



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:02 PM UTC

PDB ID : 8UBD / pdb_00008ubd
EMDB ID : EMD-42083
Title : Diversity-generating retroelement (DGR) ribonucleoprotein reverse transcriptase - Pre-active State 2
Authors : Biswas, T.; Handa, S.; Ghosh, P.
Deposited on : 2023-09-22
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

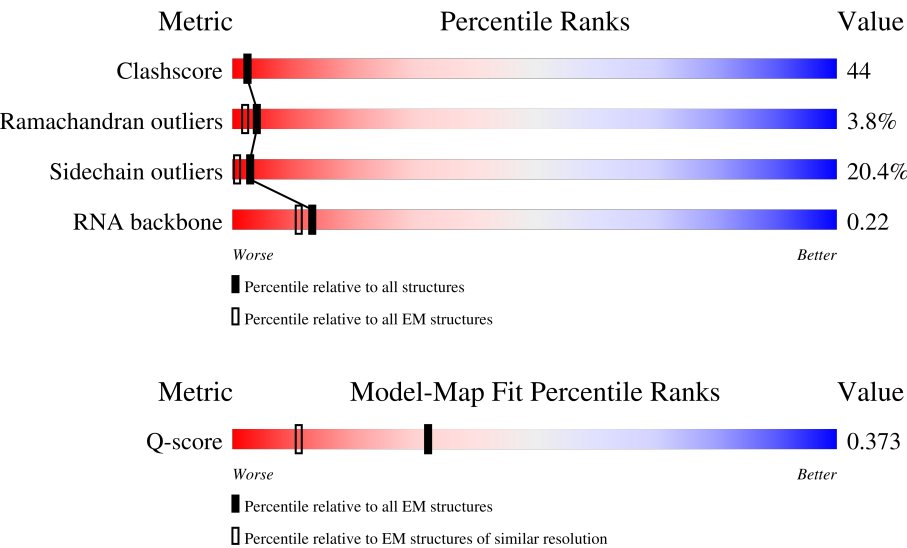
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13971 (2.55 - 3.55)

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

Mol	Chain	Length	Quality of chain
1	A	328	
2	B	290	
2	C	290	

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Mol	Chain	Length	Quality of chain
2	D	290	13%22%62%
2	E	290	12%22%62%
2	F	290	12%22%62%
3	G	19	26%32%11%32%
4	H	36	6%22%8%64%
5	I	140	17%38%28%5%12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10368 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 Reverse transcriptase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	0	0
			2665	1707	491	458	9		

- Molecule 2 is a protein called Avd.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	122	Total	C	N	O	S	0	0
			976	631	172	166	7		
2	C	111	Total	C	N	O	S	0	0
			888	578	157	148	5		
2	D	111	Total	C	N	O	S	0	0
			888	577	161	145	5		
2	E	110	Total	C	N	O	S	0	0
			876	569	156	146	5		
2	F	111	Total	C	N	O	S	0	0
			888	577	161	145	5		

- Molecule 3 is a RNA chain called Diversity-generating retroelement (DGR) RNA avd.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	13	Total	C	N	O	P	0	0
			289	127	58	91	13		

- Molecule 4 is a RNA chain called Diversity-generating retroelement (DGR) RNA TR.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	13	Total	C	N	O	P	0	0
			270	121	44	92	13		

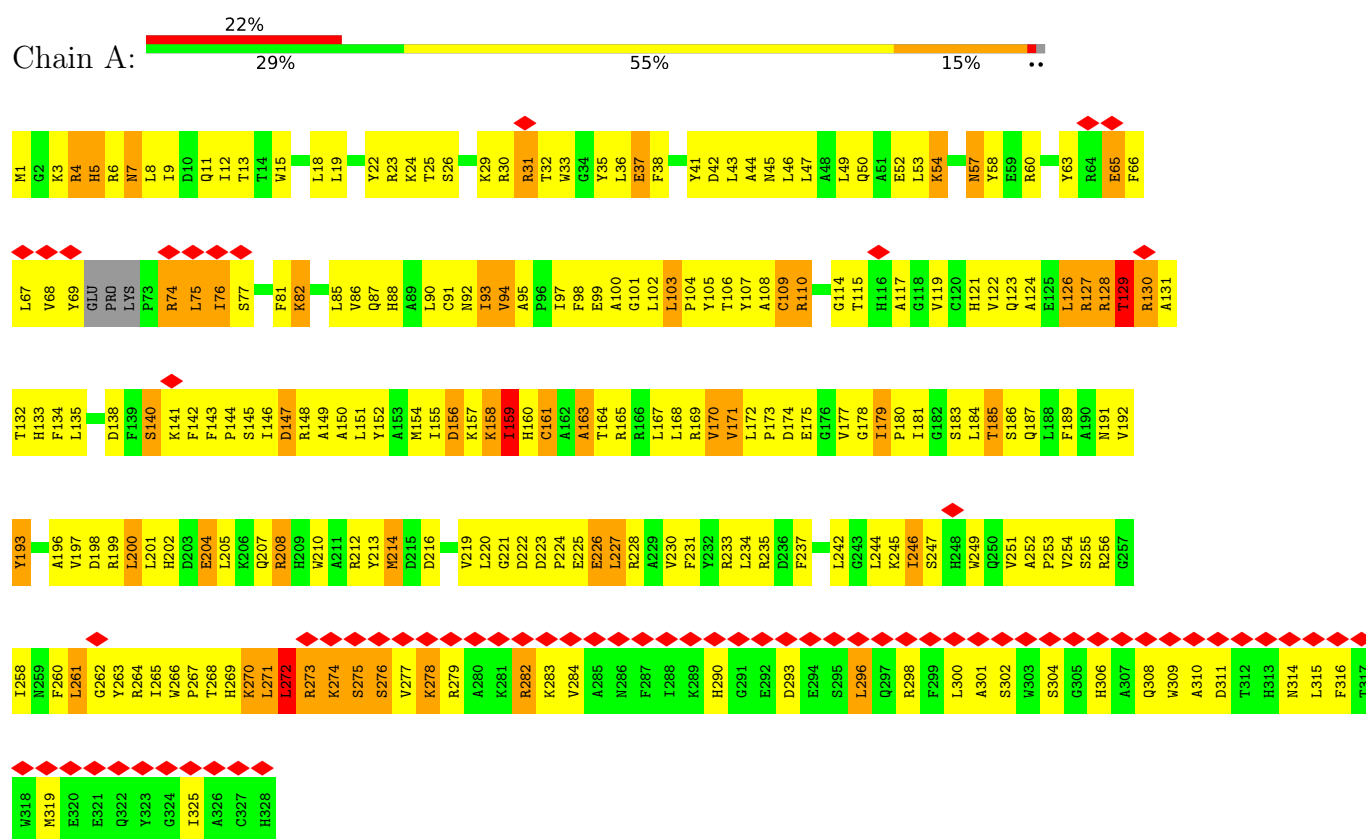
- Molecule 5 is a RNA chain called Diversity-generating retroelement (DGR) RNA Sp.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	123	Total	C	N	O	P	0	0
			2628	1171	469	865	123		

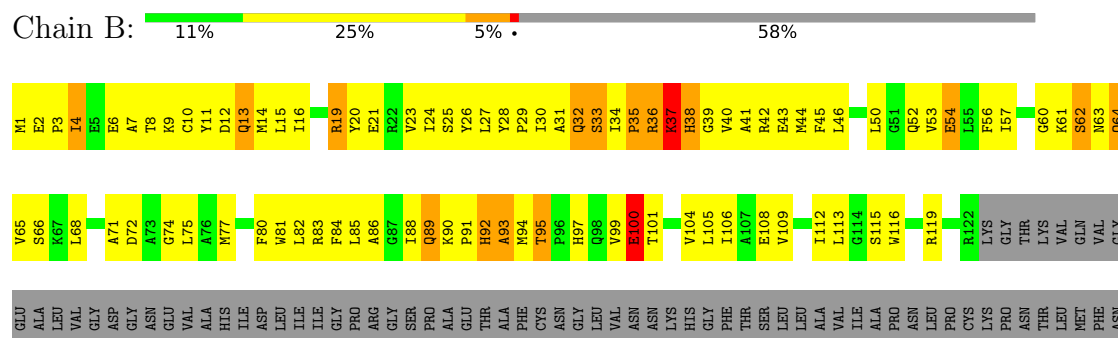
3 Residue-property plots

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

• Molecule 1: Reverse transcriptase



• Molecule 2: Avd



LYS	VAL	THR	ILE	ASN	TYR	GLY	ASP	ALA	ARG	GLN	LYS	VAL	GLN	MET	PHE	GLY	VAL	PRO	ASN	GLN	GLY	HIS	GLY	PRO	LYS	VAL	ALA	MET	ALA	VAL	GLN	ASP	VAL	ALA	GLY	THR	GLN	ASP	VAL	ALA	ASP	GLY	ASP	ASP	ALA	ASN	ALA	ILE
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● Molecule 2: Avd



MET	GLU	PRO	ILE	GLY	ARG	GLU	ALA	THR	LYS	VAL	CYS	Y11	D12	Q13	M14	L15	I16	V17	E18	R19	Y20	E21	I24	S25	Y26	L27	Y28	P29	I30	A31	Q32	S33	I34	P35	R36	K37	H38	G39	V40	A41	E42	M44	F45	L46	L50	G51	Q52	V53	E54	L55	F56	I57	V58	A59	S62	N63	Q64
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● Molecule 2: Avd



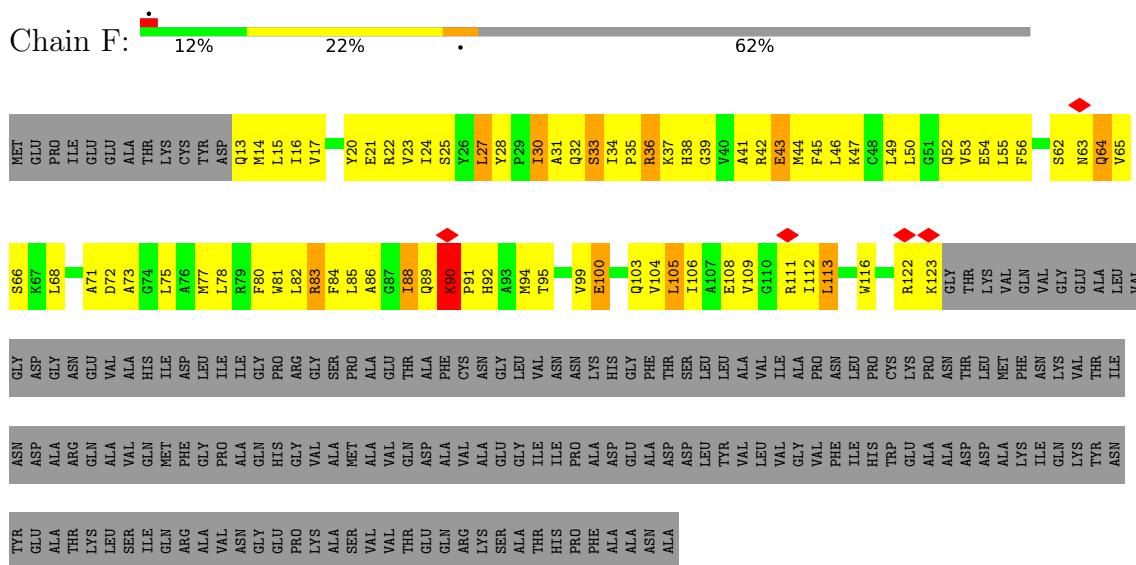
MET	GLU	PRO	ILE	GLY	ARG	GLU	ALA	THR	LYS	CYS	ASP	Q13	M14	L15	I16	V17	E18	R19	Y20	E21	I24	S25	Y26	L27	Y28	P29	I30	A31	Q32	S33	I34	P35	R36	K37	H38	G39	V40	A41	E42	M44	F45	L50	G51	Q52	V53	E54	L55	F56	I57	S62	N63	Q64	V65	L68
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● Molecule 2: Avd

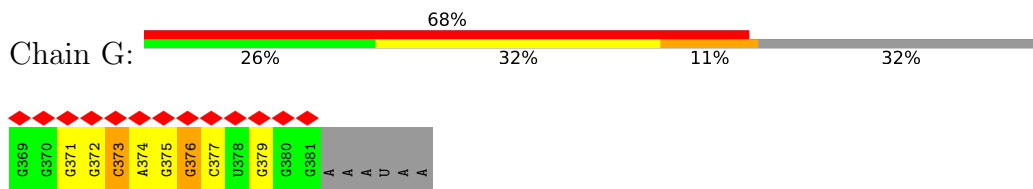


MET	GLU	PRO	ILE	GLY	ARG	GLU	ALA	THR	LYS	CYS	TYR	D12	Q13	M14	L15	I16	V17	E18	R19	Y20	E21	I24	S25	Y26	L27	Y28	P29	I30	A31	Q32	S33	I34	P35	R36	K37	H38	G39	V40	A41	E42	M44	F45	L46	K47	L50	G51	Q52	V53	E54	L55	F56	I57	V58	A59	G60	K61	S62
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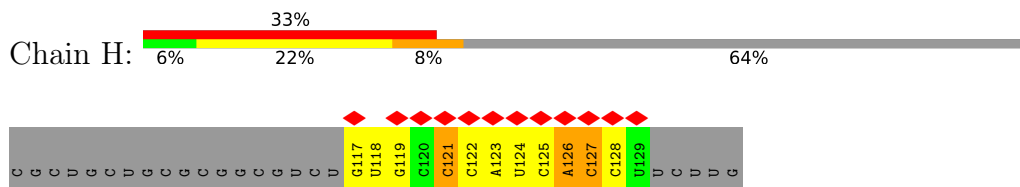
- Molecule 2: Avd



- Molecule 3: Diversity-generating retroelement (DGR) RNA and

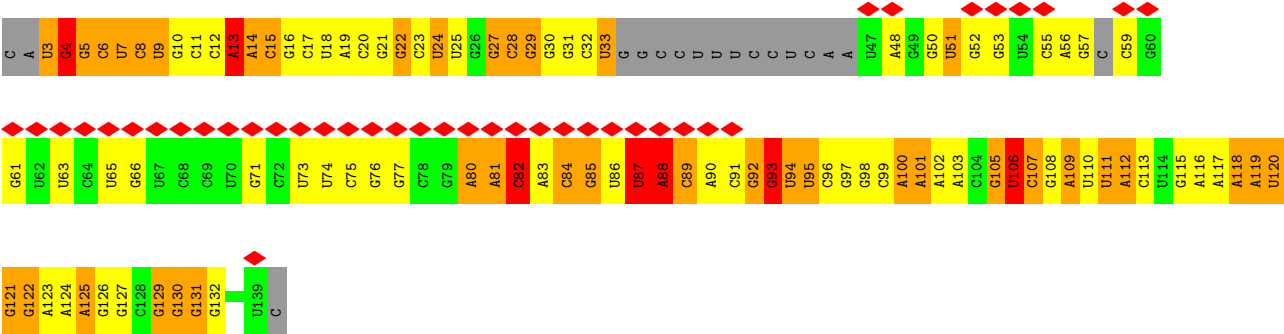


- Molecule 4: Diversity-generating retroelement (DGR) RNA TR



- Molecule 5: Diversity-generating retroelement (DGR) RNA Sp





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	202034	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.259	Depositor
Minimum map value	-1.363	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	320.0, 320.0, 320.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.68	0/2734	1.01	6/3692 (0.2%)
2	B	0.87	1/996 (0.1%)	1.01	3/1345 (0.2%)
2	C	0.89	1/907 (0.1%)	1.03	0/1226
2	D	0.70	0/906	0.88	0/1222
2	E	0.77	0/894	0.93	1/1208 (0.1%)
2	F	0.81	0/906	0.89	0/1222
3	G	0.70	0/324	0.93	1/506 (0.2%)
4	H	0.65	0/299	0.96	0/462
5	I	0.60	0/2935	1.02	22/4570 (0.5%)
All	All	0.72	2/10901 (0.0%)	0.99	33/15453 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	63	ASN	CA-CB	6.33	1.64	1.53
2	B	100	GLU	CA-CB	5.91	1.62	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	3	U	P-O3'-C3'	-10.96	103.76	120.20
5	I	88	A	O5'-P-OP2	-8.44	82.68	108.00
5	I	122	G	P-O3'-C3'	-8.13	108.00	120.20
5	I	105	G	P-O3'-C3'	-7.81	108.49	120.20
5	I	13	A	C4'-C3'-O3'	-7.06	102.41	113.00
5	I	11	C	P-O3'-C3'	-6.79	110.02	120.20
2	E	32	GLN	CB-CG-CD	-6.72	101.17	112.60
5	I	125	A	P-O3'-C3'	-6.72	110.12	120.20
1	A	159	ILE	N-CA-C	-6.57	106.39	112.96
2	B	32	GLN	N-CA-C	-6.52	105.72	113.21
5	I	111	U	P-O3'-C3'	-6.49	110.46	120.20
5	I	82	C	P-O3'-C3'	-6.46	110.51	120.20
5	I	106	U	P-O3'-C3'	-6.43	110.55	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	33	SER	N-CA-C	-6.37	106.15	114.04
1	A	31	ARG	N-CA-C	-6.30	102.73	110.61
5	I	13	A	O3'-P-O5'	-6.23	94.65	104.00
5	I	87	U	OP2-P-O3'	6.10	126.31	108.00
5	I	88	A	O5'-C5'-C4'	-6.09	102.56	111.70
5	I	121	G	P-O3'-C3'	-5.87	111.39	120.20
2	B	36	ARG	N-CA-C	-5.81	104.14	111.11
1	A	126	LEU	N-CA-C	-5.76	104.60	111.69
5	I	93	G	C2'-C3'-O3'	5.75	118.13	109.50
5	I	24	U	P-O3'-C3'	-5.72	111.62	120.20
3	G	376	G	P-O3'-C3'	-5.62	111.77	120.20
1	A	261	LEU	CA-C-N	-5.61	115.51	123.08
1	A	261	LEU	C-N-CA	-5.61	115.51	123.08
1	A	193	TYR	CB-CA-C	-5.58	102.08	110.90
5	I	88	A	P-O5'-C5'	-5.52	112.62	120.90
5	I	4	G	P-O5'-C5'	-5.29	112.97	120.90
5	I	112	A	O3'-P-O5'	-5.27	96.09	104.00
5	I	87	U	O3'-P-O5'	-5.12	96.32	104.00
5	I	81	A	P-O3'-C3'	-5.11	112.53	120.20
5	I	107	C	P-O3'-C3'	-5.07	112.59	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2665	0	2660	307	0
2	B	976	0	1014	137	0
2	C	888	0	923	129	0
2	D	888	0	936	96	0
2	E	876	0	914	95	0
2	F	888	0	936	90	0
3	G	289	0	143	2	0
4	H	270	0	141	21	0
5	I	2628	0	1328	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10368	0	8995	827	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 44.

All (827) 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)
5:I:92:G:H4'	5:I:93:G:OP1	1.35	1.16
1:A:168:LEU:HD22	1:A:189:PHE:HZ	1.27	0.96
2:E:86:ALA:HB2	2:E:99:VAL:HG21	1.48	0.95
1:A:311:ASP:HB2	5:I:87:U:H4'	1.51	0.91
2:B:9:LYS:HE2	2:B:14:MET:HE1	1.51	0.91
2:B:21:GLU:OE2	2:C:83:ARG:HD2	1.69	0.91
2:C:50:LEU:O	2:D:77:MET:HE1	1.69	0.91
2:C:86:ALA:HB2	2:C:99:VAL:HG21	1.53	0.90
5:I:13:A:H61	5:I:25:U:H3	1.16	0.89
2:E:53:VAL:HG11	2:F:80:PHE:CG	2.07	0.89
1:A:208:ARG:HG2	5:I:130:G:OP1	1.72	0.89
5:I:92:G:C4'	5:I:93:G:OP1	2.21	0.89
1:A:147:ASP:HB2	1:A:193:TYR:OH	1.73	0.88
2:C:25:SER:HA	2:D:88:ILE:HG23	1.54	0.87
1:A:124:ALA:HB2	5:I:94:U:H1'	1.56	0.86
1:A:163:ALA:HB2	5:I:120:U:O4	1.75	0.86
1:A:168:LEU:HD22	1:A:189:PHE:CZ	2.10	0.86
2:C:34:ILE:HG12	2:C:93:ALA:HB1	1.58	0.85
2:E:75:LEU:HD21	2:E:109:VAL:HG23	1.60	0.84
1:A:123:GLN:OE1	1:A:270:LYS:HB2	1.78	0.83
2:C:90:LYS:HB2	2:C:91:PRO:CD	2.08	0.83
2:B:25:SER:HA	2:C:88:ILE:HG23	1.61	0.82
2:E:53:VAL:HB	2:F:77:MET:HE1	1.61	0.82
2:E:13:GLN:HB3	2:E:60:GLY:HA3	1.61	0.81
1:A:45:ASN:O	2:B:1:MET:HE2	1.79	0.81
1:A:126:LEU:HD12	1:A:131:ALA:HB3	1.61	0.81
1:A:263:TYR:CZ	1:A:306:HIS:CD2	2.70	0.80
1:A:66:PHE:CZ	4:H:117:G:OP2	2.35	0.79
2:B:10:CYS:SG	2:B:13:GLN:N	2.54	0.78
1:A:311:ASP:HB3	5:I:88:A:P	2.22	0.78
1:A:200:LEU:HD13	1:A:237:PHE:CD1	2.18	0.78
1:A:126:LEU:HD13	1:A:220:LEU:HD22	1.67	0.77
2:F:23:VAL:HG22	2:F:105:LEU:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:HH2	2:B:9:LYS:HB2	1.50	0.77
1:A:205:LEU:HD21	1:A:233:ARG:HG2	1.66	0.76
2:C:34:ILE:HG23	2:C:89:GLN:HE21	1.50	0.76
2:F:34:ILE:HG22	2:F:38:HIS:HB2	1.67	0.76
2:F:35:PRO:HG3	2:F:92:HIS:CG	2.21	0.76
1:A:140:SER:HA	1:A:247:SER:HB3	1.67	0.75
1:A:11:GLN:HB2	1:A:93:ILE:HG12	1.67	0.75
1:A:213:TYR:CD1	1:A:261:LEU:HD21	2.22	0.75
2:E:95:THR:HG21	5:I:18:U:H4'	1.67	0.75
2:D:92:HIS:NE2	2:D:96:PRO:HD3	2.02	0.74
2:B:68:LEU:HD21	2:B:116:TRP:CE2	2.22	0.74
2:C:82:LEU:HD22	2:C:94:MET:SD	2.26	0.74
2:B:77:MET:HE1	2:F:50:LEU:O	1.86	0.74
1:A:171:VAL:HG13	1:A:185:THR:HG21	1.69	0.74
2:D:92:HIS:CE1	2:D:95:THR:HA	2.23	0.74
2:E:98:GLN:NE2	5:I:17:C:O3'	2.22	0.73
2:C:86:ALA:CB	2:C:99:VAL:HG21	2.18	0.72
2:D:82:LEU:HD11	2:D:106:ILE:HD12	1.70	0.72
1:A:213:TYR:CG	1:A:261:LEU:HD21	2.25	0.72
2:B:89:GLN:HG2	2:B:93:ALA:HB2	1.72	0.72
2:D:43:GLU:HG2	2:E:40:VAL:HG22	1.71	0.72
2:E:85:LEU:HB3	2:E:94:MET:HG3	1.72	0.72
1:A:100:ALA:O	5:I:105:G:H4'	1.89	0.72
2:B:24:ILE:HG22	2:C:88:ILE:HG21	1.70	0.72
2:B:82:LEU:HD11	2:B:106:ILE:HD12	1.72	0.72
1:A:311:ASP:CB	5:I:87:U:H4'	2.20	0.71
1:A:264:ARG:N	1:A:272:LEU:O	2.23	0.71
5:I:13:A:N6	5:I:25:U:H3	1.88	0.71
2:E:37:LYS:HA	5:I:7:U:O4'	1.89	0.71
1:A:168:LEU:CD2	1:A:189:PHE:HZ	2.01	0.71
1:A:159:ILE:O	1:A:161:CYS:N	2.22	0.70
2:F:75:LEU:HD12	2:F:113:LEU:HD12	1.72	0.70
2:B:43:GLU:HA	2:C:40:VAL:HG21	1.73	0.70
2:C:38:HIS:NE2	2:C:91:PRO:HD2	2.06	0.70
1:A:202:HIS:NE2	5:I:129:G:O3'	2.21	0.70
5:I:85:G:H1'	5:I:89:C:N4	2.05	0.70
2:F:34:ILE:HB	2:F:42:ARG:HB2	1.72	0.70
1:A:141:LYS:O	1:A:145:SER:N	2.25	0.69
5:I:9:U:H3	5:I:29:G:H1	1.37	0.69
1:A:271:LEU:HB3	5:I:83:A:C2	2.28	0.69
2:B:86:ALA:HB2	2:B:99:VAL:HG21	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:LYS:HA	5:I:3:U:H5''	1.74	0.69
1:A:196:ALA:HB3	1:A:242:LEU:HD11	1.73	0.69
2:C:57:ILE:HG21	2:D:76:ALA:HB3	1.74	0.69
2:E:21:GLU:OE2	2:F:83:ARG:HD2	1.93	0.68
2:B:9:LYS:CE	2:B:14:MET:HE1	2.21	0.68
2:E:40:VAL:HG23	5:I:7:U:C4	2.28	0.68
1:A:272:LEU:HB3	1:A:306:HIS:CE1	2.28	0.68
1:A:53:LEU:HD21	1:A:86:VAL:HG22	1.74	0.68
1:A:315:LEU:HD12	5:I:83:A:O4'	1.94	0.68
2:B:68:LEU:HD21	2:B:116:TRP:CD2	2.30	0.67
1:A:128:ARG:C	1:A:130:ARG:H	2.02	0.67
2:D:36:ARG:HB3	5:I:8:C:OP1	1.95	0.67
2:B:43:GLU:HG2	2:C:40:VAL:CG2	2.25	0.67
2:B:84:PHE:CE1	2:F:50:LEU:HD21	2.30	0.67
2:D:75:LEU:HD22	2:D:106:ILE:HG23	1.76	0.66
2:C:86:ALA:HB2	2:C:99:VAL:CG2	2.26	0.66
1:A:265:ILE:HG12	1:A:270:LYS:HG3	1.77	0.66
2:C:89:GLN:NE2	2:C:93:ALA:HB2	2.11	0.66
2:F:86:ALA:HB2	2:F:99:VAL:HG21	1.76	0.66
2:B:25:SER:HB2	2:C:88:ILE:HD12	1.77	0.66
2:B:50:LEU:HD21	2:C:84:PHE:CE1	2.31	0.66
2:B:81:TRP:HH2	2:F:50:LEU:HD13	1.60	0.66
1:A:41:TYR:CD1	2:B:4:ILE:HG22	2.31	0.66
1:A:6:ARG:NH1	5:I:122:G:N7	2.44	0.66
5:I:13:A:H3'	5:I:14:A:H8	1.60	0.66
1:A:278:LYS:HB3	3:G:373:C:H5'	1.76	0.66
2:E:87:GLY:N	5:I:19:A:H61	1.93	0.66
1:A:115:THR:HG23	1:A:261:LEU:HD22	1.77	0.66
2:D:45:PHE:CD2	2:D:85:LEU:HD11	2.30	0.66
2:D:98:GLN:HA	2:D:101:THR:HG23	1.77	0.66
1:A:90:LEU:HD13	1:A:168:LEU:HD23	1.78	0.65
1:A:147:ASP:HB2	1:A:193:TYR:HH	1.62	0.65
2:C:24:ILE:HG22	2:D:88:ILE:HG21	1.79	0.65
5:I:83:A:H8	5:I:84:C:H5	1.45	0.65
1:A:258:ILE:HG22	1:A:260:PHE:HB2	1.79	0.65
1:A:301:ALA:HB1	4:H:123:A:H4'	1.79	0.65
1:A:104:PRO:HG3	5:I:130:G:H4'	1.77	0.64
2:C:68:LEU:HD11	2:C:120:VAL:HG21	1.79	0.64
1:A:202:HIS:HE2	5:I:129:G:HO2'	1.43	0.64
2:C:34:ILE:HD13	2:C:85:LEU:HD22	1.79	0.64
2:F:68:LEU:HD21	2:F:116:TRP:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD13	1:A:50:GLN:HB2	1.79	0.64
5:I:82:C:H1'	5:I:84:C:N3	2.13	0.64
2:C:84:PHE:CD1	2:C:88:ILE:HB	2.33	0.63
2:E:52:GLN:OE1	2:E:75:LEU:HD13	1.97	0.63
2:B:81:TRP:CH2	2:F:50:LEU:HD13	2.33	0.63
2:E:53:VAL:HG21	2:F:80:PHE:CZ	2.32	0.63
1:A:122:VAL:O	1:A:126:LEU:HB2	1.98	0.63
5:I:82:C:H1'	5:I:84:C:C4	2.33	0.63
1:A:221:GLY:N	1:A:227:LEU:HD21	2.13	0.63
1:A:119:VAL:HG11	1:A:263:TYR:CD1	2.33	0.63
1:A:163:ALA:CB	5:I:120:U:O4	2.47	0.63
1:A:151:LEU:HD21	1:A:189:PHE:HB3	1.79	0.62
2:B:92:HIS:O	2:B:94:MET:N	2.31	0.62
2:C:82:LEU:HD11	2:C:106:ILE:HD12	1.81	0.62
2:F:31:ALA:C	2:F:33:SER:H	2.07	0.62
2:C:82:LEU:HD11	2:C:106:ILE:CD1	2.30	0.62
2:E:53:VAL:HG11	2:F:80:PHE:CD1	2.35	0.62
5:I:112:A:C6	5:I:113:C:C2	2.87	0.62
4:H:122:C:H2'	4:H:123:A:C8	2.35	0.62
1:A:98:PHE:HB3	1:A:192:VAL:CG2	2.29	0.61
2:C:50:LEU:HD13	2:D:81:TRP:CH2	2.35	0.61
2:F:31:ALA:HB2	2:F:45:PHE:CE2	2.35	0.61
1:A:264:ARG:HB3	1:A:266:TRP:CZ3	2.35	0.61
1:A:98:PHE:HB3	1:A:192:VAL:HG22	1.81	0.61
1:A:140:SER:HA	1:A:247:SER:CB	2.30	0.61
2:B:53:VAL:HG21	2:C:80:PHE:CZ	2.35	0.61
1:A:36:LEU:HB3	2:B:14:MET:HB3	1.83	0.61
1:A:172:LEU:HD11	1:A:179:ILE:HG12	1.80	0.61
2:E:40:VAL:HG23	5:I:7:U:O4	2.00	0.61
1:A:103:LEU:HD23	1:A:104:PRO:HD2	1.82	0.61
2:B:16:ILE:HD11	2:B:113:LEU:HB2	1.83	0.61
1:A:45:ASN:OD1	2:B:4:ILE:N	2.34	0.61
5:I:111:U:H2'	5:I:112:A:H8	1.66	0.61
2:C:38:HIS:HE1	2:C:90:LYS:HG3	1.64	0.61
3:G:371:G:H21	5:I:81:A:H8	1.48	0.61
2:D:31:ALA:O	2:D:42:ARG:HG3	2.01	0.60
1:A:269:HIS:CD2	1:A:271:LEU:HG	2.36	0.60
2:E:35:PRO:HA	5:I:24:U:H5'	1.82	0.60
5:I:95:U:H2'	5:I:96:C:C6	2.37	0.60
1:A:41:TYR:CG	2:B:4:ILE:HG21	2.37	0.60
2:C:28:TYR:CZ	2:D:41:ALA:HB2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:87:GLY:H	5:I:19:A:H61	1.47	0.60
1:A:8:LEU:CD1	1:A:159:ILE:HD12	2.32	0.60
1:A:271:LEU:O	1:A:272:LEU:C	2.44	0.60
2:F:42:ARG:NH1	5:I:4:G:C2	2.70	0.60
2:E:20:TYR:HA	2:E:109:VAL:HG11	1.84	0.60
2:C:16:ILE:HD13	2:C:112:ILE:HB	1.84	0.60
2:F:27:LEU:HD21	2:F:82:LEU:HD21	1.83	0.60
2:D:38:HIS:NE2	2:D:91:PRO:HD2	2.16	0.60
1:A:98:PHE:CZ	1:A:155:ILE:HA	2.36	0.59
2:C:31:ALA:HB2	2:C:45:PHE:CE2	2.37	0.59
2:F:68:LEU:HD21	2:F:116:TRP:CE2	2.37	0.59
1:A:8:LEU:HB2	1:A:164:THR:OG1	2.02	0.59
2:B:7:ALA:O	2:B:61:LYS:HE3	2.02	0.59
1:A:159:ILE:HG13	1:A:168:LEU:HD11	1.84	0.59
2:E:92:HIS:CE1	5:I:19:A:C4	2.90	0.59
1:A:53:LEU:HD21	1:A:86:VAL:CG2	2.32	0.59
1:A:155:ILE:HG22	1:A:155:ILE:O	2.03	0.59
2:C:90:LYS:HB2	2:C:91:PRO:HD3	1.83	0.59
2:E:24:ILE:HD11	2:E:53:VAL:CG2	2.32	0.59
2:B:10:CYS:HB3	2:B:13:GLN:HG2	1.85	0.59
2:B:53:VAL:HG11	2:C:80:PHE:CG	2.37	0.59
2:C:90:LYS:HB2	2:C:91:PRO:HD2	1.84	0.59
2:D:91:PRO:O	2:D:93:ALA:N	2.36	0.59
2:C:24:ILE:HD13	2:D:80:PHE:CZ	2.37	0.59
1:A:41:TYR:CD1	2:B:4:ILE:CG2	2.85	0.58
1:A:187:GLN:HG2	4:H:118:U:O2'	2.01	0.58
1:A:41:TYR:CE2	2:C:79:ARG:HD3	2.39	0.58
2:F:36:ARG:O	2:F:39:GLY:N	2.36	0.58
1:A:103:LEU:HD12	1:A:199:ARG:HG2	1.85	0.58
1:A:122:VAL:HG21	1:A:260:PHE:CD2	2.39	0.58
1:A:202:HIS:HE2	5:I:129:G:C3'	2.15	0.58
2:C:41:ALA:HB1	2:C:84:PHE:HE2	1.69	0.58
1:A:135:LEU:O	1:A:219:VAL:N	2.35	0.58
1:A:146:ILE:HG12	1:A:193:TYR:HD2	1.69	0.58
2:B:33:SER:O	2:B:34:ILE:C	2.45	0.58
2:B:43:GLU:HG2	2:C:40:VAL:HG22	1.85	0.58
1:A:13:THR:HA	1:A:18:LEU:HD11	1.85	0.58
2:B:80:PHE:CG	2:F:53:VAL:HG11	2.39	0.58
2:C:40:VAL:HG23	5:I:3:U:C4	2.39	0.58
4:H:122:C:H2'	4:H:123:A:H8	1.69	0.58
1:A:158:LYS:O	1:A:159:ILE:HD13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG11	1:A:230:VAL:HG11	1.84	0.57
2:D:31:ALA:HB2	2:D:45:PHE:CE2	2.39	0.57
2:C:40:VAL:HG23	5:I:3:U:O4	2.04	0.57
2:C:53:VAL:HG11	2:D:80:PHE:CG	2.39	0.57
1:A:58:TYR:CE2	1:A:86:VAL:HG11	2.39	0.57
2:D:16:ILE:HG12	2:D:109:VAL:HG23	1.86	0.57
1:A:106:THR:OG1	1:A:198:ASP:OD2	2.22	0.57
2:D:54:GLU:OE1	2:E:77:MET:HB2	2.04	0.57
2:E:36:ARG:C	5:I:7:U:H5''	2.30	0.57
5:I:5:G:N2	5:I:33:U:H1'	2.20	0.57
5:I:8:C:C2	5:I:31:G:C2	2.92	0.57
5:I:14:A:H2	5:I:15:C:H5	1.53	0.57
1:A:108:ALA:HB2	1:A:214:MET:H	1.69	0.57
1:A:134:PHE:CD1	1:A:258:ILE:HG12	2.40	0.57
1:A:7:ASN:HA	5:I:120:U:O2	2.05	0.57
1:A:41:TYR:HB3	1:A:44:ALA:HB3	1.87	0.57
1:A:134:PHE:CE1	1:A:258:ILE:HG12	2.40	0.56
2:C:90:LYS:O	2:C:92:HIS:N	2.38	0.56
2:D:82:LEU:HD11	2:D:106:ILE:CD1	2.34	0.56
2:D:92:HIS:CE1	2:D:96:PRO:HD3	2.40	0.56
5:I:6:C:N4	5:I:8:C:N4	2.53	0.56
1:A:94:VAL:HG11	1:A:168:LEU:HD21	1.87	0.56
2:B:31:ALA:HB2	2:B:45:PHE:CE2	2.40	0.56
5:I:16:G:N2	5:I:24:U:H1'	2.21	0.56
1:A:108:ALA:O	1:A:110:ARG:N	2.38	0.56
1:A:193:TYR:CE1	1:A:242:LEU:HD22	2.41	0.56
1:A:88:HIS:CE1	1:A:184:LEU:HD22	2.40	0.56
2:B:37:LYS:C	2:B:39:GLY:N	2.60	0.56
2:C:38:HIS:HD1	2:C:89:GLN:HG2	1.70	0.56
2:B:7:ALA:HB3	2:C:72:ASP:OD2	2.04	0.56
2:B:24:ILE:HD11	2:B:53:VAL:CG2	2.35	0.56
5:I:83:A:H8	5:I:84:C:C5	2.24	0.56
1:A:87:GLN:CD	1:A:185:THR:HB	2.31	0.56
1:A:158:LYS:NZ	5:I:106:U:OP1	2.38	0.56
2:B:62:SER:O	2:B:64:GLN:N	2.39	0.56
2:D:86:ALA:CB	2:D:99:VAL:HG21	2.36	0.56
1:A:49:LEU:HB2	2:B:1:MET:HE3	1.88	0.56
2:B:21:GLU:CD	2:C:83:ARG:HH11	2.14	0.56
2:F:35:PRO:CD	2:F:92:HIS:HB3	2.35	0.56
2:B:38:HIS:HA	2:F:28:TYR:OH	2.06	0.56
2:C:16:ILE:HD12	2:C:109:VAL:HG13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:HG22	1:A:53:LEU:HB2	1.87	0.55
1:A:41:TYR:CZ	2:C:79:ARG:HD3	2.41	0.55
1:A:142:PHE:CZ	1:A:146:ILE:HD11	2.41	0.55
1:A:308:GLN:HE21	1:A:309:TRP:CD1	2.23	0.55
2:C:30:ILE:HG22	2:C:93:ALA:O	2.05	0.55
5:I:10:G:C6	5:I:29:G:C6	2.94	0.55
1:A:41:TYR:CE1	2:B:4:ILE:HG22	2.42	0.55
2:C:62:SER:C	2:C:64:GLN:H	2.14	0.55
1:A:172:LEU:HD22	1:A:189:PHE:HD2	1.71	0.55
2:B:60:GLY:HA2	2:B:116:TRP:HZ2	1.70	0.55
2:D:21:GLU:OE2	2:E:80:PHE:CD1	2.59	0.55
2:F:34:ILE:HD12	2:F:42:ARG:HA	1.88	0.55
5:I:14:A:H2	5:I:15:C:C5	2.25	0.55
1:A:44:ALA:HB1	2:B:4:ILE:CD1	2.37	0.55
1:A:219:VAL:HG12	1:A:219:VAL:O	2.06	0.55
1:A:91:CYS:SG	1:A:185:THR:HA	2.47	0.55
1:A:135:LEU:HD13	1:A:231:PHE:HB2	1.89	0.55
2:D:13:GLN:NE2	2:D:119:ARG:HH12	2.05	0.55
2:E:33:SER:O	5:I:23:C:O2'	2.20	0.55
2:C:37:LYS:CA	5:I:3:U:H5''	2.36	0.55
2:F:62:SER:C	2:F:64:GLN:H	2.13	0.55
2:C:37:LYS:C	2:C:39:GLY:N	2.65	0.55
2:D:19:ARG:HG3	2:D:112:ILE:HD11	1.89	0.55
2:C:45:PHE:CG	2:C:85:LEU:HD11	2.42	0.54
2:D:68:LEU:HB3	2:D:117:ILE:CD1	2.37	0.54
5:I:13:A:H2'	5:I:14:A:O4'	2.07	0.54
1:A:30:ARG:HA	1:A:35:TYR:CD2	2.42	0.54
1:A:124:ALA:O	1:A:128:ARG:HG2	2.07	0.54
1:A:128:ARG:O	1:A:129:THR:HG22	2.07	0.54
1:A:207:GLN:CD	1:A:230:VAL:HG21	2.32	0.54
5:I:23:C:H2'	5:I:24:U:O4'	2.07	0.54
1:A:7:ASN:N	1:A:161:CYS:HB2	2.22	0.54
2:D:50:LEU:HD21	2:E:84:PHE:CZ	2.42	0.54
2:D:57:ILE:HG21	2:E:76:ALA:HB3	1.89	0.54
2:E:57:ILE:CD1	2:F:77:MET:HA	2.38	0.54
5:I:112:A:C2	5:I:113:C:H1'	2.43	0.54
1:A:33:TRP:HH2	2:B:9:LYS:CB	2.19	0.54
2:B:88:ILE:HG23	2:F:25:SER:HA	1.88	0.54
2:D:27:LEU:HD23	2:D:30:ILE:HD12	1.90	0.54
2:F:20:TYR:CZ	2:F:52:GLN:HG2	2.43	0.54
5:I:5:G:C2	5:I:33:U:H1'	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:GLU:OE1	2:C:79:ARG:NH2	2.38	0.54
2:C:37:LYS:C	2:C:39:GLY:H	2.16	0.54
2:E:53:VAL:HG11	2:F:80:PHE:CD2	2.43	0.54
2:F:38:HIS:CE1	2:F:88:ILE:HG12	2.43	0.54
1:A:223:ASP:HB3	1:A:226:GLU:HB2	1.88	0.54
2:D:28:TYR:CD2	2:E:84:PHE:HZ	2.26	0.54
2:D:65:VAL:HG11	2:D:121:ASN:ND2	2.23	0.54
2:F:31:ALA:C	2:F:33:SER:N	2.65	0.54
1:A:134:PHE:CE2	1:A:252:ALA:HB3	2.43	0.54
1:A:262:GLY:C	1:A:273:ARG:HE	2.15	0.54
2:B:21:GLU:OE2	2:C:83:ARG:CD	2.50	0.54
2:D:53:VAL:HG11	2:E:80:PHE:CG	2.43	0.54
1:A:277:VAL:HG13	1:A:315:LEU:HD11	1.90	0.53
5:I:29:G:H2'	5:I:30:G:O4'	2.08	0.53
1:A:13:THR:O	1:A:50:GLN:NE2	2.41	0.53
1:A:44:ALA:CB	2:B:4:ILE:CD1	2.87	0.53
1:A:263:TYR:CD1	1:A:263:TYR:N	2.75	0.53
2:E:12:ASP:O	2:E:16:ILE:HG13	2.09	0.53
1:A:69:TYR:O	5:I:59:C:H4'	2.08	0.53
2:B:37:LYS:O	2:B:39:GLY:N	2.42	0.53
2:B:45:PHE:CD2	2:B:85:LEU:HD11	2.44	0.53
2:E:64:GLN:HB2	2:E:67:LYS:HZ2	1.73	0.53
2:E:82:LEU:HB3	2:E:99:VAL:HG13	1.91	0.53
1:A:296:LEU:HD21	1:A:325:ILE:HG21	1.91	0.53
5:I:85:G:O2'	5:I:86:U:H5'	2.08	0.53
1:A:30:ARG:HG2	1:A:35:TYR:CE2	2.44	0.53
2:D:28:TYR:CZ	2:E:88:ILE:HD11	2.44	0.53
2:D:86:ALA:HB2	2:D:99:VAL:CG2	2.39	0.53
4:H:126:A:H61	5:I:48:A:H61	1.57	0.53
1:A:235:ARG:HG3	1:A:246:ILE:HG13	1.91	0.53
1:A:269:HIS:HB2	1:A:271:LEU:HG	1.91	0.53
2:B:15:LEU:HG	2:B:112:ILE:HD13	1.91	0.53
2:D:24:ILE:HD11	2:D:53:VAL:CG2	2.38	0.53
2:D:85:LEU:HB2	2:D:94:MET:HE3	1.89	0.53
2:F:82:LEU:HD11	2:F:106:ILE:HD12	1.89	0.53
2:E:37:LYS:HD2	5:I:7:U:O4'	2.09	0.52
4:H:126:A:H61	5:I:48:A:N6	2.06	0.52
2:C:28:TYR:CE1	2:D:41:ALA:HB2	2.44	0.52
2:C:38:HIS:ND1	2:C:89:GLN:HG2	2.24	0.52
2:E:26:TYR:CE2	2:E:101:THR:HB	2.44	0.52
1:A:38:PHE:HZ	1:A:46:LEU:HD23	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:HG12	1:A:193:TYR:CD2	2.44	0.52
1:A:198:ASP:HB3	1:A:210:TRP:CH2	2.44	0.52
1:A:204:GLU:O	1:A:205:LEU:HB2	2.10	0.52
1:A:263:TYR:CZ	1:A:306:HIS:HD2	2.25	0.52
2:B:31:ALA:C	2:B:33:SER:H	2.18	0.52
5:I:25:U:C6	5:I:25:U:H3'	2.44	0.52
2:C:50:LEU:HD21	2:D:84:PHE:CE1	2.45	0.52
2:C:85:LEU:HB3	2:C:93:ALA:HB3	1.92	0.52
2:E:31:ALA:HB2	2:E:45:PHE:CE2	2.45	0.52
1:A:25:THR:OG1	1:A:85:LEU:HA	2.10	0.52
2:B:56:PHE:HE1	2:B:113:LEU:HD22	1.73	0.52
5:I:29:G:C6	5:I:30:G:C5	2.96	0.52
1:A:53:LEU:HD23	1:A:58:TYR:HB2	1.92	0.52
1:A:15:TRP:CZ2	1:A:43:LEU:HD22	2.44	0.52
1:A:193:TYR:OH	1:A:242:LEU:HA	2.08	0.52
2:C:50:LEU:HD13	2:D:81:TRP:HH2	1.75	0.52
2:F:20:TYR:OH	2:F:78:LEU:HD22	2.09	0.52
1:A:143:PHE:HB2	1:A:144:PRO:HD3	1.92	0.52
1:A:269:HIS:HD2	1:A:271:LEU:HG	1.75	0.52
2:F:36:ARG:HB2	5:I:5:G:OP1	2.09	0.52
1:A:272:LEU:CB	1:A:306:HIS:CE1	2.92	0.52
2:D:85:LEU:HD22	2:D:89:GLN:NE2	2.25	0.52
2:F:42:ARG:HD2	5:I:4:G:C6	2.45	0.52
1:A:104:PRO:HD3	5:I:131:G:C5	2.45	0.51
2:C:75:LEU:HD11	2:C:109:VAL:HG12	1.93	0.51
2:D:86:ALA:HB2	2:D:99:VAL:HG21	1.91	0.51
2:F:35:PRO:HD3	2:F:92:HIS:HB3	1.92	0.51
5:I:83:A:C8	5:I:84:C:C5	2.98	0.51
2:C:72:ASP:N	2:C:113:LEU:HD21	2.26	0.51
2:C:25:SER:HA	2:D:88:ILE:CG2	2.34	0.51
2:C:37:LYS:O	2:C:39:GLY:N	2.41	0.51
2:E:50:LEU:O	2:F:44:MET:HE1	2.10	0.51
1:A:154:MET:CE	1:A:196:ALA:HB2	2.41	0.51
2:B:37:LYS:O	2:B:38:HIS:C	2.51	0.51
2:B:83:ARG:NE	2:F:21:GLU:OE1	2.44	0.51
2:C:53:VAL:HG11	2:D:80:PHE:CD1	2.46	0.51
5:I:121:G:C6	5:I:122:G:C4	2.98	0.51
1:A:126:LEU:HD11	1:A:254:VAL:HG11	1.92	0.51
1:A:221:GLY:HA3	1:A:227:LEU:CD1	2.40	0.51
2:B:10:CYS:HB3	2:B:13:GLN:CG	2.41	0.51
2:F:45:PHE:CD1	2:F:81:TRP:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:8:C:N3	5:I:31:G:N1	2.59	0.51
1:A:268:THR:HB	5:I:90:A:N6	2.26	0.51
2:B:28:TYR:CE2	2:B:32:GLN:HG3	2.46	0.51
2:C:46:LEU:CD1	2:D:40:VAL:HG11	2.41	0.51
5:I:25:U:H3'	5:I:25:U:H6	1.76	0.51
1:A:146:ILE:HG23	1:A:193:TYR:CD2	2.46	0.51
1:A:128:ARG:C	1:A:130:ARG:N	2.67	0.51
2:C:31:ALA:O	2:C:42:ARG:HG3	2.11	0.51
2:D:17:VAL:O	2:D:21:GLU:HG2	2.10	0.51
2:E:45:PHE:CD1	2:E:81:TRP:HB3	2.45	0.51
2:F:35:PRO:HG3	2:F:92:HIS:CD2	2.46	0.51
5:I:28:C:H2'	5:I:29:G:C8	2.46	0.51
1:A:263:TYR:HA	1:A:272:LEU:O	2.10	0.51
2:B:42:ARG:NH2	5:I:3:U:O2'	2.43	0.51
2:D:21:GLU:OE2	2:E:80:PHE:HD1	1.93	0.51
2:D:45:PHE:CD1	2:D:81:TRP:HB3	2.46	0.51
1:A:132:THR:C	1:A:254:VAL:HG23	2.36	0.50
1:A:133:HIS:CD2	1:A:253:PRO:HA	2.45	0.50
2:F:30:ILE:HG13	2:F:94:MET:HE2	1.93	0.50
1:A:49:LEU:HD23	1:A:85:LEU:HD22	1.93	0.50
1:A:141:LYS:HB3	1:A:144:PRO:HB2	1.93	0.50
1:A:142:PHE:HD1	1:A:244:LEU:HD22	1.77	0.50
1:A:148:ARG:HD3	1:A:178:GLY:O	2.10	0.50
1:A:159:ILE:C	1:A:161:CYS:H	2.17	0.50
1:A:172:LEU:HD12	1:A:180:PRO:HD2	1.94	0.50
2:B:72:ASP:HA	2:B:113:LEU:HD21	1.94	0.50
2:C:24:ILE:HD11	2:C:53:VAL:CG2	2.41	0.50
2:E:86:ALA:HB2	2:E:99:VAL:CG2	2.30	0.50
5:I:105:G:H2'	5:I:106:U:O4'	2.11	0.50
5:I:108:G:H3'	5:I:109:A:H5''	1.93	0.50
1:A:187:GLN:CG	4:H:118:U:O2'	2.60	0.50
2:B:20:TYR:CE2	2:B:52:GLN:HB3	2.46	0.50
4:H:121:C:H2'	4:H:122:C:C6	2.46	0.50
1:A:272:LEU:HD23	1:A:310:ALA:HB3	1.92	0.50
4:H:123:A:H2'	4:H:124:U:C6	2.47	0.50
1:A:99:GLU:O	1:A:110:ARG:NH1	2.45	0.50
2:B:34:ILE:HG23	2:B:89:GLN:NE2	2.27	0.50
2:B:41:ALA:HB2	2:F:28:TYR:CE1	2.47	0.50
2:C:16:ILE:CD1	2:C:109:VAL:HG13	2.41	0.50
2:D:50:LEU:HD21	2:E:84:PHE:CE1	2.46	0.50
2:E:40:VAL:HG23	5:I:7:U:C5	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:HIS:N	1:A:254:VAL:HG23	2.26	0.50
1:A:159:ILE:HG13	1:A:168:LEU:CD1	2.42	0.50
2:B:45:PHE:CD1	2:B:81:TRP:HB3	2.46	0.50
2:C:17:VAL:O	2:C:21:GLU:HG2	2.11	0.50
2:F:36:ARG:O	2:F:37:LYS:C	2.54	0.50
5:I:124:A:H2'	5:I:125:A:C8	2.47	0.50
1:A:76:ILE:HG21	4:H:117:G:N9	2.27	0.49
2:E:82:LEU:HD11	2:E:106:ILE:CD1	2.42	0.49
5:I:111:U:C5	5:I:122:G:N2	2.80	0.49
1:A:29:LYS:HE3	1:A:32:THR:HG21	1.94	0.49
1:A:45:ASN:OD1	2:B:3:PRO:HA	2.12	0.49
1:A:66:PHE:HZ	4:H:117:G:OP2	1.93	0.49
1:A:141:LYS:C	1:A:144:PRO:HD2	2.36	0.49
5:I:50:G:H2'	5:I:51:U:O4'	2.12	0.49
1:A:133:HIS:CD2	1:A:224:PRO:HB3	2.47	0.49
2:D:87:GLY:HA2	2:D:92:HIS:HB2	1.94	0.49
2:B:92:HIS:CE1	2:B:95:THR:HA	2.47	0.49
2:C:90:LYS:C	2:C:92:HIS:H	2.21	0.49
2:E:64:GLN:C	2:E:66:SER:H	2.21	0.49
1:A:183:SER:HB2	1:A:186:SER:HB2	1.94	0.49
2:C:90:LYS:C	2:C:92:HIS:N	2.71	0.49
2:D:28:TYR:CE2	2:E:84:PHE:HZ	2.30	0.49
1:A:90:LEU:CD1	1:A:168:LEU:HD23	2.43	0.49
2:B:37:LYS:C	2:B:39:GLY:H	2.21	0.49
2:C:28:TYR:OH	2:D:41:ALA:HB2	2.13	0.49
2:C:64:GLN:HB3	2:C:67:LYS:HG2	1.95	0.49
1:A:41:TYR:CG	2:B:4:ILE:CG2	2.96	0.49
1:A:108:ALA:O	1:A:109:CYS:C	2.55	0.49
1:A:154:MET:C	1:A:156:ASP:H	2.20	0.49
1:A:308:GLN:HE21	1:A:309:TRP:NE1	2.10	0.49
2:B:56:PHE:CD1	2:B:71:ALA:HB1	2.47	0.49
2:F:82:LEU:HD11	2:F:106:ILE:CD1	2.43	0.49
5:I:27:G:C5	5:I:28:C:C5	3.00	0.49
1:A:13:THR:OG1	1:A:54:LYS:HG3	2.13	0.48
1:A:152:TYR:CE2	1:A:172:LEU:HD23	2.48	0.48
2:C:31:ALA:HB1	2:C:46:LEU:HG	1.94	0.48
2:D:68:LEU:HD11	2:D:116:TRP:CD2	2.48	0.48
2:E:34:ILE:HG23	2:E:93:ALA:HB1	1.95	0.48
2:E:35:PRO:HA	5:I:24:U:C5'	2.43	0.48
2:E:40:VAL:HB	5:I:7:U:O4	2.13	0.48
1:A:141:LYS:O	1:A:145:SER:OG	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:HG2	1:A:173:PRO:O	2.13	0.48
1:A:271:LEU:HD21	5:I:87:U:H4'	1.94	0.48
1:A:311:ASP:HB3	5:I:87:U:O3'	2.14	0.48
2:D:56:PHE:HE1	2:D:113:LEU:HD22	1.78	0.48
2:E:57:ILE:HD12	2:F:77:MET:SD	2.52	0.48
2:E:87:GLY:H	5:I:19:A:N6	2.12	0.48
1:A:104:PRO:HB3	5:I:131:G:H5'	1.96	0.48
1:A:123:GLN:HE22	1:A:270:LYS:H	1.60	0.48
2:B:82:LEU:HD11	2:B:106:ILE:CD1	2.39	0.48
2:C:52:GLN:OE1	2:C:74:GLY:C	2.56	0.48
2:F:23:VAL:HG11	2:F:106:ILE:HG12	1.95	0.48
2:F:90:LYS:HB3	2:F:91:PRO:HD2	1.96	0.48
1:A:76:ILE:HG21	4:H:117:G:C8	2.48	0.48
2:C:20:TYR:CZ	2:C:52:GLN:HG2	2.48	0.48
2:D:27:LEU:HD11	2:D:82:LEU:HD21	1.96	0.48
2:D:113:LEU:O	2:D:117:ILE:HG12	2.14	0.48
1:A:103:LEU:CD1	1:A:199:ARG:HG2	2.44	0.48
1:A:314:ASN:ND2	5:I:84:C:OP1	2.46	0.48
2:B:10:CYS:SG	2:B:12:ASP:HB2	2.53	0.48
2:C:17:VAL:HG11	2:D:83:ARG:NH2	2.28	0.48
2:C:32:GLN:NE2	2:D:37:LYS:HG2	2.28	0.48
2:F:20:TYR:HA	2:F:109:VAL:HG21	1.95	0.48
1:A:26:SER:HB3	1:A:81:PHE:HZ	1.78	0.48
1:A:108:ALA:HB3	1:A:191:ASN:OD1	2.14	0.48
2:C:45:PHE:CD1	2:C:81:TRP:HB3	2.48	0.48
5:I:27:G:C6	5:I:28:C:C4	3.02	0.48
1:A:108:ALA:HA	1:A:213:TYR:CE2	2.47	0.48
2:F:62:SER:C	2:F:64:GLN:N	2.72	0.48
5:I:29:G:H5''	5:I:29:G:H8	1.78	0.48
1:A:102:LEU:HD11	1:A:191:ASN:HB3	1.96	0.48
1:A:260:PHE:CE2	1:A:261:LEU:HD12	2.49	0.48
2:B:32:GLN:CD	5:I:3:U:H3	2.22	0.48
2:B:100:GLU:O	2:B:104:VAL:HG23	2.14	0.48
2:E:31:ALA:O	2:E:42:ARG:HG3	2.13	0.48
5:I:29:G:C6	5:I:30:G:C6	3.01	0.48
2:E:40:VAL:CG2	5:I:7:U:O4	2.61	0.48
2:F:20:TYR:CG	2:F:56:PHE:HE2	2.32	0.48
1:A:31:ARG:O	2:B:11:TYR:OH	2.32	0.47
1:A:296:LEU:O	1:A:300:LEU:HB2	2.14	0.47
1:A:19:LEU:HD21	1:A:43:LEU:CD2	2.44	0.47
2:B:97:HIS:HE1	4:H:127:C:OP1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:GLU:HG3	2:C:44:MET:N	2.28	0.47
2:C:68:LEU:HD12	2:C:117:ILE:HA	1.94	0.47
1:A:43:LEU:HB2	2:C:100:GLU:HA	1.96	0.47
1:A:69:TYR:HB2	5:I:59:C:O2'	2.14	0.47
2:C:19:ARG:HG2	2:C:108:GLU:HG3	1.97	0.47
2:E:89:GLN:HB3	2:E:91:PRO:HD2	1.96	0.47
1:A:12:ILE:CD1	1:A:164:THR:HG23	2.44	0.47
1:A:101:GLY:HA2	5:I:105:G:O3'	2.13	0.47
1:A:142:PHE:CE2	1:A:146:ILE:HD11	2.50	0.47
2:B:25:SER:CB	2:C:88:ILE:HD12	2.44	0.47
2:C:41:ALA:HB1	2:C:84:PHE:CE2	2.48	0.47
2:E:53:VAL:HB	2:F:77:MET:CE	2.38	0.47
2:F:31:ALA:O	2:F:33:SER:N	2.38	0.47
1:A:304:SER:HA	1:A:316:PHE:HZ	1.80	0.47
2:B:37:LYS:HD3	2:B:38:HIS:CD2	2.50	0.47
2:D:53:VAL:HG21	2:E:80:PHE:CZ	2.49	0.47
1:A:12:ILE:HD11	1:A:164:THR:HG23	1.96	0.47
1:A:58:TYR:CD2	1:A:170:VAL:HG11	2.50	0.47
2:F:72:ASP:HA	2:F:113:LEU:CD1	2.45	0.47
1:A:88:HIS:HA	1:A:184:LEU:HD23	1.96	0.47
1:A:200:LEU:HD13	1:A:237:PHE:CG	2.49	0.47
1:A:260:PHE:HB3	1:A:265:ILE:HD12	1.96	0.47
2:E:57:ILE:HD13	2:F:77:MET:HA	1.95	0.47
2:F:37:LYS:HD2	5:I:25:U:O2'	2.14	0.47
5:I:115:G:H1'	5:I:119:A:H61	1.80	0.47
1:A:109:CYS:SG	1:A:214:MET:HE1	2.55	0.47
1:A:263:TYR:CE1	1:A:306:HIS:CD2	3.03	0.47
2:B:72:ASP:HA	2:B:113:LEU:CD2	2.45	0.47
2:C:85:LEU:HB2	2:C:94:MET:HE3	1.97	0.47
2:D:28:TYR:OH	2:D:32:GLN:NE2	2.48	0.47
2:E:59:ALA:C	2:E:116:TRP:HH2	2.23	0.47
1:A:127:ARG:NE	1:A:267:PRO:O	2.48	0.47
2:B:20:TYR:HA	2:B:109:VAL:HG21	1.97	0.47
2:C:34:ILE:HB	2:C:42:ARG:HB2	1.97	0.47
2:C:36:ARG:O	2:C:39:GLY:HA3	2.15	0.47
1:A:266:TRP:CZ3	1:A:271:LEU:HB2	2.50	0.46
2:B:44:MET:CE	2:F:47:LYS:HA	2.45	0.46
2:B:53:VAL:HG11	2:C:80:PHE:CD1	2.49	0.46
2:C:94:MET:HG3	2:C:98:GLN:CB	2.46	0.46
2:D:65:VAL:HG11	2:D:121:ASN:HD21	1.80	0.46
2:E:75:LEU:HD12	2:E:75:LEU:HA	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:LEU:HG	2:F:45:PHE:HZ	1.80	0.46
1:A:11:GLN:CB	1:A:93:ILE:HG12	2.42	0.46
1:A:90:LEU:C	1:A:92:ASN:H	2.23	0.46
1:A:271:LEU:HD11	5:I:87:U:H5'	1.98	0.46
2:B:31:ALA:O	2:B:42:ARG:HD3	2.15	0.46
2:C:34:ILE:O	2:C:35:PRO:C	2.59	0.46
2:C:82:LEU:CD2	2:C:94:MET:SD	3.00	0.46
2:C:91:PRO:O	2:C:92:HIS:HB2	2.14	0.46
2:E:106:ILE:HA	2:E:109:VAL:HG22	1.97	0.46
1:A:74:ARG:NH1	5:I:57:G:C8	2.83	0.46
1:A:108:ALA:HB2	1:A:214:MET:N	2.30	0.46
1:A:134:PHE:HB2	1:A:220:LEU:HD23	1.98	0.46
1:A:200:LEU:HD22	1:A:237:PHE:CB	2.45	0.46
1:A:33:TRP:O	1:A:37:GLU:HB3	2.16	0.46
1:A:49:LEU:HB2	2:B:1:MET:CE	2.45	0.46
2:D:85:LEU:CD2	2:D:89:GLN:NE2	2.79	0.46
5:I:13:A:N1	5:I:25:U:O2	2.49	0.46
1:A:114:GLY:H	1:A:117:ALA:HB3	1.79	0.46
2:C:34:ILE:HG23	2:C:89:GLN:NE2	2.25	0.46
2:F:24:ILE:HD11	2:F:53:VAL:CG2	2.46	0.46
1:A:76:ILE:O	1:A:76:ILE:HG22	2.14	0.46
1:A:228:ARG:HA	1:A:251:VAL:HG21	1.97	0.46
5:I:83:A:C8	5:I:84:C:H5	2.30	0.46
2:D:69:TYR:OH	2:D:121:ASN:ND2	2.49	0.46
5:I:111:U:H2'	5:I:112:A:C8	2.50	0.46
1:A:134:PHE:HA	1:A:220:LEU:HA	1.97	0.46
1:A:142:PHE:O	1:A:146:ILE:N	2.48	0.46
1:A:270:LYS:O	1:A:272:LEU:N	2.49	0.46
2:E:37:LYS:HE3	5:I:7:U:O2	2.16	0.46
1:A:45:ASN:ND2	2:B:3:PRO:HB3	2.30	0.45
2:B:26:TYR:CE2	2:B:101:THR:HB	2.51	0.45
2:B:80:PHE:CE1	2:F:53:VAL:HG21	2.51	0.45
4:H:118:U:H2'	4:H:119:G:C8	2.51	0.45
1:A:123:GLN:HG2	1:A:127:ARG:CZ	2.46	0.45
2:B:34:ILE:O	2:B:42:ARG:NH1	2.50	0.45
2:B:44:MET:HE2	2:B:44:MET:HB3	1.80	0.45
2:C:52:GLN:OE1	2:C:75:LEU:N	2.49	0.45
5:I:115:G:N2	5:I:118:A:C8	2.84	0.45
5:I:121:G:C2	5:I:122:G:H1'	2.51	0.45
1:A:105:TYR:HD2	1:A:210:TRP:CE2	2.34	0.45
2:B:36:ARG:C	2:B:37:LYS:O	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASP:HB3	1:A:150:ALA:H	1.79	0.45
2:B:80:PHE:CZ	2:F:53:VAL:HG21	2.51	0.45
1:A:22:TYR:CE1	1:A:38:PHE:CD1	3.04	0.45
1:A:208:ARG:HE	5:I:129:G:H5'	1.82	0.45
2:F:27:LEU:HD12	2:F:30:ILE:HD11	1.98	0.45
5:I:113:C:N4	5:I:122:G:N2	2.64	0.45
1:A:4:ARG:HG3	1:A:6:ARG:CD	2.47	0.45
1:A:202:HIS:CE1	5:I:130:G:C5'	3.00	0.45
1:A:202:HIS:CE1	5:I:130:G:H5'	2.51	0.45
2:B:86:ALA:HB2	2:B:99:VAL:CG2	2.44	0.45
1:A:135:LEU:CD1	1:A:231:PHE:HB2	2.46	0.45
2:B:54:GLU:HB2	2:C:77:MET:HE2	1.99	0.45
2:E:37:LYS:N	5:I:7:U:H5''	2.32	0.45
5:I:8:C:O4'	5:I:31:G:N2	2.50	0.45
1:A:44:ALA:HB1	2:B:4:ILE:HD11	1.99	0.45
2:E:82:LEU:HD11	2:E:106:ILE:HD12	1.98	0.45
2:E:95:THR:HA	5:I:19:A:N7	2.32	0.45
5:I:102:A:H2'	5:I:103:A:C8	2.51	0.45
1:A:41:TYR:HB2	2:B:4:ILE:HB	1.97	0.45
1:A:272:LEU:CB	1:A:306:HIS:HE1	2.29	0.45
5:I:107:C:N4	5:I:108:G:C6	2.85	0.45
1:A:198:ASP:CG	1:A:212:ARG:HE	2.25	0.45
1:A:269:HIS:C	1:A:271:LEU:H	2.25	0.45
1:A:138:ASP:O	1:A:246:ILE:HG23	2.17	0.44
2:B:57:ILE:O	2:B:61:LYS:HG2	2.18	0.44
2:C:62:SER:C	2:C:64:GLN:N	2.75	0.44
5:I:111:U:C2	5:I:112:A:C8	3.05	0.44
1:A:4:ARG:O	1:A:5:HIS:CB	2.65	0.44
1:A:82:LYS:HE2	1:A:82:LYS:HB2	1.61	0.44
1:A:126:LEU:HD22	1:A:258:ILE:HD12	1.99	0.44
1:A:155:ILE:CG2	1:A:168:LEU:HD13	2.46	0.44
1:A:284:VAL:HG21	1:A:319:MET:HE3	1.99	0.44
1:A:296:LEU:HD11	1:A:325:ILE:HD13	1.97	0.44
2:C:56:PHE:CE1	2:C:71:ALA:HB1	2.52	0.44
2:C:57:ILE:HD12	2:D:76:ALA:HB1	1.98	0.44
2:C:87:GLY:O	2:C:89:GLN:N	2.50	0.44
2:D:65:VAL:HG11	2:D:121:ASN:CG	2.41	0.44
2:E:28:TYR:HB3	2:E:29:PRO:HD3	1.99	0.44
5:I:29:G:H3'	5:I:30:G:H8	1.82	0.44
1:A:269:HIS:C	1:A:271:LEU:N	2.76	0.44
1:A:315:LEU:O	1:A:315:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:42:ARG:HD2	5:I:4:G:O6	2.18	0.44
5:I:9:U:C2	5:I:30:G:N2	2.85	0.44
5:I:25:U:C6	5:I:25:U:C3'	3.01	0.44
1:A:49:LEU:HD13	2:B:1:MET:HE3	1.99	0.44
1:A:263:TYR:CD2	1:A:270:LYS:HD2	2.51	0.44
1:A:271:LEU:CD1	5:I:86:U:H2'	2.47	0.44
2:D:99:VAL:HG12	2:D:103:GLN:OE1	2.16	0.44
2:F:46:LEU:HD23	2:F:46:LEU:HA	1.72	0.44
5:I:5:G:C6	5:I:33:U:O2	2.70	0.44
1:A:24:LYS:HD2	1:A:92:ASN:HD21	1.83	0.44
2:F:108:GLU:O	2:F:112:ILE:HG13	2.17	0.44
1:A:154:MET:SD	1:A:193:TYR:HA	2.58	0.44
1:A:231:PHE:CZ	1:A:249:TRP:CG	3.05	0.44
2:F:44:MET:HE2	2:F:44:MET:HB3	1.70	0.44
2:F:45:PHE:CD2	2:F:85:LEU:HD11	2.52	0.44
2:F:85:LEU:HD23	2:F:88:ILE:HD12	1.99	0.44
1:A:50:GLN:O	1:A:54:LYS:HB2	2.18	0.44
1:A:75:LEU:HD22	1:A:75:LEU:HA	1.77	0.44
1:A:126:LEU:CD1	1:A:131:ALA:HB3	2.41	0.44
2:B:82:LEU:CD1	2:B:106:ILE:HD12	2.42	0.44
2:C:24:ILE:HD13	2:D:80:PHE:HZ	1.82	0.44
2:D:106:ILE:HA	2:D:109:VAL:HG12	2.00	0.44
5:I:51:U:H2'	5:I:52:G:C8	2.53	0.44
1:A:127:ARG:NH2	5:I:92:G:O6	2.48	0.44
1:A:308:GLN:HG2	1:A:309:TRP:N	2.33	0.44
2:B:28:TYR:CE1	2:C:84:PHE:HZ	2.35	0.44
2:C:20:TYR:OH	2:C:52:GLN:HB3	2.17	0.44
2:C:44:MET:HE2	2:C:44:MET:HB3	1.85	0.44
2:D:32:GLN:NE2	5:I:7:U:N3	2.66	0.44
2:E:50:LEU:CD2	2:F:84:PHE:CE1	3.01	0.44
1:A:15:TRP:HZ2	1:A:43:LEU:HD22	1.82	0.43
1:A:274:LYS:HE3	1:A:274:LYS:HB2	1.72	0.43
2:B:28:TYR:HB3	2:B:29:PRO:HD3	1.99	0.43
2:C:100:GLU:O	2:C:104:VAL:HG23	2.17	0.43
2:D:16:ILE:HD11	2:D:113:LEU:HB2	1.99	0.43
2:E:19:ARG:HG3	2:E:112:ILE:HD11	1.99	0.43
2:E:41:ALA:HB1	2:E:84:PHE:HE2	1.83	0.43
1:A:36:LEU:HD12	2:B:11:TYR:CE1	2.53	0.43
1:A:46:LEU:HD21	1:A:85:LEU:HD11	1.99	0.43
1:A:53:LEU:HD22	1:A:167:LEU:HD11	2.00	0.43
1:A:148:ARG:NH1	1:A:178:GLY:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PHE:CE2	1:A:249:TRP:CD2	3.06	0.43
2:D:75:LEU:HD23	2:D:75:LEU:HA	1.83	0.43
2:D:81:TRP:O	2:D:85:LEU:HG	2.18	0.43
2:E:20:TYR:CA	2:E:109:VAL:HG11	2.46	0.43
1:A:265:ILE:HA	1:A:270:LYS:HA	2.00	0.43
2:B:72:ASP:CA	2:B:113:LEU:HD21	2.47	0.43
2:E:28:TYR:OH	2:F:38:HIS:HA	2.19	0.43
1:A:65:GLU:HA	1:A:77:SER:HA	2.00	0.43
1:A:272:LEU:HD12	1:A:273:ARG:H	1.83	0.43
2:E:27:LEU:HD21	2:E:102:ALA:CB	2.47	0.43
1:A:41:TYR:CD2	2:B:4:ILE:HG21	2.53	0.43
1:A:193:TYR:CE2	1:A:242:LEU:HB3	2.52	0.43
2:C:37:LYS:O	5:I:3:U:C4	2.72	0.43
2:C:38:HIS:CE1	2:C:91:PRO:HD2	2.52	0.43
2:E:13:GLN:HG3	2:E:14:MET:N	2.33	0.43
2:F:31:ALA:HB3	2:F:46:LEU:HD21	1.99	0.43
2:F:45:PHE:CG	2:F:85:LEU:HD11	2.54	0.43
5:I:80:A:N7	5:I:81:A:N6	2.67	0.43
1:A:26:SER:HB3	1:A:35:TYR:CD1	2.53	0.43
1:A:29:LYS:C	1:A:31:ARG:H	2.27	0.43
2:B:88:ILE:CG2	2:F:25:SER:HA	2.48	0.43
2:C:56:PHE:CD1	2:C:71:ALA:HB1	2.53	0.43
2:E:46:LEU:HD23	2:E:46:LEU:HA	1.84	0.43
1:A:91:CYS:O	1:A:95:ALA:HB3	2.19	0.43
2:B:105:LEU:O	2:B:109:VAL:HG23	2.18	0.43
2:F:82:LEU:HB3	2:F:99:VAL:HG13	2.01	0.43
1:A:13:THR:CG2	1:A:53:LEU:HB2	2.49	0.43
1:A:201:LEU:O	1:A:207:GLN:HB2	2.19	0.43
1:A:220:LEU:H	1:A:220:LEU:HG	1.59	0.43
2:C:94:MET:HG3	2:C:98:GLN:HB2	2.01	0.43
2:C:94:MET:O	2:C:95:THR:C	2.62	0.43
2:C:105:LEU:O	2:C:109:VAL:HG23	2.19	0.43
2:F:56:PHE:CD1	2:F:71:ALA:HB1	2.54	0.43
5:I:115:G:C2	5:I:118:A:C8	3.06	0.43
1:A:63:TYR:HB3	1:A:77:SER:HB2	2.01	0.43
1:A:200:LEU:O	1:A:205:LEU:HD12	2.19	0.43
1:A:263:TYR:HB3	1:A:270:LYS:HG2	2.01	0.43
2:B:13:GLN:HE21	2:B:61:LYS:HD3	1.83	0.43
2:C:16:ILE:CD1	2:C:112:ILE:HB	2.49	0.43
2:D:27:LEU:HD23	2:D:27:LEU:HA	1.87	0.43
4:H:123:A:H2'	4:H:124:U:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:8:C:C2	5:I:31:G:N1	2.87	0.43
5:I:123:A:H2'	5:I:124:A:O4'	2.19	0.43
1:A:41:TYR:O	1:A:45:ASN:N	2.43	0.43
2:B:19:ARG:HH22	5:I:50:G:H4'	1.84	0.43
2:B:83:ARG:NH2	2:F:17:VAL:HG11	2.33	0.43
2:D:19:ARG:HG3	2:D:112:ILE:CD1	2.49	0.43
2:E:52:GLN:HG2	2:E:55:LEU:HD12	2.00	0.43
2:B:27:LEU:HD23	2:B:27:LEU:HA	1.89	0.42
2:C:85:LEU:HA	2:C:89:GLN:HB2	2.01	0.42
2:E:57:ILE:HG21	2:F:73:ALA:O	2.19	0.42
5:I:115:G:N2	5:I:118:A:O4'	2.52	0.42
2:B:28:TYR:CD1	2:B:46:LEU:HD22	2.54	0.42
2:E:19:ARG:HG3	2:E:112:ILE:CD1	2.48	0.42
1:A:9:ILE:N	1:A:164:THR:OG1	2.53	0.42
1:A:41:TYR:CE2	2:C:107:ALA:HA	2.53	0.42
1:A:126:LEU:HD13	1:A:220:LEU:HD13	2.00	0.42
2:B:27:LEU:HD23	2:B:30:ILE:HD11	2.00	0.42
2:B:27:LEU:HD11	2:B:82:LEU:HD21	2.00	0.42
2:B:35:PRO:O	2:B:37:LYS:O	2.36	0.42
2:B:92:HIS:CE1	2:B:95:THR:HG22	2.54	0.42
2:C:35:PRO:HD2	2:C:89:GLN:HE22	1.83	0.42
5:I:107:C:H1'	5:I:127:G:N2	2.34	0.42
2:B:10:CYS:O	2:B:11:TYR:C	2.62	0.42
2:B:16:ILE:HG13	2:B:112:ILE:HB	2.01	0.42
2:D:90:LYS:HD3	2:D:90:LYS:HA	1.91	0.42
1:A:60:ARG:H	1:A:170:VAL:HG13	1.85	0.42
1:A:154:MET:HE2	1:A:196:ALA:HB2	2.01	0.42
2:B:80:PHE:CZ	2:F:24:ILE:HD13	2.54	0.42
2:B:80:PHE:CD1	2:F:53:VAL:HG11	2.55	0.42
5:I:28:C:N3	5:I:29:G:N7	2.67	0.42
1:A:22:TYR:HB2	1:A:46:LEU:HD21	2.01	0.42
2:B:35:PRO:HG2	2:B:91:PRO:HG2	2.02	0.42
2:B:84:PHE:HA	2:B:88:ILE:HD12	2.01	0.42
2:D:45:PHE:CG	2:D:85:LEU:HD11	2.54	0.42
2:E:47:LYS:HA	2:F:44:MET:SD	2.60	0.42
5:I:5:G:C6	5:I:32:C:N3	2.87	0.42
5:I:18:U:H1'	5:I:22:G:N2	2.35	0.42
1:A:208:ARG:CG	5:I:130:G:OP1	2.57	0.42
2:B:34:ILE:O	2:B:35:PRO:O	2.38	0.42
2:E:30:ILE:HG12	2:E:98:GLN:NE2	2.34	0.42
2:B:3:PRO:O	2:B:4:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:100:A:O2'	5:I:101:A:OP2	2.35	0.42
5:I:125:A:H2'	5:I:126:G:O4'	2.19	0.42
1:A:87:GLN:NE2	1:A:185:THR:HB	2.35	0.42
2:B:12:ASP:HB3	2:B:116:TRP:CG	2.54	0.42
2:B:40:VAL:HG13	2:F:43:GLU:HG3	2.02	0.42
2:D:90:LYS:O	2:D:92:HIS:N	2.53	0.42
1:A:128:ARG:O	1:A:130:ARG:N	2.53	0.42
1:A:148:ARG:HD3	1:A:178:GLY:C	2.45	0.42
1:A:169:ARG:HG2	1:A:174:ASP:HB2	2.02	0.42
2:C:82:LEU:HD11	2:C:106:ILE:HD11	2.02	0.42
2:D:32:GLN:OE1	2:E:37:LYS:HG3	2.19	0.42
2:F:37:LYS:HB2	5:I:25:U:O3'	2.19	0.42
4:H:121:C:H2'	4:H:122:C:H6	1.85	0.42
5:I:13:A:N6	5:I:14:A:N6	2.68	0.42
2:D:92:HIS:NE2	2:D:95:THR:HA	2.35	0.41
2:E:20:TYR:CZ	2:E:52:GLN:HB3	2.55	0.41
2:E:36:ARG:O	2:E:39:GLY:N	2.53	0.41
2:F:105:LEU:O	2:F:109:VAL:HG23	2.20	0.41
1:A:57:ASN:HD22	1:A:57:ASN:HA	1.42	0.41
1:A:103:LEU:CD2	1:A:104:PRO:HD2	2.49	0.41
1:A:107:TYR:OH	1:A:121:HIS:CG	2.73	0.41
1:A:202:HIS:HE1	5:I:130:G:C5'	2.33	0.41
2:B:16:ILE:HG12	2:B:109:VAL:HG13	2.02	0.41
2:D:42:ARG:HD3	5:I:7:U:N3	2.34	0.41
5:I:29:G:C4	5:I:30:G:C8	3.08	0.41
2:C:40:VAL:HG23	5:I:3:U:C5	2.55	0.41
2:D:65:VAL:HG11	2:D:121:ASN:OD1	2.19	0.41
2:D:77:MET:HE3	2:D:81:TRP:NE1	2.35	0.41
2:D:91:PRO:O	2:D:92:HIS:C	2.62	0.41
2:F:27:LEU:HB3	2:F:49:LEU:HD22	2.01	0.41
1:A:52:GLU:OE1	2:B:1:MET:HB2	2.20	0.41
1:A:98:PHE:CE1	1:A:155:ILE:HA	2.56	0.41
2:D:94:MET:HE3	2:D:94:MET:HB2	1.85	0.41
2:E:34:ILE:HG23	2:E:93:ALA:CB	2.50	0.41
2:E:86:ALA:CB	2:E:99:VAL:HG21	2.35	0.41
1:A:127:ARG:NH1	5:I:92:G:N7	2.69	0.41
2:C:25:SER:CA	2:D:88:ILE:HG23	2.39	0.41
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.91	0.41
1:A:273:ARG:HB2	1:A:276:SER:OG	2.20	0.41
2:B:52:GLN:OE1	2:B:74:GLY:C	2.64	0.41
2:C:16:ILE:HD13	2:C:16:ILE:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:26:TYR:O	2:C:30:ILE:HG12	2.20	0.41
2:C:82:LEU:CD1	2:C:106:ILE:HD12	2.50	0.41
2:E:72:ASP:HA	2:E:113:LEU:CD1	2.50	0.41
2:D:32:GLN:NE2	5:I:7:U:H3	2.19	0.41
2:D:100:GLU:O	2:D:104:VAL:HG23	2.20	0.41
5:I:10:G:C6	5:I:29:G:N1	2.89	0.41
1:A:4:ARG:O	1:A:5:HIS:HB2	2.21	0.41
1:A:172:LEU:HD22	1:A:189:PHE:CD2	2.55	0.41
1:A:263:TYR:C	1:A:272:LEU:O	2.63	0.41
2:B:34:ILE:CG2	2:B:89:GLN:NE2	2.84	0.41
2:B:85:LEU:O	2:B:93:ALA:HB3	2.21	0.41
2:D:85:LEU:HD22	2:D:89:GLN:HE21	1.86	0.41
4:H:125:C:H2'	4:H:126:A:C8	2.55	0.41
1:A:184:LEU:HD13	4:H:119:G:H5'	2.02	0.41
2:B:31:ALA:HB2	2:B:45:PHE:HE2	1.84	0.41
2:C:82:LEU:HB3	2:C:99:VAL:HG13	2.02	0.41
2:D:34:ILE:HG22	2:D:38:HIS:HB2	2.03	0.41
2:E:34:ILE:HB	2:E:42:ARG:HB2	2.02	0.41
2:E:42:ARG:HH22	5:I:24:U:H5''	1.85	0.41
2:E:96:PRO:HD3	5:I:19:A:C5	2.56	0.41
2:F:41:ALA:HB1	2:F:84:PHE:HE2	1.85	0.41
1:A:4:ARG:HG3	1:A:6:ARG:HD2	2.02	0.41
2:B:83:ARG:HE	2:F:21:GLU:CD	2.28	0.41
2:C:28:TYR:CG	2:D:84:PHE:CZ	3.09	0.41
2:C:36:ARG:HA	2:C:42:ARG:NH2	2.36	0.41
2:D:44:MET:HB3	2:D:44:MET:HE2	1.69	0.41
2:D:50:LEU:O	2:E:77:MET:HE1	2.20	0.41
2:E:30:ILE:HD13	2:E:30:ILE:HG21	1.87	0.41
2:E:100:GLU:O	2:E:104:VAL:HG23	2.21	0.41
5:I:51:U:H2'	5:I:52:G:H8	1.86	0.41
1:A:157:LYS:HE3	5:I:107:C:H5''	2.03	0.40
1:A:201:LEU:HG	1:A:234:LEU:HD11	2.03	0.40
2:B:97:HIS:CE1	4:H:127:C:OP1	2.74	0.40
2:C:31:ALA:HB2	2:C:45:PHE:CD2	2.56	0.40
2:F:100:GLU:O	2:F:104:VAL:HG23	2.21	0.40
1:A:278:LYS:O	1:A:282:ARG:HB2	2.22	0.40
2:B:23:VAL:HG12	2:B:27:LEU:HD12	2.03	0.40
5:I:56:A:C8	5:I:57:G:C8	3.09	0.40
1:A:6:ARG:NH1	5:I:121:G:C8	2.89	0.40
2:B:46:LEU:HA	2:B:46:LEU:HD23	1.75	0.40
2:C:59:ALA:HA	2:C:67:LYS:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:ILE:HD13	2:F:77:MET:CA	2.51	0.40
1:A:19:LEU:HD21	1:A:43:LEU:HD21	2.03	0.40
1:A:142:PHE:O	1:A:145:SER:N	2.42	0.40
1:A:170:VAL:HG12	1:A:171:VAL:N	2.36	0.40
2:B:85:LEU:HD12	2:B:94:MET:SD	2.62	0.40
2:E:16:ILE:HG12	2:E:112:ILE:HG22	2.02	0.40
5:I:12:C:H6	5:I:12:C:O5'	2.04	0.40
5:I:116:A:H2'	5:I:117:A:O4'	2.22	0.40
1:A:76:ILE:CG2	4:H:117:G:C4	3.04	0.40
1:A:274:LYS:O	1:A:275:SER:C	2.65	0.40
2:B:31:ALA:O	2:B:42:ARG:CD	2.70	0.40
2:C:40:VAL:HA	2:C:43:GLU:HG2	2.03	0.40
2:D:26:TYR:O	2:D:30:ILE:HG13	2.22	0.40
2:D:28:TYR:HB3	2:D:29:PRO:HD3	2.02	0.40
2:E:54:GLU:HB2	2:F:77:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/328 (98%)	263 (82%)	44 (14%)	14 (4%)	2	9
2	B	120/290 (41%)	104 (87%)	8 (7%)	8 (7%)	1	4
2	C	109/290 (38%)	94 (86%)	9 (8%)	6 (6%)	1	7
2	D	109/290 (38%)	98 (90%)	10 (9%)	1 (1%)	14	39
2	E	108/290 (37%)	99 (92%)	8 (7%)	1 (1%)	14	39
2	F	109/290 (38%)	96 (88%)	10 (9%)	3 (3%)	4	16
All	All	876/1778 (49%)	754 (86%)	89 (10%)	33 (4%)	4	12

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	7	ASN
1	A	109	CYS
1	A	160	HIS
1	A	255	SER
1	A	272	LEU
2	B	35	PRO
2	B	93	ALA
2	C	90	LYS
2	E	65	VAL
1	A	140	SER
1	A	149	ALA
1	A	163	ALA
1	A	222	ASP
1	A	271	LEU
2	B	4	ILE
2	B	37	LYS
2	B	38	HIS
2	B	63	ASN
2	C	91	PRO
2	C	93	ALA
2	D	92	HIS
1	A	214	MET
2	B	92	HIS
2	C	12	ASP
2	F	32	GLN
1	A	103	LEU
1	A	129	THR
2	B	2	GLU
2	C	63	ASN
2	C	95	THR
2	F	63	ASN
2	F	90	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/278 (99%)	213 (78%)	62 (22%)	1	3
2	B	102/232 (44%)	85 (83%)	17 (17%)	2	8
2	C	92/232 (40%)	83 (90%)	9 (10%)	7	26
2	D	92/232 (40%)	75 (82%)	17 (18%)	1	7
2	E	91/232 (39%)	71 (78%)	20 (22%)	1	4
2	F	92/232 (40%)	65 (71%)	27 (29%)	0	1
All	All	744/1438 (52%)	592 (80%)	152 (20%)	3	4

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LYS
1	A	4	ARG
1	A	23	ARG
1	A	37	GLU
1	A	42	ASP
1	A	54	LYS
1	A	57	ASN
1	A	65	GLU
1	A	67	LEU
1	A	68	VAL
1	A	74	ARG
1	A	75	LEU
1	A	76	ILE
1	A	82	LYS
1	A	93	ILE
1	A	94	VAL
1	A	97	ILE
1	A	110	ARG
1	A	127	ARG
1	A	128	ARG
1	A	129	THR
1	A	130	ARG
1	A	147	ASP
1	A	156	ASP
1	A	158	LYS
1	A	159	ILE
1	A	161	CYS
1	A	165	ARG
1	A	170	VAL

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Mol	Chain	Res	Type
1	A	171	VAL
1	A	175	GLU
1	A	177	VAL
1	A	179	ILE
1	A	181	ILE
1	A	185	THR
1	A	197	VAL
1	A	200	LEU
1	A	204	GLU
1	A	208	ARG
1	A	216	ASP
1	A	225	GLU
1	A	226	GLU
1	A	227	LEU
1	A	245	LYS
1	A	246	ILE
1	A	256	ARG
1	A	270	LYS
1	A	272	LEU
1	A	273	ARG
1	A	274	LYS
1	A	275	SER
1	A	276	SER
1	A	278	LYS
1	A	279	ARG
1	A	282	ARG
1	A	283	LYS
1	A	290	HIS
1	A	293	ASP
1	A	296	LEU
1	A	298	ARG
1	A	302	SER
2	B	8	THR
2	B	13	GLN
2	B	19	ARG
2	B	37	LYS
2	B	54	GLU
2	B	62	SER
2	B	64	GLN
2	B	65	VAL
2	B	66	SER
2	B	75	LEU

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Mol	Chain	Res	Type
2	B	89	GLN
2	B	90	LYS
2	B	95	THR
2	B	100	GLU
2	B	108	GLU
2	B	115	SER
2	B	119	ARG
2	C	14	MET
2	C	16	ILE
2	C	36	ARG
2	C	43	GLU
2	C	54	GLU
2	C	68	LEU
2	C	90	LYS
2	C	91	PRO
2	C	94	MET
2	D	14	MET
2	D	15	LEU
2	D	18	GLU
2	D	36	ARG
2	D	52	GLN
2	D	62	SER
2	D	64	GLN
2	D	65	VAL
2	D	68	LEU
2	D	89	GLN
2	D	92	HIS
2	D	95	THR
2	D	101	THR
2	D	103	GLN
2	D	119	ARG
2	D	122	ARG
2	D	123	LYS
2	E	13	GLN
2	E	16	ILE
2	E	18	GLU
2	E	36	ARG
2	E	43	GLU
2	E	50	LEU
2	E	52	GLN
2	E	62	SER
2	E	63	ASN

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Mol	Chain	Res	Type
2	E	65	VAL
2	E	66	SER
2	E	67	LYS
2	E	75	LEU
2	E	83	ARG
2	E	85	LEU
2	E	89	GLN
2	E	90	LYS
2	E	95	THR
2	E	113	LEU
2	E	119	ARG
2	F	13	GLN
2	F	14	MET
2	F	15	LEU
2	F	16	ILE
2	F	22	ARG
2	F	27	LEU
2	F	30	ILE
2	F	33	SER
2	F	36	ARG
2	F	43	GLU
2	F	54	GLU
2	F	55	LEU
2	F	64	GLN
2	F	65	VAL
2	F	66	SER
2	F	83	ARG
2	F	88	ILE
2	F	89	GLN
2	F	90	LYS
2	F	95	THR
2	F	100	GLU
2	F	103	GLN
2	F	105	LEU
2	F	111	ARG
2	F	113	LEU
2	F	122	ARG
2	F	123	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	87	GLN
1	A	286	ASN
1	A	290	HIS
1	A	306	HIS
1	A	308	GLN
2	B	13	GLN
2	B	92	HIS
2	B	97	HIS
2	C	13	GLN
2	C	64	GLN
2	C	89	GLN
2	C	97	HIS
2	C	121	ASN
2	D	13	GLN
2	D	32	GLN
2	E	89	GLN
2	F	92	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	G	12/19 (63%)	6 (50%)	2 (16%)
4	H	12/36 (33%)	4 (33%)	0
5	I	120/140 (85%)	53 (44%)	8 (6%)
All	All	144/195 (73%)	63 (43%)	10 (6%)

All (63) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	G	372	G
3	G	373	C
3	G	374	A
3	G	375	G
3	G	376	G
3	G	377	C
4	H	121	C
4	H	126	A
4	H	127	C
4	H	128	C
5	I	4	G
5	I	5	G

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Mol	Chain	Res	Type
5	I	6	C
5	I	7	U
5	I	8	C
5	I	9	U
5	I	13	A
5	I	14	A
5	I	15	C
5	I	20	C
5	I	21	G
5	I	22	G
5	I	27	G
5	I	28	C
5	I	29	G
5	I	33	U
5	I	51	U
5	I	53	G
5	I	55	C
5	I	61	G
5	I	63	U
5	I	65	U
5	I	66	G
5	I	71	G
5	I	73	U
5	I	74	U
5	I	75	C
5	I	76	G
5	I	77	G
5	I	80	A
5	I	82	C
5	I	84	C
5	I	85	G
5	I	87	U
5	I	88	A
5	I	89	C
5	I	93	G
5	I	94	U
5	I	95	U
5	I	97	G
5	I	98	G
5	I	99	C
5	I	101	A
5	I	106	U

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Mol	Chain	Res	Type
5	I	109	A
5	I	110	U
5	I	118	A
5	I	119	A
5	I	120	U
5	I	129	G
5	I	130	G
5	I	131	G
5	I	132	G

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	G	376	G
3	G	379	G
5	I	14	A
5	I	20	C
5	I	75	C
5	I	87	U
5	I	91	C
5	I	92	G
5	I	94	U
5	I	100	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

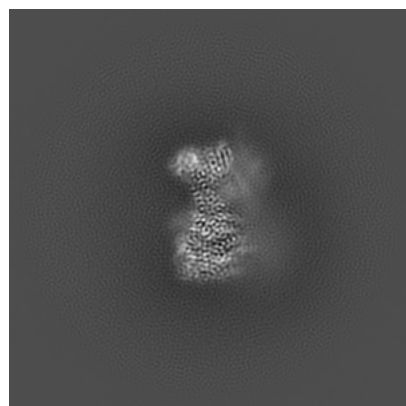
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42083. These allow visual inspection of the internal detail of the map and identification of artifacts.

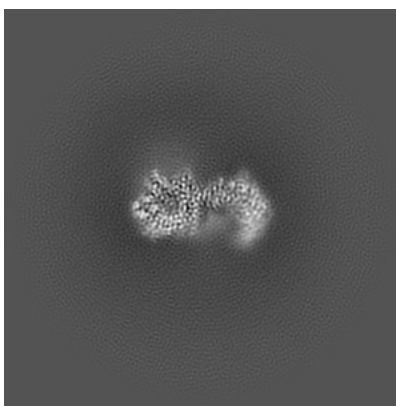
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

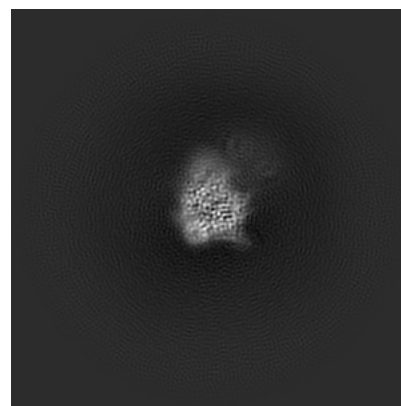
6.1.1 Primary map



X

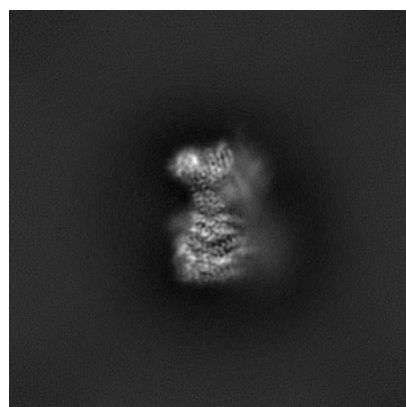


Y

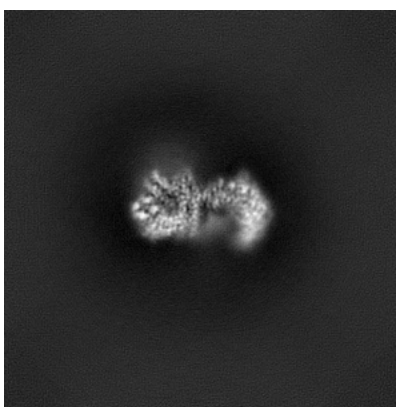


Z

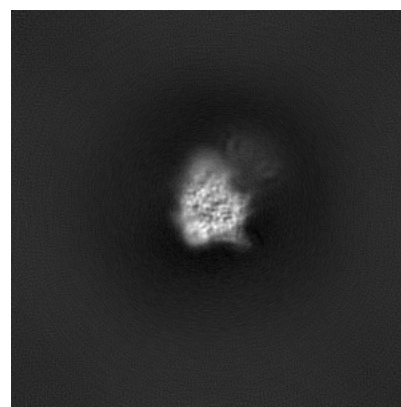
6.1.2 Raw map



X



Y

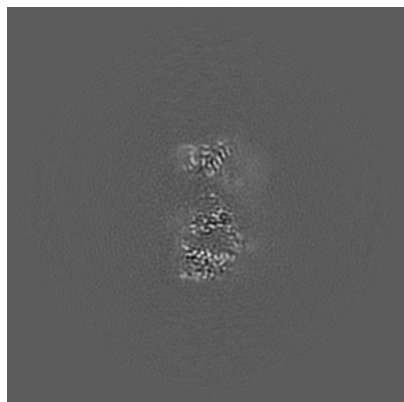


Z

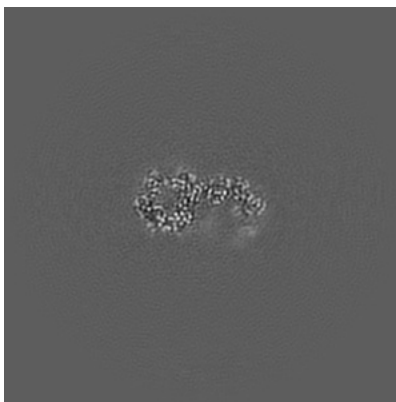
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

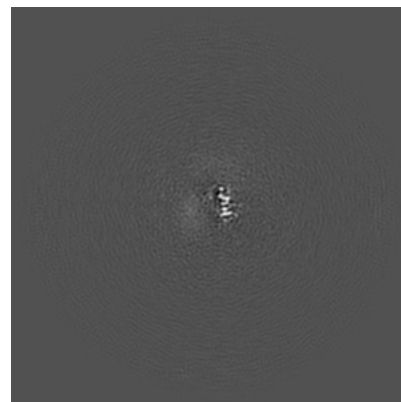
6.2.1 Primary map



X Index: 160



Y Index: 160

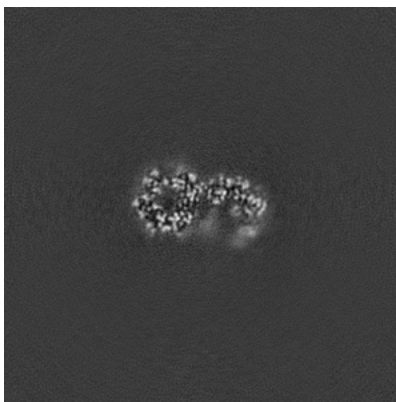


Z Index: 160

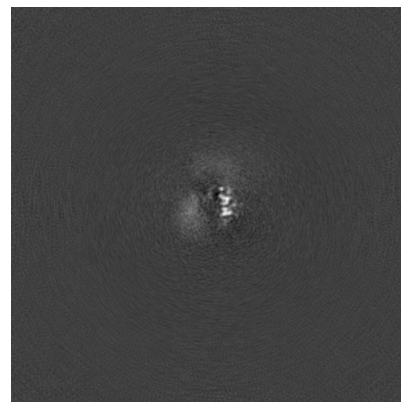
6.2.2 Raw map



X Index: 160



Y Index: 160

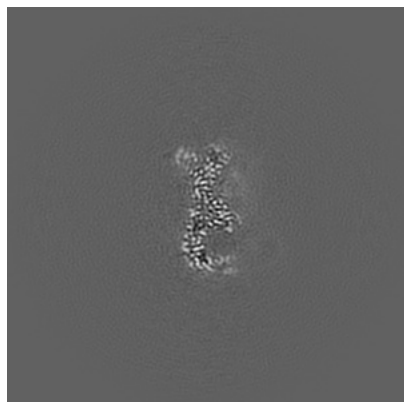


Z Index: 160

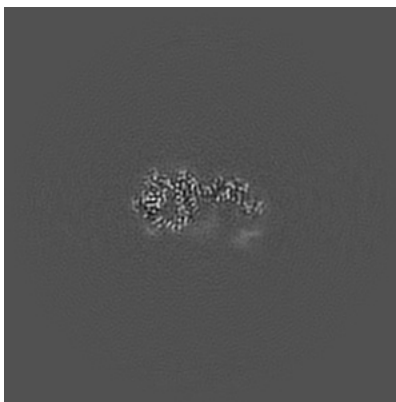
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

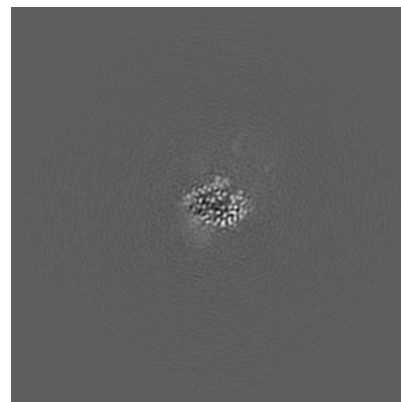
6.3.1 Primary map



X Index: 168

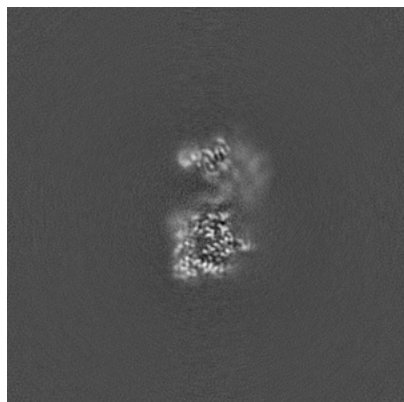


Y Index: 156

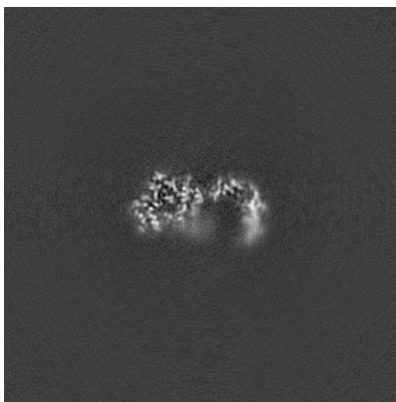


Z Index: 143

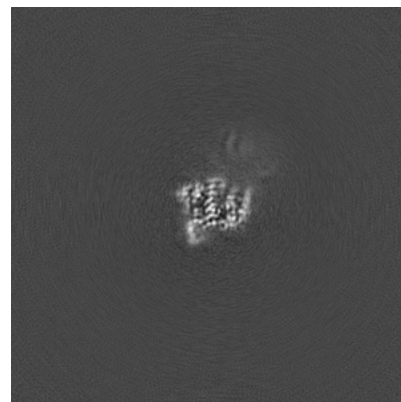
6.3.2 Raw map



X Index: 154



Y Index: 148

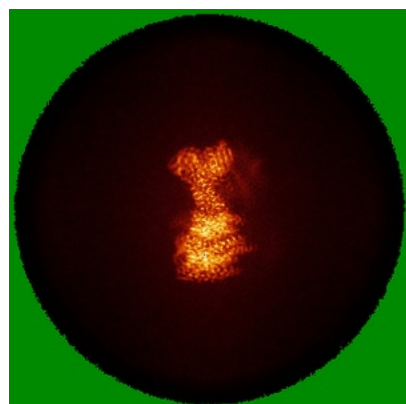


Z Index: 120

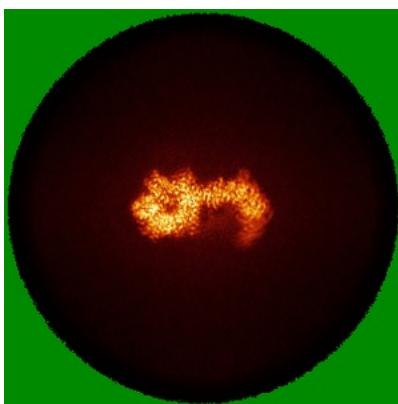
The images above show the largest variance slices of the map in three orthogonal directions.

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

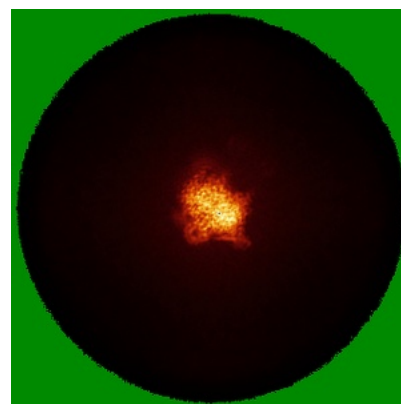
6.4.1 Primary map



X

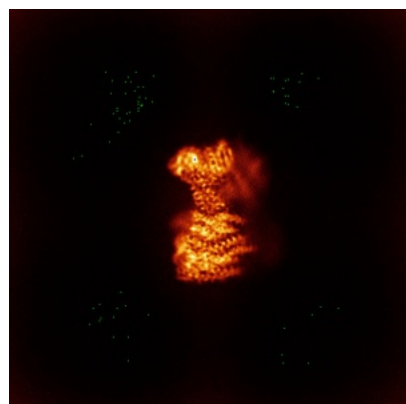


Y

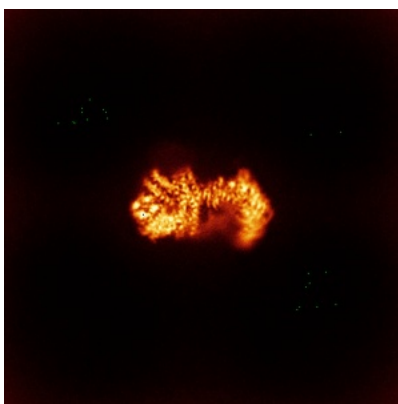


Z

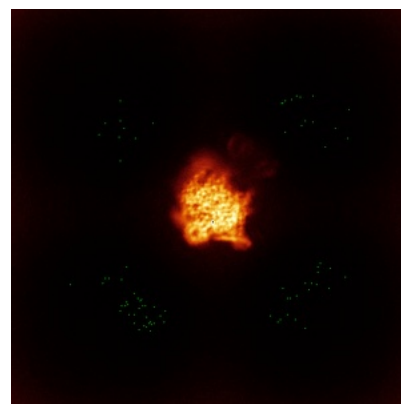
6.4.2 Raw map



X



Y

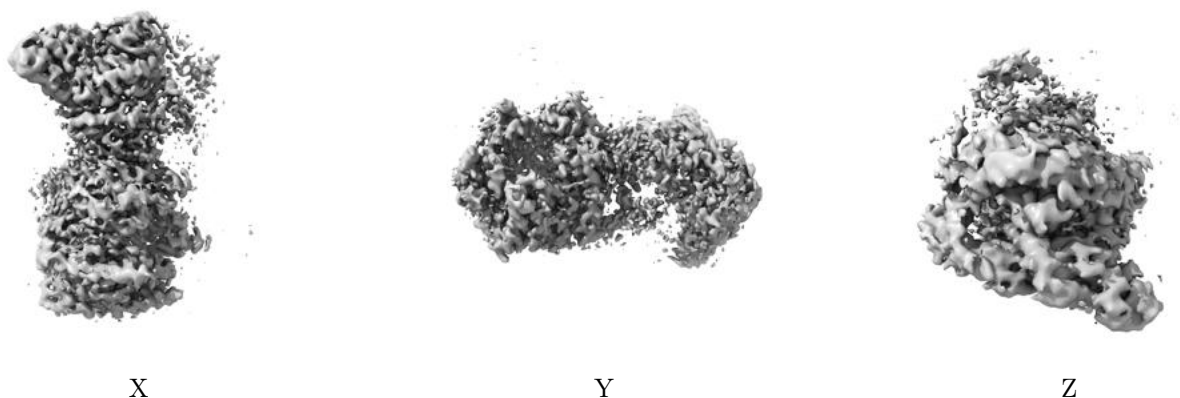


Z

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.

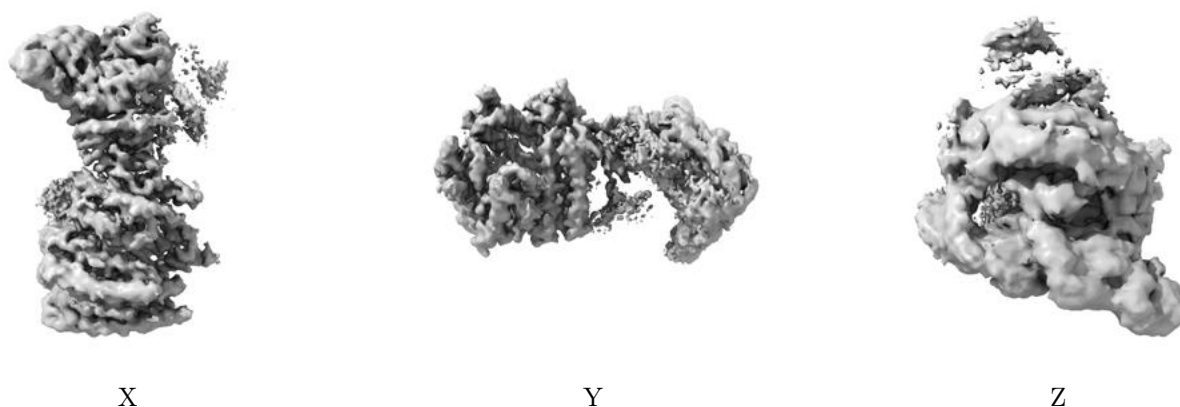
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

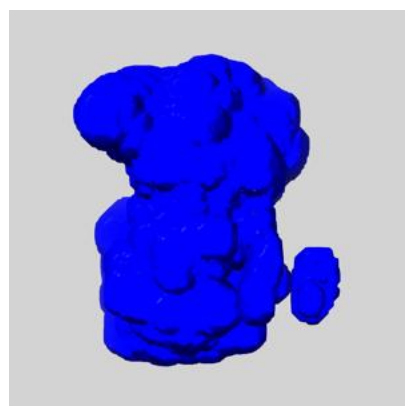
6.6 Mask visualisation [i](#)

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

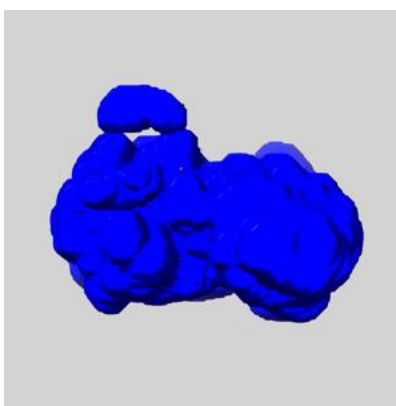
A mask typically either:

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

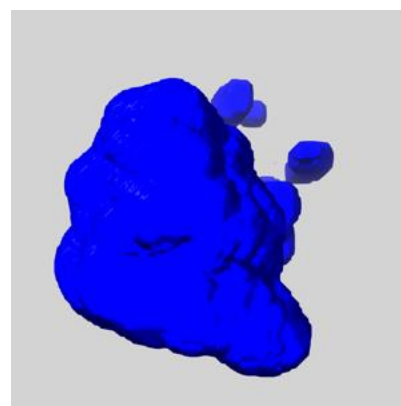
6.6.1 emd_42083_msk_1.map [i](#)



X



Y

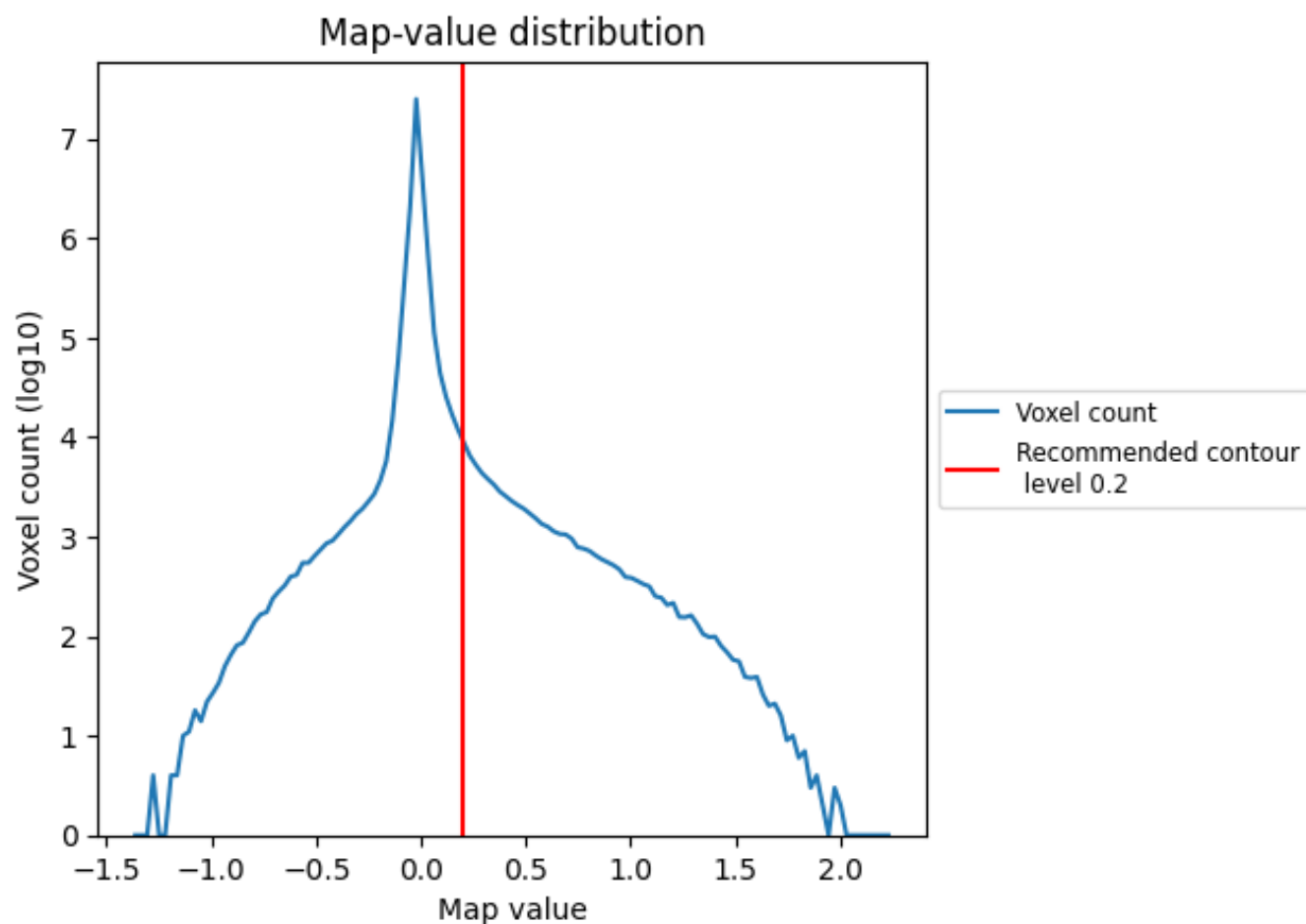


Z

7 Map analysis [i](#)

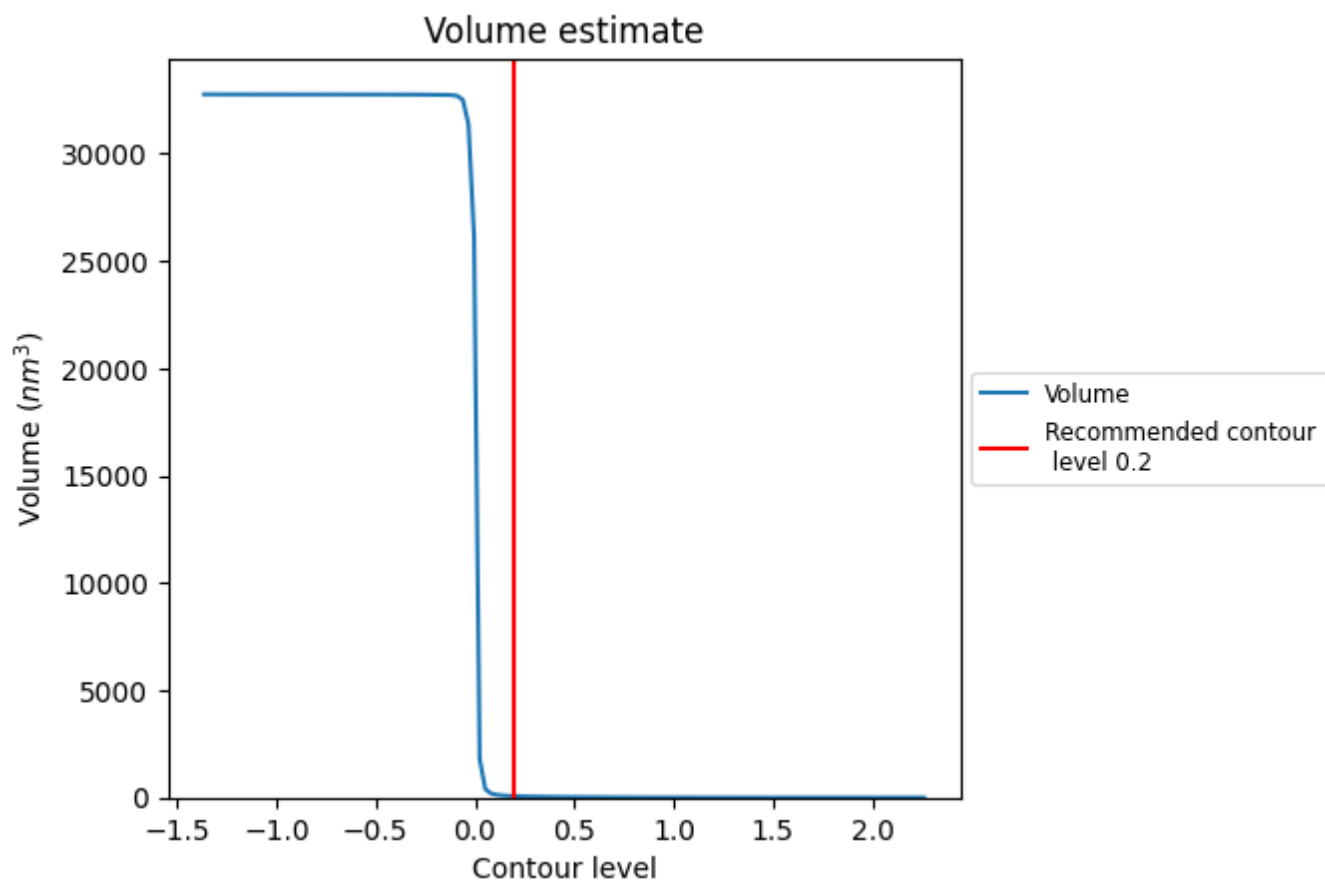
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

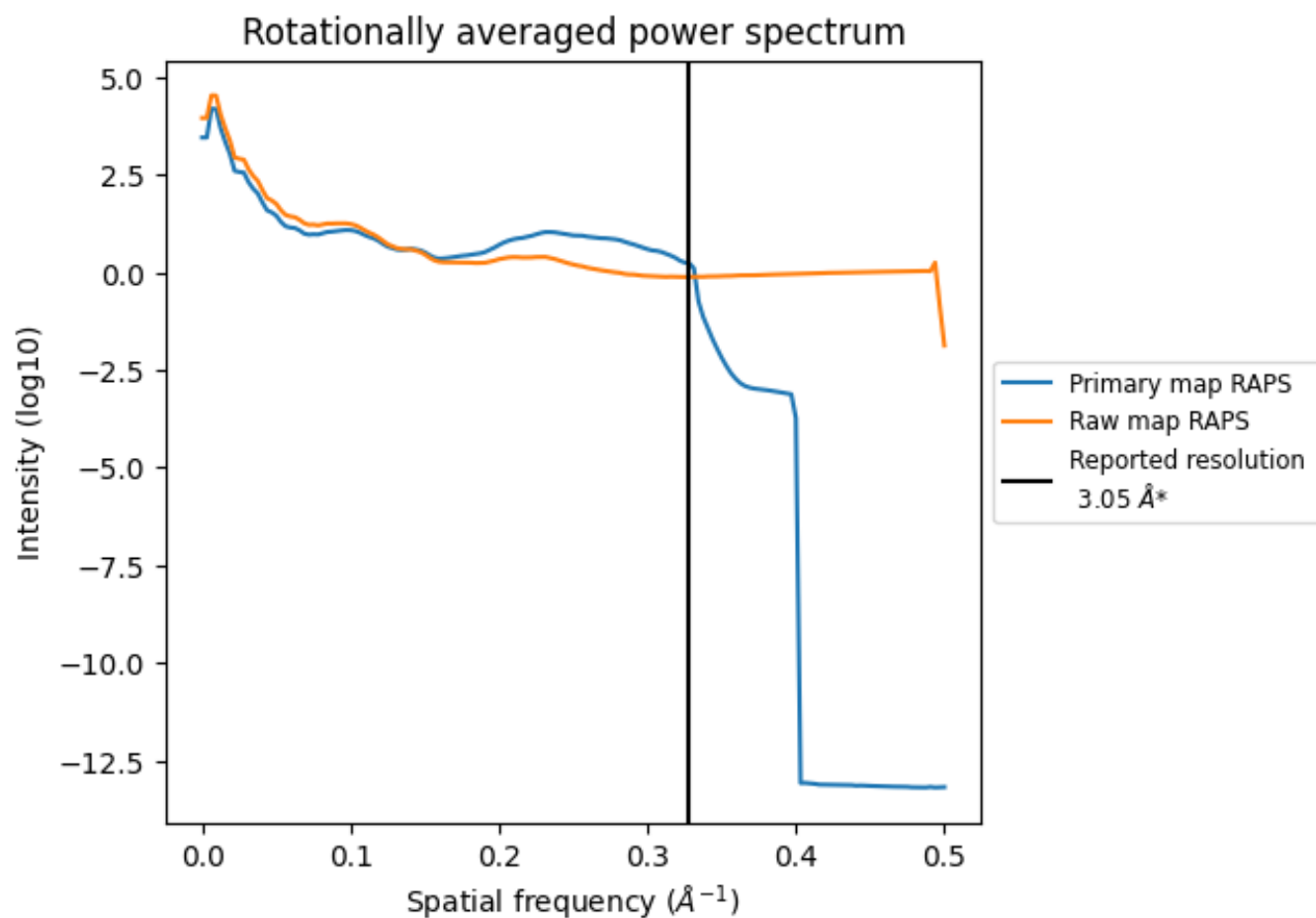
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 nm^3 ; this corresponds to an approximate mass of 59 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

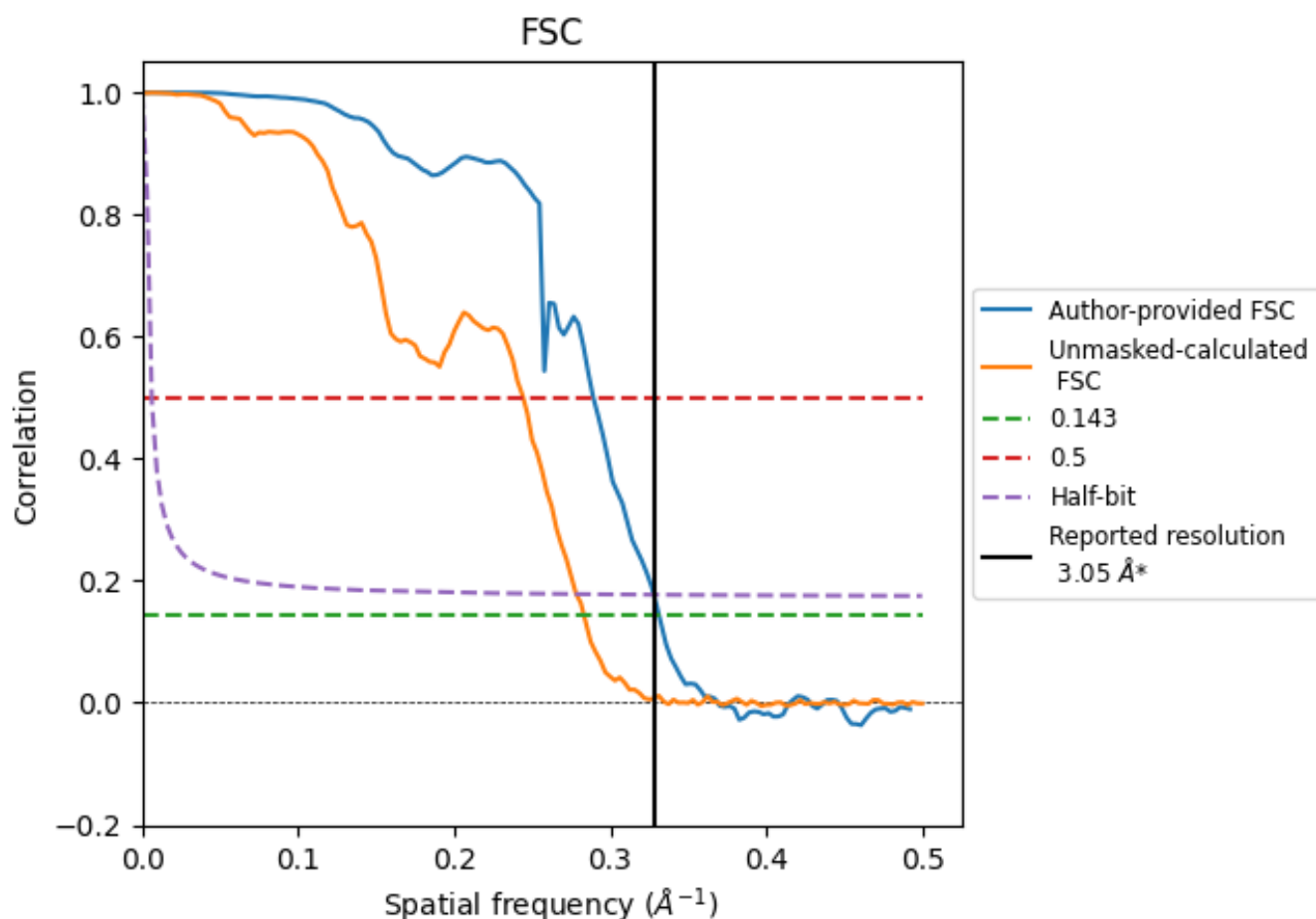


*Reported resolution corresponds to spatial frequency of 0.328 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.328 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

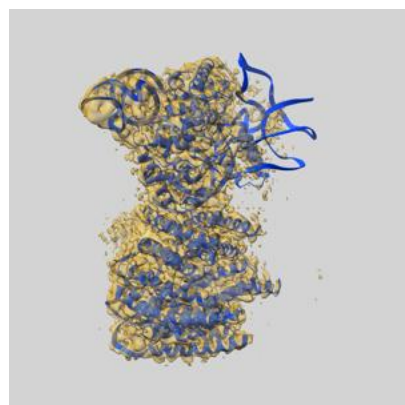
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.02	3.46	3.05
Unmasked-calculated*	3.53	4.10	3.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 3.05 by more than 10 %

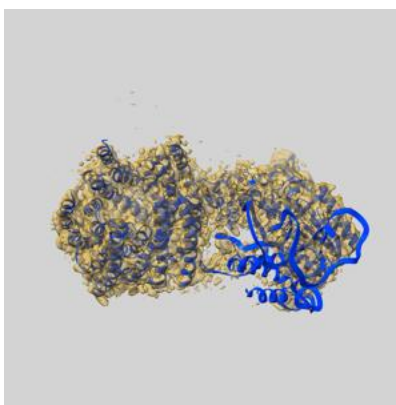
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42083 and PDB model 8UBD. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

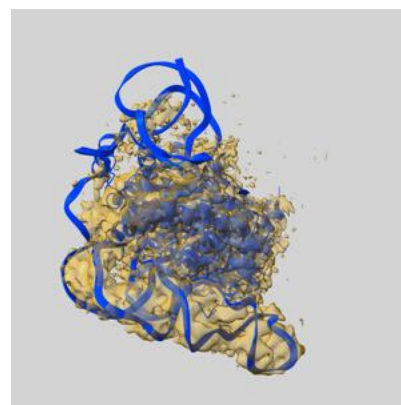
9.1 Map-model overlay [i](#)



X



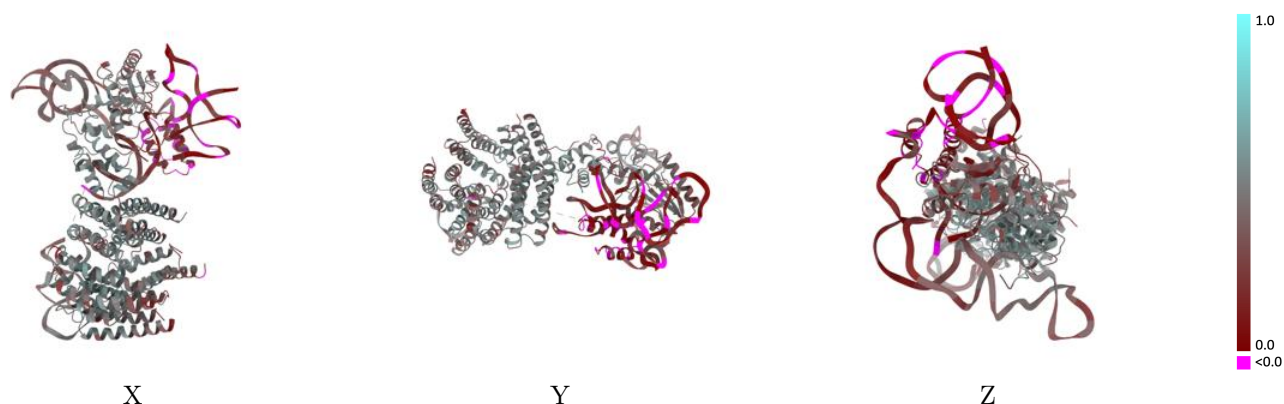
Y



Z

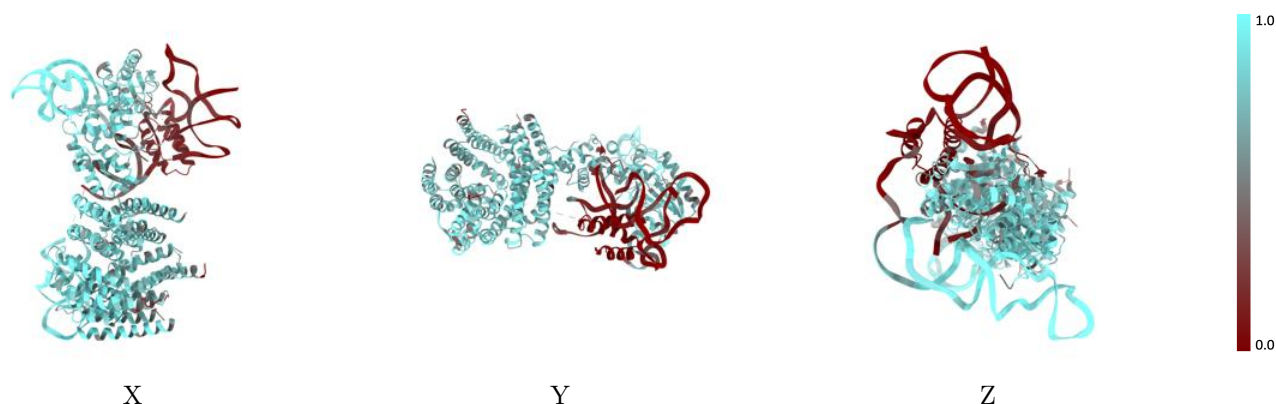
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



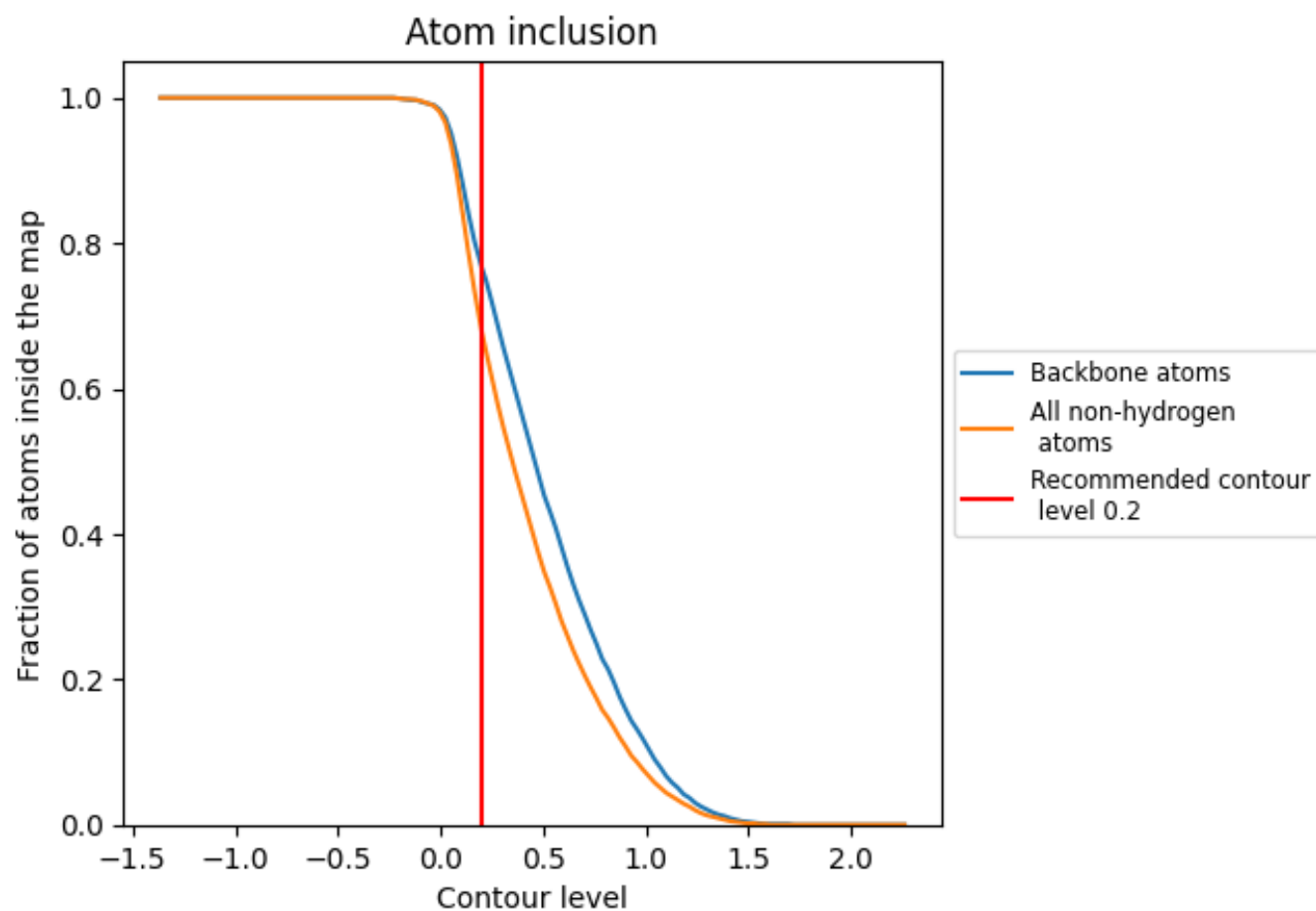
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 68% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6790	0.3730
A	0.6360	0.3740
B	0.8320	0.4890
C	0.8590	0.4900
D	0.8220	0.4560
E	0.7990	0.4540
F	0.7930	0.4470
G	0.0830	0.0820
H	0.2220	0.1640
I	0.5970	0.2650

1.0

0.0

<0.0