W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 04:57 AM JST

PDB ID	:	7W0F
EMDB ID	:	EMD-32241
Title	:	dmDicer2-LoqsPD-dsRNA Post-dicing status
Authors	:	Su, S.; Wang, J.; Wang, H.W.; Ma, J.
Deposited on	:	2021-11-18
Resolution	:	4.55 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.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.55 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.
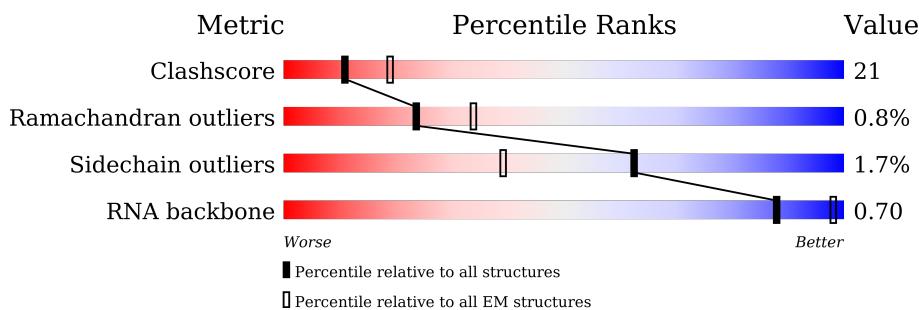
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1722	
2	B	359	
3	C	52	
3	D	52	
3	E	52	
3	F	52	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 14097 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 Dicer-2, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1476	Total 11963	C 7674	N 2038	O 2188	S 63	0	0

- Molecule 2 is a protein called Loquacious, isoform D.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	16	Total 143	C 94	N 22	O 27	0	0

- Molecule 3 is a RNA chain called siRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	21	Total 451	C 202	N 84	O 145	P 20	0	0
3	D	21	Total 437	C 196	N 70	O 150	P 21	0	0
3	E	26	Total 544	C 244	N 91	O 183	P 26	0	0
3	F	26	Total 559	C 249	N 101	O 183	P 26	0	0

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: Dicer-2, isoform A
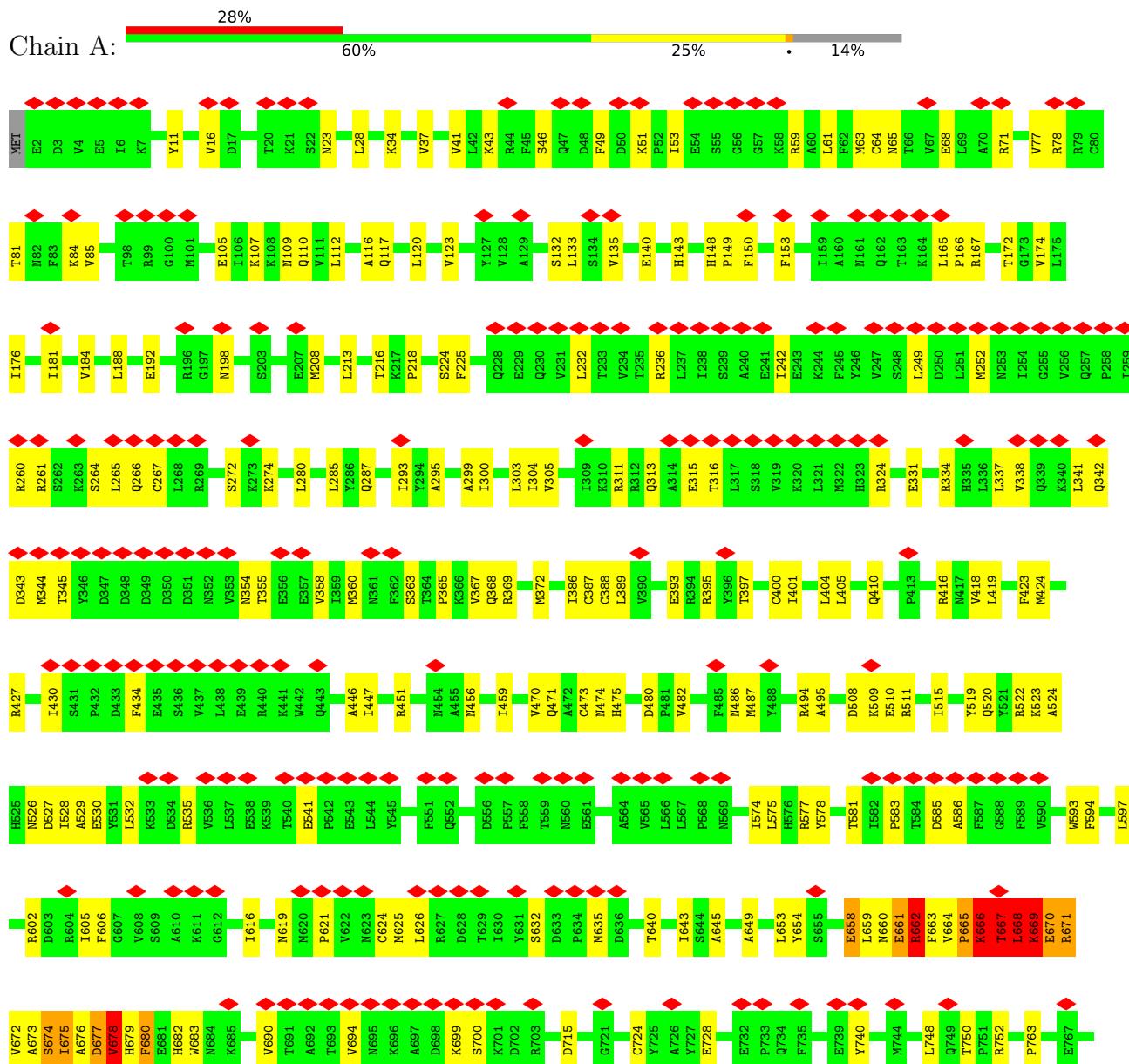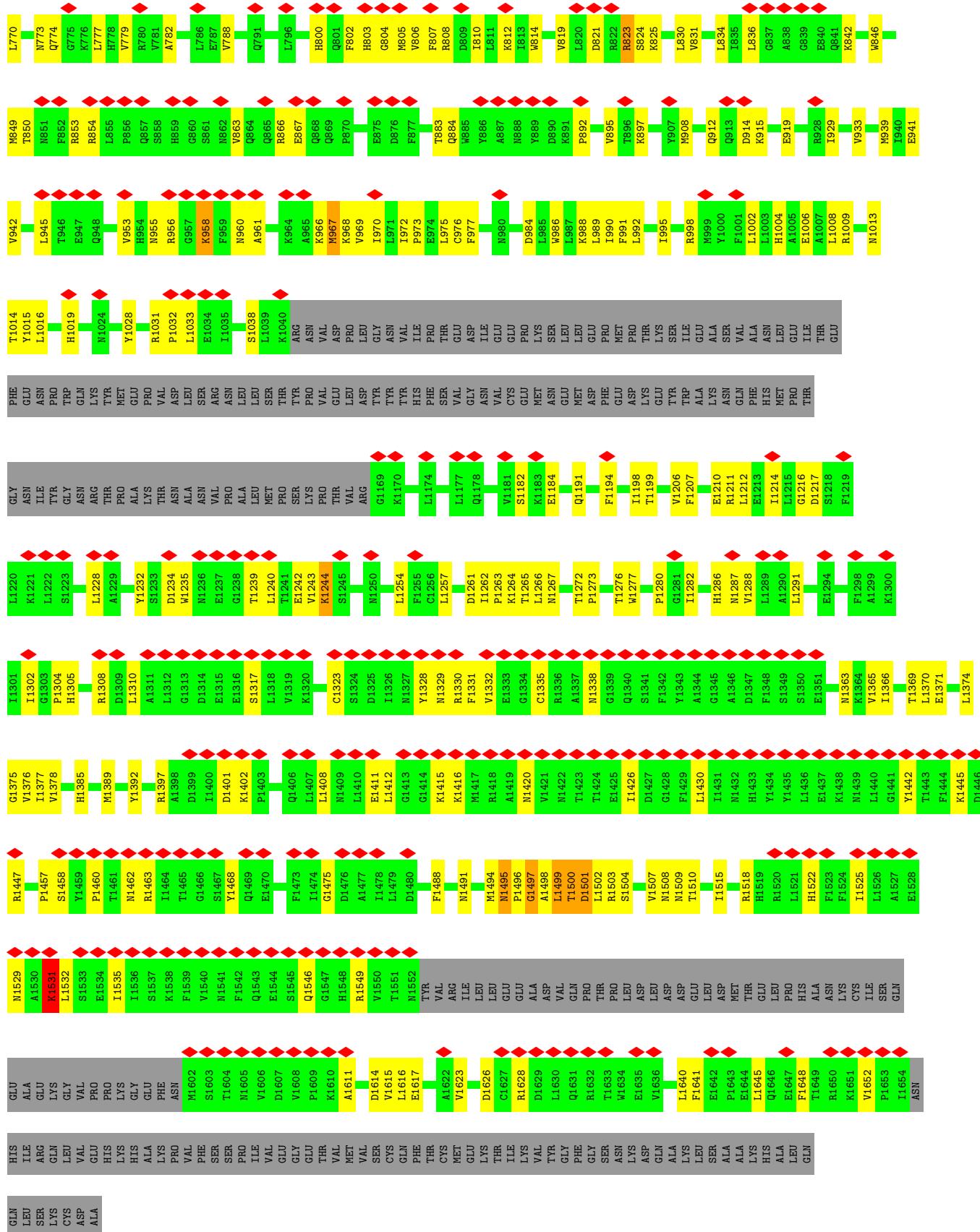
Chain A:

• Molecule 2: Loquacious, isoform D

Chain B: 96%

MET ASP GLN GLU ASN PHE HIS GLY SER SER LEU PRO GLN GLN LEU GLN ASN LEU HIS ILE GLN PRO GLN GLN GLN ALA SER PRO ASN PRO VAL GLN THR GLY PHE ALA PRO ARG ARG HIS TYR ASN ASN LEU VAL GLY LEU GLY LEU GLY ASN ASN ALA VAL SER GLY SER PRO VAL LYS GLY ALA

PRO LEU GLY GLN ARG HIS VAL LYS LEU LYS LYS GLU GLY LYS ILE SER ALA VAL GLN LEU GLN LEU SER GLN GLN PRO GLY GLN LEU GLN GLN SER ASP VAL GLY ASP PRO ALA LEU ALA GLY GLY SER LEU GLN GLY GLY VAL LEU MET GLY VAL ILE LEU PRO SER ASP GLU ALA LEU

LYS PHE VAL SER GLU THR ASP ALA ASN GLY LEU ALA MET LYS THR PRO VAL SER ILE LEU GLN GLU LEU LEU SER ARG GLY ILE THR PRO GLY TYR GLU LEU VAL GLN ILE GLY LEU ALA ILE HIS GLU PRO THR PHE ARG PHE ARG VAL SER PHE LYS ASP LYS ASP THR PRO PHE

THR ALA MET GLY ALA GLY LYS SER LYS LYS GLU ALA LYS HIS ALA ALA ALA ARG ALA LEU ILE ASP LYS LEU ILE GLY ALA GLN LEU PRO GLU GLY SER PRO SER SER ALA GLY PRO SER VAL THR GLY LEU THR VAL ALA GLY SER GLY ASP GLY ALA ASN ALA ASN THR GLY GLY

GLY ASP ALA SER ASP LYS THR VAL GLY ASN PRO ILE GLY TRP LEU GLN GLU LEU GLU MET CYS MET GLN ARG TRP PRO PRO PRO SER TYR GLU THR GLU THR GLU VAL GLY LEU PRO HIS GLU ARG LEU PHE THR ILE ALA CYS SER LEU LEU TYR ARG GLU GLU MET GLY LYS GLY LYS SER

LYS LYS ILE ALA LYS ARG LEU ALA ALA HIS ARG MET TRP MET ARG LEU GLN GLU THR PRO ILE ASP SER GLY LYS ILE SER SER ASP SER ILE CYS GLY LEU GLU GLU GLU GLY VAL SER ILE ILE GLN ASP **I344 D345 R346 Y347 E348 Q349 V350 S351 K352 D353 F354 E355 F356 I357 K358 I359**

- Molecule 3: siRNA

Chain C: 17% 21% 60%

G1 A2 G3 A4 C5 U6 U7 C11 A12 A13 U20 G21 C U G A U C A G C A G U C A C A U U G C C C A A G U U C U C U U

- Molecule 3: siRNA

Chain D: 15% 19% 6% 60%

G A G A C U U G G G C A A U G U G A C U G C U G A U C A G C A G32 U33 A37 U38 U39 C42 C43 A44 A45 C48 U49 C50 U51 U52

- Molecule 3: siRNA

Chain E: 10% 35% 15% 50%

G A G A C U U G G G C A A U G U G A C U G C U G A U C27 G32 U33 C34 A35 C36 A37 U49 C50 U51 U52

- Molecule 3: siRNA

Chain F: 13% 12% 37% 50%

G1 A2 C5 U6 U7 G8 G9 G10 C11 A12 A13 U14 G15 U16 G17 A18 C19 U20 G21 C22 U23 G24 A25 U26 C A G C A G U C A C A U U G C C C A A G U U C U C U U
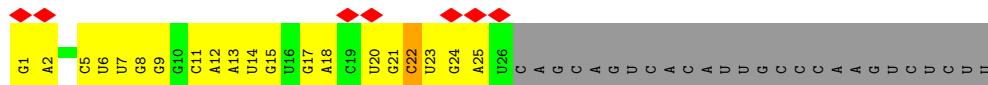
4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82469	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 $(e^-/Å^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.816	Depositor
Minimum map value	-0.269	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	259.2, 259.2, 259.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	0.26	0/12222	0.51	2/16539 (0.0%)
2	B	0.25	0/145	0.50	0/192
3	C	0.14	0/505	0.65	0/787
3	D	0.17	0/485	0.70	0/751
3	E	0.11	0/605	0.66	0/938
3	F	0.18	0/625	0.69	0/973
All	All	0.24	0/14587	0.54	2/20180 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1531	LYS	CB-CA-C	-8.04	94.31	110.40
1	A	1531	LYS	CB-CG-CD	5.55	126.04	111.60

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	11963	0	12026	529	0
2	B	143	0	140	4	0
3	C	451	0	228	41	0
3	D	437	0	225	74	0
3	E	544	0	280	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	559	0	280	56	0
All	All	14097	0	13179	553	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 21.

All (553) 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:1038:SER:OG	3:C:11:C:C5'	1.65	1.42
1:A:1509:ASN:N	3:C:21:G:H5''	1.35	1.39
1:A:1508:ASN:CA	3:C:21:G:H5'	1.60	1.28
1:A:1509:ASN:N	3:C:21:G:C5'	1.99	1.24
1:A:315:GLU:CB	1:A:1460:PRO:HB2	1.68	1.22
1:A:969:VAL:CG2	3:D:51:U:H2'	1.68	1.22
1:A:1458:SER:CB	3:F:21:G:H4'	1.69	1.21
1:A:1038:SER:OG	3:C:11:C:C4'	1.92	1.17
1:A:969:VAL:HG11	3:D:51:U:O2'	1.45	1.17
1:A:967:MET:CE	3:D:51:U:O4	1.94	1.16
1:A:953:VAL:HG11	3:D:42:C:C5'	1.76	1.15
1:A:953:VAL:HG11	3:D:42:C:H5'	1.16	1.14
1:A:1038:SER:OG	3:C:11:C:H4'	1.46	1.14
1:A:1508:ASN:HA	3:C:21:G:C5'	1.79	1.12
1:A:1509:ASN:N	3:C:21:G:OP1	1.85	1.10
1:A:1509:ASN:H	3:C:21:G:P	1.75	1.09
1:A:1038:SER:OG	3:C:11:C:H5''	1.32	1.09
1:A:315:GLU:HB3	1:A:1460:PRO:CB	1.83	1.07
1:A:967:MET:SD	3:D:51:U:N3	2.27	1.06
1:A:969:VAL:HG21	3:D:51:U:C2'	1.86	1.05
1:A:956:ARG:HA	3:D:42:C:O3'	1.57	1.04
1:A:967:MET:HE1	3:D:51:U:O4	1.55	1.03
1:A:1457:PRO:HB2	3:F:21:G:OP1	1.58	1.03
1:A:1038:SER:CB	3:C:11:C:H4'	1.87	1.02
1:A:1458:SER:HB3	3:F:21:G:H4'	1.39	1.02
1:A:958:LYS:CE	3:D:43:C:H5'	1.91	0.99
1:A:969:VAL:HG21	3:D:51:U:H2'	1.01	0.99
1:A:1507:VAL:O	3:C:21:G:H4'	1.61	0.99
1:A:660:ASN:HB3	1:A:664:VAL:H	1.27	0.98
1:A:583:PRO:C	1:A:1415:LYS:HE3	1.85	0.97
1:A:958:LYS:HE2	3:D:43:C:C4'	1.97	0.95
1:A:958:LYS:HE3	3:D:43:C:H5'	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PRO:O	1:A:1415:LYS:HE3	1.67	0.94
1:A:1508:ASN:C	3:C:21:G:H5"	1.88	0.94
1:A:315:GLU:HB3	1:A:1460:PRO:HB2	0.95	0.94
1:A:953:VAL:HG11	3:D:42:C:C4'	1.97	0.94
1:A:1509:ASN:H	3:C:21:G:C5'	1.68	0.93
1:A:677:ASP:C	1:A:679:HIS:H	1.71	0.91
1:A:578:TYR:HA	1:A:665:PRO:HA	1.53	0.91
1:A:1529:ASN:HD21	3:F:22:C:C4'	1.83	0.90
1:A:956:ARG:HA	3:D:43:C:P	2.10	0.90
1:A:969:VAL:HG11	3:D:51:U:C2'	2.01	0.89
1:A:1531:LYS:CG	1:A:1532:LEU:HD22	2.02	0.89
1:A:1508:ASN:C	3:C:21:G:C5'	2.40	0.88
1:A:953:VAL:CG1	3:D:42:C:H5'	2.02	0.88
1:A:956:ARG:HB3	3:D:42:C:H5"	1.55	0.88
1:A:958:LYS:HE2	3:D:43:C:C5'	2.05	0.87
1:A:967:MET:SD	3:D:51:U:C4	2.68	0.86
1:A:1531:LYS:HG3	1:A:1532:LEU:N	1.92	0.84
1:A:1457:PRO:HB2	3:F:21:G:P	2.17	0.84
1:A:1458:SER:HB3	3:F:21:G:C4'	2.08	0.83
1:A:1531:LYS:HB3	3:F:23:U:OP1	1.79	0.83
1:A:1038:SER:HB3	3:C:11:C:H4'	1.61	0.82
1:A:1457:PRO:CB	3:F:21:G:OP1	2.28	0.81
1:A:165:LEU:HD12	1:A:166:PRO:HD2	1.61	0.81
1:A:677:ASP:C	1:A:679:HIS:N	2.30	0.81
1:A:958:LYS:HE2	3:D:43:C:O3'	1.80	0.81
1:A:1531:LYS:CD	1:A:1535:ILE:HD12	2.12	0.80
1:A:1531:LYS:HD2	1:A:1535:ILE:HD12	1.63	0.80
1:A:1508:ASN:HA	3:C:21:G:H5'	0.82	0.80
1:A:1504:SER:OG	3:C:20:U:H1'	1.82	0.80
1:A:1508:ASN:CA	3:C:21:G:C5'	2.44	0.80
1:A:675:ILE:HD12	1:A:1232:TYR:CZ	2.17	0.79
1:A:1529:ASN:HD21	3:F:22:C:H4'	1.47	0.79
1:A:773:ASN:ND2	3:C:2:A:OP1	2.15	0.79
1:A:1502:LEU:HD13	1:A:1652:VAL:HG23	1.66	0.78
1:A:1531:LYS:HG2	1:A:1532:LEU:HD22	1.63	0.78
1:A:586:ALA:CB	1:A:1420:ASN:HB3	2.13	0.78
1:A:1038:SER:OG	3:C:11:C:H5'	1.81	0.77
1:A:1210:GLU:HG3	1:A:1496:PRO:HG2	1.67	0.77
1:A:671:ARG:HH11	1:A:1239:THR:HG21	1.49	0.77
1:A:660:ASN:HB3	1:A:664:VAL:N	1.97	0.77
1:A:958:LYS:CE	3:D:43:C:C5'	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ARG:HH11	1:A:662:ARG:HB3	1.50	0.76
1:A:1531:LYS:CG	1:A:1532:LEU:N	2.47	0.76
1:A:1211:ARG:HA	1:A:1496:PRO:HG3	1.68	0.76
1:A:672:VAL:HG13	1:A:1243:VAL:HG22	1.68	0.76
1:A:1497:GLY:HA2	3:D:33:U:H5"	1.67	0.76
1:A:1458:SER:CB	3:F:21:G:C4'	2.60	0.75
1:A:586:ALA:HB1	1:A:1420:ASN:HB3	1.69	0.75
1:A:958:LYS:HE2	3:D:43:C:C3'	2.17	0.75
1:A:810:ILE:HD13	1:A:989:LEU:HD23	1.69	0.74
1:A:1529:ASN:ND2	3:F:22:C:H4'	2.02	0.74
1:A:1458:SER:CA	3:F:21:G:H4'	2.18	0.74
1:A:1500:THR:OG1	3:D:33:U:H5'	1.88	0.73
1:A:578:TYR:CA	1:A:665:PRO:HA	2.17	0.73
1:A:583:PRO:CG	1:A:1234:ASP:HB2	2.18	0.73
1:A:805:MET:HE2	1:A:854:ARG:HA	1.70	0.73
1:A:1458:SER:HB2	3:F:21:G:H4'	1.65	0.72
1:A:955:ASN:HB2	3:D:42:C:O2'	1.88	0.72
1:A:527:ASP:HA	1:A:530:GLU:HG2	1.71	0.72
1:A:1531:LYS:HD2	1:A:1535:ILE:CD1	2.18	0.72
1:A:578:TYR:HA	1:A:665:PRO:CA	2.19	0.72
1:A:574:ILE:HD11	1:A:664:VAL:CA	2.20	0.72
1:A:675:ILE:HG23	1:A:1232:TYR:OH	1.90	0.71
1:A:967:MET:CE	3:D:51:U:C4	2.74	0.71
1:A:1509:ASN:CA	3:C:21:G:OP1	2.38	0.71
1:A:1531:LYS:CG	1:A:1535:ILE:HD12	2.21	0.71
1:A:956:ARG:CZ	3:D:42:C:OP1	2.38	0.70
1:A:1257:LEU:HB2	1:A:1370:LEU:HD12	1.73	0.70
1:A:671:ARG:HB2	1:A:1235:TRP:CZ2	2.27	0.69
1:A:967:MET:HE2	3:D:51:U:O4	1.92	0.69
1:A:360:MET:O	1:A:368:GLN:NE2	2.25	0.69
1:A:664:VAL:CG2	1:A:666:LYS:H	2.06	0.69
1:A:1457:PRO:CB	3:F:20:U:O3'	2.41	0.69
1:A:1502:LEU:HD11	1:A:1648:PHE:HB3	1.75	0.69
1:A:49:PHE:O	1:A:59:ARG:NH1	2.26	0.68
1:A:953:VAL:CG1	3:D:42:C:H4'	2.22	0.68
1:A:1462:ASN:HD22	3:F:20:U:H4'	1.57	0.68
1:A:1509:ASN:CA	3:C:21:G:H5"	2.23	0.68
1:A:597:LEU:O	1:A:602:ARG:NH1	2.27	0.68
1:A:955:ASN:CB	3:D:42:C:O2'	2.40	0.68
1:A:678:VAL:O	1:A:1397:ARG:HG3	1.94	0.68
1:A:1214:ILE:HD11	3:D:33:U:OP1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1531:LYS:CD	1:A:1535:ILE:CD1	2.72	0.67
1:A:969:VAL:CG1	3:D:51:U:C2'	2.72	0.67
1:A:1509:ASN:N	3:C:21:G:P	2.57	0.67
1:A:583:PRO:HG2	1:A:1234:ASP:HB2	1.76	0.67
1:A:1031:ARG:HD3	1:A:1032:PRO:HD2	1.77	0.67
1:A:1257:LEU:HD22	1:A:1366:ILE:HG23	1.76	0.67
1:A:315:GLU:CB	1:A:1460:PRO:CB	2.56	0.66
1:A:1377:ILE:HD13	1:A:1389:MET:HG3	1.78	0.66
1:A:653:LEU:O	1:A:658:GLU:HB3	1.94	0.66
1:A:192:GLU:OE2	1:A:535:ARG:NH1	2.27	0.66
1:A:700:SER:O	1:A:1363:ASN:ND2	2.28	0.66
1:A:961:ALA:HB2	3:D:44:A:OP1	1.96	0.66
1:A:1009:ARG:NH2	1:A:1028:TYR:OH	2.28	0.66
1:A:1458:SER:N	3:F:21:G:H5'	2.11	0.66
1:A:958:LYS:HE2	3:D:43:C:H4'	1.77	0.66
1:A:953:VAL:HG11	3:D:42:C:H4'	1.75	0.65
1:A:78:ARG:NH2	1:A:85:VAL:O	2.28	0.65
1:A:658:GLU:O	1:A:659:LEU:C	2.34	0.65
1:A:956:ARG:CA	3:D:42:C:O3'	2.39	0.65
1:A:1457:PRO:HB3	3:F:20:U:O3'	1.95	0.65
1:A:662:ARG:HB3	1:A:662:ARG:NH1	2.10	0.65
1:A:654:TYR:CE1	1:A:661:GLU:HA	2.32	0.65
1:A:419:LEU:HA	1:A:456:ASN:HD21	1.60	0.65
1:A:660:ASN:HD22	1:A:666:LYS:HA	1.62	0.65
1:A:680:PHE:HD2	1:A:690:VAL:HG12	1.61	0.65
1:A:967:MET:SD	3:D:51:U:O4	2.54	0.65
1:A:1529:ASN:ND2	3:F:22:C:C4'	2.57	0.65
1:A:669:LYS:HZ3	1:A:670:GLU:H	1.45	0.64
1:A:953:VAL:CG1	3:D:42:C:C4'	2.74	0.64
1:A:401:ILE:HD13	1:A:404:LEU:HD21	1.78	0.64
1:A:774:GLN:HE22	3:C:1:G:H5'	1.61	0.64
1:A:1214:ILE:HG21	1:A:1500:THR:HG22	1.79	0.64
1:A:632:SER:HB3	1:A:645:ALA:HB2	1.80	0.64
1:A:956:ARG:CB	3:D:42:C:H5"	2.26	0.64
1:A:956:ARG:NH2	3:D:42:C:OP1	2.30	0.64
1:A:176:ILE:HD11	1:A:188:LEU:HD12	1.78	0.64
3:D:44:A:O2'	3:D:45:A:H5'	1.98	0.64
1:A:585:ASP:HA	1:A:1415:LYS:HD3	1.79	0.64
1:A:1496:PRO:O	1:A:1500:THR:HG23	1.97	0.64
1:A:671:ARG:O	1:A:674:SER:HB3	1.98	0.64
1:A:958:LYS:CE	3:D:43:C:O3'	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1509:ASN:CB	3:C:21:G:OP1	2.47	0.63
1:A:1457:PRO:O	1:A:1462:ASN:ND2	2.31	0.63
1:A:1531:LYS:CG	3:F:23:U:OP1	2.47	0.63
1:A:51:LYS:O	1:A:59:ARG:NH1	2.31	0.63
1:A:1458:SER:CA	3:F:21:G:C5'	2.77	0.62
1:A:260:ARG:NH1	1:A:272:SER:OG	2.32	0.62
1:A:1038:SER:CB	3:C:11:C:C4'	2.68	0.62
1:A:969:VAL:CG2	3:D:51:U:C2'	2.61	0.62
1:A:1531:LYS:CB	3:F:23:U:OP1	2.46	0.62
1:A:581:THR:HG21	1:A:665:PRO:HB2	1.80	0.62
1:A:939:MET:HA	1:A:973:PRO:HD3	1.82	0.62
1:A:661:GLU:C	1:A:663:PHE:H	2.03	0.62
1:A:676:ALA:O	1:A:680:PHE:N	2.33	0.62
1:A:912:GLN:NE2	3:D:52:U:O3'	2.33	0.62
1:A:64:CYS:SG	1:A:65:ASN:N	2.73	0.61
1:A:331:GLU:OE1	1:A:334:ARG:NH1	2.33	0.61
1:A:750:THR:OG1	1:A:988:LYS:NZ	2.34	0.61
1:A:1006:GLU:OE1	1:A:1191:GLN:NE2	2.32	0.61
2:B:346:ARG:NH1	2:B:347:TYR:O	2.34	0.61
1:A:249:LEU:O	1:A:274:LYS:NZ	2.33	0.61
1:A:969:VAL:HG11	3:D:51:U:HO2'	1.65	0.61
1:A:311:ARG:HH12	1:A:324:ARG:HH21	1.49	0.61
1:A:1457:PRO:CB	3:F:21:G:P	2.88	0.61
1:A:574:ILE:HD11	1:A:664:VAL:HA	1.83	0.60
1:A:671:ARG:HG2	1:A:672:VAL:N	2.16	0.60
1:A:1507:VAL:O	3:C:21:G:C4'	2.44	0.60
1:A:1302:ILE:HG12	1:A:1335:CYS:HB3	1.83	0.60
1:A:1458:SER:CA	3:F:21:G:H5'	2.31	0.60
1:A:105:GLU:OE1	1:A:109:ASN:ND2	2.35	0.60
1:A:59:ARG:HH21	1:A:107:LYS:HA	1.67	0.60
1:A:287:GLN:NE2	1:A:397:THR:OG1	2.35	0.60
1:A:995:ILE:HD13	1:A:998:ARG:HH22	1.66	0.60
1:A:956:ARG:NH1	3:D:42:C:OP1	2.35	0.59
1:A:972:ILE:HG23	1:A:975:LEU:HB2	1.84	0.59
1:A:410:GLN:O	1:A:416:ARG:NH1	2.35	0.59
1:A:577:ARG:HB3	1:A:665:PRO:HG3	1.82	0.59
1:A:958:LYS:HG3	3:D:43:C:OP1	2.03	0.59
1:A:280:LEU:HD21	1:A:303:LEU:HD22	1.85	0.59
1:A:694:VAL:HG11	1:A:699:LYS:HB3	1.84	0.58
1:A:677:ASP:O	1:A:679:HIS:N	2.36	0.58
1:A:953:VAL:CG1	3:D:42:C:C5'	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1468:TYR:HE1	1:A:1614:ASP:HB3	1.68	0.58
1:A:969:VAL:CG1	3:D:51:U:O3'	2.52	0.58
1:A:1531:LYS:CD	3:F:23:U:OP1	2.52	0.58
1:A:1263:PRO:HA	1:A:1266:LEU:HD23	1.85	0.58
1:A:1008:LEU:HD21	1:A:1265:THR:HG21	1.86	0.58
1:A:574:ILE:CD1	1:A:664:VAL:HA	2.33	0.57
1:A:654:TYR:N	1:A:659:LEU:HB3	2.19	0.57
1:A:969:VAL:HA	3:D:52:U:H1'	1.86	0.57
1:A:941:GLU:HG2	1:A:970:ILE:HG13	1.86	0.57
1:A:958:LYS:HE2	3:D:43:C:H5'	1.66	0.57
1:A:654:TYR:HB2	1:A:659:LEU:HD23	1.84	0.57
1:A:1458:SER:N	3:F:21:G:C5'	2.67	0.57
1:A:300:ILE:O	1:A:304:ILE:HD12	2.04	0.57
1:A:578:TYR:HD1	1:A:665:PRO:O	1.88	0.57
1:A:581:THR:HG21	1:A:665:PRO:CB	2.34	0.57
1:A:625:MET:HE3	1:A:626:LEU:HG	1.85	0.57
1:A:664:VAL:C	1:A:666:LYS:H	2.07	0.57
1:A:969:VAL:HA	3:D:52:U:C1'	2.34	0.57
1:A:1462:ASN:ND2	3:F:20:U:H4'	2.20	0.57
1:A:1509:ASN:HB3	3:C:21:G:OP1	2.05	0.57
1:A:1199:THR:HA	1:A:1267:ASN:HB3	1.86	0.57
1:A:1458:SER:HA	3:F:21:G:H5'	1.87	0.57
1:A:1458:SER:HB3	3:F:21:G:C5'	2.35	0.56
1:A:578:TYR:CB	1:A:665:PRO:HA	2.36	0.56
1:A:969:VAL:CG1	3:D:51:U:O2'	2.37	0.56
1:A:345:THR:HB	1:A:354:ASN:HD21	1.71	0.56
1:A:266:GLN:CD	1:A:267:CYS:H	2.08	0.56
1:A:664:VAL:HG22	1:A:666:LYS:H	1.70	0.56
1:A:669:LYS:O	1:A:672:VAL:HB	2.06	0.56
1:A:667:THR:C	1:A:668:LEU:HD23	2.26	0.55
3:F:22:C:H5"	3:F:22:C:H6	1.70	0.55
1:A:427:ARG:NE	3:F:15:G:OP2	2.39	0.55
1:A:966:LYS:HE2	3:C:1:G:C5	2.39	0.55
1:A:995:ILE:HD13	1:A:998:ARG:NH2	2.21	0.55
1:A:653:LEU:HB3	1:A:659:LEU:H	1.71	0.55
1:A:676:ALA:HB1	1:A:690:VAL:HG11	1.87	0.55
1:A:395:ARG:HH12	1:A:430:ILE:HB	1.72	0.55
1:A:821:ASP:OD2	1:A:824:SER:OG	2.18	0.55
1:A:967:MET:HG3	3:D:52:U:C4	2.42	0.55
1:A:671:ARG:HG2	1:A:672:VAL:H	1.72	0.55
1:A:969:VAL:HG22	3:D:52:U:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1494:MET:SD	1:A:1499:LEU:N	2.80	0.55
1:A:135:VAL:HG12	1:A:167:ARG:HB3	1.88	0.55
1:A:583:PRO:C	1:A:1415:LYS:CE	2.68	0.55
1:A:1458:SER:HA	3:F:21:G:C4'	2.37	0.55
1:A:578:TYR:HA	1:A:665:PRO:HB3	1.89	0.55
1:A:895:VAL:HA	1:A:942:VAL:HG12	1.89	0.55
1:A:1495:ASN:HD21	1:A:1498:ALA:H	1.53	0.55
1:A:68:GLU:OE2	1:A:71:ARG:NH2	2.40	0.55
1:A:1194:PHE:O	1:A:1198:ILE:HG12	2.07	0.55
1:A:218:PRO:HG3	1:A:495:ALA:HB3	1.88	0.54
1:A:594:PHE:HB3	1:A:616:ILE:HD11	1.89	0.54
1:A:148:HIS:HD2	1:A:150:PHE:HD2	1.53	0.54
1:A:1214:ILE:HG13	1:A:1496:PRO:HB3	1.90	0.54
1:A:1262:ILE:O	1:A:1264:LYS:N	2.41	0.54
1:A:653:LEU:HB2	1:A:659:LEU:HB2	1.90	0.54
1:A:808:ARG:HG3	1:A:814:TRP:CD2	2.43	0.54
1:A:883:THR:O	1:A:977:PHE:N	2.40	0.54
1:A:640:THR:HA	1:A:643:ILE:HG12	1.90	0.54
1:A:836:LEU:HD23	1:A:842:LYS:HG2	1.89	0.54
1:A:1531:LYS:CD	1:A:1532:LEU:HD22	2.37	0.54
1:A:1182:SER:OG	1:A:1184:GLU:OE1	2.26	0.54
1:A:184:VAL:HG22	1:A:188:LEU:HD13	1.90	0.54
1:A:123:VAL:HG21	1:A:153:PHE:CZ	2.43	0.54
1:A:16:VAL:HG23	1:A:41:VAL:HG22	1.91	0.53
1:A:672:VAL:O	1:A:673:ALA:C	2.45	0.53
1:A:213:LEU:O	1:A:216:THR:OG1	2.25	0.53
1:A:1529:ASN:OD1	3:F:22:C:H4'	2.08	0.53
1:A:1015:TYR:HD2	1:A:1016:LEU:HD12	1.73	0.53
1:A:814:TRP:HZ3	1:A:1282:ILE:HD13	1.73	0.53
1:A:929:ILE:HD13	1:A:975:LEU:HD21	1.90	0.53
1:A:969:VAL:HG13	3:D:51:U:O3'	2.09	0.53
3:F:8:G:H2'	3:F:9:G:C8	2.44	0.53
1:A:1458:SER:HA	3:F:21:G:H4'	1.90	0.53
3:F:23:U:H2'	3:F:24:G:C8	2.43	0.53
1:A:664:VAL:C	1:A:666:LYS:N	2.61	0.53
1:A:669:LYS:HZ3	1:A:670:GLU:N	2.06	0.53
1:A:578:TYR:HA	1:A:665:PRO:CB	2.39	0.53
1:A:966:LYS:HE2	3:C:1:G:N7	2.24	0.53
1:A:664:VAL:HG23	1:A:666:LYS:H	1.72	0.52
1:A:912:GLN:HB2	1:A:915:LYS:HB3	1.89	0.52
1:A:1305:HIS:NE2	1:A:1338:ASN:OD1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1458:SER:CA	3:F:21:G:C4'	2.85	0.52
1:A:49:PHE:HB3	1:A:110:GLN:HG2	1.91	0.52
1:A:668:LEU:HD12	1:A:669:LYS:HE3	1.91	0.52
1:A:715:ASP:H	1:A:825:LYS:HB3	1.74	0.52
1:A:586:ALA:HA	1:A:1420:ASN:ND2	2.24	0.52
1:A:867:GLU:HG3	1:A:933:VAL:HG11	1.92	0.52
1:A:1508:ASN:ND2	3:C:20:U:O2'	2.42	0.52
1:A:1328:TYR:HA	1:A:1331:PHE:CE1	2.45	0.52
1:A:482:VAL:HA	1:A:487:MET:HE1	1.91	0.52
1:A:658:GLU:HA	1:A:666:LYS:HE2	1.92	0.52
1:A:451:ARG:HG2	1:A:471:GLN:HE22	1.74	0.52
1:A:1254:LEU:HD22	1:A:1363:ASN:ND2	2.25	0.52
1:A:1310:LEU:HD21	1:A:1331:PHE:HB3	1.92	0.52
1:A:1529:ASN:CG	3:F:22:C:H4'	2.30	0.52
1:A:892:PRO:HG2	1:A:945:LEU:HD21	1.90	0.51
1:A:1214:ILE:HG21	1:A:1500:THR:CG2	2.40	0.51
1:A:1546:GLN:HG2	1:A:1549:ARG:HB3	1.93	0.51
1:A:675:ILE:HD12	1:A:1232:TYR:CE1	2.45	0.51
1:A:763:PRO:HG3	1:A:1006:GLU:HG2	1.92	0.51
1:A:1287:ASN:OD1	1:A:1288:VAL:N	2.43	0.51
1:A:1640:LEU:HD23	1:A:1641:PHE:HE1	1.74	0.51
1:A:1497:GLY:O	3:D:33:U:H4'	2.10	0.51
1:A:1494:MET:SD	1:A:1499:LEU:HA	2.51	0.51
1:A:770:LEU:N	1:A:777:LEU:O	2.38	0.51
1:A:1365:VAL:O	1:A:1369:THR:HG23	2.11	0.51
1:A:986:TRP:O	1:A:990:ILE:HG12	2.11	0.51
1:A:1500:THR:O	1:A:1503:ARG:HB3	2.12	0.51
1:A:522:ARG:O	1:A:526:ASN:ND2	2.32	0.50
1:A:1212:LEU:HD23	1:A:1488:PHE:HZ	1.76	0.50
1:A:635:MET:HG3	1:A:640:THR:HG22	1.93	0.50
1:A:664:VAL:O	1:A:666:LYS:N	2.45	0.50
1:A:1445:LYS:NZ	1:A:1626:ASP:OD1	2.36	0.50
1:A:315:GLU:HB2	1:A:1460:PRO:HB2	1.77	0.50
1:A:621:PRO:HG2	1:A:624:CYS:HB2	1.94	0.50
1:A:61:LEU:HD12	1:A:112:LEU:HB2	1.94	0.50
1:A:520:GLN:O	1:A:520:GLN:NE2	2.44	0.50
1:A:181:ILE:HD12	1:A:524:ALA:HB2	1.94	0.50
1:A:968:LYS:O	3:D:52:U:H1'	2.11	0.50
1:A:1504:SER:CB	3:D:32:G:H21	2.24	0.50
1:A:1529:ASN:HB3	1:A:1532:LEU:HB2	1.92	0.50
1:A:625:MET:HE2	1:A:658:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ALA:O	1:A:676:ALA:HB3	2.12	0.49
1:A:958:LYS:HG2	3:D:43:C:H4'	1.94	0.49
1:A:53:ILE:HD12	1:A:132:SER:HB2	1.93	0.49
3:C:11:C:H2'	3:C:12:A:C8	2.47	0.49
1:A:77:VAL:O	1:A:81:THR:OG1	2.16	0.49
3:F:11:C:H2'	3:F:12:A:C8	2.48	0.49
1:A:34:LYS:HA	1:A:37:VAL:HG12	1.94	0.49
1:A:654:TYR:CE1	1:A:661:GLU:HG2	2.47	0.49
1:A:120:LEU:HD11	1:A:149:PRO:HB3	1.95	0.49
1:A:846:TRP:HA	1:A:849:MET:HE2	1.95	0.49
1:A:1262:ILE:O	1:A:1265:THR:HG22	2.11	0.49
1:A:1401:ASP:OD1	1:A:1402:LYS:N	2.45	0.49
3:F:17:G:H2'	3:F:18:A:C8	2.47	0.49
1:A:654:TYR:HE1	1:A:661:GLU:HG2	1.78	0.49
1:A:1458:SER:HA	3:F:21:G:C5'	2.41	0.49
1:A:224:SER:OG	1:A:508:ASP:OD1	2.22	0.49
1:A:198:ASN:OD1	1:A:535:ARG:NH1	2.46	0.49
3:C:2:A:H2'	3:C:3:G:C8	2.48	0.49
1:A:427:ARG:N	3:F:14:U:OP2	2.46	0.48
1:A:524:ALA:O	1:A:528:ILE:HG12	2.12	0.48
1:A:581:THR:CG2	1:A:665:PRO:HB3	2.43	0.48
1:A:1457:PRO:HB2	3:F:20:U:O3'	2.11	0.48
1:A:242:ILE:HG21	1:A:285:LEU:HD11	1.95	0.48
1:A:305:VAL:HG21	1:A:434:PHE:O	2.13	0.48
1:A:418:VAL:O	1:A:456:ASN:ND2	2.46	0.48
1:A:123:VAL:HG11	1:A:153:PHE:HE1	1.77	0.48
1:A:249:LEU:HA	1:A:252:MET:HG2	1.95	0.48
1:A:1304:PRO:HB2	1:A:1308:ARG:HH21	1.79	0.48
1:A:261:ARG:NH2	1:A:265:LEU:O	2.47	0.48
1:A:1199:THR:HG21	1:A:1207:PHE:HE1	1.78	0.48
1:A:800:HIS:CD2	1:A:830:LEU:HD21	2.49	0.48
1:A:1214:ILE:HD12	1:A:1500:THR:HG21	1.95	0.48
1:A:574:ILE:HD11	1:A:664:VAL:N	2.28	0.48
1:A:804:GLY:HA2	1:A:1282:ILE:HD11	1.94	0.48
1:A:955:ASN:HB3	3:D:42:C:O2'	2.11	0.48
1:A:969:VAL:HG22	3:D:51:U:H2'	1.84	0.48
1:A:1525:ILE:HG12	1:A:1615:VAL:HG11	1.95	0.48
1:A:578:TYR:HB2	1:A:665:PRO:HA	1.96	0.48
3:E:34:C:H2'	3:E:35:A:C8	2.49	0.48
1:A:728:GLU:HG2	1:A:782:ALA:HB2	1.96	0.48
1:A:661:GLU:C	1:A:663:PHE:N	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:HIS:O	1:A:682:HIS:CE1	2.67	0.47
3:E:36:C:H2'	3:E:37:A:H8	1.78	0.47
1:A:884:GLN:HA	1:A:976:CYS:HA	1.96	0.47
1:A:1228:LEU:HD12	1:A:1244:LYS:HB3	1.95	0.47
1:A:1239:THR:HA	1:A:1242:GLU:HG2	1.97	0.47
1:A:1494:MET:SD	1:A:1499:LEU:CA	3.03	0.47
1:A:1531:LYS:HG3	1:A:1535:ILE:HD12	1.97	0.47
1:A:1531:LYS:HD3	3:F:23:U:OP1	2.14	0.47
1:A:1531:LYS:HE2	3:F:23:U:OP2	2.15	0.47
3:C:5:C:H2'	3:C:6:U:C6	2.50	0.47
1:A:1228:LEU:HD22	1:A:1232:TYR:HE2	1.79	0.47
1:A:1531:LYS:HG2	1:A:1532:LEU:CD2	2.41	0.47
1:A:1531:LYS:HG3	1:A:1532:LEU:CA	2.44	0.47
1:A:1640:LEU:HB3	1:A:1641:PHE:HD1	1.79	0.47
3:C:12:A:H2'	3:C:13:A:H8	1.78	0.47
1:A:117:GLN:HA	1:A:120:LEU:HD12	1.96	0.47
1:A:660:ASN:HB2	1:A:666:LYS:HB2	1.97	0.47
1:A:389:LEU:HD13	1:A:494:ARG:HB3	1.97	0.47
1:A:1015:TYR:CE2	1:A:1392:TYR:HB2	2.49	0.47
1:A:1216:GLY:HA3	1:A:1371:GLU:O	2.15	0.47
1:A:1273:PRO:HA	1:A:1277:TRP:HB3	1.96	0.47
1:A:1211:ARG:NH2	1:A:1491:ASN:O	2.34	0.47
1:A:387:CYS:O	1:A:474:ASN:N	2.41	0.46
1:A:850:THR:O	1:A:853:ARG:NH2	2.36	0.46
1:A:671:ARG:CB	1:A:1235:TRP:CZ2	2.98	0.46
1:A:669:LYS:HD2	1:A:670:GLU:OE1	2.15	0.46
1:A:819:VAL:HG22	1:A:1317:SER:HA	1.98	0.46
1:A:1458:SER:HB3	3:F:21:G:H5"	1.97	0.46
1:A:369:ARG:HD2	1:A:372:MET:HE3	1.97	0.46
1:A:1501:ASP:HB2	3:D:33:U:O2'	2.15	0.46
1:A:1531:LYS:CE	1:A:1532:LEU:HD22	2.46	0.46
1:A:365:PRO:O	1:A:369:ARG:HG2	2.15	0.46
1:A:28:LEU:HB2	1:A:34:LYS:HD3	1.98	0.46
1:A:299:ALA:O	1:A:303:LEU:HG	2.16	0.46
1:A:724:CYS:HB2	1:A:788:VAL:HG23	1.96	0.46
1:A:1462:ASN:ND2	3:F:20:U:O2'	2.49	0.46
1:A:405:LEU:HD12	1:A:459:ILE:HD11	1.98	0.46
1:A:578:TYR:CD1	1:A:665:PRO:O	2.69	0.46
1:A:1272:THR:HG1	1:A:1276:THR:HG1	1.63	0.46
1:A:1504:SER:HA	1:A:1507:VAL:HG12	1.98	0.46
1:A:1228:LEU:HB3	1:A:1240:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:12:A:H2'	3:F:13:A:C8	2.51	0.45
1:A:117:GLN:NE2	3:F:15:G:O3'	2.50	0.45
1:A:519:TYR:O	1:A:523:LYS:HG2	2.16	0.45
1:A:863:VAL:HG12	1:A:866:ARG:HH12	1.80	0.45
1:A:953:VAL:HG12	3:D:42:C:H4'	1.96	0.45
1:A:958:LYS:NZ	3:D:43:C:O3'	2.49	0.45
1:A:1475:GLY:HA3	1:A:1617:GLU:O	2.17	0.45
1:A:225:PHE:O	1:A:508:ASP:N	2.49	0.45
1:A:1328:TYR:HA	1:A:1331:PHE:HE1	1.80	0.45
1:A:264:SER:OG	3:F:7:U:OP1	2.25	0.45
1:A:581:THR:HG23	1:A:665:PRO:HB3	1.99	0.45
1:A:1531:LYS:CE	1:A:1532:LEU:CD2	2.94	0.45
1:A:1287:ASN:ND2	1:A:1323:CYS:SG	2.85	0.45
1:A:752:ARG:NH1	1:A:984:ASP:OD2	2.50	0.45
1:A:1214:ILE:HG23	1:A:1503:ARG:HH12	1.82	0.45
1:A:369:ARG:HD3	2:B:350:VAL:HG11	1.99	0.45
1:A:1291:LEU:HD21	1:A:1331:PHE:HZ	1.80	0.45
1:A:1495:ASN:O	1:A:1496:PRO:C	2.55	0.45
1:A:659:LEU:O	1:A:660:ASN:C	2.55	0.45
3:F:22:C:H5"	3:F:22:C:C6	2.51	0.44
1:A:37:VAL:O	1:A:41:VAL:HG23	2.18	0.44
1:A:675:ILE:HG23	1:A:1232:TYR:CZ	2.52	0.44
1:A:676:ALA:O	1:A:679:HIS:HB2	2.18	0.44
1:A:897:LYS:HB3	1:A:941:GLU:HB3	1.99	0.44
1:A:1199:THR:HG22	1:A:1267:ASN:HD22	1.82	0.44
1:A:1329:ASN:HA	1:A:1332:VAL:HG12	1.98	0.44
1:A:1497:GLY:HA2	3:D:33:U:C5'	2.40	0.44
1:A:337:LEU:O	1:A:341:LEU:HG	2.18	0.44
1:A:511:ARG:O	1:A:515:ILE:HG12	2.18	0.44
1:A:669:LYS:NZ	1:A:670:GLU:H	2.12	0.44
1:A:1261:ASP:O	1:A:1264:LYS:NZ	2.43	0.44
1:A:1641:PHE:HB3	1:A:1645:LEU:HD23	2.00	0.44
1:A:654:TYR:HE1	1:A:661:GLU:HA	1.79	0.44
1:A:969:VAL:HG11	3:D:51:U:O3'	2.17	0.44
1:A:1004:HIS:HB3	1:A:1265:THR:OG1	2.17	0.44
1:A:509:LYS:HG3	1:A:510:GLU:OE2	2.18	0.43
1:A:593:TRP:HB3	1:A:619:ASN:HB2	2.00	0.43
1:A:1531:LYS:HG3	1:A:1532:LEU:HD22	1.91	0.43
1:A:342:GLN:NE2	1:A:343:ASP:OD1	2.51	0.43
1:A:807:PHE:CE2	1:A:1280:PRO:HD2	2.53	0.43
1:A:225:PHE:HB3	1:A:369:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:GLU:HA	1:A:1460:PRO:CG	2.48	0.43
1:A:740:TYR:HH	3:C:1:G:H8	1.62	0.43
1:A:908:MET:HG3	1:A:914:ASP:H	1.83	0.43
1:A:1033:LEU:HD22	1:A:1206:VAL:HG21	1.99	0.43
1:A:401:ILE:HG22	1:A:459:ILE:HD13	2.01	0.43
1:A:675:ILE:HA	1:A:678:VAL:HB	2.01	0.43
1:A:1458:SER:CB	3:F:21:G:C5'	2.96	0.43
1:A:1463:ARG:CZ	3:E:33:U:O2'	2.65	0.43
1:A:671:ARG:O	1:A:1235:TRP:HH2	2.02	0.43
1:A:779:VAL:HG11	1:A:995:ILE:HD12	1.99	0.43
1:A:823:ARG:HH21	1:A:1286:HIS:CD2	2.36	0.43
1:A:1522:HIS:HA	1:A:1525:ILE:HD12	2.00	0.43
3:F:1:G:H2'	3:F:2:A:H8	1.84	0.43
1:A:133:LEU:O	1:A:166:PRO:HB3	2.19	0.43
1:A:386:ILE:HG22	1:A:456:ASN:HB2	2.00	0.43
1:A:748:LEU:HD13	1:A:988:LYS:HG2	1.99	0.43
1:A:372:MET:HB2	2:B:352:LYS:NZ	2.34	0.43
3:F:5:C:H2'	3:F:6:U:C6	2.53	0.43
1:A:393:GLU:N	1:A:480:ASP:OD2	2.52	0.43
1:A:1500:THR:HG1	3:D:33:U:H5'	1.84	0.43
1:A:578:TYR:HD1	1:A:665:PRO:C	2.21	0.43
1:A:586:ALA:CA	1:A:1420:ASN:HB3	2.48	0.43
1:A:1426:ILE:HG23	1:A:1430:LEU:HD13	2.01	0.43
3:E:50:C:H2'	3:E:51:U:C6	2.54	0.42
1:A:63:MET:SD	1:A:116:ALA:HA	2.59	0.42
1:A:423:PHE:HA	1:A:459:ILE:O	2.18	0.42
1:A:574:ILE:HD13	1:A:663:PHE:O	2.19	0.42
1:A:11:TYR:HD1	1:A:208:MET:SD	2.42	0.42
1:A:295:ALA:HB1	1:A:400:CYS:SG	2.59	0.42
1:A:1214:ILE:CD1	1:A:1500:THR:HG21	2.49	0.42
1:A:1212:LEU:HD13	1:A:1376:VAL:HG22	2.02	0.42
1:A:1611:ALA:O	1:A:1615:VAL:HG23	2.19	0.42
1:A:660:ASN:O	1:A:663:PHE:N	2.49	0.42
1:A:812:LYS:HE3	1:A:812:LYS:HB3	1.87	0.42
1:A:1014:THR:HA	1:A:1019:HIS:NE2	2.35	0.42
1:A:1198:ILE:HG23	1:A:1266:LEU:HA	2.01	0.42
3:C:6:U:H2'	3:C:7:U:C6	2.55	0.42
1:A:750:THR:OG1	1:A:984:ASP:OD1	2.26	0.42
1:A:1002:LEU:HD21	1:A:1031:ARG:NH2	2.34	0.42
1:A:1411:GLU:HA	1:A:1628:ARG:HH12	1.84	0.42
1:A:232:LEU:HD12	1:A:293:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:GLU:O	1:A:671:ARG:C	2.55	0.42
1:A:915:LYS:HE3	1:A:919:GLU:HB3	2.01	0.42
1:A:1616:LEU:HD23	1:A:1616:LEU:HA	1.93	0.42
1:A:43:LYS:O	1:A:46:SER:OG	2.27	0.42
1:A:831:VAL:HG21	1:A:992:LEU:HD11	2.02	0.42
1:A:991:PHE:O	1:A:995:ILE:HG12	2.20	0.42
1:A:1442:TYR:CD2	1:A:1623:VAL:HG13	2.55	0.42
1:A:84:LYS:HD2	1:A:84:LYS:HA	1.83	0.42
1:A:143:HIS:HB3	1:A:148:HIS:CD2	2.54	0.42
1:A:388:CYS:HA	1:A:473:CYS:HB3	2.02	0.42
1:A:960:ASN:OD1	1:A:961:ALA:N	2.52	0.42
1:A:578:TYR:CE1	1:A:658:GLU:OE2	2.73	0.42
1:A:624:CYS:SG	1:A:625:MET:N	2.92	0.42
1:A:678:VAL:O	1:A:679:HIS:CD2	2.73	0.42
1:A:969:VAL:HG11	3:D:51:U:C3'	2.50	0.42
3:F:6:U:H2'	3:F:7:U:C6	2.55	0.42
1:A:334:ARG:O	1:A:338:VAL:HG23	2.19	0.41
1:A:529:ALA:O	1:A:532:LEU:HG	2.20	0.41
1:A:803:HIS:ND1	1:A:831:VAL:HG12	2.35	0.41
1:A:958:LYS:NZ	1:A:961:ALA:HB3	2.35	0.41
1:A:1462:ASN:ND2	3:F:20:U:C4'	2.82	0.41
1:A:1510:THR:N	3:C:21:G:OP1	2.51	0.41
1:A:388:CYS:HB3	1:A:475:HIS:HB2	2.02	0.41
1:A:945:LEU:HD23	1:A:945:LEU:H	1.85	0.41
1:A:313:GLN:OE1	3:E:32:G:O2'	2.28	0.41
1:A:315:GLU:OE1	1:A:1463:ARG:NH2	2.53	0.41
1:A:668:LEU:O	1:A:670:GLU:N	2.53	0.41
1:A:1330:ARG:O	1:A:1330:ARG:NH1	2.54	0.41
1:A:1515:ILE:HD13	1:A:1518:ARG:HH12	1.84	0.41
1:A:315:GLU:HA	1:A:1460:PRO:HG3	2.02	0.41
1:A:315:GLU:CD	1:A:1463:ARG:NH2	2.73	0.41
1:A:355:THR:HA	1:A:358:VAL:HG12	2.02	0.41
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.92	0.41
3:F:24:G:H2'	3:F:25:A:C8	2.56	0.41
1:A:65:ASN:ND2	1:A:140:GLU:OE1	2.46	0.41
1:A:802:PHE:O	1:A:806:VAL:HG23	2.19	0.41
1:A:1500:THR:OG1	3:D:32:G:O2'	2.37	0.41
3:D:48:C:H2'	3:D:49:U:C6	2.56	0.41
1:A:1009:ARG:HH11	1:A:1013:ASN:ND2	2.19	0.41
1:A:1288:VAL:HG22	1:A:1331:PHE:CE2	2.54	0.41
3:C:3:G:H2'	3:C:4:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:THR:OG1	1:A:174:VAL:O	2.32	0.41
1:A:953:VAL:CB	3:D:42:C:H5'	2.50	0.41
1:A:970:ILE:O	3:D:52:U:H4'	2.21	0.41
1:A:1016:LEU:HD23	1:A:1385:HIS:HB3	2.02	0.41
3:C:2:A:H2'	3:C:3:G:H8	1.85	0.41
1:A:23:ASN:OD1	1:A:167:ARG:HD3	2.21	0.41
1:A:363:SER:OG	1:A:367:VAL:HB	2.21	0.41
1:A:424:MET:SD	1:A:446:ALA:HB3	2.61	0.41
1:A:447:ILE:HD11	1:A:470:VAL:HG22	2.02	0.41
1:A:575:LEU:HD11	1:A:649:ALA:HB3	2.03	0.41
1:A:605:ILE:HG22	1:A:606:PHE:HD1	1.85	0.41
1:A:1408:LEU:HD23	1:A:1408:LEU:H	1.85	0.41
1:A:174:VAL:HG11	1:A:486:ASN:HB2	2.03	0.41
1:A:369:ARG:HD2	1:A:369:ARG:HA	1.88	0.41
1:A:315:GLU:HG2	1:A:316:THR:H	1.85	0.40
1:A:344:MET:CE	1:A:345:THR:H	2.34	0.40
1:A:1412:LEU:HD23	1:A:1628:ARG:NH2	2.36	0.40
1:A:315:GLU:CD	1:A:1463:ARG:HH21	2.23	0.40
1:A:369:ARG:HH21	2:B:354:PHE:HB3	1.85	0.40
1:A:680:PHE:HB3	1:A:683:TRP:CD2	2.56	0.40
1:A:653:LEU:CB	1:A:659:LEU:HB2	2.50	0.40
1:A:666:LYS:O	1:A:667:THR:HG23	2.21	0.40
1:A:834:LEU:HB3	1:A:842:LYS:HB3	2.03	0.40
1:A:1257:LEU:HG	1:A:1262:ILE:HD12	2.02	0.40
1:A:1375:GLY:HA2	1:A:1378:VAL:HG12	2.03	0.40
1:A:1416:LYS:HE2	1:A:1416:LYS:HB3	1.94	0.40
1:A:1015:TYR:CZ	1:A:1392:TYR:HB2	2.56	0.40
1:A:1371:GLU:HA	1:A:1374:LEU:HB2	2.03	0.40
1:A:1463:ARG:NH1	3:E:33:U:H1'	2.36	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	1470/1722 (85%)	1392 (95%)	66 (4%)	12 (1%)	19	60
2	B	14/359 (4%)	14 (100%)	0	0	100	100
All	All	1484/2081 (71%)	1406 (95%)	66 (4%)	12 (1%)	24	60

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	658	GLU
1	A	667	THR
1	A	666	LYS
1	A	674	SER
1	A	1497	GLY
1	A	541	GLU
1	A	665	PRO
1	A	668	LEU
1	A	662	ARG
1	A	680	PHE
1	A	669	LYS
1	A	678	VAL

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	1327/1549 (86%)	1304 (98%)	23 (2%)	60	78
2	B	16/289 (6%)	16 (100%)	0	100	100
All	All	1343/1838 (73%)	1320 (98%)	23 (2%)	62	78

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	ARG
1	A	661	GLU
1	A	662	ARG
1	A	666	LYS

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Mol	Chain	Res	Type
1	A	667	THR
1	A	668	LEU
1	A	669	LYS
1	A	670	GLU
1	A	671	ARG
1	A	675	ILE
1	A	677	ASP
1	A	678	VAL
1	A	823	ARG
1	A	958	LYS
1	A	967	MET
1	A	1217	ASP
1	A	1244	LYS
1	A	1447	ARG
1	A	1495	ASN
1	A	1499	LEU
1	A	1500	THR
1	A	1501	ASP
1	A	1531	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	287	GLN
1	A	679	HIS
1	A	912	GLN
1	A	1353	ASN
1	A	1452	GLN
1	A	1462	ASN
1	A	1495	ASN
1	A	1529	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	20/52 (38%)	1 (5%)	0
3	D	20/52 (38%)	6 (30%)	0
3	E	25/52 (48%)	0	0
3	F	25/52 (48%)	1 (4%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	90/208 (43%)	8 (8%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	13	A
3	D	37	A
3	D	38	U
3	D	39	U
3	D	43	C
3	D	44	A
3	D	52	U
3	F	22	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-32241. 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 ⓘ

6.1.1 Primary map

| X | Y | Z |
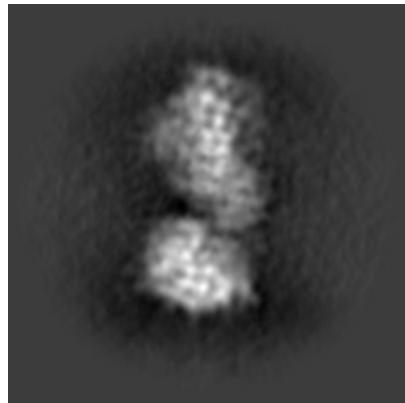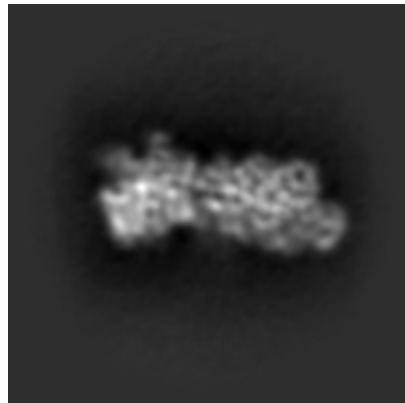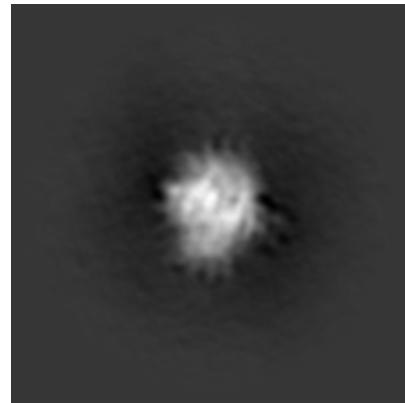
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
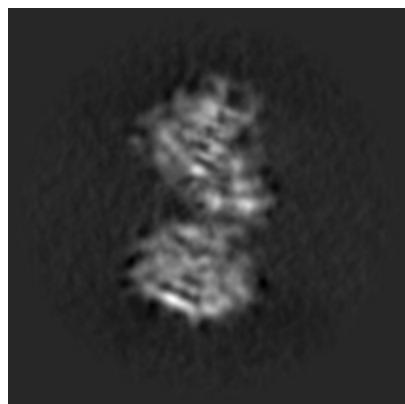
6.2.1 Primary map
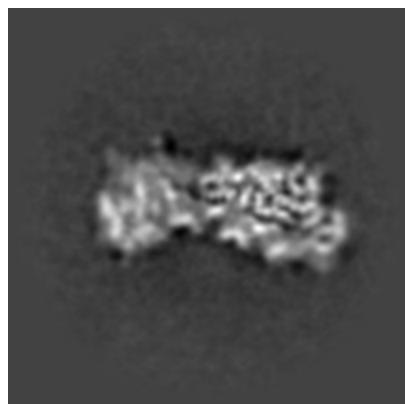
| X Index: 120 | Y Index: 120 | Z Index: 120 |
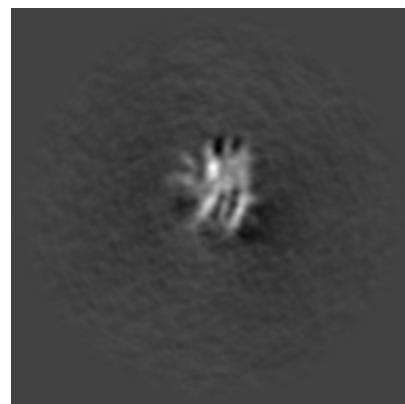
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

| X Index: 121 | Y Index: 119 | Z Index: 79 |
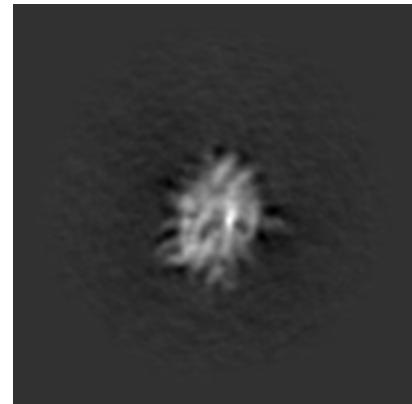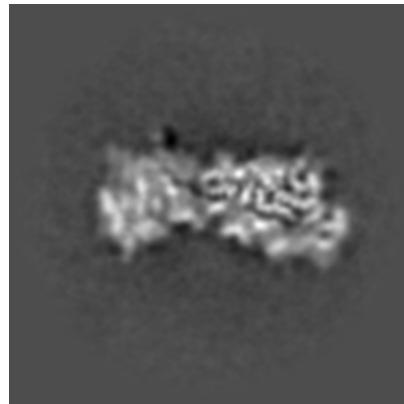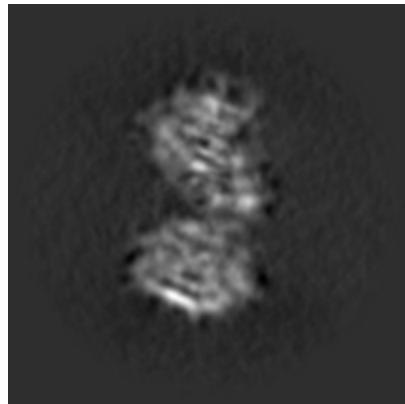
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

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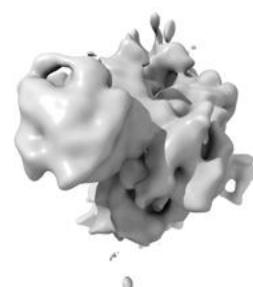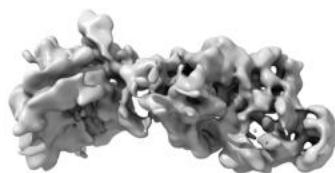
The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation ⓘ

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

7   Map analysis ⓘ

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

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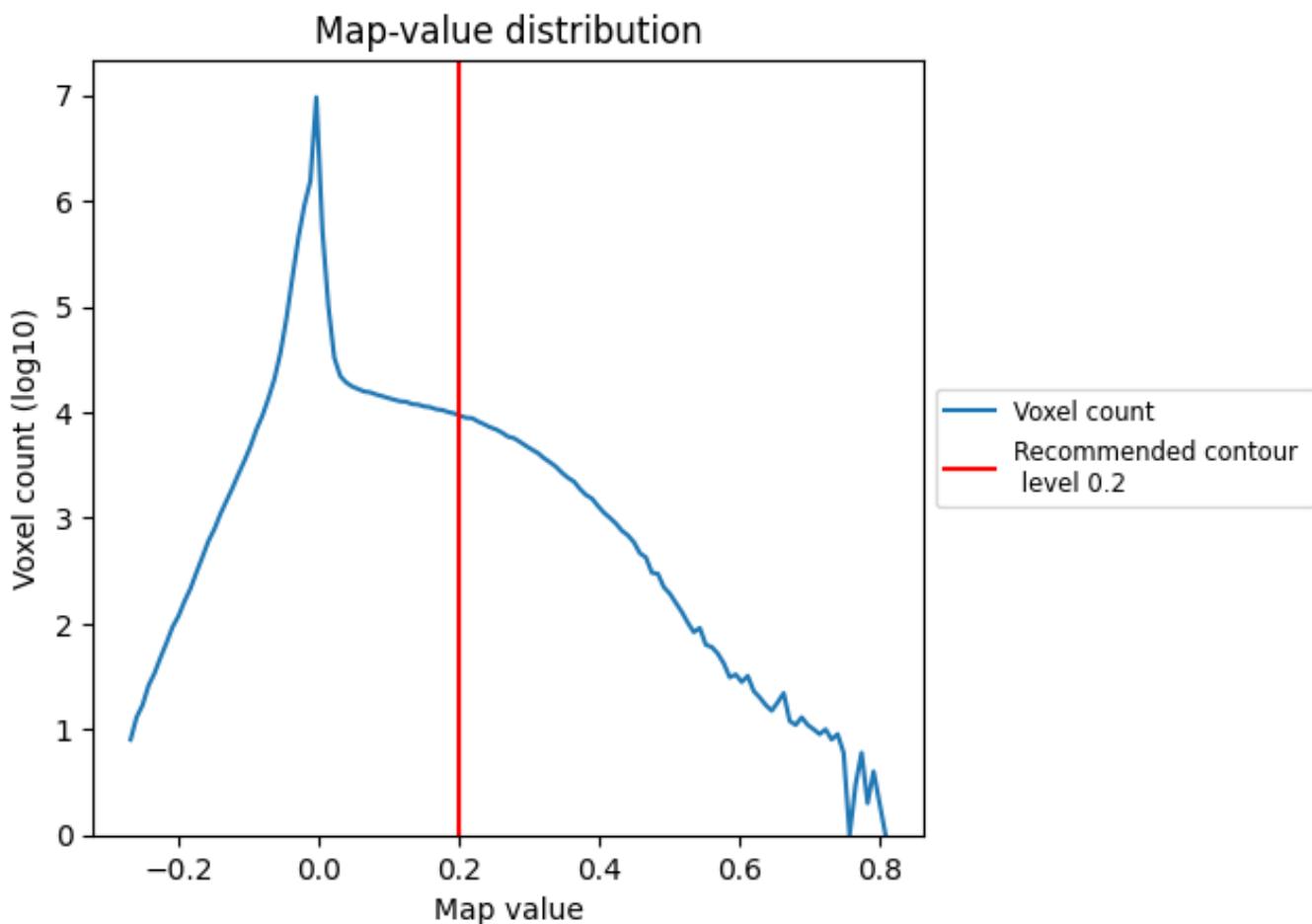
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
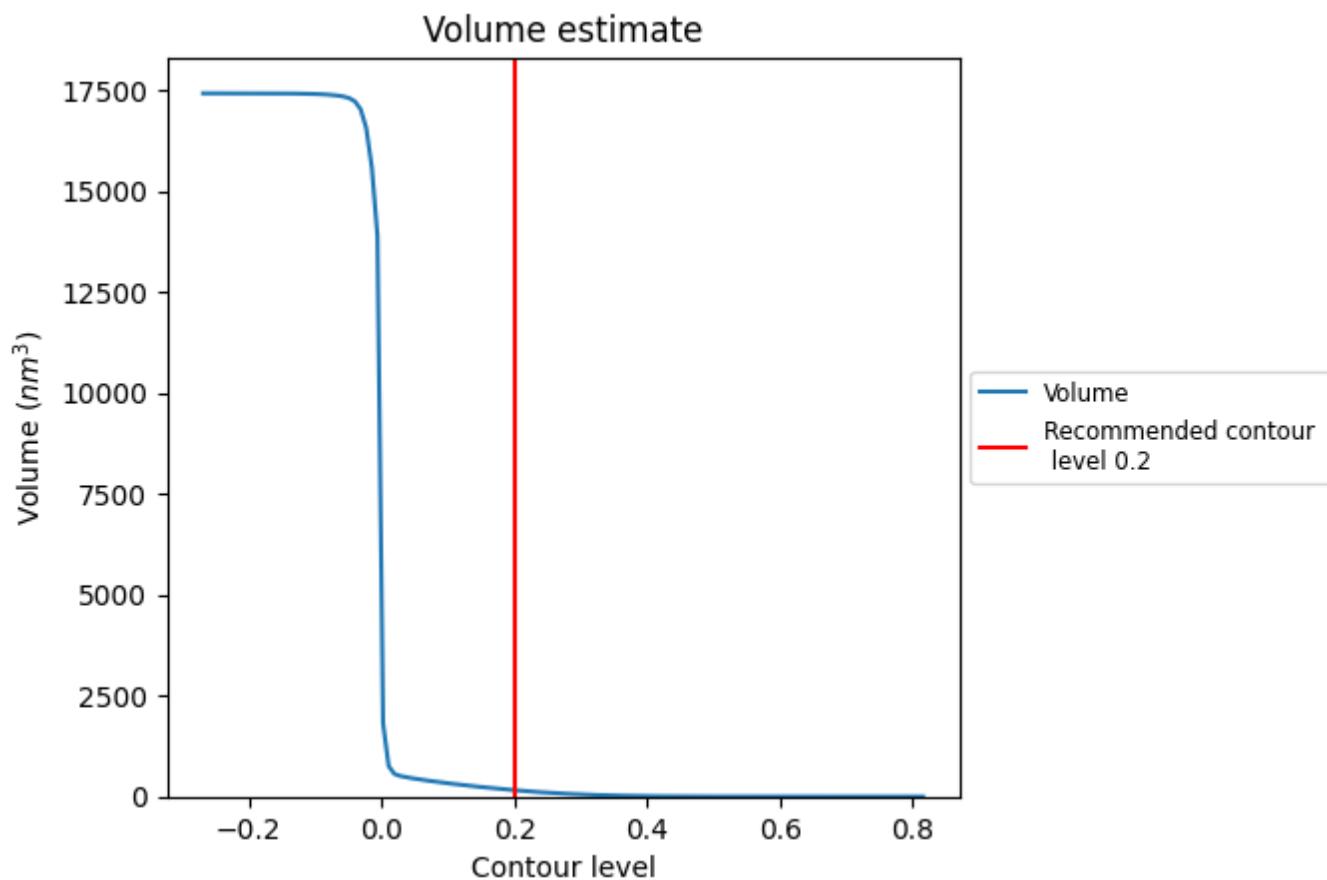
The volume at the recommended contour level is 159 nm^3; this corresponds to an approximate mass of 143 kDa.

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 ⓘ
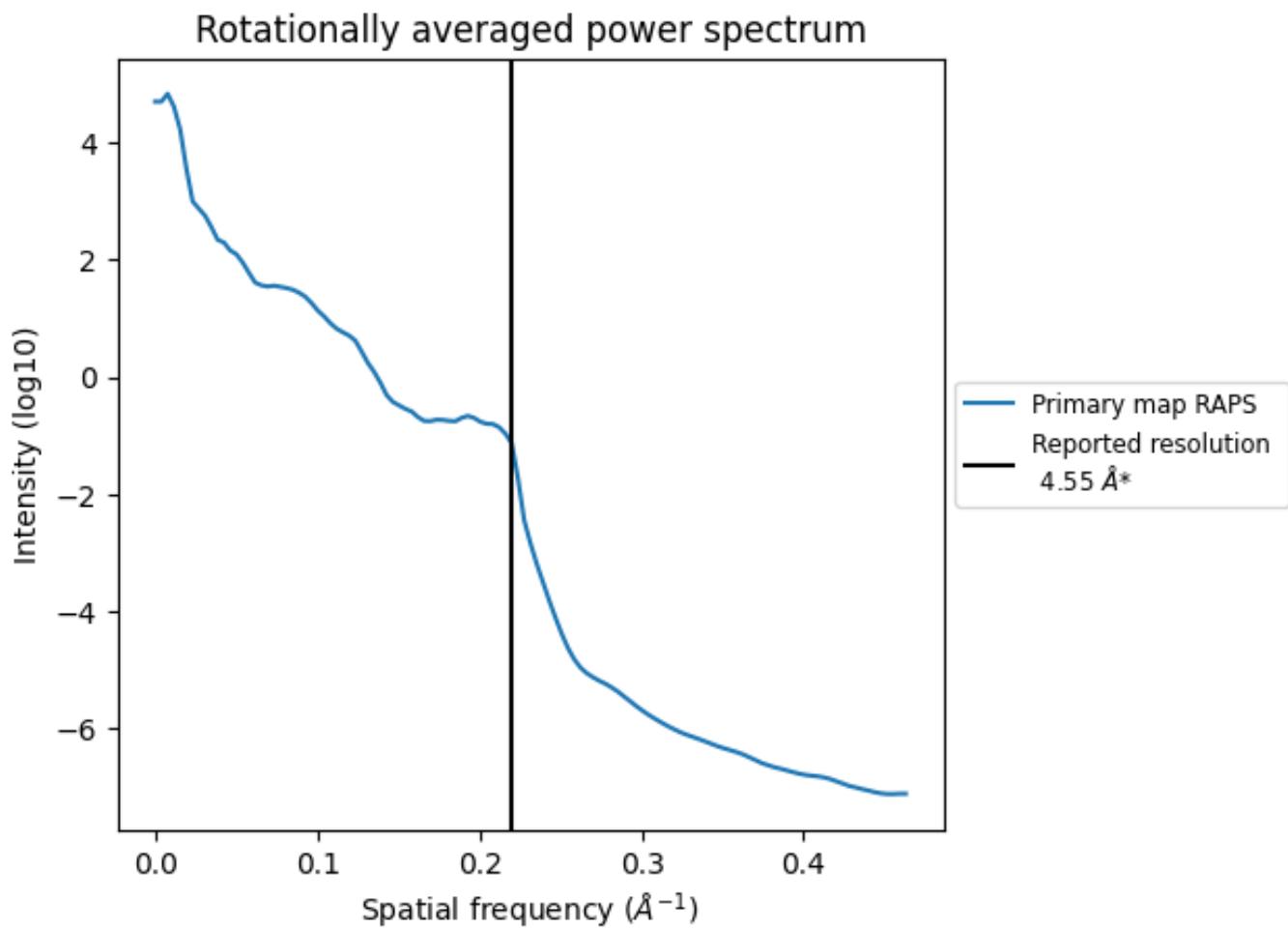
*Reported resolution corresponds to spatial frequency of 0.220 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-32241 and PDB model 7W0F. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay ⓘ

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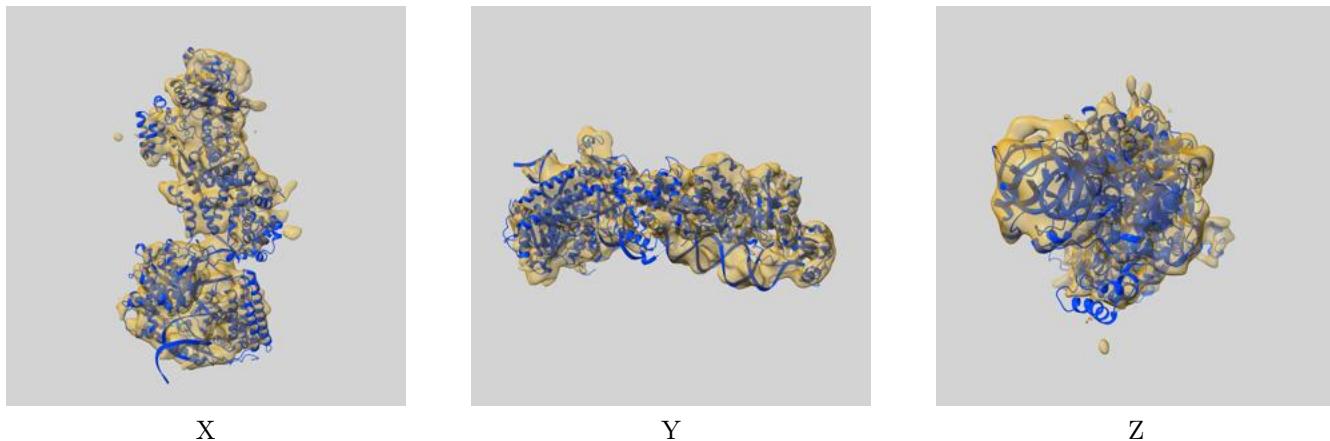
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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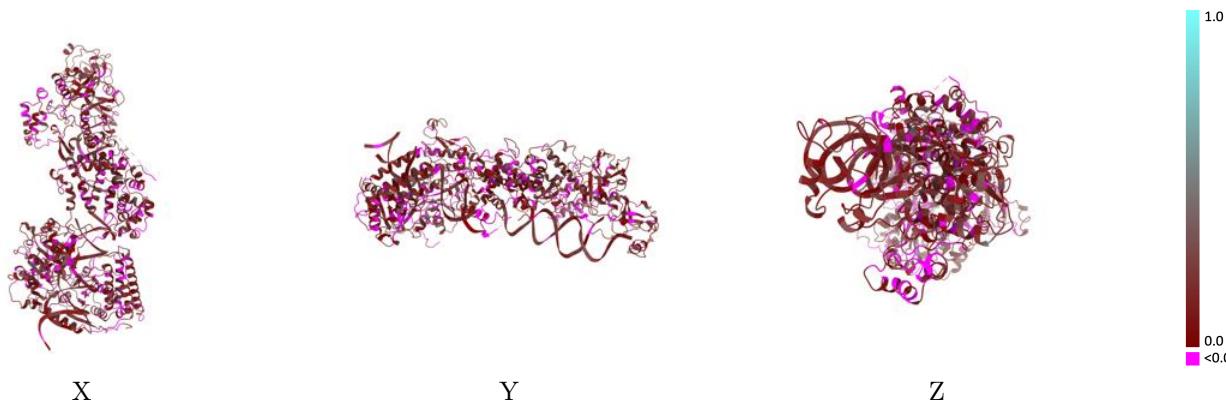
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
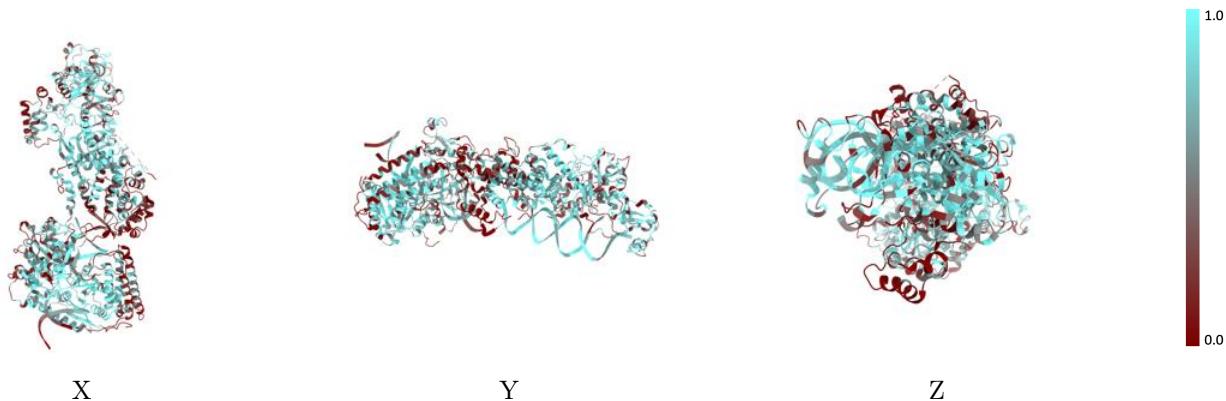
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4　Atom inclusion ⓘ
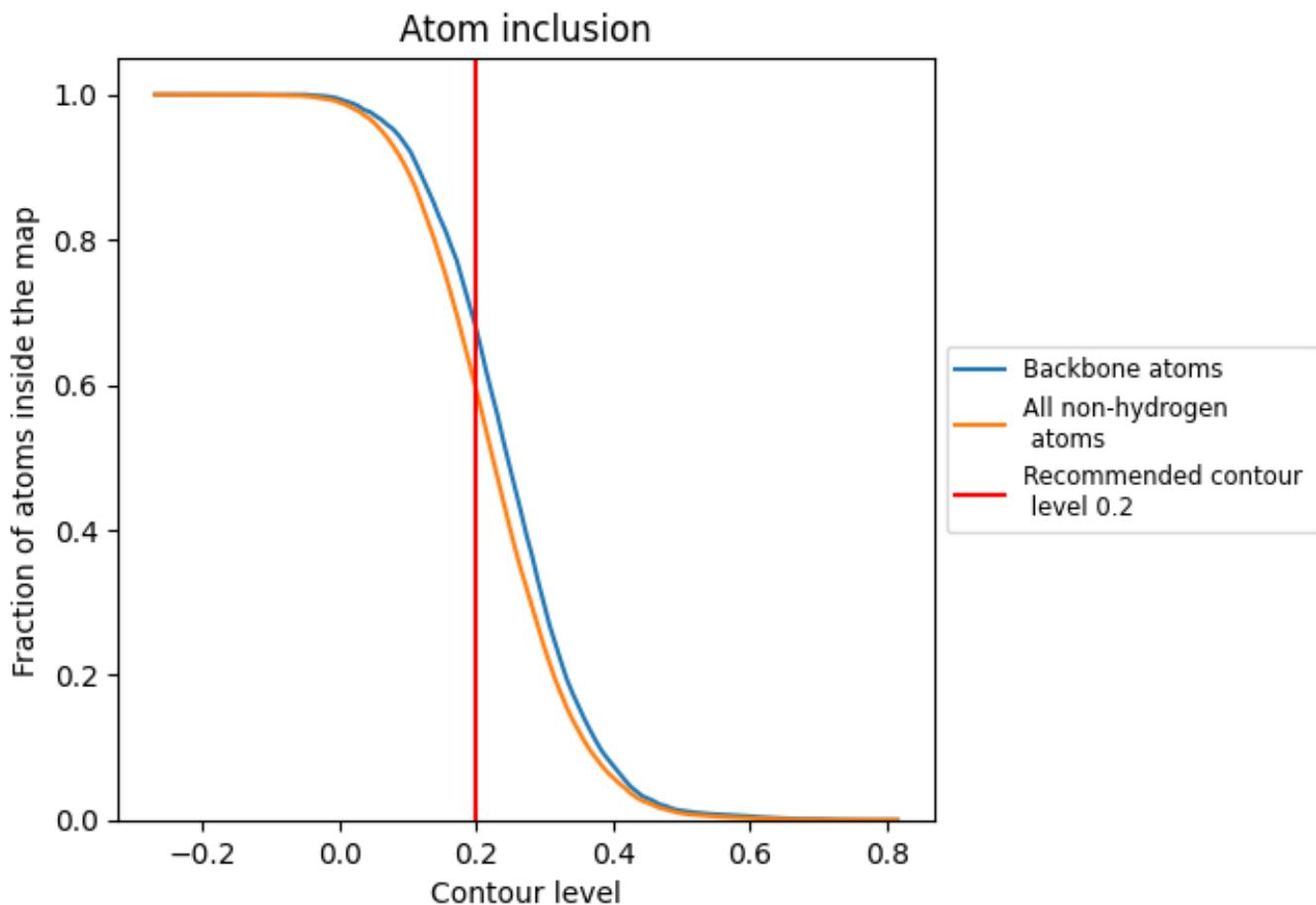
At the recommended contour level, 68% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

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	0.5933	0.1130
A	0.5792	0.1100
B	0.0571	-0.0400
C	0.7738	0.1530
D	0.7826	0.1620
E	0.6893	0.1640
F	0.6369	0.1120

1.0

0.0
<0.0