



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 04:58 PM EDT

PDB ID : 7RDX / pdb_00007rdx
EMDB ID : EMD-24426
Title : SARS-CoV-2 replication-transcription complex bound to nsp13 helicase -
nsp13(2)-RTC - open class
Authors : Chen, J.; Malone, B.; Campbell, E.A.; Darst, S.A.
Deposited on : 2021-07-12
Resolution : 3.10 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:

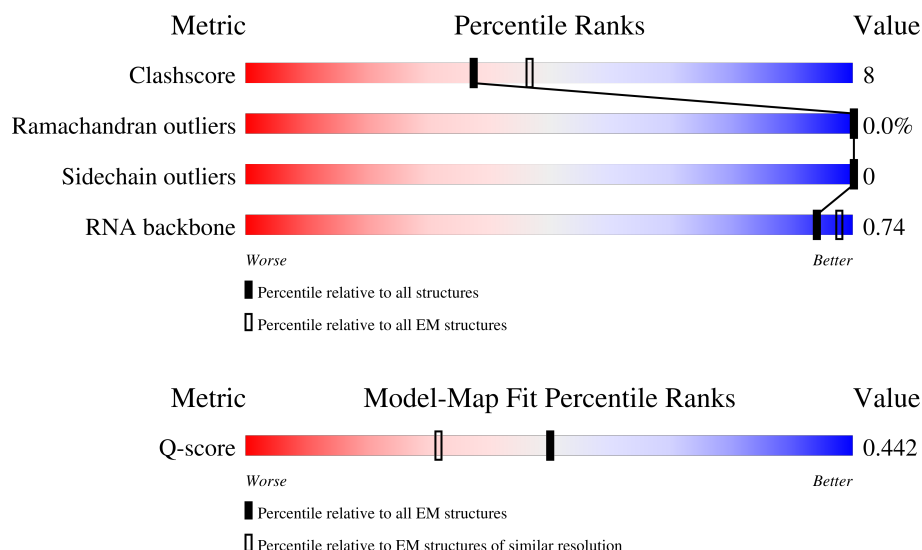
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	932	 86% 14%
2	B	199	 81% 12% 7%
2	D	199	 82% 11% 7%

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Mol	Chain	Length	Quality of chain
3	C	88	75% 10% 15%
4	E	605	10% 75% 23%
4	F	605	45% 81% 16%
5	P	35	74% 17% 6%
6	T	55	38% 38% 7% 16%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 42468 atoms, of which 20640 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	927	Total	C	H	N	O	S	0	0
			14676	4770	7206	1253	1393	54		

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	186	Total	C	H	N	O	S	0	0
			2823	884	1415	241	272	11		
2	D	185	Total	C	H	N	O	S	0	0
			2846	889	1431	242	273	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P0DTD1
D	0	MET	-	initiating methionine	UNP P0DTD1

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	75	Total	C	H	N	O	S	0	0
			1182	362	606	94	113	7		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP P0DTD1
C	-3	PRO	-	expression tag	UNP P0DTD1
C	-2	VAL	-	expression tag	UNP P0DTD1
C	-1	ASP	-	expression tag	UNP P0DTD1
C	0	MET	-	expression tag	UNP P0DTD1

- Molecule 4 is a protein called Helicase.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	590	Total	C	H	N	O	S	0	0
			8971	2861	4464	761	851	34		
4	F	590	Total	C	H	N	O	S	0	0
			9074	2896	4517	771	856	34		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP P0DTD1
E	-2	PRO	-	expression tag	UNP P0DTD1
E	-1	HIS	-	expression tag	UNP P0DTD1
E	0	MET	-	expression tag	UNP P0DTD1
F	-3	GLY	-	expression tag	UNP P0DTD1
F	-2	PRO	-	expression tag	UNP P0DTD1
F	-1	HIS	-	expression tag	UNP P0DTD1
F	0	MET	-	expression tag	UNP P0DTD1

- Molecule 5 is a RNA chain called Product RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	P	34	Total	C	H	N	O	P	0	0
			1085	322	366	125	238	34		

- Molecule 6 is a RNA chain called Template RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	T	46	Total	C	H	N	O	P	0	0
			1470	438	491	171	324	46		

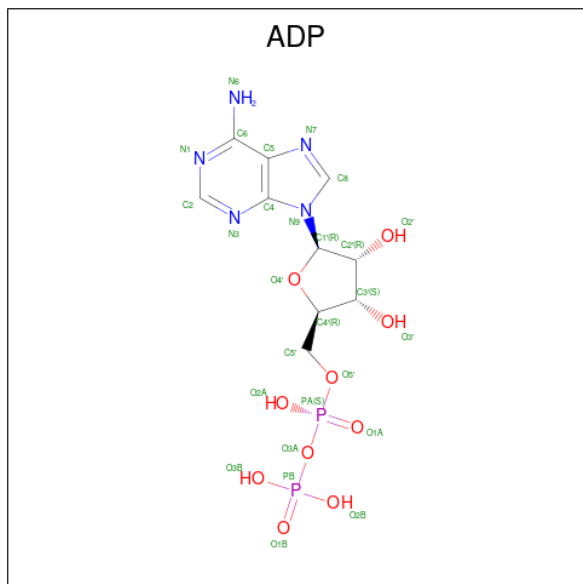
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Zn	0
			2	2	
7	E	3	Total	Zn	0
			3	3	
7	F	3	Total	Zn	0
			3	3	

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

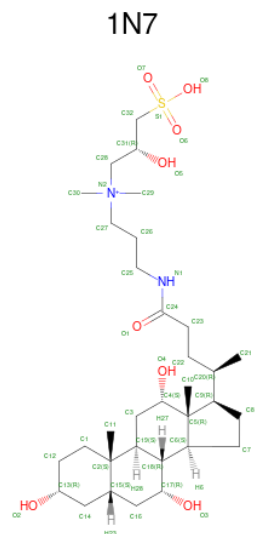
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total Mg 1 1	0
8	E	1	Total Mg 1 1	0
8	F	1	Total Mg 1 1	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



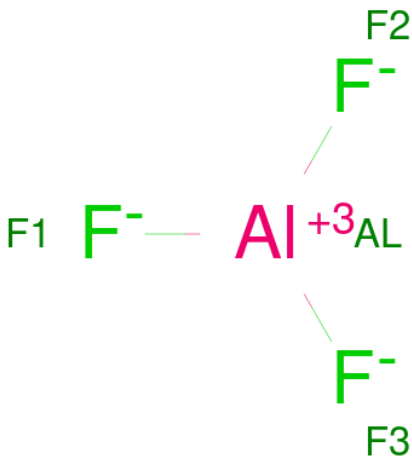
Mol	Chain	Residues	Atoms						AltConf
9	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
9	E	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
9	F	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 10 is CHAPSO (CCD ID: 1N7) (formula: $\text{C}_{32}\text{H}_{59}\text{N}_2\text{O}_8\text{S}$).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total 75	C 29	H 40	N 2	O 4	0
10	A	1	Total 52	C 23	H 26	O 3		0
10	E	1	Total 78	C 30	H 42	N 2	O 4	0

- Molecule 11 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			AltConf
11	E	1	Total 4	Al 1	F 3	0

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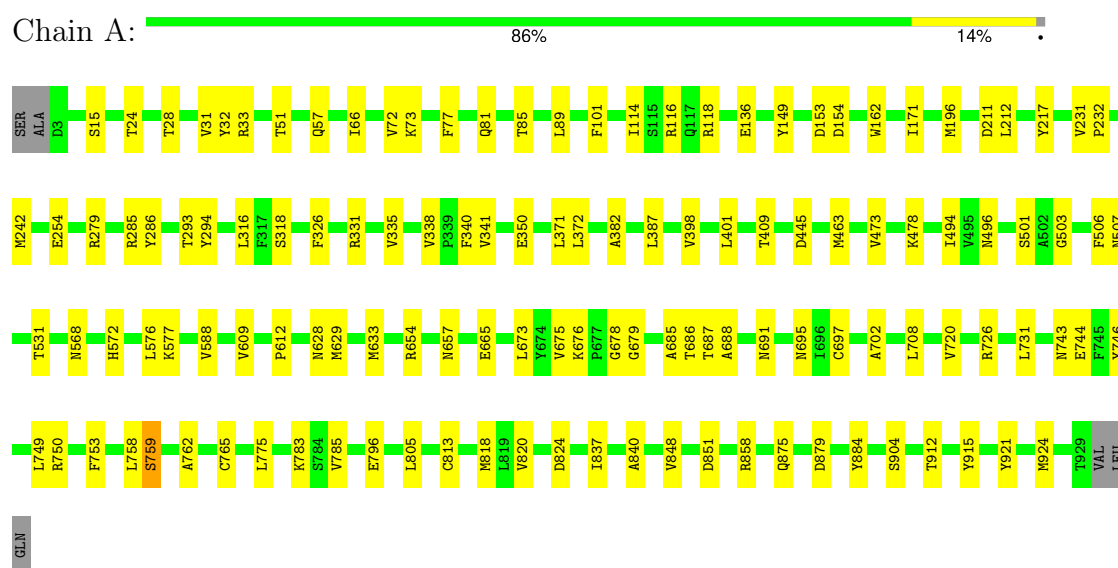
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Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
11	F	1	4	1	3	0

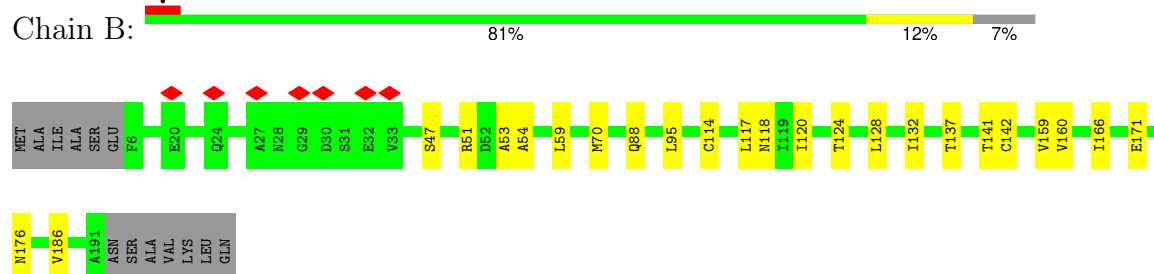
3 Residue-property plots

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.

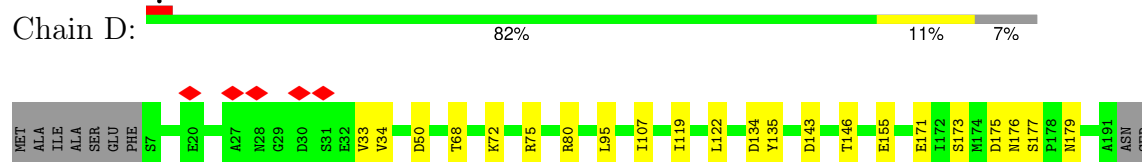
• Molecule 1: RNA-directed RNA polymerase



• Molecule 2: Non-structural protein 8



• Molecule 2: Non-structural protein 8



ALA
VAL
LYS
LEU
GLN

• Molecule 3: Non-structural protein 7

Chain C: 

GLY
PRO
VAL
ASP
MET
S1
L14
L20
E23
H36
L40
E50
S54
V58
A65
H75
LEU
ASP
ASN
ARG
ALA
THR
LEU
GLN

• Molecule 4: Helicase

Chain E: 

GLY
PRO
HIS
MET
A1
C5
V6
L7
T12
T12
A18
L25
C26
C27
C28
C29
H39
G54
D59
V60
T61
I79
T115
I116
A117
Y120
I121
C126
T127
E128
K131
L132
L138
L147
S148
Y149
G150
V154
R155
E156
V157
L158
S159
D160
R161
E162

L163
H164
L165
S166
V167
G170
K171
P172
L176
N177
R178
N179
Y180
G184
Y185
R186
V187
T188
K189
N190
S191
K192
V193
Q194
I195
G196
E197
F200
E201
K202
G203
D204
Y205
G206
D207
A208
V209
V210
V211
R212
G213
T214
T215
T216
Y217
K218
L219
N220
V221
G222
D223
Y224
F225
T228

L235
L240
V241
L249
T255
L256
N257
S259
D260
E261
Q270
L280
Q281
G282
T283
T286
G287
K288
S289
H290
A296
F300
R303
I304
V305
Y306
T307
A308
V314
A321
L325
D328
K329
R332
I333
R339
K347
T351
Q354
Y355

C358
T359
E365
I370
V371
E375
I376
K388
A389
R390
I399
G400
D401
P402
A403
L405
P406
R409
K414
Y421
F422
V425
C426
R427
L428
M429
K430
T431
L438
C441
R442
R443
A446
E447
H554
I448
V449
D450
T451
V452
V456
Y457
L461
K462
A463
H464

K485
M474
T480
T481
H482
D483
S486
V495
E498
T501
R502
A505
W506
R507
K508
A509
Y515
Q518
N519
A522
S523
L526
G527
P529
T530
T549
T550
E551
T552
A553
S555
R560
F561
N562
V563
M576
D583
R584
L585
Q586
F587
L590

GLU
ILE
PRO
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MET
ASN
VAL
ALA
THR
LEU
GLN

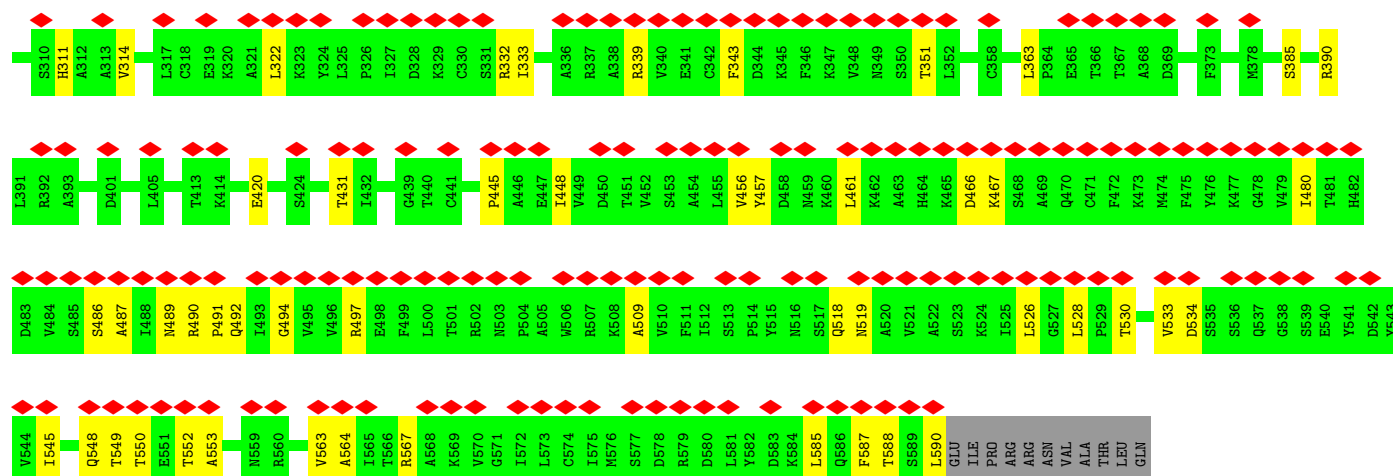
• Molecule 4: Helicase

Chain F: 

GLY
PRO
HIS
MET
A1
C5
V6
L7
T12
R15
R21
F24
L25
C26
C29
C30
V34
T37
K40
S80
F81
L92
T96
D105
F106
N107
T111
E136
K146
Y149
G150
I151
A152
T153
V154
R155
E156
V157
L158
S159
D160
R161
E162

L163
H164
L165
S166
V167
E168
V169
G170
K171
P172
R173
P174
P175
L176
N177
R178
N179
T183
G184
Y185
R186
V187
T188
K189
N190
S191
K192
V193
Q194
I195
G196
E197
Y198
E201
K202
G203
D204
Y205
G206
D207
A208
V209
V210
Y211
R212
G213
T214
T215
T216
Y217
K218
L219
N220
V221
G222
D223
Y224
F225

V226
L227
T228
S229
H230
T231
V232
L235
S236
P242
Q243
E244
H245
Y246
V247
R248
I249
T250
G251
L252
Y253
P254
T255
L256
H257
I258
S259
D260
E261
F262
G263
S264
R265
V266
A267
V272
G273
H274
L280
Q281
G282
P283
T286
G287
K288
A292
L295
A296
L297
S301
A302
R303



- Molecule 5: Product RNA

Chain P: 74% 17% 6% •



- Molecule 6: Template RNA

Chain T: 38% 38% 7% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105272	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.538	Depositor
Minimum map value	-2.297	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 1N7, ADP, AF3, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/7659	0.33	0/10394
2	B	0.17	0/1427	0.34	0/1937
2	D	0.17	0/1434	0.32	0/1943
3	C	0.23	0/579	0.31	0/779
4	E	0.15	0/4605	0.33	0/6275
4	F	0.13	0/4659	0.33	0/6344
5	P	0.15	0/802	0.24	0/1246
6	T	0.16	0/1094	0.28	0/1702
All	All	0.19	0/22259	0.32	0/30620

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	759	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7470	7206	7206	99	0
2	B	1408	1415	1407	22	0
2	D	1415	1431	1431	16	0
3	C	576	606	608	7	0
4	E	4507	4464	4429	99	0
4	F	4557	4517	4503	71	0
5	P	719	366	366	13	0
6	T	979	491	492	12	0
7	A	2	0	0	0	0
7	E	3	0	0	0	0
7	F	3	0	0	0	0
8	A	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	A	27	12	12	2	0
9	E	27	12	12	2	0
9	F	27	12	12	1	0
10	A	61	66	86	1	0
10	E	36	42	52	2	0
11	E	4	0	0	1	0
11	F	4	0	0	1	0
All	All	21828	20640	20616	319	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 8.

All (319) 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:77:PHE:HE1	1:A:81:GLN:HE21	1.19	0.90
4:E:328:ASP:O	4:E:347:LYS:NZ	2.07	0.87
4:F:519:ASN:OD1	4:F:530:THR:OG1	1.93	0.86
5:P:25:C:O2	6:T:31:G:N2	2.10	0.83
4:E:303:ARG:NH2	4:E:351:THR:O	2.11	0.83
4:F:332:ARG:NH1	4:F:333:ILE:O	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ILE:O	2:B:124:THR:OG1	2.01	0.78
4:E:300:PRO:O	4:E:354:GLN:NE2	2.18	0.77
4:E:282:GLY:O	4:E:288:LYS:NZ	2.16	0.76
4:E:438:LEU:HD12	4:E:438:LEU:O	1.87	0.75
4:E:176:LEU:HD22	4:E:201:GLU:HB3	1.69	0.74
2:D:176:ASN:OD1	2:D:179:ASN:ND2	2.20	0.74
4:E:332:ARG:NH1	4:E:333:ILE:O	2.21	0.74
1:A:387:LEU:HD23	2:B:128:LEU:HD12	1.69	0.74
4:F:489:ASN:O	4:F:518:GLN:NE2	2.21	0.74
4:F:420:GLU:OE2	4:F:431:THR:OG1	2.05	0.74
4:E:286:THR:N	9:E:704:ADP:O1B	2.21	0.74
4:E:443:ARG:NH2	9:E:704:ADP:O1A	2.22	0.73
4:E:185:TYR:O	4:E:187:VAL:HG13	1.88	0.73
4:E:448:ILE:O	4:E:451:THR:OG1	2.04	0.72
1:A:676:LYS:NZ	1:A:678:GLY:O	2.23	0.72
1:A:242:MET:SD	1:A:463:MET:HE2	2.30	0.71
1:A:720:VAL:HG11	1:A:775:LEU:HD23	1.73	0.70
1:A:758:LEU:HD23	1:A:813:CYS:SG	2.32	0.70
4:F:159:SER:OG	4:F:162:GLU:O	2.10	0.70
2:D:50:ASP:OD2	5:P:19:A:O2'	2.09	0.70
1:A:409:THR:OG1	3:C:23:GLU:OE2	2.09	0.70
1:A:915:TYR:O	1:A:921:TYR:OH	2.06	0.69
3:C:54:SER:HB2	2:D:122:LEU:HD21	1.75	0.68
4:E:328:ASP:OD1	4:E:329:LYS:N	2.26	0.67
4:E:441:CYS:HB2	4:E:449:VAL:HG21	1.77	0.67
4:E:228:THR:HG22	4:E:228:THR:O	1.94	0.66
3:C:50:GLU:HG2	2:D:122:LEU:HD22	1.77	0.66
4:F:7:LEU:HD21	4:F:29:CYS:SG	2.36	0.66
4:F:585:LEU:O	4:F:585:LEU:HD12	1.97	0.65
4:F:322:LEU:HD11	4:F:343:PHE:CZ	2.32	0.65
2:D:134:ASP:OD1	2:D:135:TYR:N	2.31	0.64
4:E:200:PHE:HB3	4:E:209:VAL:HG21	1.77	0.64
4:E:26:CYS:SG	4:E:27:CYS:N	2.71	0.64
4:F:322:LEU:HD11	4:F:343:PHE:HZ	1.63	0.63
1:A:340:PHE:CE1	2:B:95:LEU:HD11	2.33	0.63
4:F:248:ARG:NH1	4:F:249:ILE:O	2.31	0.62
4:E:201:GLU:C	4:E:209:VAL:HG23	2.25	0.62
1:A:612:PRO:CG	1:A:805:LEU:HD11	2.28	0.61
4:F:363:LEU:O	4:F:390:ARG:NH1	2.33	0.61
4:F:549:THR:HG22	4:F:550:THR:HG23	1.81	0.61
1:A:478:LYS:NZ	1:A:743:ASN:OD1	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:451:THR:HG22	4:E:586:GLN:H	1.64	0.61
4:E:554:HIS:O	4:E:560:ARG:NE	2.33	0.60
4:E:296:ALA:HB2	4:E:306:TYR:OH	2.02	0.60
1:A:568:ASN:OD1	1:A:654:ARG:NH2	2.34	0.60
1:A:72:VAL:HG12	1:A:72:VAL:O	2.02	0.60
1:A:875:GLN:NE2	1:A:879:ASP:OD1	2.35	0.59
4:F:7:LEU:H	4:F:7:LEU:HD23	1.67	0.59
4:F:96:THR:O	4:F:96:THR:HG22	2.02	0.59
4:E:376:ILE:HD11	4:E:429:MET:HE1	1.83	0.59
1:A:676:LYS:NZ	1:A:679:GLY:O	2.33	0.59
4:E:163:LEU:N	4:E:209:VAL:O	2.34	0.58
4:E:501:THR:O	4:E:507:ARG:NH2	2.36	0.58
4:E:240:LEU:HD21	4:E:425:VAL:HG22	1.86	0.58
4:E:375:GLU:OE2	11:E:706:AF3:F3	2.12	0.58
1:A:340:PHE:HE1	2:B:95:LEU:HD11	1.67	0.58
4:E:214:THR:O	4:E:214:THR:HG22	2.03	0.57
1:A:57:GLN:NE2	1:A:66:ILE:O	2.36	0.57
1:A:912:THR:O	1:A:912:THR:HG22	2.05	0.57
1:A:335:VAL:O	1:A:338:VAL:HG12	2.05	0.57
4:F:563:VAL:O	4:F:567:ARG:NH1	2.38	0.56
1:A:473:VAL:HG22	1:A:633:MET:SD	2.45	0.56
4:E:365:GLU:OE2	4:E:390:ARG:NH1	2.38	0.56
4:F:258:ILE:HG23	4:F:259:SER:N	2.20	0.56
2:B:159:VAL:HG22	2:B:186:VAL:HG12	1.86	0.56
4:E:5:CYS:SG	4:E:26:CYS:N	2.79	0.56
2:D:175:ASP:OD1	2:D:176:ASN:N	2.38	0.56
4:E:376:ILE:HD11	4:E:429:MET:CE	2.36	0.56
4:E:147:LEU:HD12	4:E:147:LEU:O	2.05	0.56
4:F:235:LEU:HD23	4:F:235:LEU:H	1.71	0.56
1:A:840:ALA:O	1:A:858:ARG:NH2	2.37	0.55
4:E:154:VAL:HG21	4:E:163:LEU:HD11	1.87	0.55
1:A:254:GLU:OE1	1:A:285:ARG:NH2	2.39	0.55
2:B:171:GLU:O	2:B:176:ASN:ND2	2.40	0.55
4:E:447:GLU:O	4:E:451:THR:HG23	2.07	0.55
4:E:515:TYR:O	4:E:519:ASN:ND2	2.40	0.55
4:E:456:VAL:HG23	4:E:457:TYR:CD2	2.42	0.55
4:E:409:ARG:NH2	4:E:422:PHE:O	2.40	0.55
4:E:576:MET:HE1	4:E:585:LEU:HD21	1.89	0.54
1:A:331:ARG:NH2	2:B:114:CYS:SG	2.81	0.54
2:D:173:SER:O	2:D:177:SER:N	2.41	0.54
4:F:518:GLN:OE1	4:F:549:THR:OG1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1006:1N7:H5	10:A:1006:1N7:H31	1.90	0.53
1:A:503:GLY:O	1:A:507:ASN:ND2	2.40	0.53
6:T:9:A:O2'	6:T:10:U:O5'	2.21	0.53
4:E:18:ALA:HB3	4:E:39:HIS:CG	2.43	0.53
4:E:280:LEU:HB3	4:E:399:ILE:HG22	1.90	0.53
1:A:904:SER:CB	10:E:707:1N7:H51	2.38	0.53
4:F:80:SER:HB3	4:F:81:PHE:HB3	1.91	0.53
4:F:492:GLN:NE2	4:F:548:GLN:O	2.42	0.53
1:A:326:PHE:O	2:B:118:ASN:ND2	2.42	0.53
4:F:105:ASP:OD1	4:F:106:PHE:N	2.42	0.53
1:A:116:ARG:NH2	9:A:1004:ADP:O3B	2.40	0.52
1:A:341:VAL:HG13	1:A:341:VAL:O	2.10	0.52
1:A:629:MET:HE3	1:A:629:MET:HA	1.90	0.52
4:E:59:ASP:OD1	4:E:61:THR:HG22	2.10	0.52
1:A:445:ASP:OD1	1:A:445:ASP:N	2.43	0.52
2:D:155:GLU:OE1	2:D:155:GLU:HA	2.10	0.52
1:A:904:SER:HB3	10:E:707:1N7:H53	1.92	0.52
1:A:686:THR:HG23	1:A:686:THR:O	2.10	0.52
4:E:154:VAL:HG21	4:E:163:LEU:CD1	2.40	0.52
1:A:77:PHE:CE1	1:A:81:GLN:NE2	2.67	0.51
4:E:441:CYS:CB	4:E:449:VAL:HG21	2.40	0.51
1:A:691:ASN:HB3	1:A:759:SER:O	2.09	0.51
1:A:858:ARG:NH1	5:P:32:G:OP1	2.43	0.51
4:E:165:LEU:HD21	4:E:167:TRP:NE1	2.24	0.51
4:E:121:ILE:HG22	4:E:421:TYR:CD2	2.45	0.51
4:F:228:THR:HG23	4:F:228:THR:O	2.10	0.51
1:A:28:THR:HG21	1:A:51:THR:O	2.12	0.50
2:B:59:LEU:C	2:B:59:LEU:HD23	2.37	0.50
4:E:79:ILE:HG23	4:E:79:ILE:O	2.11	0.50
4:E:456:VAL:HG21	4:E:562:ASN:ND2	2.26	0.50
4:F:480:ILE:HD13	4:F:550:THR:HG22	1.94	0.50
4:F:107:ASN:O	4:F:111:THR:HG22	2.11	0.50
4:F:178:ARG:NH2	4:F:534:ASP:O	2.44	0.50
1:A:279:ARG:NH1	1:A:318:SER:OG	2.42	0.50
2:B:53:ALA:O	2:B:54:ALA:HB3	2.11	0.50
1:A:720:VAL:HG11	1:A:775:LEU:CD2	2.42	0.49
4:E:120:TYR:CE2	4:E:138:LEU:HD11	2.46	0.49
1:A:28:THR:HG21	1:A:51:THR:C	2.36	0.49
1:A:350:GLU:OE1	1:A:628:ASN:ND2	2.46	0.49
4:E:554:HIS:O	4:E:560:ARG:NH2	2.45	0.49
4:F:283:PRO:HB2	4:F:461:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:37:THR:O	4:F:40:LYS:NZ	2.45	0.49
4:F:311:HIS:HA	4:F:314:VAL:HG12	1.93	0.49
1:A:372:LEU:HD12	1:A:506:PHE:CE1	2.48	0.49
2:B:159:VAL:HG13	2:B:186:VAL:HG12	1.95	0.49
4:F:585:LEU:HD13	4:F:587:PHE:CE2	2.48	0.49
6:T:37:U:C2	6:T:38:G:C8	3.01	0.48
4:F:5:CYS:SG	4:F:26:CYS:N	2.86	0.48
4:F:272:VAL:HG11	4:F:295:LEU:HD21	1.94	0.48
4:E:126:CYS:O	4:E:131:LYS:NZ	2.45	0.48
4:E:296:ALA:HB1	4:E:355:TYR:HE1	1.79	0.48
1:A:572:HIS:HB3	1:A:576:LEU:HD13	1.96	0.48
1:A:629:MET:HE3	1:A:629:MET:CA	2.44	0.48
4:E:449:VAL:HG11	4:E:463:ALA:HB2	1.95	0.48
1:A:851:ASP:OD1	2:D:75:ARG:NH2	2.44	0.47
4:F:214:THR:OG1	4:F:339:ARG:O	2.29	0.47
1:A:116:ARG:NH1	9:A:1004:ADP:O3B	2.46	0.47
1:A:612:PRO:CB	1:A:805:LEU:HD11	2.44	0.47
1:A:695:ASN:HD21	1:A:762:ALA:HB2	1.78	0.47
1:A:749:LEU:O	1:A:753:PHE:N	2.45	0.47
4:E:321:ALA:O	4:E:325:LEU:N	2.38	0.47
9:F:1003:ADP:O3B	11:F:1005:AF3:F1	2.23	0.47
1:A:77:PHE:HE1	1:A:81:GLN:NE2	2.00	0.47
1:A:531:THR:O	1:A:657:ASN:ND2	2.47	0.47
4:E:260:ASP:OD1	4:E:261:GLU:N	2.47	0.47
4:F:489:ASN:HB2	4:F:549:THR:HG23	1.97	0.47
4:E:451:THR:HG21	4:E:587:PHE:CE1	2.50	0.47
4:E:249:ILE:HD11	4:E:270:GLN:NE2	2.29	0.47
4:E:449:VAL:HA	4:E:452:VAL:HG12	1.97	0.47
5:P:24:C:O2'	5:P:25:C:P	2.72	0.47
4:E:148:SER:OG	4:E:149:TYR:N	2.48	0.47
4:E:518:GLN:OE1	4:E:549:THR:OG1	2.23	0.47
4:F:303:ARG:NH2	4:F:351:THR:O	2.47	0.47
4:E:308:ALA:HB3	4:E:314:VAL:HG13	1.97	0.46
4:E:507:ARG:O	4:E:528:LEU:HD21	2.15	0.46
4:F:258:ILE:HD11	4:F:297:LEU:HB3	1.97	0.46
5:P:24:C:HO2'	5:P:25:C:P	2.38	0.46
1:A:162:TRP:O	1:A:171:ILE:HD13	2.16	0.46
2:B:137:THR:O	2:B:141:THR:HG22	2.16	0.46
2:D:95:LEU:HD21	2:D:107:ILE:HD11	1.98	0.46
4:E:116:ASN:OD1	4:E:117:ALA:N	2.44	0.46
4:E:576:MET:HE1	4:E:585:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ARG:NH2	1:A:744:GLU:OE2	2.47	0.46
3:C:14:LEU:HD22	3:C:36:HIS:CG	2.51	0.46
4:E:228:THR:O	4:E:228:THR:CG2	2.64	0.46
4:E:464:HIS:O	4:E:465:LYS:HG3	2.15	0.46
4:F:509:ALA:HB1	4:F:545:ILE:HG12	1.98	0.46
1:A:231:VAL:HG13	1:A:231:VAL:O	2.16	0.46
4:E:255:THR:HG22	4:E:256:LEU:N	2.30	0.46
4:F:448:ILE:HG22	4:F:587:PHE:CE1	2.50	0.46
4:E:509:ALA:O	4:E:528:LEU:HD22	2.16	0.46
4:F:158:LEU:HB2	4:F:163:LEU:HD13	1.98	0.46
4:F:588:THR:HG22	4:F:590:LEU:H	1.80	0.45
3:C:58:VAL:HG22	2:D:119:ILE:HG12	1.97	0.45
1:A:316:LEU:HD22	1:A:463:MET:SD	2.56	0.45
4:E:446:ALA:HA	4:E:449:VAL:HG12	1.99	0.45
4:F:552:THR:OG1	4:F:553:ALA:N	2.49	0.45
1:A:149:TYR:HE2	1:A:212:LEU:HD13	1.81	0.45
4:E:249:ILE:HD11	4:E:270:GLN:HE22	1.81	0.45
4:E:358:CYS:SG	4:E:359:THR:N	2.89	0.45
4:F:212:ARG:NH1	4:F:339:ARG:O	2.49	0.45
4:F:255:THR:HG21	4:F:258:ILE:HD13	1.99	0.45
4:F:274:MET:HA	4:F:274:MET:HE2	1.99	0.45
1:A:496:ASN:OD1	1:A:496:ASN:C	2.60	0.45
1:A:665:GLU:OE1	1:A:665:GLU:N	2.50	0.45
4:E:449:VAL:HG22	4:E:461:LEU:HD22	1.97	0.45
4:F:216:THR:HG22	4:F:216:THR:O	2.17	0.45
1:A:494:ILE:HD11	1:A:577:LYS:HE2	1.99	0.45
4:F:456:VAL:HG23	4:F:457:TYR:N	2.32	0.45
4:F:466:ASP:OD1	4:F:467:LYS:N	2.49	0.45
4:F:283:PRO:O	4:F:286:THR:HG23	2.17	0.45
1:A:15:SER:OG	1:A:118:ARG:NH2	2.49	0.45
1:A:824:ASP:OD1	1:A:824:ASP:N	2.49	0.45
4:E:12:THR:HG21	4:E:25:LEU:O	2.17	0.45
4:E:474:MET:HE1	4:E:495:VAL:HG11	1.98	0.45
6:T:14:A:HO2'	6:T:15:U:P	2.40	0.45
4:F:192:LYS:O	4:F:192:LYS:HG2	2.17	0.44
1:A:338:VAL:CG2	2:B:95:LEU:HD13	2.48	0.44
1:A:293:THR:HG22	1:A:294:TYR:N	2.33	0.44
1:A:775:LEU:N	1:A:775:LEU:HD12	2.32	0.44
4:E:7:LEU:HD11	4:E:29:CYS:SG	2.58	0.44
4:F:486:SER:OG	4:F:487:ALA:N	2.50	0.44
2:B:160:VAL:HG12	2:B:166:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:15:ARG:HE	4:F:24:PHE:HE1	1.66	0.44
1:A:338:VAL:HG22	2:B:95:LEU:HD13	1.99	0.44
1:A:72:VAL:O	1:A:73:LYS:C	2.61	0.44
1:A:382:ALA:HB3	2:B:117:LEU:HD11	2.00	0.44
1:A:501:SER:OG	6:T:19:A:OP1	2.21	0.44
4:F:258:ILE:HG23	4:F:259:SER:H	1.82	0.44
1:A:702:ALA:HA	1:A:785:VAL:HG21	2.00	0.43
2:D:171:GLU:O	2:D:176:ASN:ND2	2.51	0.43
4:E:176:LEU:HD13	4:E:200:PHE:C	2.43	0.43
2:B:141:THR:HG23	2:B:142:CYS:N	2.33	0.43
4:E:474:MET:HE1	4:E:495:VAL:CG1	2.48	0.43
1:A:31:VAL:HG22	1:A:32:TYR:N	2.34	0.43
1:A:153:ASP:O	1:A:154:ASP:HB3	2.19	0.43
1:A:211:ASP:OD2	1:A:211:ASP:C	2.61	0.43
2:B:59:LEU:HD12	4:F:80:SER:HB2	2.00	0.43
4:E:405:LEU:HD23	4:E:563:VAL:HG11	2.01	0.43
5:P:25:C:N3	6:T:31:G:N1	2.48	0.43
4:F:80:SER:HB3	4:F:81:PHE:CA	2.49	0.43
4:F:247:VAL:HG23	4:F:248:ARG:N	2.33	0.43
5:P:26:U:C2	5:P:27:A:C8	3.06	0.43
1:A:116:ARG:HG2	1:A:217:TYR:HB2	2.01	0.43
1:A:848:VAL:HG11	2:D:80:ARG:CZ	2.49	0.43
4:F:12:THR:OG1	4:F:25:LEU:O	2.29	0.43
1:A:149:TYR:CE2	1:A:212:LEU:HD13	2.53	0.43
1:A:335:VAL:O	1:A:335:VAL:HG23	2.19	0.43
4:E:304:ILE:HG12	4:E:370:ILE:CG2	2.48	0.43
4:F:445:PRO:HD2	4:F:448:ILE:HD11	2.01	0.43
4:F:526:LEU:HD13	4:F:528:LEU:HG	2.00	0.43
1:A:401:LEU:HD11	1:A:673:LEU:HD11	2.00	0.43
4:E:283:PRO:CB	4:E:461:LEU:HD12	2.49	0.43
4:E:371:VAL:O	4:E:371:VAL:HG13	2.18	0.43
4:F:494:GLY:HA2	4:F:497:ARG:NH1	2.34	0.43
1:A:154:ASP:OD1	1:A:154:ASP:O	2.38	0.42
1:A:568:ASN:HB3	1:A:685:ALA:HB3	2.01	0.42
4:E:241:VAL:HG13	4:E:388:ASN:OD1	2.18	0.42
4:E:259:SER:OG	4:E:260:ASP:N	2.52	0.42
4:F:136:GLU:HB2	4:F:235:LEU:HD22	2.01	0.42
1:A:136:GLU:OE1	1:A:783:LYS:NZ	2.44	0.42
1:A:85:THR:O	1:A:89:LEU:HD13	2.20	0.42
4:F:80:SER:HB3	4:F:81:PHE:HA	2.01	0.42
4:F:192:LYS:O	4:F:192:LYS:CG	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:25:C:H2'	5:P:26:U:O4'	2.18	0.42
6:T:42:U:C2	6:T:43:A:C8	3.07	0.42
1:A:837:ILE:HG22	1:A:884:TYR:CE2	2.54	0.42
4:F:533:VAL:HG23	4:F:564:ALA:HB2	2.01	0.42
1:A:708:LEU:HD11	1:A:731:LEU:HD12	2.01	0.42
4:E:165:LEU:HD21	4:E:167:TRP:HE1	1.84	0.42
4:E:401:ASP:OD2	4:E:403:ALA:HB3	2.19	0.42
3:C:20:LEU:HD13	3:C:65:ALA:HB1	2.02	0.42
5:P:24:C:C2	5:P:25:C:C5	3.08	0.42
1:A:77:PHE:CD1	1:A:81:GLN:NE2	2.85	0.42
4:F:21:ARG:NE	4:F:136:GLU:OE2	2.40	0.42
2:D:33:VAL:HG13	2:D:34:VAL:N	2.35	0.42
4:E:115:THR:HG22	4:E:414:LYS:HE2	2.02	0.42
1:A:31:VAL:HG21	1:A:33:ARG:NH2	2.35	0.42
4:F:490:ARG:N	4:F:491:PRO:HD2	2.35	0.42
1:A:612:PRO:HB2	1:A:805:LEU:HD11	2.02	0.41
2:B:132:ILE:HD11	2:B:142:CYS:SG	2.60	0.41
4:E:132:LEU:HB3	4:E:235:LEU:HD11	2.02	0.41
4:E:150:GLY:N	4:E:172:PRO:O	2.54	0.41
4:E:515:TYR:OH	4:E:552:THR:HG21	2.21	0.41
6:T:47:U:C2	6:T:48:G:C8	3.08	0.41
2:D:68:THR:O	2:D:72:LYS:HG2	2.21	0.41
4:F:232:VAL:O	4:F:232:VAL:HG13	2.19	0.41
1:A:796:GLU:O	1:A:796:GLU:CD	2.64	0.41
2:D:143:ASP:O	2:D:146:THR:OG1	2.37	0.41
4:E:287:GLY:HA3	4:E:290:HIS:CE1	2.56	0.41
1:A:254:GLU:OE2	1:A:286:TYR:OH	2.28	0.41
1:A:633:MET:HE2	1:A:697:CYS:SG	2.61	0.41
1:A:746:TYR:CZ	1:A:750:ARG:HD2	2.55	0.41
5:P:24:C:C2'	5:P:25:C:O5'	2.69	0.41
6:T:45:C:C2	6:T:46:A:C8	3.09	0.41
5:P:10:U:C2	5:P:11:G:C8	3.08	0.41
1:A:101:PHE:CD2	1:A:114:ILE:HG22	2.56	0.41
3:C:36:HIS:CE1	3:C:40:LEU:HD11	2.56	0.41
4:E:154:VAL:O	4:E:154:VAL:HG13	2.21	0.41
4:E:304:ILE:HD12	4:E:355:TYR:CE1	2.56	0.41
4:F:152:ALA:O	4:F:225:PHE:N	2.51	0.41
6:T:33:A:C4	6:T:34:G:C8	3.09	0.41
1:A:196:MET:HE2	1:A:232:PRO:HB3	2.01	0.41
2:B:70:MET:HG2	4:F:92:LEU:HD21	2.02	0.41
4:E:235:LEU:HD12	4:E:235:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:405:LEU:HD12	4:E:406:PRO:O	2.21	0.41
4:E:480:ILE:CD1	4:E:550:THR:HG22	2.51	0.41
4:F:235:LEU:HD12	4:F:385:SER:CB	2.51	0.41
1:A:609:VAL:HG21	1:A:765:CYS:O	2.21	0.41
2:B:47:SER:O	2:B:51:ARG:N	2.53	0.41
4:E:287:GLY:HA3	4:E:290:HIS:HE1	1.86	0.41
4:E:555:SER:O	4:E:561:PHE:CZ	2.73	0.41
5:P:25:C:H2'	5:P:26:U:H6	1.84	0.41
6:T:50:U:H2'	6:T:51:A:H8	1.86	0.41
4:E:188:THR:O	4:E:189:LYS:HB2	2.21	0.41
4:E:258:ILE:HG23	4:E:259:SER:N	2.36	0.41
4:F:30:CYS:O	4:F:34:VAL:HG22	2.21	0.41
5:P:24:C:O2'	5:P:25:C:OP1	2.38	0.40
4:E:177:ASN:O	4:E:180:TYR:N	2.50	0.40
4:E:427:ARG:O	4:E:431:THR:OG1	2.31	0.40
1:A:24:THR:O	1:A:24:THR:OG1	2.39	0.40
1:A:588:VAL:HG23	1:A:588:VAL:O	2.21	0.40
1:A:818:MET:HE3	1:A:820:VAL:HG11	2.04	0.40
1:A:924:MET:HE2	1:A:924:MET:HB2	1.99	0.40
4:E:127:THR:HG22	4:E:128:GLU:N	2.37	0.40
4:F:162:GLU:C	4:F:163:LEU:HD22	2.45	0.40
4:F:448:ILE:HG22	4:F:587:PHE:CZ	2.56	0.40
6:T:40:C:C2	6:T:41:G:C8	3.09	0.40
1:A:371:LEU:HD21	2:B:88:GLN:HG3	2.03	0.40
1:A:398:VAL:HG23	1:A:675:VAL:HG23	2.03	0.40
1:A:687:THR:HG23	1:A:688:ALA:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	925/932 (99%)	873 (94%)	52 (6%)	0	100	100
2	B	184/199 (92%)	181 (98%)	3 (2%)	0	100	100
2	D	183/199 (92%)	178 (97%)	5 (3%)	0	100	100
3	C	73/88 (83%)	73 (100%)	0	0	100	100
4	E	588/605 (97%)	537 (91%)	50 (8%)	1 (0%)	43	73
4	F	588/605 (97%)	538 (92%)	50 (8%)	0	100	100
All	All	2541/2628 (97%)	2380 (94%)	160 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	189	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	819/823 (100%)	819 (100%)	0	100	100
2	B	149/168 (89%)	149 (100%)	0	100	100
2	D	152/168 (90%)	152 (100%)	0	100	100
3	C	70/81 (86%)	70 (100%)	0	100	100
4	E	494/526 (94%)	494 (100%)	0	100	100
4	F	504/526 (96%)	504 (100%)	0	100	100
All	All	2188/2292 (96%)	2188 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	113	HIS

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Mol	Chain	Res	Type
1	A	468	GLN
1	A	541	GLN
2	D	19	GLN
4	E	275	GLN
4	E	470	GLN
4	E	554	HIS
4	F	124	ASN
4	F	190	ASN
4	F	349	ASN
4	F	503	ASN
4	F	516	ASN
4	F	554	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	P	33/35 (94%)	1 (3%)	1 (3%)
6	T	46/55 (83%)	8 (17%)	2 (4%)
All	All	79/90 (87%)	9 (11%)	3 (3%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	P	25	C
6	T	10	U
6	T	12	U
6	T	13	G
6	T	14	A
6	T	15	U
6	T	16	U
6	T	17	U
6	T	18	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	P	24	C
6	T	9	A
6	T	13	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ADP	E	704	11,8	28,29,29	1.41	4 (14%)	43,45,45	1.91	9 (20%)
10	1N7	A	1005	-	38,38,46	2.91	21 (55%)	58,58,72	2.68	26 (44%)
11	AF3	E	706	9	0,3,3	-	-	-	-	-
10	1N7	A	1006	-	29,29,46	2.73	16 (55%)	47,47,72	2.24	16 (34%)
9	ADP	F	1003	8	28,29,29	1.41	4 (14%)	43,45,45	1.89	10 (23%)
9	ADP	A	1004	8	28,29,29	1.35	4 (14%)	43,45,45	1.85	10 (23%)
11	AF3	F	1005	-	0,3,3	-	-	-	-	-
10	1N7	E	707	-	39,39,46	2.74	22 (56%)	61,61,72	2.38	27 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	E	704	11,8	-	1/16/32/32	0/3/3/3
10	1N7	A	1005	-	-	9/16/81/92	0/4/4/4
10	1N7	A	1006	-	-	2/6/71/92	0/4/4/4
9	ADP	F	1003	8	-	3/16/32/32	0/3/3/3
9	ADP	A	1004	8	-	7/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	1N7	E	707	-	-	9/17/82/92	0/4/4/4

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1005	1N7	C2-C19	5.74	1.66	1.56
10	E	707	1N7	C18-C17	5.53	1.63	1.53
10	A	1006	1N7	C18-C17	5.52	1.63	1.53
10	A	1005	1N7	C3-C19	5.16	1.62	1.53
10	E	707	1N7	C2-C19	5.02	1.64	1.56
10	A	1005	1N7	C18-C17	4.99	1.62	1.53
10	A	1005	1N7	C23-C24	4.93	1.61	1.51
10	E	707	1N7	C23-C24	4.83	1.61	1.51
10	A	1005	1N7	C24-N1	4.71	1.44	1.33
10	E	707	1N7	C24-N1	4.70	1.44	1.33
9	F	1003	ADP	C5-C4	4.65	1.47	1.39
10	A	1006	1N7	C2-C19	4.64	1.64	1.56
9	E	704	ADP	C5-C4	4.60	1.47	1.39
9	A	1004	ADP	C5-C4	4.46	1.47	1.39
10	A	1006	1N7	C3-C19	4.44	1.60	1.53
10	E	707	1N7	C3-C19	4.33	1.60	1.53
10	A	1005	1N7	C20-C9	4.25	1.61	1.54
10	A	1006	1N7	C14-C13	4.17	1.59	1.52
10	A	1005	1N7	C28-N2	3.97	1.58	1.46
10	A	1006	1N7	C16-C17	3.96	1.60	1.52
10	A	1005	1N7	C2-C15	3.87	1.61	1.55
10	E	707	1N7	C20-C9	3.82	1.60	1.54
10	A	1006	1N7	C20-C9	3.80	1.60	1.54
10	E	707	1N7	C16-C17	3.78	1.59	1.52
10	E	707	1N7	C14-C13	3.68	1.58	1.52
10	A	1005	1N7	C14-C13	3.67	1.58	1.52
10	A	1005	1N7	C5-C4	3.60	1.60	1.54
10	A	1005	1N7	C16-C17	3.58	1.59	1.52
10	E	707	1N7	C28-N2	3.54	1.60	1.50
10	A	1006	1N7	C5-C4	3.50	1.59	1.54
10	A	1005	1N7	C1-C2	3.39	1.60	1.54
10	A	1005	1N7	C14-C15	3.36	1.59	1.53
10	E	707	1N7	C5-C4	3.36	1.59	1.54
10	A	1005	1N7	C3-C4	3.24	1.58	1.53
10	A	1006	1N7	C14-C15	3.24	1.59	1.53
10	E	707	1N7	C1-C2	3.15	1.59	1.54
10	E	707	1N7	C14-C15	3.06	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1005	1N7	C16-C15	3.05	1.58	1.53
10	A	1006	1N7	C16-C15	3.02	1.58	1.53
10	A	1005	1N7	C25-N1	3.01	1.52	1.46
10	E	707	1N7	C25-N1	3.00	1.52	1.46
10	E	707	1N7	C29-N2	2.89	1.58	1.50
10	A	1006	1N7	C1-C2	2.87	1.59	1.54
10	A	1006	1N7	C3-C4	2.82	1.57	1.53
10	E	707	1N7	C2-C15	2.81	1.59	1.55
10	E	707	1N7	C16-C15	2.76	1.58	1.53
10	E	707	1N7	C18-C19	2.70	1.59	1.53
9	F	1003	ADP	C5-C6	2.69	1.48	1.41
10	A	1006	1N7	C2-C15	2.67	1.59	1.55
10	A	1006	1N7	C18-C6	2.67	1.59	1.53
10	E	707	1N7	C3-C4	2.65	1.57	1.53
10	E	707	1N7	C18-C6	2.62	1.58	1.53
9	A	1004	ADP	C5-C6	2.62	1.48	1.41
9	E	704	ADP	C5-C6	2.62	1.48	1.41
10	A	1006	1N7	C12-C13	2.55	1.57	1.51
10	A	1005	1N7	C18-C19	2.50	1.58	1.53
10	A	1006	1N7	C18-C19	2.49	1.58	1.53
10	A	1005	1N7	C18-C6	2.48	1.58	1.53
10	A	1005	1N7	C5-C6	2.43	1.59	1.55
9	E	704	ADP	C5-N7	-2.41	1.34	1.39
10	A	1005	1N7	C12-C13	2.39	1.57	1.51
9	A	1004	ADP	C5-N7	-2.37	1.34	1.39
10	A	1006	1N7	C5-C6	2.33	1.59	1.55
10	E	707	1N7	C12-C13	2.32	1.57	1.51
9	A	1004	ADP	C8-N7	2.32	1.36	1.31
9	F	1003	ADP	C8-N7	2.31	1.36	1.31
10	E	707	1N7	C5-C6	2.29	1.59	1.55
9	F	1003	ADP	C5-N7	-2.28	1.34	1.39
9	E	704	ADP	C8-N7	2.27	1.36	1.31
10	E	707	1N7	C22-C23	2.09	1.59	1.52
10	A	1005	1N7	C22-C23	2.08	1.59	1.52

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1005	1N7	C6-C18-C17	6.93	121.05	111.85
10	A	1005	1N7	C19-C2-C15	6.30	117.26	108.51
10	A	1006	1N7	C9-C5-C4	-6.22	112.07	117.67
9	E	704	ADP	C5-C4-N3	-5.98	118.49	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1006	1N7	C8-C9-C5	-5.95	97.77	103.54
9	F	1003	ADP	C5-C4-N3	-5.89	118.61	126.72
9	A	1004	ADP	C5-C4-N3	-5.88	118.62	126.72
10	E	707	1N7	C8-C9-C5	-5.78	97.94	103.54
10	E	707	1N7	C9-C5-C4	-5.71	112.53	117.67
10	A	1005	1N7	C11-C2-C1	-5.35	99.80	108.31
10	A	1006	1N7	C6-C18-C17	5.34	118.94	111.85
10	A	1005	1N7	C9-C5-C6	5.33	105.46	100.11
10	E	707	1N7	C1-C2-C15	5.15	115.14	107.75
10	E	707	1N7	C3-C4-C5	-4.91	106.27	111.26
9	E	704	ADP	N3-C4-N9	4.87	135.44	127.17
10	A	1005	1N7	C23-C24-N1	4.85	125.18	116.34
9	F	1003	ADP	N3-C4-N9	4.81	135.36	127.17
10	A	1005	1N7	C19-C3-C4	4.69	120.42	114.29
10	E	707	1N7	C23-C24-N1	4.64	124.80	116.34
9	A	1004	ADP	N3-C4-N9	4.57	134.95	127.17
10	A	1005	1N7	C16-C17-C18	-4.54	106.55	111.50
10	A	1005	1N7	C9-C5-C4	-4.39	113.72	117.67
10	A	1005	1N7	C8-C7-C6	-4.35	96.63	105.14
9	E	704	ADP	C2-N3-C4	3.87	121.28	111.83
10	E	707	1N7	C11-C2-C1	-3.86	102.16	108.31
9	A	1004	ADP	C2-N3-C4	3.86	121.25	111.83
9	F	1003	ADP	C2-N3-C4	3.86	121.25	111.83
10	A	1006	1N7	C11-C2-C1	-3.72	102.39	108.31
9	F	1003	ADP	N3-C2-N1	-3.66	123.05	128.58
10	E	707	1N7	C2-C19-C18	3.64	115.89	111.84
10	E	707	1N7	C6-C18-C17	3.63	116.67	111.85
9	A	1004	ADP	N3-C2-N1	-3.61	123.12	128.58
9	E	704	ADP	N3-C2-N1	-3.60	123.13	128.58
10	A	1005	1N7	C6-C5-C4	-3.55	104.17	107.42
10	E	707	1N7	C16-C15-C2	-3.47	108.97	112.66
9	A	1004	ADP	C4-C5-N7	-3.45	106.63	110.58
9	E	704	ADP	C4-C5-N7	-3.45	106.64	110.58
9	F	1003	ADP	C4-C5-N7	-3.35	106.75	110.58
10	A	1005	1N7	C14-C13-C12	-3.28	106.61	110.62
10	A	1006	1N7	C3-C4-C5	-3.24	107.97	111.26
10	A	1005	1N7	C23-C22-C20	3.22	120.47	114.46
10	A	1005	1N7	C1-C2-C15	3.19	112.32	107.75
10	A	1006	1N7	C5-C9-C20	-3.17	115.64	119.48
10	A	1006	1N7	C8-C9-C20	3.16	116.97	112.18
10	A	1005	1N7	C2-C19-C18	3.15	115.35	111.84
10	E	707	1N7	C27-C26-C25	3.15	117.10	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1005	1N7	C14-C15-C2	3.11	115.97	112.66
10	A	1005	1N7	C16-C15-C14	-3.07	107.72	111.23
10	E	707	1N7	C29-N2-C28	-2.95	101.22	108.98
10	E	707	1N7	O1-C24-C23	-2.94	116.69	122.02
10	E	707	1N7	C6-C5-C4	2.94	110.10	107.42
9	F	1003	ADP	C4-N9-C8	2.91	108.80	105.74
9	E	704	ADP	C4-N9-C8	2.90	108.79	105.74
10	A	1005	1N7	O1-C24-C23	-2.88	116.79	122.02
10	A	1005	1N7	C8-C9-C5	-2.84	100.79	103.54
10	E	707	1N7	C30-N2-C28	-2.80	101.62	108.98
10	A	1005	1N7	C19-C18-C6	-2.79	105.85	109.75
10	E	707	1N7	C7-C6-C5	-2.76	100.87	103.54
10	A	1006	1N7	C6-C5-C4	2.74	109.92	107.42
9	A	1004	ADP	C5-N7-C8	2.66	107.62	103.45
10	E	707	1N7	C8-C9-C20	2.65	116.19	112.18
9	F	1003	ADP	C5-N7-C8	2.61	107.56	103.45
9	A	1004	ADP	C4-N9-C8	2.59	108.45	105.74
9	E	704	ADP	C5-N7-C8	2.56	107.47	103.45
10	A	1005	1N7	O1-C24-N1	-2.55	118.03	123.03
10	A	1005	1N7	C5-C6-C18	-2.55	111.49	114.72
10	A	1005	1N7	C11-C2-C15	-2.54	106.19	110.44
10	A	1006	1N7	C19-C3-C4	2.52	117.59	114.29
10	E	707	1N7	C10-C5-C4	2.52	111.58	109.06
10	A	1006	1N7	C1-C12-C13	2.51	113.81	110.48
10	E	707	1N7	C23-C22-C20	2.49	119.11	114.46
10	A	1005	1N7	C11-C2-C19	-2.48	107.85	111.18
10	A	1005	1N7	C3-C4-C5	-2.46	108.77	111.26
10	A	1006	1N7	C10-C5-C4	2.41	111.46	109.06
9	E	704	ADP	C3'-C2'-C1'	2.40	106.01	101.46
9	F	1003	ADP	C3'-C2'-C1'	2.38	105.96	101.46
10	E	707	1N7	C7-C8-C9	2.34	109.72	105.14
10	A	1006	1N7	C1-C2-C19	2.33	114.96	111.34
10	E	707	1N7	C1-C12-C13	2.31	113.55	110.48
10	E	707	1N7	O1-C24-N1	-2.30	118.51	123.03
10	A	1006	1N7	C11-C2-C19	-2.29	108.10	111.18
10	A	1006	1N7	C19-C2-C15	2.26	111.66	108.51
10	A	1006	1N7	C7-C8-C9	2.25	109.54	105.14
10	E	707	1N7	C5-C9-C20	-2.24	116.78	119.48
10	E	707	1N7	C19-C2-C15	2.23	111.61	108.51
10	A	1006	1N7	C15-C16-C17	2.22	117.04	114.40
10	E	707	1N7	C25-N1-C24	2.22	126.96	122.82
9	A	1004	ADP	N9-C8-N7	-2.17	110.85	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	1003	ADP	N9-C8-N7	-2.17	110.86	113.94
10	E	707	1N7	C11-C2-C15	-2.14	106.86	110.44
10	A	1005	1N7	C25-N1-C24	2.09	126.71	122.82
10	A	1005	1N7	C1-C12-C13	2.08	113.24	110.48
9	A	1004	ADP	O2A-PA-O1A	2.08	122.14	112.44
9	A	1004	ADP	C6-C5-N7	2.07	136.07	132.09
9	F	1003	ADP	C2-N1-C6	2.06	122.12	118.73
9	E	704	ADP	N9-C8-N7	-2.04	111.04	113.94
10	E	707	1N7	C15-C16-C17	-2.03	111.99	114.40
10	E	707	1N7	C12-C1-C2	2.03	116.16	112.74

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1004	ADP	C5'-O5'-PA-O1A
9	A	1004	ADP	C5'-O5'-PA-O2A
9	A	1004	ADP	C5'-O5'-PA-O3A
9	F	1003	ADP	PB-O3A-PA-O5'
10	A	1005	1N7	C26-C27-N2-C29
10	E	707	1N7	C26-C27-N2-C28
10	E	707	1N7	C26-C27-N2-C30
10	A	1005	1N7	C22-C20-C9-C5
10	A	1005	1N7	C22-C23-C24-O1
10	A	1005	1N7	C26-C27-N2-C28
10	A	1005	1N7	C22-C23-C24-N1
10	A	1005	1N7	C21-C20-C9-C5
10	A	1006	1N7	C21-C20-C22-C23
10	A	1005	1N7	C21-C20-C9-C8
10	E	707	1N7	C26-C27-N2-C29
10	E	707	1N7	C21-C20-C22-C23
10	A	1006	1N7	C9-C20-C22-C23
9	F	1003	ADP	O4'-C4'-C5'-O5'
9	E	704	ADP	PA-O3A-PB-O1B
9	F	1003	ADP	C3'-C4'-C5'-O5'
10	E	707	1N7	C21-C20-C9-C5
10	A	1005	1N7	C22-C20-C9-C8
10	E	707	1N7	C22-C20-C9-C5
9	A	1004	ADP	C2'-C1'-N9-C8
9	A	1004	ADP	PB-O3A-PA-O1A
10	A	1005	1N7	N1-C25-C26-C27
9	A	1004	ADP	O4'-C1'-N9-C8

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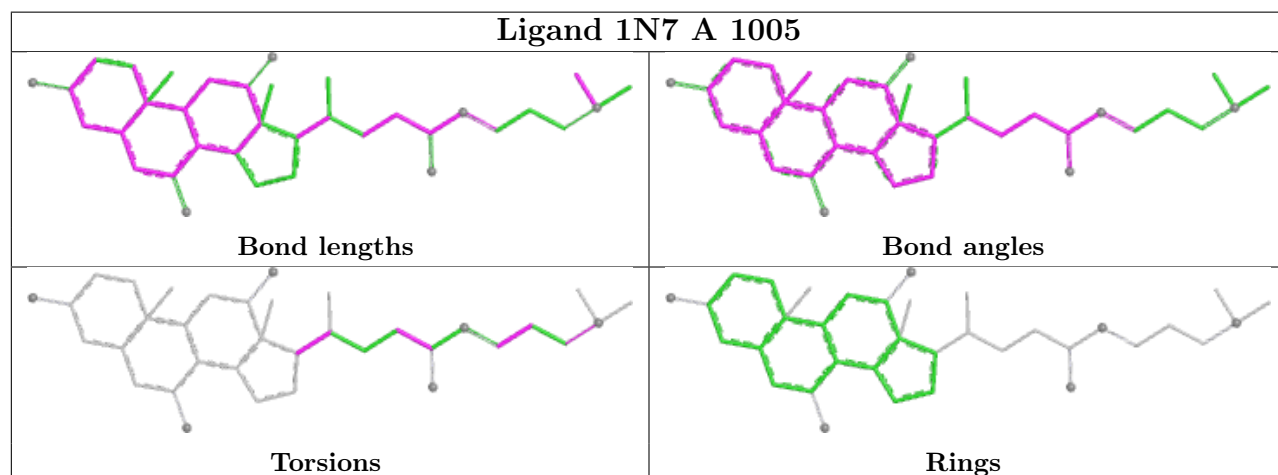
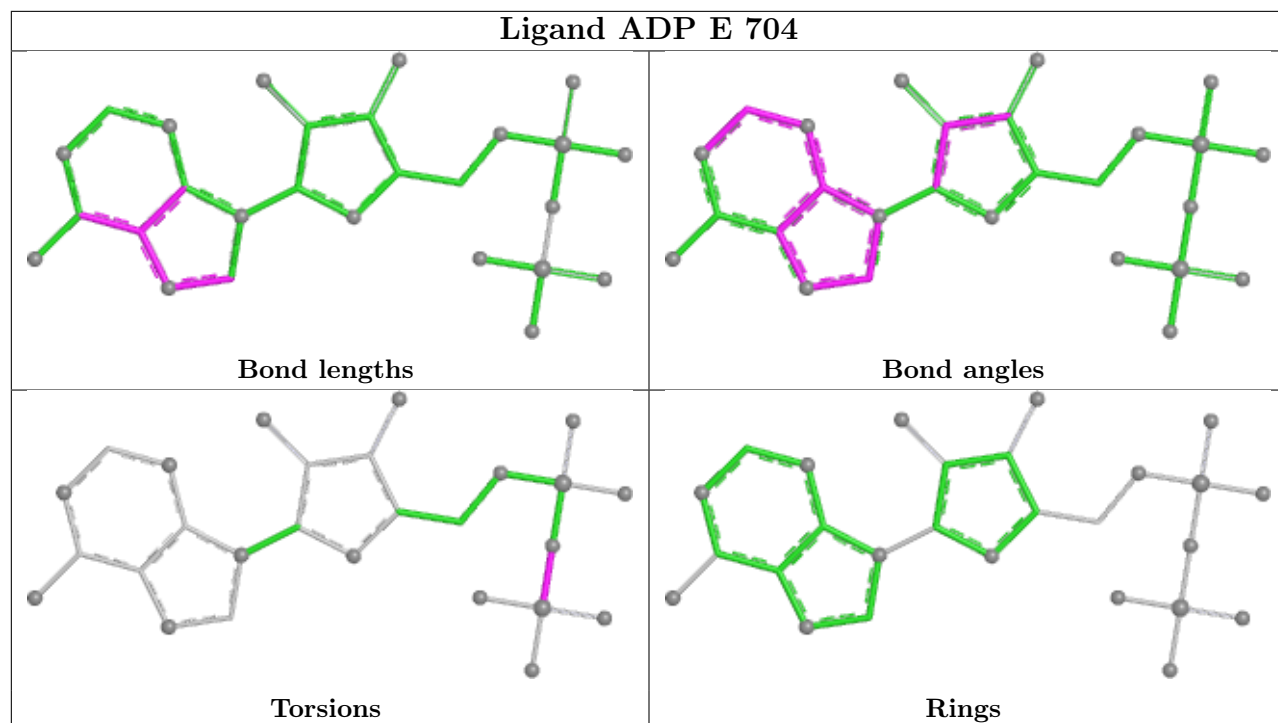
Mol	Chain	Res	Type	Atoms
9	A	1004	ADP	PB-O3A-PA-O2A
10	E	707	1N7	C22-C20-C9-C8
10	E	707	1N7	C22-C23-C24-O1
10	E	707	1N7	C22-C23-C24-N1

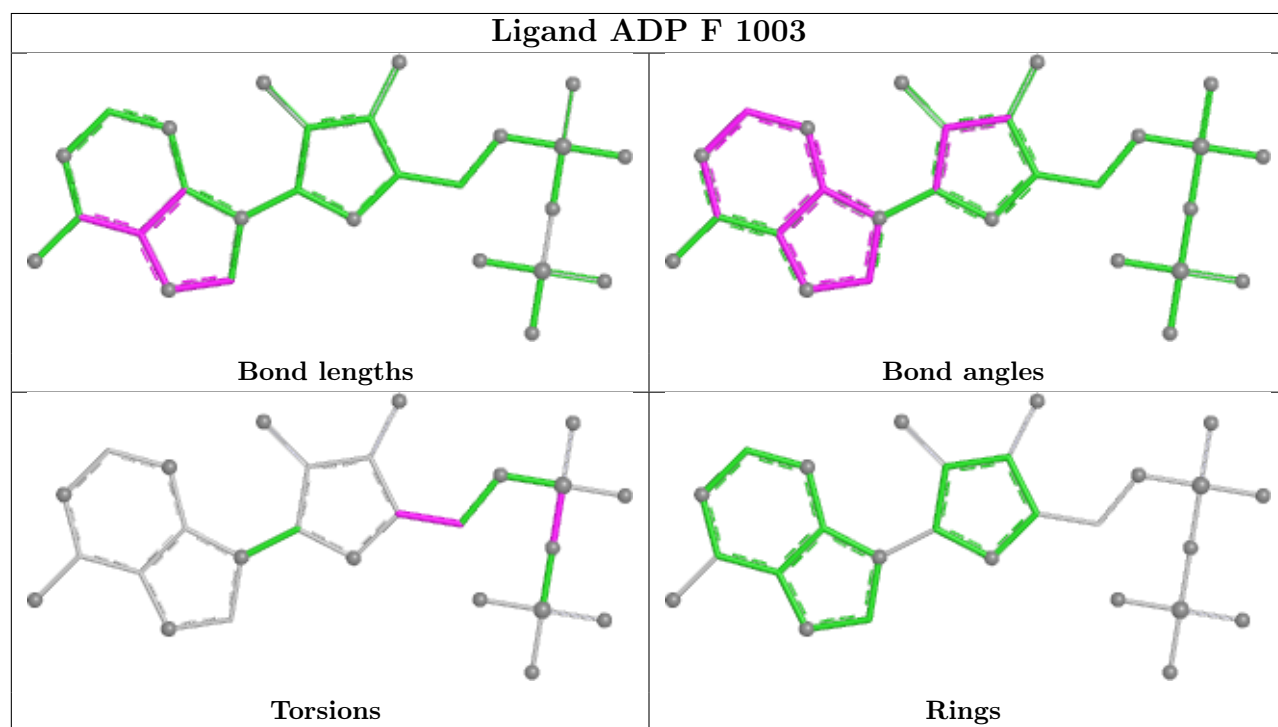
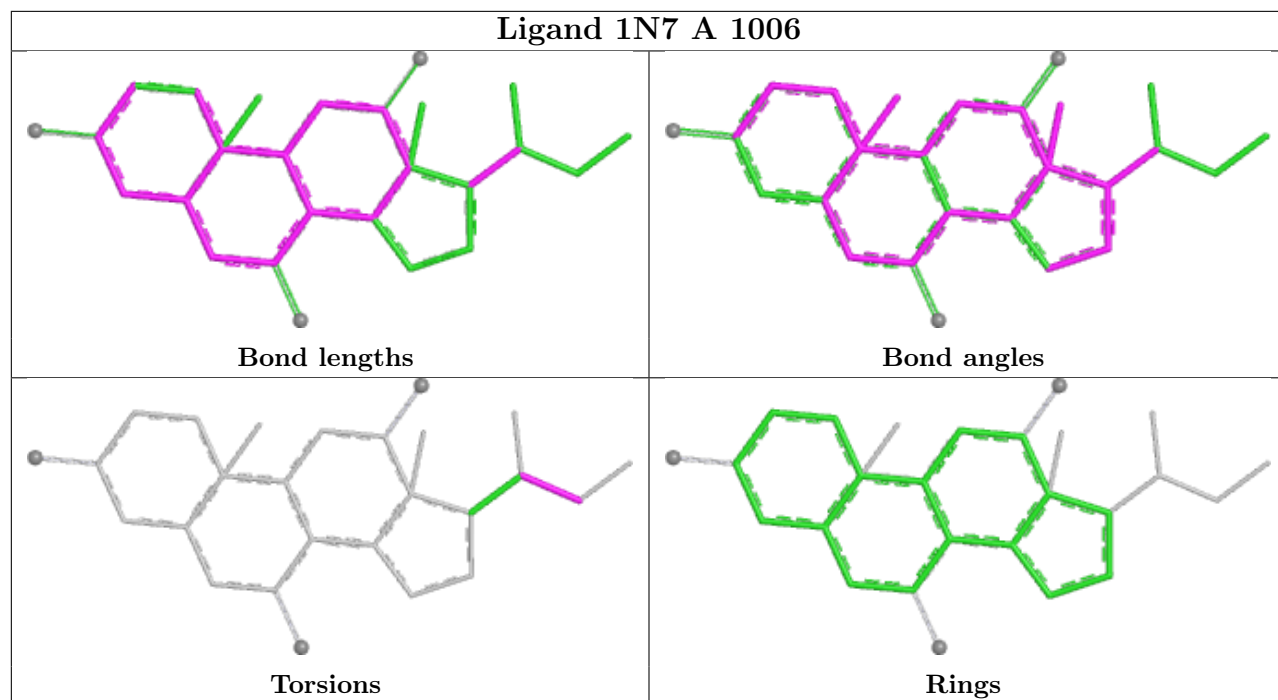
There are no ring outliers.

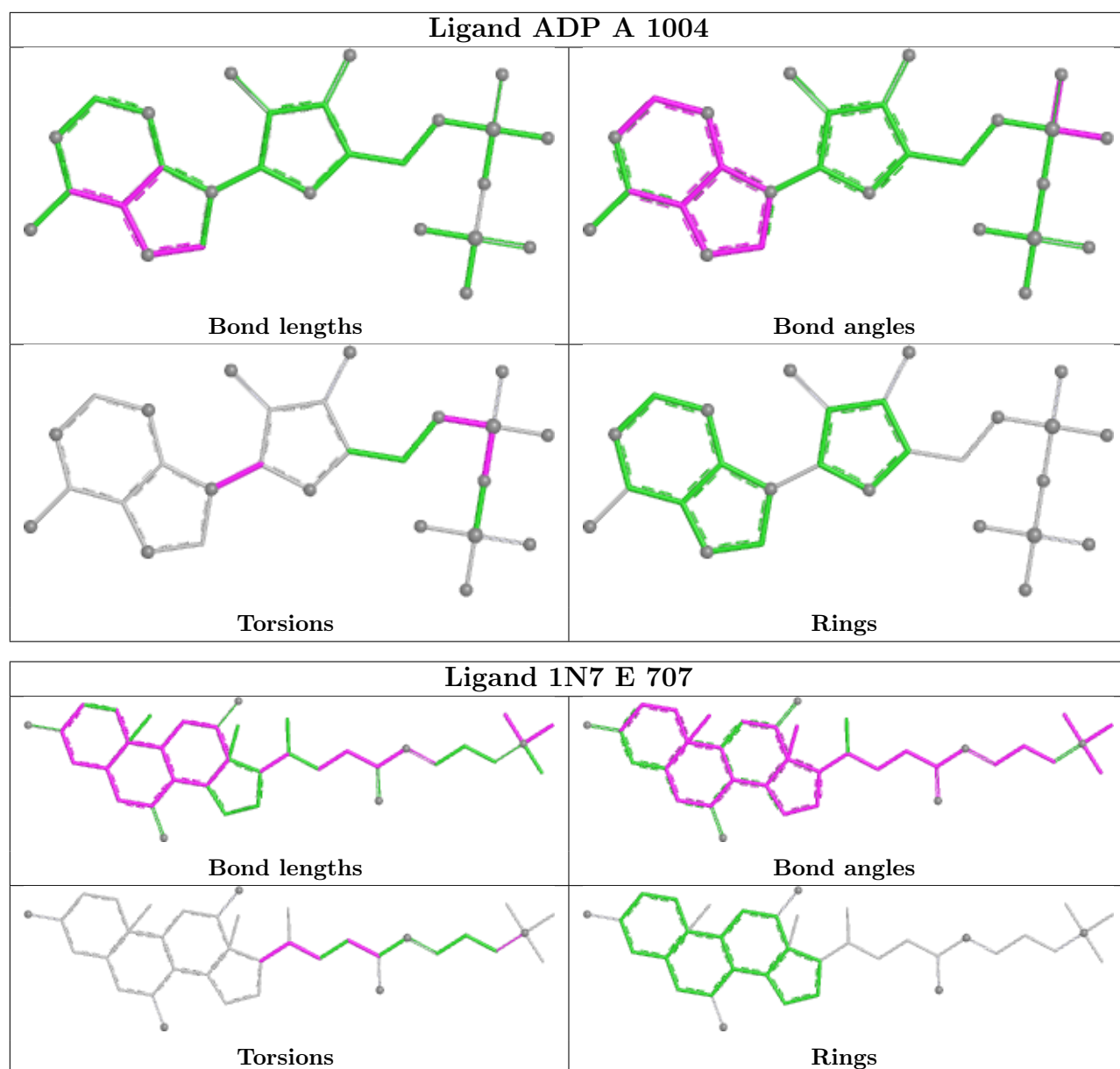
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	704	ADP	2	0
11	E	706	AF3	1	0
10	A	1006	1N7	1	0
9	F	1003	ADP	1	0
9	A	1004	ADP	2	0
11	F	1005	AF3	1	0
10	E	707	1N7	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

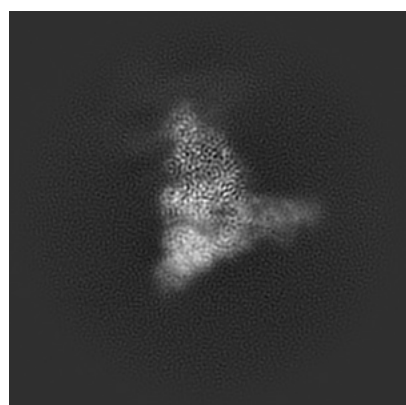
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24426. These allow visual inspection of the internal detail of the map and identification of artifacts.

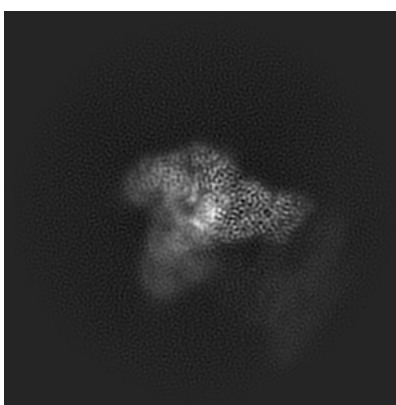
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

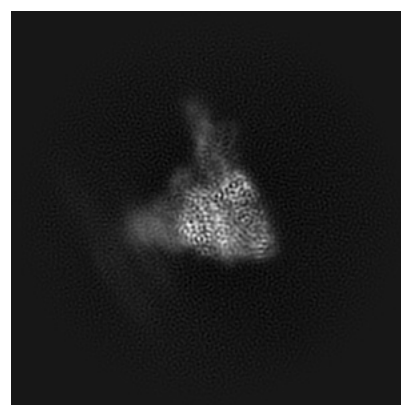
6.1.1 Primary map



X



Y

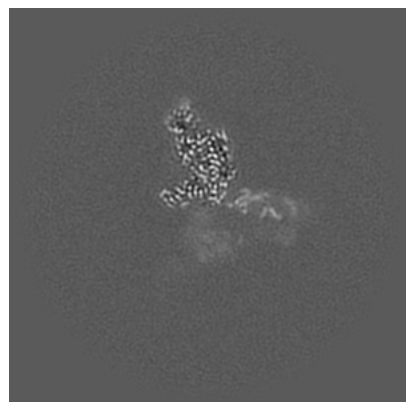


Z

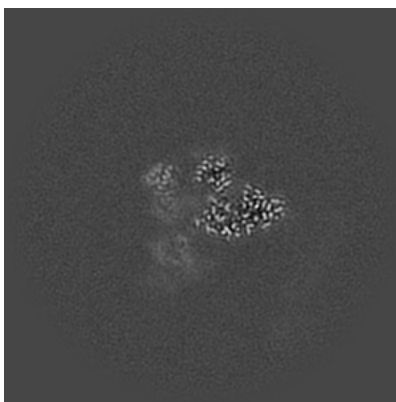
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

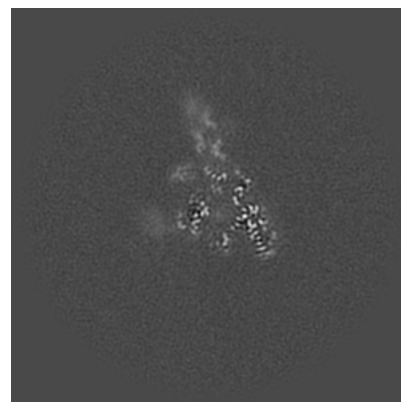
6.2.1 Primary map



X Index: 160



Y Index: 160

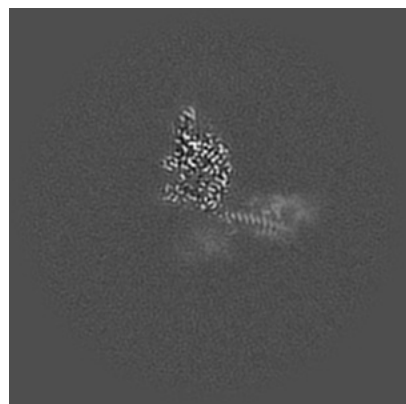


Z Index: 160

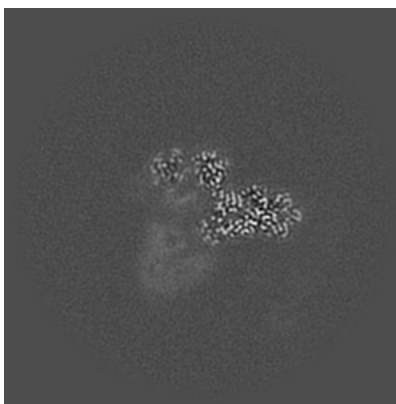
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

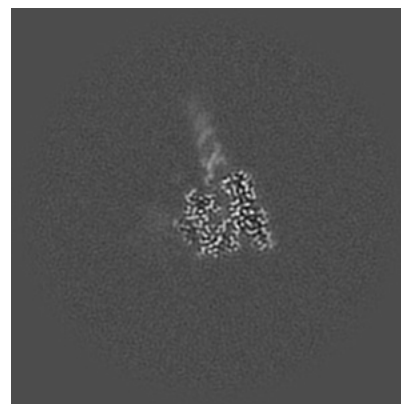
6.3.1 Primary map



X Index: 152



Y Index: 148

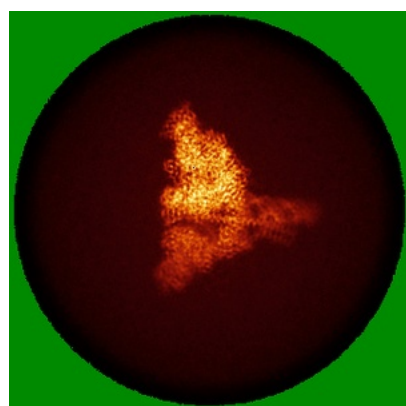


Z Index: 167

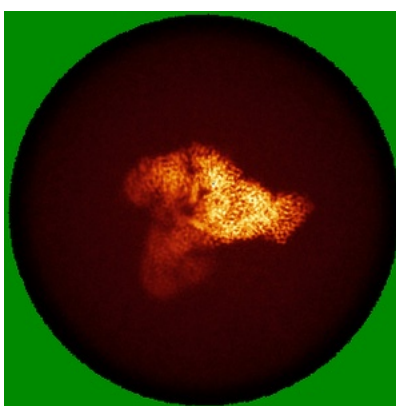
The images above show the largest variance slices of the map in three orthogonal directions.

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

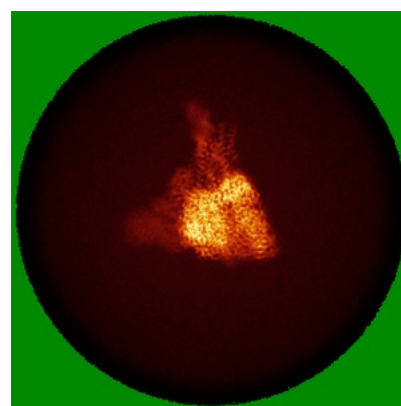
6.4.1 Primary map



X



Y

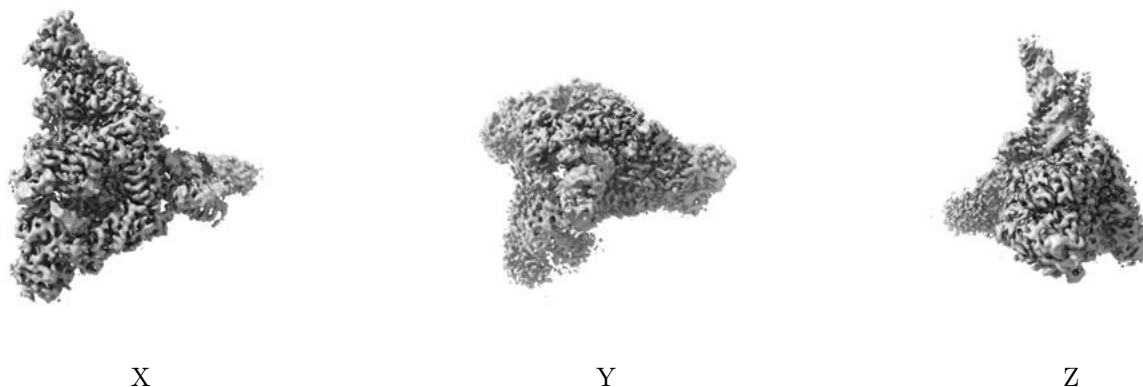


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

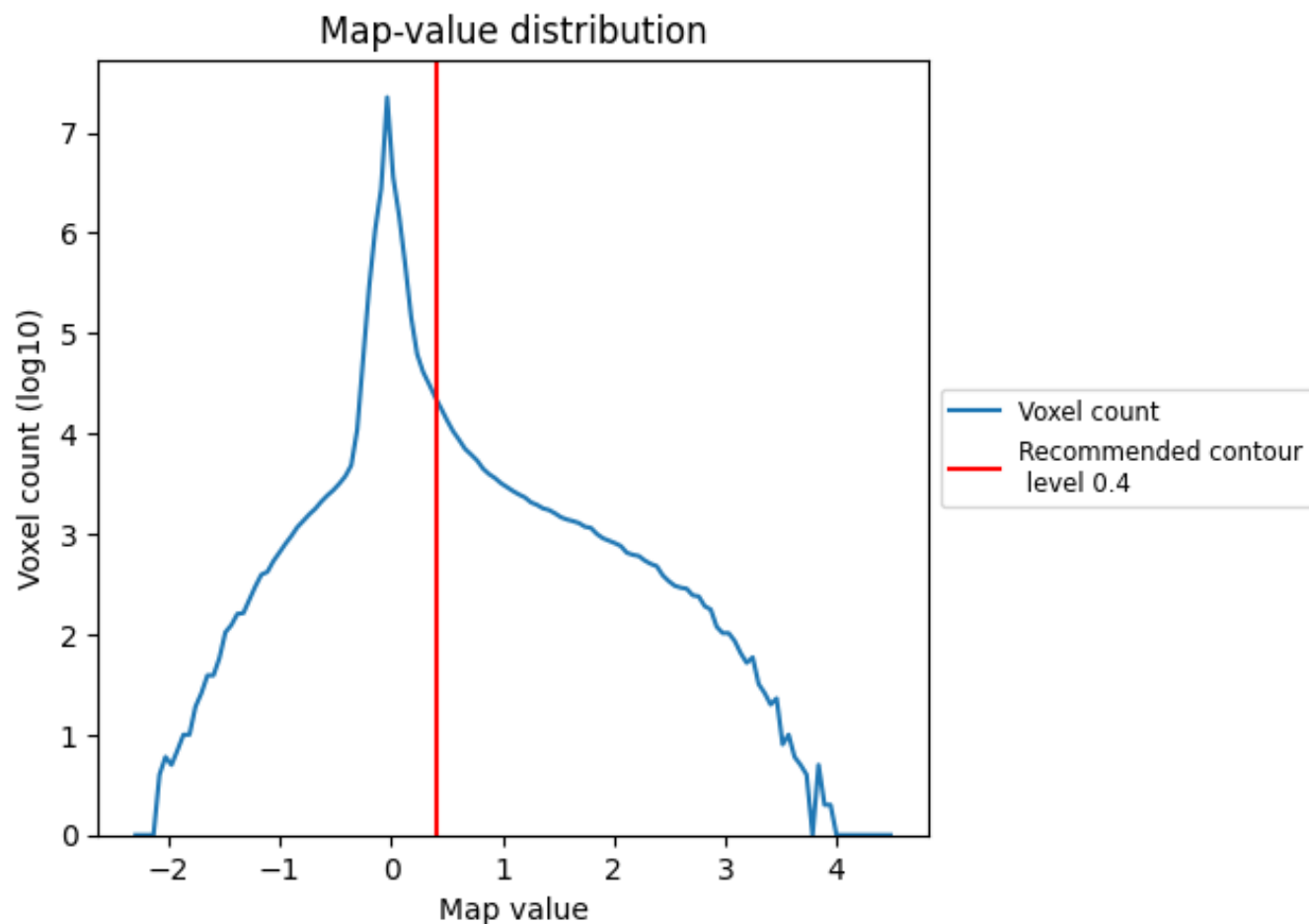
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

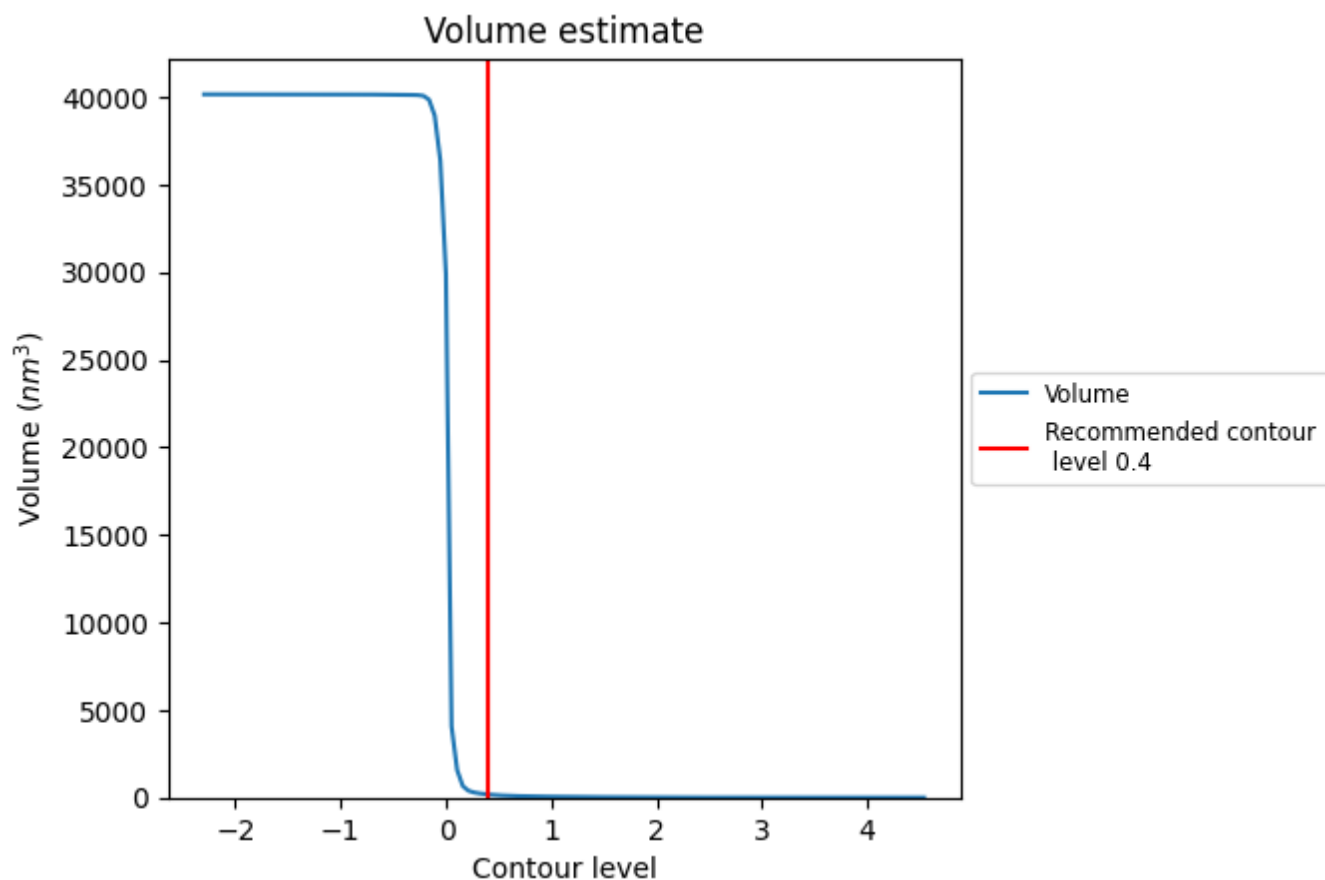
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

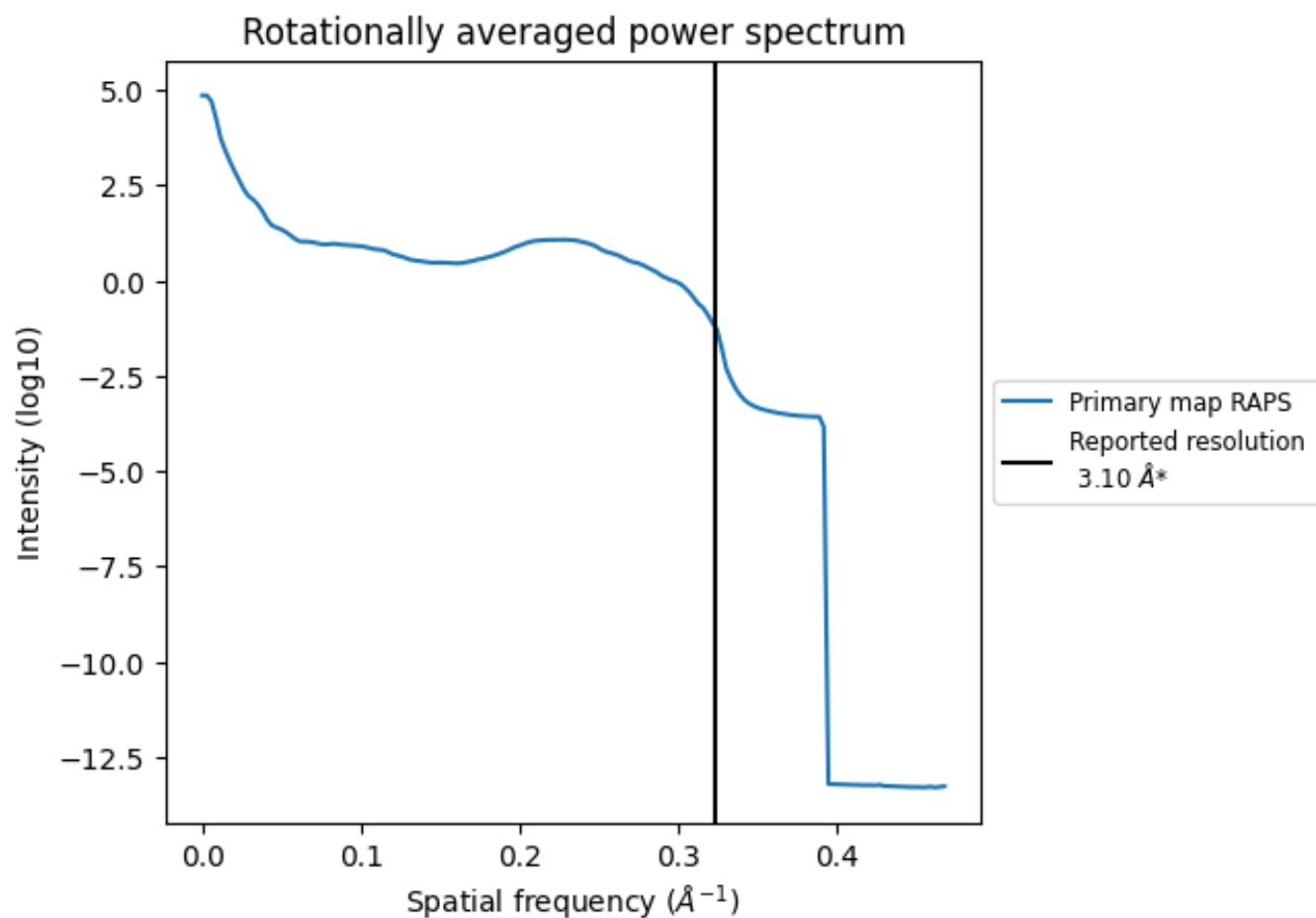
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 160 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 ⓘ

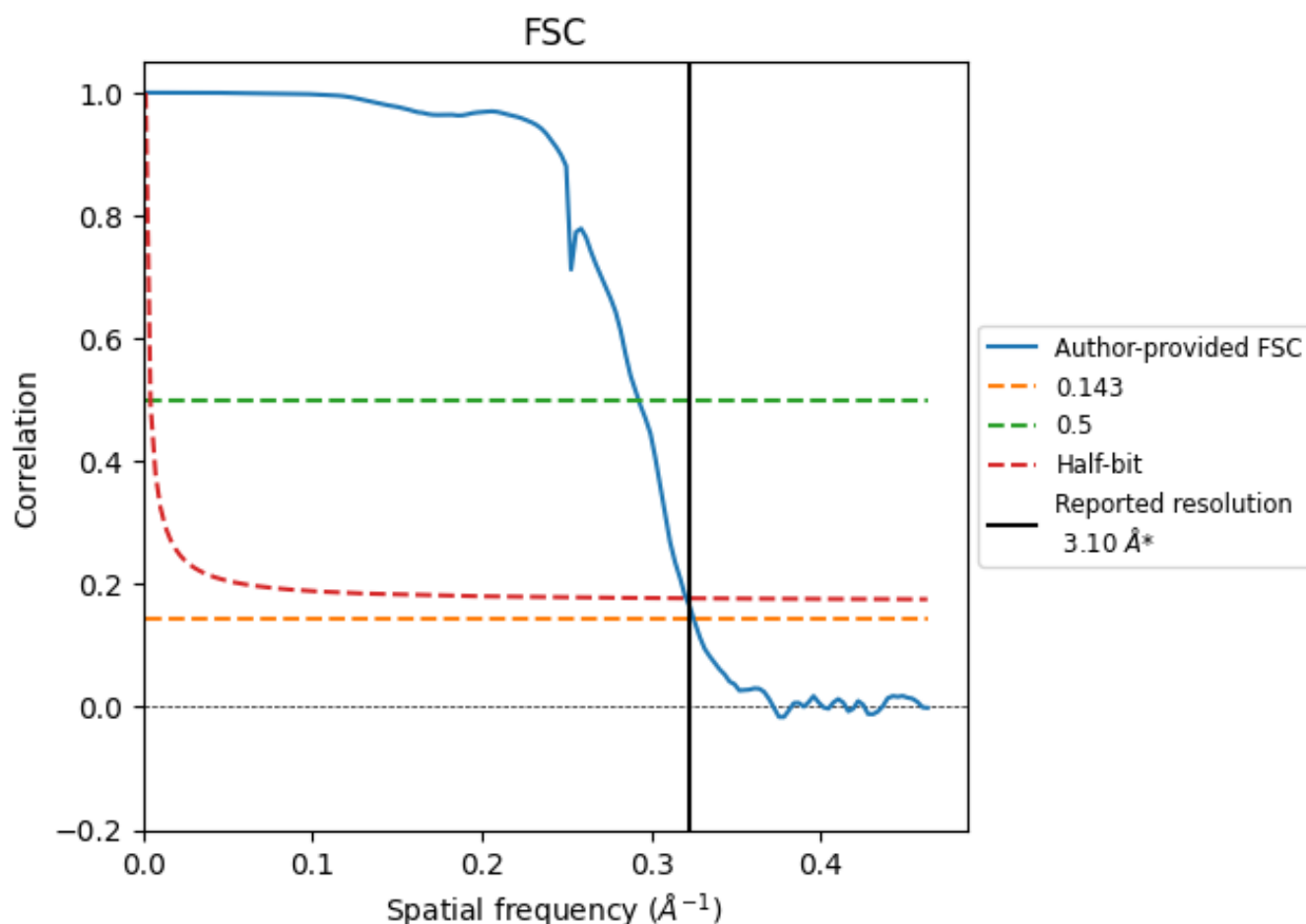


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

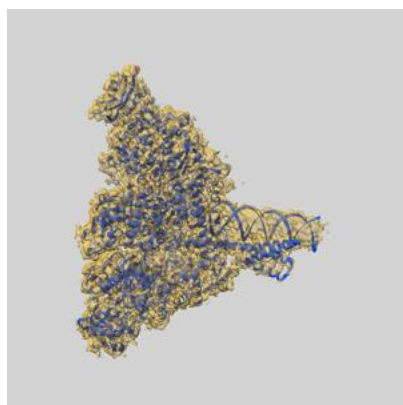
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.42	3.12
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

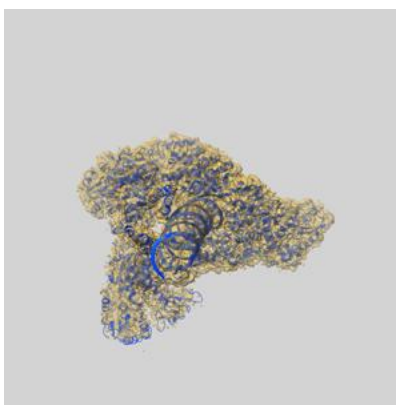
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24426 and PDB model 7RDX. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

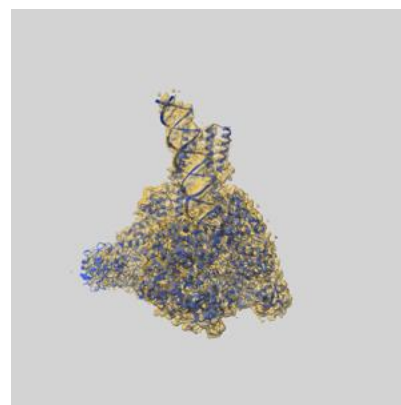
9.1 Map-model overlay [i](#)



X



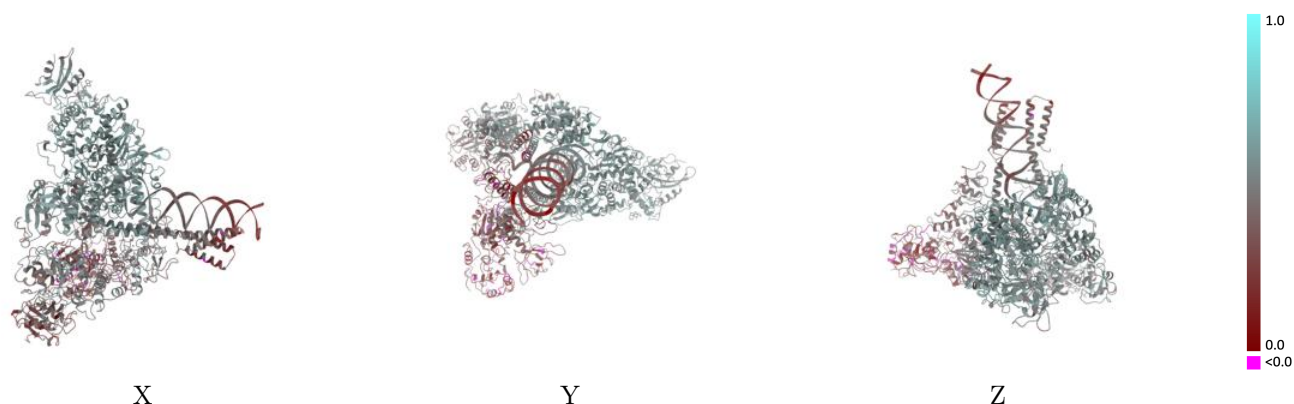
Y



Z

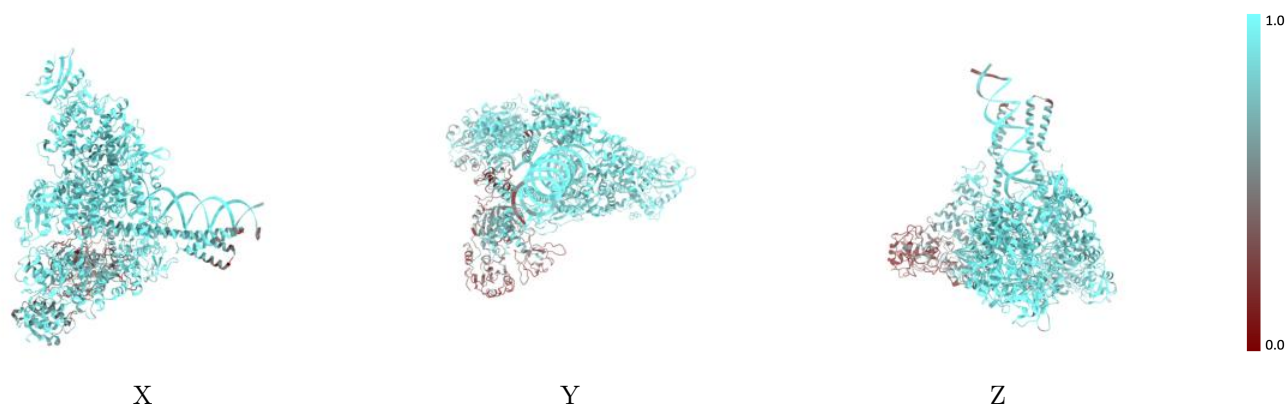
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



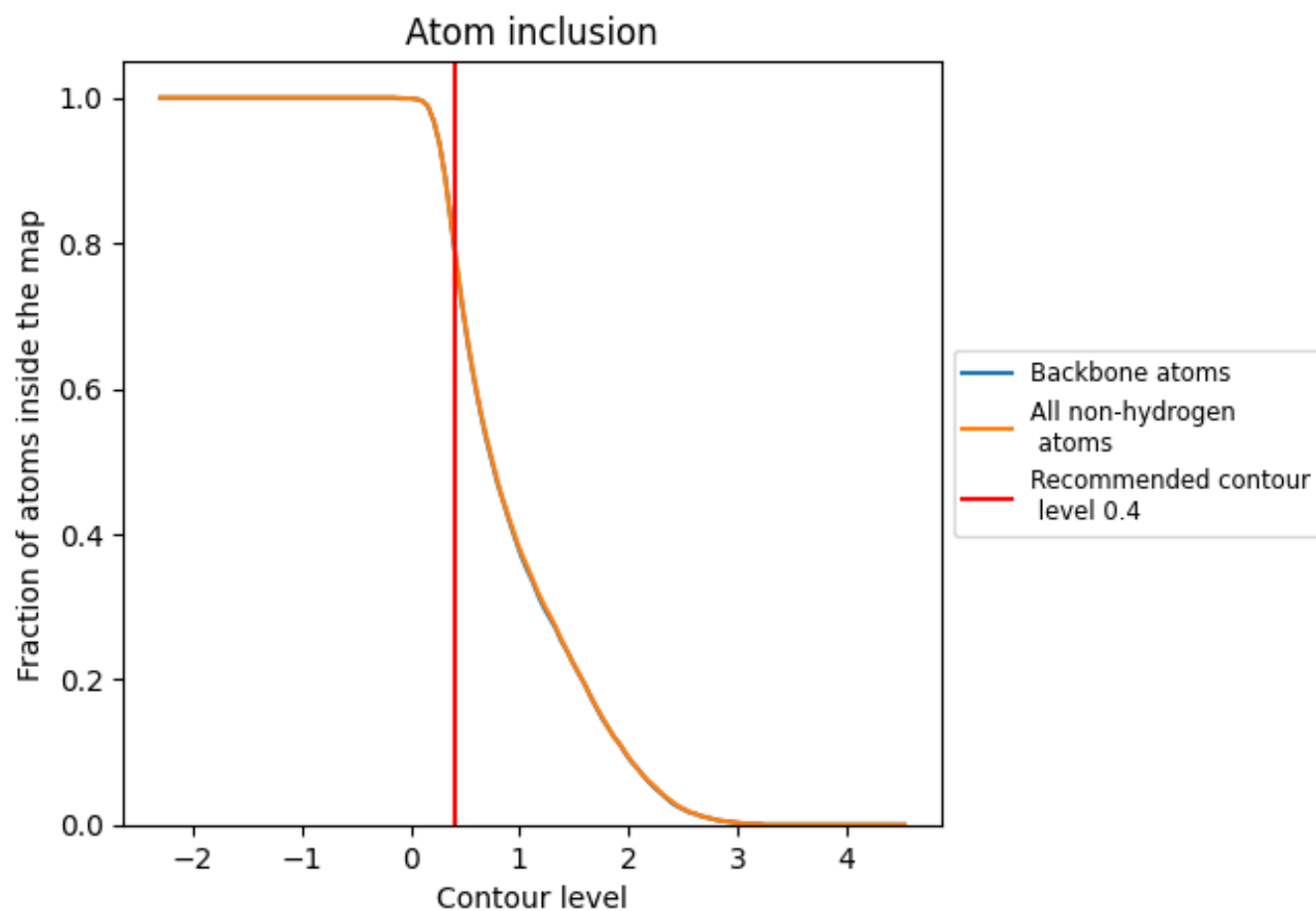
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.4420
A	0.9470	0.5540
B	0.8770	0.4790
C	0.9130	0.5350
D	0.8900	0.4780
E	0.7950	0.4240
F	0.4660	0.2670
P	0.9300	0.3740
T	0.8850	0.3780

1.0

0.0

<0.0