Full wwPDB EM Validation Report (i)

Nov 6, 2023 – 12:54 pm GMT

PDB ID	:	7AHH
EMDB ID	:	EMD-11786
Title	:	OpuA inhibited inward-facing, SBD docked
Authors	:	Sikkema, H.R.; Rheinberger, J.; Paulino, C.; Poolman, B.
Deposited on	:	2020-09-24
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

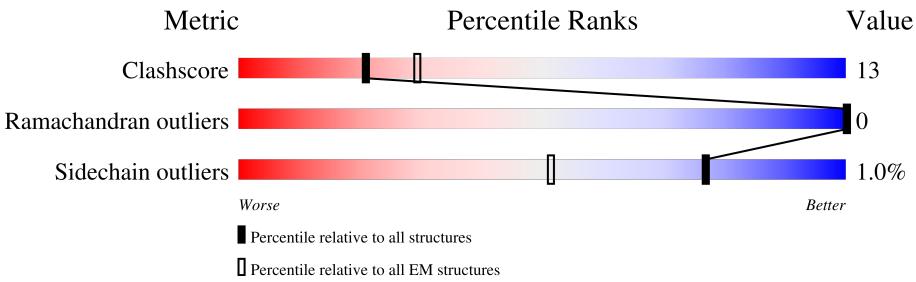
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	585	19% 68% 22% 10%
1	B	585	• 34% 12% 54%
2	C	408	20% 66% 27% • 6%
2	D	408	18% 63% 29% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12125 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ABC transporter permease subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	526	4011	2603	653	734	21	0	0
1	B	272	2016	1335	318	352	11	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	574	GLY	-	expression tag	UNP A0A0V8ETW8
A	575	SER	-	expression tag	UNP A0A0V8ETW8
A	576	ILE	-	expression tag	UNP A0A0V8ETW8
A	577	GLU	-	expression tag	UNP A0A0V8ETW8
A	578	GLY	-	expression tag	UNP A0A0V8ETW8
A	579	ARG	-	expression tag	UNP A0A0V8ETW8
A	580	HIS	-	expression tag	UNP A0A0V8ETW8
A	581	HIS	-	expression tag	UNP A0A0V8ETW8
A	582	HIS	-	expression tag	UNP A0A0V8ETW8
A	583	HIS	-	expression tag	UNP A0A0V8ETW8
A	584	HIS	-	expression tag	UNP A0A0V8ETW8
A	585	HIS	-	expression tag	UNP A0A0V8ETW8
B	574	GLY	-	expression tag	UNP A0A0V8ETW8
B	575	SER	-	expression tag	UNP A0A0V8ETW8
B	576	ILE	-	expression tag	UNP A0A0V8ETW8
B	577	GLU	-	expression tag	UNP A0A0V8ETW8
B	578	GLY	-	expression tag	UNP A0A0V8ETW8
B	579	ARG	-	expression tag	UNP A0A0V8ETW8
B	580	HIS	-	expression tag	UNP A0A0V8ETW8
B	581	HIS	-	expression tag	UNP A0A0V8ETW8
B	582	HIS	-	expression tag	UNP A0A0V8ETW8
B	583	HIS	-	expression tag	UNP A0A0V8ETW8
B	584	HIS	-	expression tag	UNP A0A0V8ETW8
B	585	HIS	-	expression tag	UNP A0A0V8ETW8

- Molecule 2 is a protein called ABC-type proline/glycine betaine transport system ATPase

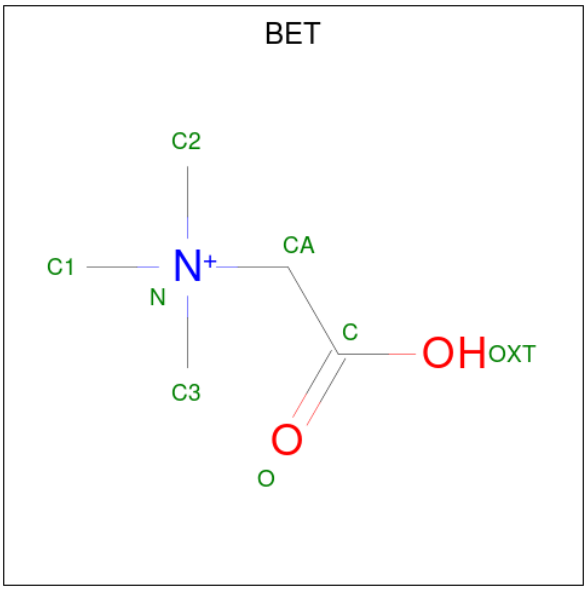
component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	382	2992	1890	515	573	14	0	0
2	D	382	2992	1890	515	573	14	0	0

There are 4 discrepancies between the modelled and reference sequences:

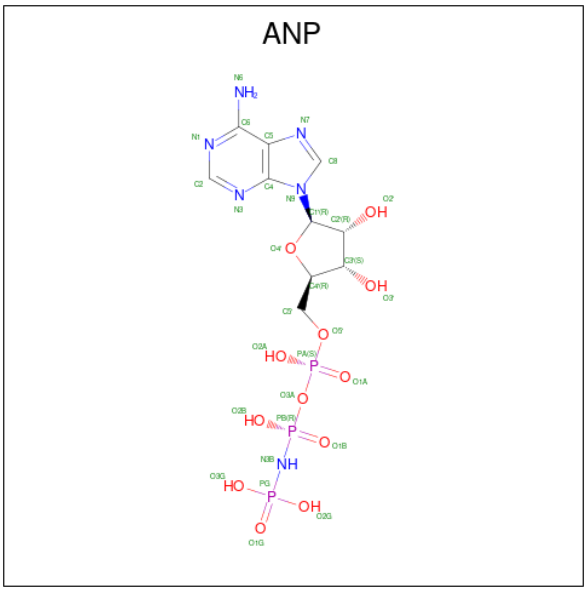
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP A0A0R2NIU5
C	2	ALA	-	expression tag	UNP A0A0R2NIU5
D	1	MET	-	initiating methionine	UNP A0A0R2NIU5
D	2	ALA	-	expression tag	UNP A0A0R2NIU5

- Molecule 3 is TRIMETHYL GLYCINE (three-letter code: BET) (formula: $C_5H_{12}NO_2$).



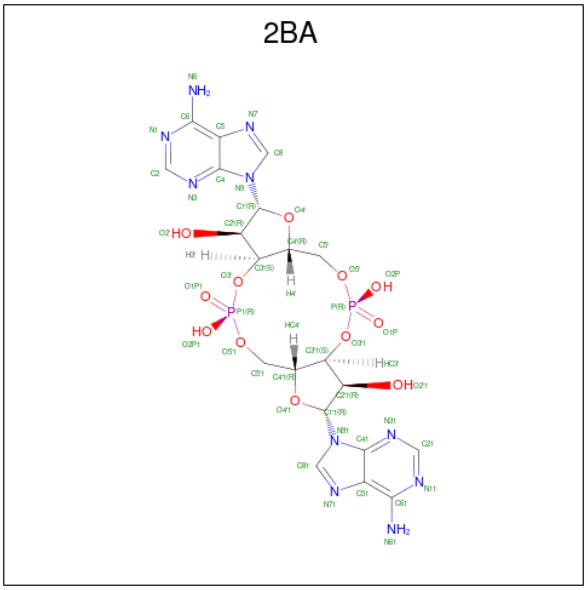
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	8	5	1	2	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	C	1	31	10	6	12	3	0
			Total	C	N	O	P	
4	D	1	31	10	6	12	3	0

- Molecule 5 is (2R,3R,3aS,5R,7aR,9R,10R,10aS,12R,14aR)-2,9-bis(6-amino-9H-purin-9-yl)octahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-3,5,10,12-tetrol 5,12-dioxide (three-letter code: 2BA) (formula: $C_{20}H_{24}N_{10}O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



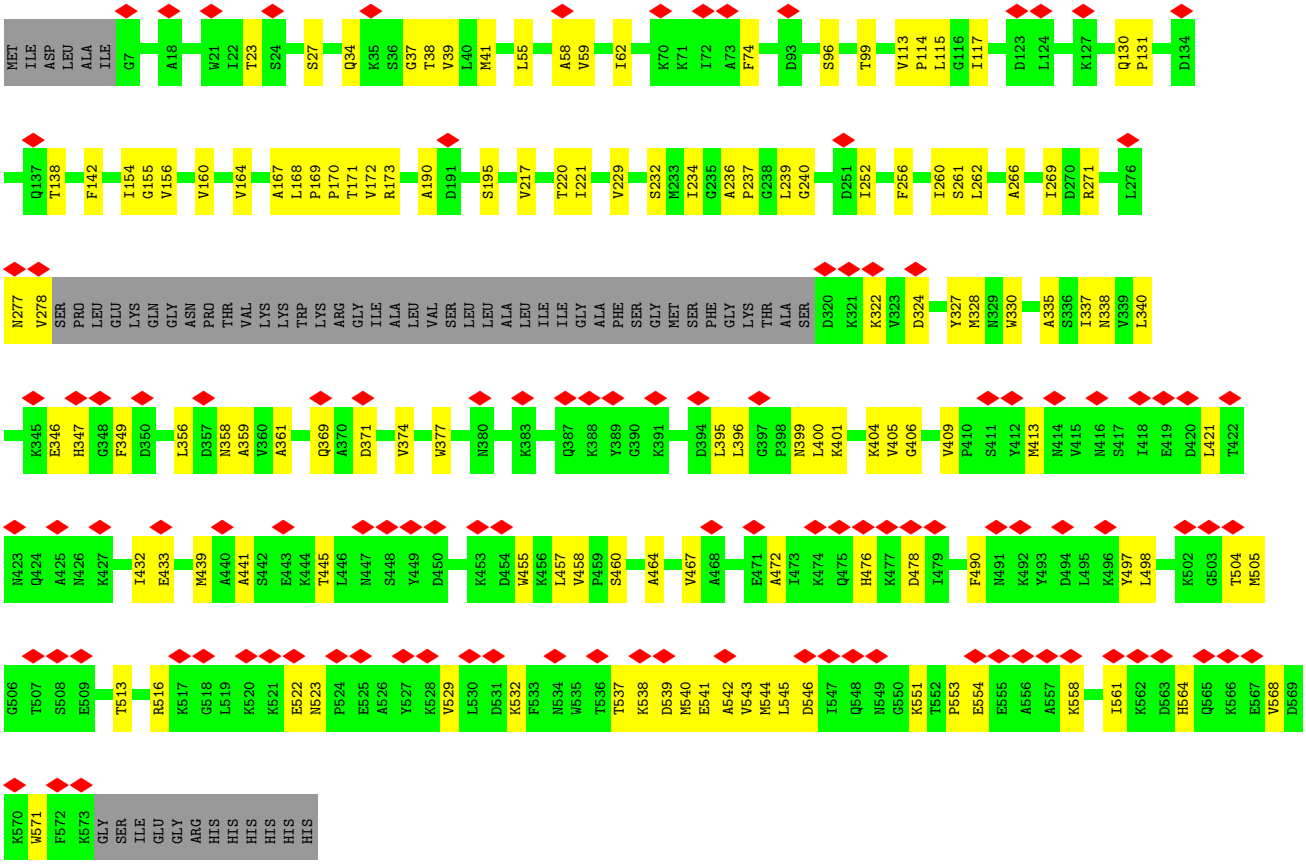
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	D	1	44	20	10	12	2	0

3 Residue-property plots (i)

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

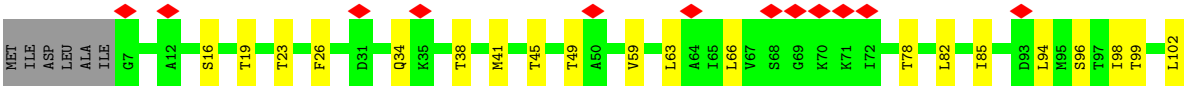
• Molecule 1: ABC transporter permease subunit

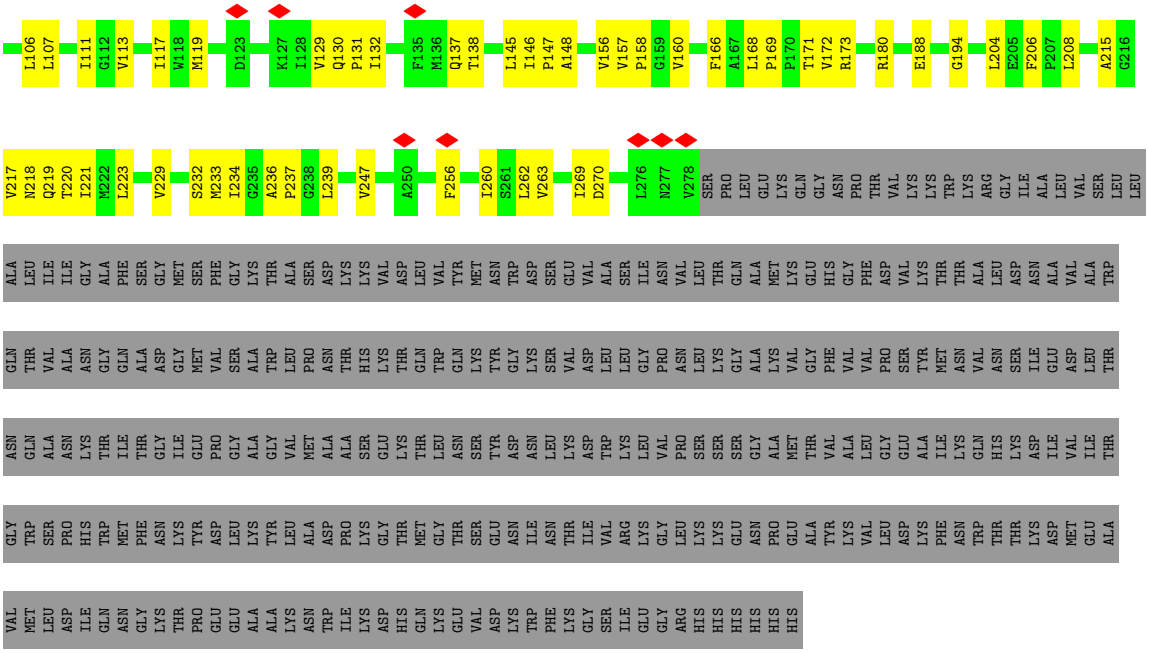
Chain A:



• Molecule 1: ABC transporter permease subunit

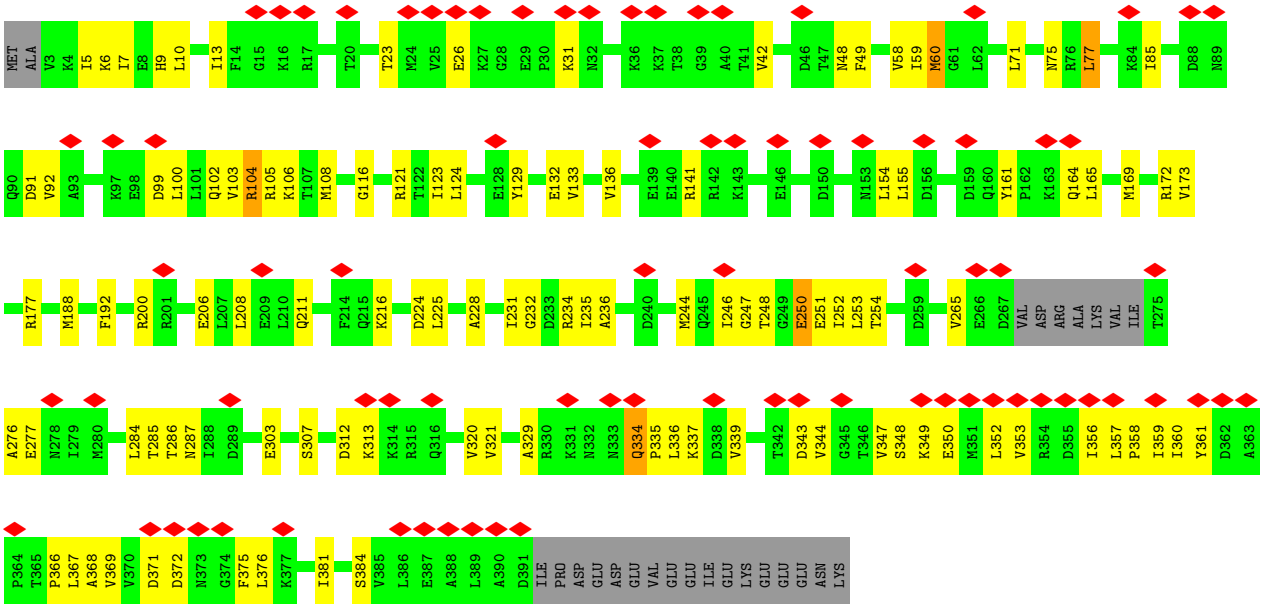
Chain B:





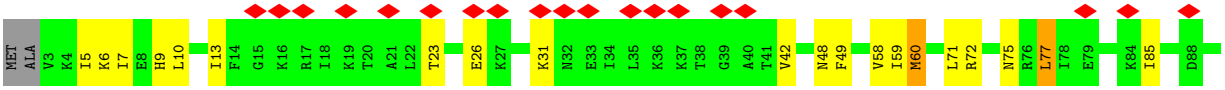
• Molecule 2: ABC-type proline/glycine betaine transport system ATPase component

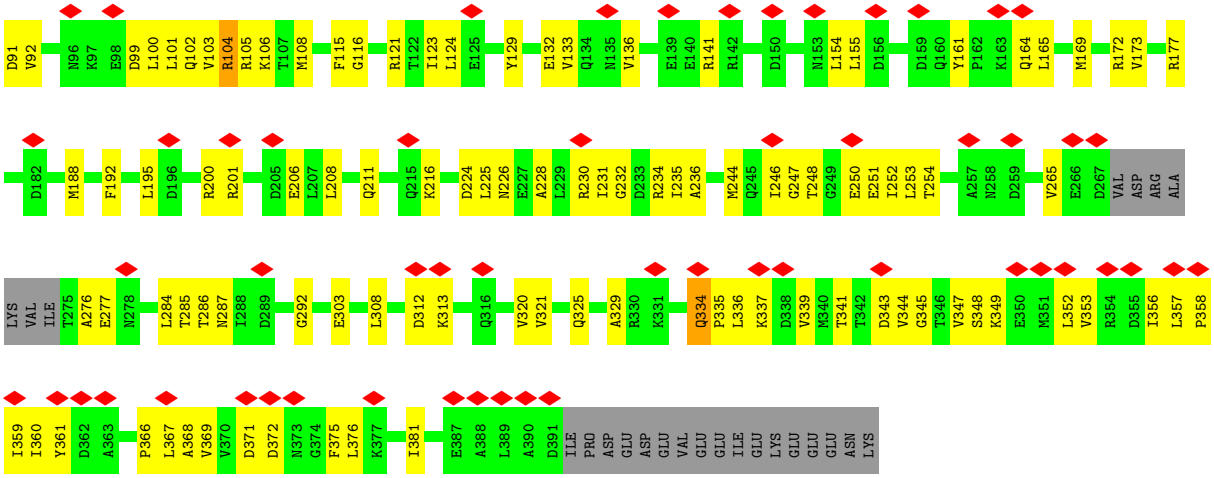
Chain C:



• Molecule 2: ABC-type proline/glycine betaine transport system ATPase component

Chain D:




D91
V92
N96
K97
E98
D99
L100
L101
Q102
V103
R104
R105
K106
T107
M108
F115
G116
R121
T122
I123
L124
E125
Y129
E132
V133
Q134
N135
V136
E139
E140
R141
R142
D150
N153
L154
L155
D156
D159
Q160
Y161
P162
K163
Q164
L165
M169
R172
V173
R177
D182
M188
F192
L195
D196
R200
R201
D205
E206
L207
L208
Q211
Q215
K216
D224
L225
N226
E227
A228
L229
R230
I231
G232
D233
R234
I235
A236
M244
Q245
I246
G247
T248
G249
E250
E251
I252
L253
T254
A257
N258
D259
V265
E266
D267
VAL
ASP
ARG
ALA
LYS
VAL
ILE
T275
A276
E277
N278
L284
T285
T286
N287
I288
D289
G292
E303
L308
D312
K313
Q316
V320
V321
Q325
A329
R330
K331
Q334
P335
L336
K337
D338
V339
M340
T341
T342
D343
V344
G345
T346
V347
S348
K349
E350
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L352
V353
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I356
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P358
I359
I360
Y361
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A363
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A368
V369
V370
D371
D372
N373
G374
F375
L376
K377
I381
E387
A388
L389
A390
D391
ILE
PRO
ASP
GLU
ASP
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VAL
GLU
GLU
GLU
ILE
GLU
LYS
GLU
GLU
GLU
GLU
ASN
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110161	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	49407	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0416	Depositor
Map size (Å)	259.072, 259.072, 259.072	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.012, 1.012, 1.012	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: 2BA, BET, ANP

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	0.35	0/4095	0.49	0/5565
1	B	0.36	0/2055	0.46	0/2800
2	C	0.37	0/3026	0.58	0/4075
2	D	0.37	0/3026	0.58	0/4075
All	All	0.36	0/12202	0.53	0/16515

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4011	0	4133	102	0
1	B	2016	0	2155	65	0
2	C	2992	0	3105	81	0
2	D	2992	0	3105	89	0
3	A	8	0	11	0	0
4	C	31	0	13	0	0
4	D	31	0	13	0	0
5	D	44	0	23	2	0
All	All	12125	0	12558	328	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 13.

All (328) 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:217:VAL:O	1:A:220:THR:HG22	1.44	1.14
1:A:168:LEU:O	1:A:171:THR:HG22	1.62	1.00
1:B:217:VAL:O	1:B:220:THR:HG22	1.67	0.94
1:B:168:LEU:O	1:B:171:THR:HG22	1.68	0.91
1:A:421:LEU:HD21	1:A:455:TRP:CH2	2.08	0.88
2:D:235:ILE:HB	2:D:252:ILE:HD11	1.56	0.87
2:D:360:ILE:HG22	2:D:367:LEU:CD1	2.05	0.86
1:A:217:VAL:O	1:A:220:THR:CG2	2.24	0.86
2:C:235:ILE:HB	2:C:252:ILE:HD11	1.56	0.86
1:A:217:VAL:C	1:A:220:THR:HG22	2.04	0.77
1:B:217:VAL:C	1:B:220:THR:HG22	2.04	0.77
1:A:421:LEU:HD21	1:A:455:TRP:CZ3	2.20	0.77
2:C:123:ILE:HD11	2:C:165:LEU:HD11	1.68	0.76
2:D:123:ILE:HD11	2:D:165:LEU:HD11	1.68	0.75
1:A:138:THR:OG1	1:B:263:VAL:HG23	1.87	0.74
2:C:360:ILE:HD13	2:C:384:SER:OG	1.88	0.74
1:A:472:ALA:O	1:A:476:HIS:N	2.22	0.73
2:C:250:GLU:O	2:C:253:LEU:N	2.21	0.72
2:C:91:ASP:OD1	2:C:92:VAL:N	2.23	0.72
1:A:421:LEU:CD2	1:A:455:TRP:CH2	2.74	0.71
2:D:91:ASP:OD1	2:D:92:VAL:N	2.23	0.71
2:C:276:ALA:HA	2:C:353:VAL:HG22	1.73	0.70
1:B:217:VAL:O	1:B:220:THR:CG2	2.38	0.70
1:A:160:VAL:O	1:A:164:VAL:HG23	1.91	0.70
2:D:276:ALA:HA	2:D:353:VAL:HG22	1.73	0.70
2:D:250:GLU:O	2:D:253:LEU:N	2.25	0.69
2:C:250:GLU:O	2:C:254:THR:N	2.27	0.68
2:D:250:GLU:O	2:D:254:THR:N	2.24	0.68
1:B:168:LEU:O	1:B:171:THR:CG2	2.40	0.68
1:B:171:THR:HG23	1:B:172:VAL:N	2.09	0.67
1:A:541:GLU:O	1:A:545:LEU:N	2.22	0.67
2:D:235:ILE:HB	2:D:252:ILE:CD1	2.26	0.66
1:A:433:GLU:N	1:A:460:SER:O	2.29	0.65
2:D:102:GLN:OE1	2:D:106:LYS:NZ	2.30	0.65
2:C:102:GLN:OE1	2:C:106:LYS:NZ	2.30	0.65
2:D:371:ASP:N	2:D:375:PHE:O	2.30	0.65
1:A:337:ILE:HD11	1:A:374:VAL:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:HG23	1:A:172:VAL:N	2.12	0.64
2:C:371:ASP:N	2:C:375:PHE:O	2.30	0.64
1:A:564:HIS:O	1:A:568:VAL:HG23	1.98	0.64
2:D:169:MET:O	2:D:173:VAL:HG23	1.98	0.63
2:C:9:HIS:N	2:C:48:ASN:OD1	2.23	0.63
1:B:119:MET:O	1:B:180:ARG:NH2	2.31	0.63
1:A:395:LEU:HD12	1:A:396:LEU:N	2.14	0.63
1:B:85:ILE:HD13	1:B:94:LEU:HD12	1.79	0.63
2:C:169:MET:O	2:C:173:VAL:HG23	1.98	0.63
1:A:395:LEU:HD12	1:A:396:LEU:H	1.62	0.62
2:C:235:ILE:HB	2:C:252:ILE:CD1	2.27	0.62
1:B:221:ILE:HG21	1:B:269:ILE:HG21	1.82	0.62
1:B:188:GLU:OE1	2:D:72:ARG:NH2	2.34	0.61
1:A:154:ILE:N	1:A:369:GLN:OE1	2.34	0.60
1:A:439:MET:SD	1:A:457:LEU:HD21	2.41	0.60
1:A:458:VAL:HG13	1:A:458:VAL:O	2.01	0.60
1:B:217:VAL:CA	1:B:220:THR:HG22	2.31	0.60
1:A:358:ASN:OD1	1:A:359:ALA:N	2.33	0.60
1:A:400:LEU:HD11	1:A:540:MET:SD	2.42	0.60
2:D:320:VAL:HB	2:D:341:THR:OG1	2.02	0.60
2:D:9:HIS:N	2:D:48:ASN:OD1	2.23	0.59
1:B:204:LEU:HD12	1:B:208:LEU:HD12	1.83	0.59
2:D:369:VAL:O	2:D:369:VAL:HG23	2.03	0.59
1:A:409:VAL:HG22	1:A:498:LEU:HD11	1.85	0.59
2:D:105:ARG:NH2	2:D:133:VAL:O	2.35	0.59
1:A:221:ILE:HG21	1:A:269:ILE:HG21	1.85	0.59
1:B:137:GLN:OE1	1:B:173:ARG:NH2	2.35	0.59
1:B:217:VAL:HA	1:B:220:THR:HG22	1.83	0.58
2:C:369:VAL:HG23	2:C:369:VAL:O	2.03	0.58
2:D:201:ARG:HG2	2:D:230:ARG:NH1	2.19	0.58
2:D:381:ILE:HG13	2:D:381:ILE:O	2.04	0.57
2:C:105:ARG:NH2	2:C:133:VAL:O	2.36	0.57
1:A:561:ILE:HG23	1:A:568:VAL:HG21	1.87	0.57
1:B:85:ILE:HD13	1:B:94:LEU:CD1	2.35	0.57
2:C:75:ASN:HA	2:C:108:MET:SD	2.45	0.57
2:C:381:ILE:HG13	2:C:381:ILE:O	2.04	0.56
1:A:542:ALA:O	1:A:546:ASP:HB2	2.06	0.56
2:D:75:ASN:HA	2:D:108:MET:SD	2.45	0.56
1:A:538:LYS:HG3	1:A:539:ASP:N	2.21	0.56
1:A:217:VAL:HA	1:A:220:THR:HG22	1.88	0.56
1:A:115:LEU:HD23	1:A:172:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:366:PRO:HB3	2:C:381:ILE:HG22	1.88	0.56
1:B:217:VAL:HA	1:B:220:THR:CG2	2.35	0.55
2:D:248:THR:O	2:D:248:THR:HG22	2.06	0.55
2:D:366:PRO:HB3	2:D:381:ILE:HG22	1.89	0.55
1:A:217:VAL:CA	1:A:220:THR:HG22	2.37	0.55
2:C:248:THR:HG22	2:C:248:THR:O	2.06	0.55
1:A:277:ASN:OD1	1:A:278:VAL:N	2.39	0.55
1:B:219:GLN:O	1:B:223:LEU:HD13	2.07	0.55
2:C:350:GLU:O	2:C:350:GLU:HG3	2.07	0.55
1:A:409:VAL:CG2	1:A:498:LEU:HD11	2.38	0.54
1:A:401:LYS:O	1:A:537:THR:OG1	2.26	0.54
2:C:211:GLN:NE2	2:C:216:LYS:O	2.40	0.54
1:A:347:HIS:O	1:A:347:HIS:ND1	2.39	0.54
2:D:325:GLN:HE22	2:D:341:THR:HG23	1.73	0.54
1:A:168:LEU:O	1:A:171:THR:CG2	2.46	0.54
1:B:59:VAL:O	1:B:63:LEU:HD23	2.07	0.54
2:D:211:GLN:NE2	2:D:216:LYS:O	2.40	0.54
2:D:284:LEU:HD13	2:D:303:GLU:OE1	2.08	0.54
2:C:360:ILE:CD1	2:C:384:SER:OG	2.55	0.53
1:A:542:ALA:HA	1:A:545:LEU:HG	1.89	0.53
1:B:41:MET:HE2	1:B:160:VAL:HG11	1.90	0.53
2:D:75:ASN:HB3	2:D:77:LEU:HD12	1.90	0.53
2:D:371:ASP:OD1	2:D:372:ASP:N	2.42	0.53
2:C:250:GLU:OE1	2:D:292:GLY:N	2.42	0.53
1:B:234:ILE:HG13	1:B:234:ILE:O	2.08	0.53
1:A:541:GLU:O	1:A:544:MET:N	2.42	0.53
2:C:284:LEU:HD13	2:C:303:GLU:OE1	2.08	0.53
2:C:371:ASP:OD1	2:C:372:ASP:N	2.42	0.52
1:B:94:LEU:CD2	1:B:98:ILE:HD11	2.39	0.52
2:D:339:VAL:HG13	2:D:339:VAL:O	2.10	0.52
1:A:234:ILE:HG13	1:A:234:ILE:O	2.10	0.52
2:C:75:ASN:HB3	2:C:77:LEU:HD12	1.90	0.52
2:D:284:LEU:HD22	2:D:303:GLU:OE1	2.10	0.52
1:B:171:THR:CG2	1:B:172:VAL:N	2.72	0.52
2:D:121:ARG:NH1	2:D:132:GLU:OE2	2.38	0.52
1:A:190:ALA:O	1:A:195:SER:OG	2.26	0.52
1:B:102:LEU:O	1:B:106:LEU:HD13	2.10	0.52
1:B:129:VAL:O	1:B:132:ILE:N	2.42	0.52
2:C:121:ARG:NH1	2:C:132:GLU:OE2	2.38	0.52
2:C:284:LEU:HD22	2:C:303:GLU:OE1	2.10	0.52
2:C:208:LEU:HD11	2:C:231:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:ILE:HG22	2:D:367:LEU:HD13	1.88	0.52
1:A:546:ASP:OD1	1:A:551:LYS:HD2	2.09	0.52
2:C:116:GLY:O	2:C:177:ARG:NH1	2.42	0.51
1:B:41:MET:CE	1:B:160:VAL:HG11	2.41	0.51
2:D:116:GLY:O	2:D:177:ARG:NH1	2.42	0.51
1:A:142:PHE:HB3	1:B:247:VAL:HG21	1.92	0.51
1:A:266:ALA:HB3	1:B:138:THR:HG21	1.92	0.51
2:C:339:VAL:O	2:C:339:VAL:HG13	2.10	0.51
1:A:217:VAL:HA	1:A:220:THR:CG2	2.40	0.51
2:C:7:ILE:HD12	2:C:49:PHE:CZ	2.45	0.51
2:D:208:LEU:HD11	2:D:231:ILE:HG22	1.92	0.51
2:D:343:ASP:O	2:D:344:VAL:HG23	2.11	0.50
1:B:156:VAL:HG12	1:B:237:PRO:HD2	1.92	0.50
2:C:312:ASP:OD1	2:C:313:LYS:N	2.44	0.50
2:C:343:ASP:O	2:C:344:VAL:HG23	2.11	0.50
1:A:545:LEU:HD12	1:A:546:ASP:N	2.27	0.50
1:A:239:LEU:N	1:A:239:LEU:HD12	2.26	0.50
2:D:334:GLN:HG3	2:D:335:PRO:HD2	1.94	0.50
2:D:7:ILE:HD12	2:D:49:PHE:CZ	2.46	0.50
1:A:405:VAL:HG12	1:A:406:GLY:N	2.27	0.50
2:C:334:GLN:HG3	2:C:335:PRO:HD2	1.94	0.49
2:D:234:ARG:HG2	2:D:247:GLY:HA3	1.95	0.49
1:A:171:THR:CG2	1:A:172:VAL:N	2.74	0.49
1:A:37:GLY:O	1:A:41:MET:HG3	2.13	0.49
2:D:228:ALA:O	2:D:232:GLY:N	2.43	0.49
2:C:234:ARG:HG2	2:C:247:GLY:HA3	1.95	0.49
2:C:123:ILE:HD11	2:C:165:LEU:CD1	2.40	0.49
2:D:226:ASN:O	2:D:230:ARG:HG3	2.13	0.49
1:A:327:TYR:HB3	1:A:337:ILE:HG13	1.95	0.49
1:A:413:MET:SD	1:A:478:ASP:HB2	2.53	0.48
1:A:322:LYS:O	1:A:523:ASN:ND2	2.43	0.48
1:A:554:GLU:O	1:A:558:LYS:HG3	2.13	0.48
2:C:307:SER:HG	5:D:502:2BA:HO2A	1.54	0.48
2:D:352:LEU:HB3	2:D:356:ILE:HG23	1.95	0.48
1:A:239:LEU:HD21	1:A:261:SER:OG	2.13	0.48
1:A:538:LYS:HG3	1:A:539:ASP:H	1.78	0.48
2:D:10:LEU:HD11	2:D:85:ILE:HD11	1.96	0.48
1:A:356:LEU:HD11	1:A:361:ALA:HB2	1.95	0.48
2:D:123:ILE:HD11	2:D:165:LEU:CD1	2.40	0.47
2:D:248:THR:HB	2:D:251:GLU:OE1	2.14	0.47
1:A:335:ALA:HB1	1:A:543:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:LEU:HD11	2:C:85:ILE:HD11	1.96	0.47
2:C:352:LEU:HB3	2:C:356:ILE:HG23	1.95	0.47
2:D:312:ASP:OD1	2:D:313:LYS:N	2.44	0.47
2:C:228:ALA:O	2:C:232:GLY:N	2.43	0.47
1:B:256:PHE:CE2	1:B:260:ILE:HD11	2.50	0.47
2:C:248:THR:HB	2:C:251:GLU:OE1	2.14	0.47
1:B:188:GLU:HG2	2:D:77:LEU:HD22	1.97	0.46
1:A:23:THR:O	1:A:27:SER:HB3	2.16	0.46
1:B:157:VAL:N	1:B:158:PRO:HD2	2.30	0.46
2:D:71:LEU:HD11	2:D:188:MET:O	2.16	0.46
1:A:58:ALA:O	1:A:62:ILE:HG12	2.16	0.46
1:B:239:LEU:H	1:B:239:LEU:HD12	1.81	0.46
2:C:60:MET:HE3	2:C:60:MET:HB3	1.77	0.46
1:A:156:VAL:HG12	1:A:237:PRO:HD2	1.98	0.46
2:C:347:VAL:HG12	2:C:348:SER:N	2.31	0.45
1:A:167:ALA:O	1:A:170:PRO:HD2	2.16	0.45
2:C:10:LEU:CD1	2:C:85:ILE:HD11	2.46	0.45
2:C:172:ARG:NH1	2:C:206:GLU:OE1	2.49	0.45
2:D:10:LEU:CD1	2:D:85:ILE:HD11	2.46	0.45
1:A:34:GLN:O	1:A:38:THR:HG22	2.16	0.45
1:A:55:LEU:O	1:A:59:VAL:HG23	2.16	0.45
1:A:232:SER:HA	1:A:236:ALA:HB3	1.98	0.45
1:A:399:ASN:ND2	1:A:513:THR:HB	2.32	0.45
1:B:145:LEU:O	1:B:148:ALA:HB3	2.17	0.45
2:C:360:ILE:HA	2:C:367:LEU:HD11	1.99	0.45
2:D:58:VAL:HG12	2:D:59:ILE:N	2.32	0.45
2:D:347:VAL:HG12	2:D:348:SER:N	2.31	0.45
1:A:256:PHE:O	1:A:260:ILE:HG12	2.16	0.45
1:A:349:PHE:HE2	1:A:529:VAL:HG21	1.82	0.45
2:D:155:LEU:C	2:D:155:LEU:HD23	2.37	0.45
2:D:172:ARG:NH1	2:D:206:GLU:OE1	2.49	0.45
1:B:146:ILE:N	1:B:147:PRO:HD2	2.32	0.45
1:A:220:THR:HG23	1:A:221:ILE:N	2.31	0.45
1:A:266:ALA:HB3	1:B:138:THR:CG2	2.47	0.45
2:D:320:VAL:HG23	2:D:344:VAL:HG21	1.99	0.45
1:B:19:THR:O	1:B:23:THR:HG22	2.16	0.45
1:A:400:LEU:CD1	1:A:540:MET:SD	3.05	0.44
1:A:497:TYR:C	1:A:498:LEU:HD12	2.38	0.44
1:B:119:MET:SD	1:B:129:VAL:HG11	2.57	0.44
2:C:58:VAL:HG12	2:C:59:ILE:N	2.32	0.44
2:D:235:ILE:HG22	2:D:236:ALA:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:155:LEU:HD23	2:C:155:LEU:C	2.37	0.44
1:A:113:VAL:O	1:A:117:ILE:HG12	2.17	0.44
1:A:173:ARG:HG2	1:A:173:ARG:HH21	1.81	0.44
2:C:71:LEU:HD11	2:C:188:MET:O	2.16	0.44
2:D:123:ILE:CD1	2:D:165:LEU:HD11	2.45	0.44
1:A:168:LEU:N	1:A:169:PRO:CD	2.81	0.44
1:A:516:ARG:NH1	1:A:522:GLU:OE1	2.50	0.44
2:C:23:THR:O	2:C:26:GLU:HB2	2.18	0.44
1:A:229:VAL:HG21	1:A:262:LEU:HD13	1.98	0.44
2:D:23:THR:O	2:D:26:GLU:HB2	2.18	0.44
2:D:360:ILE:HA	2:D:367:LEU:HD11	1.99	0.44
1:A:432:ILE:H	1:A:439:MET:CE	2.30	0.44
1:B:166:PHE:O	1:B:223:LEU:HD23	2.18	0.44
1:B:229:VAL:HG21	1:B:262:LEU:HD13	1.99	0.44
2:C:307:SER:OG	5:D:502:2BA:O2'1	2.27	0.44
1:A:328:MET:SD	1:A:330:TRP:CZ3	3.10	0.44
2:D:161:TYR:O	2:D:164:GLN:HG2	2.18	0.44
1:B:168:LEU:C	1:B:171:THR:HG22	2.35	0.44
2:C:276:ALA:HB1	2:C:350:GLU:HB2	2.00	0.44
1:B:217:VAL:O	1:B:217:VAL:HG12	2.18	0.43
1:B:232:SER:HA	1:B:236:ALA:HB3	1.99	0.43
2:D:100:LEU:HD21	2:D:104:ARG:NH2	2.34	0.43
1:B:107:LEU:O	1:B:111:ILE:HG22	2.18	0.43
1:B:194:GLY:HA2	2:D:101:LEU:HD12	2.00	0.43
2:C:161:TYR:O	2:C:164:GLN:HG2	2.18	0.43
2:C:235:ILE:HG22	2:C:236:ALA:N	2.33	0.43
2:D:60:MET:HE3	2:D:60:MET:HB3	1.78	0.43
1:A:478:ASP:OD1	1:A:478:ASP:O	2.36	0.43
2:C:31:LYS:HD2	2:C:42:VAL:HG13	2.00	0.43
2:C:100:LEU:HD21	2:C:104:ARG:NH2	2.34	0.43
2:D:357:LEU:N	2:D:358:PRO:CD	2.81	0.43
1:A:539:ASP:C	1:A:541:GLU:N	2.71	0.43
1:B:148:ALA:HB1	1:B:158:PRO:CB	2.47	0.43
2:C:123:ILE:CD1	2:C:165:LEU:HD11	2.45	0.43
1:A:252:ILE:HG21	1:B:16:SER:HA	2.01	0.43
1:B:233:MET:HG3	1:B:234:ILE:HG23	1.99	0.43
2:C:320:VAL:HG23	2:C:344:VAL:HG21	1.99	0.43
2:D:124:LEU:O	2:D:124:LEU:HD23	2.19	0.43
1:B:96:SER:O	1:B:99:THR:HG22	2.18	0.43
2:D:244:MET:SD	2:D:246:ILE:HD12	2.59	0.43
1:A:340:LEU:O	1:A:340:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:276:ALA:HA	2:C:353:VAL:CG2	2.47	0.43
1:A:377:TRP:HZ3	1:A:405:VAL:HG22	1.84	0.43
1:B:168:LEU:N	1:B:169:PRO:CD	2.82	0.43
2:C:357:LEU:N	2:C:358:PRO:CD	2.81	0.43
1:B:156:VAL:HG12	1:B:237:PRO:CD	2.49	0.42
1:B:220:THR:HG23	1:B:221:ILE:N	2.33	0.42
1:B:113:VAL:O	1:B:117:ILE:HG12	2.20	0.42
2:C:366:PRO:HB3	2:C:381:ILE:CG2	2.49	0.42
1:A:154:ILE:HG22	1:A:155:GLY:N	2.35	0.42
1:B:26:PHE:N	1:B:26:PHE:CD1	2.87	0.42
1:B:78:THR:O	1:B:82:LEU:HG	2.19	0.42
2:C:13:ILE:HD13	2:C:42:VAL:HG23	2.01	0.42
2:C:244:MET:SD	2:C:246:ILE:HD12	2.59	0.42
2:D:336:LEU:O	2:D:337:LYS:HB3	2.19	0.42
1:A:346:GLU:OE2	1:A:346:GLU:HA	2.19	0.42
1:A:532:LYS:HB2	1:A:571:TRP:HA	2.01	0.42
1:B:215:ALA:O	1:B:219:GLN:HG3	2.19	0.42
2:D:116:GLY:O	2:D:177:ARG:NH2	2.51	0.42
1:A:239:LEU:HD12	1:A:239:LEU:H	1.85	0.42
2:C:124:LEU:HD23	2:C:124:LEU:O	2.19	0.42
2:C:320:VAL:HG12	2:C:321:VAL:N	2.34	0.42
2:D:154:LEU:HD23	2:D:154:LEU:H	1.84	0.42
2:D:287:ASN:OD1	2:D:313:LYS:HA	2.20	0.42
2:C:99:ASP:O	2:C:103:VAL:HG23	2.19	0.42
2:D:13:ILE:HD13	2:D:42:VAL:HG23	2.01	0.42
2:D:31:LYS:HD2	2:D:42:VAL:HG13	2.00	0.42
2:D:285:THR:HG22	2:D:286:THR:N	2.35	0.42
1:A:96:SER:O	1:A:99:THR:HG22	2.20	0.42
2:C:5:ILE:HG22	2:C:6:LYS:N	2.35	0.42
2:C:287:ASN:OD1	2:C:313:LYS:HA	2.20	0.42
2:D:5:ILE:HG22	2:D:6:LYS:N	2.35	0.42
2:D:99:ASP:O	2:D:103:VAL:HG23	2.19	0.42
2:D:192:PHE:HB3	2:D:200:ARG:HG3	2.02	0.42
1:A:338:ASN:ND2	1:A:553:PRO:HB2	2.35	0.42
2:C:154:LEU:HD23	2:C:154:LEU:H	1.84	0.42
2:C:336:LEU:O	2:C:337:LYS:HB3	2.19	0.42
2:D:225:LEU:HD22	2:D:265:VAL:HG12	2.02	0.42
2:C:356:ILE:O	2:C:359:ILE:HG12	2.20	0.41
2:D:366:PRO:HB3	2:D:381:ILE:CG2	2.49	0.41
2:D:334:GLN:HG3	2:D:335:PRO:CD	2.50	0.41
1:B:204:LEU:HD12	1:B:208:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASN:ND2	1:B:270:ASP:OD1	2.52	0.41
2:C:116:GLY:O	2:C:177:ARG:NH2	2.51	0.41
2:D:277:GLU:HB2	2:D:349:LYS:O	2.20	0.41
2:D:320:VAL:HG12	2:D:321:VAL:N	2.34	0.41
1:A:113:VAL:HB	1:A:114:PRO:HD3	2.01	0.41
1:A:232:SER:HB3	1:A:240:GLY:HA3	2.03	0.41
1:A:337:ILE:CD1	1:A:374:VAL:HG22	2.50	0.41
1:B:66:LEU:C	1:B:66:LEU:HD23	2.41	0.41
2:C:136:VAL:HG23	2:C:141:ARG:HG3	2.03	0.41
2:C:277:GLU:HB2	2:C:349:LYS:O	2.20	0.41
2:C:285:THR:HG22	2:C:286:THR:N	2.35	0.41
2:C:368:ALA:HB1	2:C:376:LEU:HD13	2.02	0.41
1:A:540:MET:O	1:A:543:VAL:HB	2.21	0.41
2:C:192:PHE:HB3	2:C:200:ARG:HG3	2.02	0.41
2:C:129:TYR:CE1	2:C:133:VAL:HG11	2.56	0.41
2:D:201:ARG:HG2	2:D:230:ARG:HH12	1.83	0.41
1:A:490:PHE:HZ	1:A:497:TYR:CE1	2.39	0.41
1:B:45:THR:O	1:B:49:THR:HG22	2.21	0.41
1:B:260:ILE:O	1:B:263:VAL:HG12	2.21	0.41
2:D:356:ILE:O	2:D:359:ILE:HG12	2.20	0.41
1:A:399:ASN:HD21	1:A:513:THR:HB	1.86	0.41
1:B:34:GLN:O	1:B:38:THR:HG22	2.20	0.41
1:B:219:GLN:O	1:B:223:LEU:CD1	2.69	0.41
2:C:334:GLN:HG3	2:C:335:PRO:CD	2.50	0.41
2:D:286:THR:OG1	2:D:308:LEU:HD13	2.21	0.41
2:D:368:ALA:HB1	2:D:376:LEU:HD13	2.01	0.41
1:A:74:PHE:CE1	1:A:271:ARG:HB2	2.55	0.41
1:A:504:THR:HG23	1:A:505:MET:N	2.36	0.41
2:C:329:ALA:HB1	2:C:334:GLN:O	2.21	0.41
2:D:100:LEU:HD21	2:D:104:ARG:HH21	1.87	0.41
2:D:345:GLY:O	2:D:347:VAL:HG23	2.21	0.41
1:A:324:ASP:N	1:A:371:ASP:OD2	2.43	0.40
2:C:225:LEU:HD22	2:C:265:VAL:HG12	2.02	0.40
1:A:404:LYS:CG	1:A:497:TYR:HE2	2.34	0.40
1:A:38:THR:HG23	1:A:39:VAL:N	2.37	0.40
1:A:441:ALA:O	1:A:445:THR:N	2.47	0.40
2:D:115:PHE:HE1	2:D:195:LEU:HD21	1.87	0.40
1:A:130:GLN:N	1:A:131:PRO:CD	2.84	0.40
1:B:130:GLN:N	1:B:131:PRO:CD	2.84	0.40
1:B:206:PHE:O	1:B:208:LEU:N	2.54	0.40
2:D:129:TYR:CE1	2:D:133:VAL:HG11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:VAL:HG23	2:D:141:ARG:HG3	2.03	0.40
1:A:464:ALA:O	1:A:467:VAL:HG12	2.21	0.40
2:D:329:ALA:HB1	2:D:334:GLN:O	2.21	0.40
2:D:357:LEU:O	2:D:360:ILE:HG13	2.22	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	522/585 (89%)	487 (93%)	35 (7%)	0	100	100
1	B	270/585 (46%)	259 (96%)	11 (4%)	0	100	100
2	C	378/408 (93%)	342 (90%)	36 (10%)	0	100	100
2	D	378/408 (93%)	342 (90%)	36 (10%)	0	100	100
All	All	1548/1986 (78%)	1430 (92%)	118 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	437/484 (90%)	437 (100%)	0	100	100
1	B	221/484 (46%)	221 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	332/356 (93%)	325 (98%)	7 (2%)	53	79
2	D	332/356 (93%)	326 (98%)	6 (2%)	59	81
All	All	1322/1680 (79%)	1309 (99%)	13 (1%)	77	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	60	MET
2	C	77	LEU
2	C	104	ARG
2	C	224	ASP
2	C	250	GLU
2	C	334	GLN
2	C	361	TYR
2	D	60	MET
2	D	77	LEU
2	D	104	ARG
2	D	224	ASP
2	D	334	GLN
2	D	361	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
1	A	382	HIS
1	A	399	ASN
2	D	325	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
4	ANP	C	501	-	29,33,33	1.19	5 (17%)	31,52,52	1.11	2 (6%)
3	BET	A	601	-	7,7,7	1.03	1 (14%)	10,10,10	0.49	0
5	2BA	D	502	-	44,50,50	1.38	9 (20%)	50,78,78	1.17	2 (4%)
4	ANP	D	501	-	29,33,33	1.19	5 (17%)	31,52,52	1.11	2 (6%)

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
4	ANP	C	501	-	-	4/14/38/38	0/3/3/3
3	BET	A	601	-	-	5/5/5/5	-
5	2BA	D	502	-	-	8/22/62/62	0/6/7/7
4	ANP	D	501	-	-	4/14/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	ANP	PG-O1G	3.10	1.51	1.46
4	D	501	ANP	PG-O1G	3.06	1.51	1.46
4	D	501	ANP	PB-O1B	2.98	1.50	1.46
4	C	501	ANP	PB-O1B	2.92	1.50	1.46
5	D	502	2BA	P-O3'1	2.70	1.67	1.60
3	A	601	BET	OXT-C	-2.68	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	2BA	P1-O3'	2.64	1.67	1.60
5	D	502	2BA	O5'1-C5'1	-2.36	1.35	1.44
5	D	502	2BA	O3'-C3'	-2.26	1.35	1.44
5	D	502	2BA	O2'-C2'	-2.25	1.37	1.43
5	D	502	2BA	O3'1-C3'1	-2.24	1.36	1.44
4	C	501	ANP	PB-O2B	-2.23	1.50	1.56
4	D	501	ANP	PB-O2B	-2.22	1.50	1.56
5	D	502	2BA	O5'-C5'	-2.20	1.36	1.44
5	D	502	2BA	C2-N1	2.18	1.38	1.33
5	D	502	2BA	O2'1-C2'1	-2.17	1.37	1.43
4	C	501	ANP	PG-O2G	-2.14	1.51	1.56
4	D	501	ANP	PG-O2G	-2.11	1.51	1.56
4	C	501	ANP	PG-O3G	-2.10	1.51	1.56
4	D	501	ANP	PG-O3G	-2.07	1.51	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	501	ANP	O2B-PB-O1B	4.15	118.63	109.92
4	D	501	ANP	O2B-PB-O1B	4.12	118.56	109.92
5	D	502	2BA	O2P-P-O1P	3.38	128.95	112.24
5	D	502	2BA	O2P1-P1-O1P1	3.30	128.56	112.24
4	C	501	ANP	C5-C6-N6	2.24	123.76	120.35
4	D	501	ANP	C5-C6-N6	2.21	123.71	120.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	BET	O-C-CA-N
3	A	601	BET	OXT-C-CA-N
4	C	501	ANP	PG-N3B-PB-O1B
4	C	501	ANP	PG-N3B-PB-O3A
4	D	501	ANP	PG-N3B-PB-O1B
4	D	501	ANP	PG-N3B-PB-O3A
5	D	502	2BA	C5'-O5'-P-O1P
5	D	502	2BA	C5'1-O5'1-P1-O1P1
4	C	501	ANP	O4'-C4'-C5'-O5'
4	C	501	ANP	C3'-C4'-C5'-O5'
4	D	501	ANP	O4'-C4'-C5'-O5'
4	D	501	ANP	C3'-C4'-C5'-O5'
5	D	502	2BA	O4'1-C4'1-C5'1-O5'1

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Mol	Chain	Res	Type	Atoms
3	A	601	BET	C-CA-N-C2
3	A	601	BET	C-CA-N-C3
3	A	601	BET	C-CA-N-C1
5	D	502	2BA	C3'1-C4'1-C5'1-O5'1
5	D	502	2BA	C5'1-O5'1-P1-O3'
5	D	502	2BA	C5'-O5'-P-O3'1
5	D	502	2BA	O4'-C4'-C5'-O5'
5	D	502	2BA	C3'1-O3'1-P-O5'

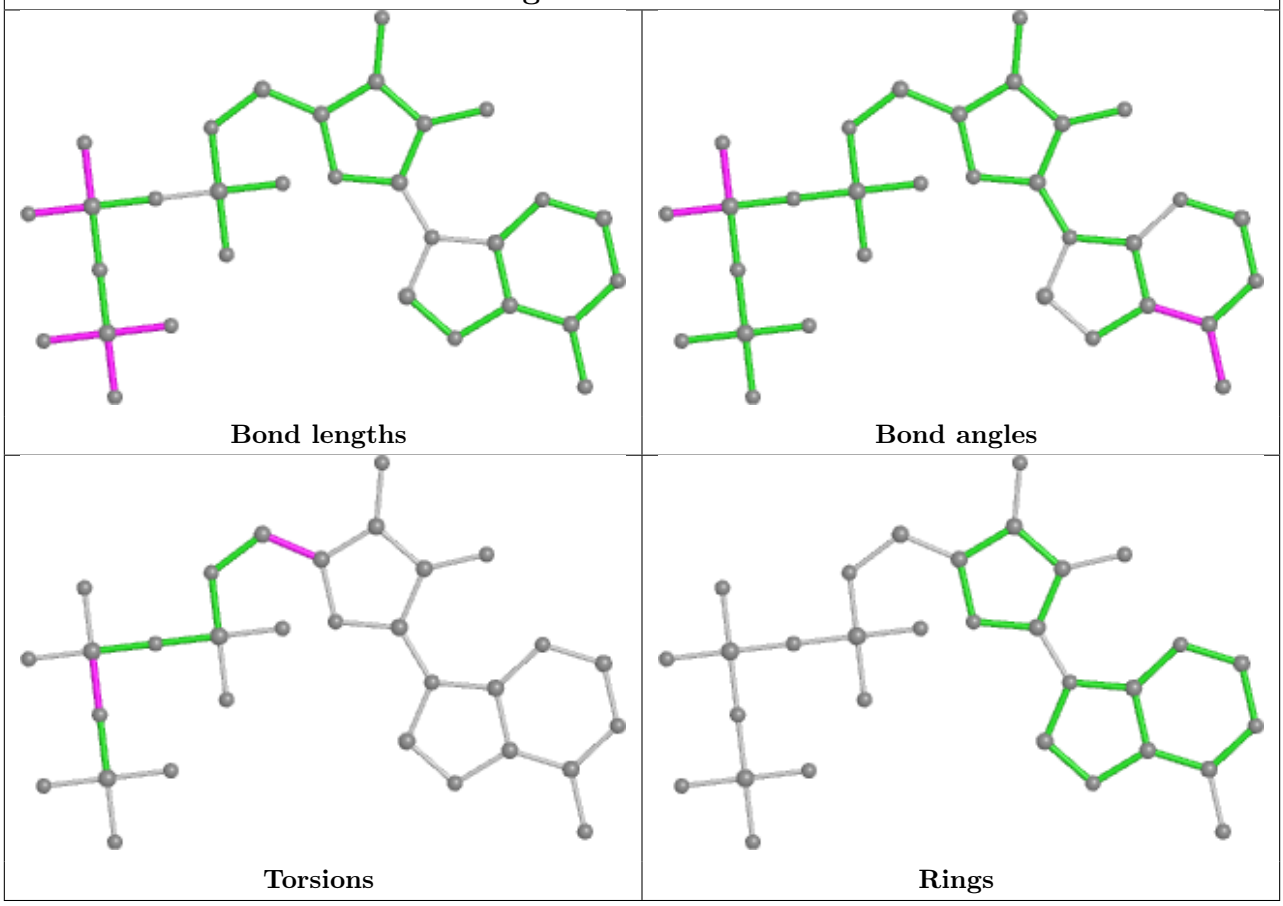
There are no ring outliers.

1 monomer is involved in 2 short contacts:

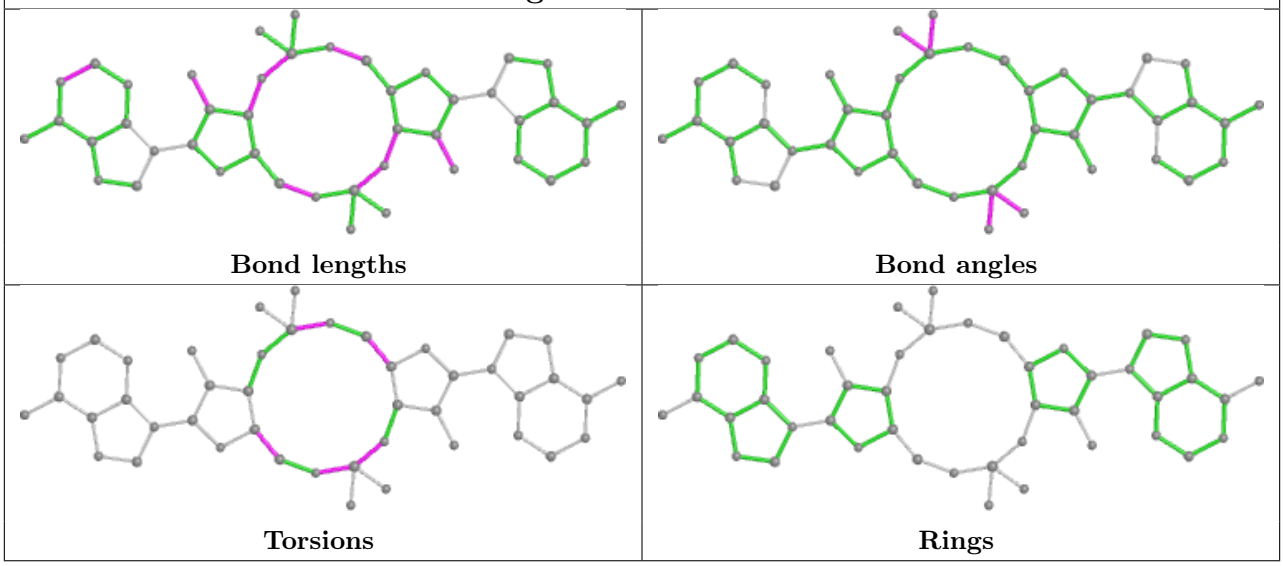
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	2BA	2	0

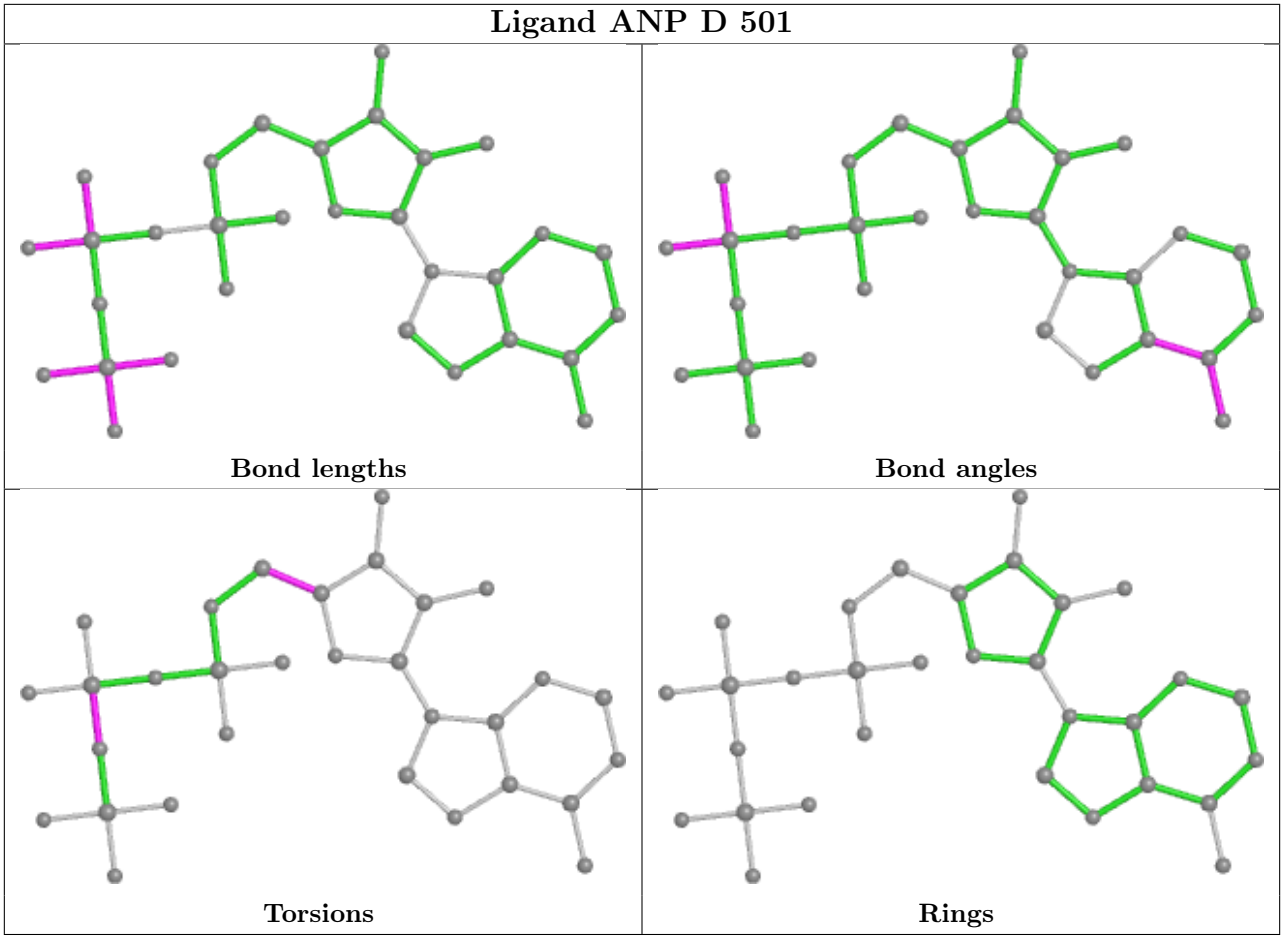
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand ANP C 501



Ligand 2BA D 502





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.

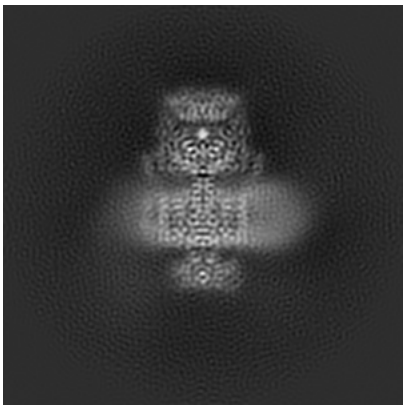
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11786. These allow visual inspection of the internal detail of the map and identification of artifacts.

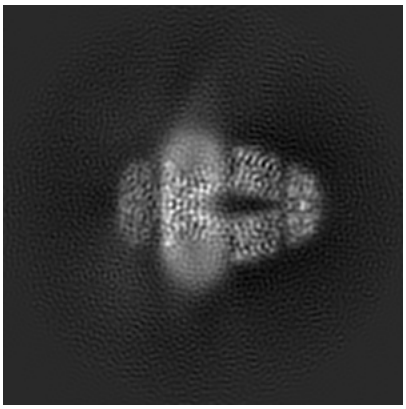
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

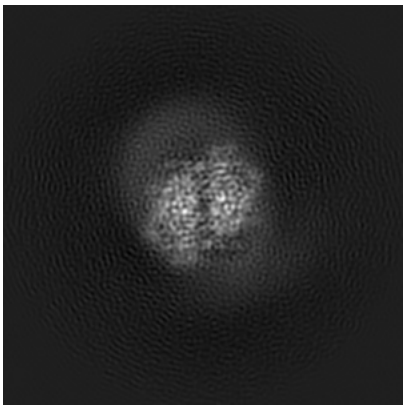
6.1.1 Primary map



X

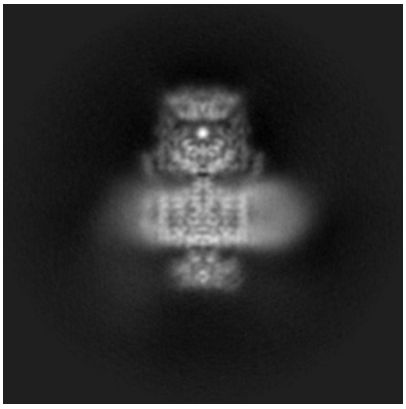


Y

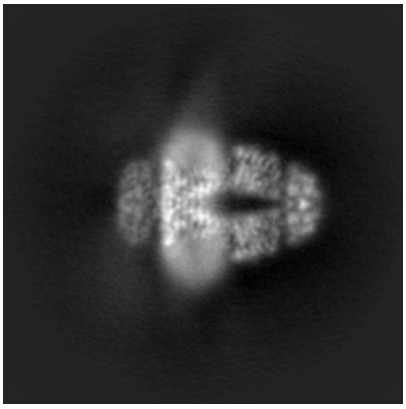


Z

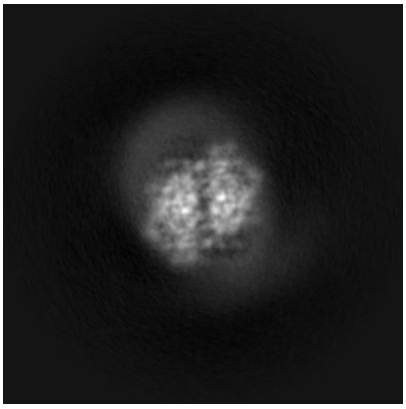
6.1.2 Raw map



X



Y

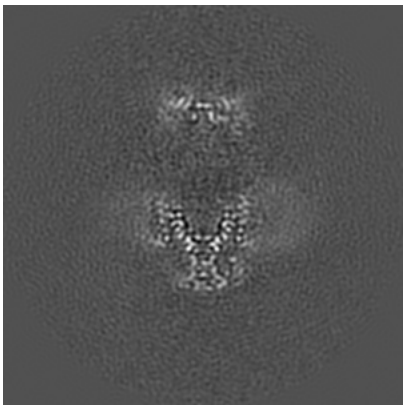


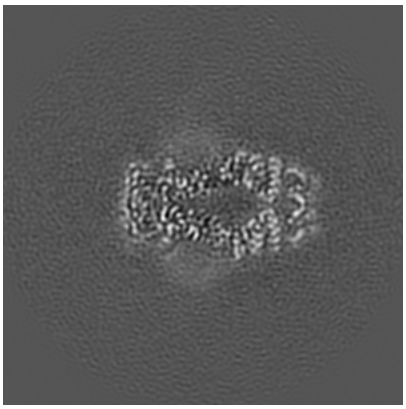
Z

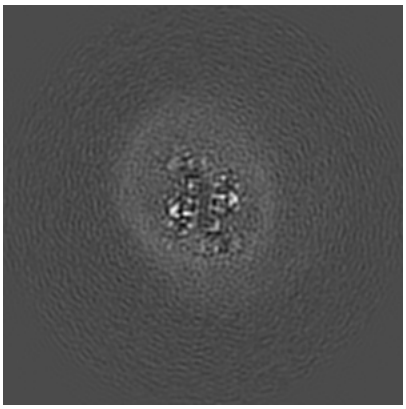
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

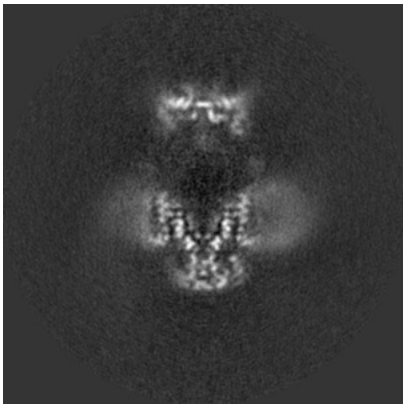
6.2.1 Primary map

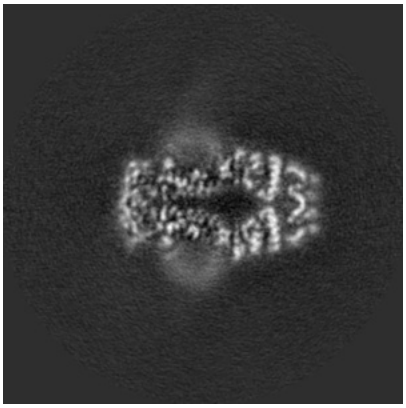

X Index: 128

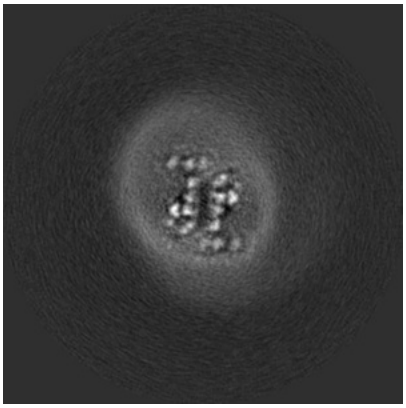

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

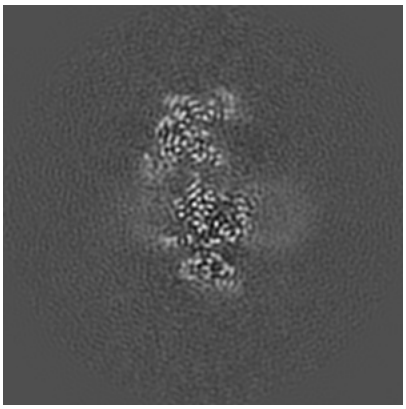

Y Index: 128

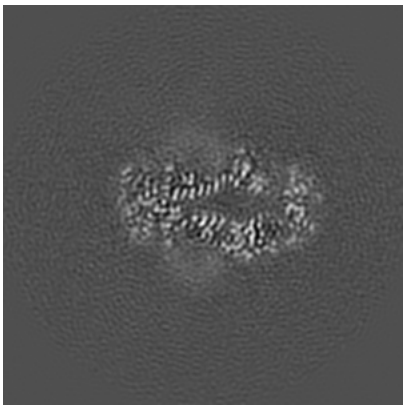

Z Index: 128

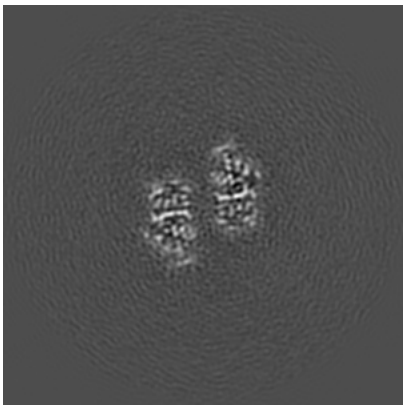
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

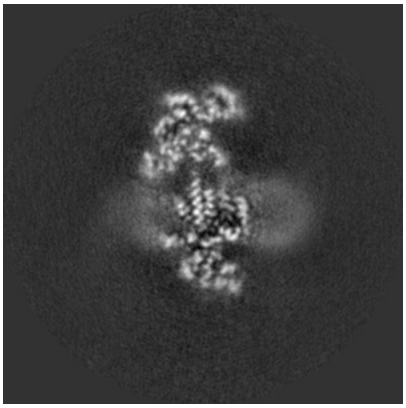
6.3.1 Primary map

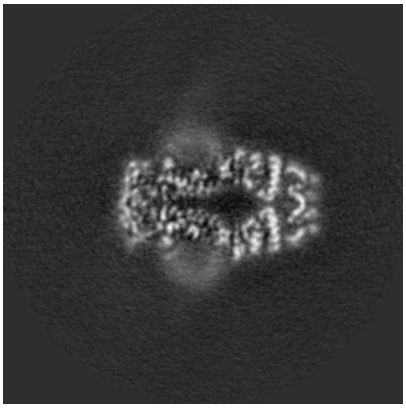

X Index: 117

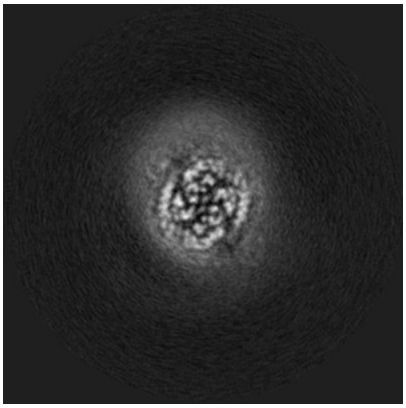

Y Index: 122


Z Index: 159

6.3.2 Raw map


X Index: 118

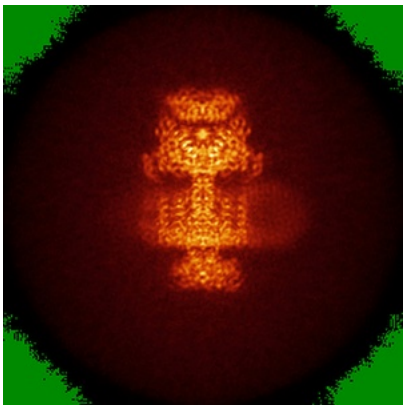

Y Index: 128

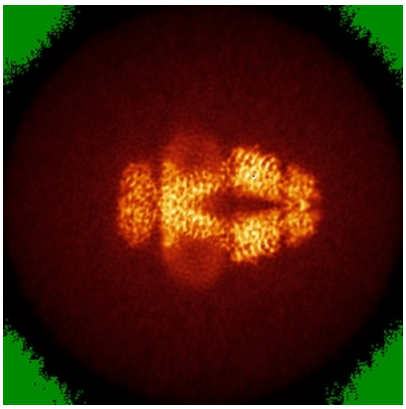

Z Index: 106

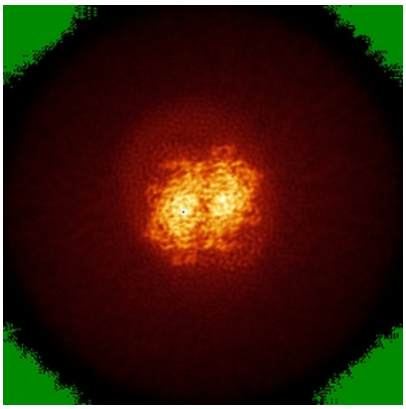
The images above show the largest variance slices of the map in three orthogonal directions.

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

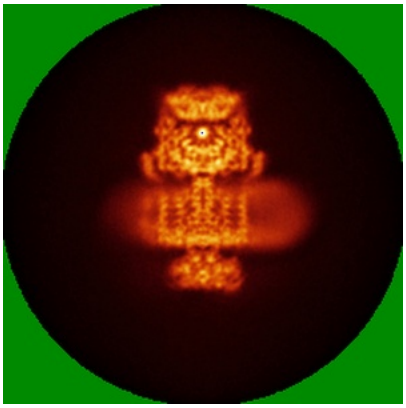
6.4.1 Primary map

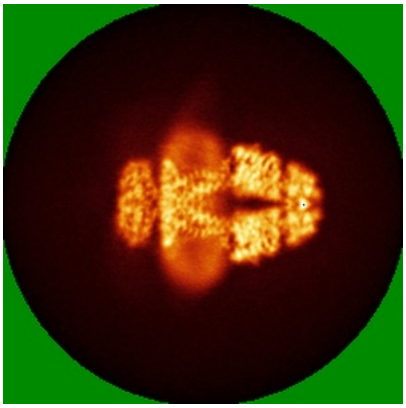

X

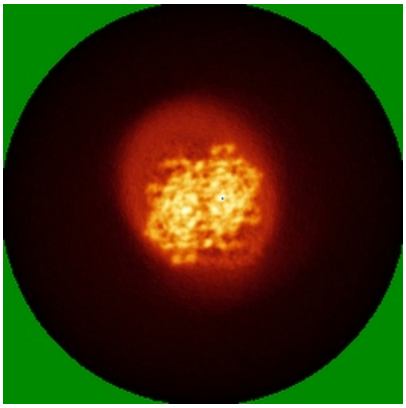

Y


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.

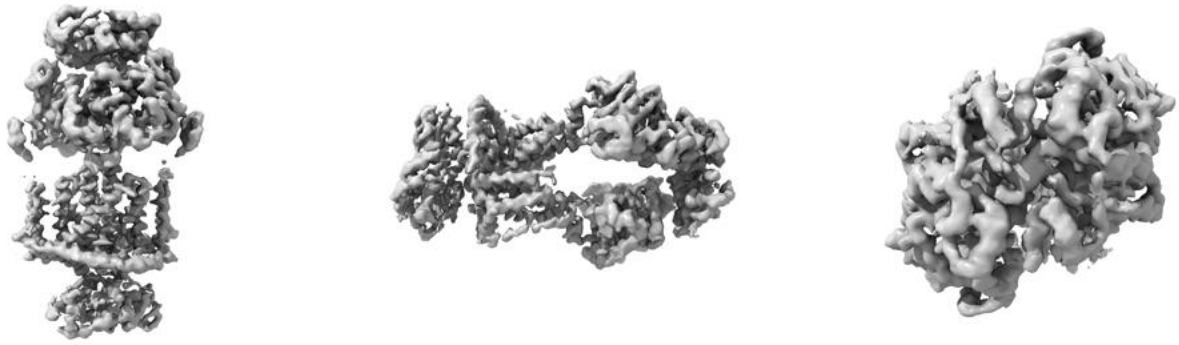
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0416. 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



X Y Z

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

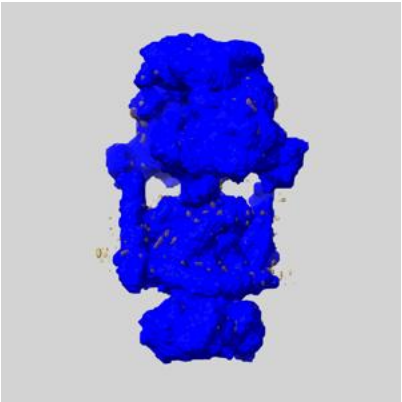
6.6 Mask visualisation (i)

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

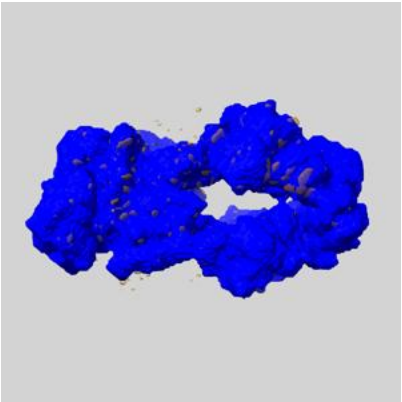
A mask typically either:

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

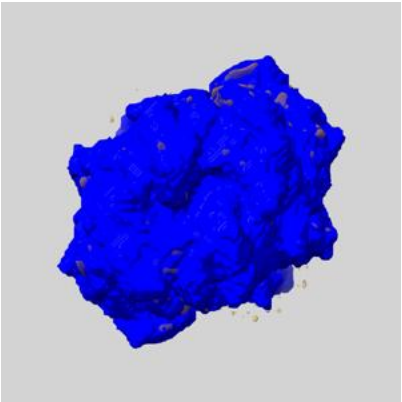
6.6.1 emd_11786_msk_1.map (i)



X



Y

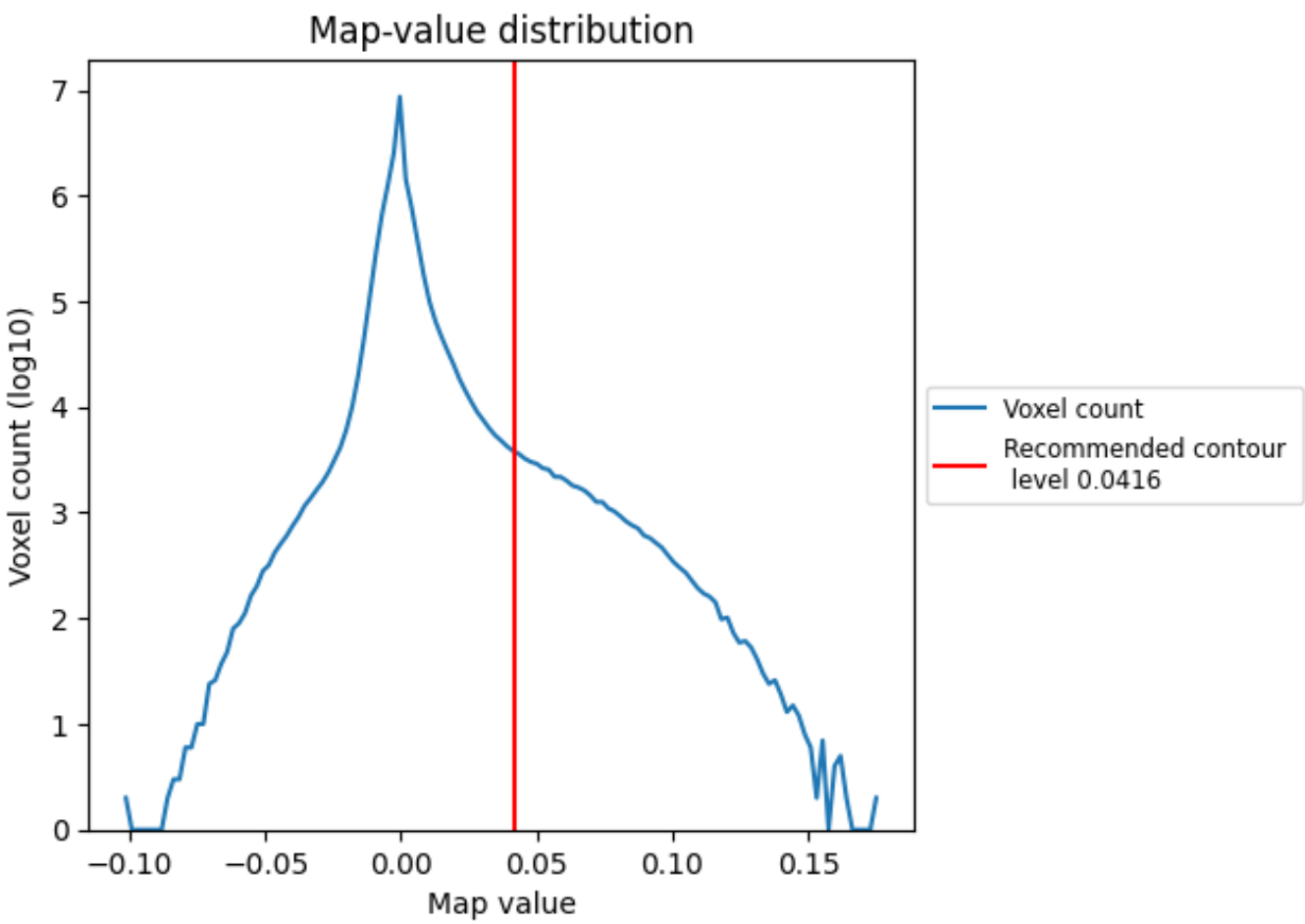


Z

7 Map analysis (i)

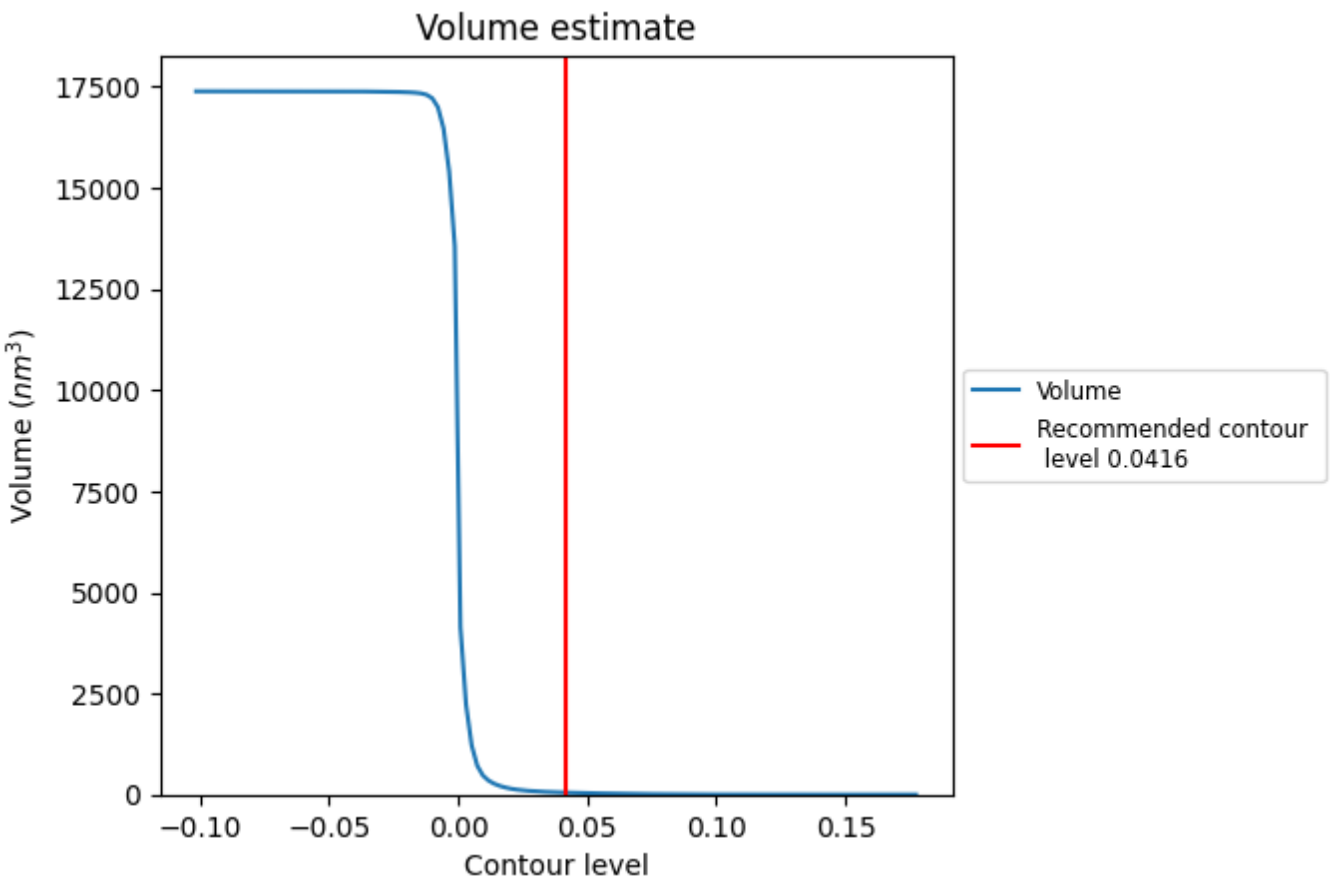
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

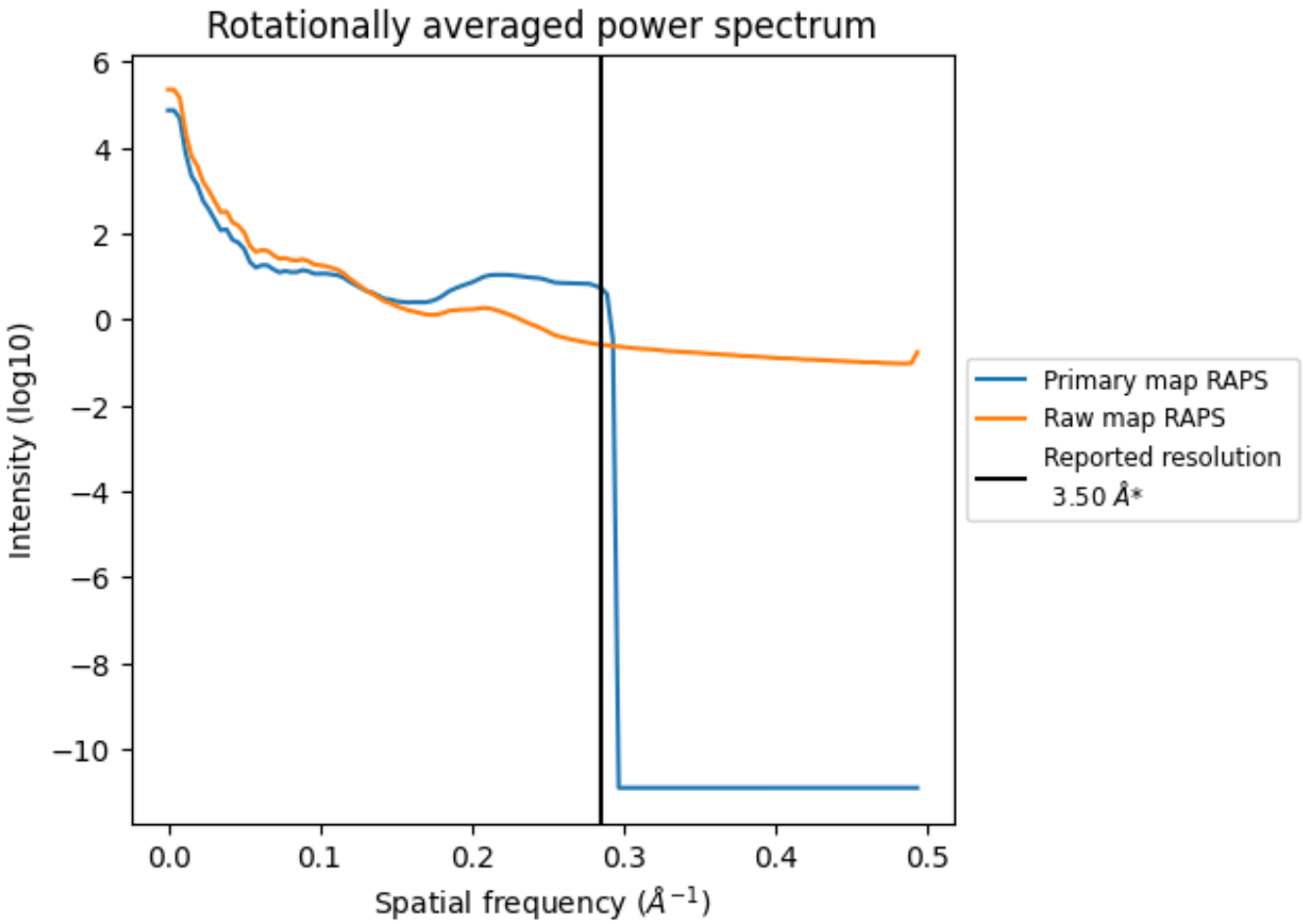
7.2 Volume estimate (i)



The volume at the recommended contour level is 49 nm^3; this corresponds to an approximate mass of 44 kDa.

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

7.3 Rotationally averaged power spectrum (i)

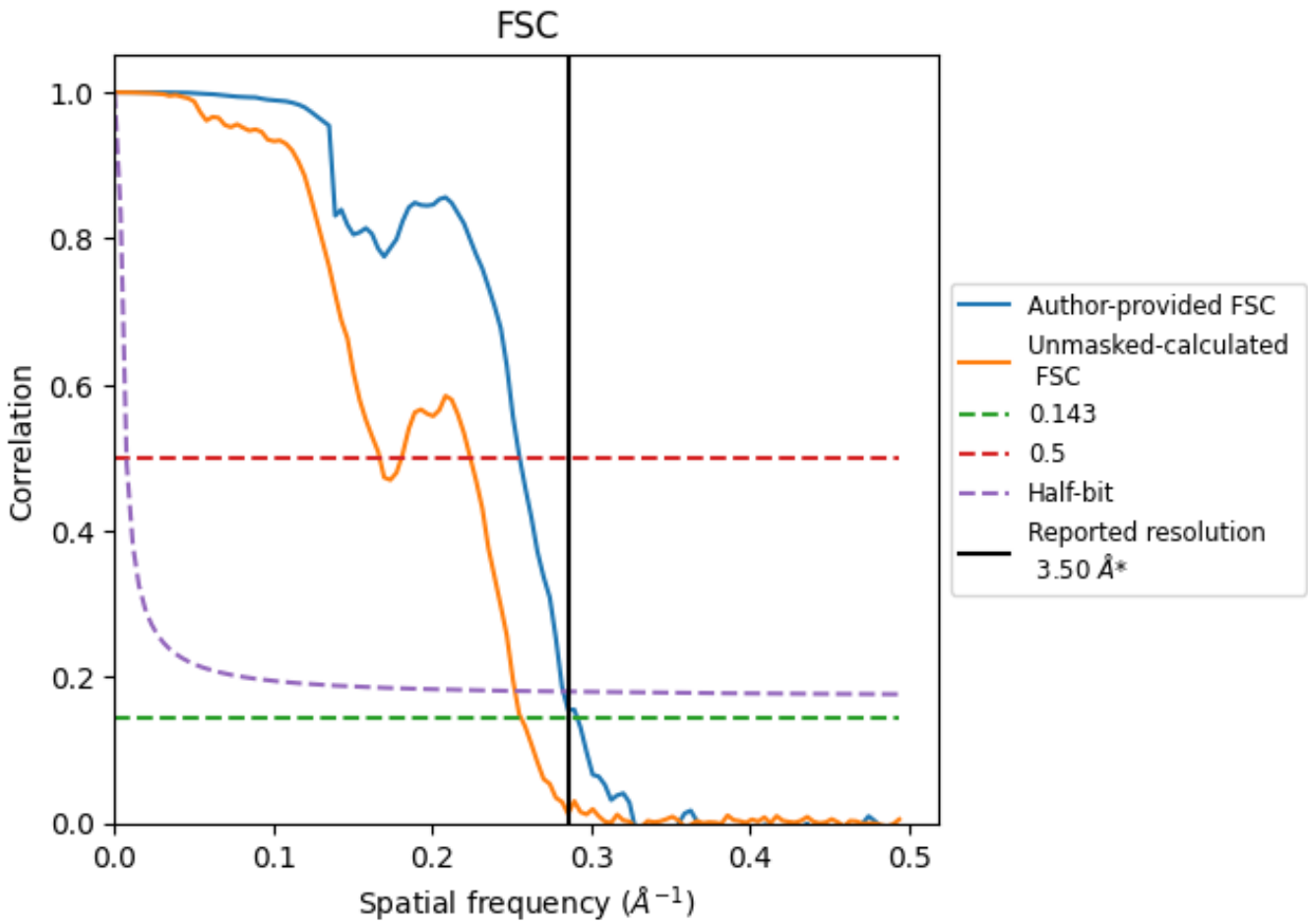


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

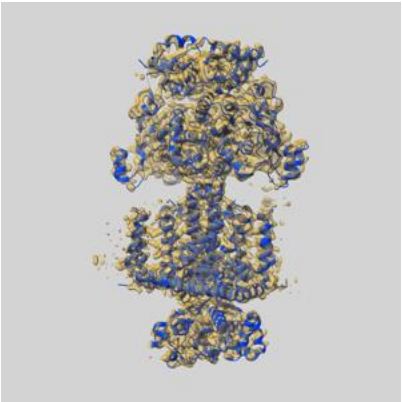
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.43	3.92	3.54
Unmasked-calculated*	3.90	5.99	3.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 3.5 by more than 10 %

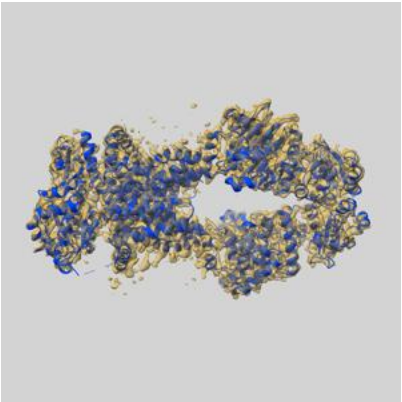
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11786 and PDB model 7AHH. Per-residue inclusion information can be found in section 3 on page 7.

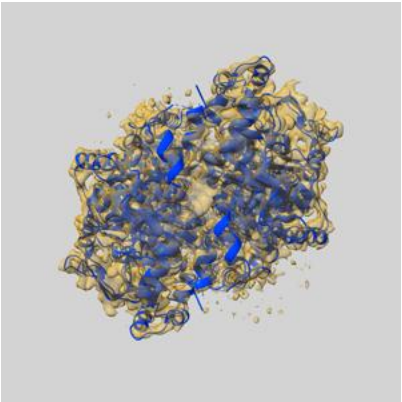
9.1 Map-model overlay (i)



X



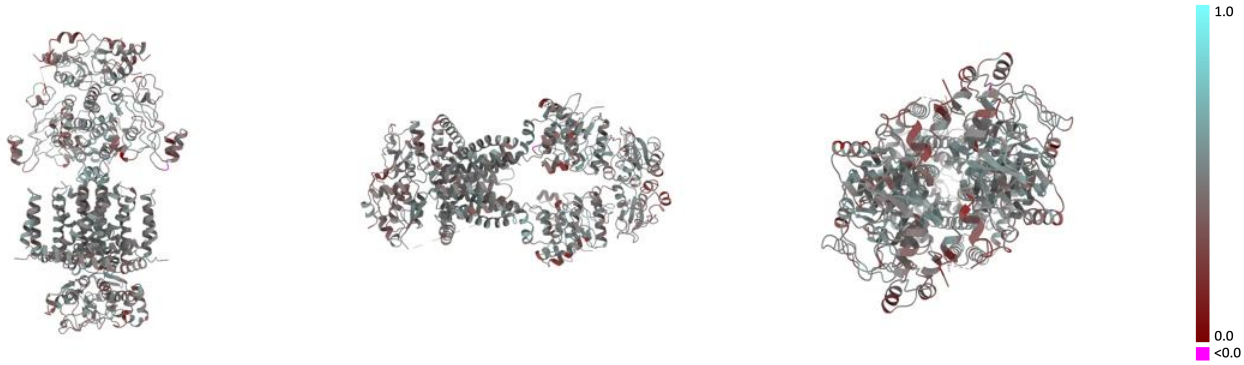
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0416 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

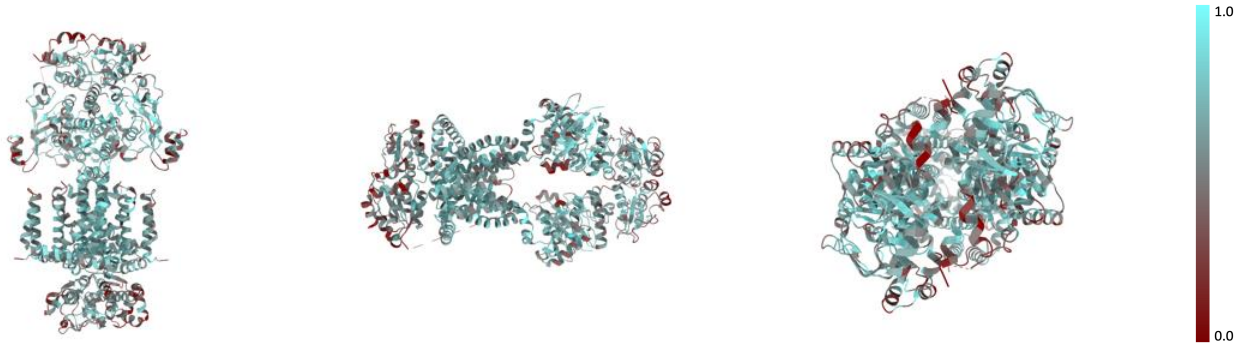
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

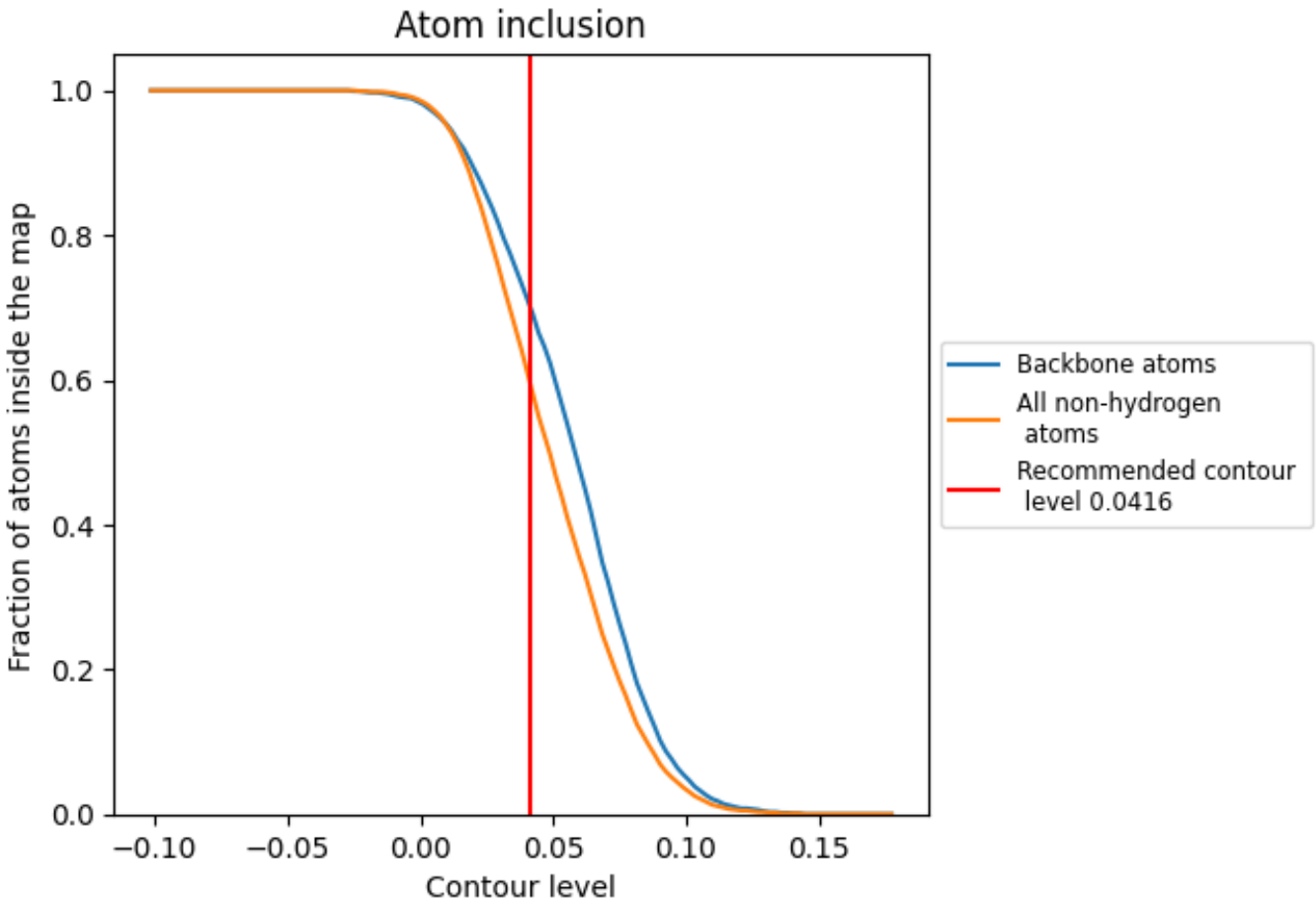
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0416).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0416) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5920	0.4630
A	0.5700	0.4680
B	0.6430	0.4870
C	0.5850	0.4560
D	0.5940	0.4480