79
1:C:1006:LEU:HA	1:C:1009:ILE:HG22	1.64	0.78
2:D:167:ARG:HE	2:D:172:TRP:HA	1.48	0.78
2:B:277:TYR:HH	2:B:317:TRP:H	1.31	0.77
1:C:1026:GLU:HA	1:C:1029:LYS:HE3	1.66	0.77
2:D:218:PHE:HB2	2:D:234:ILE:HB	1.67	0.77
3:E:9:DC:N4	4:F:42:DG:O6	2.17	0.76
1:A:486:CYS:SG	1:A:500:TYR:OH	2.44	0.76
2:D:152:ALA:HB2	2:D:240:LEU:HD21	1.67	0.76
1:A:465:LYS:NZ	4:F:23:DT:OP1	2.19	0.76
1:A:903:LYS:HZ3	1:A:907:LEU:HD11	1.51	0.75
2:D:86:LYS:HZ1	2:D:123:ARG:HD3	1.50	0.75
1:A:447:LYS:NZ	1:C:463:GLU:OE2	2.12	0.75
1:C:877:ARG:NE	1:C:916:ARG:HH12	1.85	0.74
2:B:65:ASN:O	2:B:123:ARG:NH1	2.21	0.74
2:B:235:ARG:HB3	2:B:250:THR:HG23	1.69	0.74
1:A:590:GLU:OE2	1:A:714:GLY:N	2.15	0.74
1:A:735:ARG:HH11	1:A:735:ARG:HB3	1.52	0.74
2:B:58:ARG:NH1	2:B:118:ARG:O	2.20	0.74
2:D:331:ILE:O	2:D:343:TYR:HA	1.87	0.74
1:A:897:ARG:HH12	1:A:948:TYR:HE2	1.34	0.73
2:D:43:THR:HG22	2:D:45:ILE:H	1.54	0.73
1:C:1023:LYS:O	1:C:1027:ALA:CB	2.37	0.73
2:B:167:ARG:NH2	2:B:172:TRP:O	2.22	0.73
1:C:486:CYS:HG	1:C:500:TYR:HH	1.34	0.73
2:D:50:ILE:HD12	2:D:322:LEU:HD11	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:LEU:HD21	2:B:347:GLN:HB2	1.69	0.72
3:E:29:DG:N2	4:F:23:DT:O2	2.22	0.72
2:B:281:THR:HG22	2:B:315:ARG:HH12	1.55	0.72
1:A:903:LYS:NZ	1:A:907:LEU:HD11	2.03	0.72
2:B:114:ARG:HB2	2:B:120:VAL:HG13	1.72	0.72
1:C:501:HIS:CE1	1:C:505:ARG:HH11	2.07	0.72
1:A:553:ILE:HG13	1:A:576:PHE:HE1	1.55	0.72
1:C:523:ARG:HH12	3:E:25:DT:H71	1.53	0.72
1:A:485:VAL:HG12	1:A:1024:PHE:HB3	1.71	0.72
2:B:281:THR:HG22	2:B:315:ARG:NH1	2.04	0.72
2:D:341:GLU:OE2	2:D:343:TYR:N	2.23	0.71
2:B:283:LYS:NZ	2:B:314:SER:O	2.23	0.71
1:A:892:VAL:O	1:A:898:ARG:NH2	2.23	0.71
1:C:760:SER:HB2	1:C:954:ILE:HD11	1.72	0.71
1:C:518:PRO:CG	1:C:520:HIS:CE1	2.73	0.71
1:C:616:LYS:NZ	1:C:979:ALA:O	2.24	0.71
2:D:99:ASN:O	2:D:101:GLU:N	2.23	0.71
2:B:72:LEU:HB3	2:B:95:GLY:HA3	1.72	0.70
3:E:34:DG:O6	4:F:17:DC:N4	2.25	0.70
2:B:188:GLU:OE2	2:B:189:PHE:HD1	1.73	0.70
1:C:749:CYS:SG	1:C:752:CYS:N	2.59	0.70
2:D:339:PRO:HB2	2:D:341:GLU:H	1.57	0.70
2:B:219:LEU:HD21	2:B:256:LEU:HB3	1.73	0.70
2:D:22:LEU:HD11	2:D:92:ILE:HD11	1.74	0.70
1:A:585:ALA:HB2	1:A:675:ARG:HH12	1.57	0.70
3:E:8:DC:OP2	3:E:8:DC:H6	1.74	0.69
1:C:486:CYS:SG	1:C:500:TYR:OH	2.48	0.69
2:B:51:LYS:HB3	2:B:52:LYS:HE2	1.74	0.69
1:C:518:PRO:HG2	1:C:520:HIS:CE1	2.28	0.69
2:B:142:LEU:HD12	2:B:155:LEU:HB2	1.74	0.69
2:B:96:ARG:NH2	2:B:100:ASN:OD1	2.25	0.69
4:F:42:DG:H2'	4:F:43:DG:OP2	1.92	0.69
1:A:548:SER:OG	1:A:550:ASP:OD1	2.10	0.69
1:A:885:VAL:HG21	1:A:905:MET:HG2	1.75	0.69
1:A:908:TYR:O	1:A:912:LYS:HB3	1.93	0.69
1:A:756:ARG:HD2	1:A:954:ILE:H	1.58	0.68
1:A:651:ILE:HD11	1:A:653:LEU:HB2	1.75	0.68
1:A:849:ARG:O	1:A:849:ARG:NH2	2.27	0.68
1:C:687:HIS:NE2	1:C:736:GLU:O	2.25	0.68
4:F:21:DT:H2'	4:F:21:DT:OP2	1.93	0.68
1:A:683:ASP:OD1	1:A:684:GLU:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:GLU:CG	1:A:713:VAL:HG23	2.23	0.68
3:E:28:DA:OP2	3:E:28:DA:H8	1.77	0.68
2:B:281:THR:HA	2:B:315:ARG:HH22	1.59	0.68
1:C:858:GLN:NE2	1:C:887:ALA:O	2.26	0.68
2:B:66:SER:HA	2:B:123:ARG:HH11	1.59	0.67
1:C:762:ASN:ND2	1:C:765:LEU:HB3	2.09	0.67
2:D:212:ARG:HH11	2:D:269:HIS:CE1	2.12	0.67
1:A:590:GLU:HG3	1:A:713:VAL:HG23	1.77	0.67
1:A:737:MET:HB3	1:A:807:MET:HB3	1.76	0.67
2:B:272:ILE:HG22	2:B:289:TYR:HB2	1.77	0.67
1:C:523:ARG:HH22	3:E:24:DC:H6	1.43	0.67
1:C:730:ASP:OD2	1:C:732:LYS:HB3	1.95	0.67
1:C:958:LEU:O	1:C:962:LEU:HG	1.93	0.67
2:D:308:THR:HG22	2:D:310:GLU:H	1.59	0.67
1:A:961:THR:HA	1:A:965:VAL:HG23	1.77	0.67
4:F:10:DT:H2"	4:F:11:DT:OP2	1.95	0.67
1:A:913:PRO:HA	1:A:916:ARG:HB3	1.78	0.66
1:C:954:ILE:HG22	1:C:955:THR:H	1.60	0.66
2:D:314:SER:OG	2:D:316:THR:O	2.11	0.66
1:C:749:CYS:HA	1:C:960:LYS:NZ	2.10	0.66
1:C:624:ASP:OD1	1:C:991:ARG:NH1	2.28	0.66
1:A:555:ASP:HB2	1:A:557:LEU:HD12	1.78	0.66
1:A:762:ASN:HD21	1:A:765:LEU:HB3	1.59	0.66
1:A:836:GLU:OE1	1:A:839:GLN:N	2.26	0.66
1:C:762:ASN:HD21	1:C:765:LEU:HB3	1.60	0.66
1:C:901:LEU:HA	1:C:904:LEU:HB3	1.78	0.66
2:B:309:SER:O	2:B:313:HIS:ND1	2.29	0.66
1:C:490:ARG:NH1	1:C:497:CYS:SG	2.69	0.66
4:F:43:DG:OP2	4:F:43:DG:H8	1.78	0.66
1:A:748:ILE:HD12	1:A:749:CYS:H	1.60	0.66
1:A:641:ARG:NH1	1:A:987:ASN:OD1	2.16	0.66
1:A:778:ARG:HH21	1:A:799:LYS:HB2	1.61	0.65
1:C:706:GLU:N	1:C:706:GLU:OE1	2.29	0.65
2:D:273:ILE:HG22	2:D:275:GLY:H	1.61	0.65
1:A:441:GLU:O	1:C:412:ARG:NH1	2.29	0.65
1:A:997:ASN:OD1	1:A:1012:HIS:NE2	2.29	0.65
2:B:76:ALA:CB	2:B:93:HIS:O	2.40	0.65
2:B:267:GLY:H	2:B:270:GLU:HB2	1.62	0.65
1:A:609:SER:H	1:A:653:LEU:HD12	1.62	0.65
2:B:150:LYS:HG3	2:B:240:LEU:HD23	1.79	0.65
1:C:641:ARG:NH1	1:C:983:ASN:O	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:24:DG:OP2	4:F:24:DG:H8	1.79	0.64
1:A:882:ARG:HH21	1:A:902:LEU:HB3	1.62	0.64
2:D:183:TYR:HA	2:D:193:THR:O	1.97	0.64
2:B:279:SER:OG	2:B:282:GLN:N	2.31	0.64
1:C:865:LEU:HG	1:C:878:ARG:NH1	2.13	0.64
1:A:479:PHE:HA	1:A:513:ARG:NH1	2.12	0.64
2:B:2:SER:HA	2:B:305:PRO:HB3	1.79	0.64
1:C:496:SER:OG	3:E:23:DG:OP2	2.09	0.64
2:D:99:ASN:HB3	2:D:101:GLU:OE2	1.97	0.64
2:D:290:VAL:HG22	2:D:299:MET:HB2	1.80	0.64
2:D:97:THR:OG1	2:D:99:ASN:O	2.12	0.64
1:C:1022:GLN:HA	1:C:1025:MET:HG2	1.78	0.63
4:F:18:DC:H2'	4:F:19:DA:C8	2.33	0.63
1:A:1020:TYR:HD1	1:A:1021:LEU:HD12	1.62	0.63
2:B:323:GLY:O	2:B:326:THR:OG1	2.14	0.63
1:A:833:GLU:OE2	1:A:897:ARG:NH1	2.32	0.63
1:A:860:ARG:NH1	1:A:864:LYS:HA	2.13	0.63
1:C:877:ARG:HH21	1:C:916:ARG:NH1	1.97	0.63
2:B:278:GLN:HB3	2:B:284:ARG:NH1	2.14	0.63
2:D:238:VAL:HG12	2:D:247:LEU:HG	1.80	0.63
2:B:322:LEU:H	2:B:327:ALA:HA	1.64	0.63
1:C:789:GLU:HB3	1:C:793:GLU:HG3	1.81	0.63
2:D:102:LEU:HB2	2:D:136:ALA:HB1	1.80	0.63
2:D:256:LEU:HD21	2:D:284:ARG:HH12	1.64	0.63
2:D:284:ARG:NE	2:D:286:GLU:O	2.30	0.63
2:B:310:GLU:OE1	2:B:346:TYR:OH	2.17	0.62
1:C:638:LYS:NZ	1:C:683:ASP:OD2	2.21	0.62
2:D:157:GLY:HA3	2:D:207:HIS:HE1	1.63	0.62
1:C:665:GLU:OE2	1:C:666:GLN:N	2.33	0.62
1:C:1023:LYS:HB3	1:C:1027:ALA:HB2	1.81	0.62
2:D:150:LYS:HD3	2:D:240:LEU:HB3	1.81	0.62
4:F:11:DT:C6	4:F:12:DT:H72	2.34	0.62
1:A:672:LEU:O	1:A:1022:GLN:NE2	2.33	0.62
2:B:338:THR:HG22	2:B:340:PRO:HA	1.80	0.62
2:D:284:ARG:NH2	2:D:288:THR:OG1	2.33	0.62
1:A:878:ARG:NH1	1:A:878:ARG:HB2	2.15	0.62
1:C:651:ILE:HD11	1:C:653:LEU:HB2	1.82	0.62
1:C:487:LEU:HD13	1:C:522:LEU:HB3	1.82	0.61
1:A:430:LEU:HD21	1:C:434:VAL:HG13	1.82	0.61
1:A:665:GLU:OE2	1:A:667:LYS:N	2.25	0.61
2:B:278:GLN:HB3	2:B:284:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:ARG:HB2	1:C:426:ARG:HH12	1.64	0.61
1:C:493:THR:HG23	1:C:495:LEU:HG	1.82	0.61
1:C:418:LEU:HB2	1:C:423:GLN:HG3	1.82	0.61
1:C:555:ASP:OD2	1:C:557:LEU:HD23	2.01	0.61
2:D:137:ARG:NE	2:D:178:CYS:SG	2.73	0.61
1:C:748:ILE:O	1:C:960:LYS:NZ	2.30	0.61
2:B:16:GLN:NE2	2:B:73:ARG:HG3	2.15	0.61
1:A:835:GLY:HA3	1:A:851:TRP:CE2	2.35	0.60
2:B:293:ASP:OD1	2:B:294:ASP:N	2.34	0.60
2:B:331:ILE:O	2:B:343:TYR:HA	2.01	0.60
1:A:688:GLU:OE2	2:B:16:GLN:NE2	2.33	0.60
1:C:942:LEU:O	1:C:947:LYS:N	2.34	0.60
1:C:955:THR:HG1	1:C:957:TYR:HD1	1.49	0.60
1:C:562:VAL:HG23	1:C:569:ALA:HB3	1.82	0.60
2:D:226:SER:OG	2:D:228:CYS:SG	2.59	0.60
1:A:558:SER:OG	2:B:173:ASN:N	2.33	0.60
1:C:675:ARG:NH1	1:C:1014:TRP:CD2	2.69	0.60
3:E:19:DC:H4'	3:E:20:DA:H5'	1.82	0.60
3:E:26:DA:H2''	3:E:27:DC:OP2	2.00	0.60
2:B:293:ASP:HB3	2:B:296:GLY:H	1.67	0.60
2:D:4:GLN:OE1	2:D:347:GLN:NE2	2.34	0.60
3:E:25:DT:H2''	3:E:26:DA:OP2	2.00	0.60
4:F:20:DG:H2'	4:F:21:DT:C6	2.37	0.60
1:C:955:THR:OG1	1:C:957:TYR:HD1	1.85	0.59
1:C:502:LYS:O	1:C:506:THR:OG1	2.19	0.59
1:C:958:LEU:O	1:C:961:THR:HG22	2.01	0.59
1:C:1018:SER:HB3	1:C:1021:LEU:HD13	1.83	0.59
1:A:779:TYR:CE2	1:A:804:LYS:HB2	2.37	0.59
1:C:728:GLY:HA2	1:C:980:SER:HB3	1.83	0.59
1:C:745:SER:C	1:C:756:ARG:HH11	2.06	0.59
1:C:752:CYS:SG	1:C:753:ASP:N	2.74	0.59
3:E:26:DA:OP2	3:E:26:DA:H8	1.86	0.59
1:A:863:MET:HG3	1:A:884:ALA:HA	1.84	0.59
1:A:753:ASP:HA	1:A:770:ARG:HH21	1.67	0.59
1:C:788:SER:HB2	2:D:65:ASN:HA	1.82	0.59
2:B:160:SER:C	2:B:175:VAL:HG23	2.23	0.59
1:C:741:GLU:CD	1:C:795:ARG:HH11	2.04	0.59
2:D:308:THR:HB	2:D:311:ILE:HG22	1.84	0.59
2:B:28:VAL:HG13	2:B:48:VAL:HB	1.85	0.59
1:C:546:SER:O	1:C:577:ARG:NH2	2.35	0.59
1:C:969:VAL:HG12	1:C:975:ILE:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:ARG:NH1	2:D:58:ARG:HD3	2.18	0.58
3:E:36:DA:H2''	3:E:37:DC:OP2	2.01	0.58
1:A:620:ASP:OD1	1:A:621:GLY:N	2.37	0.58
1:C:540:PRO:HD2	1:C:707:SER:HA	1.85	0.58
2:D:1:MET:HB3	2:D:305:PRO:HG3	1.84	0.58
2:D:132:ASP:OD2	2:D:193:THR:HA	2.03	0.58
1:A:713:VAL:HG13	1:A:718:ARG:CD	2.32	0.58
1:A:773:ASP:OD1	1:A:773:ASP:N	2.36	0.58
2:B:232:ARG:HA	2:B:255:GLY:N	2.19	0.58
1:A:538:TRP:CD2	1:A:542:LEU:HD21	2.38	0.58
1:A:571:THR:HG21	1:A:682:VAL:HG13	1.86	0.58
1:A:1011:LYS:O	1:A:1015:LEU:HG	2.04	0.58
2:B:283:LYS:HD2	2:B:317:TRP:HE1	1.67	0.58
2:D:249:CYS:SG	2:D:250:THR:N	2.76	0.58
1:A:578:TYR:HH	1:A:724:PHE:HE2	1.52	0.58
2:B:78:ALA:HB3	2:B:91:LEU:HB2	1.86	0.58
1:C:587:LYS:NZ	1:C:712:SER:O	2.36	0.58
3:E:1:DG:H2''	3:E:2:DA:N7	2.18	0.58
1:A:590:GLU:CD	1:A:713:VAL:HG23	2.24	0.58
2:B:132:ASP:OD2	2:B:194:ALA:N	2.28	0.58
2:B:66:SER:HB3	2:B:123:ARG:HB2	1.85	0.58
1:C:741:GLU:OE1	1:C:795:ARG:NH1	2.22	0.58
4:F:28:DC:H2''	4:F:29:DA:N7	2.19	0.58
1:C:893:PRO:O	1:C:898:ARG:NH2	2.34	0.57
3:E:9:DC:H2''	3:E:10:DT:OP2	2.04	0.57
1:C:1023:LYS:O	1:C:1027:ALA:HB3	2.04	0.57
4:F:11:DT:H2''	4:F:12:DT:OP2	2.04	0.57
4:F:23:DT:H2''	4:F:24:DG:C8	2.39	0.57
1:A:585:ALA:CB	1:A:675:ARG:HH12	2.17	0.57
2:B:249:CYS:SG	2:B:250:THR:N	2.75	0.57
1:C:520:HIS:NE2	4:F:23:DT:P	2.77	0.57
1:C:751:LEU:HD12	1:C:964:HIS:CG	2.40	0.57
2:D:96:ARG:NH1	2:D:138:TYR:CZ	2.69	0.57
1:C:938:PHE:O	1:C:942:LEU:HG	2.04	0.57
1:C:795:ARG:NH1	2:D:39:ARG:NH1	2.52	0.57
1:A:872:ASN:OD1	3:E:18:DA:N6	2.38	0.57
2:B:284:ARG:NH1	2:B:284:ARG:HB2	2.20	0.57
3:E:38:DA:H2''	3:E:39:DA:H8	1.70	0.57
2:D:282:GLN:NE2	2:D:283:LYS:O	2.37	0.57
1:A:676:PRO:HG3	1:A:1013:HIS:CD2	2.40	0.57
1:A:912:LYS:HG3	1:A:913:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:PRO:HG2	2:B:98:PRO:HG3	1.86	0.57
2:D:159:ARG:HH12	2:D:206:PHE:HD2	1.53	0.57
1:A:774:GLU:OE2	1:A:778:ARG:NH1	2.37	0.56
1:A:895:GLU:OE2	1:A:898:ARG:NH2	2.37	0.56
1:C:709:LEU:O	1:C:719:SER:HA	2.05	0.56
1:C:877:ARG:HE	1:C:916:ARG:NH1	1.97	0.56
2:D:47:GLY:H	2:D:60:ILE:HD11	1.69	0.56
1:C:575:ARG:NH1	1:C:577:ARG:HA	2.18	0.56
1:C:999:ARG:N	1:C:1000:GLN:HA	2.20	0.56
2:D:159:ARG:NH1	2:D:206:PHE:HD2	2.03	0.56
4:F:24:DG:H2''	4:F:25:DT:OP2	2.04	0.56
1:A:439:GLU:HA	1:A:444:GLY:H	1.70	0.56
1:A:534:HIS:CE1	1:A:587:LYS:NZ	2.74	0.56
1:C:750:THR:H	1:C:960:LYS:NZ	2.03	0.56
2:B:117:ASN:HB3	3:E:6:DG:H5''	1.87	0.56
2:B:148:ARG:N	2:B:149:GLY:HA2	2.21	0.56
2:D:33:GLN:NE2	2:D:35:GLY:O	2.39	0.56
2:D:269:HIS:HB3	2:D:292:LEU:HG	1.88	0.56
1:A:612:THR:N	1:A:650:SER:O	2.34	0.56
1:A:862:LYS:NZ	1:A:862:LYS:HB3	2.20	0.56
1:A:795:ARG:CZ	2:B:39:ARG:NH1	2.69	0.56
4:F:34:DG:H2''	4:F:35:DT:OP2	2.06	0.56
1:A:735:ARG:HH12	1:A:741:GLU:C	2.08	0.56
2:B:7:THR:N	2:B:53:GLY:O	2.38	0.56
2:B:168:THR:HG22	2:B:170:GLN:H	1.70	0.56
1:C:757:ALA:O	1:C:761:GLN:N	2.38	0.56
1:C:930:GLN:O	1:C:934:ASN:ND2	2.34	0.56
2:D:272:ILE:HD11	2:D:287:CYS:HB2	1.88	0.56
1:A:502:LYS:O	1:A:506:THR:OG1	2.19	0.56
1:C:603:ASP:OD1	1:C:604:ASP:N	2.39	0.56
1:A:687:HIS:HD2	2:B:36:TRP:CD1	2.24	0.56
2:B:51:LYS:O	2:B:54:GLU:HB2	2.05	0.56
1:C:687:HIS:CD2	1:C:736:GLU:HG2	2.41	0.56
1:A:653:LEU:HD22	1:A:654:GLU:HA	1.89	0.55
2:B:273:ILE:HB	2:B:288:THR:OG1	2.05	0.55
4:F:2:DT:H2'	4:F:3:DG:C8	2.41	0.55
1:A:553:ILE:HG21	1:A:1007:GLU:HG3	1.88	0.55
2:B:221:GLY:HA2	2:B:258:ILE:O	2.06	0.55
2:D:330:ALA:HB1	2:D:343:TYR:HB3	1.89	0.55
2:D:339:PRO:HB2	2:D:341:GLU:N	2.21	0.55
3:E:41:DA:H8	3:E:41:DA:OP2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:ARG:NH1	2:B:39:ARG:NH1	2.55	0.55
1:A:590:GLU:O	1:A:593:ILE:HG13	2.05	0.55
2:B:317:TRP:HB3	2:B:331:ILE:HD13	1.89	0.55
1:C:687:HIS:HD2	1:C:736:GLU:HG2	1.71	0.55
2:D:77:ILE:HG23	2:D:90:TYR:HE1	1.72	0.55
2:D:278:GLN:HB2	2:D:284:ARG:HB2	1.89	0.55
3:E:27:DC:H2''	3:E:28:DA:C8	2.41	0.55
2:B:219:LEU:HD11	2:B:256:LEU:N	2.21	0.55
2:D:231:SER:O	2:D:255:GLY:N	2.34	0.55
1:A:509:ALA:HB1	1:C:1028:HIS:HB3	1.87	0.55
2:B:49:ARG:NH1	2:B:58:ARG:HB3	2.21	0.55
1:C:583:VAL:HG12	1:C:709:LEU:HD21	1.88	0.55
1:C:795:ARG:HH12	2:D:39:ARG:NH1	2.04	0.55
2:B:234:ILE:HD12	2:B:251:ILE:HA	1.89	0.55
1:C:577:ARG:HG3	1:C:579:ASP:OD1	2.06	0.55
1:C:619:CYS:HB3	1:C:642:PHE:HD1	1.72	0.55
2:D:156:PHE:HB2	2:D:182:VAL:HG12	1.88	0.55
1:A:558:SER:OG	1:A:558:SER:O	2.21	0.55
2:B:312:SER:OG	2:B:313:HIS:ND1	2.40	0.55
4:F:25:DT:H2''	4:F:26:DA:H8	1.72	0.55
1:C:621:GLY:HA2	1:C:640:VAL:HA	1.88	0.55
3:E:3:DT:H2''	3:E:4:DC:C5	2.42	0.55
3:E:41:DA:OP2	3:E:41:DA:H2'	2.07	0.55
1:C:807:MET:SD	1:C:808:GLU:N	2.80	0.54
1:A:585:ALA:HB2	1:A:675:ARG:NH1	2.20	0.54
2:B:134:PRO:HA	2:B:183:TYR:CZ	2.43	0.54
1:C:683:ASP:OD1	1:C:684:GLU:N	2.40	0.54
1:A:540:PRO:HD2	1:A:707:SER:HA	1.89	0.54
1:A:534:HIS:CE1	1:A:587:LYS:HZ2	2.25	0.54
2:B:163:PRO:HB2	2:B:166:GLU:OE2	2.08	0.54
2:B:300:GLU:OE2	2:B:302:ARG:HG2	2.07	0.54
1:C:420:ARG:HA	1:C:423:GLN:HB2	1.89	0.54
1:A:748:ILE:HD12	1:A:749:CYS:N	2.23	0.54
2:B:233:LEU:HB3	2:B:252:LEU:HD23	1.89	0.54
1:A:555:ASP:OD1	1:A:555:ASP:N	2.40	0.54
1:A:811:PRO:HG2	1:A:971:ARG:HH12	1.72	0.54
1:C:553:ILE:HG13	1:C:576:PHE:HE1	1.71	0.54
1:C:557:LEU:O	2:D:173:ASN:ND2	2.40	0.54
2:D:229:ARG:HH12	2:D:280:GLU:N	2.06	0.54
2:B:118:ARG:NH1	4:F:48:DA:O3'	2.40	0.54
1:C:518:PRO:HB2	1:C:520:HIS:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:PHE:CE1	1:C:549:TRP:HB2	2.43	0.54
2:D:94:GLY:H	2:D:140:HIS:CE1	2.26	0.54
1:C:574:ARG:NH2	1:C:1003:THR:O	2.41	0.54
1:A:831:GLN:NE2	1:A:848:ARG:O	2.41	0.53
1:C:590:GLU:HA	1:C:593:ILE:HG22	1.90	0.53
4:F:13:DT:H4'	4:F:14:DG:OP1	2.06	0.53
4:F:25:DT:H2''	4:F:26:DA:C8	2.43	0.53
1:A:823:ALA:HB1	1:A:879:LEU:HD23	1.89	0.53
1:C:412:ARG:HB2	1:C:426:ARG:NH1	2.23	0.53
1:C:858:GLN:HE21	1:C:888:VAL:HA	1.74	0.53
2:D:265:PRO:HB3	2:D:271:TYR:CE2	2.42	0.53
4:F:17:DC:H2''	4:F:18:DC:C6	2.43	0.53
1:A:508:LYS:HE3	1:A:514:GLN:HB2	1.91	0.53
1:A:840:LYS:HE3	1:A:847:GLU:OE2	2.08	0.53
1:A:980:SER:O	1:A:983:ASN:HB3	2.07	0.53
1:C:579:ASP:OD1	1:C:579:ASP:N	2.40	0.53
4:F:46:DA:H2''	4:F:47:DG:C8	2.44	0.53
1:A:603:ASP:OD1	1:A:605:SER:N	2.39	0.53
1:A:735:ARG:HB3	1:A:735:ARG:NH1	2.20	0.53
1:C:997:ASN:ND2	3:E:23:DG:OP1	2.42	0.53
2:B:212:ARG:NH1	2:B:293:ASP:HA	2.23	0.53
1:C:1023:LYS:O	1:C:1027:ALA:CA	2.57	0.53
1:C:955:THR:OG1	1:C:957:TYR:CD1	2.62	0.53
2:D:16:GLN:HB3	2:D:34:LYS:HZ3	1.74	0.53
2:B:257:THR:HG23	2:B:257:THR:O	2.09	0.53
2:B:286:GLU:OE1	2:B:286:GLU:N	2.40	0.53
1:C:650:SER:OG	1:C:651:ILE:N	2.42	0.53
3:E:3:DT:H2''	3:E:4:DC:C6	2.44	0.53
1:A:779:TYR:CZ	1:A:804:LYS:HB2	2.44	0.53
1:C:798:VAL:HG22	1:C:801:VAL:HB	1.91	0.53
4:F:7:DG:H2'	4:F:8:DG:C8	2.44	0.53
2:B:217:TYR:HB3	2:B:233:LEU:HD11	1.91	0.52
2:B:273:ILE:O	2:B:288:THR:OG1	2.19	0.52
1:C:671:GLU:OE2	1:C:986:GLY:N	2.43	0.52
2:B:47:GLY:N	2:B:60:ILE:HD11	2.24	0.52
1:C:871:MET:HG3	1:C:875:TYR:HB3	1.91	0.52
2:D:232:ARG:HD3	2:D:232:ARG:H	1.74	0.52
4:F:24:DG:OP2	4:F:24:DG:C8	2.62	0.52
2:B:104:SER:OG	2:B:134:PRO:O	2.28	0.52
1:A:747:TYR:HE2	1:A:799:LYS:HZ2	1.58	0.52
2:D:16:GLN:HB3	2:D:34:LYS:NZ	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:PHE:CA	1:A:513:ARG:HH11	2.19	0.52
1:C:683:ASP:OD1	1:C:685:SER:N	2.38	0.52
1:C:951:ASP:OD1	1:C:951:ASP:N	2.43	0.52
2:D:338:THR:CG2	2:D:340:PRO:HA	2.30	0.52
3:E:27:DC:OP2	3:E:27:DC:H6	1.93	0.52
1:A:613:VAL:HB	1:A:722:PHE:CD2	2.45	0.52
1:A:753:ASP:HB3	1:A:770:ARG:HE	1.75	0.52
2:B:232:ARG:HB2	2:B:252:LEU:O	2.09	0.52
1:C:644:PHE:O	1:C:675:ARG:HB2	2.10	0.52
1:C:974:SER:OG	1:C:975:ILE:N	2.43	0.52
4:F:38:DG:H2''	4:F:39:DA:OP2	2.09	0.52
2:B:113:SER:N	2:B:121:THR:OG1	2.38	0.51
1:C:650:SER:HA	1:C:662:ILE:HG13	1.91	0.51
1:C:863:MET:O	1:C:878:ARG:NH1	2.43	0.51
1:A:583:VAL:HG12	1:A:709:LEU:HD21	1.92	0.51
1:A:687:HIS:CG	1:A:736:GLU:OE2	2.63	0.51
1:A:863:MET:HE2	1:A:884:ALA:HB2	1.93	0.51
1:C:538:TRP:CZ3	1:C:709:LEU:HB2	2.45	0.51
2:D:230:PRO:HB2	2:D:232:ARG:CD	2.41	0.51
1:C:649:ILE:HG22	1:C:663:PHE:HD2	1.75	0.51
1:C:1029:LYS:O	1:C:1029:LYS:HG2	2.11	0.51
2:D:159:ARG:NH1	2:D:206:PHE:CD2	2.78	0.51
3:E:16:DA:H2''	3:E:17:DC:H5'	1.92	0.51
4:F:9:DT:H2'	4:F:10:DT:C6	2.45	0.51
1:A:926:ASP:OD1	1:A:926:ASP:N	2.43	0.51
2:B:96:ARG:NH2	2:B:161:TYR:OH	2.44	0.51
2:B:211:ALA:HB2	2:B:216:VAL:HG13	1.93	0.51
1:A:512:GLY:HA2	1:A:513:ARG:C	2.31	0.51
1:A:731:GLU:HG3	1:A:735:ARG:HD2	1.92	0.51
1:A:735:ARG:HH11	1:A:735:ARG:CB	2.21	0.51
1:A:778:ARG:HB2	1:A:801:VAL:HG11	1.93	0.51
2:B:226:SER:OG	2:B:228:CYS:SG	2.48	0.51
1:C:617:GLU:HA	1:C:644:PHE:HA	1.93	0.51
1:C:787:PHE:CE1	1:C:797:ARG:NH1	2.78	0.51
2:D:129:LEU:HB3	2:D:192:CYS:SG	2.50	0.51
1:A:671:GLU:OE1	1:A:671:GLU:N	2.43	0.51
1:A:834:ILE:HD12	1:A:891:LEU:HB2	1.92	0.51
2:D:206:PHE:HD1	2:D:260:SER:HB2	1.75	0.51
4:F:10:DT:H1'	4:F:11:DT:H5'	1.92	0.51
2:D:283:LYS:HD2	2:D:317:TRP:NE1	2.26	0.51
1:A:492:ASN:ND2	1:C:502:LYS:NZ	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:MET:O	1:A:598:ARG:HG3	2.10	0.51
1:C:751:LEU:HA	1:C:770:ARG:HB2	1.93	0.51
1:C:752:CYS:HB2	1:C:767:SER:O	2.11	0.51
3:E:5:DT:H1'	3:E:6:DG:C5	2.45	0.51
1:A:991:ARG:HH21	1:A:991:ARG:HB2	1.76	0.51
2:D:130:VAL:N	2:D:190:GLY:O	2.30	0.51
2:D:131:GLY:HA3	2:D:132:ASP:C	2.32	0.51
1:A:538:TRP:CZ3	1:A:709:LEU:HB2	2.46	0.50
1:A:546:SER:O	1:A:577:ARG:NH2	2.43	0.50
1:A:992:ARG:HH22	3:E:21:DG:H3'	1.77	0.50
1:C:579:ASP:OD1	1:C:580:VAL:N	2.44	0.50
3:E:37:DC:OP2	3:E:37:DC:H6	1.94	0.50
1:A:641:ARG:NH1	1:A:987:ASN:N	2.59	0.50
2:D:6:LEU:HD22	2:D:53:GLY:HA2	1.93	0.50
1:A:958:LEU:HA	1:A:961:THR:HG22	1.92	0.50
2:B:279:SER:HG	2:B:282:GLN:H	1.57	0.50
3:E:44:DC:H4'	3:E:45:DC:OP1	2.11	0.50
2:B:258:ILE:HD13	2:B:284:ARG:HD2	1.94	0.50
1:C:912:LYS:HA	1:C:915:TRP:CZ3	2.45	0.50
1:C:1001:SER:O	1:C:1005:GLU:N	2.44	0.50
1:C:1025:MET:N	1:C:1025:MET:SD	2.85	0.50
1:A:557:LEU:O	1:A:560:TRP:HB2	2.12	0.50
1:A:795:ARG:NH1	2:B:39:ARG:HH11	2.10	0.50
2:B:47:GLY:H	2:B:60:ILE:HD11	1.76	0.50
1:C:856:ASP:OD2	1:C:867:PRO:HB3	2.11	0.50
3:E:34:DG:H1'	3:E:35:DA:H5'	1.93	0.50
3:E:47:DG:H2''	3:E:48:DC:C6	2.47	0.50
1:A:558:SER:HG	2:B:173:ASN:H	1.58	0.50
2:B:109:LEU:HD12	2:B:124:CYS:SG	2.51	0.50
2:D:106:LEU:HB2	2:D:129:LEU:HD11	1.93	0.50
2:D:321:SER:HA	2:D:327:ALA:HA	1.94	0.50
1:A:611:PHE:HA	1:A:651:ILE:HA	1.93	0.50
1:A:833:GLU:OE2	1:A:948:TYR:OH	2.16	0.50
1:A:865:LEU:HD21	1:A:878:ARG:HG2	1.93	0.50
1:C:856:ASP:CG	1:C:867:PRO:HB3	2.31	0.50
3:E:35:DA:H2''	3:E:36:DA:C8	2.46	0.50
1:A:439:GLU:HA	1:A:444:GLY:N	2.27	0.50
2:B:229:ARG:HB3	2:B:257:THR:OG1	2.12	0.50
1:C:931:TYR:CD1	1:C:966:PRO:HG3	2.47	0.50
1:C:942:LEU:HD22	1:C:950:TYR:CE2	2.47	0.50
2:D:73:ARG:HH21	2:D:96:ARG:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:4:DC:H2''	4:F:5:DA:C8	2.46	0.50
2:B:8:ALA:HA	2:B:55:LEU:HB3	1.92	0.50
1:C:675:ARG:HD2	1:C:1014:TRP:CZ3	2.46	0.50
1:C:919:CYS:SG	1:C:922:ARG:NH1	2.85	0.50
2:D:159:ARG:HH21	2:D:224:LEU:HB2	1.77	0.50
1:A:1002:LYS:O	1:A:1005:GLU:HG2	2.12	0.49
2:B:131:GLY:HA3	2:B:132:ASP:C	2.32	0.49
2:B:138:TYR:CE1	2:B:159:ARG:HB2	2.47	0.49
2:B:168:THR:O	2:B:172:TRP:N	2.46	0.49
2:D:147:SER:HB2	2:D:240:LEU:HB2	1.94	0.49
1:A:465:LYS:NZ	4:F:23:DT:P	2.86	0.49
1:A:898:ARG:O	1:A:902:LEU:HG	2.12	0.49
1:C:520:HIS:CD2	4:F:23:DT:OP2	2.65	0.49
3:E:28:DA:H2''	3:E:29:DG:C8	2.47	0.49
1:C:696:PRO:HG3	2:D:172:TRP:HB3	1.94	0.49
2:D:197:LEU:HB2	2:D:200:LEU:HB2	1.94	0.49
2:B:293:ASP:HB3	2:B:298:HIS:HE1	1.78	0.49
4:F:12:DT:OP2	4:F:12:DT:H6	1.96	0.49
1:A:697:VAL:O	1:A:700:GLU:HG2	2.12	0.49
1:A:988:LYS:HE3	3:E:20:DA:H3'	1.94	0.49
1:A:820:ILE:HG23	1:A:871:MET:HG2	1.94	0.49
1:C:851:TRP:HA	1:C:854:THR:HG22	1.94	0.49
1:C:939:ALA:HA	1:C:942:LEU:HD12	1.94	0.49
1:C:946:PHE:HA	1:C:948:TYR:HD1	1.77	0.49
1:A:491:VAL:HG11	1:A:1015:LEU:HD13	1.94	0.49
1:A:577:ARG:HB3	1:A:580:VAL:HG23	1.94	0.49
1:A:579:ASP:O	1:A:583:VAL:HG13	2.12	0.49
1:A:727:THR:O	1:A:729:TYR:N	2.46	0.49
1:A:778:ARG:O	1:A:781:ILE:HG22	2.13	0.49
1:A:856:ASP:HA	1:A:859:LEU:HD12	1.94	0.49
1:C:577:ARG:NH1	1:C:577:ARG:HG2	2.28	0.49
1:C:667:LYS:HB3	1:C:670:SER:HB3	1.95	0.49
2:B:265:PRO:HB3	2:B:271:TYR:CE2	2.48	0.49
1:C:616:LYS:HZ1	1:C:978:TRP:C	2.15	0.49
1:C:618:SER:HB2	1:C:728:GLY:HA3	1.93	0.49
1:C:686:ASP:OD2	1:C:689:THR:OG1	2.29	0.49
1:C:798:VAL:HG13	1:C:801:VAL:H	1.78	0.49
2:B:83:GLN:NE2	2:B:84:ASP:O	2.46	0.48
2:B:138:TYR:HE1	2:B:159:ARG:HB2	1.79	0.48
1:C:712:SER:O	1:C:712:SER:OG	2.30	0.48
1:C:779:TYR:CZ	1:C:804:LYS:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:877:ARG:HH21	1:C:916:ARG:HH12	1.59	0.48
2:B:38:LYS:NZ	4:F:38:DG:H5''	2.28	0.48
1:C:421:ARG:NH2	4:F:14:DG:O6	2.46	0.48
2:D:134:PRO:HB2	2:D:137:ARG:NH1	2.28	0.48
1:C:708:ARG:HA	1:C:708:ARG:HD3	1.66	0.48
4:F:1:DC:H3'	4:F:2:DT:H71	1.96	0.48
1:A:843:PRO:HD2	1:A:848:ARG:NH1	2.29	0.48
1:A:898:ARG:O	1:A:901:LEU:HG	2.13	0.48
1:C:651:ILE:O	1:C:659:GLY:HA2	2.13	0.48
2:D:2:SER:O	2:D:348:VAL:HA	2.13	0.48
2:D:229:ARG:HD2	2:D:278:GLN:O	2.13	0.48
2:B:182:VAL:HG22	2:B:195:HIS:HB2	1.96	0.48
1:C:762:ASN:HD21	1:C:765:LEU:CB	2.26	0.48
1:C:877:ARG:CZ	1:C:916:ARG:HH12	2.26	0.48
2:D:37:PRO:HB3	2:D:41:CYS:O	2.13	0.48
2:D:135:SER:OG	2:D:137:ARG:NH2	2.46	0.48
2:D:167:ARG:NH1	2:D:172:TRP:CD2	2.81	0.48
2:D:212:ARG:HB2	2:D:269:HIS:CD2	2.48	0.48
2:B:22:LEU:HD13	2:B:90:TYR:CG	2.48	0.48
2:B:115:GLY:H	2:B:116:CYS:HA	1.79	0.48
1:C:751:LEU:HD22	1:C:811:PRO:HB2	1.96	0.48
1:C:819:ASP:OD1	1:C:915:TRP:NE1	2.47	0.48
2:D:1:MET:HG2	2:D:350:PHE:HA	1.96	0.48
3:E:26:DA:OP2	3:E:26:DA:H2'	2.13	0.48
1:A:735:ARG:HH12	1:A:740:LEU:C	2.17	0.48
2:B:135:SER:N	2:B:137:ARG:HH12	2.12	0.48
2:B:211:ALA:HA	2:B:216:VAL:HA	1.95	0.48
1:C:523:ARG:HH12	3:E:25:DT:C7	2.22	0.48
2:D:148:ARG:N	2:D:149:GLY:HA2	2.29	0.48
1:A:878:ARG:HB2	1:A:878:ARG:HH11	1.78	0.48
2:B:75:PRO:HG2	2:B:77:ILE:HD11	1.94	0.48
2:B:210:LEU:HD13	2:B:292:LEU:HD21	1.95	0.48
2:B:228:CYS:SG	2:B:230:PRO:HD3	2.54	0.48
2:B:266:ILE:HD13	2:B:350:PHE:CD2	2.49	0.48
1:C:657:ASP:OD1	1:C:657:ASP:N	2.46	0.48
2:D:87:PRO:HA	2:D:88:GLU:HA	1.53	0.48
3:E:20:DA:C4	3:E:21:DG:C6	3.02	0.48
1:A:818:CYS:SG	1:A:819:ASP:N	2.87	0.48
2:B:290:VAL:HG13	2:B:298:HIS:H	1.79	0.47
2:D:97:THR:HB	2:D:98:PRO:HD2	1.96	0.47
1:A:465:LYS:HZ1	4:F:22:DC:H3'	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:GLN:HG3	2:B:207:HIS:CD2	2.48	0.47
1:C:518:PRO:CB	1:C:520:HIS:CE1	2.96	0.47
1:C:410:ARG:NH1	3:E:41:DA:C4	2.80	0.47
1:C:696:PRO:HG3	2:D:172:TRP:CB	2.45	0.47
1:C:877:ARG:HH21	1:C:916:ARG:CZ	2.27	0.47
4:F:22:DC:OP2	4:F:22:DC:H2'	2.14	0.47
2:B:69:LEU:HD22	2:B:124:CYS:SG	2.54	0.47
1:C:877:ARG:NH2	1:C:916:ARG:HH12	2.11	0.47
3:E:41:DA:H2''	3:E:42:DA:C8	2.49	0.47
4:F:44:DC:H2''	4:F:45:DC:C6	2.49	0.47
1:A:760:SER:HB2	1:A:952:GLY:HA2	1.97	0.47
1:C:575:ARG:HB2	1:C:678:CYS:HB2	1.97	0.47
1:C:651:ILE:HB	1:C:662:ILE:HD11	1.97	0.47
1:C:961:THR:HA	1:C:965:VAL:HG23	1.97	0.47
2:D:146:ASN:HA	2:D:150:LYS:O	2.14	0.47
2:D:202:ASP:OD1	2:D:203:GLY:N	2.48	0.47
2:D:206:PHE:CD1	2:D:260:SER:HB2	2.50	0.47
2:D:229:ARG:HH12	2:D:280:GLU:H	1.62	0.47
1:A:492:ASN:O	1:C:502:LYS:NZ	2.47	0.47
1:A:828:LYS:HD3	1:A:949:ARG:HH22	1.79	0.47
1:A:835:GLY:HA3	1:A:851:TRP:CD2	2.49	0.47
2:B:306:GLN:N	2:B:306:GLN:OE1	2.48	0.47
1:C:590:GLU:O	1:C:593:ILE:HG22	2.15	0.47
1:A:542:LEU:HB2	1:A:545:VAL:HB	1.95	0.47
1:A:553:ILE:HD12	1:A:553:ILE:H	1.80	0.47
2:B:94:GLY:H	2:B:140:HIS:CE1	2.33	0.47
1:C:415:LEU:HD21	1:C:427:LEU:HD11	1.96	0.47
4:F:7:DG:H2'	4:F:8:DG:H8	1.80	0.47
1:A:698:VAL:HG23	1:A:701:ARG:NH2	2.30	0.47
1:A:742:ALA:O	4:F:39:DA:H5''	2.15	0.47
1:C:913:PRO:O	1:C:917:SER:N	2.48	0.47
1:A:675:ARG:HD2	1:A:1014:TRP:CZ3	2.50	0.47
1:C:428:ARG:O	1:C:432:ASN:ND2	2.44	0.47
1:C:924:CYS:HB2	1:C:927:GLN:HB2	1.95	0.47
2:D:164:PRO:HA	2:D:167:ARG:HB2	1.97	0.47
4:F:47:DG:C5	4:F:48:DA:C6	3.02	0.47
1:A:555:ASP:HA	1:A:574:ARG:HD3	1.97	0.46
2:B:232:ARG:HD2	2:B:232:ARG:O	2.15	0.46
1:A:511:SER:O	1:A:513:ARG:HB3	2.16	0.46
1:A:871:MET:O	3:E:18:DA:N6	2.47	0.46
1:A:957:TYR:OH	3:E:16:DA:OP1	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ARG:HA	2:B:115:GLY:HA2	1.65	0.46
2:B:150:LYS:HE3	2:B:242:LEU:HD21	1.97	0.46
1:C:652:ARG:NH1	1:C:655:GLY:O	2.47	0.46
2:D:332:PRO:HA	2:D:342:ALA:O	2.15	0.46
4:F:27:DG:C5	4:F:28:DC:C4	3.04	0.46
1:A:645:THR:OG1	1:A:674:CYS:HA	2.15	0.46
1:A:748:ILE:HG21	1:A:756:ARG:HD3	1.97	0.46
1:A:897:ARG:NH1	1:A:948:TYR:HE2	2.09	0.46
1:C:742:ALA:HA	1:C:743:SER:HA	1.54	0.46
2:D:217:TYR:HD1	2:D:233:LEU:HD21	1.80	0.46
1:A:849:ARG:HH22	1:A:852:ARG:HB3	1.81	0.46
2:B:242:LEU:HA	2:B:243:GLY:HA2	1.54	0.46
1:A:590:GLU:HG3	1:A:713:VAL:CG2	2.44	0.46
1:C:645:THR:HG21	1:C:673:SER:HB2	1.96	0.46
1:A:989:LEU:HD22	1:A:1016:TYR:HE2	1.80	0.46
2:D:229:ARG:HH22	2:D:280:GLU:HB2	1.80	0.46
1:A:742:ALA:HA	1:A:743:SER:HA	1.52	0.46
2:D:140:HIS:HB2	2:D:155:LEU:HD11	1.98	0.46
2:D:180:PRO:HB3	2:D:202:ASP:C	2.36	0.46
1:A:426:ARG:NE	1:C:442:GLU:OE1	2.41	0.46
2:B:314:SER:HB3	2:B:331:ILE:HD12	1.98	0.46
1:C:913:PRO:HA	1:C:916:ARG:HB2	1.97	0.46
4:F:26:DA:H2"	4:F:27:DG:H8	1.80	0.46
1:A:603:ASP:OD2	1:A:606:MET:HB2	2.16	0.46
1:A:995:LYS:HB3	1:A:996:MET:SD	2.56	0.46
2:B:135:SER:O	2:B:137:ARG:HG2	2.15	0.46
2:B:168:THR:HB	2:B:171:ASN:HB2	1.98	0.46
1:C:579:ASP:O	1:C:583:VAL:HG13	2.15	0.46
1:C:643:SER:OG	1:C:644:PHE:N	2.49	0.46
1:C:749:CYS:HB2	1:C:959:HIS:NE2	2.31	0.46
2:D:39:ARG:HA	2:D:39:ARG:HD2	1.62	0.46
2:D:73:ARG:HH21	2:D:96:ARG:HH21	1.64	0.46
3:E:7:DG:N2	4:F:45:DC:O2	2.49	0.46
1:A:536:PHE:HB3	1:A:711:ILE:HD11	1.99	0.46
1:A:687:HIS:HD2	2:B:36:TRP:HD1	1.64	0.46
1:A:731:GLU:OE1	1:A:750:THR:OG1	2.34	0.46
1:A:876:ALA:HA	1:A:879:LEU:HB3	1.98	0.46
1:A:944:SER:OG	1:A:945:MET:N	2.48	0.46
2:B:132:ASP:CG	2:B:194:ALA:H	2.14	0.46
1:C:557:LEU:HD12	1:C:560:TRP:HE3	1.81	0.46
1:C:993:PHE:HE2	1:C:1013:HIS:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:LEU:HD21	2:D:306:GLN:O	2.16	0.46
2:D:66:SER:HB2	2:D:124:CYS:H	1.81	0.46
3:E:30:DA:OP2	3:E:30:DA:H8	1.99	0.46
1:A:687:HIS:ND1	1:A:736:GLU:OE2	2.48	0.45
2:B:289:TYR:HD2	2:B:300:GLU:HG3	1.81	0.45
1:C:513[A]:ARG:CZ	1:C:513[A]:ARG:HB3	2.46	0.45
1:C:523:ARG:NH2	3:E:24:DC:H2'	2.31	0.45
1:A:795:ARG:NH1	4:F:40:DC:OP1	2.48	0.45
1:A:882:ARG:NH1	1:A:906:ASP:CG	2.63	0.45
1:A:971:ARG:NE	1:A:972:ASP:OD1	2.43	0.45
2:B:231:SER:O	2:B:256:LEU:N	2.50	0.45
1:C:419:THR:HG23	4:F:13:DT:OP2	2.16	0.45
1:C:513[B]:ARG:CZ	1:C:513[B]:ARG:HB3	2.46	0.45
1:C:954:ILE:HG22	1:C:955:THR:N	2.30	0.45
3:E:28:DA:H2''	3:E:29:DG:H8	1.81	0.45
4:F:40:DC:C2	4:F:41:DA:N7	2.84	0.45
1:A:956:ASN:O	1:A:960:LYS:HG3	2.15	0.45
1:C:615:VAL:CG1	1:C:644:PHE:HD2	2.29	0.45
1:C:817:HIS:O	1:C:820:ILE:HG22	2.16	0.45
4:F:45:DC:H2''	4:F:46:DA:N7	2.32	0.45
1:A:435:LYS:HG3	1:A:439:GLU:OE2	2.16	0.45
1:A:566:ASP:OD1	1:A:567:VAL:N	2.41	0.45
1:A:590:GLU:HA	1:A:593:ILE:HG12	1.99	0.45
1:A:919:CYS:O	1:A:923:ASP:N	2.36	0.45
1:A:927:GLN:O	1:A:931:TYR:N	2.49	0.45
2:B:38:LYS:NZ	4:F:38:DG:P	2.90	0.45
2:B:135:SER:N	2:B:137:ARG:NH1	2.64	0.45
2:D:159:ARG:HH11	2:D:205:SER:HG	1.61	0.45
4:F:29:DA:C8	4:F:29:DA:OP2	2.69	0.45
1:A:493:THR:O	1:A:493:THR:OG1	2.35	0.45
1:A:539:GLN:HG2	1:A:710:ILE:HD11	1.98	0.45
1:A:594:MET:SD	1:A:718:ARG:NH1	2.89	0.45
2:B:12:GLY:O	2:B:341:GLU:HA	2.16	0.45
2:B:333:SER:OG	2:B:344:HIS:N	2.49	0.45
1:C:1001:SER:O	1:C:1005:GLU:HG3	2.16	0.45
3:E:21:DG:H4'	3:E:22:DT:OP1	2.16	0.45
1:A:560:TRP:CD1	2:B:173:ASN:HB3	2.51	0.45
1:A:749:CYS:HB2	1:A:959:HIS:CD2	2.50	0.45
1:C:936:GLN:O	1:C:936:GLN:NE2	2.48	0.45
3:E:29:DG:H2''	3:E:30:DA:C8	2.52	0.45
1:A:1029:LYS:HB3	1:A:1029:LYS:HE2	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:ASP:HB3	2:B:298:HIS:CE1	2.51	0.45
1:C:493:THR:O	1:C:493:THR:OG1	2.29	0.45
4:F:24:DG:OP2	4:F:24:DG:H2'	2.16	0.45
1:A:430:LEU:HD11	1:C:434:VAL:HG22	1.98	0.45
1:A:536:PHE:HB3	1:A:711:ILE:CD1	2.46	0.45
1:A:696:PRO:HG3	2:B:172:TRP:CG	2.51	0.45
1:A:860:ARG:HA	1:A:860:ARG:HD2	1.86	0.45
1:A:862:LYS:HB3	1:A:862:LYS:HZ3	1.81	0.45
1:C:675:ARG:HD2	1:C:1014:TRP:CE3	2.51	0.45
1:A:735:ARG:NH1	1:A:741:GLU:C	2.70	0.45
2:B:316:THR:OG1	2:B:317:TRP:N	2.50	0.45
2:B:327:ALA:HB3	2:B:348:VAL:HG23	1.97	0.45
1:C:558:SER:O	1:C:558:SER:OG	2.34	0.45
2:D:144:VAL:HG22	2:D:153:CYS:SG	2.56	0.45
2:D:236:LEU:HD12	2:D:238:VAL:HG11	1.98	0.45
2:D:328:LEU:HD11	2:D:345:PHE:HD2	1.82	0.45
1:A:538:TRP:CZ2	1:A:709:LEU:HD13	2.52	0.45
1:A:640:VAL:HG23	1:A:682:VAL:O	2.17	0.45
1:C:538:TRP:HB3	1:C:707:SER:OG	2.17	0.45
1:C:883:GLU:OE1	1:C:883:GLU:N	2.45	0.45
1:C:922:ARG:NH1	1:C:922:ARG:HB3	2.32	0.45
1:C:926:ASP:OD1	1:C:926:ASP:N	2.50	0.45
4:F:49:DT:H2''	4:F:50:DC:C5	2.52	0.45
1:A:762:ASN:OD1	1:A:763:MET:N	2.50	0.44
2:B:235:ARG:HE	2:B:250:THR:HG21	1.82	0.44
2:D:93:HIS:HA	2:D:94:GLY:HA2	1.66	0.44
2:D:137:ARG:NH1	2:D:183:TYR:CE2	2.85	0.44
4:F:39:DA:C5	4:F:40:DC:C4	3.05	0.44
1:A:955:THR:OG1	1:A:958:LEU:HB2	2.18	0.44
2:B:36:TRP:HZ2	2:B:99:ASN:HB3	1.81	0.44
2:B:317:TRP:HB3	2:B:331:ILE:CD1	2.47	0.44
1:C:753:ASP:N	1:C:753:ASP:OD1	2.50	0.44
4:F:18:DC:H2'	4:F:19:DA:H8	1.81	0.44
2:B:80:PHE:HZ	2:B:83:GLN:HE21	1.65	0.44
1:C:523:ARG:HH22	3:E:24:DC:H2'	1.81	0.44
1:C:574:ARG:NE	1:C:1007:GLU:OE1	2.34	0.44
2:D:338:THR:HG22	2:D:340:PRO:CA	2.32	0.44
3:E:29:DG:H2''	3:E:30:DA:OP2	2.17	0.44
1:C:410:ARG:HG2	1:C:411:PRO:HD2	1.99	0.44
1:C:502:LYS:HA	1:C:505:ARG:NH1	2.33	0.44
1:C:646:ILE:H	1:C:646:ILE:HG13	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:230:PRO:HB2	2:D:232:ARG:HD2	2.00	0.44
1:A:751:LEU:HD22	1:A:811:PRO:HB2	1.99	0.44
2:B:49:ARG:CZ	2:B:58:ARG:HD2	2.47	0.44
2:B:70:PRO:HG2	2:B:72:LEU:HD21	1.99	0.44
2:B:322:LEU:N	2:B:326:THR:O	2.50	0.44
1:C:835:GLY:HA3	1:C:851:TRP:CZ2	2.52	0.44
2:D:218:PHE:CE1	2:D:236:LEU:HD21	2.52	0.44
4:F:40:DC:H2''	4:F:41:DA:OP2	2.16	0.44
1:A:804:LYS:NZ	2:B:101:GLU:OE2	2.50	0.44
1:A:430:LEU:HB2	1:C:437:PHE:CG	2.53	0.44
1:A:905:MET:O	1:A:909:LEU:HG	2.18	0.44
1:A:911:MET:HE1	1:A:935:SER:HB3	1.99	0.44
1:A:1012:HIS:HA	1:A:1015:LEU:HD12	2.00	0.44
2:B:39:ARG:HH11	2:B:39:ARG:HG3	1.82	0.44
1:C:419:THR:O	1:C:423:GLN:N	2.33	0.44
1:A:625:VAL:HG23	1:A:637:GLU:HB2	1.99	0.44
1:A:735:ARG:O	1:A:739:GLY:N	2.49	0.44
1:A:845:ARG:NH1	1:A:845:ARG:HB2	2.33	0.44
1:A:858:GLN:HB3	1:A:888:VAL:HG22	1.99	0.44
2:B:9:VAL:HG13	2:B:10:ASN:H	1.83	0.44
1:C:966:PRO:HA	1:C:969:VAL:HG22	2.00	0.44
1:A:834:ILE:HD13	1:A:834:ILE:HA	1.85	0.44
2:B:150:LYS:HE2	2:B:240:LEU:HB3	1.98	0.44
1:C:564:VAL:HG21	2:D:315:ARG:HH12	1.82	0.44
2:D:47:GLY:N	2:D:60:ILE:HD11	2.31	0.44
1:A:747:TYR:OH	1:A:796:ASP:HA	2.17	0.43
1:C:555:ASP:N	1:C:555:ASP:OD1	2.51	0.43
1:A:539:GLN:CD	1:A:710:ILE:HD11	2.38	0.43
1:A:708:ARG:NH2	1:A:719:SER:OG	2.51	0.43
1:A:798:VAL:HG23	1:A:801:VAL:H	1.83	0.43
2:B:9:VAL:HG13	2:B:10:ASN:OD1	2.18	0.43
2:B:159:ARG:HH22	2:B:206:PHE:HE2	1.64	0.43
2:B:269:HIS:HA	2:B:271:TYR:HE1	1.84	0.43
2:B:310:GLU:OE2	2:B:344:HIS:CG	2.69	0.43
1:C:588:ASP:OD2	1:C:1018:SER:OG	2.18	0.43
1:C:894:SER:O	1:C:898:ARG:HG3	2.18	0.43
4:F:30:DC:H2''	4:F:31:DT:C6	2.53	0.43
1:A:560:TRP:CZ3	1:A:569:ALA:HA	2.53	0.43
1:A:870:ARG:NH1	3:E:17:DC:H2''	2.33	0.43
2:B:115:GLY:N	2:B:116:CYS:HA	2.33	0.43
1:C:576:PHE:HB2	1:C:677:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:676:PRO:HG3	1:C:1013:HIS:CG	2.53	0.43
1:C:753:ASP:OD1	1:C:769:THR:OG1	2.35	0.43
1:C:912:LYS:HA	1:C:915:TRP:CH2	2.53	0.43
3:E:4:DC:H1'	3:E:5:DT:C6	2.52	0.43
1:A:991:ARG:HB2	1:A:991:ARG:NH2	2.33	0.43
1:C:858:GLN:NE2	1:C:891:LEU:HG	2.34	0.43
2:D:3:LEU:HB3	2:D:348:VAL:HG12	2.01	0.43
3:E:9:DC:C2	4:F:43:DG:N2	2.86	0.43
3:E:38:DA:H2''	3:E:39:DA:C8	2.51	0.43
4:F:15:DT:H2'	4:F:16:DT:C6	2.53	0.43
1:A:429:ASP:HB2	1:C:437:PHE:HE2	1.83	0.43
1:A:674:CYS:H	1:A:1017:THR:HG21	1.83	0.43
2:B:75:PRO:HA	2:B:95:GLY:HA2	2.00	0.43
1:C:447:LYS:HE2	1:C:474:MET:HE1	2.01	0.43
1:C:675:ARG:HD3	1:C:1017:THR:HG23	1.99	0.43
2:D:6:LEU:HD11	2:D:347:GLN:HB2	2.00	0.43
2:D:79:HIS:NE2	2:D:88:GLU:OE2	2.47	0.43
4:F:4:DC:H2''	4:F:5:DA:H8	1.84	0.43
1:A:783:ARG:HH21	1:A:784:LYS:HG2	1.83	0.43
1:C:762:ASN:HD21	1:C:765:LEU:CA	2.31	0.43
3:E:19:DC:O2	3:E:19:DC:H5'	2.18	0.43
1:A:533:PHE:HD2	1:A:534:HIS:CE1	2.37	0.43
1:A:544:ASN:HB3	2:B:167:ARG:O	2.19	0.43
1:A:619:CYS:HB2	1:A:642:PHE:CD2	2.54	0.43
2:B:87:PRO:HA	2:B:88:GLU:HA	1.69	0.43
4:F:29:DA:H1'	4:F:30:DC:O4'	2.18	0.43
4:F:48:DA:H1'	4:F:49:DT:O4'	2.18	0.43
1:A:849:ARG:NH1	1:A:853:SER:HB3	2.34	0.43
1:A:889:CYS:SG	1:A:902:LEU:HD21	2.58	0.43
2:B:86:LYS:HA	2:B:86:LYS:HD2	1.89	0.43
2:B:237:HIS:CD2	2:B:239:GLU:OE2	2.71	0.43
1:C:676:PRO:HG3	1:C:1013:HIS:CD2	2.54	0.43
1:C:810:GLN:O	1:C:812:THR:N	2.52	0.43
1:A:568:PRO:HB2	1:A:570:ASP:OD2	2.19	0.43
1:A:795:ARG:NE	2:B:39:ARG:HD3	2.33	0.43
1:A:810:GLN:OE1	1:A:971:ARG:NH1	2.52	0.43
1:A:814:ASP:OD2	1:A:817:HIS:N	2.46	0.43
1:A:849:ARG:NH2	1:A:852:ARG:HB3	2.34	0.43
2:B:180:PRO:HG3	2:B:202:ASP:HA	2.00	0.43
2:B:290:VAL:HG22	2:B:299:MET:HB2	2.01	0.43
1:C:615:VAL:HG11	1:C:644:PHE:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:785:ASN:ND2	1:C:789:GLU:H	2.16	0.43
1:C:903:LYS:HD2	1:C:906:ASP:OD2	2.19	0.43
2:D:113:SER:H	2:D:121:THR:HG1	1.62	0.43
2:D:167:ARG:NH1	2:D:172:TRP:CG	2.86	0.43
2:D:259:THR:H	2:D:277:TYR:H	1.65	0.43
1:A:415:LEU:HD13	1:A:426:ARG:NE	2.34	0.43
1:A:621:GLY:N	1:A:684:GLU:OE2	2.42	0.43
1:A:992:ARG:NH2	3:E:21:DG:O5'	2.52	0.43
1:C:534:HIS:ND1	1:C:587:LYS:HG2	2.34	0.43
1:C:716:LEU:HD12	1:C:718:ARG:NH2	2.34	0.43
1:C:739:GLY:CA	1:C:803:ALA:HB3	2.49	0.43
4:F:10:DT:OP2	4:F:10:DT:H6	2.02	0.43
2:B:102:LEU:HD12	2:B:102:LEU:HA	1.86	0.42
2:B:168:THR:HG22	2:B:170:GLN:N	2.34	0.42
1:C:751:LEU:HD12	1:C:964:HIS:CD2	2.53	0.42
2:D:322:LEU:H	2:D:327:ALA:HA	1.84	0.42
2:B:145:ILE:HB	2:B:214:ASP:HA	2.00	0.42
2:B:159:ARG:HA	2:B:177:ASP:HA	2.00	0.42
2:D:43:THR:HG21	2:D:62:PHE:HE1	1.83	0.42
4:F:21:DT:H2''	4:F:22:DC:C5	2.53	0.42
1:A:603:ASP:OD1	1:A:604:ASP:N	2.52	0.42
2:B:82:ALA:HB2	2:B:88:GLU:HB2	2.01	0.42
2:B:188:GLU:HA	2:B:189:PHE:HA	1.64	0.42
1:C:786:PRO:HG2	1:C:787:PHE:CD1	2.54	0.42
1:C:787:PHE:CD1	1:C:797:ARG:NH1	2.88	0.42
2:D:179:PRO:O	2:D:181:GLN:N	2.52	0.42
1:A:993:PHE:HB3	1:A:1009:ILE:HG13	2.01	0.42
2:B:290:VAL:HG12	2:B:292:LEU:HD12	2.01	0.42
4:F:34:DG:N3	4:F:34:DG:H2'	2.35	0.42
1:A:1027:ALA:O	1:C:509:ALA:HB1	2.19	0.42
2:B:38:LYS:HZ1	4:F:38:DG:H5''	1.83	0.42
2:B:119:LYS:HB2	3:E:6:DG:O3'	2.19	0.42
2:B:134:PRO:HA	2:B:137:ARG:HH12	1.85	0.42
2:B:295:VAL:HB	2:B:298:HIS:CE1	2.54	0.42
1:C:764:VAL:HG11	1:C:936:GLN:HA	2.01	0.42
2:D:113:SER:N	2:D:121:THR:OG1	2.50	0.42
1:A:420:ARG:NH1	1:C:459:ARG:CZ	2.82	0.42
1:A:730:ASP:OD1	1:A:732:LYS:N	2.53	0.42
1:A:748:ILE:HG23	1:A:756:ARG:HB2	2.02	0.42
1:A:869:MET:HG2	1:A:870:ARG:N	2.35	0.42
2:B:119:LYS:HE2	2:B:119:LYS:HB3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:LEU:HD11	2:B:284:ARG:NH2	2.35	0.42
2:B:318:PHE:CE2	2:B:330:ALA:HB3	2.54	0.42
1:C:708:ARG:HB3	1:C:719:SER:OG	2.19	0.42
1:C:762:ASN:HD21	1:C:765:LEU:H	1.67	0.42
4:F:46:DA:C4	4:F:47:DG:C6	3.07	0.42
1:A:496:SER:HB3	1:A:499:GLN:HG3	2.01	0.42
1:A:877:ARG:NH2	1:A:916:ARG:NH1	2.67	0.42
1:A:971:ARG:HE	1:A:972:ASP:CG	2.23	0.42
2:B:127:LYS:NZ	2:B:187:LEU:O	2.40	0.42
2:B:322:LEU:HD21	2:B:328:LEU:HB3	2.02	0.42
1:C:895:GLU:OE1	1:C:895:GLU:N	2.46	0.42
2:D:228:CYS:SG	2:D:230:PRO:HD3	2.60	0.42
2:D:242:LEU:HA	2:D:243:GLY:HA2	1.51	0.42
1:A:487:LEU:HB2	1:A:522:LEU:HD22	2.02	0.42
1:A:732:LYS:HB3	1:A:732:LYS:HE2	1.69	0.42
1:A:878:ARG:HH11	1:A:878:ARG:HD3	1.65	0.42
1:A:946:PHE:HA	1:A:948:TYR:CE2	2.55	0.42
2:B:212:ARG:HG3	2:B:269:HIS:ND1	2.34	0.42
2:D:167:ARG:HH11	2:D:172:TRP:C	2.18	0.42
2:D:236:LEU:HA	2:D:249:CYS:HA	2.01	0.42
3:E:49:DA:H2	4:F:2:DT:H3	1.68	0.42
1:A:532:GLY:H	1:A:580:VAL:CG1	2.33	0.42
1:A:713:VAL:CG1	1:A:718:ARG:HD2	2.41	0.42
1:A:731:GLU:O	1:A:735:ARG:HG3	2.20	0.42
1:A:825:GLU:OE1	1:A:955:THR:HG21	2.19	0.42
1:A:1017:THR:HA	1:A:1022:GLN:NE2	2.35	0.42
2:B:197:LEU:HD23	2:B:197:LEU:HA	1.77	0.42
1:C:570:ASP:N	1:C:570:ASP:OD1	2.45	0.42
1:C:838:TYR:CZ	1:C:897:ARG:HG3	2.55	0.42
2:D:69:LEU:HD13	2:D:107:TYR:CZ	2.55	0.42
2:D:310:GLU:OE2	2:D:344:HIS:CE1	2.73	0.42
3:E:22:DT:H2'	3:E:23:DG:C8	2.55	0.42
4:F:3:DG:H2'	4:F:4:DC:C6	2.55	0.42
1:A:688:GLU:OE1	2:B:73:ARG:NH2	2.51	0.42
2:B:155:LEU:HB3	2:B:183:TYR:HB2	2.01	0.42
2:B:284:ARG:HH11	2:B:284:ARG:HB2	1.85	0.42
1:C:526:GLU:C	1:C:530:LEU:HG	2.39	0.42
1:C:708:ARG:CZ	1:C:721:ARG:HG3	2.50	0.42
2:D:294:ASP:OD1	2:D:295:VAL:N	2.53	0.42
1:A:492:ASN:ND2	1:A:492:ASN:O	2.38	0.41
1:A:616:LYS:HE2	1:A:616:LYS:HB3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:GLU:HA	1:A:902:LEU:HD12	2.02	0.41
2:B:1:MET:O	2:B:1:MET:HG2	2.19	0.41
2:B:258:ILE:HD11	2:B:276:GLY:HA3	2.02	0.41
1:C:693:ILE:O	1:C:696:PRO:HD2	2.20	0.41
1:C:1029:LYS:HZ3	1:C:1030:ASN:ND2	2.18	0.41
3:E:12:DT:H2''	3:E:13:DC:OP2	2.19	0.41
1:A:975:ILE:HG12	1:A:976:GLY:H	1.85	0.41
1:C:572:ILE:HD13	1:C:1002:LYS:HB3	2.02	0.41
2:D:166:GLU:O	2:D:168:THR:OG1	2.32	0.41
4:F:27:DG:C2	4:F:28:DC:C2	3.08	0.41
1:C:795:ARG:NH1	2:D:39:ARG:CZ	2.83	0.41
1:A:451:LEU:HB2	1:C:454:PHE:CE1	2.56	0.41
1:A:535:GLN:HA	1:A:549:TRP:CD2	2.56	0.41
1:A:608:THR:HB	1:A:718:ARG:HG2	2.01	0.41
1:C:985:SER:O	1:C:988:LYS:HB3	2.19	0.41
4:F:5:DA:H2''	4:F:6:DG:C8	2.55	0.41
4:F:38:DG:C2	4:F:39:DA:C5	3.08	0.41
1:A:537:GLU:CD	1:A:710:ILE:HD12	2.41	0.41
1:A:870:ARG:HH11	3:E:17:DC:H2''	1.85	0.41
1:A:947:LYS:HE3	1:A:947:LYS:HB2	1.87	0.41
1:A:1013:HIS:O	1:A:1016:TYR:N	2.50	0.41
1:C:499:GLN:H	1:C:499:GLN:HG3	1.55	0.41
1:C:679:LEU:C	1:C:680:MET:HG3	2.40	0.41
1:C:698:VAL:HG12	1:C:702:LYS:HE2	2.00	0.41
1:C:865:LEU:HG	1:C:878:ARG:HH11	1.80	0.41
1:A:500:TYR:HD2	1:A:519:LEU:HD23	1.85	0.41
1:A:870:ARG:NH1	3:E:18:DA:C2	2.89	0.41
2:B:79:HIS:CD2	2:B:79:HIS:C	2.93	0.41
2:B:134:PRO:CA	2:B:137:ARG:HH12	2.33	0.41
1:C:564:VAL:CG2	2:D:315:ARG:HH12	2.33	0.41
3:E:16:DA:H2''	3:E:17:DC:C6	2.56	0.41
3:E:28:DA:OP2	3:E:28:DA:H2'	2.21	0.41
3:E:33:DG:OP2	3:E:33:DG:H8	2.04	0.41
4:F:41:DA:C6	4:F:42:DG:C6	3.09	0.41
1:A:716:LEU:HB3	1:A:718:ARG:HE	1.86	0.41
2:B:1:MET:SD	2:B:302:ARG:NH1	2.93	0.41
2:B:6:LEU:HD12	2:B:328:LEU:HD13	2.03	0.41
2:B:93:HIS:HA	2:B:94:GLY:HA2	1.64	0.41
1:C:840:LYS:O	1:C:843:PRO:HD3	2.20	0.41
1:A:709:LEU:O	1:A:719:SER:HA	2.21	0.41
1:A:735:ARG:CZ	1:A:742:ALA:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:PRO:HB2	2:B:199:GLU:OE2	2.20	0.41
1:A:456:LEU:HD13	1:C:424:LYS:HG2	2.02	0.41
1:A:459:ARG:HH12	1:A:464:HIS:HD2	1.69	0.41
1:A:555:ASP:HB3	1:A:574:ARG:CZ	2.50	0.41
1:A:612:THR:O	1:A:650:SER:N	2.42	0.41
1:A:749:CYS:HB3	1:A:752:CYS:O	2.20	0.41
1:A:814:ASP:OD1	1:A:979:ALA:HB1	2.21	0.41
1:A:864:LYS:HB2	1:A:864:LYS:HE3	1.88	0.41
1:A:927:GLN:H	1:A:927:GLN:CD	2.23	0.41
1:A:1028:HIS:ND1	1:A:1029:LYS:HE3	2.36	0.41
2:B:289:TYR:HB3	2:B:300:GLU:OE2	2.20	0.41
2:B:331:ILE:HD13	2:B:331:ILE:HA	1.95	0.41
1:C:582:LEU:HD23	1:C:582:LEU:HA	1.89	0.41
1:C:814:ASP:OD1	1:C:816:LEU:N	2.51	0.41
1:C:829:ILE:O	1:C:833:GLU:HG2	2.21	0.41
1:C:908:TYR:CZ	1:C:915:TRP:HH2	2.39	0.41
3:E:18:DA:H2'	3:E:19:DC:O2	2.21	0.41
1:A:459:ARG:NH1	1:A:464:HIS:HD2	2.19	0.41
1:A:479:PHE:HD1	1:A:480:GLY:H	1.68	0.41
1:A:571:THR:CG2	1:A:682:VAL:HG13	2.50	0.41
1:A:1002:LYS:HA	1:A:1005:GLU:OE2	2.21	0.41
1:A:1018:SER:OG	1:A:1020:TYR:HB3	2.21	0.41
2:B:108:MET:HB3	2:B:108:MET:HE2	2.01	0.41
1:C:600:ARG:HD3	1:C:600:ARG:HA	1.67	0.41
1:C:751:LEU:O	1:C:770:ARG:N	2.34	0.41
2:D:16:GLN:NE2	2:D:32:GLY:O	2.53	0.41
2:B:7:THR:O	2:B:54:GLU:HA	2.21	0.40
1:C:766:HIS:HB2	1:C:963:ALA:HB1	2.03	0.40
2:D:9:VAL:HG13	2:D:10:ASN:H	1.86	0.40
1:A:990:PHE:CE1	1:A:1009:ILE:HD13	2.57	0.40
1:A:1025:MET:HG3	1:A:1026:GLU:OE2	2.21	0.40
2:B:229:ARG:HH22	2:B:280:GLU:HG3	1.87	0.40
2:D:106:LEU:HD22	2:D:127:LYS:HB3	2.02	0.40
2:D:217:TYR:CD1	2:D:235:ARG:HB2	2.55	0.40
3:E:39:DA:C6	3:E:40:DA:C6	3.09	0.40
1:A:882:ARG:O	1:A:886:GLU:HG2	2.22	0.40
1:A:1020:TYR:CE2	1:A:1024:PHE:HE2	2.40	0.40
2:B:277:TYR:OH	2:B:316:THR:OG1	2.33	0.40
1:C:543:LYS:O	1:C:545:VAL:HG23	2.21	0.40
1:C:785:ASN:CG	1:C:789:GLU:H	2.24	0.40
1:C:915:TRP:NE1	1:C:916:ARG:HG2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:GLN:O	2:D:214:ASP:OD1	2.40	0.40
3:E:27:DC:C2	3:E:28:DA:C5	3.09	0.40
2:D:73:ARG:HE	2:D:96:ARG:HD2	1.85	0.40
2:D:82:ALA:HB2	2:D:88:GLU:HG3	2.03	0.40
2:D:142:LEU:HA	2:D:154:VAL:O	2.21	0.40
2:D:147:SER:CB	2:D:240:LEU:H	2.34	0.40
2:D:188:GLU:HA	2:D:189:PHE:HA	1.74	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	610/1159 (53%)	557 (91%)	53 (9%)	0	100	100
1	C	613/1159 (53%)	557 (91%)	56 (9%)	0	100	100
2	B	349/533 (66%)	316 (90%)	32 (9%)	1 (0%)	41	76
2	D	349/533 (66%)	324 (93%)	25 (7%)	0	100	100
All	All	1921/3384 (57%)	1754 (91%)	166 (9%)	1 (0%)	54	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	341	GLU

#### 5.3.2 Protein sidechains [i](#)

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	543/1000 (54%)	511 (94%)	32 (6%)	19	47
1	C	546/1000 (55%)	517 (95%)	29 (5%)	22	49
2	B	303/465 (65%)	284 (94%)	19 (6%)	18	44
2	D	303/465 (65%)	284 (94%)	19 (6%)	18	44
All	All	1695/2930 (58%)	1596 (94%)	99 (6%)	24	47

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	PHE
1	A	492	ASN
1	A	494	PHE
1	A	511	SER
1	A	526	GLU
1	A	537	GLU
1	A	546	SER
1	A	558	SER
1	A	597	LEU
1	A	622	MET
1	A	654	GLU
1	A	702	LYS
1	A	730	ASP
1	A	735	ARG
1	A	752	CYS
1	A	818	CYS
1	A	848	ARG
1	A	869	MET
1	A	874	ASN
1	A	878	ARG
1	A	906	ASP
1	A	912	LYS
1	A	933	TYR
1	A	937	GLN
1	A	940	ASP
1	A	981	GLU
1	A	992	ARG
1	A	996	MET
1	A	1013	HIS
1	A	1016	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1018	SER
1	A	1029	LYS
2	B	1	MET
2	B	96	ARG
2	B	103	SER
2	B	104	SER
2	B	123	ARG
2	B	132	ASP
2	B	137	ARG
2	B	167	ARG
2	B	189	PHE
2	B	197	LEU
2	B	202	ASP
2	B	210	LEU
2	B	212	ARG
2	B	232	ARG
2	B	236	LEU
2	B	249	CYS
2	B	279	SER
2	B	285	MET
2	B	312	SER
1	C	479	PHE
1	C	486	CYS
1	C	490	ARG
1	C	513[A]	ARG
1	C	513[B]	ARG
1	C	542	LEU
1	C	558	SER
1	C	577	ARG
1	C	582	LEU
1	C	624	ASP
1	C	626	SER
1	C	654	GLU
1	C	663	PHE
1	C	670	SER
1	C	674	CYS
1	C	680	MET
1	C	708	ARG
1	C	721	ARG
1	C	745	SER
1	C	753	ASP
1	C	770	ARG

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Mol	Chain	Res	Type
1	C	818	CYS
1	C	860	ARG
1	C	878	ARG
1	C	956	ASN
1	C	957	TYR
1	C	994	ARG
1	C	1013	HIS
1	C	1015	LEU
2	D	1	MET
2	D	16	GLN
2	D	90	TYR
2	D	148	ARG
2	D	153	CYS
2	D	160	SER
2	D	178	CYS
2	D	205	SER
2	D	214	ASP
2	D	227	ASP
2	D	232	ARG
2	D	236	LEU
2	D	237	HIS
2	D	282	GLN
2	D	284	ARG
2	D	287	CYS
2	D	292	LEU
2	D	299	MET
2	D	302	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	492	ASN
1	A	517	GLN
1	A	687	HIS
1	A	775	ASN
2	B	83	GLN
1	C	858	GLN
1	C	997	ASN
1	C	1030	ASN
2	D	99	ASN
2	D	269	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

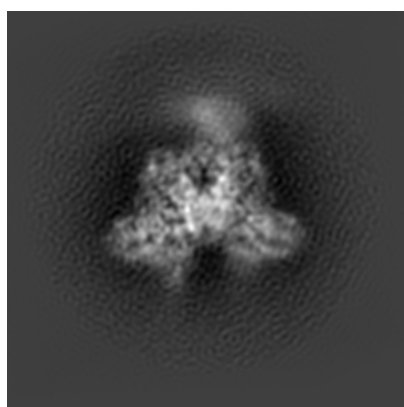
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7852. These allow visual inspection of the internal detail of the map and identification of artifacts.

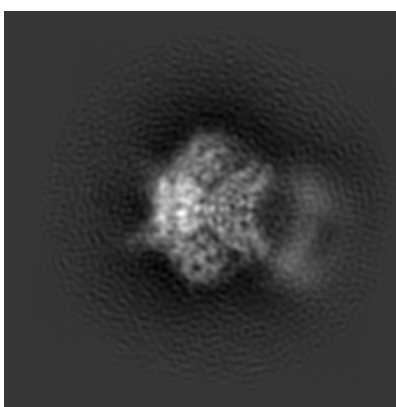
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

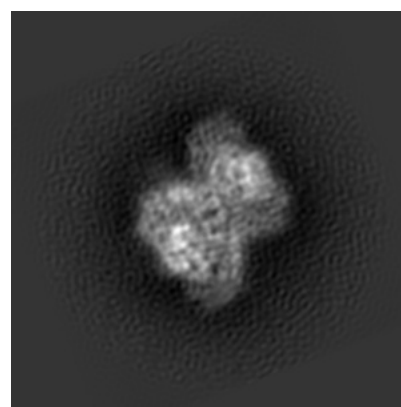
#### 6.1.1 Primary map



X



Y

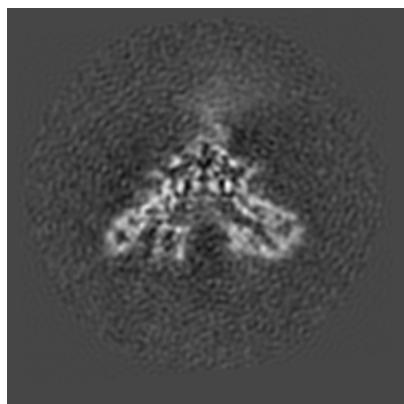


Z

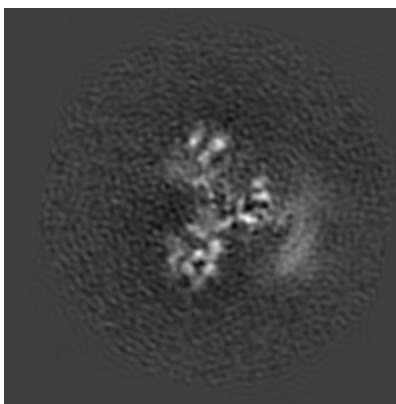
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

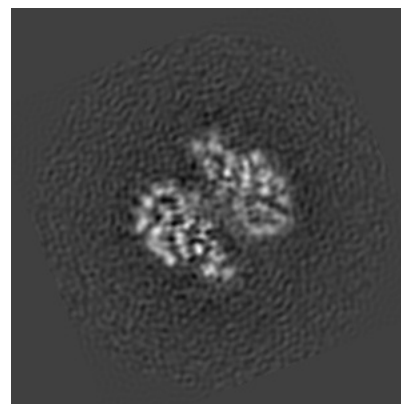
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

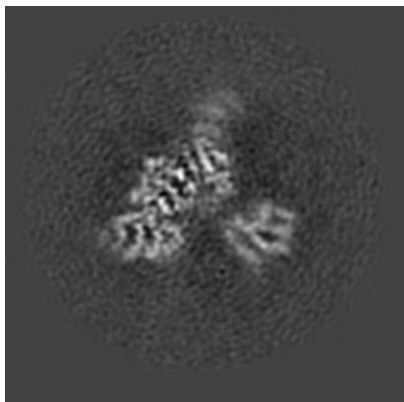


Z Index: 128

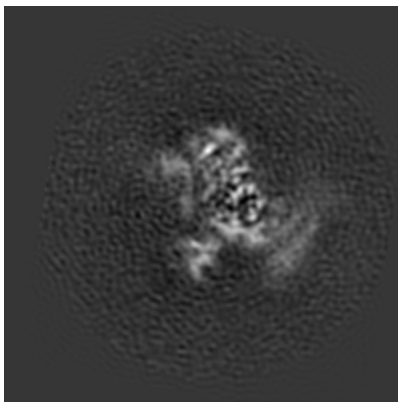
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

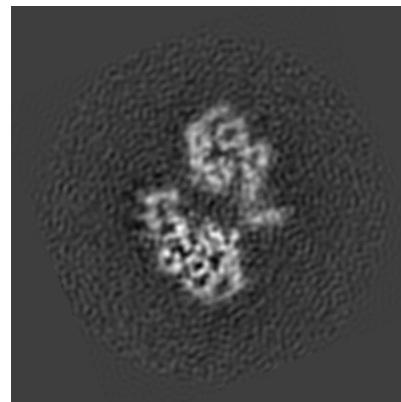
### 6.3.1 Primary map



X Index: 121



Y Index: 138

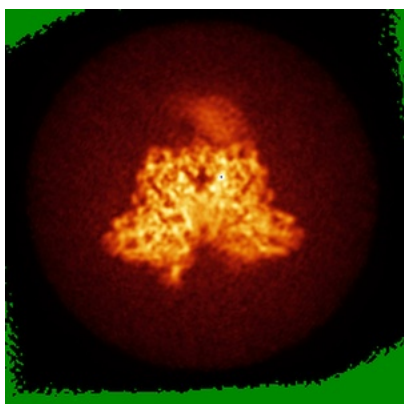


Z Index: 114

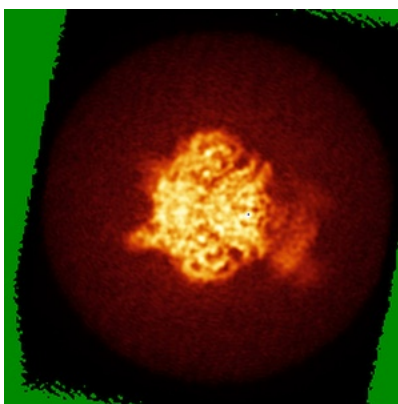
The images above show the largest variance slices of the map in three orthogonal directions.

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

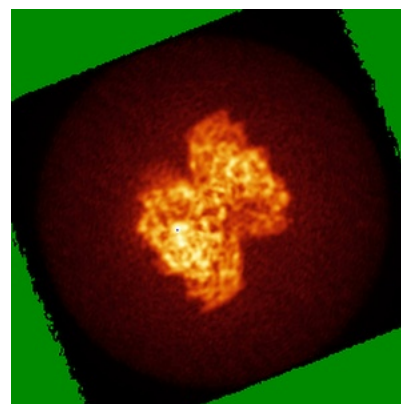
### 6.4.1 Primary map



X



Y

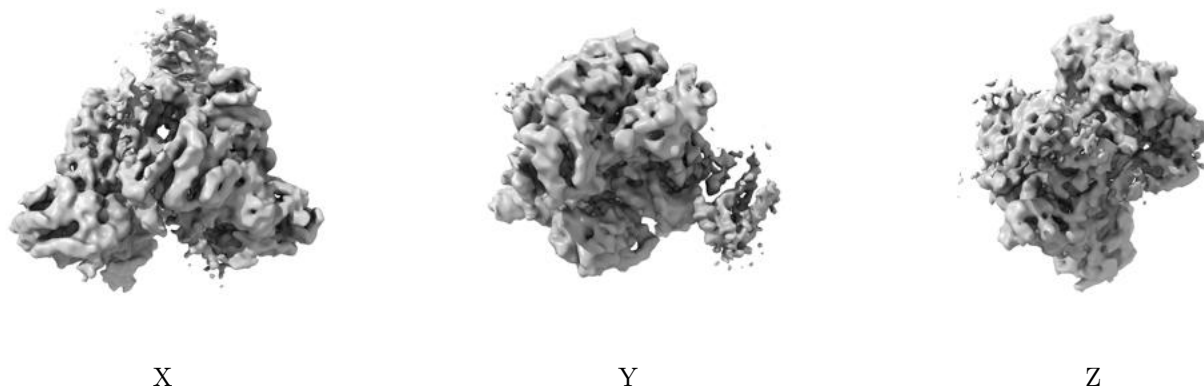


Z

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

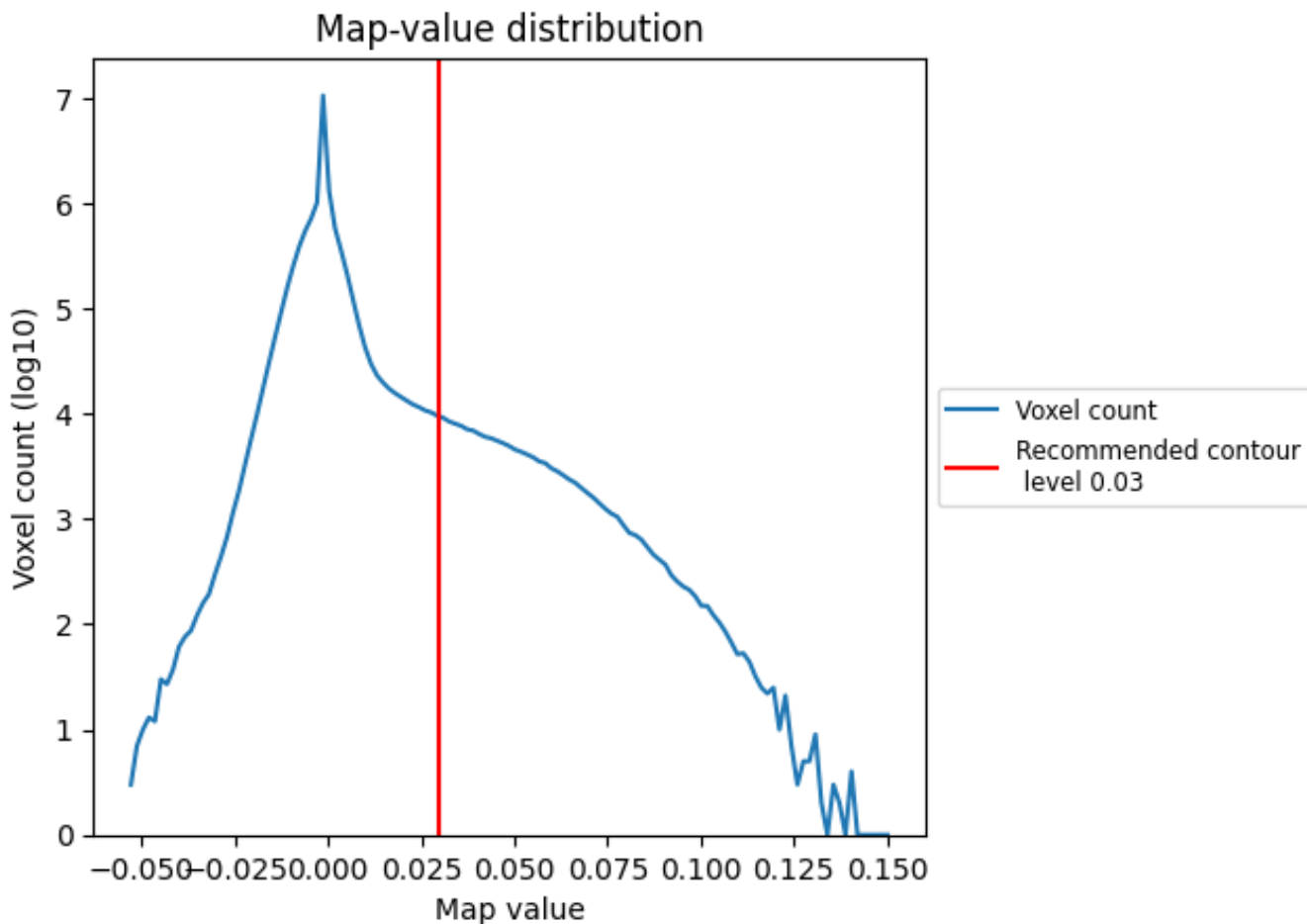
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

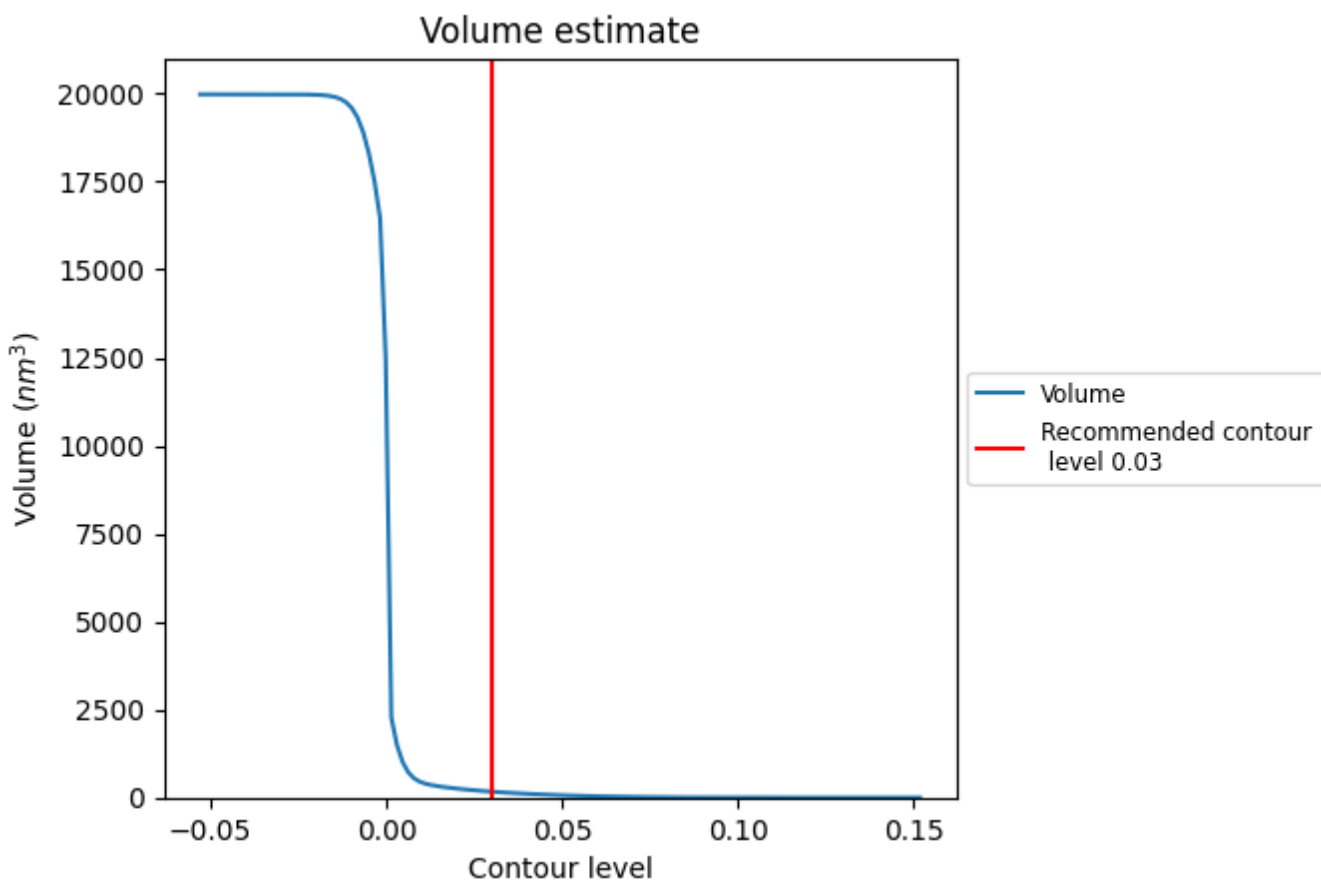
### 7.1 Map-value distribution [i](#)



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



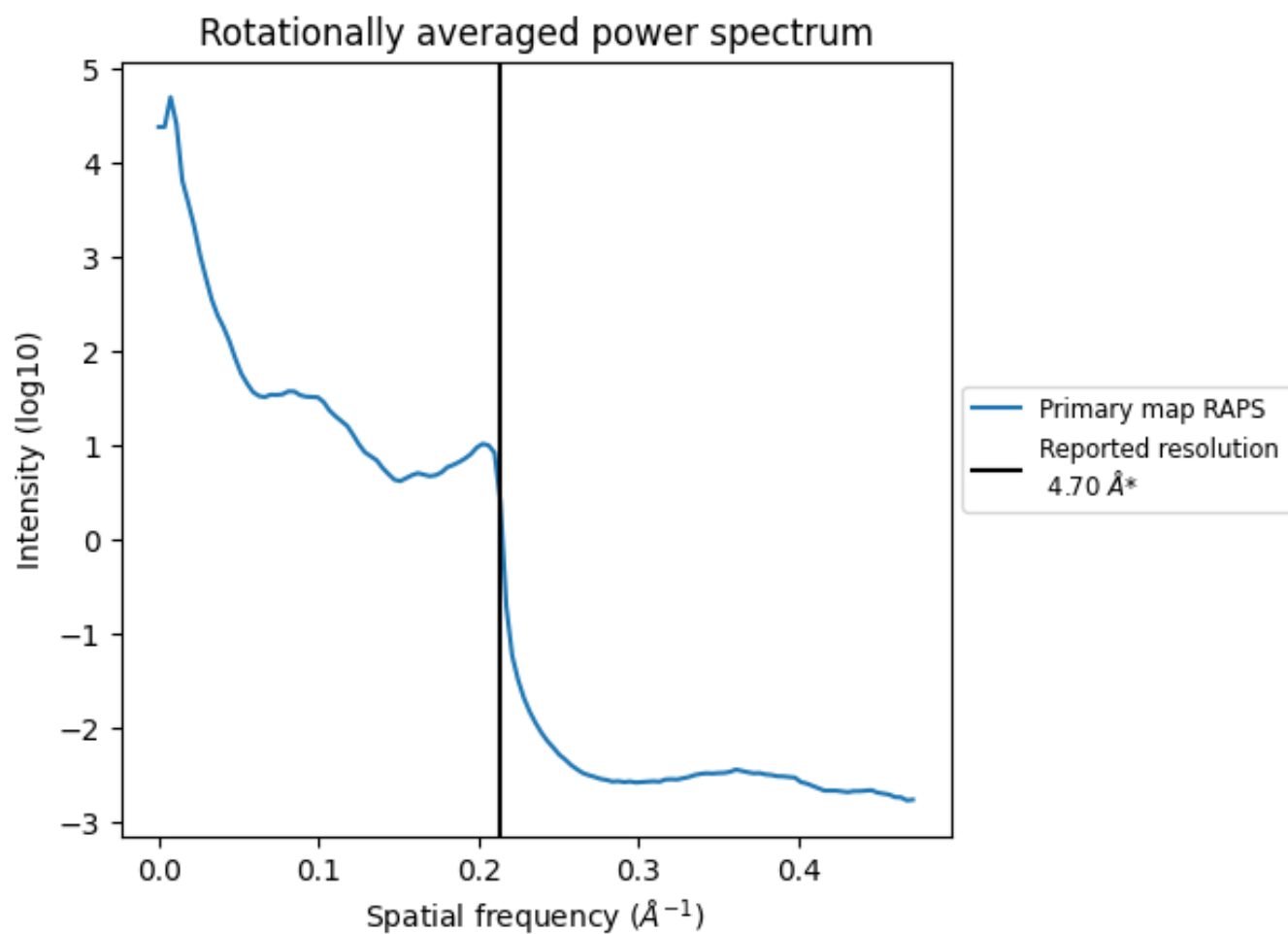
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm<sup>3</sup>; this corresponds to an approximate mass of 151 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  $0.213 \text{\AA}^{-1}$

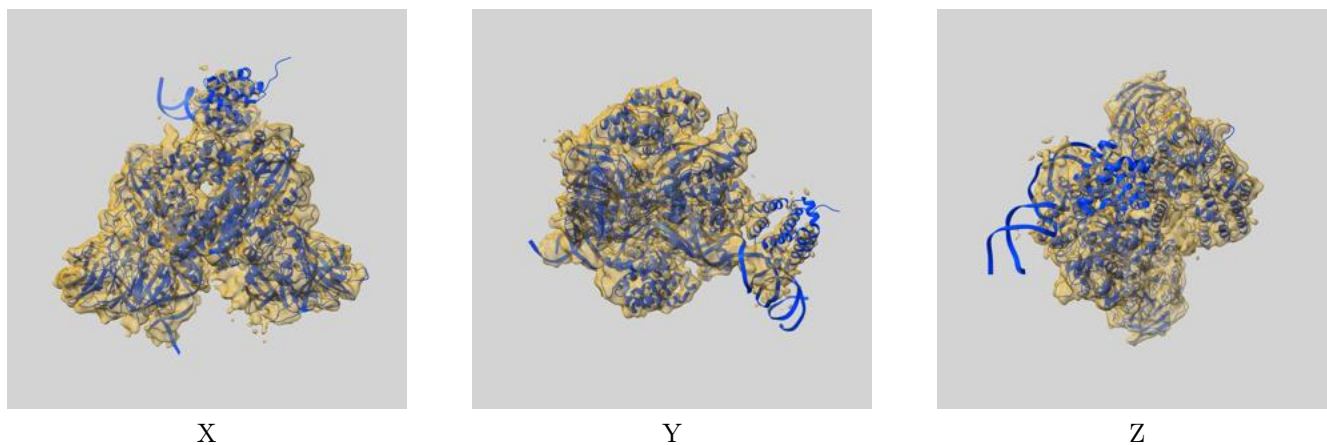
## 8 Fourier-Shell correlation

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-7852 and PDB model 6DBW. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



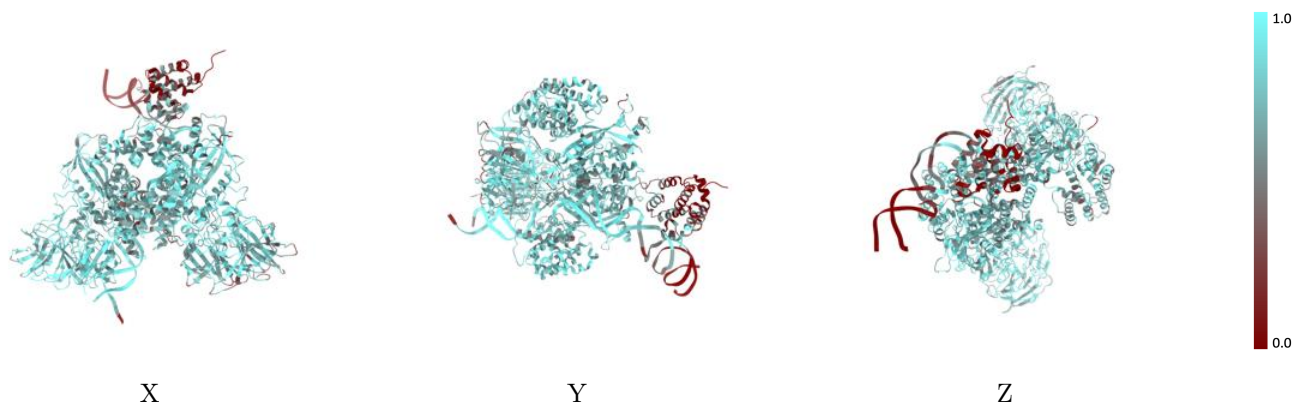
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



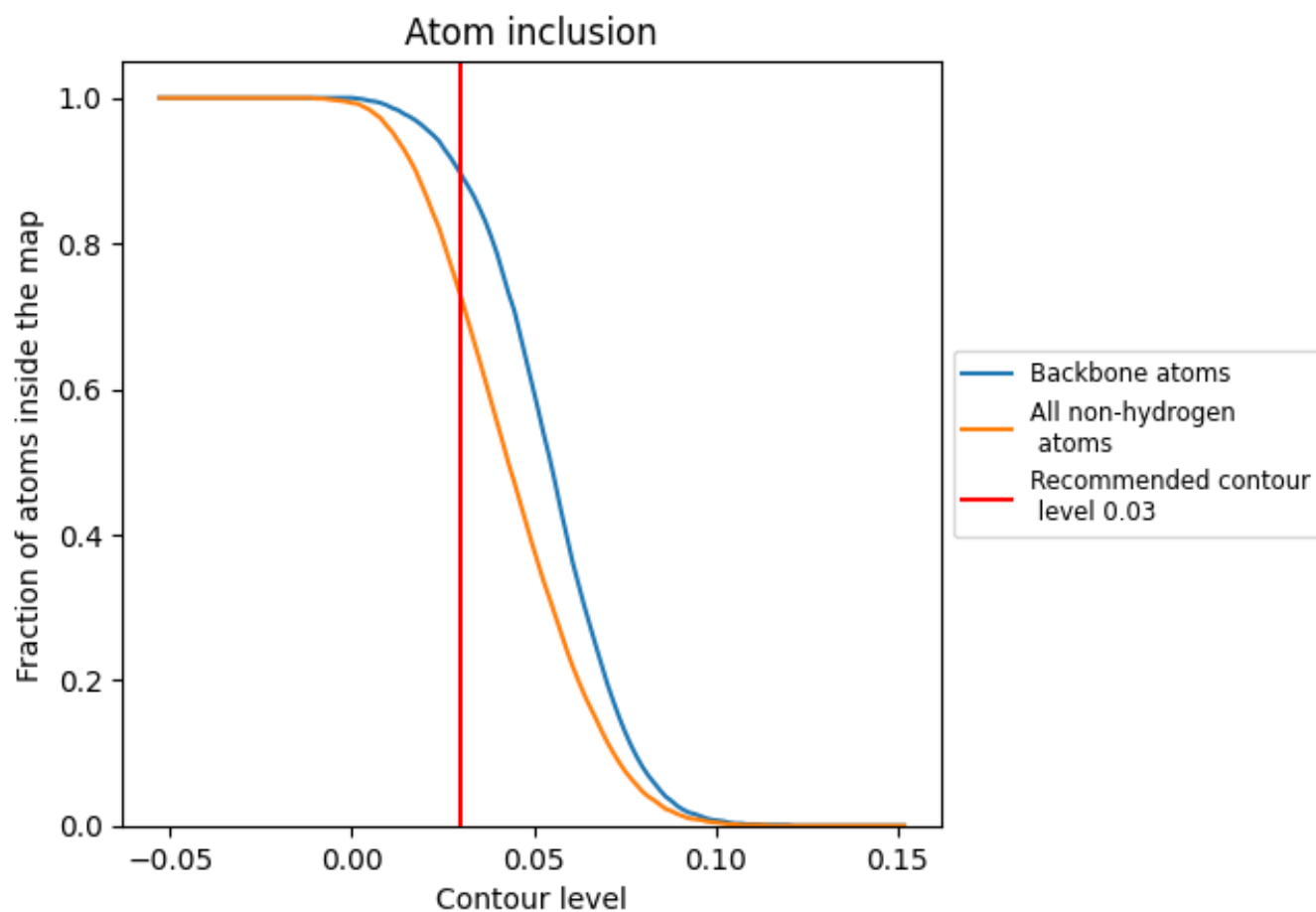
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 73% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7260	 0.2650
A	 0.7300	 0.2810
B	 0.8090	 0.2970
C	 0.6970	 0.2550
D	 0.7320	 0.2570
E	 0.6760	 0.2170
F	 0.6560	 0.2190

