Full wwPDB EM Validation Report (i)

Mar 4, 2024 – 07:12 AM EST

PDB ID	:	6CG0
EMDB ID	:	EMD-7470
Title	:	Cryo-EM structure of mouse RAG1/2 HFC complex (3.17 A)
Authors	:	Chen, X.; Kim, M.; Chuenchor, W.; Cui, Y.; Zhang, X.; Zhou, Z.H.; Gellert, M.; Yang, W.
Deposited on	:	2018-02-19
Resolution	:	3.17 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 (i) 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 (i)) were used in the production of this report:

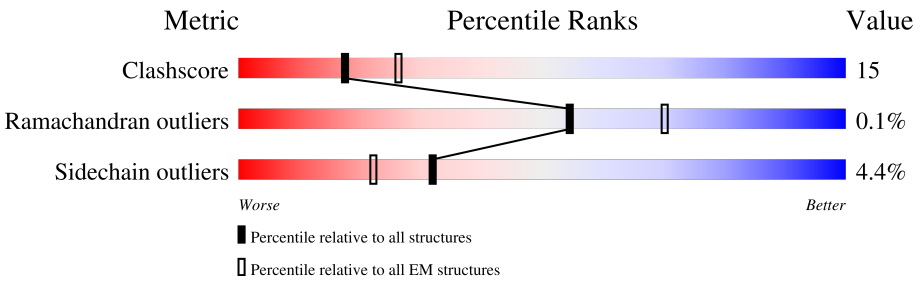
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.17 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	775	60% 18% • 21%
1	C	775	56% 19% • 21%
2	B	520	52% 13% • 34%
2	D	520	51% 13% • 34%
3	F	46	7% 50% 50%
4	I	16	62% 38%
5	J	19	5% 47% 53%
6	G	60	10% 30% 70%

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Mol	Chain	Length	Quality of chain
7	L	30	10% 47% 53%
8	M	41	12% 32% 68%
9	N	126	14% 50% 10% 40%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 20080 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
			Total	C	N	O	S		
1	A	614	4921	3097	876	914	34	0	0
1	C	616	4944	3111	881	918	34	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	962	GLN	GLU	conflict	UNP P15919
C	962	GLN	GLU	conflict	UNP P15919

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	342	2664	1701	452	493	18	2	0
2	B	342	2672	1706	453	494	19	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	490	ALA	THR	conflict	UNP P21784
B	490	ALA	THR	conflict	UNP P21784

- Molecule 3 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	F	46	947	452	172	278	45	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	I	16	323	156	54	98	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	J	19	387	185	64	119	19	0	0

- Molecule 6 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	G	60	1225	586	215	365	59	0	0

- Molecule 7 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	L	30	610	290	118	172	30	0	0

- Molecule 8 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	M	41	845	400	170	234	41	0	0

- Molecule 9 is a protein called High mobility group protein B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	N	75	538	346	92	96	4	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

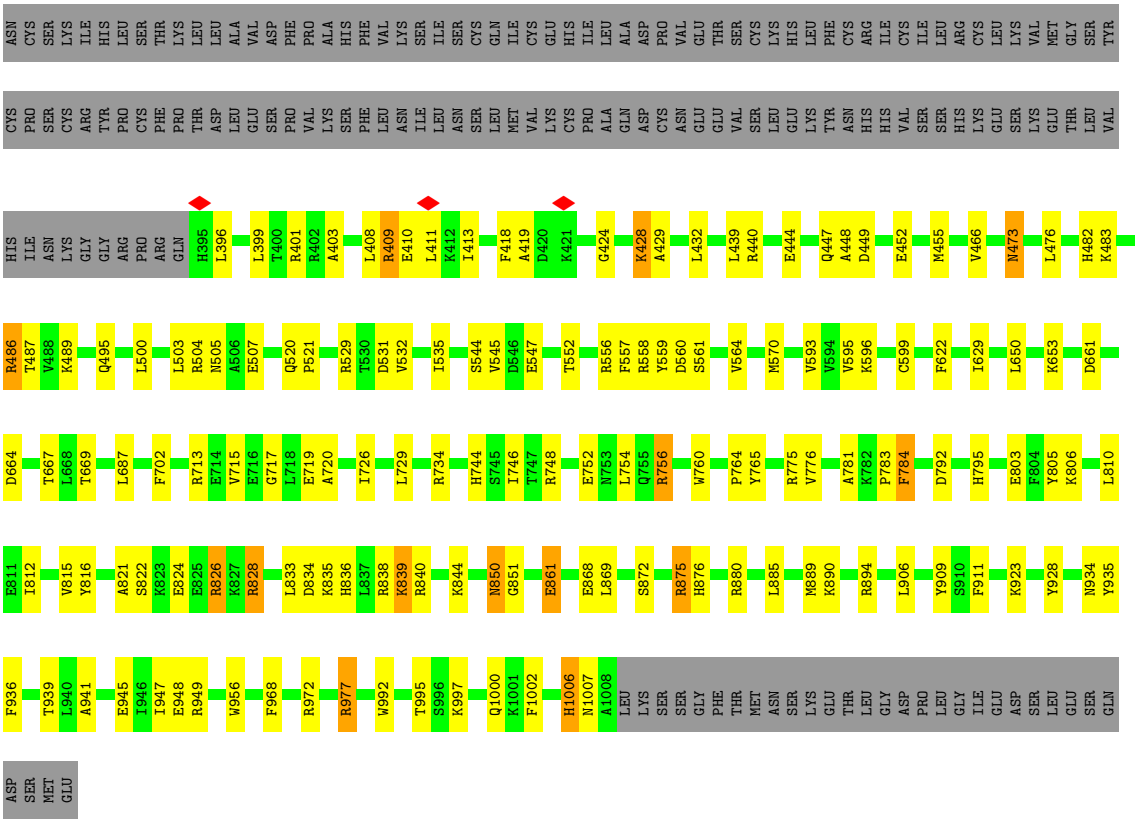
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
11	A	1	1	1	0
11	C	1	1	1	0

3 Residue-property plots (i)

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.

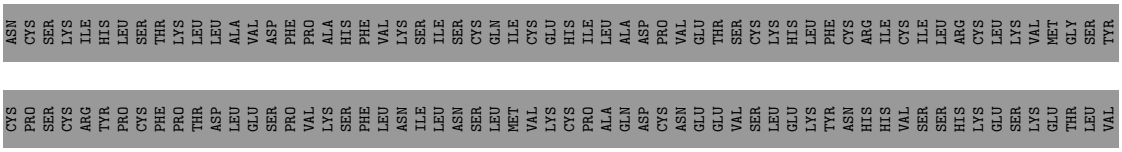
• Molecule 1: V(D)J recombination-activating protein 1

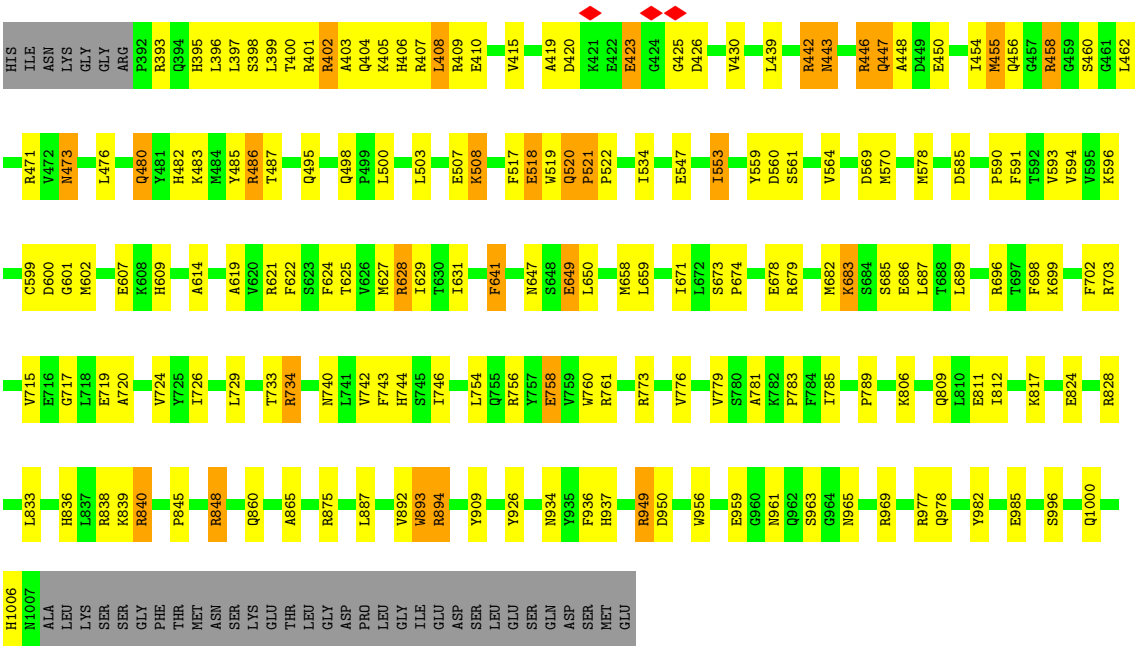
Chain A:



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

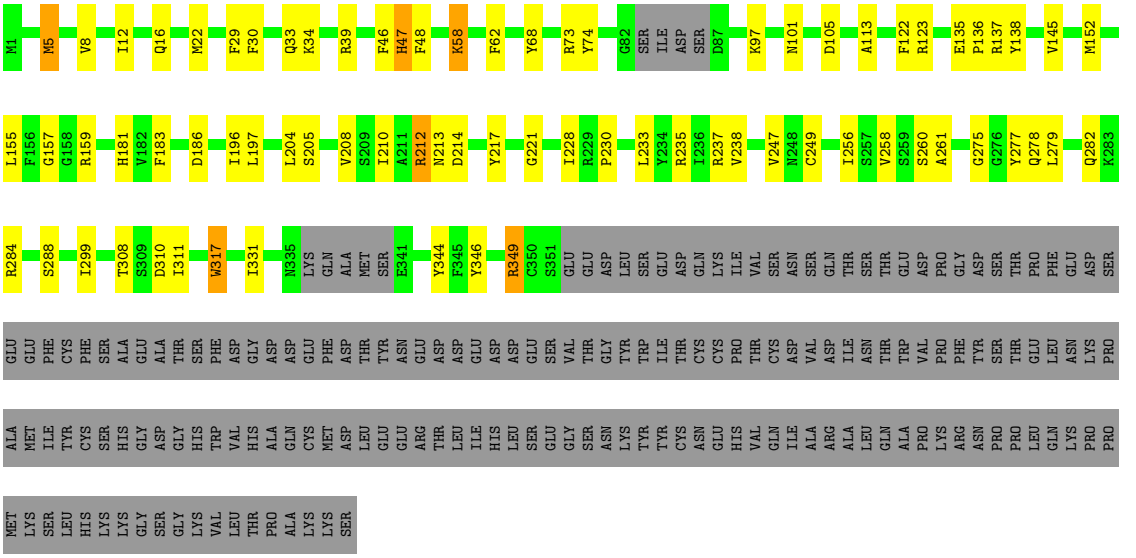
Chain C:





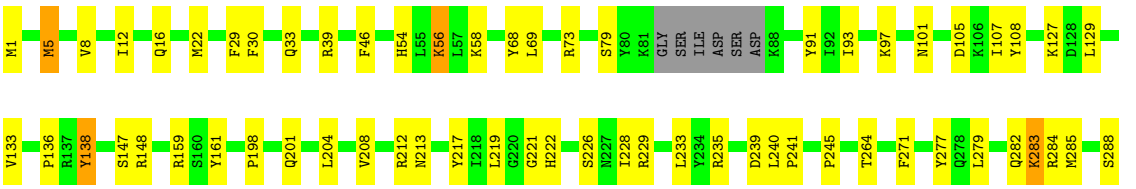
- Molecule 2: V(D)J recombination-activating protein 2

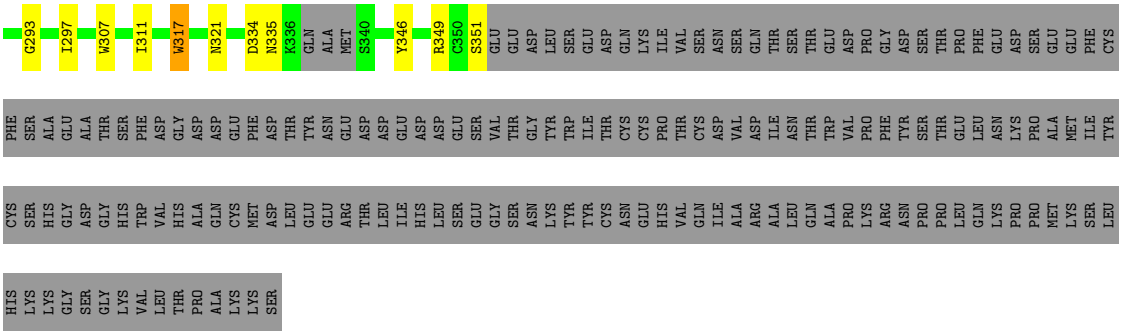
Chain D: 51% 13% • 34%



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

Chain B: 52% 13% • 34%



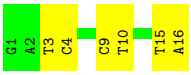


• Molecule 3: DNA (46-MER)

Chain F: 7% 50% 50%

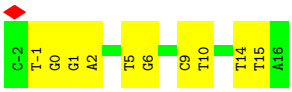
• Molecule 4: DNA (5'-D(*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3')

Chain I: 62% 38%



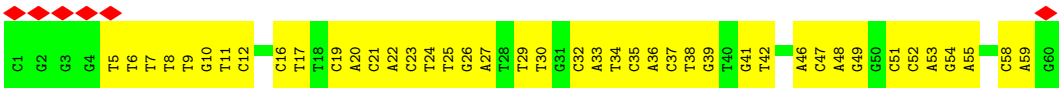
• Molecule 5: DNA (5'-D(P*CP*TP*GP*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3')

Chain J: 5% 47% 53%



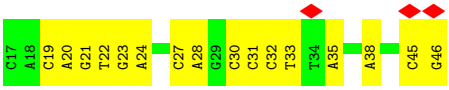
• Molecule 6: DNA (60-MER)

Chain G: 10% 30% 70%



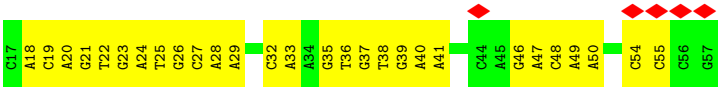
• Molecule 7: DNA (30-MER)

Chain L: 10% 47% 53%



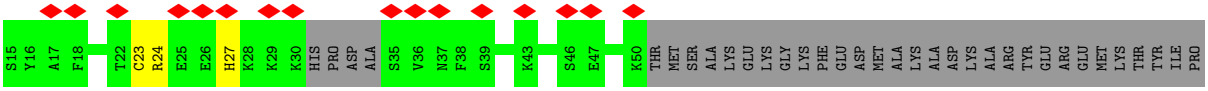
- Molecule 8: DNA (41-MER)

Chain M:



- Molecule 9: High mobility group protein B1

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	139781	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 ($e^-/Å^2$)	57.6	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	0.121	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0136	Depositor
Map size (Å)	308.16, 308.16, 308.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: CA, 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	0.24	0/5022	0.41	0/6767
1	C	0.24	0/5046	0.42	0/6798
2	B	0.25	0/2740	0.44	0/3716
2	D	0.25	0/2735	0.43	0/3712
3	F	0.59	0/1062	0.96	0/1640
4	I	0.49	0/360	0.97	0/554
5	J	0.54	0/431	1.08	0/663
6	G	0.52	0/1371	0.94	0/2115
7	L	0.59	0/685	0.84	0/1052
8	M	0.53	0/952	0.84	0/1466
9	N	0.24	0/553	0.37	0/748
All	All	0.34	0/20957	0.59	0/29231

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4921	0	4887	166	0
1	C	4944	0	4918	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2672	0	2605	63	0
2	D	2664	0	2585	65	0
3	F	947	0	522	24	0
4	I	323	0	184	5	0
5	J	387	0	217	7	0
6	G	1225	0	681	39	0
7	L	610	0	335	16	0
8	M	845	0	457	24	0
9	N	538	0	458	11	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
11	A	1	0	0	0	0
11	C	1	0	0	0	0
All	All	20080	0	17849	566	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 15.

All (566) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ARG:HG3	1:C:1006:HIS:NE2	1.46	1.29
2:B:283:LYS:HD2	2:B:317:TRP:CE2	1.82	1.14
1:A:486:ARG:CZ	1:C:1006:HIS:HE1	1.61	1.14
1:A:439:LEU:HD23	1:A:448:ALA:HB2	1.31	1.13
1:C:520:GLN:HB3	1:C:521:PRO:HD3	1.22	1.13
1:A:432:LEU:HD21	1:A:455:MET:SD	1.92	1.09
1:C:726:ILE:HG22	1:C:734:ARG:NH2	1.73	1.02
1:A:486:ARG:CZ	1:C:1006:HIS:CE1	2.42	1.01
1:A:532:VAL:HG21	1:A:558:ARG:HD3	1.44	0.99
1:A:409:ARG:HD2	1:A:413:ILE:HD11	1.46	0.97
1:A:977:ARG:HD3	8:M:23:DG:H1'	1.48	0.96
1:C:649:GLU:HG2	1:C:963:SER:HB3	1.49	0.95
1:C:726:ILE:CG2	1:C:734:ARG:NH2	2.30	0.94
2:B:283:LYS:HD2	2:B:317:TRP:CZ2	2.01	0.94
1:A:466:VAL:HG22	1:A:1002:PHE:CE1	2.03	0.94
1:A:432:LEU:CD2	1:A:455:MET:SD	2.57	0.93
2:D:256:ILE:HD11	2:D:299:ILE:HG21	1.50	0.92
2:D:349:ARG:HH21	2:D:349:ARG:HG3	1.34	0.92
1:C:726:ILE:CG2	1:C:734:ARG:HH21	1.82	0.92
1:A:439:LEU:HD23	1:A:448:ALA:CB	1.98	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ARG:HH21	1:C:407:ARG:HG3	1.35	0.91
1:A:466:VAL:HG22	1:A:1002:PHE:CD1	2.07	0.89
1:A:409:ARG:HG2	1:A:409:ARG:HH21	1.38	0.89
1:C:458:ARG:HH21	1:C:458:ARG:HB2	1.37	0.88
1:C:456:GLN:HG2	1:C:458:ARG:HD2	1.56	0.88
1:C:486:ARG:HH11	1:C:486:ARG:CB	1.88	0.87
1:A:483:LYS:HA	1:A:486:ARG:HD2	1.58	0.84
1:C:520:GLN:CB	1:C:521:PRO:HD3	2.05	0.84
1:A:486:ARG:CB	1:A:486:ARG:HH11	1.91	0.84
1:A:486:ARG:HG3	1:C:1006:HIS:CE1	2.13	0.83
1:C:892:VAL:HG21	1:C:909:TYR:HD1	1.42	0.83
1:A:1006:HIS:HD2	1:A:1007:ASN:N	1.76	0.83
1:C:520:GLN:HB3	1:C:521:PRO:CD	2.05	0.82
1:C:439:LEU:HD11	1:C:447:GLN:HB3	1.61	0.81
1:A:408:LEU:HD23	1:C:423:GLU:OE1	1.80	0.81
1:A:439:LEU:HD12	1:A:444:GLU:OE1	1.79	0.81
2:D:8:VAL:HG11	2:D:12:ILE:HD12	1.62	0.81
1:A:439:LEU:CD1	1:A:444:GLU:OE1	2.30	0.79
1:A:824:GLU:O	1:A:828:ARG:HG2	1.82	0.79
1:C:456:GLN:CG	1:C:458:ARG:HD2	2.13	0.79
1:C:458:ARG:HB2	1:C:458:ARG:NH2	1.98	0.79
1:A:822:SER:O	1:A:826:ARG:HD3	1.83	0.78
1:A:418:PHE:CZ	1:C:410:GLU:OE1	2.37	0.78
1:A:409:ARG:HG2	1:A:409:ARG:NH2	1.98	0.77
1:A:1006:HIS:ND1	1:C:486:ARG:HG3	1.98	0.77
1:A:826:ARG:HH11	1:A:826:ARG:HG2	1.49	0.76
1:A:439:LEU:HD23	1:A:448:ALA:CA	2.16	0.76
2:B:212:ARG:HG3	2:B:213:ASN:H	1.51	0.76
1:A:1006:HIS:CD2	1:A:1007:ASN:N	2.53	0.75
2:B:283:LYS:CD	2:B:317:TRP:CE2	2.68	0.75
1:A:466:VAL:CG2	1:A:1002:PHE:HE1	1.99	0.75
1:C:559:TYR:HH	1:C:702:PHE:HE1	1.36	0.74
1:C:848:ARG:HD2	6:G:42:DT:C2	2.24	0.73
2:D:212:ARG:CG	2:D:213:ASN:H	2.00	0.73
2:B:264:THR:O	2:B:271:PHE:HD1	1.72	0.73
1:A:466:VAL:CG2	1:A:1002:PHE:CE1	2.72	0.73
1:A:547:GLU:OE2	2:B:159:ARG:NH1	2.23	0.72
2:D:152:MET:SD	2:D:186:ASP:OD1	2.47	0.72
1:C:934:ASN:HD22	5:J:15:DT:H5'	1.54	0.72
2:D:258:VAL:HG22	2:D:284:ARG:HD3	1.72	0.72
1:A:409:ARG:HD2	1:A:413:ILE:CD1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:ASP:HB3	2:B:136:PRO:HG3	1.72	0.72
2:B:222:HIS:HD2	2:B:229:ARG:HE	1.39	0.71
2:D:47[A]:HIS:HB2	2:D:58:LYS:HG2	1.72	0.71
8:M:36:DT:H2"	8:M:37:DG:C8	2.26	0.71
1:C:559:TYR:OH	1:C:702:PHE:HE1	1.74	0.71
1:C:658:MET:SD	1:C:671:ILE:HG21	2.32	0.70
1:A:1006:HIS:CE1	1:C:486:ARG:CZ	2.75	0.70
1:A:440:ARG:NH1	1:C:401:ARG:CZ	2.55	0.69
1:A:483:LYS:HA	1:A:486:ARG:CD	2.22	0.69
1:A:752:GLU:O	1:A:756:ARG:HG2	1.92	0.69
1:C:407:ARG:HG3	1:C:407:ARG:NH2	2.07	0.69
1:A:1006:HIS:HE1	1:C:486:ARG:NH2	1.90	0.69
1:C:591:PHE:HE1	1:C:631:ILE:HD12	1.58	0.69
1:C:758:GLU:HA	1:C:758:GLU:OE2	1.90	0.69
1:C:439:LEU:HA	1:C:442:ARG:HE	1.57	0.69
2:D:284:ARG:NH1	2:D:288:SER:OG	2.26	0.68
8:M:49:DA:H2'	8:M:50:DA:C8	2.28	0.68
1:C:726:ILE:HG21	1:C:734:ARG:HH21	1.58	0.68
1:A:775:ARG:HG3	1:A:775:ARG:HH11	1.57	0.68
1:C:406:HIS:O	1:C:409:ARG:NH1	2.26	0.68
6:G:37:DC:H2'	6:G:38:DT:H71	1.76	0.68
6:G:6:DT:H2'	6:G:7:DT:H72	1.76	0.68
1:C:480:GLN:HA	1:C:480:GLN:OE1	1.93	0.68
1:C:559:TYR:CE2	1:C:702:PHE:HE1	2.11	0.68
1:C:442:ARG:C	1:C:443:ASN:OD1	2.32	0.68
7:L:20:DA:H2"	7:L:21:DG:H5"	1.74	0.67
1:C:559:TYR:HE2	1:C:702:PHE:CE1	2.13	0.67
1:C:519:TRP:HZ2	1:C:560:ASP:HB2	1.58	0.67
1:C:559:TYR:CE2	1:C:702:PHE:CE1	2.82	0.67
1:C:949:ARG:HG2	1:C:949:ARG:NH2	2.09	0.67
9:N:110:ARG:HG3	9:N:129:LEU:CD2	2.25	0.67
3:F:12:DT:H73	3:F:13:DA:N6	2.10	0.67
2:B:148:ARG:NH1	2:B:239:ASP:OD1	2.28	0.66
2:B:30:PHE:HB3	2:B:46:PHE:HB2	1.77	0.66
1:C:848:ARG:HG2	1:C:848:ARG:HH11	1.61	0.66
1:A:556:ARG:HD2	1:A:557:PHE:O	1.95	0.66
1:C:977:ARG:HH12	7:L:24:DA:H5'	1.61	0.66
1:A:486:ARG:CG	1:C:1006:HIS:NE2	2.42	0.66
2:D:279:LEU:HB2	2:D:282:GLN:HB3	1.77	0.66
1:A:411:LEU:HD21	1:C:415:VAL:HG13	1.77	0.65
1:A:713:ARG:NH2	1:A:726:ILE:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:106:CYS:HB3	9:N:110:ARG:HE	1.60	0.65
1:C:740:ASN:HD21	1:C:743:PHE:HB2	1.61	0.65
1:C:828:ARG:HH12	2:B:5:MET:HE2	1.61	0.65
8:M:20:DA:H2"	8:M:21:DG:H5"	1.78	0.65
1:A:836:HIS:CD2	1:A:869:LEU:HD11	2.32	0.65
2:D:145:VAL:HG13	2:D:214:ASP:HA	1.79	0.65
1:C:726:ILE:HG21	1:C:734:ARG:NH2	2.12	0.65
2:B:198:PRO:O	2:B:201:GLN:NE2	2.29	0.65
1:C:828:ARG:HH12	2:B:5:MET:CE	2.09	0.64
1:A:775:ARG:HG3	1:A:775:ARG:NH1	2.11	0.64
6:G:19:DC:H2"	6:G:20:DA:H5'	1.80	0.64
8:M:35:DG:H2'	8:M:36:DT:H5'	1.80	0.64
1:A:396:LEU:HD11	1:C:426:ASP:HB3	1.80	0.64
1:A:486:ARG:NH1	1:C:1006:HIS:CE1	2.65	0.64
1:C:949:ARG:HG2	1:C:949:ARG:HH21	1.60	0.64
9:N:23:CYS:O	9:N:27:HIS:ND1	2.30	0.64
2:D:212:ARG:HG3	2:D:213:ASN:H	1.63	0.64
1:A:828:ARG:NH2	1:A:828:ARG:HG3	2.13	0.63
2:D:152:MET:CE	2:D:186:ASP:OD1	2.46	0.63
1:C:977:ARG:HH21	1:C:982:TYR:HB3	1.64	0.63
1:C:848:ARG:HG2	1:C:848:ARG:NH1	2.14	0.63
1:A:838:ARG:HH21	1:C:614:ALA:HA	1.63	0.63
1:C:419:ALA:HA	1:C:423:GLU:HG3	1.80	0.63
1:A:836:HIS:CD2	1:A:869:LEU:CD1	2.82	0.63
1:C:399:LEU:HD23	1:C:403:ALA:HB1	1.80	0.63
1:C:483:LYS:HA	1:C:486:ARG:HD2	1.79	0.63
1:A:486:ARG:HG2	1:A:487:THR:N	2.12	0.63
7:L:45:DC:H2'	7:L:46:DG:C8	2.34	0.63
1:C:518:GLU:O	1:C:518:GLU:HG3	1.99	0.63
1:C:485:TYR:OH	1:C:495:GLN:NE2	2.31	0.62
1:A:1006:HIS:HD2	1:A:1007:ASN:H	1.47	0.62
2:D:349:ARG:HG3	2:D:349:ARG:NH2	2.04	0.62
1:C:462:LEU:O	1:C:498:GLN:NE2	2.22	0.62
1:C:806:LYS:HD2	1:C:809:GLN:HE21	1.65	0.62
1:A:418:PHE:HZ	1:C:410:GLU:OE1	1.82	0.61
1:C:404:GLN:O	1:C:408:LEU:HG	1.99	0.61
1:C:596:LYS:HG3	1:C:956:TRP:CE3	2.35	0.61
1:A:844:LYS:NZ	1:C:607:GLU:O	2.25	0.61
1:A:803:GLU:OE2	1:A:803:GLU:HA	2.00	0.61
1:C:578:MET:HE1	1:C:591:PHE:HZ	1.66	0.61
6:G:23:DC:H2'	6:G:24:DT:C6	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ARG:HH12	1:C:401:ARG:CZ	2.14	0.61
1:C:486:ARG:HH11	1:C:486:ARG:CG	2.14	0.61
1:A:408:LEU:CD2	1:C:423:GLU:OE1	2.49	0.61
1:A:419:ALA:O	1:A:424:GLY:N	2.31	0.60
1:A:486:ARG:HH11	1:A:486:ARG:CG	2.13	0.60
6:G:35:DC:H2"	6:G:36:DA:C8	2.36	0.60
1:A:826:ARG:HH11	1:A:826:ARG:CG	2.14	0.60
2:B:349:ARG:NH1	2:B:351:SER:OG	2.33	0.60
1:C:399:LEU:HD22	1:C:407:ARG:HH21	1.66	0.60
1:C:649:GLU:CG	1:C:963:SER:HB3	2.29	0.60
1:C:828:ARG:NH2	2:B:5:MET:SD	2.73	0.60
1:A:504:ARG:HG3	1:A:504:ARG:HH11	1.67	0.60
1:C:828:ARG:NH1	2:B:5:MET:HE2	2.15	0.60
1:C:678:GLU:O	1:C:682:MET:HG3	2.01	0.59
1:C:892:VAL:HG21	1:C:909:TYR:CD1	2.31	0.59
1:C:949:ARG:HH21	1:C:949:ARG:CG	2.13	0.59
1:C:482:HIS:HB2	1:C:500:LEU:HD11	1.84	0.59
1:A:828:ARG:CG	1:A:828:ARG:HH21	2.14	0.59
1:C:534:ILE:HG21	1:C:985:GLU:HG3	1.85	0.59
8:M:36:DT:O4'	9:N:122:ILE:HD13	2.03	0.59
2:D:258:VAL:CG2	2:D:284:ARG:HD3	2.31	0.59
2:B:1:MET:N	2:B:349:ARG:O	2.36	0.59
1:A:486:ARG:NE	1:C:1006:HIS:HE1	2.01	0.59
1:A:828:ARG:HG3	1:A:828:ARG:HH21	1.68	0.59
1:C:593:VAL:HG22	1:C:629:ILE:HG12	1.83	0.59
1:C:559:TYR:CZ	1:C:702:PHE:HE1	2.21	0.58
2:B:54:HIS:HD2	2:B:56:LYS:NZ	2.01	0.58
1:C:559:TYR:HD2	1:C:682:MET:SD	2.26	0.58
1:A:483:LYS:CA	1:A:486:ARG:HD2	2.32	0.58
1:C:969:ARG:NH2	6:G:41:DG:OP1	2.37	0.58
1:A:570:MET:HG2	1:A:997:LYS:HD2	1.85	0.58
3:F:6:DT:H2'	3:F:7:DT:C6	2.38	0.58
1:C:578:MET:CE	1:C:591:PHE:CZ	2.87	0.58
1:C:520:GLN:O	1:C:520:GLN:NE2	2.37	0.58
1:C:860:GLN:HE21	1:C:887:LEU:HD12	1.68	0.58
1:A:1006:HIS:HE1	1:C:486:ARG:CZ	2.14	0.58
1:C:508:LYS:N	1:C:508:LYS:HD3	2.17	0.58
1:C:836:HIS:NE2	1:C:865:ALA:O	2.37	0.58
1:A:440:ARG:HE	1:A:448:ALA:HB3	1.69	0.58
1:A:803:GLU:HG3	1:A:928:TYR:OH	2.04	0.58
7:L:45:DC:H2'	7:L:46:DG:H8	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:MET:CE	1:C:702:PHE:HZ	2.17	0.57
1:A:483:LYS:O	1:A:486:ARG:CD	2.52	0.57
2:D:210:ILE:HB	2:D:217:TYR:HB2	1.87	0.57
2:D:212:ARG:CG	2:D:213:ASN:N	2.68	0.57
1:A:520:GLN:HB3	1:A:521:PRO:HD3	1.87	0.56
1:C:839:LYS:HE2	1:C:840:ARG:HH12	1.68	0.56
2:B:317:TRP:N	2:B:317:TRP:CD1	2.73	0.56
1:A:428:LYS:HG2	1:A:429:ALA:N	2.19	0.56
1:A:552:THR:HG21	1:A:667:THR:HG21	1.87	0.56
6:G:9:DT:H2"	6:G:10:DG:C8	2.40	0.56
6:G:26:DG:H2"	6:G:27:DA:H5"	1.86	0.56
7:L:21:DG:H2'	7:L:22:DT:H71	1.88	0.56
1:C:720:ALA:HB3	6:G:46:DA:H5'	1.85	0.56
1:A:466:VAL:HG22	1:A:1002:PHE:HD1	1.65	0.56
1:C:517:PHE:CD1	1:C:564:VAL:HG21	2.40	0.56
1:A:803:GLU:HG2	1:A:936:PHE:HE2	1.71	0.56
2:B:212:ARG:NH1	2:B:293:GLY:O	2.37	0.56
3:F:5:DT:H2'	3:F:6:DT:H71	1.88	0.56
6:G:29:DT:H2"	6:G:30:DT:H5"	1.87	0.56
2:B:283:LYS:CD	2:B:317:TRP:NE1	2.70	0.55
6:G:23:DC:C2	8:M:35:DG:N2	2.74	0.55
2:D:5:MET:HG2	2:D:346:TYR:CE1	2.42	0.55
2:B:284:ARG:NH2	2:B:288:SER:OG	2.37	0.55
2:D:155:LEU:HB3	2:D:183:PHE:HB2	1.88	0.55
2:D:311:ILE:HD11	2:D:346:TYR:HD2	1.71	0.55
9:N:110:ARG:CG	9:N:129:LEU:CD2	2.84	0.55
1:A:486:ARG:NH2	1:C:1006:HIS:HE1	2.02	0.55
1:C:719:GLU:OE1	1:C:773:ARG:NH2	2.40	0.55
1:C:578:MET:CE	1:C:591:PHE:HZ	2.20	0.55
1:A:483:LYS:NZ	8:M:21:DG:OP1	2.40	0.55
1:A:872:SER:HB3	1:A:875:ARG:HG3	1.89	0.55
1:A:593:VAL:HG22	1:A:629:ILE:HG12	1.89	0.55
1:C:650:LEU:HB3	1:C:1000:GLN:HE22	1.72	0.54
9:N:110:ARG:HG3	9:N:129:LEU:HD23	1.88	0.54
1:A:729:LEU:HB3	1:A:746:ILE:HG22	1.88	0.54
1:C:828:ARG:NH1	2:B:5:MET:CE	2.71	0.54
1:C:585:ASP:O	1:C:696:ARG:NH1	2.39	0.54
2:B:129:LEU:HG	2:B:133:VAL:HG12	1.88	0.54
6:G:7:DT:H2'	6:G:8:DT:H71	1.89	0.54
1:A:885:LEU:O	1:A:889:MET:HG3	2.08	0.54
1:C:602:MET:N	1:C:619:ALA:O	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:ILE:HD11	2:D:346:TYR:CD2	2.43	0.54
2:D:308:THR:OG1	2:D:310:ASP:OD1	2.21	0.54
2:B:16:GLN:NE2	2:B:33:GLN:O	2.41	0.54
1:A:439:LEU:HD11	1:A:444:GLU:OE1	2.05	0.53
1:C:443:ASN:OD1	1:C:443:ASN:N	2.40	0.53
2:B:208:VAL:HB	2:B:219:LEU:HB2	1.90	0.53
1:A:466:VAL:HG23	1:A:1002:PHE:HE1	1.72	0.53
2:B:39:ARG:HG3	3:F:35:DA:H3'	1.89	0.53
1:C:758:GLU:OE1	1:C:761:ARG:NH2	2.42	0.53
9:N:131:GLU:O	9:N:135:ASN:ND2	2.42	0.53
1:A:440:ARG:HH12	1:C:401:ARG:NH2	2.07	0.53
1:C:649:GLU:HG2	1:C:963:SER:CB	2.30	0.53
1:C:726:ILE:HG21	1:C:734:ARG:HE	1.74	0.53
3:F:10:DG:H1'	3:F:11:DT:H5'	1.91	0.53
3:F:43:DG:H2"	3:F:44:DA:N7	2.23	0.53
1:A:826:ARG:N	1:A:826:ARG:HD2	2.24	0.53
1:C:602:MET:SD	1:C:965:ASN:ND2	2.81	0.53
1:A:754:LEU:HD23	1:A:783:PRO:HD2	1.89	0.53
8:M:35:DG:C2'	8:M:36:DT:H5'	2.38	0.53
1:A:840:ARG:NH1	1:A:868:GLU:OE1	2.42	0.52
1:C:682:MET:HE2	1:C:702:PHE:CZ	2.43	0.52
6:G:5:DT:H2"	6:G:6:DT:C6	2.44	0.52
1:A:428:LYS:HB2	1:C:442:ARG:NH1	2.25	0.52
5:J:14:DT:H2'	5:J:15:DT:C6	2.45	0.52
1:A:720:ALA:HB3	3:F:35:DA:H5'	1.91	0.52
1:C:486:ARG:HH11	1:C:486:ARG:HB3	1.74	0.52
6:G:8:DT:H1'	6:G:9:DT:H5"	1.90	0.52
1:A:805:TYR:OH	1:A:834:ASP:OD1	2.26	0.52
1:A:726:ILE:HG22	1:A:734:ARG:NH1	2.25	0.52
2:D:197:LEU:HD21	2:D:247:VAL:HG23	1.92	0.52
1:A:599:CYS:HB2	1:A:622:PHE:HD1	1.75	0.52
3:F:36:DC:H2"	3:F:37:DA:C8	2.45	0.52
8:M:18:DA:C8	8:M:18:DA:H5'	2.44	0.52
1:C:399:LEU:HG	3:F:8:DT:H3'	1.92	0.52
1:C:486:ARG:HH11	1:C:486:ARG:HB2	1.70	0.51
2:D:277:TYR:HE1	2:D:317:TRP:CD1	2.28	0.51
2:B:93:ILE:HB	2:B:108:TYR:HB2	1.92	0.51
1:A:650:LEU:HB3	1:A:1000:GLN:HE22	1.76	0.51
2:B:147:SER:HB3	2:B:240:LEU:HD23	1.91	0.51
1:A:826:ARG:CG	1:A:826:ARG:NH1	2.73	0.51
1:C:578:MET:HE1	1:C:591:PHE:CZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:828:ARG:NH1	2:B:5:MET:SD	2.83	0.51
1:A:812:ILE:HD11	1:A:833:LEU:HD13	1.92	0.51
1:C:726:ILE:HG21	1:C:734:ARG:NE	2.26	0.51
1:C:776:VAL:HG22	1:C:779:VAL:HB	1.91	0.51
1:C:978:GLN:HE21	3:F:27:DT:H4'	1.75	0.51
2:B:229:ARG:HH22	2:B:277:TYR:HB2	1.76	0.51
2:B:334:ASP:OD1	2:B:335:ASN:N	2.43	0.51
1:A:532:VAL:HB	1:A:535:ILE:HD11	1.92	0.51
1:A:560:ASP:OD1	1:A:561:SER:N	2.44	0.51
1:C:439:LEU:HD22	1:C:448:ALA:HB2	1.93	0.51
1:A:418:PHE:CE1	1:C:410:GLU:OE1	2.64	0.51
1:C:520:GLN:NE2	1:C:520:GLN:HA	2.25	0.51
5:J:-1:DT:H2"	5:J:0:DG:C8	2.46	0.51
1:C:520:GLN:CB	1:C:521:PRO:CD	2.78	0.50
1:C:520:GLN:NE2	1:C:520:GLN:CA	2.73	0.50
2:D:275:GLY:CA	2:D:284:ARG:HG2	2.41	0.50
1:C:717:GLY:HA2	1:C:781:ALA:HB3	1.92	0.50
2:B:54:HIS:CD2	2:B:56:LYS:NZ	2.79	0.50
3:F:41:DC:H2"	3:F:42:DA:C8	2.46	0.50
1:A:486:ARG:CG	1:A:486:ARG:NH1	2.73	0.50
1:C:407:ARG:NH2	1:C:407:ARG:CG	2.73	0.50
1:C:703:ARG:NH1	1:C:950:ASP:OD1	2.37	0.50
2:D:159:ARG:HH21	2:D:205:SER:HB2	1.76	0.50
2:D:204:LEU:HD11	2:D:221:GLY:HA3	1.93	0.50
1:A:440:ARG:NH2	1:A:449:ASP:OD1	2.44	0.50
1:A:760:TRP:HB2	1:A:776:VAL:HG11	1.93	0.50
1:C:473:ASN:ND2	1:C:473:ASN:O	2.44	0.50
1:C:726:ILE:CG2	1:C:734:ARG:CZ	2.90	0.50
2:D:217:TYR:HE1	2:D:235:ARG:HG3	1.77	0.50
8:M:46:DG:H1'	8:M:47:DA:H5'	1.92	0.50
1:C:560:ASP:OD1	1:C:561:SER:N	2.45	0.50
2:B:107:ILE:HG23	2:B:127:LYS:HB3	1.93	0.50
1:A:726:ILE:HG21	1:A:734:ARG:CZ	2.42	0.49
1:A:1006:HIS:CD2	1:A:1006:HIS:C	2.86	0.49
2:D:39:ARG:HG3	6:G:46:DA:H3'	1.94	0.49
6:G:38:DT:H2'	6:G:39:DG:N7	2.27	0.49
1:A:968:PHE:C	1:A:968:PHE:CD2	2.85	0.49
1:A:486:ARG:HH11	1:A:486:ARG:HB3	1.72	0.49
1:C:458:ARG:NH2	1:C:458:ARG:CB	2.73	0.49
1:C:893:TRP:CD1	1:C:893:TRP:C	2.85	0.49
2:D:73:ARG:NH2	2:D:97:LYS:HD3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:51:DC:H2"	6:G:52:DC:C6	2.48	0.49
1:A:764:PRO:HG2	1:A:765:TYR:CD2	2.47	0.49
1:A:876:HIS:O	1:A:880:ARG:HG2	2.12	0.49
1:A:909:TYR:OH	1:A:939:THR:O	2.26	0.49
1:C:641:PHE:C	1:C:641:PHE:CD2	2.86	0.49
1:C:729:LEU:HD23	1:C:746:ILE:HG12	1.95	0.49
2:B:138:TYR:C	2:B:138:TYR:CD2	2.85	0.49
2:B:311:ILE:HD11	2:B:346:TYR:HE2	1.78	0.49
1:A:483:LYS:O	1:A:486:ARG:HD2	2.12	0.49
1:C:569:ASP:OD1	1:C:996:SER:OG	2.30	0.49
1:C:740:ASN:ND2	1:C:743:PHE:HB2	2.27	0.49
2:D:105:ASP:HB3	2:D:136:PRO:HB3	1.93	0.49
1:C:517:PHE:C	1:C:517:PHE:CD2	2.86	0.49
1:A:803:GLU:HG2	1:A:936:PHE:CE2	2.48	0.49
1:A:810:LEU:HD22	1:A:815:VAL:HG21	1.95	0.49
3:F:11:DT:H73	7:L:35:DA:N6	2.28	0.49
1:C:405:LYS:NZ	7:L:33:DT:OP2	2.46	0.48
1:C:590:PRO:HB2	1:C:699:LYS:HE3	1.94	0.48
4:I:3:DT:H2"	4:I:4:DC:C6	2.48	0.48
5:J:5:DT:H2"	5:J:6:DG:C8	2.48	0.48
8:M:25:DT:H2"	8:M:26:DG:C8	2.48	0.48
8:M:32:DC:H2"	8:M:33:DA:C8	2.48	0.48
1:A:844:LYS:HG2	1:C:609:HIS:CE1	2.48	0.48
5:J:9:DC:H4'	5:J:10:DT:OP1	2.13	0.48
1:C:420:ASP:HA	1:C:425:GLY:HA2	1.93	0.48
1:C:812:ILE:HD11	1:C:833:LEU:HD13	1.94	0.48
8:M:54:DC:H2'	8:M:55:DC:C6	2.49	0.48
1:A:473:ASN:O	1:A:473:ASN:ND2	2.47	0.48
1:A:822:SER:O	1:A:826:ARG:CD	2.59	0.48
1:C:443:ASN:HD21	6:G:17:DT:H1'	1.78	0.48
1:C:486:ARG:CG	1:C:486:ARG:NH1	2.73	0.48
5:J:5:DT:H2"	5:J:6:DG:N7	2.28	0.48
6:G:22:DA:H2'	6:G:23:DC:C6	2.47	0.48
1:A:564:VAL:HG22	1:A:687:LEU:HD21	1.95	0.48
1:C:724:VAL:HG22	1:C:733:THR:HB	1.95	0.48
3:F:45:DT:H2"	3:F:46:DC:C5	2.49	0.48
9:N:110:ARG:CG	9:N:129:LEU:HD23	2.43	0.48
1:A:503:LEU:O	1:A:507:GLU:HG3	2.14	0.48
1:A:821:ALA:CB	1:A:826:ARG:HE	2.27	0.48
1:C:682:MET:CE	1:C:702:PHE:CZ	2.96	0.48
2:B:97:LYS:NZ	2:B:161:TYR:OH	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:LEU:HD11	2:B:221:GLY:HA3	1.96	0.48
6:G:23:DC:H2'	6:G:24:DT:C5	2.49	0.48
7:L:32:DC:H2'	7:L:33:DT:H71	1.94	0.48
6:G:32:DC:H2"	6:G:33:DA:C8	2.49	0.47
1:A:483:LYS:O	1:A:486:ARG:HD3	2.13	0.47
1:C:503:LEU:O	1:C:507:GLU:HG3	2.14	0.47
1:A:428:LYS:HB2	1:C:442:ARG:HH12	1.79	0.47
2:D:47[A]:HIS:HB2	2:D:58:LYS:CG	2.44	0.47
2:D:238:VAL:HG12	2:D:247:VAL:HG12	1.96	0.47
2:B:212:ARG:HG3	2:B:213:ASN:N	2.25	0.47
6:G:47:DC:H2"	6:G:48:DA:C8	2.49	0.47
6:G:52:DC:H2"	6:G:53:DA:C8	2.49	0.47
7:L:20:DA:C4	7:L:21:DG:C8	3.03	0.47
8:M:47:DA:H2"	8:M:48:DC:C4	2.49	0.47
1:C:811:GLU:OE2	1:C:926:TYR:OH	2.21	0.47
4:I:9:DC:H2'	4:I:10:DT:C6	2.49	0.47
6:G:11:DT:H2'	6:G:12:DC:C6	2.50	0.47
1:A:838:ARG:NH2	1:C:607:GLU:OE2	2.34	0.47
1:C:553:ILE:HG12	1:C:553:ILE:O	2.14	0.47
1:C:679:ARG:NH2	1:C:683:LYS:NZ	2.62	0.47
1:C:848:ARG:HD2	6:G:42:DT:O2	2.15	0.47
6:G:54:DG:H2"	6:G:55:DA:C8	2.48	0.47
1:A:439:LEU:CD2	1:A:448:ALA:CA	2.91	0.47
1:C:760:TRP:CZ2	2:D:68:TYR:CD2	3.02	0.47
1:C:894:ARG:HD3	1:C:894:ARG:HA	1.58	0.47
2:D:208:VAL:HG21	2:D:261:ALA:HB3	1.96	0.47
2:D:275:GLY:HA2	2:D:284:ARG:HG2	1.97	0.47
6:G:32:DC:H2"	6:G:33:DA:H8	1.80	0.47
1:A:653:LYS:NZ	1:A:995:THR:O	2.45	0.47
8:M:21:DG:C8	8:M:22:DT:H72	2.49	0.47
2:B:233:LEU:HD11	2:B:297:ILE:HD13	1.95	0.47
2:B:311:ILE:HD11	2:B:346:TYR:CE2	2.49	0.47
1:C:715:VAL:HG11	1:C:785:ILE:HB	1.97	0.46
1:A:596:LYS:HB2	1:A:956:TRP:CZ3	2.50	0.46
1:A:935:TYR:OH	4:I:16:DA:OP1	2.33	0.46
1:C:396:LEU:HD11	1:C:408:LEU:HD21	1.97	0.46
1:C:547:GLU:OE2	2:D:159:ARG:NH1	2.47	0.46
6:G:16:DC:H2'	6:G:17:DT:C6	2.50	0.46
1:C:744:HIS:CE1	1:C:937:HIS:HE1	2.33	0.46
1:C:828:ARG:HH22	2:B:5:MET:CE	2.29	0.46
3:F:12:DT:H73	3:F:13:DA:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:GLN:C	1:C:520:GLN:HE21	2.19	0.46
2:B:285:MET:CE	2:B:307:TRP:CD1	2.98	0.46
6:G:21:DC:N3	6:G:22:DA:N6	2.64	0.46
8:M:25:DT:H2"	8:M:26:DG:H8	1.81	0.46
8:M:47:DA:H2"	8:M:48:DC:C5	2.51	0.46
1:A:861:GLU:H	1:A:861:GLU:HG2	1.46	0.46
1:A:911:PHE:CD1	1:A:911:PHE:C	2.87	0.46
2:D:62:PHE:CD1	2:D:122:PHE:HB2	2.51	0.46
2:D:113:ALA:HB2	2:D:123:ARG:HB2	1.97	0.46
2:D:137:ARG:HH11	2:D:157:GLY:HA2	1.81	0.46
2:D:235:ARG:NH1	2:D:237:ARG:HE	2.13	0.46
7:L:31:DC:H2'	7:L:32:DC:H6	1.81	0.46
1:C:679:ARG:CZ	1:C:683:LYS:HZ3	2.29	0.46
1:C:687:LEU:HB3	1:C:698:PHE:HB2	1.98	0.46
5:J:1:DG:H2"	5:J:2:DA:C8	2.51	0.46
1:C:596:LYS:N	1:C:625:THR:O	2.46	0.46
4:I:9:DC:H2"	4:I:10:DT:O5'	2.16	0.46
1:A:439:LEU:CD2	1:A:448:ALA:N	2.80	0.45
1:A:803:GLU:CG	1:A:928:TYR:OH	2.64	0.45
1:C:407:ARG:HD3	3:F:8:DT:H71	1.98	0.45
1:C:471:ARG:HG2	1:C:471:ARG:HH11	1.82	0.45
1:C:726:ILE:HG21	1:C:734:ARG:CZ	2.46	0.45
2:D:30:PHE:HB3	2:D:46:PHE:HB2	1.98	0.45
2:D:181:HIS:CE1	2:D:196:ILE:HG12	2.51	0.45
1:C:773:ARG:HA	1:C:776:VAL:HG12	1.96	0.45
2:D:16:GLN:NE2	2:D:33:GLN:O	2.49	0.45
1:A:482:HIS:HB2	1:A:500:LEU:HD11	1.98	0.45
1:A:744:HIS:HB2	1:A:941:ALA:HB1	1.99	0.45
1:C:403:ALA:O	1:C:407:ARG:HG2	2.16	0.45
1:C:519:TRP:HA	1:C:686:GLU:O	2.17	0.45
1:C:553:ILE:HD11	1:C:659:LEU:HD12	1.97	0.45
6:G:20:DA:C4	6:G:21:DC:C5	3.05	0.45
1:A:447:GLN:OE1	1:C:455:MET:CE	2.64	0.45
1:C:600:ASP:OD1	1:C:601:GLY:N	2.49	0.45
1:C:754:LEU:HD23	1:C:783:PRO:HD2	1.97	0.45
2:B:217:TYR:HE1	2:B:235:ARG:HG3	1.81	0.45
2:B:279:LEU:HB2	2:B:282:GLN:HB3	1.98	0.45
1:A:717:GLY:HA2	1:A:781:ALA:HB3	1.98	0.45
2:D:74:TYR:HB2	2:D:138:TYR:HB2	1.97	0.45
3:F:12:DT:C7	3:F:13:DA:N6	2.79	0.45
1:A:476:LEU:HD21	1:C:476:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ARG:NE	1:C:1006:HIS:CE1	2.80	0.45
1:C:402:ARG:HD3	1:C:402:ARG:N	2.32	0.45
1:A:911:PHE:CD1	1:A:911:PHE:O	2.70	0.45
2:D:152:MET:HE3	2:D:186:ASP:OD1	2.17	0.45
2:D:331:ILE:N	2:D:344:TYR:O	2.43	0.45
7:L:23:DG:H2"	7:L:24:DA:C8	2.53	0.45
1:A:396:LEU:HD13	1:C:423:GLU:O	2.17	0.44
1:A:935:TYR:CE2	4:I:15:DT:H5'	2.52	0.44
1:C:594:VAL:HG13	1:C:627:MET:HB2	1.98	0.44
1:A:595:VAL:HB	1:A:702:PHE:HD1	1.82	0.44
2:B:69:LEU:HB2	2:B:108:TYR:CE2	2.52	0.44
3:F:7:DT:H2"	3:F:8:DT:C6	2.53	0.44
1:C:621:ARG:HD3	1:C:965:ASN:ND2	2.33	0.44
2:B:229:ARG:NH2	2:B:277:TYR:O	2.50	0.44
1:A:396:LEU:HD23	1:A:396:LEU:H	1.82	0.44
1:C:410:GLU:H	1:C:410:GLU:HG2	1.61	0.44
2:B:8:VAL:HB	2:B:12:ILE:HD12	2.00	0.44
8:M:38:DT:H2"	8:M:39:DG:H5'	1.99	0.44
1:A:850:ASN:ND2	1:A:851:GLY:H	2.14	0.44
1:A:906:LEU:HD11	1:A:947:ILE:HG21	1.98	0.44
1:C:400:THR:HG23	1:C:403:ALA:H	1.82	0.44
1:C:450:GLU:O	1:C:454:ILE:HG12	2.17	0.44
6:G:48:DA:H2"	6:G:49:DG:H8	1.82	0.44
9:N:24:ARG:HA	9:N:27:HIS:CE1	2.53	0.44
1:C:399:LEU:HD22	1:C:407:ARG:NH2	2.33	0.44
2:D:310:ASP:OD1	2:D:311:ILE:N	2.51	0.44
2:D:317:TRP:CD1	2:D:317:TRP:O	2.70	0.44
1:C:519:TRP:HB3	1:C:685:SER:OG	2.18	0.44
2:B:264:THR:HA	2:B:321:ASN:ND2	2.33	0.44
7:L:30:DC:H2"	7:L:31:DC:H6	1.83	0.44
1:C:599:CYS:HB2	1:C:622:PHE:HD1	1.82	0.43
6:G:6:DT:H2'	6:G:7:DT:C7	2.44	0.43
1:A:669:THR:HG22	1:A:784:PHE:CE2	2.53	0.43
1:A:715:VAL:HA	1:A:784:PHE:HE1	1.83	0.43
2:D:58:LYS:HE3	2:D:58:LYS:HB3	1.73	0.43
2:B:73:ARG:HH22	2:B:101:ASN:ND2	2.17	0.43
1:A:945:GLU:HA	1:A:948:GLU:HG2	2.01	0.43
1:C:628:ARG:HE	1:C:628:ARG:HB3	1.57	0.43
1:A:449:ASP:HA	1:A:452:GLU:HG2	2.01	0.43
1:A:792:ASP:OD2	1:A:795:HIS:ND1	2.51	0.43
1:C:578:MET:HE3	1:C:591:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:PRO:HD2	2:B:245:PRO:HA	2.00	0.43
9:N:110:ARG:N	9:N:111:PRO:HD2	2.34	0.43
1:A:544:SER:OG	1:A:545:VAL:N	2.51	0.43
1:A:726:ILE:HB	1:A:934:ASN:OD1	2.19	0.43
1:C:402:ARG:HH22	7:L:33:DT:H72	1.84	0.43
2:D:233:LEU:H	2:D:233:LEU:HD23	1.83	0.43
2:D:278:GLN:HG2	2:D:279:LEU:HD12	2.00	0.43
3:F:41:DC:H2"	3:F:42:DA:N7	2.34	0.43
1:C:486:ARG:HG2	1:C:487:THR:N	2.33	0.43
6:G:23:DC:H2'	6:G:24:DT:H71	2.00	0.43
1:C:439:LEU:HA	1:C:442:ARG:NE	2.27	0.43
1:A:447:GLN:OE1	1:C:455:MET:HE1	2.19	0.43
1:A:821:ALA:HB3	1:A:826:ARG:HE	1.84	0.43
2:D:256:ILE:HD11	2:D:299:ILE:CG2	2.36	0.43
2:B:285:MET:HE2	2:B:307:TRP:CD1	2.54	0.43
2:D:22:MET:HG3	2:D:29:PHE:HB2	2.01	0.42
2:D:30:PHE:HB2	2:D:48:PHE:HD1	1.84	0.42
2:D:228:ILE:O	2:D:230:PRO:HD3	2.19	0.42
1:A:529:ARG:NE	1:A:531:ASP:OD1	2.51	0.42
1:A:726:ILE:CG2	1:A:734:ARG:NH1	2.83	0.42
1:C:624:PHE:CD2	1:C:624:PHE:C	2.93	0.42
1:C:520:GLN:NE2	1:C:520:GLN:C	2.73	0.42
1:C:647:ASN:HB3	1:C:959:GLU:HB2	2.00	0.42
2:B:317:TRP:N	2:B:317:TRP:HD1	2.17	0.42
3:F:2:DG:H2"	3:F:3:DG:C8	2.54	0.42
3:F:27:DT:H2'	3:F:28:DG:C8	2.55	0.42
1:C:689:LEU:HB3	1:C:698:PHE:HE2	1.84	0.42
2:D:212:ARG:HG2	2:D:213:ASN:H	1.83	0.42
2:B:226:SER:HB3	2:B:228:ILE:HD12	2.02	0.42
1:A:399:LEU:HD23	1:A:403:ALA:HB1	2.00	0.42
1:C:742:VAL:HG23	1:C:743:PHE:CD2	2.54	0.42
3:F:10:DG:C5	3:F:11:DT:N3	2.88	0.42
2:D:256:ILE:CD1	2:D:299:ILE:HD13	2.50	0.42
1:A:439:LEU:HD23	1:A:448:ALA:N	2.35	0.42
1:A:532:VAL:CG2	1:A:558:ARG:HD3	2.32	0.42
6:G:24:DT:H2'	6:G:25:DT:C5	2.54	0.42
1:A:486:ARG:HH11	1:A:486:ARG:HB2	1.78	0.42
1:C:673:SER:OG	1:C:674:PRO:HD3	2.20	0.42
2:D:135:GLU:CD	2:D:136:PRO:HD2	2.39	0.41
2:B:222:HIS:HD2	2:B:229:ARG:NE	2.13	0.41
1:A:734:ARG:HE	1:A:734:ARG:HB2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:GLU:H	1:C:423:GLU:HG2	1.55	0.41
1:C:824:GLU:O	1:C:828:ARG:HG2	2.19	0.41
2:B:22:MET:HB2	2:B:91:TYR:CE2	2.55	0.41
2:B:283:LYS:CD	2:B:317:TRP:CZ2	2.90	0.41
2:B:317:TRP:HD1	2:B:317:TRP:H	1.69	0.41
3:F:10:DG:N2	7:L:38:DA:N3	2.68	0.41
8:M:19:DC:H2"	8:M:20:DA:C8	2.56	0.41
8:M:40:DA:H2"	8:M:41:DA:C8	2.55	0.41
1:A:839:LYS:O	1:A:839:LYS:HG3	2.14	0.41
1:C:789:PRO:O	1:C:949:ARG:NH1	2.53	0.41
2:B:22:MET:O	2:B:29:PHE:N	2.45	0.41
6:G:19:DC:H2"	6:G:20:DA:H8	1.84	0.41
1:A:408:LEU:HD13	1:C:430:VAL:HG13	2.02	0.41
1:C:760:TRP:CE2	2:D:68:TYR:HD2	2.38	0.41
2:D:73:ARG:HH22	2:D:101:ASN:ND2	2.19	0.41
8:M:27:DC:H2"	8:M:28:DA:C8	2.55	0.41
8:M:24:DA:H2'	8:M:25:DT:H71	2.03	0.41
1:A:440:ARG:HE	1:A:448:ALA:CB	2.34	0.41
2:B:79:SER:HA	2:B:91:TYR:CD1	2.55	0.41
2:B:283:LYS:HB3	2:B:283:LYS:HE2	1.48	0.41
3:F:6:DT:H2'	3:F:7:DT:H71	2.03	0.41
1:C:401:ARG:HH11	1:C:401:ARG:HG3	1.85	0.41
1:C:442:ARG:C	1:C:443:ASN:CG	2.79	0.41
1:C:446:ARG:O	1:C:450:GLU:HG3	2.21	0.41
1:C:679:ARG:NH2	1:C:683:LYS:HZ3	2.18	0.41
1:C:838:ARG:NH1	1:C:845:PRO:HD2	2.36	0.41
2:D:34:LYS:HZ3	2:D:34:LYS:HG3	1.62	0.41
2:D:137:ARG:NH1	2:D:157:GLY:HA2	2.36	0.41
2:D:197:LEU:HD13	2:D:249:CYS:HB2	2.03	0.41
3:F:23:DT:H2"	3:F:24:DC:C6	2.56	0.41
1:A:489:LYS:NZ	1:A:495:GLN:HE21	2.19	0.41
1:C:734:ARG:O	1:C:734:ARG:HG3	2.20	0.41
1:A:595:VAL:HB	1:A:702:PHE:CD1	2.54	0.40
1:C:483:LYS:O	1:C:486:ARG:HD2	2.19	0.40
1:C:811:GLU:CD	1:C:875:ARG:HH21	2.25	0.40
1:A:661:ASP:HB3	1:A:664:ASP:HB2	2.03	0.40
1:A:821:ALA:HB3	1:A:826:ARG:NE	2.36	0.40
2:B:212:ARG:CG	2:B:213:ASN:H	2.28	0.40
1:C:395:HIS:ND1	1:C:397:LEU:HG	2.37	0.40
1:C:703:ARG:HH22	1:C:950:ASP:CG	2.25	0.40
2:D:47[B]:HIS:HB3	2:D:58:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:19:DC:C2	6:G:20:DA:C8	3.10	0.40
6:G:58:DC:H2"	6:G:59:DA:C8	2.57	0.40
8:M:28:DA:H2"	8:M:29:DA:H8	1.86	0.40
1:A:760:TRP:CZ2	2:B:68:TYR:CD2	3.10	0.40
1:A:826:ARG:HG2	1:A:826:ARG:NH1	2.26	0.40
7:L:19:DC:H2"	7:L:20:DA:C8	2.57	0.40
7:L:27:DC:H2"	7:L:28:DA:C8	2.56	0.40
9:N:100:SER:OG	9:N:101:ALA:N	2.55	0.40
1:A:653:LYS:HB3	1:A:992:TRP:CZ3	2.56	0.40
1:C:627:MET:HG3	1:C:956:TRP:CH2	2.56	0.40
1:C:726:ILE:HB	1:C:934:ASN:OD1	2.21	0.40
2:D:47[B]:HIS:HB3	2:D:58:LYS:HG2	2.03	0.40
6:G:33:DA:H2'	6:G:34:DT:H71	2.04	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	612/775 (79%)	595 (97%)	17 (3%)	0	100	100
1	C	614/775 (79%)	595 (97%)	17 (3%)	2 (0%)	41	73
2	B	337/520 (65%)	330 (98%)	7 (2%)	0	100	100
2	D	338/520 (65%)	332 (98%)	6 (2%)	0	100	100
9	N	69/126 (55%)	67 (97%)	2 (3%)	0	100	100
All	All	1970/2716 (72%)	1919 (97%)	49 (2%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	521	PRO

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Mol	Chain	Res	Type
1	C	522	PRO

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	536/691 (78%)	508 (95%)	28 (5%)	23	56
1	C	540/691 (78%)	505 (94%)	35 (6%)	17	48
2	B	297/461 (64%)	291 (98%)	6 (2%)	55	79
2	D	294/461 (64%)	286 (97%)	8 (3%)	44	74
9	N	48/109 (44%)	48 (100%)	0	100	100
All	All	1715/2413 (71%)	1638 (96%)	77 (4%)	32	61

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	401	ARG
1	A	409	ARG
1	A	410	GLU
1	A	428	LYS
1	A	473	ASN
1	A	486	ARG
1	A	505	ASN
1	A	559	TYR
1	A	719	GLU
1	A	748	ARG
1	A	756	ARG
1	A	784	PHE
1	A	806	LYS
1	A	816	TYR
1	A	826	ARG
1	A	828	ARG
1	A	835	LYS
1	A	839	LYS

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Mol	Chain	Res	Type
1	A	850	ASN
1	A	861	GLU
1	A	875	ARG
1	A	890	LYS
1	A	894	ARG
1	A	923	LYS
1	A	949	ARG
1	A	972	ARG
1	A	977	ARG
1	A	1006	HIS
1	C	393	ARG
1	C	398	SER
1	C	402	ARG
1	C	408	LEU
1	C	423	GLU
1	C	442	ARG
1	C	443	ASN
1	C	446	ARG
1	C	447	GLN
1	C	455	MET
1	C	458	ARG
1	C	460	SER
1	C	473	ASN
1	C	480	GLN
1	C	486	ARG
1	C	508	LYS
1	C	518	GLU
1	C	520	GLN
1	C	553	ILE
1	C	570	MET
1	C	628	ARG
1	C	641	PHE
1	C	649	GLU
1	C	683	LYS
1	C	734	ARG
1	C	756	ARG
1	C	758	GLU
1	C	817	LYS
1	C	840	ARG
1	C	848	ARG
1	C	893	TRP
1	C	894	ARG

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Mol	Chain	Res	Type
1	C	936	PHE
1	C	949	ARG
1	C	961	ASN
2	D	5	MET
2	D	47[A]	HIS
2	D	47[B]	HIS
2	D	58	LYS
2	D	212	ARG
2	D	260	SER
2	D	317	TRP
2	D	349	ARG
2	B	5	MET
2	B	56	LYS
2	B	58	LYS
2	B	138	TYR
2	B	283	LYS
2	B	317	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	495	GLN
1	A	505	ASN
1	A	850	ASN
1	A	978	GLN
1	A	990	HIS
1	A	1000	GLN
1	A	1006	HIS
1	C	406	HIS
1	C	495	GLN
1	C	520	GLN
1	C	800	ASN
1	C	809	GLN
1	C	860	GLN
1	C	934	ASN
1	C	962	GLN
1	C	978	GLN
1	C	990	HIS
1	C	1000	GLN
1	C	1006	HIS
2	D	94	HIS
2	B	222	HIS

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Mol	Chain	Res	Type
9	N	135	ASN

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 4 ligands modelled in this entry, 4 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.

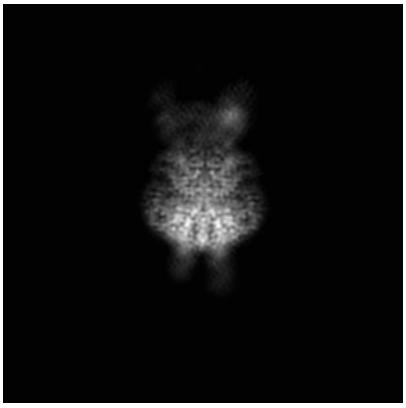
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7470. These allow visual inspection of the internal detail of the map and identification of artifacts.

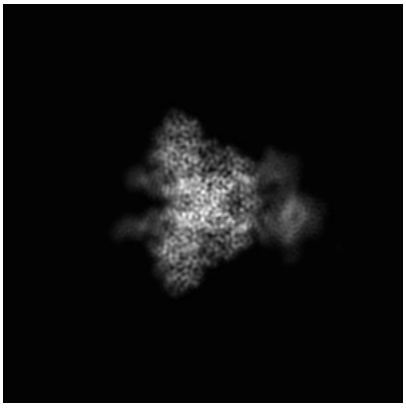
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

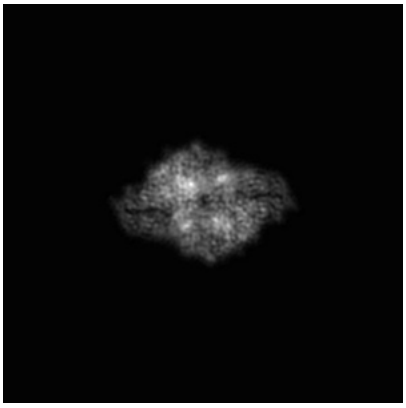
6.1.1 Primary map



X



Y



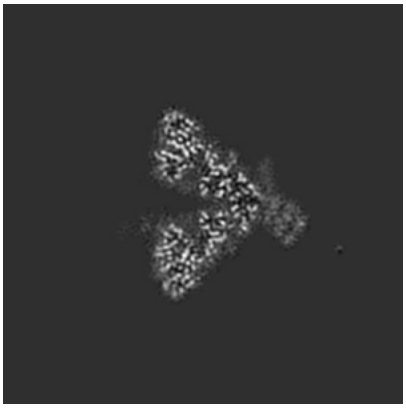
Z

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

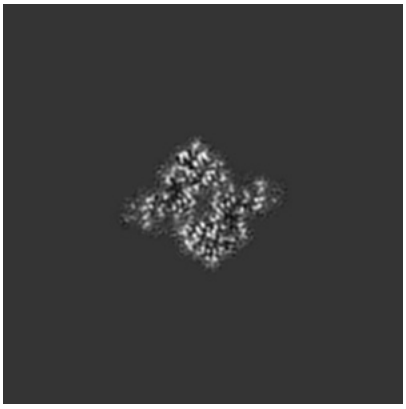
6.2 Central slices (i)

6.2.1 Primary map

X Index: 144



Y Index: 144



Z Index: 144

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: 136

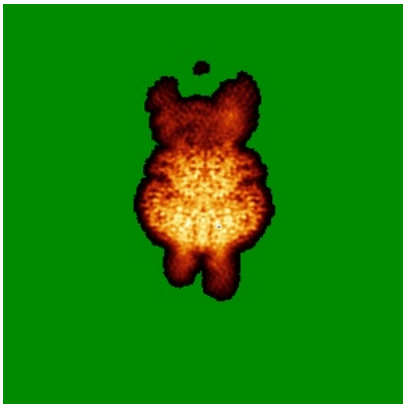
Y Index: 155

Z Index: 130

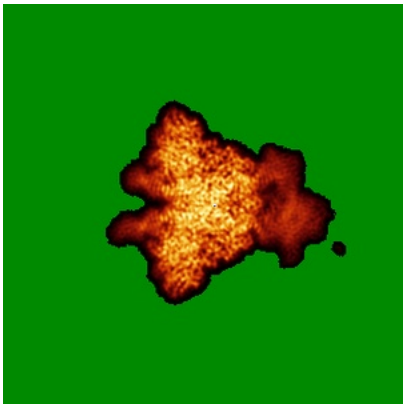
The images above show the largest variance slices of the map in three orthogonal directions.

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

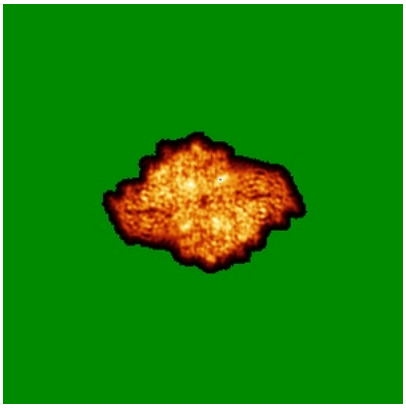
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0136. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

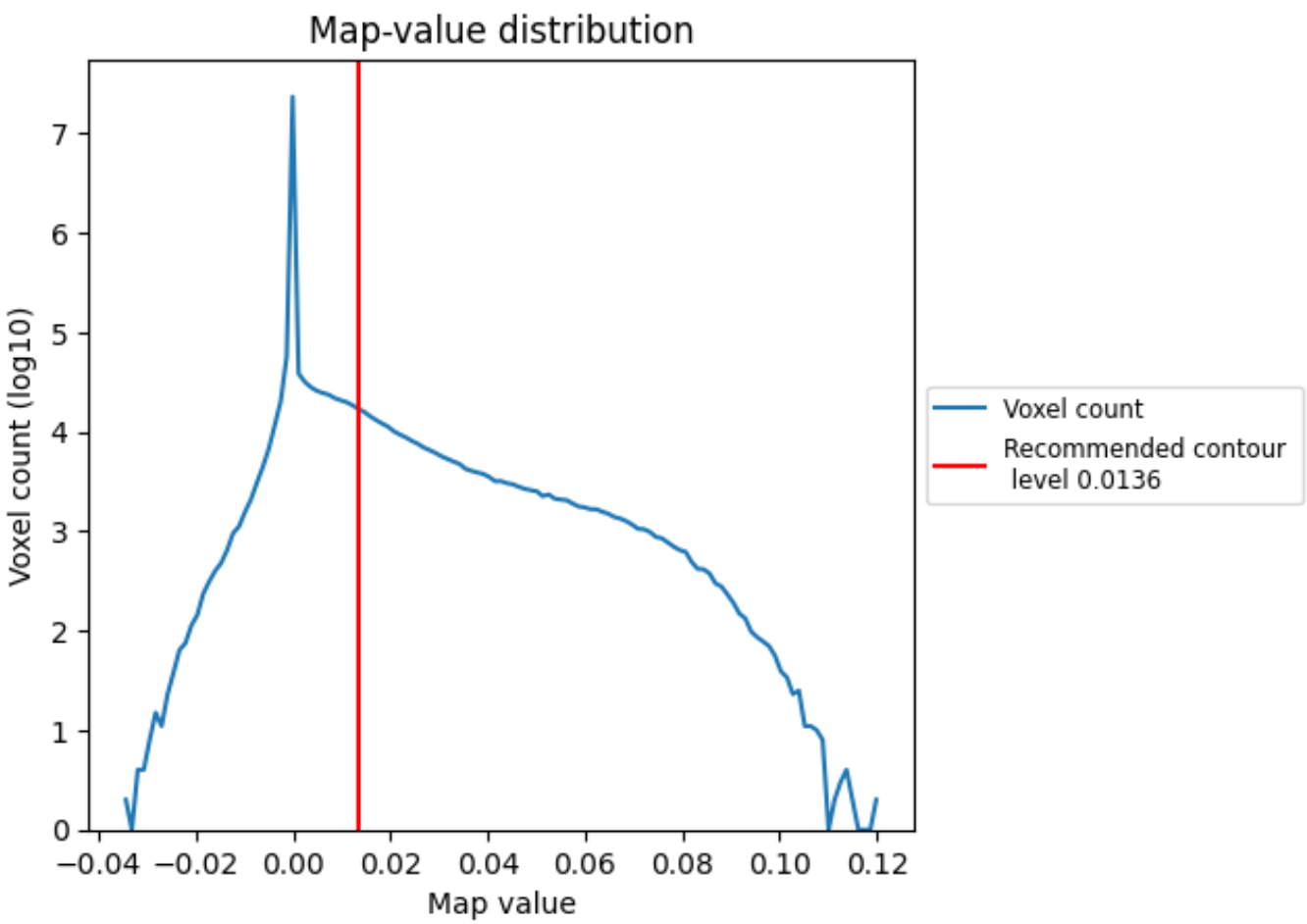
6.6 Mask visualisation (i)

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

7 Map analysis (i)

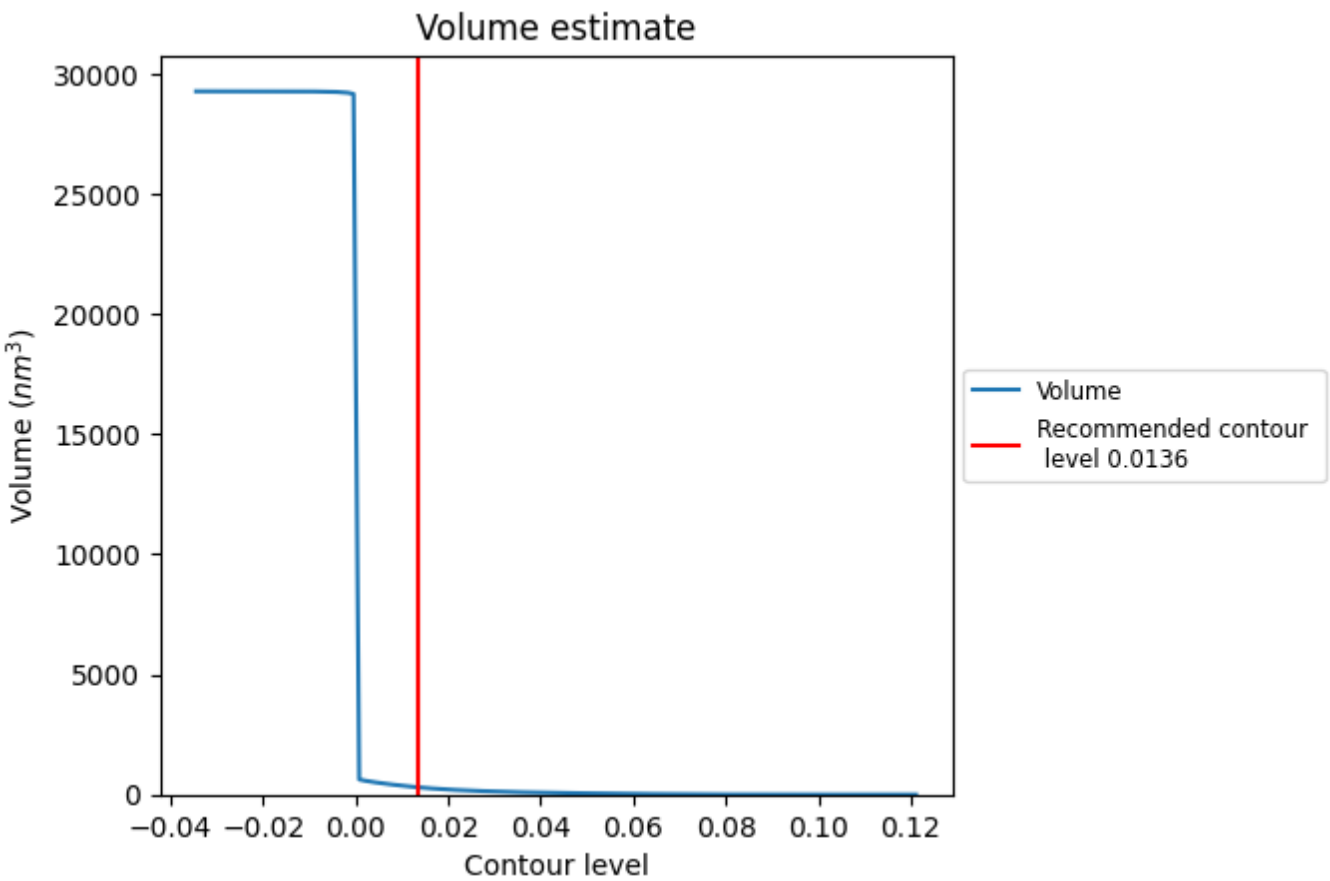
This section contains the results of statistical analysis of the map.

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.

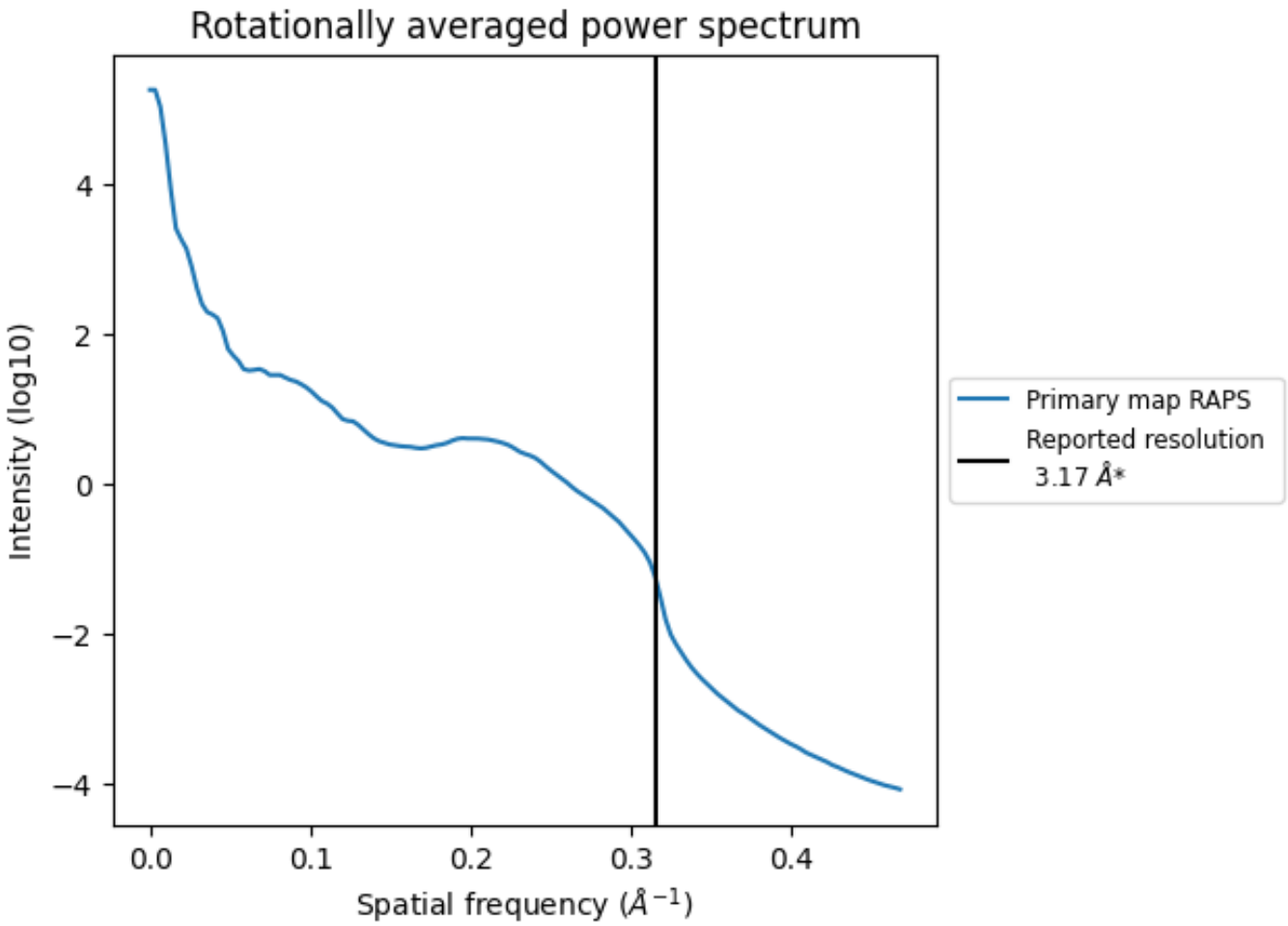
7.2 Volume estimate (i)



The volume at the recommended contour level is 301 nm^3; this corresponds to an approximate mass of 272 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 0.315 Å^{-1}

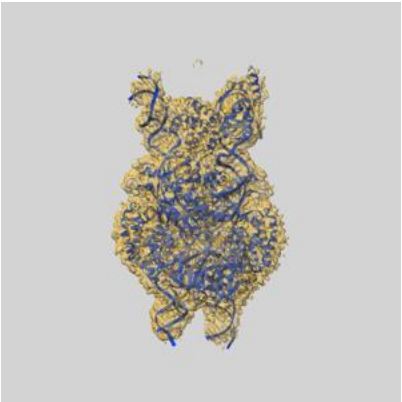
8 Fourier-Shell correlation (i)

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

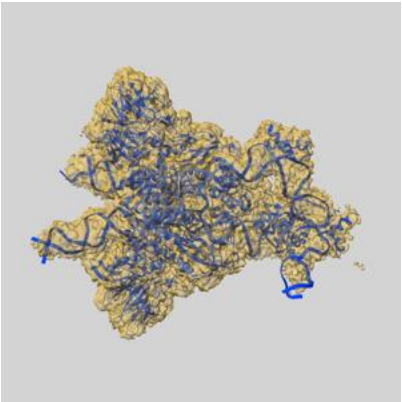
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7470 and PDB model 6CG0. Per-residue inclusion information can be found in section 3 on page 7.

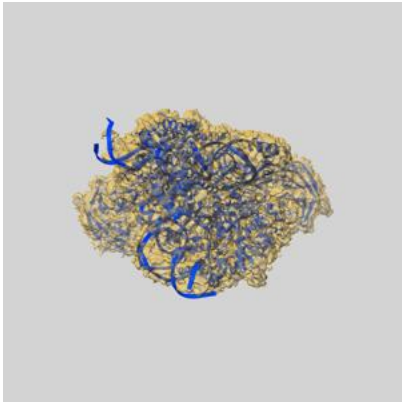
9.1 Map-model overlay (i)



X



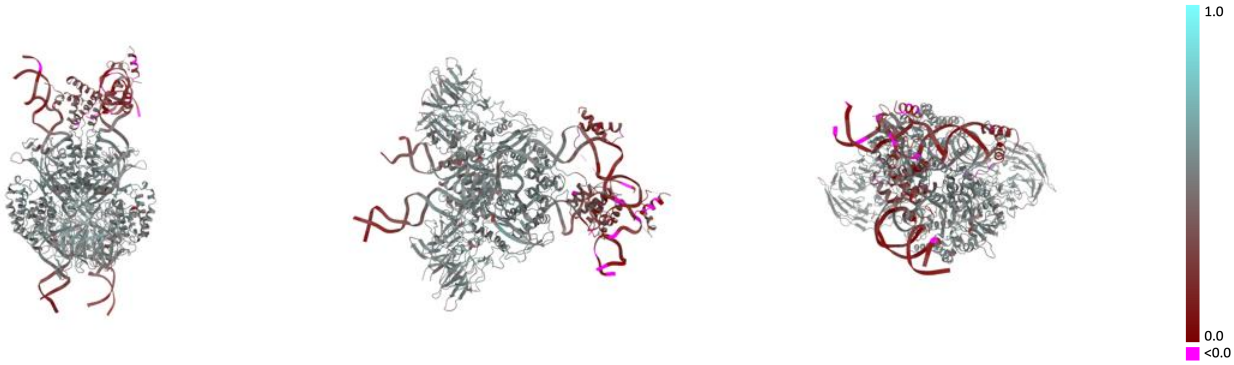
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0136 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.

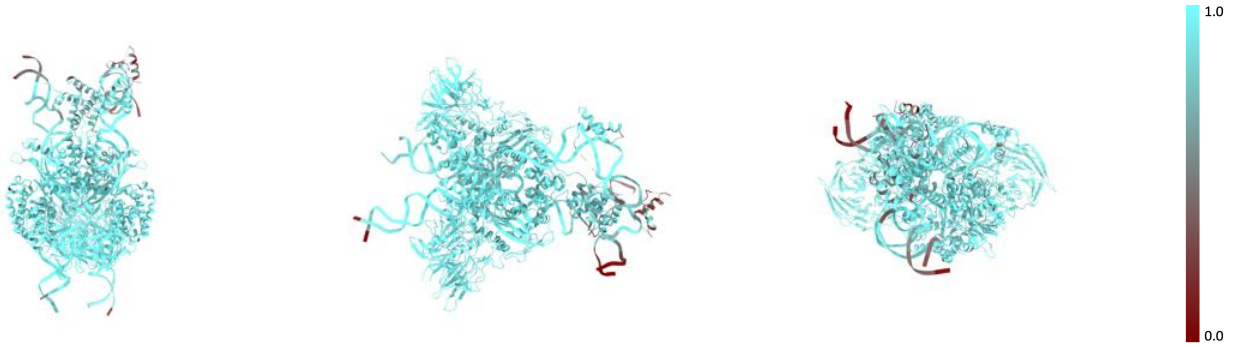
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

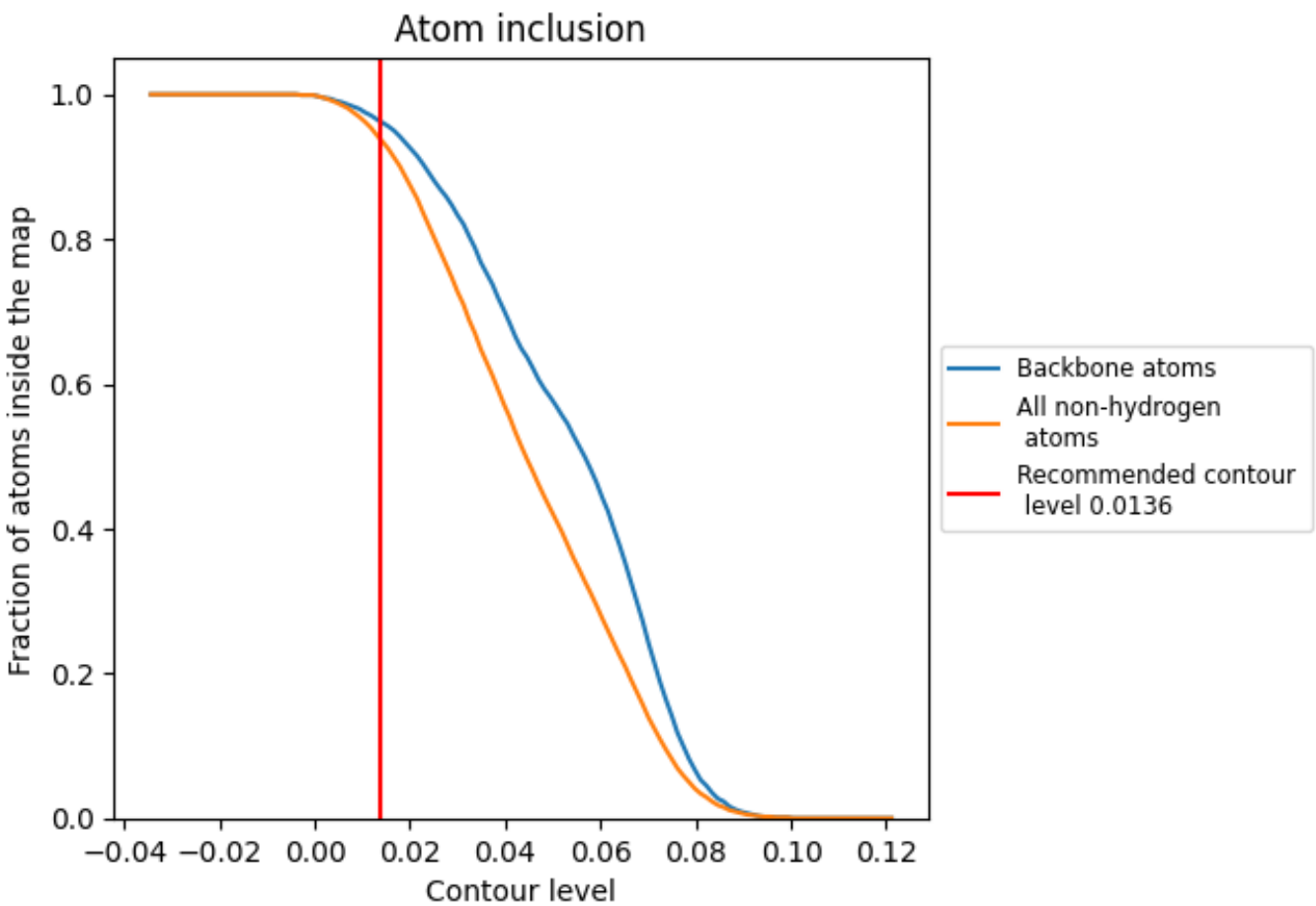
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0136).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0136) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9390	0.4520
A	0.9650	0.4880
B	0.9760	0.5090
C	0.9670	0.4850
D	0.9780	0.5100
F	0.8820	0.3690
G	0.8470	0.3270
I	0.9750	0.3800
J	0.9120	0.3580
L	0.8440	0.3170
M	0.8340	0.2900
N	0.6790	0.1850