



Full wwPDB EM Validation Report ⓘ

Jul 5, 2026 – 01:32 AM JST

PDB ID : 9W XF / pdb_00009wxf
EMDB ID : EMD-66345
Title : cryo-electron microscopy structure of Dandelion
Authors : Yu, Y.; Chen, Q.; Tang, Y.
Deposited on : 2025-09-25
Resolution : 3.33 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.dev133
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) : 2.50

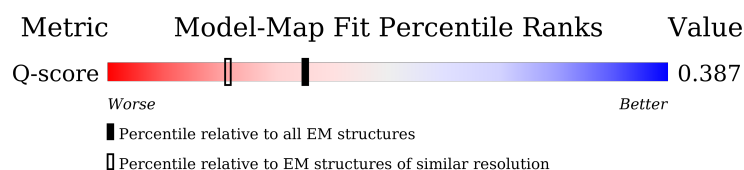
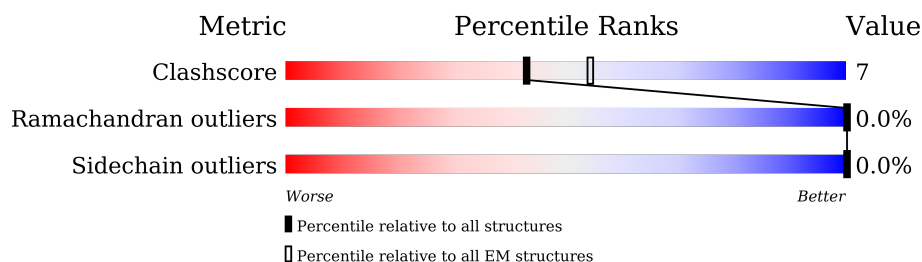
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14484 (2.83 - 3.83)

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	460	 80% 15% 5%
1	B	460	 83% 13% .
1	C	460	 82% 13% 5%
1	D	460	 82% 13% 6%

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Mol	Chain	Length	Quality of chain
1	E	460	77%19%.
1	F	460	78%17%. .
1	G	460	28%6%66%
1	H	460	30%.66%
1	I	460	82%13%5%
1	J	460	7%78%17%5%
1	K	460	76%20%.
1	L	460	78%18%. .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 77260 atoms, of which 38424 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.

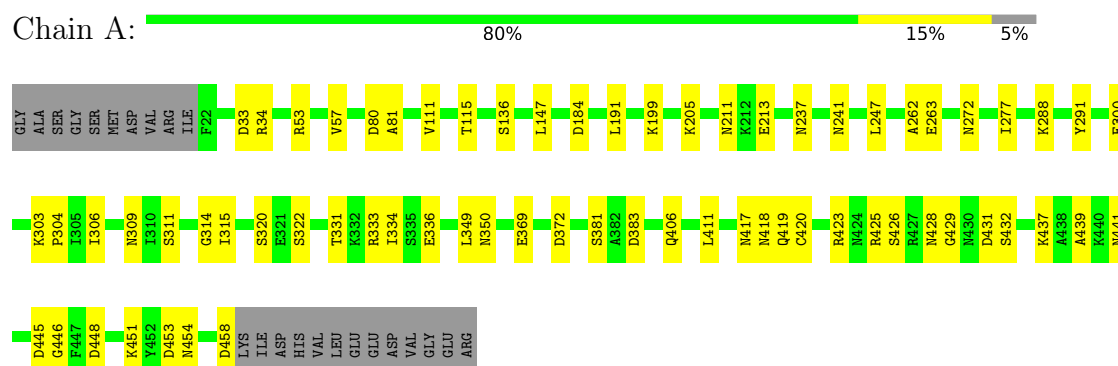
- Molecule 1 is a protein called Dandelion.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	437	Total 7199	C 2308	H 3589	N 610	O 680	S 12	0	0
1	B	442	Total 7276	C 2335	H 3624	N 618	O 687	S 12	0	0
1	C	437	Total 7208	C 2308	H 3598	N 610	O 680	S 12	0	0
1	D	433	Total 7143	C 2285	H 3567	N 606	O 673	S 12	0	0
1	E	441	Total 7263	C 2326	H 3622	N 617	O 686	S 12	0	0
1	F	441	Total 7256	C 2326	H 3615	N 617	O 686	S 12	0	0
1	G	155	Total 2526	C 818	H 1239	N 223	O 241	S 5	0	0
1	H	155	Total 2526	C 818	H 1239	N 223	O 241	S 5	0	0
1	I	438	Total 7229	C 2312	H 3611	N 614	O 680	S 12	0	0
1	J	437	Total 7199	C 2308	H 3589	N 610	O 680	S 12	0	0
1	K	442	Total 7236	C 2334	H 3584	N 618	O 687	S 13	0	0
1	L	442	Total 7199	C 2334	H 3547	N 618	O 687	S 13	0	0

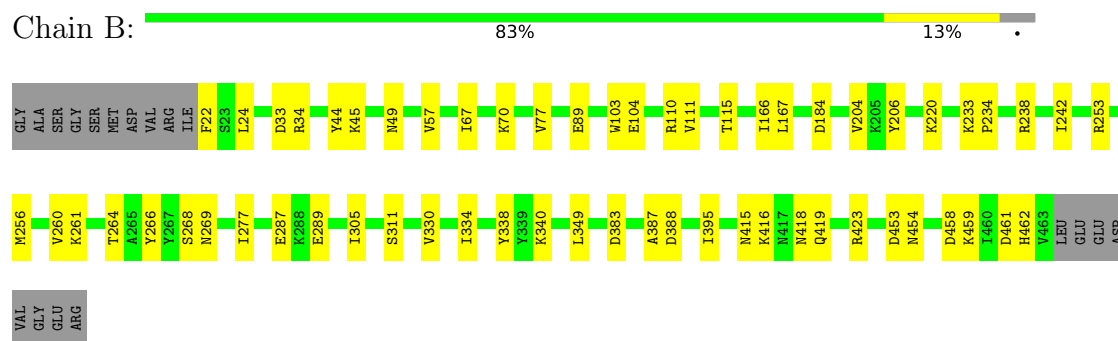
3 Residue-property plots

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.

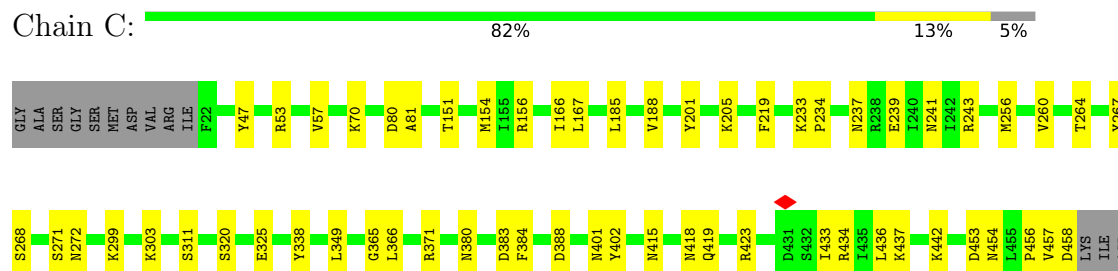
• Molecule 1: Dandelion



• Molecule 1: Dandelion



• Molecule 1: Dandelion



HIS
VAL
LEU
GLY
GLU
ASP
VAL
GLY
ARG

● Molecule 1: Dandelion

Chain D:  82% 13% 6%

GLY
ALA
SER
GLY
SER
MET
ASP
VAL
ARG
ILE
PHE
SER
LEU
GLU

N273
H274
I277
F283
I284
S285
R286
E287
V298
I302
I305
I315
F318
I319
T331
I334
S335
K340
E363
E367
Y370
T115
I166
I167
P171
D194
K200
V204
K205
Y206
L215
K233
P234
M245
R253
S271
N272

LYS
ILE
ASP
HIS
VAL
LEU
GLU
ASP
ARG
VAL
GLY
GLU
ARG

● Molecule 1: Dandelion

Chain E:  77% 19% 4%

GLY
ALA
SER
GLY
SER
MET
ASP
VAL
ARG
ILE
PHE
S23
L24
E25
K28
E41
F42
V43
A55
M58
L59
W60
S61
V62
V63
I67
K70
D80
A81
E104
V111
T115
L113
I122
I166
M173
I177
L178
F181
L185
V188

S194
D195
V204
L210
W211
K212
E213
V214
K217
R238
I242
R243
A244
N245
K255
M256
V260
T264
D311
Y267
S268
S271
N272
N273
H274
F283
D295
D296
K299
I306
I310
F313
P323
I327
I334
S335
E336
Y342
N350
Q351

D383
F384
E385
Y402
S403
Q406
A414
N417
N418
Q419
C420
Y421
V422
R423
N424
R425
S426
R427
N428
G429
K430
D431
S432
L436
K442
D448
F449
S450
K451
Y452
D453
N454
L455
D461
H462
V463
LEU
GLU
ASP
VAL
GLY
ARG

● Molecule 1: Dandelion

Chain F:  78% 17% 5%

GLY
ALA
SER
GLY
SER
MET
ASP
VAL
ARG
ILE
PHE
S23
D33
R34
K45
N49
R53
S54
W60
V64
I67
L71
R75
D76
L87
S142
D143
E144
L147
I166
L167
F172
M173
S174
Q175
L178
V182
A183
D184
L185
E186
S194
D195

Y206
N211
K212
R228
E231
N237
R238
E239
I240
N241
R242
R243
E250
R253
N269
I270
S271
N272
N273
H274
K278
E282
E287
K303
K307
I310
S311
Y312
F313
S320
E324
E325
H326
I327
N328
R329
V330
T331
K332
R333
I334
K337
Y338

Y339
K340
K341
D344
F348
L366
F373
E385
D392
K397
L411
E412
N415
D431
K437
K440
D448
K451
Y452
D453
N454
V457
V463
LEU
GLU
ASP
VAL
GLY
ARG

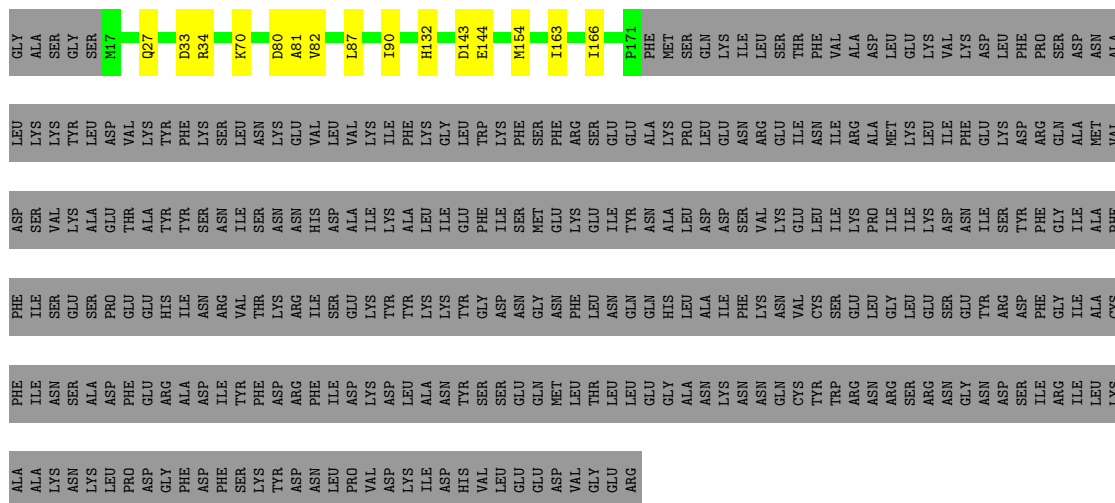
● Molecule 1: Dandelion

Chain G:  28% 6% 66%

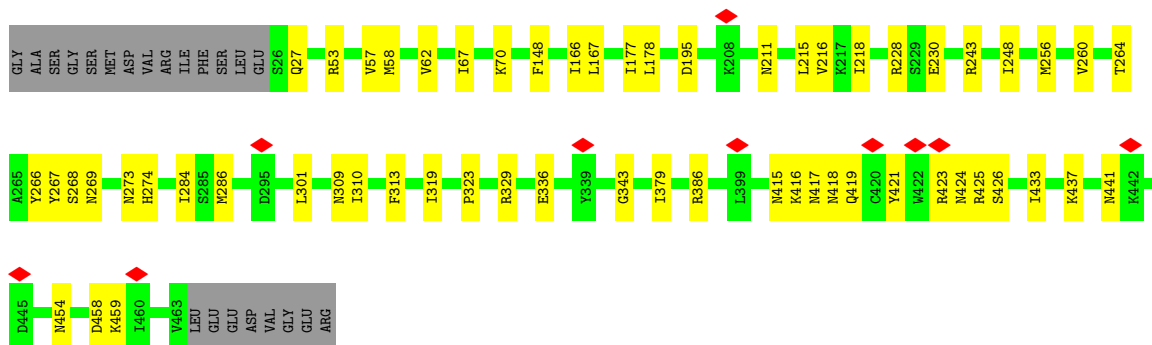
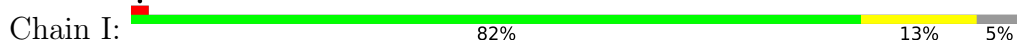
GLY
ALA
SER
GLY
SER
M17
I21
F22
T36
R53
S54
V57
W60
V64
C65
D66
I67
I68
L71
L87
E91
E104
L107
V111
T115
L127
R133
D143
E144
D145
P150
M154
I166
L167
P171
PHE
MET
SER
GLN
LYS



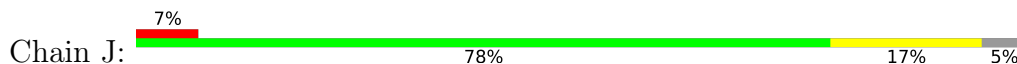
- Molecule 1: Dandelion

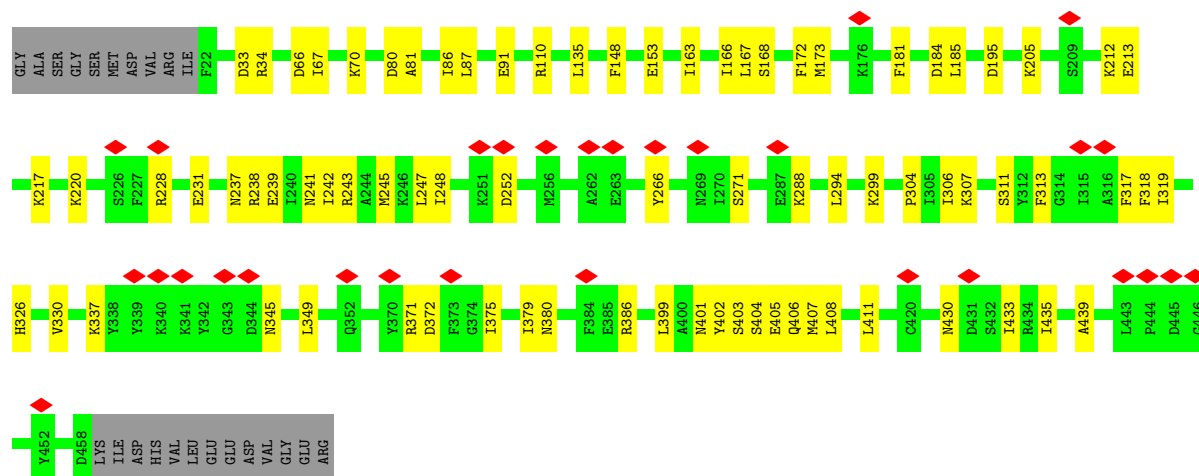


- Molecule 1: Dandelion

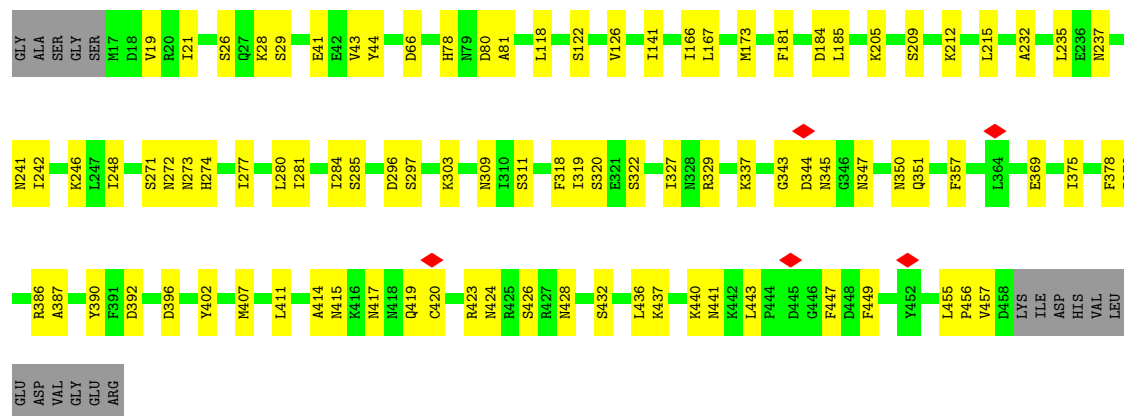
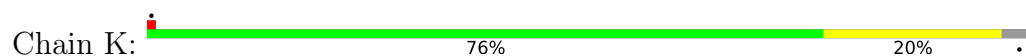


- Molecule 1: Dandelion

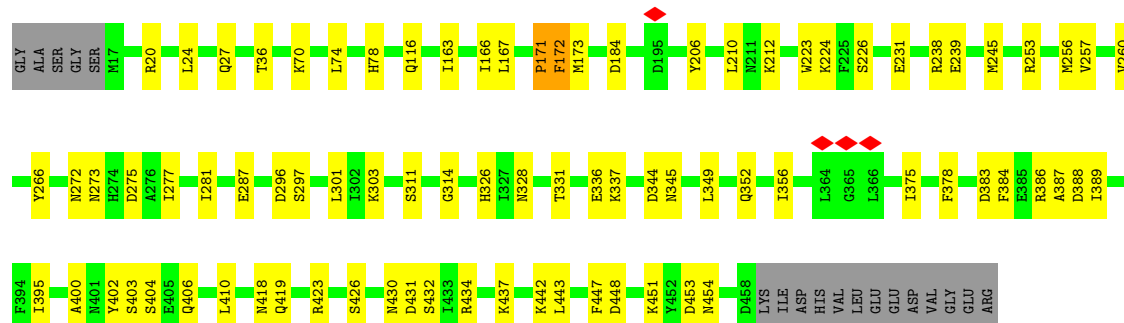
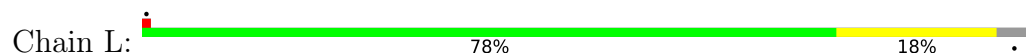




• Molecule 1: Dandelion



• Molecule 1: Dandelion



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70976	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.68	Depositor
Minimum defocus (nm)	404	Depositor
Maximum defocus (nm)	4966	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.072	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.0225	Depositor
Map size ($\text{\AA}$)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	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	0.23	0/3683	0.37	0/4957
1	B	0.29	0/3726	0.35	0/5015
1	C	0.23	0/3683	0.34	0/4957
1	D	0.28	0/3648	0.40	2/4910 (0.0%)
1	E	0.27	0/3714	0.40	2/4999 (0.0%)
1	F	0.20	0/3714	0.34	0/4999
1	G	0.24	0/1312	0.38	0/1772
1	H	0.26	0/1312	0.34	0/1772
1	I	0.23	0/3691	0.35	0/4968
1	J	0.20	0/3683	0.33	0/4957
1	K	0.21	0/3725	0.33	0/5013
1	L	0.21	0/3725	0.39	0/5013
All	All	0.24	0/39616	0.36	4/53332 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	171	PRO	CA-C-N	8.20	133.72	120.60
1	D	171	PRO	C-N-CA	8.20	133.72	120.60
1	E	336	GLU	CA-C-N	7.55	135.55	122.56
1	E	336	GLU	C-N-CA	7.55	135.55	122.56

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	3610	3589	3597	39	0
1	B	3652	3624	3641	40	0
1	C	3610	3598	3597	35	0
1	D	3576	3567	3566	41	0
1	E	3641	3622	3632	59	0
1	F	3641	3615	3632	52	0
1	G	1287	1239	1298	23	0
1	H	1287	1239	1298	8	0
1	I	3618	3611	3610	47	0
1	J	3610	3589	3597	52	0
1	K	3652	3584	3643	66	0
1	L	3652	3547	3643	60	0
All	All	38836	38424	38754	508	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 7.

All (508) 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:D:70:LYS:NZ	1:D:166:ILE:O	2.05	0.90
1:E:402:TYR:O	1:E:442:LYS:NZ	2.06	0.89
1:C:402:TYR:O	1:C:442:LYS:NZ	2.08	0.87
1:F:250:GLU:O	1:F:253:ARG:NH2	2.09	0.86
1:F:172:PHE:O	1:F:173:MET:HG2	1.74	0.86
1:B:266:TYR:O	1:B:269:ASN:ND2	2.10	0.85
1:C:388:ASP:OD1	1:C:423:ARG:NH1	2.09	0.85
1:C:264:THR:O	1:C:268:SER:OG	1.96	0.83
1:D:111:VAL:O	1:D:115:THR:OG1	1.96	0.83
1:J:372:ASP:OD1	1:J:406:GLN:NE2	2.11	0.83
1:F:448:ASP:O	1:F:451:LYS:NZ	2.12	0.83
1:B:70:LYS:NZ	1:B:166:ILE:O	2.14	0.80
1:E:70:LYS:NZ	1:E:166:ILE:O	2.14	0.79
1:K:343:GLY:N	1:K:347:ASN:OD1	2.15	0.79
1:I:273:ASN:OD1	1:I:274:HIS:N	2.16	0.79
1:E:383:ASP:OD2	1:E:384:PHE:N	2.15	0.79
1:G:36:THR:OG1	1:G:66:ASP:OD1	2.01	0.78
1:I:228:ARG:NH2	1:I:266:TYR:O	2.17	0.78
1:E:80:ASP:OD2	1:E:81:ALA:N	2.18	0.77
1:G:60:TRP:NE1	1:G:104:GLU:OE2	2.18	0.77
1:F:339:TYR:O	1:F:341:LYS:NZ	2.18	0.77
1:H:80:ASP:OD1	1:H:81:ALA:N	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:294:LEU:O	1:J:299:LYS:NZ	2.19	0.75
1:B:383:ASP:O	1:B:419:GLN:NE2	2.20	0.75
1:H:70:LYS:NZ	1:H:166:ILE:O	2.20	0.74
1:F:320:SER:OG	1:F:325:GLU:OE1	2.04	0.74
1:B:388:ASP:OD1	1:B:423:ARG:NH1	2.21	0.74
1:E:273:ASN:OD1	1:E:274:HIS:N	2.21	0.73
1:I:228:ARG:NE	1:I:269:ASN:O	2.22	0.73
1:E:28:LYS:NZ	1:E:41:GLU:OE1	2.16	0.73
1:E:111:VAL:O	1:E:115:THR:OG1	2.06	0.72
1:J:345:ASN:OD1	1:J:386:ARG:NH2	2.22	0.72
1:K:443:LEU:HD13	1:K:447:PHE:CG	2.24	0.72
1:K:28:LYS:NZ	1:K:41:GLU:OE2	2.18	0.71
1:A:372:ASP:OD1	1:A:406:GLN:NE2	2.23	0.71
1:B:184:ASP:OD2	1:B:206:TYR:OH	2.09	0.71
1:D:335:SER:OG	1:D:380:ASN:OD1	2.09	0.70
1:F:184:ASP:OD2	1:F:206:TYR:OH	2.09	0.70
1:C:201:TYR:OH	1:C:205:LYS:NZ	2.21	0.70
1:I:70:LYS:NZ	1:I:166:ILE:O	2.24	0.70
1:C:320:SER:OG	1:C:325:GLU:OE1	2.08	0.70
1:K:426:SER:O	1:K:432:SER:OG	2.02	0.69
1:C:436:LEU:HD22	1:C:456:PRO:O	1.92	0.69
1:K:320:SER:OG	1:K:322:SER:O	2.11	0.68
1:D:184:ASP:OD2	1:D:206:TYR:OH	2.08	0.68
1:L:314:GLY:O	1:L:326:HIS:NE2	2.26	0.68
1:F:273:ASN:OD1	1:F:274:HIS:N	2.26	0.68
1:L:184:ASP:OD1	1:L:206:TYR:OH	2.10	0.67
1:J:407:MET:HE2	1:J:439:ALA:HB2	1.75	0.67
1:K:379:ILE:O	1:K:417:ASN:ND2	2.28	0.67
1:E:417:ASN:OD1	1:E:420:CYS:N	2.26	0.67
1:F:142:SER:OG	1:G:91:GLU:OE2	2.10	0.67
1:G:111:VAL:O	1:G:115:THR:OG1	2.12	0.67
1:L:418:ASN:OD1	1:L:419:GLN:N	2.28	0.67
1:B:45:LYS:O	1:B:49:ASN:ND2	2.28	0.67
1:F:415:ASN:O	1:F:454:ASN:ND2	2.29	0.66
1:I:433:ILE:HD11	1:I:459:LYS:HD3	1.77	0.66
1:J:181:PHE:HE1	1:J:185:LEU:HD11	1.60	0.66
1:I:264:THR:O	1:I:268:SER:OG	2.14	0.66
1:A:309:ASN:OD1	1:A:311:SER:N	2.29	0.66
1:A:437:LYS:NZ	1:A:458:ASP:O	2.28	0.66
1:C:70:LYS:NZ	1:C:166:ILE:O	2.29	0.66
1:K:237:ASN:O	1:K:241:ASN:ND2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:ASN:O	1:F:241:ASN:ND2	2.29	0.65
1:K:296:ASP:OD2	1:K:297:SER:N	2.28	0.65
1:D:245:MET:HE3	1:D:283:PHE:CE1	2.32	0.65
1:E:194:SER:O	1:E:243:ARG:NH2	2.29	0.65
1:D:253:ARG:NH2	1:D:287:GLU:OE2	2.29	0.65
1:K:402:TYR:HB2	1:K:407:MET:HE2	1.78	0.65
1:I:418:ASN:OD1	1:I:419:GLN:N	2.29	0.65
1:A:311:SER:O	1:A:314:GLY:N	2.31	0.64
1:B:256:MET:O	1:B:260:VAL:HG23	1.98	0.64
1:F:60:TRP:O	1:F:64:VAL:HG23	1.98	0.64
1:K:424:ASN:O	1:K:428:ASN:N	2.29	0.64
1:F:324:GLU:O	1:F:328:ASN:ND2	2.31	0.64
1:A:211:ASN:OD1	1:A:213:GLU:N	2.31	0.64
1:F:71:LEU:HD23	1:F:71:LEU:O	1.98	0.64
1:A:445:ASP:OD1	1:A:446:GLY:N	2.31	0.64
1:I:379:ILE:O	1:I:417:ASN:ND2	2.31	0.64
1:I:424:ASN:OD1	1:I:425:ARG:N	2.31	0.63
1:B:330:VAL:O	1:B:334:ILE:HD12	1.98	0.63
1:C:383:ASP:OD2	1:C:384:PHE:N	2.31	0.63
1:J:403:SER:OG	1:J:405:GLU:OE1	2.17	0.63
1:K:350:ASN:OD1	1:K:351:GLN:N	2.31	0.63
1:D:363:GLU:OE1	1:K:19:VAL:HG12	1.99	0.62
1:B:415:ASN:OD1	1:B:416:LYS:N	2.32	0.62
1:E:67:ILE:HG13	1:E:166:ILE:HD11	1.81	0.62
1:L:231:GLU:N	1:L:231:GLU:OE1	2.33	0.62
1:I:53:ARG:NH1	1:I:148:PHE:O	2.32	0.61
1:F:143:ASP:OD2	1:F:144:GLU:N	2.33	0.61
1:C:260:VAL:HG22	1:C:267:TYR:CE1	2.36	0.61
1:C:338:TYR:O	1:C:380:ASN:ND2	2.34	0.61
1:G:64:VAL:O	1:G:68:ILE:HD12	2.01	0.61
1:I:260:VAL:HG22	1:I:267:TYR:CE2	2.34	0.61
1:J:306:ILE:HG23	1:J:313:PHE:CD2	2.37	0.60
1:E:25:GLU:OE2	1:I:27:GLN:NE2	2.35	0.59
1:J:337:LYS:NZ	1:J:380:ASN:O	2.23	0.59
1:L:448:ASP:OD1	1:L:451:LYS:NZ	2.35	0.59
1:A:369:GLU:N	1:A:369:GLU:OE1	2.36	0.59
1:F:71:LEU:HD22	1:F:87:LEU:HG	1.85	0.58
1:A:288:LYS:O	1:A:291:TYR:N	2.33	0.58
1:B:458:ASP:OD1	1:B:459:LYS:N	2.37	0.58
1:D:285:SER:OG	1:D:315:ILE:O	2.20	0.58
1:F:328:ASN:O	1:F:331:THR:OG1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:173:MET:HB3	1:L:210:LEU:HD23	1.85	0.58
1:A:437:LYS:O	1:A:441:ASN:ND2	2.37	0.58
1:H:132:HIS:CE1	1:H:154:MET:HE2	2.38	0.58
1:J:153:GLU:N	1:J:153:GLU:OE2	2.35	0.58
1:L:406:GLN:N	1:L:406:GLN:OE1	2.36	0.58
1:A:411:LEU:HD11	1:A:439:ALA:HB1	1.86	0.58
1:C:260:VAL:HG22	1:C:267:TYR:HE1	1.69	0.58
1:D:453:ASP:OD1	1:D:454:ASN:N	2.35	0.58
1:L:328:ASN:O	1:L:331:THR:OG1	2.19	0.58
1:C:47:TYR:OH	1:C:156:ARG:NH1	2.37	0.57
1:F:311:SER:OG	1:F:348:PHE:O	2.22	0.57
1:L:443:LEU:HD13	1:L:447:PHE:CD1	2.39	0.57
1:L:453:ASP:OD1	1:L:454:ASN:N	2.37	0.57
1:D:67:ILE:CG1	1:D:166:ILE:HD11	2.35	0.57
1:L:314:GLY:C	1:L:326:HIS:HE2	2.11	0.57
1:C:271:SER:OG	1:C:272:ASN:N	2.38	0.57
1:F:287:GLU:OE2	1:F:287:GLU:N	2.38	0.57
1:B:238:ARG:O	1:B:242:ILE:HD12	2.05	0.56
1:A:417:ASN:OD1	1:A:420:CYS:N	2.39	0.56
1:F:453:ASP:OD1	1:F:454:ASN:N	2.38	0.56
1:I:67:ILE:HG13	1:I:166:ILE:HD11	1.86	0.56
1:D:395:ILE:HG22	1:D:399:LEU:HD21	1.88	0.56
1:A:453:ASP:OD1	1:A:454:ASN:N	2.39	0.56
1:J:407:MET:HE1	1:J:435:ILE:HG23	1.87	0.56
1:B:57:VAL:HG11	1:I:57:VAL:HG11	1.89	0.56
1:E:173:MET:HE1	1:E:214:VAL:HG21	1.87	0.56
1:B:395:ILE:HG22	1:B:395:ILE:O	2.05	0.55
1:F:228:ARG:NH1	1:F:269:ASN:OD1	2.39	0.55
1:E:181:PHE:HE1	1:E:185:LEU:HD11	1.71	0.55
1:K:443:LEU:HD13	1:K:447:PHE:CD1	2.40	0.55
1:E:428:ASN:OD1	1:E:429:GLY:N	2.40	0.55
1:A:199:LYS:HG2	1:A:247:LEU:HD22	1.89	0.55
1:L:426:SER:O	1:L:432:SER:OG	2.13	0.55
1:L:253:ARG:O	1:L:257:VAL:HG23	2.05	0.55
1:A:418:ASN:OD1	1:A:419:GLN:N	2.38	0.55
1:D:388:ASP:OD1	1:D:423:ARG:NH1	2.40	0.54
1:F:211:ASN:OD1	1:F:212:LYS:N	2.40	0.54
1:K:166:ILE:HG23	1:K:167:LEU:N	2.22	0.54
1:F:303:LYS:O	1:F:307:LYS:NZ	2.33	0.54
1:F:310:ILE:HD11	1:F:334:ILE:HG12	1.88	0.54
1:K:327:ILE:HG23	1:K:357:PHE:HZ	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:THR:O	1:E:268:SER:OG	2.16	0.54
1:K:181:PHE:CE2	1:K:185:LEU:HD11	2.43	0.54
1:K:319:ILE:HD12	1:K:329:ARG:NH1	2.23	0.54
1:H:33:ASP:OD1	1:H:34:ARG:N	2.41	0.54
1:E:60:TRP:NE1	1:E:104:GLU:OE2	2.35	0.54
1:F:53:ARG:HD3	1:F:147:LEU:HD21	1.89	0.54
1:A:184:ASP:OD2	1:A:205:LYS:NZ	2.34	0.53
1:F:54:SER:HB3	1:G:54:SER:HB2	1.89	0.53
1:K:378:PHE:CE2	1:K:387:ALA:HB1	2.43	0.53
1:L:78:HIS:ND1	1:L:173:MET:SD	2.81	0.53
1:J:304:PRO:HA	1:J:307:LYS:HG2	1.89	0.53
1:C:151:THR:OG1	1:C:154:MET:SD	2.64	0.53
1:I:67:ILE:CG1	1:I:166:ILE:HD11	2.39	0.53
1:I:230:GLU:N	1:I:230:GLU:OE1	2.41	0.53
1:J:318:PHE:CE2	1:J:319:ILE:HG23	2.44	0.53
1:E:177:ILE:HG13	1:E:178:LEU:N	2.24	0.53
1:J:87:LEU:O	1:J:91:GLU:HG2	2.09	0.53
1:C:437:LYS:NZ	1:C:458:ASP:O	2.36	0.52
1:K:440:LYS:HA	1:K:443:LEU:HD12	1.91	0.52
1:E:177:ILE:HD11	1:E:217:LYS:HD2	1.91	0.52
1:F:385:GLU:OE1	1:F:385:GLU:N	2.42	0.52
1:H:80:ASP:OD1	1:H:82:VAL:N	2.41	0.52
1:L:239:GLU:OE1	1:L:239:GLU:N	2.38	0.52
1:B:204:VAL:HG12	1:B:204:VAL:O	2.09	0.52
1:I:260:VAL:HG13	1:I:267:TYR:HD2	1.73	0.52
1:K:417:ASN:OD1	1:K:420:CYS:N	2.40	0.52
1:F:313:PHE:CE2	1:F:330:VAL:HG22	2.45	0.52
1:E:58:MET:O	1:E:62:VAL:HG23	2.10	0.52
1:G:143:ASP:OD1	1:G:144:GLU:N	2.43	0.52
1:C:80:ASP:OD1	1:C:81:ALA:N	2.43	0.52
1:G:166:ILE:HG23	1:G:167:LEU:N	2.25	0.51
1:K:375:ILE:HD11	1:K:402:TYR:CE2	2.45	0.51
1:F:33:ASP:OD1	1:F:34:ARG:N	2.39	0.51
1:B:277:ILE:HG21	1:B:305:ILE:HD12	1.92	0.51
1:K:375:ILE:HD11	1:K:402:TYR:CZ	2.45	0.51
1:L:400:ALA:O	1:L:442:LYS:NZ	2.41	0.51
1:D:331:THR:HA	1:D:334:ILE:HD12	1.92	0.51
1:G:71:LEU:CD2	1:G:87:LEU:HD12	2.41	0.51
1:J:91:GLU:OE2	1:K:141:ILE:HG21	2.11	0.51
1:L:272:ASN:OD1	1:L:273:ASN:N	2.43	0.51
1:F:75:ARG:NE	1:F:76:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:LEU:HD23	1:H:90:ILE:HD11	1.92	0.51
1:E:63:VAL:HG13	1:E:166:ILE:HD13	1.93	0.51
1:J:407:MET:HE1	1:J:435:ILE:CG2	2.40	0.51
1:E:238:ARG:O	1:E:242:ILE:HD12	2.10	0.50
1:E:271:SER:OG	1:E:272:ASN:N	2.44	0.50
1:F:271:SER:OG	1:F:272:ASN:N	2.45	0.50
1:I:343:GLY:O	1:I:386:ARG:NE	2.44	0.50
1:J:166:ILE:HG23	1:J:167:LEU:N	2.26	0.50
1:J:195:ASP:OD1	1:J:243:ARG:NH2	2.38	0.50
1:E:295:ASP:OD1	1:E:296:ASP:N	2.45	0.50
1:A:303:LYS:O	1:A:306:ILE:HG22	2.11	0.50
1:B:261:LYS:NZ	1:B:289:GLU:OE2	2.44	0.50
1:B:340:LYS:NZ	1:B:418:ASN:OD1	2.40	0.50
1:C:437:LYS:NZ	1:C:457:VAL:O	2.40	0.50
1:D:204:VAL:HG12	1:D:204:VAL:O	2.11	0.50
1:L:70:LYS:NZ	1:L:166:ILE:O	2.43	0.50
1:L:431:ASP:OD1	1:L:432:SER:N	2.42	0.50
1:F:194:SER:OG	1:F:195:ASP:N	2.44	0.50
1:L:419:GLN:O	1:L:423:ARG:HG3	2.11	0.50
1:J:163:ILE:O	1:J:168:SER:OG	2.25	0.50
1:J:181:PHE:CE1	1:J:185:LEU:HD11	2.43	0.50
1:L:256:MET:O	1:L:260:VAL:HG23	2.12	0.50
1:A:333:ARG:O	1:A:336:GLU:O	2.29	0.49
1:E:350:ASN:OD1	1:E:351:GLN:N	2.40	0.49
1:E:418:ASN:OD1	1:E:419:GLN:N	2.43	0.49
1:G:143:ASP:OD1	1:G:145:ASP:N	2.43	0.49
1:K:80:ASP:OD2	1:K:81:ALA:N	2.45	0.49
1:L:443:LEU:HD13	1:L:447:PHE:CG	2.47	0.49
1:E:323:PRO:O	1:E:327:ILE:HD12	2.12	0.49
1:I:284:ILE:O	1:I:284:ILE:HG13	2.12	0.49
1:L:430:ASN:O	1:L:434:ARG:N	2.46	0.49
1:F:337:LYS:O	1:F:337:LYS:NZ	2.35	0.49
1:F:392:ASP:O	1:F:397:LYS:NZ	2.33	0.49
1:L:383:ASP:OD1	1:L:383:ASP:N	2.45	0.49
1:A:331:THR:HA	1:A:334:ILE:HG22	1.94	0.49
1:J:70:LYS:NZ	1:J:166:ILE:O	2.44	0.49
1:K:414:ALA:CB	1:K:455:LEU:HD11	2.43	0.49
1:L:311:SER:HB2	1:L:349:LEU:HD12	1.93	0.49
1:D:383:ASP:OD1	1:D:384:PHE:N	2.45	0.49
1:I:195:ASP:OD1	1:I:243:ARG:NE	2.45	0.49
1:L:311:SER:CB	1:L:349:LEU:HD12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143:ASP:OD1	1:H:144:GLU:N	2.46	0.49
1:I:177:ILE:HD11	1:I:218:ILE:HD11	1.94	0.49
1:K:369:GLU:OE2	1:K:369:GLU:N	2.38	0.48
1:B:387:ALA:HB2	1:B:419:GLN:NE2	2.28	0.48
1:E:245:MET:HE3	1:E:283:PHE:CE2	2.48	0.48
1:G:57:VAL:HG13	1:G:133:ARG:CG	2.44	0.48
1:K:327:ILE:HG23	1:K:357:PHE:CZ	2.48	0.48
1:K:437:LYS:O	1:K:441:ASN:ND2	2.46	0.48
1:J:231:GLU:N	1:J:231:GLU:OE1	2.46	0.48
1:J:243:ARG:O	1:J:247:LEU:HG	2.13	0.48
1:K:122:SER:O	1:K:126:VAL:HG23	2.14	0.48
1:L:74:LEU:HD21	1:L:172:PHE:O	2.13	0.48
1:L:287:GLU:OE1	1:L:287:GLU:N	2.45	0.48
1:I:319:ILE:HD12	1:I:329:ARG:NH1	2.28	0.48
1:L:27:GLN:HB3	1:L:163:ILE:HD13	1.94	0.48
1:A:431:ASP:OD1	1:A:432:SER:N	2.42	0.48
1:C:237:ASN:O	1:C:241:ASN:ND2	2.44	0.48
1:D:166:ILE:HG23	1:D:167:LEU:N	2.29	0.48
1:E:436:LEU:HD21	1:E:455:LEU:HD13	1.94	0.48
1:J:33:ASP:OD1	1:J:34:ARG:N	2.44	0.48
1:K:318:PHE:CE2	1:K:319:ILE:HG23	2.48	0.48
1:B:67:ILE:CG1	1:B:166:ILE:HD11	2.43	0.48
1:K:449:PHE:HB2	1:K:457:VAL:HG22	1.96	0.48
1:D:77:VAL:HG12	1:D:77:VAL:O	2.13	0.48
1:J:318:PHE:CD2	1:J:319:ILE:HG23	2.49	0.48
1:K:184:ASP:OD2	1:K:205:LYS:NZ	2.42	0.48
1:A:453:ASP:OD1	1:A:454:ASN:ND2	2.47	0.48
1:C:365:GLY:C	1:C:366:LEU:HD12	2.37	0.48
1:E:448:ASP:OD2	1:E:450:SER:OG	2.30	0.48
1:J:238:ARG:CG	1:J:242:ILE:HD11	2.44	0.48
1:L:344:ASP:OD1	1:L:345:ASN:N	2.46	0.48
1:D:63:VAL:HG13	1:D:166:ILE:HD13	1.94	0.47
1:F:412:GLU:N	1:F:412:GLU:OE1	2.46	0.47
1:J:184:ASP:OD1	1:J:205:LYS:NZ	2.45	0.47
1:K:277:ILE:H	1:K:277:ILE:HD12	1.78	0.47
1:G:22:PHE:CD1	1:I:286:MET:SD	3.07	0.47
1:L:296:ASP:OD1	1:L:297:SER:N	2.47	0.47
1:C:219:PHE:CD2	1:C:256:MET:HE2	2.49	0.47
1:F:178:LEU:HD23	1:F:178:LEU:O	2.15	0.47
1:I:58:MET:O	1:I:62:VAL:HG23	2.14	0.47
1:F:166:ILE:HG23	1:F:167:LEU:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:SER:OG	1:A:322:SER:O	2.24	0.47
1:E:334:ILE:HD11	1:E:342:TYR:CD1	2.49	0.47
1:K:386:ARG:H	1:K:386:ARG:HD2	1.80	0.47
1:H:27:GLN:HB3	1:H:163:ILE:HD13	1.96	0.47
1:L:226:SER:O	1:L:238:ARG:NH1	2.47	0.47
1:L:275:ASP:N	1:L:275:ASP:OD1	2.44	0.47
1:E:212:LYS:HD2	1:E:255:ALA:HB2	1.97	0.47
1:A:111:VAL:O	1:A:115:THR:HG22	2.15	0.47
1:K:423:ARG:O	1:K:426:SER:OG	2.13	0.47
1:I:458:ASP:OD1	1:I:459:LYS:N	2.48	0.47
1:L:78:HIS:CG	1:L:173:MET:HE1	2.50	0.47
1:A:448:ASP:O	1:A:451:LYS:NZ	2.48	0.46
1:B:461:ASP:OD2	1:B:462:HIS:ND1	2.47	0.46
1:F:175:GLN:OE1	1:F:175:GLN:N	2.47	0.46
1:A:80:ASP:OD2	1:A:81:ALA:N	2.48	0.46
1:E:403:SER:HG	1:E:406:GLN:CD	2.16	0.46
1:F:326:HIS:O	1:F:330:VAL:HG23	2.15	0.46
1:C:415:ASN:OD1	1:C:454:ASN:ND2	2.47	0.46
1:E:453:ASP:OD1	1:E:453:ASP:N	2.48	0.46
1:K:43:VAL:HG12	1:K:43:VAL:O	2.15	0.46
1:F:327:ILE:HD12	1:F:366:LEU:HD12	1.97	0.46
1:L:403:SER:OG	1:L:404:SER:N	2.48	0.46
1:A:33:ASP:OD1	1:A:34:ARG:N	2.46	0.46
1:A:315:ILE:O	1:A:315:ILE:HG13	2.15	0.46
1:B:89:GLU:OE2	1:B:110:ARG:NH1	2.48	0.46
1:I:177:ILE:HG23	1:I:178:LEU:N	2.31	0.46
1:L:171:PRO:O	1:L:172:PHE:CG	2.68	0.46
1:D:423:ARG:O	1:D:426:SER:N	2.47	0.46
1:F:411:LEU:O	1:F:415:ASN:OD1	2.34	0.46
1:L:277:ILE:HD12	1:L:277:ILE:H	1.81	0.46
1:C:418:ASN:OD1	1:C:419:GLN:N	2.49	0.46
1:B:33:ASP:OD1	1:B:34:ARG:N	2.49	0.46
1:I:216:VAL:HG22	1:I:256:MET:SD	2.56	0.46
1:K:273:ASN:OD1	1:K:274:HIS:N	2.49	0.46
1:L:36:THR:HG21	1:L:167:LEU:HD22	1.97	0.46
1:D:395:ILE:HG22	1:D:399:LEU:CD2	2.45	0.45
1:A:381:SER:O	1:A:417:ASN:ND2	2.50	0.45
1:B:264:THR:O	1:B:268:SER:OG	2.19	0.45
1:D:378:PHE:CG	1:D:378:PHE:O	2.69	0.45
1:L:383:ASP:OD1	1:L:386:ARG:HB2	2.16	0.45
1:A:53:ARG:O	1:A:57:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:TRP:O	1:D:422:TRP:CD1	2.69	0.45
1:K:212:LYS:HD2	1:K:212:LYS:N	2.31	0.45
1:L:375:ILE:HG23	1:L:410:LEU:HD13	1.98	0.45
1:L:395:ILE:HG23	1:L:402:TYR:OH	2.16	0.45
1:E:425:ARG:O	1:E:429:GLY:N	2.50	0.45
1:G:71:LEU:HD22	1:G:87:LEU:HD12	1.99	0.45
1:D:33:ASP:OD1	1:D:34:ARG:N	2.50	0.45
1:E:67:ILE:CG1	1:E:166:ILE:HD11	2.47	0.45
1:K:215:LEU:HD11	1:K:248:ILE:HG23	1.99	0.45
1:C:53:ARG:O	1:C:57:VAL:HG23	2.17	0.44
1:C:256:MET:O	1:C:260:VAL:HG23	2.16	0.44
1:E:260:VAL:HG22	1:E:267:TYR:CD2	2.52	0.44
1:G:22:PHE:HZ	1:I:323:PRO:HG3	1.81	0.44
1:E:296:ASP:O	1:E:299:LYS:N	2.50	0.44
1:F:67:ILE:HG12	1:F:166:ILE:HD11	1.98	0.44
1:J:311:SER:HA	1:J:349:LEU:HD12	2.00	0.44
1:K:411:LEU:O	1:K:415:ASN:ND2	2.50	0.44
1:K:281:ILE:O	1:K:285:SER:N	2.51	0.44
1:D:200:LYS:O	1:D:204:VAL:HG23	2.17	0.44
1:I:309:ASN:OD1	1:I:310:ILE:N	2.48	0.44
1:A:349:LEU:HD23	1:A:350:ASN:N	2.33	0.44
1:D:277:ILE:HG21	1:D:305:ILE:HD12	2.00	0.44
1:F:45:LYS:O	1:F:49:ASN:ND2	2.50	0.44
1:G:57:VAL:HG13	1:G:133:ARG:HG3	2.00	0.44
1:J:326:HIS:O	1:J:330:VAL:HG23	2.18	0.44
1:B:24:LEU:HD22	1:B:44:TYR:CE2	2.52	0.44
1:K:390:TYR:N	1:K:390:TYR:CD2	2.86	0.44
1:B:453:ASP:OD1	1:B:454:ASN:N	2.51	0.44
1:J:212:LYS:HD2	1:J:212:LYS:N	2.33	0.44
1:C:371:ARG:NH1	1:C:401:ASN:O	2.51	0.44
1:I:437:LYS:O	1:I:441:ASN:ND2	2.51	0.44
1:J:399:LEU:HA	1:J:402:TYR:HD2	1.83	0.44
1:A:300:GLU:O	1:A:304:PRO:HD3	2.18	0.43
1:G:21:ILE:HD12	1:G:21:ILE:H	1.82	0.43
1:K:66:ASP:OD2	1:K:167:LEU:HD23	2.17	0.43
1:K:173:MET:HE3	1:K:209:SER:HB2	2.00	0.43
1:K:242:ILE:O	1:K:246:LYS:HG3	2.17	0.43
1:L:172:PHE:HD1	1:L:172:PHE:HA	1.65	0.43
1:B:166:ILE:HG23	1:B:167:LEU:N	2.33	0.43
1:B:387:ALA:HB2	1:B:419:GLN:HE22	1.83	0.43
1:L:388:ASP:OD1	1:L:423:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:417:ASN:OD1	1:I:419:GLN:N	2.51	0.43
1:B:22:PHE:HB2	1:D:27:GLN:HB3	2.01	0.43
1:C:166:ILE:HG23	1:C:167:LEU:N	2.33	0.43
1:J:238:ARG:HG3	1:J:242:ILE:HD11	2.00	0.43
1:K:78:HIS:CE1	1:K:173:MET:HE2	2.54	0.43
1:J:237:ASN:O	1:J:241:ASN:ND2	2.51	0.43
1:E:177:ILE:HD11	1:E:217:LYS:CD	2.49	0.43
1:G:107:LEU:O	1:G:111:VAL:HG23	2.18	0.43
1:B:103:TRP:O	1:B:104:GLU:C	2.62	0.43
1:C:185:LEU:HA	1:C:188:VAL:HG22	2.01	0.43
1:C:433:ILE:O	1:C:434:ARG:C	2.62	0.43
1:I:195:ASP:OD1	1:I:243:ARG:NH2	2.51	0.43
1:J:430:ASN:O	1:J:433:ILE:N	2.51	0.43
1:K:350:ASN:OD1	1:K:350:ASN:C	2.62	0.43
1:A:272:ASN:HA	1:A:277:ILE:HD11	2.01	0.43
1:B:461:ASP:OD2	1:B:462:HIS:N	2.51	0.43
1:E:173:MET:HE2	1:E:210:LEU:CD2	2.49	0.43
1:A:383:ASP:C	1:A:383:ASP:OD1	2.62	0.43
1:C:260:VAL:HG13	1:C:267:TYR:HD1	1.83	0.43
1:D:273:ASN:OD1	1:D:274:HIS:N	2.48	0.43
1:E:306:ILE:HG23	1:E:313:PHE:HD2	1.84	0.43
1:F:173:MET:HA	1:F:175:GLN:OE1	2.19	0.43
1:I:248:ILE:HG22	1:I:256:MET:HE3	2.01	0.43
1:B:415:ASN:OD1	1:B:415:ASN:C	2.60	0.43
1:C:264:THR:O	1:C:264:THR:HG22	2.19	0.43
1:D:271:SER:OG	1:D:272:ASN:N	2.51	0.43
1:I:336:GLU:OE1	1:I:336:GLU:N	2.51	0.43
1:K:271:SER:OG	1:K:272:ASN:N	2.49	0.43
1:E:194:SER:OG	1:E:195:ASP:N	2.50	0.42
1:G:22:PHE:CD2	1:I:286:MET:HG3	2.54	0.42
1:J:252:ASP:OD2	1:J:252:ASP:N	2.52	0.42
1:C:233:LYS:HB3	1:C:234:PRO:HD3	2.01	0.42
1:D:298:VAL:O	1:D:302:ILE:HG13	2.19	0.42
1:D:423:ARG:NH2	1:D:431:ASP:OD2	2.52	0.42
1:K:274:HIS:HD1	1:K:274:HIS:H	1.67	0.42
1:L:378:PHE:CB	1:L:395:ILE:HD11	2.48	0.42
1:C:239:GLU:O	1:C:243:ARG:HG3	2.20	0.42
1:D:166:ILE:HG23	1:D:167:LEU:HG	2.02	0.42
1:D:340:LYS:C	1:D:382:ALA:HB2	2.43	0.42
1:G:17:MET:SD	1:G:17:MET:N	2.92	0.42
1:I:421:TYR:O	1:I:426:SER:OG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:80:ASP:OD1	1:J:81:ALA:N	2.53	0.42
1:J:212:LYS:HD2	1:J:212:LYS:H	1.84	0.42
1:K:21:ILE:HG23	1:K:44:TYR:OH	2.19	0.42
1:L:116:GLN:O	1:L:172:PHE:HD2	2.03	0.42
1:D:318:PHE:CE2	1:D:319:ILE:HG23	2.55	0.42
1:I:301:LEU:HD12	1:I:301:LEU:H	1.85	0.42
1:L:224:LYS:HB2	1:L:266:TYR:OH	2.20	0.42
1:L:297:SER:O	1:L:301:LEU:HG	2.20	0.42
1:E:424:ASN:OD1	1:E:425:ARG:N	2.53	0.42
1:F:166:ILE:CG2	1:F:167:LEU:N	2.82	0.42
1:K:375:ILE:O	1:K:379:ILE:HG23	2.20	0.42
1:E:256:MET:O	1:E:260:VAL:HG23	2.20	0.42
1:E:306:ILE:HG23	1:E:313:PHE:CD2	2.54	0.42
1:F:334:ILE:HD11	1:F:373:PHE:CE1	2.55	0.42
1:J:213:GLU:O	1:J:217:LYS:HG3	2.19	0.42
1:K:277:ILE:O	1:K:281:ILE:HG13	2.20	0.42
1:B:111:VAL:O	1:B:115:THR:OG1	2.37	0.42
1:E:431:ASP:OD1	1:E:432:SER:N	2.51	0.42
1:G:71:LEU:O	1:G:71:LEU:HD23	2.19	0.42
1:I:423:ARG:O	1:I:426:SER:OG	2.28	0.42
1:J:228:ARG:O	1:J:271:SER:OG	2.38	0.42
1:J:245:MET:HA	1:J:248:ILE:HG22	2.01	0.42
1:L:20:ARG:O	1:L:24:LEU:HD13	2.20	0.42
1:L:384:PHE:O	1:L:387:ALA:HB3	2.19	0.42
1:C:453:ASP:OD1	1:C:453:ASP:N	2.52	0.42
1:J:371:ARG:NH1	1:J:401:ASN:O	2.53	0.42
1:J:404:SER:O	1:J:408:LEU:HG	2.20	0.42
1:K:319:ILE:HD12	1:K:329:ARG:CZ	2.50	0.42
1:E:118:LEU:HD23	1:E:122:SER:HB3	2.01	0.41
1:J:172:PHE:C	1:J:173:MET:HG2	2.45	0.41
1:J:288:LYS:NZ	1:J:317:PHE:O	2.39	0.41
1:D:233:LYS:N	1:D:234:PRO:CD	2.83	0.41
1:E:185:LEU:HA	1:E:188:VAL:HG22	2.01	0.41
1:K:303:LYS:HD2	1:K:303:LYS:O	2.20	0.41
1:K:417:ASN:OD1	1:K:419:GLN:N	2.53	0.41
1:B:334:ILE:O	1:B:338:TYR:O	2.38	0.41
1:D:53:ARG:O	1:D:57:VAL:HG23	2.20	0.41
1:E:181:PHE:CE1	1:E:185:LEU:HD11	2.54	0.41
1:E:334:ILE:HD11	1:E:342:TYR:CE1	2.54	0.41
1:K:232:ALA:HA	1:K:235:LEU:HD12	2.01	0.41
1:A:136:SER:O	1:A:147:LEU:HD22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:ALA:O	1:E:421:TYR:HD1	2.03	0.41
1:K:280:LEU:O	1:K:284:ILE:HG12	2.21	0.41
1:K:337:LYS:N	1:K:337:LYS:HD3	2.35	0.41
1:K:449:PHE:CB	1:K:457:VAL:HG22	2.50	0.41
1:L:223:TRP:HA	1:L:245:MET:SD	2.60	0.41
1:B:311:SER:HA	1:B:349:LEU:HD23	2.02	0.41
1:D:318:PHE:CD2	1:D:319:ILE:HG23	2.55	0.41
1:E:43:VAL:HG13	1:E:55:ALA:HB1	2.03	0.41
1:E:452:TYR:HB3	1:E:455:LEU:HD12	2.02	0.41
1:F:457:VAL:HG12	1:F:457:VAL:O	2.21	0.41
1:I:416:LYS:O	1:I:416:LYS:HD3	2.21	0.41
1:J:66:ASP:OD2	1:J:167:LEU:HD23	2.20	0.41
1:K:392:ASP:HA	1:K:396:ASP:HB2	2.02	0.41
1:B:220:LYS:HG2	1:B:266:TYR:CE1	2.56	0.41
1:B:233:LYS:HB3	1:B:234:PRO:HD3	2.02	0.41
1:B:253:ARG:NH2	1:B:287:GLU:OE1	2.54	0.41
1:B:269:ASN:O	1:B:269:ASN:CG	2.64	0.41
1:D:215:LEU:HD12	1:D:215:LEU:H	1.86	0.41
1:F:437:LYS:O	1:F:440:LYS:HG2	2.20	0.41
1:I:211:ASN:O	1:I:215:LEU:HD13	2.20	0.41
1:K:26:SER:O	1:K:29:SER:OG	2.36	0.41
1:L:336:GLU:HG3	1:L:337:LYS:N	2.36	0.41
1:C:311:SER:HA	1:C:349:LEU:HD23	2.03	0.41
1:E:423:ARG:O	1:E:426:SER:N	2.51	0.41
1:F:53:ARG:NH1	1:F:147:LEU:HD22	2.35	0.41
1:I:260:VAL:HG13	1:I:267:TYR:CD2	2.55	0.41
1:J:86:ILE:HG23	1:J:110:ARG:HD2	2.03	0.41
1:J:375:ILE:O	1:J:379:ILE:HG12	2.21	0.41
1:K:436:LEU:HD12	1:K:456:PRO:O	2.21	0.41
1:F:182:VAL:O	1:F:186:GLU:HG3	2.20	0.41
1:J:239:GLU:HA	1:J:242:ILE:HD12	2.01	0.41
1:A:191:LEU:HD21	1:E:204:VAL:HG12	2.03	0.41
1:A:262:ALA:HB3	1:A:263:GLU:OE1	2.21	0.41
1:A:423:ARG:O	1:A:426:SER:N	2.48	0.41
1:A:425:ARG:O	1:A:429:GLY:HA3	2.20	0.41
1:A:428:ASN:ND2	1:E:385:GLU:OE1	2.54	0.41
1:B:77:VAL:O	1:B:77:VAL:HG12	2.20	0.41
1:F:332:LYS:N	1:F:332:LYS:HD3	2.36	0.41
1:G:127:LEU:HD23	1:G:127:LEU:O	2.21	0.41
1:G:150:PRO:HA	1:G:154:MET:SD	2.60	0.41
1:J:407:MET:HE3	1:J:411:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:389:ILE:O	1:L:393:ARG:HG2	2.21	0.41
1:C:299:LYS:O	1:C:303:LYS:HG2	2.21	0.41
1:E:327:ILE:HD12	1:E:327:ILE:H	1.85	0.41
1:E:403:SER:OG	1:E:406:GLN:OE1	2.14	0.41
1:L:212:LYS:N	1:L:212:LYS:HD3	2.36	0.41
1:L:437:LYS:HD3	1:L:437:LYS:HA	1.90	0.41
1:B:22:PHE:HB2	1:D:27:GLN:CB	2.51	0.40
1:E:310:ILE:CD1	1:E:334:ILE:HD13	2.51	0.40
1:J:220:LYS:O	1:J:266:TYR:OH	2.36	0.40
1:L:74:LEU:HD23	1:L:74:LEU:HA	1.96	0.40
1:E:461:ASP:OD1	1:E:462:HIS:N	2.54	0.40
1:I:53:ARG:O	1:I:57:VAL:HG23	2.22	0.40
1:J:67:ILE:CG1	1:J:166:ILE:HD11	2.51	0.40
1:L:277:ILE:HG22	1:L:281:ILE:HD11	2.02	0.40
1:D:215:LEU:HD12	1:D:215:LEU:N	2.36	0.40
1:D:363:GLU:CD	1:K:19:VAL:HG12	2.46	0.40
1:I:166:ILE:HG23	1:I:167:LEU:N	2.37	0.40
1:I:260:VAL:HG22	1:I:267:TYR:HE2	1.80	0.40
1:J:135:LEU:HB3	1:J:148:PHE:CE1	2.56	0.40
1:K:344:ASP:OD2	1:K:345:ASN:N	2.55	0.40
1:L:418:ASN:OD1	1:L:419:GLN:HG2	2.21	0.40
1:A:237:ASN:O	1:A:241:ASN:ND2	2.54	0.40
1:D:367:GLU:O	1:D:370:TYR:N	2.53	0.40
1:F:239:GLU:O	1:F:243:ARG:HG3	2.21	0.40
1:G:53:ARG:O	1:G:57:VAL:HG23	2.21	0.40
1:I:273:ASN:OD1	1:I:273:ASN:C	2.65	0.40
1:J:166:ILE:CG2	1:J:167:LEU:N	2.83	0.40
1:K:118:LEU:HD22	1:K:122:SER:HB3	2.04	0.40
1:L:303:LYS:O	1:L:303:LYS:HD2	2.21	0.40
1:L:352:GLN:O	1:L:356:ILE:HG13	2.21	0.40
1:F:278:LYS:O	1:F:282:GLU:HG3	2.21	0.40
1:I:313:PHE:CD1	1:I:313:PHE:C	2.99	0.40
1:I:415:ASN:OD1	1:I:454:ASN:ND2	2.53	0.40
1:K:309:ASN:OD1	1:K:311:SER:N	2.55	0.40
1:L:223:TRP:CD1	1:L:223:TRP:C	2.99	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	435/460 (95%)	419 (96%)	16 (4%)	0	100	100
1	B	440/460 (96%)	425 (97%)	15 (3%)	0	100	100
1	C	435/460 (95%)	418 (96%)	17 (4%)	0	100	100
1	D	431/460 (94%)	407 (94%)	24 (6%)	0	100	100
1	E	439/460 (95%)	414 (94%)	25 (6%)	0	100	100
1	F	439/460 (95%)	421 (96%)	18 (4%)	0	100	100
1	G	153/460 (33%)	150 (98%)	3 (2%)	0	100	100
1	H	153/460 (33%)	148 (97%)	5 (3%)	0	100	100
1	I	436/460 (95%)	427 (98%)	9 (2%)	0	100	100
1	J	435/460 (95%)	425 (98%)	10 (2%)	0	100	100
1	K	440/460 (96%)	429 (98%)	11 (2%)	0	100	100
1	L	440/460 (96%)	434 (99%)	4 (1%)	2 (0%)	24	55
All	All	4676/5520 (85%)	4517 (97%)	157 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	171	PRO
1	L	172	PHE

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	401/420 (96%)	401 (100%)	0	100	100
1	B	406/420 (97%)	406 (100%)	0	100	100
1	C	401/420 (96%)	401 (100%)	0	100	100
1	D	397/420 (94%)	397 (100%)	0	100	100
1	E	405/420 (96%)	404 (100%)	1 (0%)	87	87
1	F	405/420 (96%)	405 (100%)	0	100	100
1	G	147/420 (35%)	147 (100%)	0	100	100
1	H	147/420 (35%)	147 (100%)	0	100	100
1	I	402/420 (96%)	402 (100%)	0	100	100
1	J	401/420 (96%)	401 (100%)	0	100	100
1	K	406/420 (97%)	406 (100%)	0	100	100
1	L	406/420 (97%)	406 (100%)	0	100	100
All	All	4324/5040 (86%)	4323 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	242	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	138	HIS
1	A	241	ASN
1	A	292	ASN
1	A	347	ASN
1	A	353	HIS
1	A	401	ASN
1	A	415	ASN
1	B	124	HIS
1	B	134	HIS
1	B	237	ASN
1	C	49	ASN
1	C	138	HIS
1	C	196	ASN
1	C	353	HIS
1	D	130	GLN

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Mol	Chain	Res	Type
1	D	347	ASN
1	D	415	ASN
1	D	419	GLN
1	F	49	ASN
1	F	95	ASN
1	F	241	ASN
1	F	326	HIS
1	F	353	HIS
1	G	27	GLN
1	G	124	HIS
1	H	132	HIS
1	I	134	HIS
1	I	138	HIS
1	I	196	ASN
1	I	353	HIS
1	I	454	ASN
1	J	78	HIS
1	J	123	ASN
1	J	328	ASN
1	J	430	ASN
1	K	116	GLN
1	K	132	HIS
1	K	272	ASN
1	K	428	ASN
1	K	441	ASN
1	K	454	ASN
1	L	27	GLN
1	L	132	HIS
1	L	273	ASN
1	L	347	ASN
1	L	380	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 [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 [i](#)

There are no chain breaks in this entry.

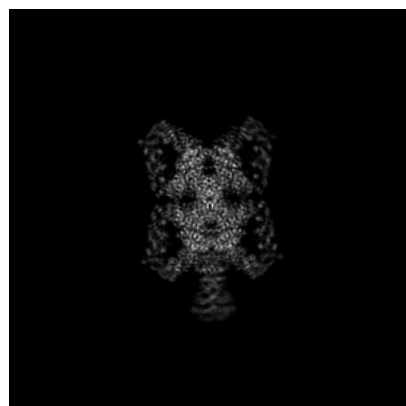
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66345. These allow visual inspection of the internal detail of the map and identification of artifacts.

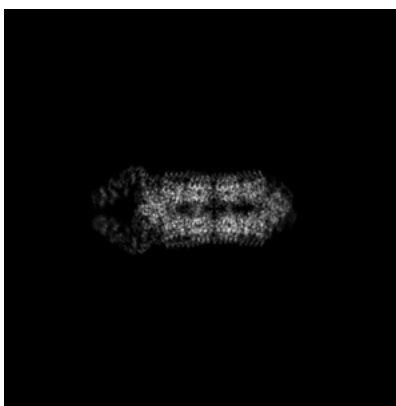
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

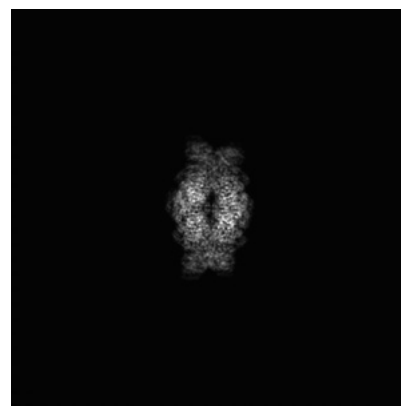
6.1.1 Primary map



X

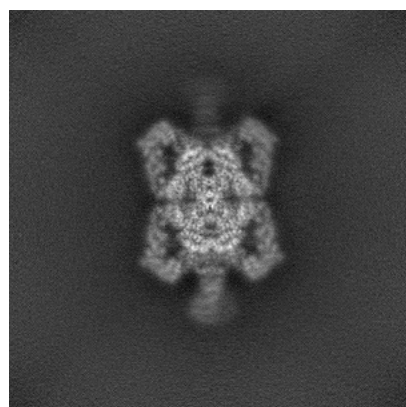


Y

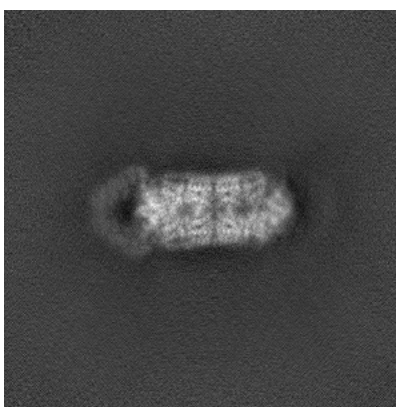


Z

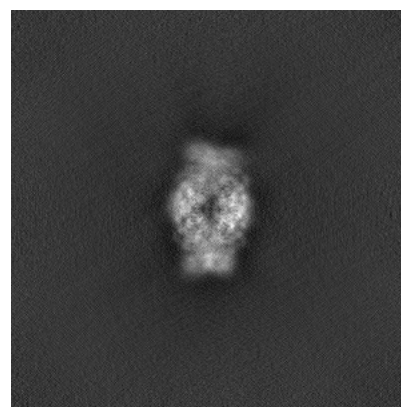
6.1.2 Raw map



X



Y

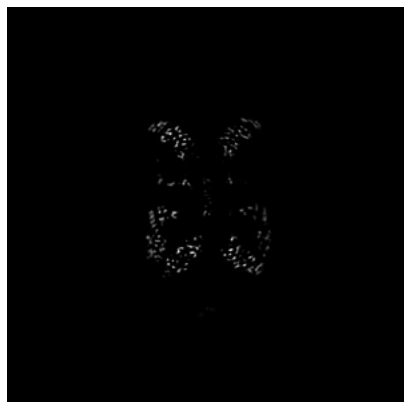


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256

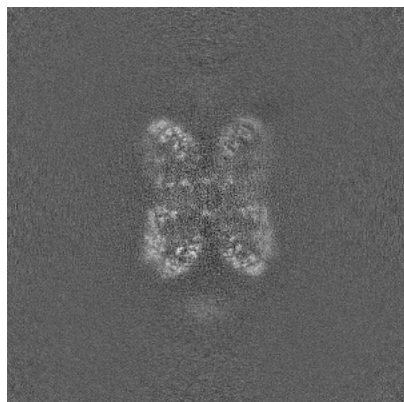


Y Index: 256

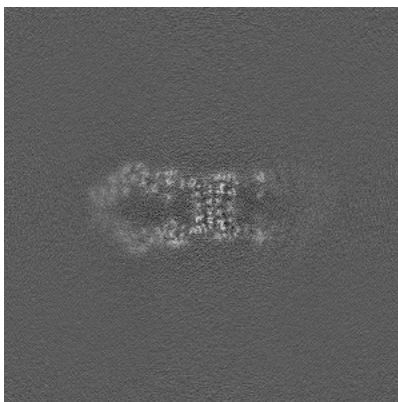


Z Index: 256

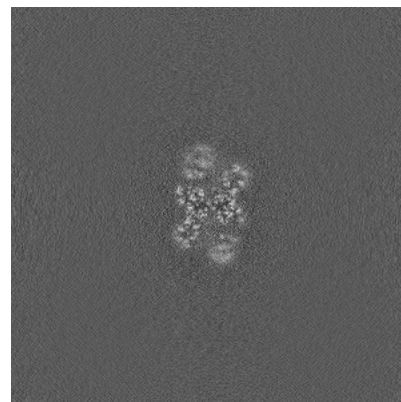
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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

6.3 Largest variance slices [i](#)

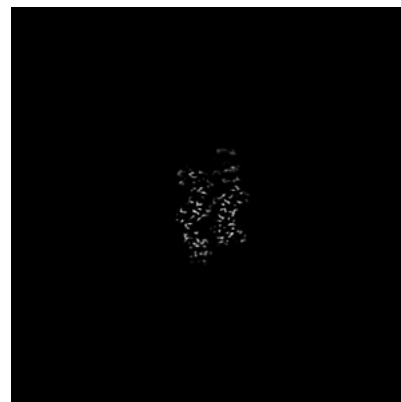
6.3.1 Primary map



X Index: 240

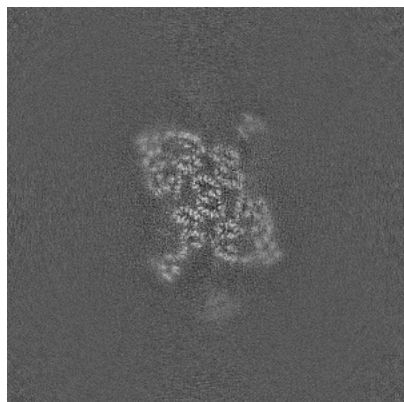


Y Index: 238

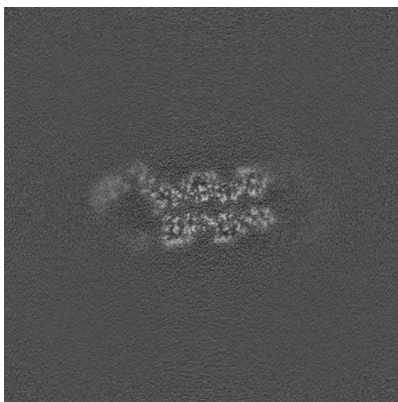


Z Index: 291

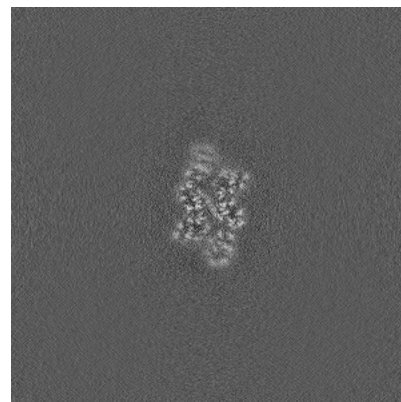
6.3.2 Raw map



X Index: 240



Y Index: 243



Z Index: 246

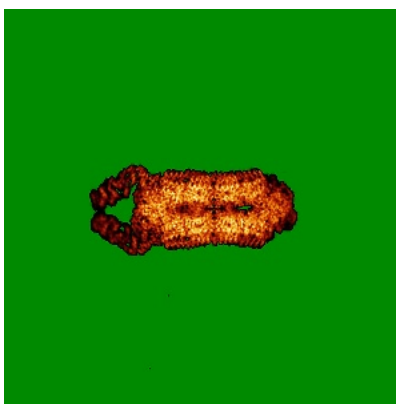
The images above show the largest variance slices of the map in three orthogonal directions.

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

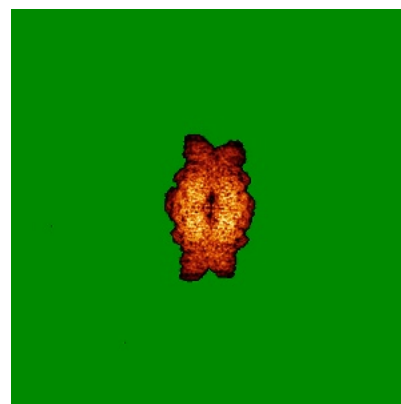
6.4.1 Primary map



X

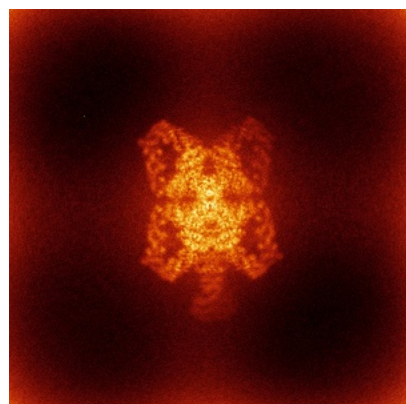


Y

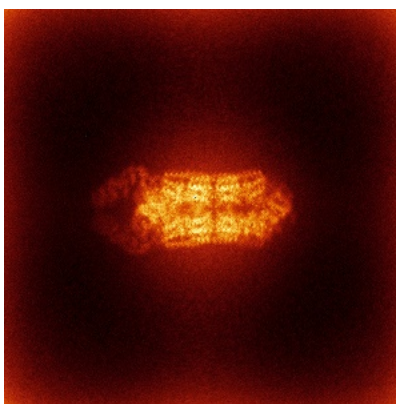


Z

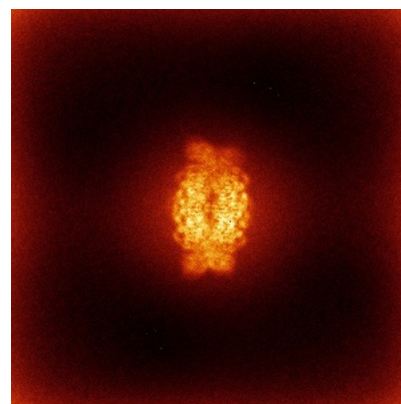
6.4.2 Raw map



X



Y

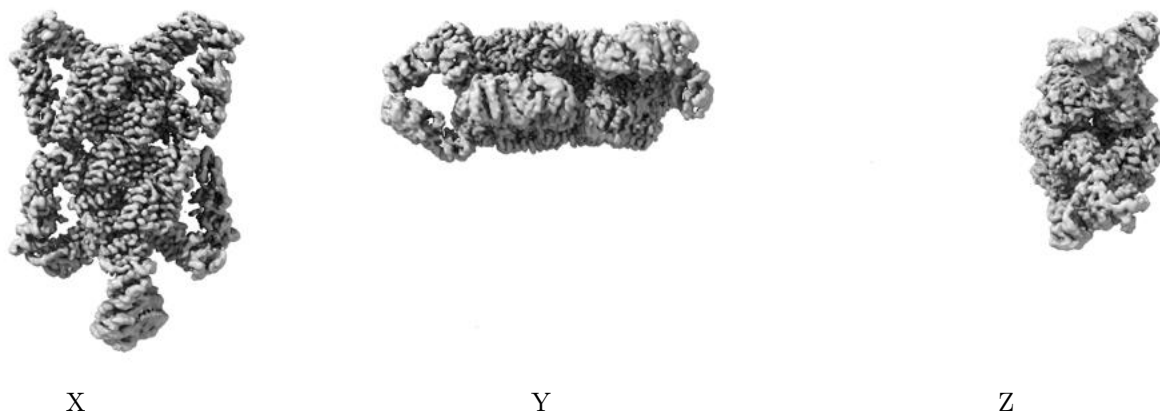


Z

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.

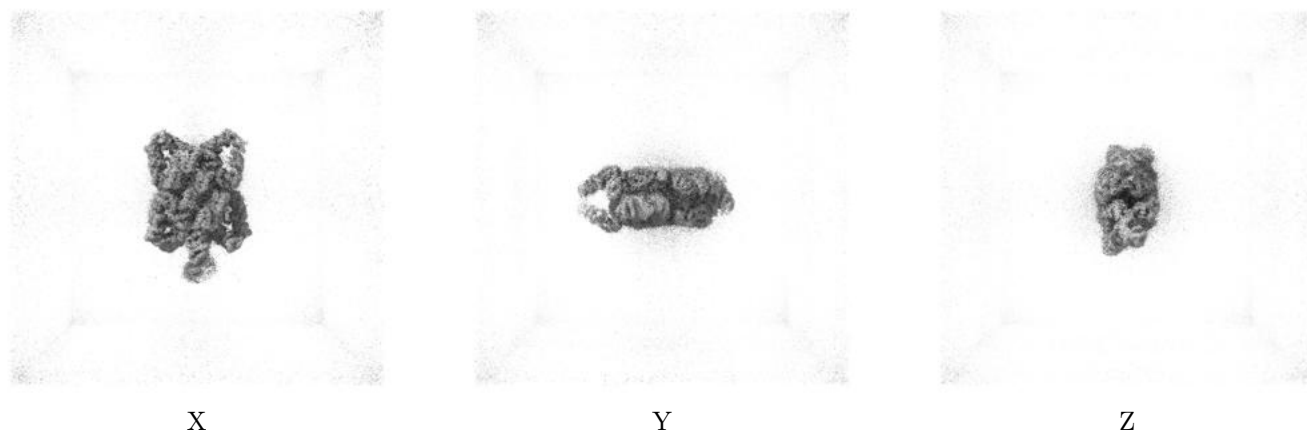
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0225. 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.

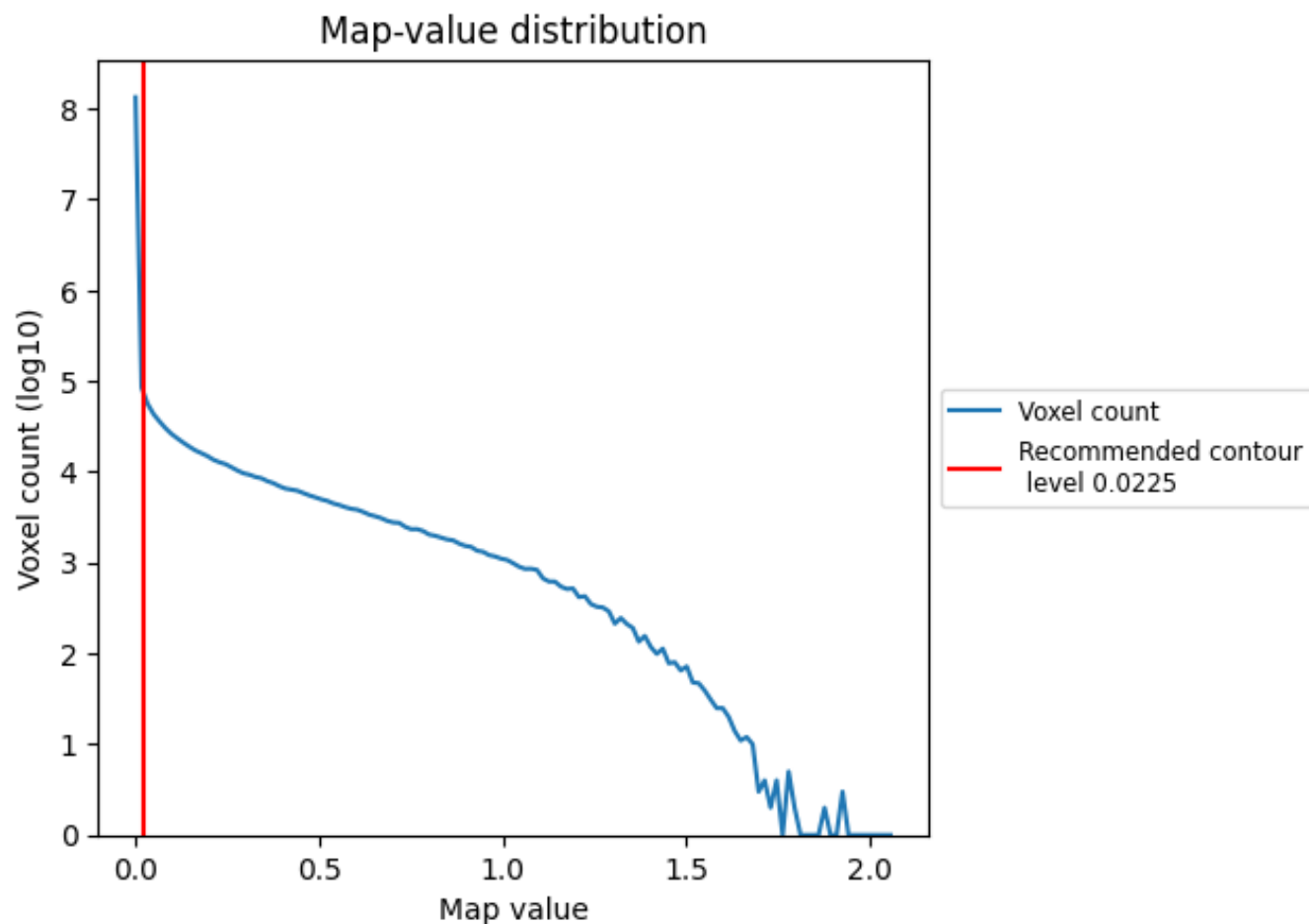
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

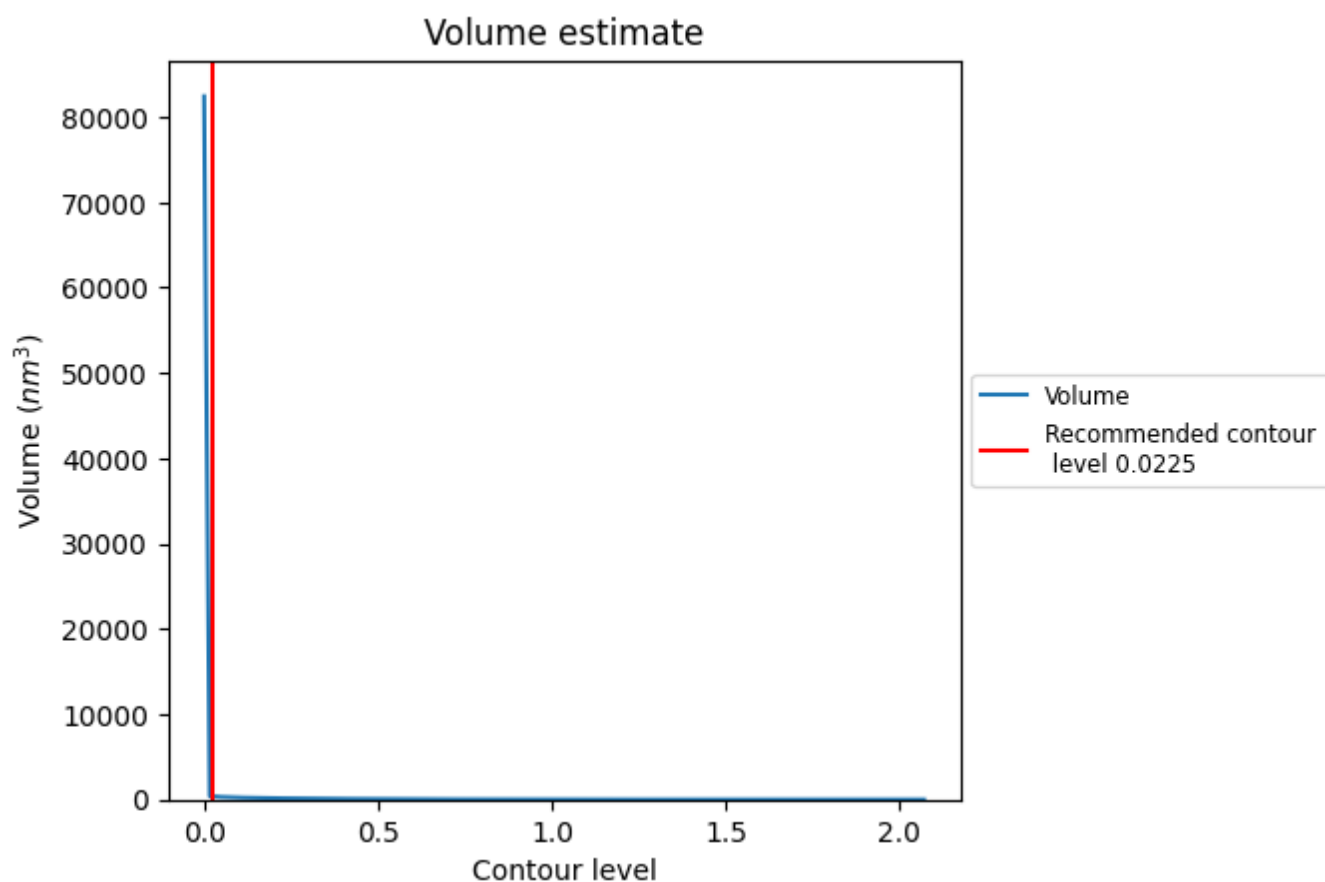
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

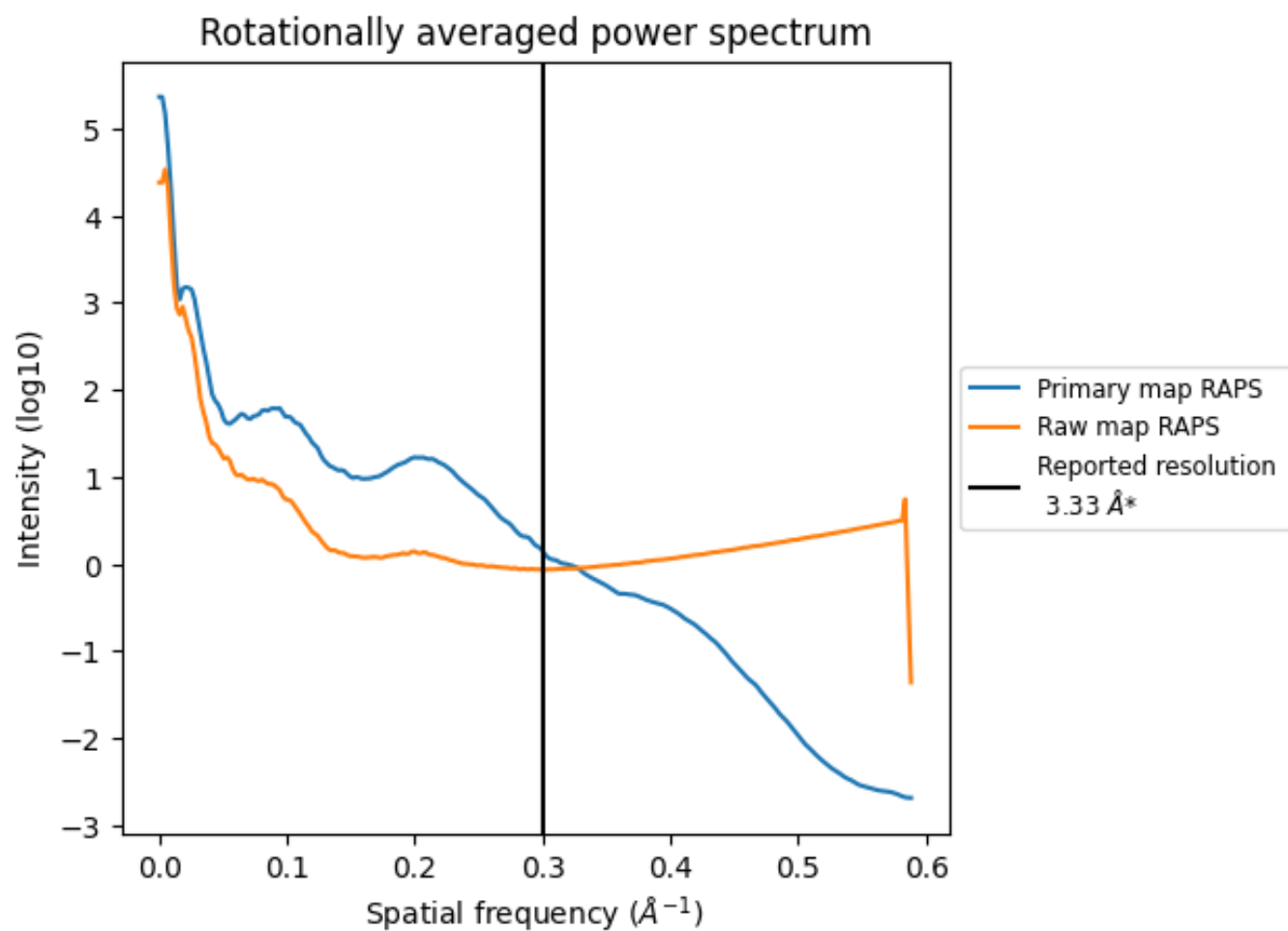
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 367 nm³; this corresponds to an approximate mass of 331 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 ⓘ

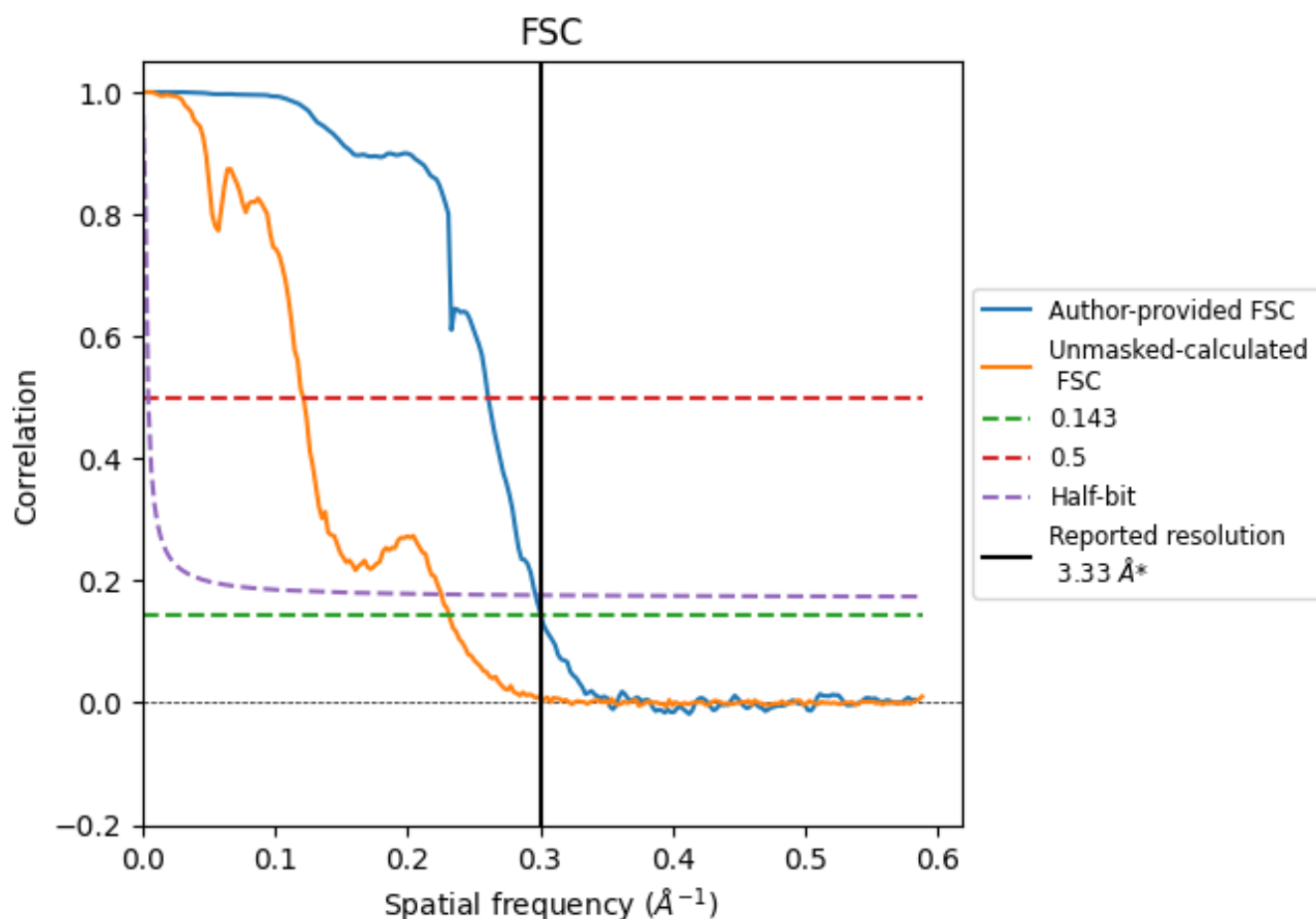


*Reported resolution corresponds to spatial frequency of $0.300 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.300 $\text{\AA}^{-1}$

8.2 Resolution estimates

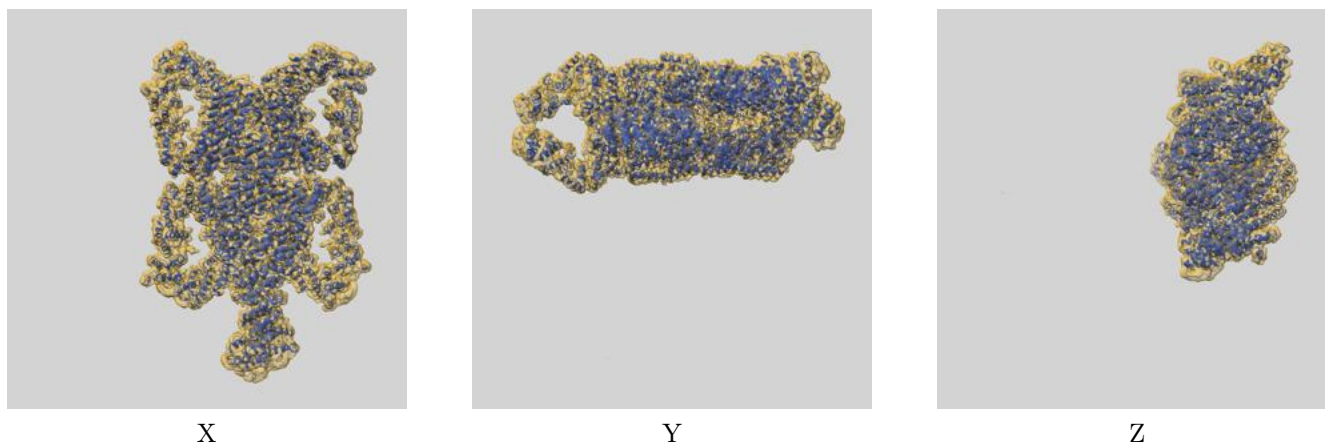
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.33	3.83	3.37
Unmasked-calculated*	4.32	8.23	4.43

*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 4.32 differs from the reported value 3.33 by more than 10 %

9 Map-model fit [i](#)

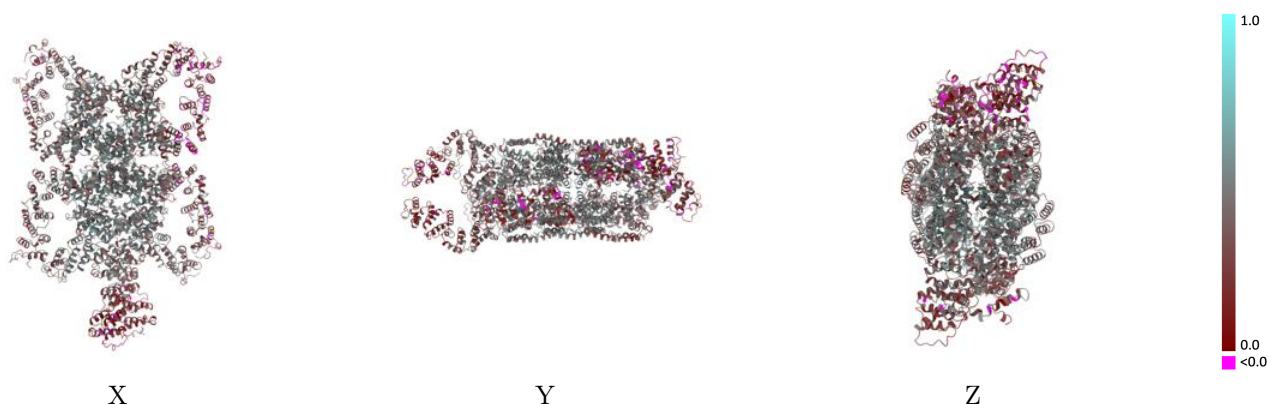
This section contains information regarding the fit between EMDB map EMD-66345 and PDB model 9WXF. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



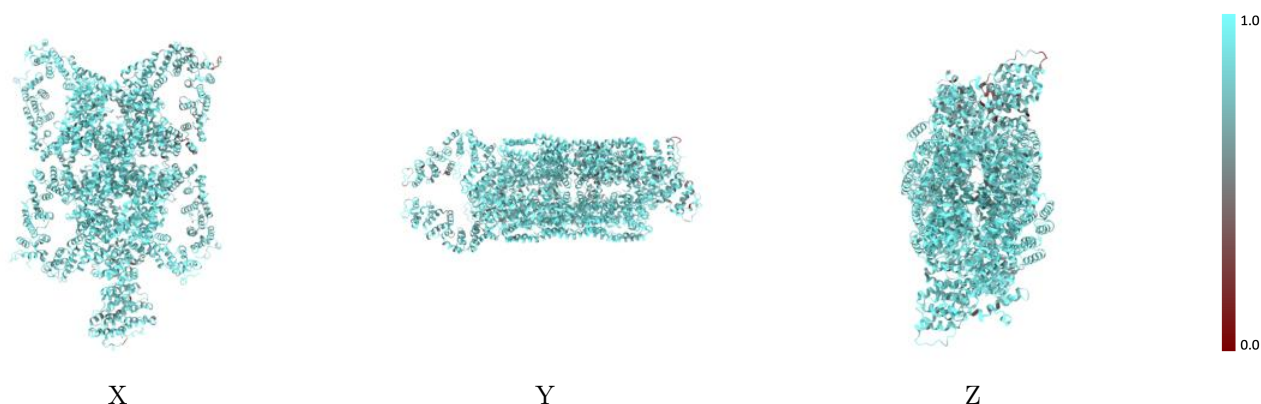
The images above show the 3D surface view of the map at the recommended contour level 0.0225 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



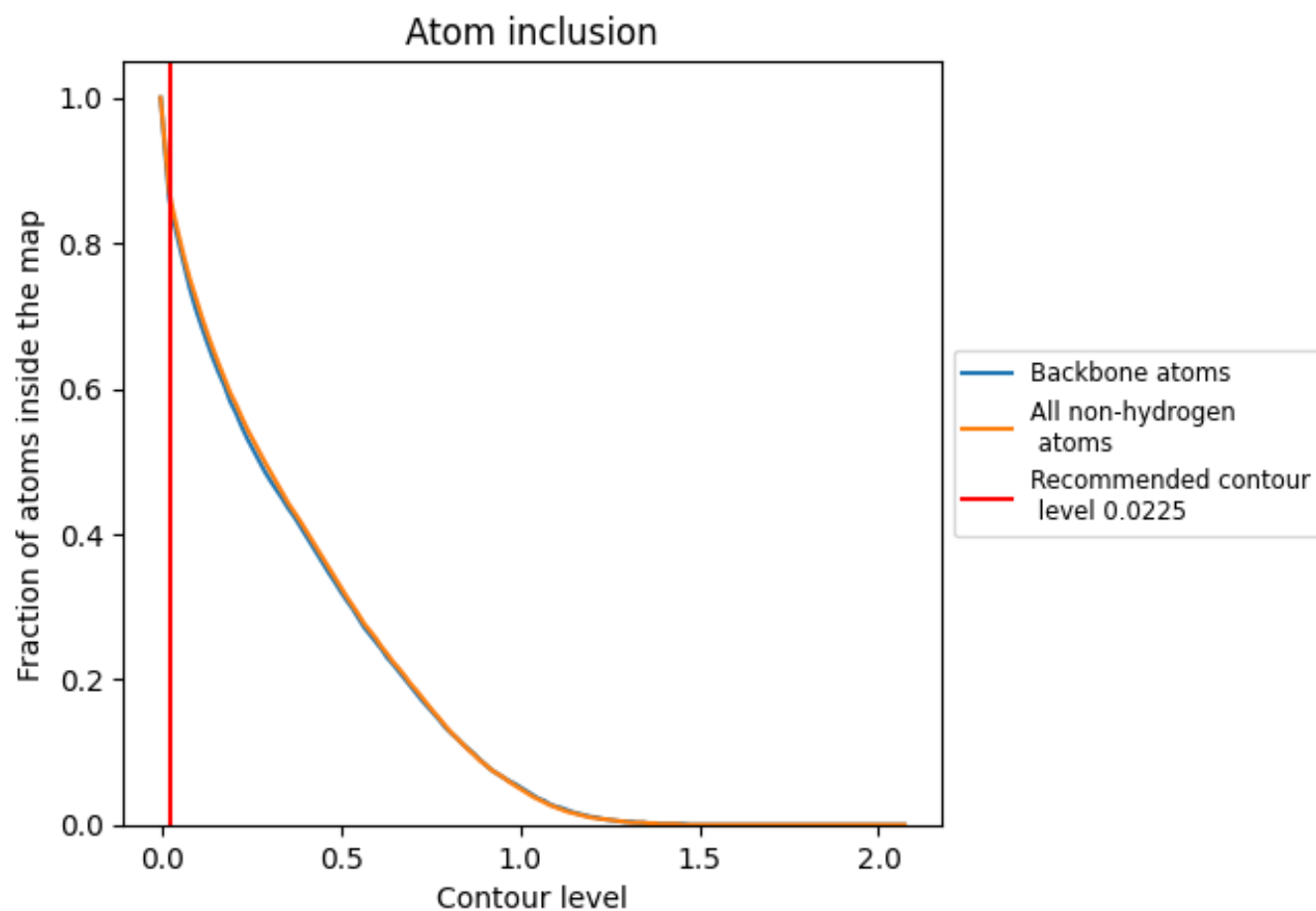
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0225).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 87% 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 (0.0225) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.3870
A	0.8770	0.3870
B	0.9100	0.4560
C	0.8840	0.4030
D	0.9140	0.4580
E	0.9100	0.4400
F	0.8490	0.3340
G	0.8790	0.3890
H	0.9130	0.4400
I	0.8590	0.3860
J	0.7990	0.3050
K	0.8600	0.3410
L	0.8650	0.3370

1.0

0.0

<0.0