



Full wwPDB EM Validation Report ⓘ

Jul 23, 2026 – 05:04 PM JST

PDB ID : 9UKF / pdb_00009ukf
EMDB ID : EMD-64237
Title : CryoEM structure of Brucella melitensis CobS(E142Q)-CobT complex with ATP (conformation 1)
Authors : Zhou, Y.L.; Chen, X.; Liu, L.
Deposited on : 2025-04-17
Resolution : 3.30 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:

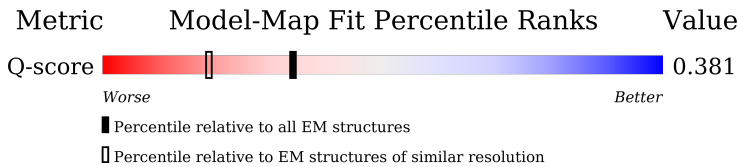
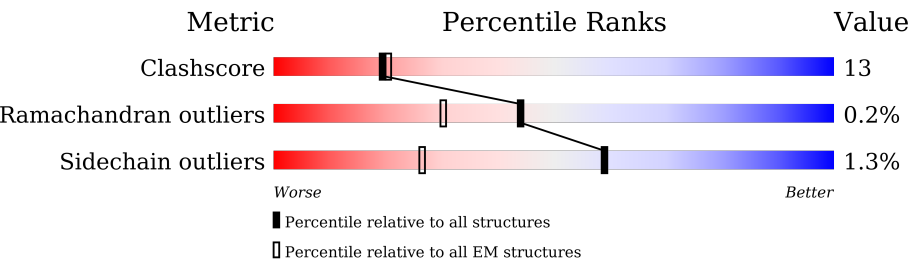
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	328	67%24%8%
1	B	328	63%28%9%
1	C	328	67%26%5%
1	D	328	73%23%

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Mol	Chain	Length	Quality of chain
1	E	328	74% 23%
1	F	328	67% 30%
2	G	637	19% 33% 14% 52%
2	a	637	24% 8% 68%
2	c	637	9% 23% 8% 68%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20302 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 Cobaltochelatase subunit CobS.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	320	Total	C	N	O	S	0	0
			2519	1596	442	471	10		
1	F	319	Total	C	N	O	S	0	0
			2514	1593	441	470	10		
1	A	302	Total	C	N	O	S	0	0
			2390	1515	420	445	10		
1	B	297	Total	C	N	O	S	0	0
			2357	1497	414	436	10		
1	C	312	Total	C	N	O	S	0	0
			2457	1556	431	460	10		
1	D	319	Total	C	N	O	S	0	0
			2514	1593	441	470	10		

There are 6 discrepancies between the modelled and reference sequences:

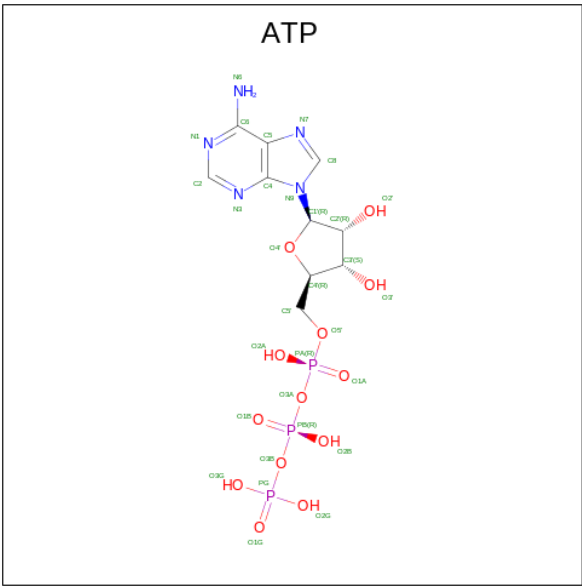
Chain	Residue	Modelled	Actual	Comment	Reference
E	142	GLN	GLU	engineered mutation	UNP A0AB36PZV1
F	142	GLN	GLU	engineered mutation	UNP A0AB36PZV1
A	142	GLN	GLU	engineered mutation	UNP A0AB36PZV1
B	142	GLN	GLU	engineered mutation	UNP A0AB36PZV1
C	142	GLN	GLU	engineered mutation	UNP A0AB36PZV1
D	142	GLN	GLU	engineered mutation	UNP A0AB36PZV1

- Molecule 2 is a protein called Cobaltochelatase subunit CobT.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	304	Total	C	N	O	S	0	0
			2423	1508	448	457	10		
2	a	201	Total	C	N	O	S	0	0
			1462	906	267	281	8		
2	c	203	Total	C	N	O	S	0	0
			1475	913	269	285	8		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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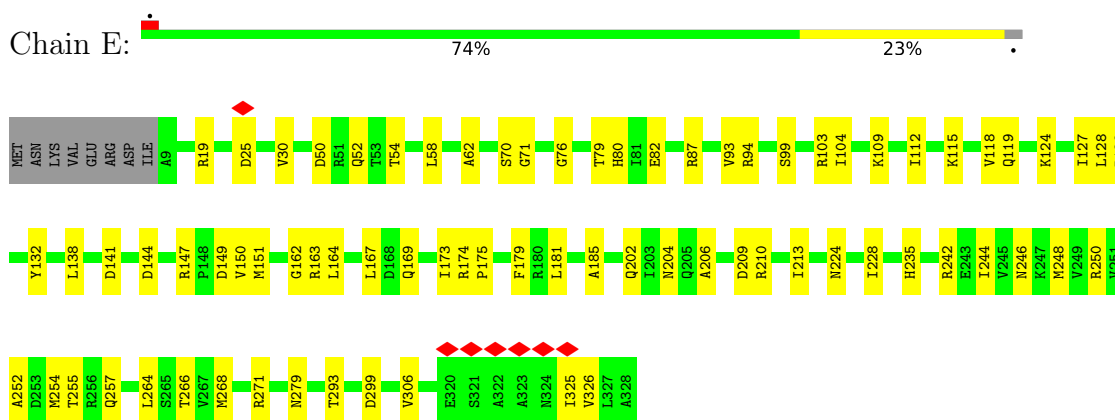
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	D	1	1	1	0

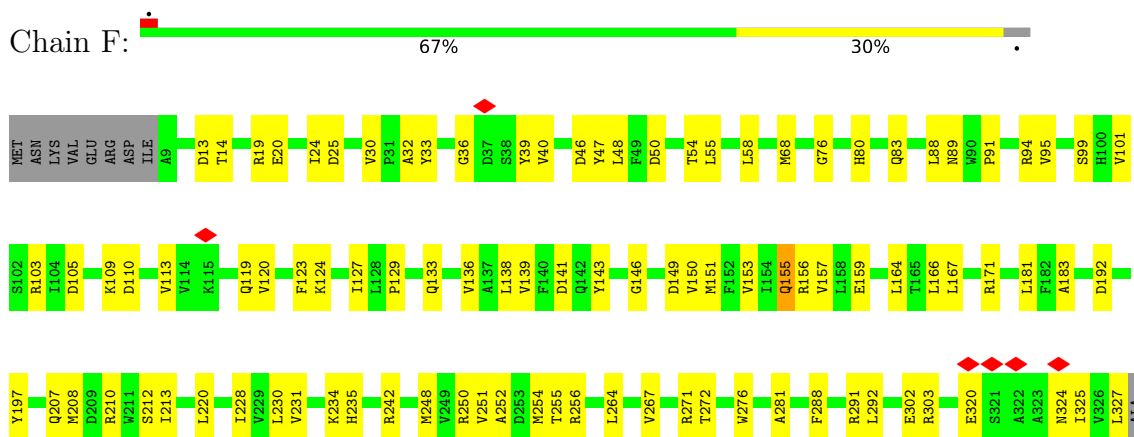
3 Residue-property plots

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.

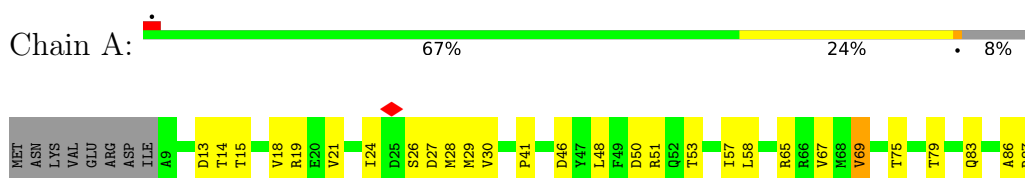
• Molecule 1: Cobaltochelatase subunit CobS



• Molecule 1: Cobaltochelatase subunit CobS

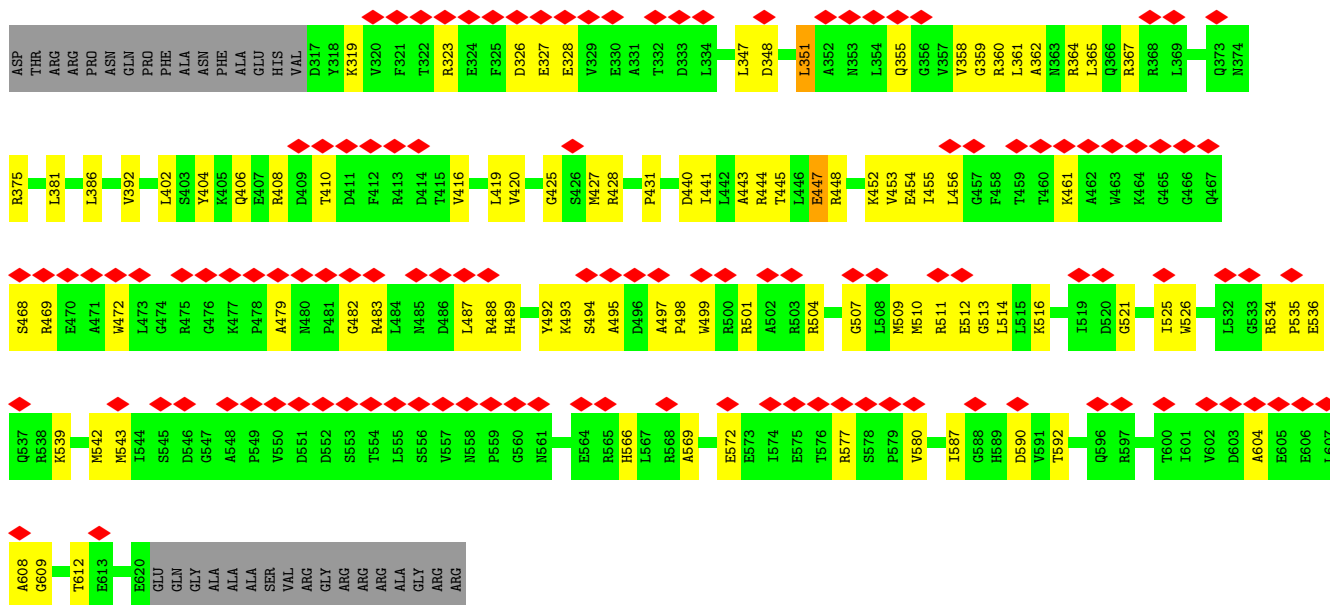


• Molecule 1: Cobaltochelatase subunit CobS



Chain G:

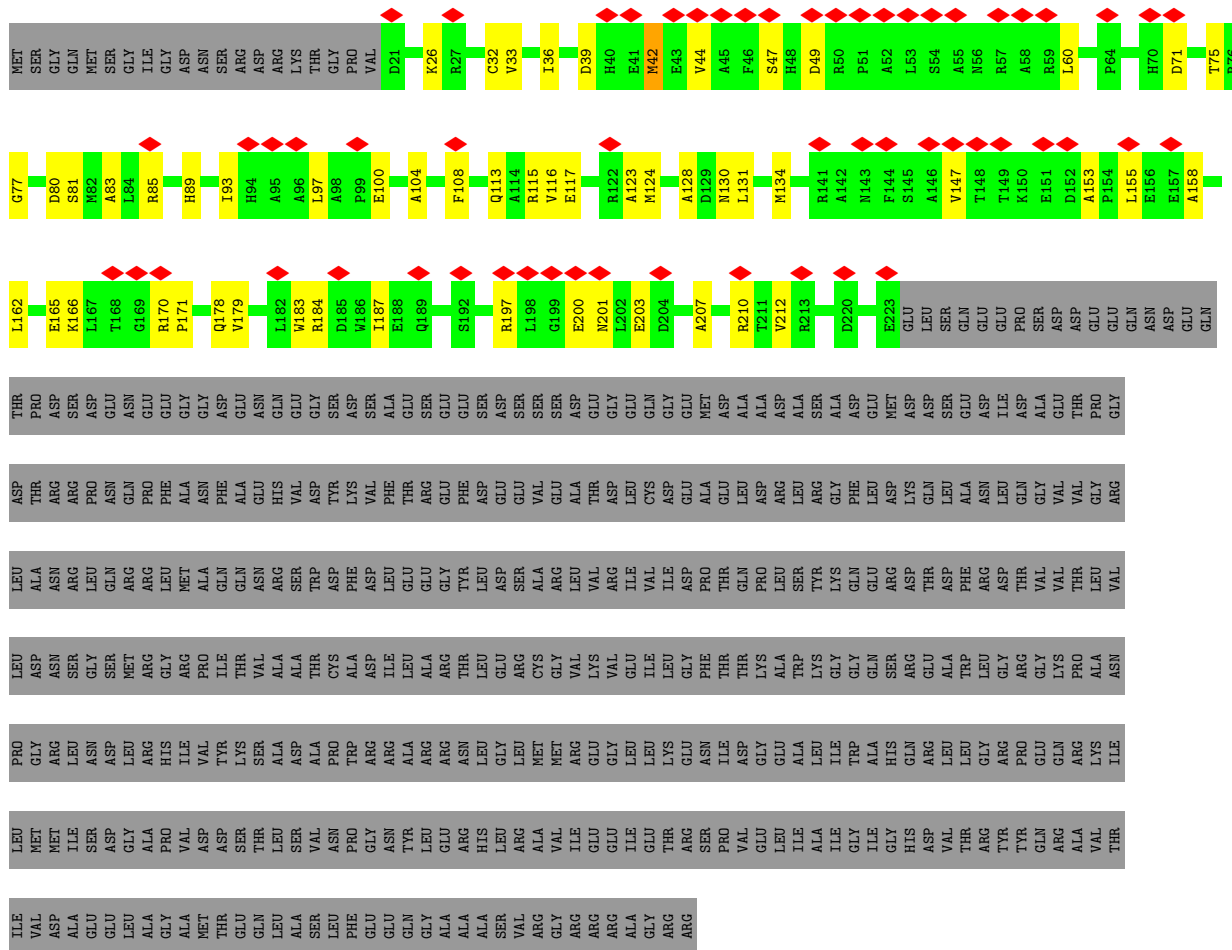
THR	GLU	ALA	PRO	MET
PRO	LEU	ARG	ASP	SER
ASP	TRP	ALA	LEU	GLY
SER	ARG	MET	PRO	GLN
ASP	ASP	GLY	LYS	MET
GLU	TRP	VAL	PRO	SER
ASN	ILE	VAL	THR	GLY
GLU	GLU	ASP	ALA	GLY
GLY	GLN	ASN	HIS	ASP
GLY	LYS	LEU	ASP	ASN
ASP	SER	SER	ILE	SER
GLU	ALA	THR	ALA	ARG
ASN	ASP	MET	VAL	ASP
GLN	ILE	LEU	THR	ARG
GLY	ALA	ALA	ARG	LYS
GLY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



Chain a:

Position	Amino Acid	Frequency (approx.)
1	MET	0.24
2	SER	0.08
3	GLY	0.08
4	GLN	0.08
5	MET	0.08
6	SER	0.08
7	GLY	0.08
8	ILE	0.08
9	GLY	0.08
10	ASP	0.08
11	ASN	0.08
12	SER	0.08
13	ARG	0.08
14	ASP	0.08
15	ARG	0.08
16	LYS	0.08
17	THR	0.08
18	GLY	0.08
19	PRO	0.08
20	VAL	0.08
21	ASP	0.08
22	S22	0.08
23	E23	0.08
24	C32	0.08
25	V33	0.08
26	R34	0.08
27	S37	0.08
28	G38	0.08
29	D39	0.08
30	H40	0.08
31	E41	0.08
32	M42	0.08
33	S47	0.08
34	L53	0.08
35	R57	0.08
36	L63	0.08
37	P67	0.08
38	D71	0.08
39	I72	0.08
40	A73	0.08
41	R76	0.08
42	S81	0.08
43	V111	0.08
44	E112	0.08
45	V116	0.08
46	E117	0.08
47	A123	0.08
48	L131	0.08
49	M134	0.08
50	K138	0.08
51	R141	0.08
52	A142	0.08
53	A146	0.08
54	V147	0.08
55	T148	0.08
56	E151	0.08
57	E156	0.08
58	E157	0.08
59	A158	0.08
60	V159	0.08
61	L163	0.08
62	R164	0.08
63	R170	0.08
64	Q178	0.08
65	V179	0.08
66	L180	0.08
67	E181	0.08
68	L182	0.08
69	W183	0.08
70	R184	0.08
71	D185	0.08
72	W186	0.08
73	L187	0.08
74	D194	0.08
75	I195	0.08
76	A196	0.08
77	R197	0.08
78	L198	0.08
79	C199	0.08
80	E200	0.08

- Molecule 2: Cobaltochelatase subunit CobT



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66428	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.061	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	293.16, 293.16, 293.16	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.698, 0.698, 0.698	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: ATP, 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	0.21	0/2440	0.34	0/3320
1	B	0.18	0/2407	0.34	0/3275
1	C	0.27	0/2507	0.39	0/3411
1	D	0.28	0/2567	0.38	0/3495
1	E	0.18	0/2572	0.32	0/3502
1	F	0.22	0/2567	0.35	0/3495
2	G	0.21	0/2460	0.39	0/3323
2	a	0.11	0/1486	0.32	0/2022
2	c	0.11	0/1499	0.31	0/2040
All	All	0.21	0/20505	0.35	0/27883

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	2390	0	2350	58	0
1	B	2357	0	2324	70	0
1	C	2457	0	2419	77	0
1	D	2514	0	2473	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2519	0	2478	63	0
1	F	2514	0	2474	71	0
2	G	2423	0	2428	76	0
2	a	1462	0	1402	36	0
2	c	1475	0	1408	38	0
3	A	31	0	12	1	0
3	B	31	0	12	2	0
3	C	31	0	12	3	0
3	D	31	0	12	2	0
3	E	31	0	12	2	0
3	F	31	0	12	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	20302	0	19828	506	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 (506) 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)
2:G:359:GLY:HA2	2:G:448:ARG:HH12	1.12	1.14
1:C:311:GLN:HB2	1:C:317:GLU:HA	1.50	0.90
2:G:359:GLY:HA2	2:G:448:ARG:NH1	1.88	0.89
1:F:155:GLN:HG3	1:F:207:GLN:HG3	1.63	0.80
1:D:287:GLY:HA3	1:D:319:PRO:HD2	1.64	0.79
2:G:362:ALA:CB	2:G:448:ARG:HH11	1.96	0.78
2:a:110:ALA:HB2	2:a:156:GLU:HG2	1.67	0.75
1:D:255:THR:HG21	1:D:268:MET:HB2	1.68	0.75
2:G:416:VAL:HG22	2:G:452:LYS:HB2	1.69	0.74
2:G:359:GLY:CA	2:G:448:ARG:HH12	1.97	0.74
1:C:53:THR:HA	1:C:215:THR:HG21	1.71	0.72
2:G:452:LYS:HE3	2:G:495:ALA:HB1	1.71	0.72
1:B:317:GLU:OE1	1:B:318:LEU:N	2.23	0.72
1:B:246:ASN:OD1	1:B:250:ARG:NH2	2.24	0.70
2:G:326:ASP:HA	2:G:487:LEU:O	1.90	0.70
1:D:290:PHE:HD2	1:D:318:LEU:HD21	1.56	0.70
2:a:32:CYS:SG	1:A:312:ARG:NH1	2.65	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ASP:OD2	1:D:271:ARG:NH1	2.25	0.69
1:E:255:THR:HG21	1:E:268:MET:HB2	1.74	0.69
1:F:76:GLY:O	1:F:80:HIS:ND1	2.26	0.69
1:C:24:ILE:HD11	1:C:51:ARG:HA	1.74	0.69
1:E:164:LEU:HD23	1:E:173:ILE:HD11	1.75	0.68
1:A:65:ARG:NH1	1:B:278:GLU:OE1	2.27	0.68
2:G:455:ILE:HB	2:G:492:TYR:HB2	1.75	0.68
1:E:271:ARG:NH1	1:D:209:ASP:OD2	2.26	0.68
2:a:81:SER:OG	2:a:134:MET:SD	2.51	0.67
2:a:221:MET:SD	2:a:221:MET:N	2.68	0.67
1:B:163:ARG:NH2	1:C:92:CYS:O	2.28	0.67
1:D:19:ARG:NH2	1:D:27:ASP:OD1	2.27	0.67
2:G:362:ALA:CB	2:G:448:ARG:NH1	2.59	0.66
1:F:123:PHE:HE2	1:F:167:LEU:HD12	1.59	0.66
2:G:493:LYS:HE3	2:G:501:ARG:HE	1.60	0.66
1:D:42:GLU:OE1	1:D:42:GLU:N	2.26	0.66
1:E:149:ASP:OD1	1:E:150:VAL:N	2.28	0.66
2:G:362:ALA:HB3	2:G:448:ARG:HH11	1.58	0.66
2:a:111:VAL:HG11	2:a:212:VAL:HG11	1.78	0.65
2:G:362:ALA:HA	2:G:365:LEU:HD12	1.79	0.65
1:B:251:VAL:HA	1:B:254:MET:HE2	1.77	0.65
2:a:212:VAL:O	2:a:216:LEU:HD12	1.96	0.65
2:G:493:LYS:HD2	2:G:501:ARG:HH21	1.63	0.64
2:G:493:LYS:HE2	2:G:498:PRO:HA	1.78	0.64
1:A:99:SER:O	1:A:147:ARG:NH1	2.31	0.64
2:G:534:ARG:NH2	2:G:536:GLU:OE2	2.30	0.63
1:A:13:ASP:OD1	1:A:14:THR:N	2.32	0.63
1:B:112:ILE:HD13	1:C:119:GLN:HE22	1.62	0.63
2:G:362:ALA:HB1	2:G:448:ARG:HD2	1.79	0.63
1:F:153:VAL:O	1:F:157:VAL:HG23	1.99	0.62
2:G:347:LEU:HG	2:G:351:LEU:HD22	1.80	0.62
2:G:454:GLU:HA	2:G:494:SER:HA	1.80	0.62
2:c:80:ASP:OD1	1:C:312:ARG:NH1	2.31	0.62
1:B:154:ILE:HD12	1:B:154:ILE:H	1.64	0.62
1:C:225:GLU:OE2	1:C:256:ARG:NH2	2.32	0.62
1:A:94:ARG:HH12	1:A:141:ASP:HB2	1.65	0.62
1:A:107:VAL:HG12	1:A:166:LEU:HD13	1.81	0.62
1:C:28:MET:HE3	1:D:326:VAL:HG11	1.80	0.61
1:C:187:THR:HG22	1:C:194:THR:HG21	1.81	0.61
1:C:46:ASP:HB3	1:C:231:VAL:HG22	1.81	0.61
1:A:242:ARG:O	1:A:246:ASN:ND2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:85:ARG:O	2:c:89:HIS:HB2	2.02	0.60
1:A:79:THR:OG1	3:A:401:ATP:O1A	2.20	0.60
1:B:243:GLU:HG3	1:B:247:LYS:HZ1	1.66	0.60
1:A:128:LEU:HD22	1:A:157:VAL:HG21	1.82	0.60
1:B:138:LEU:HB3	1:B:181:LEU:HD12	1.83	0.60
1:D:232:LYS:HG3	1:D:274:ILE:HD13	1.83	0.60
1:F:230:LEU:HD11	1:F:242:ARG:HG2	1.84	0.60
1:B:13:ASP:OD1	1:B:14:THR:N	2.35	0.60
1:F:19:ARG:NH2	1:F:25:ASP:O	2.34	0.60
1:F:256:ARG:HG2	1:F:267:VAL:HG23	1.84	0.59
1:E:209:ASP:OD1	1:F:272:THR:OG1	2.20	0.59
2:a:148:THR:HB	2:a:178:GLN:H	1.66	0.59
2:c:128:ALA:O	2:c:170:ARG:NH1	2.36	0.59
1:E:79:THR:HA	1:E:82:GLU:HG2	1.84	0.59
1:A:30:VAL:HG21	1:A:58:LEU:HD13	1.84	0.59
1:B:210:ARG:NH2	3:C:401:ATP:O3G	2.35	0.59
1:E:224:ASN:O	1:E:228:ILE:HG13	2.03	0.59
1:C:10:ASN:OD1	1:C:135:ASN:ND2	2.36	0.59
2:G:362:ALA:CB	2:G:448:ARG:HD2	2.32	0.59
1:E:50:ASP:O	1:E:54:THR:HG22	2.03	0.58
2:c:39:ASP:HB3	2:c:42:MET:HB2	1.85	0.58
1:E:30:VAL:HG13	1:E:62:ALA:HB2	1.86	0.58
1:C:18:VAL:HG21	1:C:28:MET:HG3	1.85	0.58
1:F:113:VAL:HG13	1:F:120:VAL:HG23	1.85	0.58
1:F:291:ARG:NH2	1:F:320:GLU:OE2	2.36	0.58
1:D:165:THR:HG22	1:D:172:VAL:HG22	1.85	0.58
1:C:167:LEU:HD23	1:D:127:ILE:HG13	1.85	0.58
1:A:300:GLU:HA	1:A:303:ARG:HD2	1.85	0.58
1:B:128:LEU:HD11	1:B:140:PHE:HZ	1.68	0.58
2:G:386:LEU:HD12	2:G:402:LEU:HD21	1.85	0.58
2:c:123:ALA:HB1	1:C:250:ARG:HD3	1.85	0.58
1:B:74:GLY:HA3	1:B:269:SER:HB3	1.85	0.57
1:D:48:LEU:O	3:D:401:ATP:N6	2.37	0.57
1:E:299:ASP:OD1	1:E:299:ASP:N	2.37	0.57
1:B:76:GLY:O	1:B:80:HIS:ND1	2.34	0.57
1:E:162:GLY:O	1:E:163:ARG:HD2	2.05	0.57
1:B:245:VAL:HA	1:B:248:MET:HE3	1.87	0.57
2:G:456:LEU:HD22	2:G:526:TRP:HH2	1.69	0.57
1:A:146:GLY:HA3	1:A:151:MET:HE3	1.87	0.57
1:A:236:TYR:HB3	1:A:241:GLY:HA3	1.86	0.57
1:E:250:ARG:O	1:E:254:MET:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:358:VAL:O	2:G:448:ARG:NH1	2.37	0.57
2:G:511:ARG:NH2	2:G:512:GLU:OE2	2.38	0.56
1:E:325:ILE:HG13	1:E:326:VAL:HG22	1.86	0.56
2:G:364:ARG:NH1	2:G:612:THR:OG1	2.39	0.56
1:C:74:GLY:N	3:C:401:ATP:O1G	2.34	0.56
1:C:155:GLN:OE1	1:C:210:ARG:NH1	2.37	0.56
1:F:50:ASP:O	1:F:54:THR:HG22	2.05	0.56
1:A:155:GLN:HG3	1:A:207:GLN:HE21	1.70	0.56
1:D:144:ASP:HB2	1:D:200:THR:HG23	1.88	0.56
2:G:604:ALA:HB1	2:G:608:ALA:HB2	1.87	0.56
1:E:202:GLN:OE1	2:G:367:ARG:HG2	2.05	0.56
1:D:79:THR:OG1	3:D:401:ATP:O2A	2.24	0.56
2:a:159:VAL:O	2:a:163:LEU:HG	2.06	0.55
2:c:36:ILE:HB	2:c:83:ALA:HB1	1.87	0.55
1:C:52:GLN:HE21	1:D:324:ASN:HD21	1.54	0.55
1:E:151:MET:HE2	1:E:151:MET:HA	1.87	0.55
1:E:76:GLY:O	1:E:80:HIS:ND1	2.40	0.55
2:a:219:MET:HG3	2:a:221:MET:SD	2.47	0.55
2:G:521:GLY:HA2	2:G:566:HIS:CE1	2.42	0.55
1:B:43:LEU:HD12	1:B:43:LEU:H	1.71	0.55
2:c:200:GLU:O	2:c:201:ASN:ND2	2.40	0.55
1:E:30:VAL:HG21	1:E:58:LEU:HD12	1.89	0.55
1:F:192:ASP:HB3	1:F:197:TYR:HB2	1.87	0.55
1:B:53:THR:O	1:B:57:ILE:HD12	2.06	0.55
1:E:279:ASN:ND2	1:E:293:THR:OG1	2.40	0.54
1:F:146:GLY:HA3	1:F:151:MET:HE3	1.89	0.54
1:A:67:VAL:HG22	1:A:182:PHE:CD1	2.42	0.54
1:B:256:ARG:HH21	1:B:270:PRO:HD3	1.72	0.54
1:D:235:HIS:CE1	1:D:281:ALA:HB2	2.41	0.54
1:F:20:GLU:OE1	1:F:20:GLU:N	2.40	0.54
1:C:165:THR:HG22	1:C:172:VAL:HG22	1.88	0.54
2:c:32:CYS:O	2:c:36:ILE:HG13	2.07	0.54
2:G:358:VAL:O	2:G:445:THR:HG22	2.06	0.54
1:C:13:ASP:OD1	1:C:14:THR:N	2.41	0.54
1:B:48:LEU:HB3	3:B:401:ATP:HN62	1.73	0.54
1:C:141:ASP:HA	1:C:184:THR:HG23	1.89	0.54
1:F:151:MET:SD	1:F:207:GLN:NE2	2.74	0.54
2:a:22:SER:OG	2:a:23:GLU:N	2.41	0.54
1:C:93:VAL:HG13	1:C:136:VAL:HG21	1.89	0.53
1:A:30:VAL:HG11	1:A:58:LEU:HD22	1.89	0.53
1:B:311:GLN:NE2	1:B:315:GLY:O	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:HG23	1:A:29:MET:HE2	1.90	0.53
1:F:220:LEU:HD12	1:F:220:LEU:H	1.73	0.53
2:G:360:ARG:NH1	2:G:609:GLY:O	2.41	0.53
1:C:29:MET:HE2	1:C:29:MET:HA	1.90	0.53
1:E:242:ARG:O	1:E:246:ASN:ND2	2.41	0.53
1:B:50:ASP:O	1:B:54:THR:HG22	2.08	0.53
1:F:213:ILE:HG23	1:A:292:LEU:HB3	1.91	0.53
2:c:124:MET:HG3	1:C:250:ARG:HD2	1.91	0.53
2:G:375:ARG:NH1	2:G:410:THR:OG1	2.42	0.53
1:E:204:ASN:N	1:E:204:ASN:OD1	2.41	0.52
1:A:113:VAL:HG23	1:A:120:VAL:HG23	1.91	0.52
1:F:212:SER:OG	1:F:213:ILE:N	2.42	0.52
1:B:271:ARG:HB2	3:B:401:ATP:H4'	1.90	0.52
1:E:206:ALA:O	1:E:210:ARG:NH1	2.40	0.52
1:F:103:ARG:HH12	1:F:167:LEU:HD23	1.73	0.52
1:E:70:SER:HA	1:E:185:ALA:O	2.10	0.52
2:G:362:ALA:HB2	2:G:448:ARG:NH1	2.25	0.52
1:F:48:LEU:HD11	1:F:231:VAL:HG21	1.92	0.52
2:c:184:ARG:NE	2:c:184:ARG:HA	2.24	0.52
1:B:263:ASP:HB3	1:B:264:LEU:HD23	1.92	0.52
1:B:112:ILE:HG21	1:C:119:GLN:HE22	1.74	0.52
1:F:30:VAL:HG21	1:F:58:LEU:HD22	1.91	0.52
1:D:252:ALA:O	1:D:256:ARG:HG3	2.10	0.52
1:D:143:TYR:HB3	1:D:185:ALA:HB2	1.92	0.51
1:E:112:ILE:HD11	2:G:392:VAL:HG13	1.90	0.51
2:G:441:ILE:O	2:G:445:THR:HG23	2.11	0.51
1:E:94:ARG:NH2	1:E:141:ASP:OD2	2.38	0.51
1:E:244:ILE:O	1:E:248:MET:HG3	2.10	0.51
2:G:497:ALA:HB1	2:G:499:TRP:HD1	1.75	0.51
1:B:226:VAL:HG11	1:B:242:ARG:HH21	1.74	0.51
1:C:238:ASN:OD1	1:C:240:GLU:N	2.39	0.51
1:D:219:TYR:CD2	1:D:256:ARG:HD3	2.46	0.51
1:F:228:ILE:HG12	3:F:401:ATP:N6	2.25	0.51
2:G:361:LEU:HD23	2:G:445:THR:HG21	1.91	0.51
1:B:270:PRO:O	1:B:274:ILE:HG13	2.09	0.51
1:E:174:ARG:HH11	1:E:175:PRO:HD2	1.75	0.51
1:E:264:LEU:HD23	1:E:266:THR:H	1.74	0.51
2:a:194:ASP:N	2:a:194:ASP:OD1	2.43	0.51
1:E:99:SER:HB3	1:D:149:ASP:HB3	1.92	0.51
1:E:326:VAL:O	1:D:51:ARG:NH2	2.43	0.51
1:A:128:LEU:HD23	1:A:138:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ILE:O	1:B:278:GLU:HG3	2.10	0.51
1:A:316:VAL:O	1:A:317:GLU:C	2.54	0.50
1:E:179:PHE:CZ	1:E:181:LEU:HD13	2.46	0.50
2:c:93:ILE:O	2:c:97:LEU:HB2	2.11	0.50
1:D:194:THR:HG22	1:D:196:LEU:HG	1.93	0.50
2:a:34:ARG:HH21	1:A:261:ASN:HB3	1.76	0.50
1:B:311:GLN:NE2	1:B:311:GLN:O	2.45	0.50
1:D:11:LEU:HD21	1:D:177:PRO:HB2	1.93	0.50
2:G:590:ASP:OD2	2:G:592:THR:OG1	2.27	0.50
1:B:243:GLU:O	1:B:247:LYS:NZ	2.44	0.50
2:a:164:ARG:C	2:a:164:ARG:HD2	2.37	0.50
2:c:131:LEU:HB2	2:c:170:ARG:HH12	1.76	0.50
1:E:149:ASP:HB2	1:F:99:SER:HB3	1.93	0.50
1:E:209:ASP:OD2	1:F:271:ARG:NE	2.38	0.50
1:F:103:ARG:HD3	1:F:149:ASP:OD1	2.12	0.50
1:B:291:ARG:HA	1:B:295:LEU:HB2	1.93	0.50
1:F:46:ASP:OD2	1:F:234:LYS:NZ	2.44	0.50
2:G:362:ALA:HB3	2:G:448:ARG:NH1	2.22	0.50
1:D:132:TYR:HE1	1:D:157:VAL:HG13	1.76	0.50
1:E:30:VAL:HG11	1:E:58:LEU:HD12	1.94	0.49
1:C:167:LEU:HB3	1:D:105:ASP:OD1	2.11	0.49
2:G:347:LEU:HG	2:G:351:LEU:CD2	2.42	0.49
1:A:41:PRO:HG2	1:A:86:ALA:HB2	1.94	0.49
2:a:85:ARG:HH12	2:a:112:GLU:HG3	1.78	0.49
2:c:153:ALA:HB1	2:c:179:VAL:HG13	1.94	0.49
1:A:226:VAL:HG22	1:A:245:VAL:HG12	1.94	0.49
1:D:223:ASP:N	1:D:223:ASP:OD1	2.43	0.49
1:D:263:ASP:N	1:D:263:ASP:OD1	2.46	0.49
2:a:123:ALA:O	1:A:250:ARG:NH1	2.45	0.49
1:E:118:VAL:HB	1:F:119:GLN:HE21	1.78	0.49
1:D:132:TYR:CE1	1:D:157:VAL:HG13	2.47	0.49
1:B:301:LEU:HD12	1:B:302:GLU:HG3	1.94	0.49
1:D:125:ASP:HB3	1:D:129:PRO:HG2	1.93	0.49
1:A:103:ARG:O	1:A:107:VAL:HG22	2.12	0.49
1:B:26:SER:OG	1:B:27:ASP:N	2.45	0.49
2:c:36:ILE:HD11	1:C:312:ARG:HD2	1.94	0.49
1:F:159:GLU:HG2	1:F:210:ARG:HD3	1.95	0.48
1:F:303:ARG:HE	1:F:303:ARG:HB2	1.48	0.48
2:G:348:ASP:HA	2:G:351:LEU:HB2	1.93	0.48
2:a:72:ILE:HD11	1:A:324:ASN:HB2	1.96	0.48
1:C:110:ASP:OD1	1:C:121:THR:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:HB2	1:C:129:PRO:HD3	1.95	0.48
1:E:94:ARG:O	1:D:165:THR:HG21	2.13	0.48
1:C:167:LEU:HD13	1:D:105:ASP:OD2	2.13	0.48
1:F:208:MET:HE3	1:A:297:LYS:HG2	1.94	0.48
1:A:320:GLU:C	1:A:322:ALA:H	2.22	0.48
1:F:103:ARG:HH12	1:F:167:LEU:CD2	2.26	0.48
2:a:184:ARG:O	2:a:187:ILE:HG13	2.12	0.48
1:C:11:LEU:HD11	1:C:177:PRO:HG2	1.96	0.48
2:a:86:GLN:O	2:a:86:GLN:NE2	2.47	0.48
1:C:252:ALA:HA	1:C:268:MET:HG3	1.94	0.48
1:E:128:LEU:HB3	1:E:129:PRO:HD3	1.95	0.48
1:E:169:GLN:HG2	1:F:124:LYS:HG2	1.96	0.48
1:F:143:TYR:OH	1:F:207:GLN:NE2	2.40	0.48
1:A:24:ILE:HD12	1:A:51:ARG:HA	1.96	0.48
1:F:24:ILE:HD12	1:F:55:LEU:HD13	1.96	0.48
2:a:204:ASP:HB3	2:a:207:ALA:HB3	1.95	0.48
1:F:95:VAL:HG21	1:F:127:ILE:HG21	1.95	0.47
1:B:154:ILE:HA	1:B:157:VAL:HG12	1.95	0.47
1:F:109:LYS:HB3	1:F:109:LYS:HE3	1.66	0.47
2:G:425:GLY:O	2:G:428:ARG:NH1	2.46	0.47
1:B:310:TYR:HD2	1:B:318:LEU:HG	1.79	0.47
2:c:113:GLN:HA	2:c:116:VAL:HG12	1.96	0.47
1:B:57:ILE:HD12	1:B:57:ILE:H	1.80	0.47
1:B:153:VAL:HG22	1:B:166:LEU:HD22	1.95	0.47
1:B:248:MET:HG2	1:B:276:TRP:CE3	2.49	0.47
1:D:132:TYR:CZ	1:D:175:PRO:HB3	2.49	0.47
1:E:138:LEU:HB3	1:E:181:LEU:HD12	1.97	0.47
1:E:213:ILE:HG23	1:F:292:LEU:HB3	1.97	0.47
2:G:328:GLU:HG3	2:G:489:HIS:HB2	1.95	0.47
1:B:155:GLN:OE1	1:B:207:GLN:NE2	2.48	0.47
1:C:320:GLU:HB3	1:C:321:SER:H	1.51	0.47
2:G:319:LYS:NZ	2:G:482:GLY:O	2.29	0.47
1:A:234:LYS:HD2	1:A:234:LYS:HA	1.70	0.47
1:B:152:PHE:HD1	1:C:99:SER:HB2	1.78	0.47
1:F:101:VAL:HG12	1:F:150:VAL:HG21	1.97	0.47
1:A:18:VAL:HG23	1:A:28:MET:H	1.80	0.47
1:B:243:GLU:HG3	1:B:247:LYS:NZ	2.30	0.47
1:D:143:TYR:OH	1:D:207:GLN:OE1	2.21	0.47
2:c:155:LEU:HD13	2:c:183:TRP:CE3	2.50	0.46
1:C:125:ASP:HB3	1:C:129:PRO:HB2	1.97	0.46
1:F:129:PRO:HG3	1:F:166:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:77:GLY:HA2	2:c:130:ASN:HB3	1.96	0.46
1:E:264:LEU:HD11	1:E:306:VAL:HG22	1.97	0.46
1:B:310:TYR:CD2	1:B:318:LEU:HG	2.50	0.46
2:G:493:LYS:HD2	2:G:501:ARG:NH2	2.28	0.46
1:C:51:ARG:NH2	1:D:324:ASN:O	2.48	0.46
1:D:248:MET:HG2	1:D:276:TRP:CE3	2.50	0.46
2:G:497:ALA:HB1	2:G:499:TRP:CD1	2.51	0.46
1:C:153:VAL:HG13	1:D:98:ASP:OD2	2.16	0.46
1:D:166:LEU:HD12	1:D:173:ILE:HD11	1.98	0.46
1:D:290:PHE:CD2	1:D:318:LEU:HD21	2.44	0.46
1:E:104:ILE:HG23	1:E:109:LYS:HB3	1.97	0.46
1:F:110:ASP:OD1	1:F:110:ASP:N	2.39	0.46
1:F:248:MET:HG2	1:F:276:TRP:CE3	2.51	0.46
2:G:569:ALA:O	2:G:572:GLU:HG3	2.15	0.46
1:B:248:MET:HG2	1:B:276:TRP:CZ3	2.50	0.46
1:F:13:ASP:OD1	1:F:14:THR:N	2.47	0.46
1:A:53:THR:HG21	1:A:217:LEU:HD22	1.97	0.46
1:B:9:ALA:HB1	1:B:11:LEU:HD23	1.97	0.46
1:B:256:ARG:NH2	1:B:270:PRO:HD3	2.30	0.46
2:G:514:LEU:HD12	2:G:514:LEU:O	2.14	0.46
1:C:65:ARG:HE	1:C:212:SER:HB3	1.80	0.46
1:D:259:PHE:HA	1:D:263:ASP:O	2.15	0.46
1:E:257:GLN:HA	1:E:257:GLN:OE1	2.16	0.46
1:C:320:GLU:O	1:C:321:SER:C	2.59	0.46
2:c:71:ASP:O	2:c:75:THR:HG22	2.16	0.45
2:c:165:GLU:HG2	2:c:171:PRO:HA	1.97	0.45
1:A:311:GLN:HB2	1:A:317:GLU:HA	1.98	0.45
1:C:57:ILE:HG21	1:C:84:VAL:HG11	1.99	0.45
1:D:320:GLU:O	1:D:321:SER:C	2.60	0.45
1:F:91:PRO:HB2	1:F:136:VAL:HG12	1.97	0.45
2:G:402:LEU:HD22	2:G:404:TYR:CZ	2.51	0.45
2:c:44:VAL:HG21	2:c:60:LEU:HD21	1.98	0.45
1:C:52:GLN:OE1	1:C:215:THR:HG23	2.16	0.45
1:F:19:ARG:HB3	1:F:19:ARG:HH11	1.82	0.45
1:B:238:ASN:HD22	1:B:238:ASN:HA	1.66	0.45
1:C:307:ALA:HA	1:C:318:LEU:HD12	1.97	0.45
1:D:283:PHE:CE2	1:D:292:LEU:HD12	2.52	0.45
1:F:129:PRO:O	1:F:133:GLN:HG3	2.17	0.45
1:F:39:TYR:HB2	1:F:91:PRO:HB3	1.99	0.45
2:a:53:LEU:HD12	2:a:53:LEU:HA	1.86	0.45
2:c:32:CYS:SG	1:C:312:ARG:NE	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLN:O	1:A:87:ARG:HG2	2.17	0.45
1:D:99:SER:O	1:D:147:ARG:HG3	2.17	0.45
1:F:33:TYR:HB2	1:F:89:ASN:HB2	1.99	0.45
2:G:504:ARG:HH11	2:G:504:ARG:HG3	1.82	0.45
2:a:37:SER:HA	2:a:87:ALA:HB2	1.99	0.45
2:a:180:LEU:HD23	2:a:180:LEU:H	1.82	0.45
1:B:52:GLN:HG3	1:C:288:PHE:HE1	1.81	0.45
1:D:255:THR:CG2	1:D:268:MET:HB2	2.44	0.45
1:E:124:LYS:HA	1:E:124:LYS:HD3	1.71	0.45
1:A:57:ILE:HD11	1:A:69:VAL:HG11	1.99	0.45
2:c:115:ARG:NH1	2:c:203:GLU:O	2.50	0.44
1:A:21:VAL:O	1:A:87:ARG:NH1	2.49	0.44
2:a:138:LYS:O	2:a:142:ALA:N	2.49	0.44
1:B:67:VAL:HB	1:B:182:PHE:HD1	1.82	0.44
1:F:55:LEU:HD12	1:F:55:LEU:HA	1.77	0.44
2:a:39:ASP:HB3	2:a:42:MET:HG2	1.99	0.44
1:A:205:GLN:HE22	1:B:267:VAL:HG22	1.82	0.44
1:A:311:GLN:NE2	1:A:312:ARG:HG2	2.33	0.44
1:C:144:ASP:OD1	1:C:144:ASP:N	2.43	0.44
1:C:268:MET:O	1:C:269:SER:OG	2.25	0.44
2:a:198:LEU:HA	2:a:201:ASN:HB2	2.00	0.44
1:F:32:ALA:HB2	1:F:88:LEU:HD22	2.00	0.44
1:D:98:ASP:N	1:D:98:ASP:OD1	2.50	0.44
2:c:147:VAL:HG11	2:c:178:GLN:H	1.81	0.44
1:B:239:ALA:C	1:B:241:GLY:H	2.26	0.44
1:E:167:LEU:HB3	1:F:105:ASP:OD1	2.18	0.44
2:G:381:LEU:HD12	2:G:406:GLN:HB2	2.00	0.44
2:c:162:LEU:HD12	2:c:166:LYS:HD3	1.99	0.44
1:D:167:LEU:HD23	1:D:167:LEU:HA	1.80	0.44
1:F:94:ARG:NH2	1:F:141:ASP:OD2	2.49	0.44
1:D:268:MET:HE3	1:D:272:THR:HG22	2.00	0.44
1:E:52:GLN:HG3	1:F:288:PHE:HZ	1.83	0.43
1:E:326:VAL:H	1:D:51:ARG:HH22	1.66	0.43
1:F:36:GLY:HA3	1:F:40:VAL:HG21	2.00	0.43
1:F:230:LEU:HD23	1:F:230:LEU:HA	1.86	0.43
2:G:534:ARG:HB3	2:G:536:GLU:OE1	2.18	0.43
1:D:26:SER:OG	1:D:27:ASP:N	2.50	0.43
1:D:252:ALA:O	1:D:255:THR:HG22	2.18	0.43
2:G:327:GLU:H	2:G:327:GLU:HG3	1.63	0.43
2:G:468:SER:OG	2:G:483:ARG:NH2	2.35	0.43
2:G:525:ILE:HD11	2:G:566:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ILE:CG2	1:C:84:VAL:HG11	2.48	0.43
1:F:151:MET:HB3	1:F:207:GLN:OE1	2.18	0.43
2:G:427:MET:HA	2:G:431:PRO:HB2	2.00	0.43
1:B:242:ARG:HH22	1:B:246:ASN:HB2	1.82	0.43
1:C:156:ARG:HD3	1:C:164:LEU:HD11	1.99	0.43
2:G:492:TYR:HE1	2:G:507:GLY:HA3	1.83	0.43
2:c:49:ASP:OD1	2:c:49:ASP:N	2.47	0.43
1:B:39:TYR:HB2	1:B:91:PRO:HB3	2.00	0.43
1:F:250:ARG:O	1:F:254:MET:HG3	2.19	0.43
1:F:251:VAL:O	1:F:255:THR:HG22	2.19	0.43
2:G:419:LEU:HD23	2:G:542:MET:HE2	2.00	0.43
2:c:158:ALA:HB2	2:c:179:VAL:HG12	2.01	0.43
1:C:129:PRO:O	1:C:133:GLN:NE2	2.50	0.43
1:D:46:ASP:HB2	1:D:231:VAL:HG13	2.01	0.43
1:E:132:TYR:CZ	1:E:175:PRO:HB3	2.53	0.43
1:B:112:ILE:HD13	1:C:119:GLN:NE2	2.32	0.43
1:D:208:MET:HA	1:D:211:TRP:HD1	1.83	0.43
1:E:87:ARG:HH11	1:E:87:ARG:HG3	1.84	0.43
2:G:355:GLN:O	2:G:358:VAL:HG22	2.19	0.43
2:a:117:GLU:N	2:a:117:GLU:OE1	2.51	0.43
1:B:146:GLY:HA3	1:B:151:MET:HE1	2.00	0.43
1:B:155:GLN:O	1:B:159:GLU:HG3	2.19	0.43
1:C:51:ARG:HG3	1:C:51:ARG:HH11	1.84	0.43
1:C:274:ILE:HD12	3:C:401:ATP:H1'	2.00	0.43
1:D:158:LEU:HB2	1:D:210:ARG:HD3	2.01	0.43
1:D:166:LEU:O	1:D:168:ASP:N	2.51	0.43
1:D:268:MET:HE2	1:D:273:VAL:HG22	1.99	0.43
1:E:19:ARG:NH2	1:E:25:ASP:OD1	2.46	0.43
1:A:115:LYS:HD2	1:A:115:LYS:HA	1.75	0.43
1:C:159:GLU:HG2	1:C:161:SER:H	1.84	0.43
1:E:70:SER:OG	1:E:71:GLY:N	2.52	0.43
1:F:156:ARG:HG2	1:F:164:LEU:HD11	2.00	0.43
1:F:264:LEU:HD12	1:F:302:GLU:OE1	2.19	0.43
1:F:94:ARG:HG2	1:F:139:VAL:HB	2.00	0.43
1:C:17:SER:O	1:C:21:VAL:HG12	2.19	0.43
1:E:138:LEU:HB3	1:E:181:LEU:CD1	2.49	0.42
2:a:198:LEU:HD11	2:a:208:PHE:HA	1.99	0.42
1:A:75:THR:CG2	1:A:217:LEU:HG	2.49	0.42
1:C:204:ASN:ND2	1:D:197:TYR:HA	2.34	0.42
2:G:358:VAL:HG23	2:G:448:ARG:HH22	1.84	0.42
1:F:252:ALA:O	1:F:256:ARG:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:131:LEU:HD12	2:a:131:LEU:HA	1.88	0.42
1:A:106:LEU:HD23	1:A:127:ILE:HB	2.02	0.42
1:B:111:ALA:HB3	1:B:124:LYS:HD2	2.00	0.42
1:F:264:LEU:HD12	1:F:264:LEU:HA	1.91	0.42
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.71	0.42
1:F:68:MET:HG3	1:F:183:ALA:HB3	2.02	0.42
2:G:510:MET:SD	2:G:510:MET:N	2.93	0.42
2:G:539:LYS:HB2	2:G:580:VAL:HG22	1.99	0.42
2:a:73:ALA:HA	2:a:76:ARG:HB3	2.01	0.42
2:c:113:GLN:HE21	2:c:113:GLN:HB3	1.66	0.42
1:E:144:ASP:OD1	1:E:144:ASP:N	2.51	0.42
1:E:181:LEU:HD12	1:E:181:LEU:HA	1.83	0.42
1:F:47:TYR:CD2	1:F:83:GLN:HG3	2.55	0.42
1:B:268:MET:HE3	1:B:294:PHE:HD2	1.85	0.42
2:G:577:ARG:H	2:G:577:ARG:HG2	1.72	0.42
2:c:81:SER:HB3	2:c:134:MET:HE2	2.01	0.42
1:B:283:PHE:CE2	1:B:292:LEU:HD12	2.55	0.42
1:C:190:LEU:HB2	1:C:191:GLY:H	1.68	0.42
1:E:252:ALA:O	1:E:255:THR:HG22	2.19	0.42
1:F:235:HIS:CE1	1:F:281:ALA:HB2	2.55	0.42
1:C:28:MET:HB2	1:C:30:VAL:HG13	2.02	0.42
1:C:166:LEU:HA	1:C:166:LEU:HD23	1.74	0.42
1:C:207:GLN:HA	1:C:210:ARG:HG3	2.01	0.42
2:a:63:LEU:HB3	2:a:67:PRO:HB3	2.01	0.42
2:a:85:ARG:HA	2:a:116:VAL:HG21	2.02	0.42
1:A:295:LEU:HA	1:A:295:LEU:HD12	1.83	0.42
1:E:115:LYS:HB3	1:E:115:LYS:HE3	1.90	0.42
1:E:235:HIS:CD2	1:E:235:HIS:C	2.97	0.42
2:G:461:LYS:HA	2:G:488:ARG:HE	1.84	0.42
2:a:184:ARG:HE	2:a:187:ILE:HD11	1.83	0.42
2:c:117:GLU:HB3	2:c:131:LEU:HD13	2.02	0.42
1:A:69:VAL:HG23	1:A:184:THR:HG22	2.02	0.42
1:B:128:LEU:HD11	1:B:140:PHE:CZ	2.52	0.42
1:C:66:ARG:HB3	1:C:211:TRP:CE3	2.54	0.42
1:C:70:SER:HB2	1:C:188:VAL:HG13	2.01	0.42
1:C:204:ASN:HD22	1:D:197:TYR:HA	1.85	0.42
1:E:202:GLN:H	1:E:202:GLN:HG3	1.62	0.41
2:G:447:GLU:HG2	2:G:453:VAL:HG23	2.01	0.41
1:A:50:ASP:OD1	1:A:50:ASP:N	2.53	0.41
1:D:144:ASP:OD1	1:D:144:ASP:N	2.53	0.41
2:G:469:ARG:HA	2:G:469:ARG:HD2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:47:SER:HB3	2:c:60:LEU:H	1.85	0.41
1:A:46:ASP:OD1	1:A:46:ASP:N	2.39	0.41
1:A:248:MET:HG2	1:A:276:TRP:CE3	2.55	0.41
1:B:94:ARG:HG2	1:B:139:VAL:HB	2.01	0.41
1:C:213:ILE:HG23	1:D:292:LEU:HB3	2.02	0.41
1:E:127:ILE:HD12	1:E:127:ILE:HA	1.89	0.41
1:F:156:ARG:HH21	1:A:100:HIS:CE1	2.39	0.41
2:a:170:ARG:H	2:a:170:ARG:HG2	1.73	0.41
1:B:31:PRO:HD2	1:B:62:ALA:HA	2.01	0.41
1:B:104:ILE:HD13	1:B:104:ILE:HA	1.91	0.41
1:B:286:VAL:HG11	1:B:314:PHE:CE2	2.55	0.41
1:E:103:ARG:NH2	1:E:167:LEU:HB2	2.36	0.41
2:G:443:ALA:O	2:G:501:ARG:NH1	2.52	0.41
2:a:157:GLU:H	2:a:157:GLU:HG3	1.65	0.41
1:F:138:LEU:HB3	1:F:181:LEU:HD12	2.01	0.41
2:G:427:MET:HE1	2:G:587:ILE:HG13	2.02	0.41
2:G:516:LYS:HA	2:G:516:LYS:HD3	1.84	0.41
2:G:534:ARG:HA	2:G:535:PRO:HD3	1.93	0.41
1:A:212:SER:OG	1:A:213:ILE:HG13	2.20	0.41
2:G:509:MET:SD	2:G:513:GLY:HA2	2.61	0.41
1:A:263:ASP:OD1	1:A:263:ASP:N	2.54	0.41
1:C:285:ASP:OD1	1:C:285:ASP:N	2.53	0.41
1:E:93:VAL:HG11	1:E:127:ILE:HD11	2.03	0.41
1:E:119:GLN:HE21	1:D:118:VAL:HG13	1.86	0.41
2:c:26:LYS:HA	2:c:26:LYS:HD3	1.75	0.41
1:E:147:ARG:NH2	2:G:375:ARG:O	2.54	0.41
2:a:184:ARG:NE	2:a:187:ILE:HD11	2.36	0.41
2:c:108:PHE:CG	2:c:212:VAL:HG11	2.56	0.41
2:c:183:TRP:O	2:c:187:ILE:HG13	2.19	0.41
2:c:197:ARG:HD3	2:c:197:ARG:HA	1.84	0.41
1:A:138:LEU:HD12	1:A:138:LEU:HA	1.94	0.41
1:D:284:ASN:OD1	1:D:284:ASN:N	2.53	0.41
1:E:228:ILE:HD13	3:E:401:ATP:N1	2.36	0.41
1:F:103:ARG:HG3	1:F:153:VAL:HG21	2.03	0.41
2:G:323:ARG:HH22	2:G:526:TRP:CD1	2.38	0.41
1:A:67:VAL:HG12	1:A:213:ILE:HB	2.03	0.41
1:A:295:LEU:HD22	1:A:318:LEU:HD12	2.03	0.41
1:B:127:ILE:HG22	1:B:128:LEU:HD12	2.03	0.41
1:C:81:ILE:O	1:C:84:VAL:HG12	2.20	0.41
1:C:141:ASP:OD1	1:C:141:ASP:N	2.54	0.41
1:C:268:MET:HE3	1:C:273:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ARG:HH11	1:D:87:ARG:HG3	1.86	0.41
1:D:151:MET:HE3	1:D:151:MET:HA	2.02	0.41
1:F:47:TYR:CE1	3:F:401:ATP:C6	3.09	0.41
2:G:472:TRP:HD1	2:G:482:GLY:HA3	1.86	0.41
1:C:167:LEU:HD21	1:D:95:VAL:HG13	2.02	0.41
1:D:93:VAL:HG21	1:D:130:TRP:HH2	1.86	0.41
3:E:401:ATP:O1G	1:D:210:ARG:NH1	2.54	0.40
2:a:108:PHE:O	2:a:111:VAL:HG12	2.21	0.40
2:c:100:GLU:N	2:c:104:ALA:HB2	2.36	0.40
2:c:207:ALA:O	2:c:210:ARG:HG3	2.21	0.40
1:A:19:ARG:NH1	1:A:26:SER:O	2.54	0.40
1:A:238:ASN:OD1	1:A:241:GLY:N	2.34	0.40
1:B:52:GLN:HG3	1:C:288:PHE:CE1	2.56	0.40
1:B:67:VAL:HB	1:B:182:PHE:CD1	2.56	0.40
1:B:152:PHE:O	1:B:156:ARG:HG3	2.21	0.40
1:B:232:LYS:HD3	1:B:274:ILE:HG21	2.03	0.40
1:C:54:THR:C	1:C:56:ALA:H	2.29	0.40
1:C:196:LEU:H	1:C:196:LEU:HD23	1.87	0.40
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.77	0.40
1:D:32:ALA:HB2	1:D:88:LEU:HD22	2.03	0.40
1:F:235:HIS:CD2	1:F:235:HIS:C	2.99	0.40
2:G:444:ARG:O	2:G:448:ARG:NE	2.55	0.40
2:c:33:VAL:HG12	2:c:42:MET:HE2	2.03	0.40
1:C:244:ILE:HD13	1:C:244:ILE:HA	1.92	0.40
1:F:171:ARG:HA	1:F:171:ARG:HD2	1.72	0.40
2:G:408:ARG:O	2:G:408:ARG:HG2	2.22	0.40
2:G:472:TRP:HE1	2:G:479:ALA:HA	1.86	0.40
2:c:162:LEU:HD22	2:c:187:ILE:HG21	2.04	0.40
1:A:94:ARG:NH1	1:A:141:ASP:HB2	2.35	0.40
1:B:46:ASP:HB2	1:B:231:VAL:HG11	2.04	0.40
1:B:77:LYS:NZ	1:B:186:ASN:OD1	2.46	0.40
1:C:186:ASN:O	1:C:187:THR:C	2.64	0.40
2:G:420:VAL:HB	2:G:543:MET:HB2	2.04	0.40
1:A:247:LYS:O	1:A:251:VAL:HG23	2.22	0.40
1:C:113:VAL:HG11	1:C:122:GLU:OE1	2.22	0.40
1:C:158:LEU:HD21	1:C:211:TRP:CH2	2.56	0.40
1:C:318:LEU:O	1:C:320:GLU:N	2.55	0.40
1:D:235:HIS:ND1	1:D:281:ALA:HB2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/328 (91%)	273 (92%)	24 (8%)	1 (0%)	36	65
1	B	293/328 (89%)	273 (93%)	20 (7%)	0	100	100
1	C	308/328 (94%)	291 (94%)	14 (4%)	3 (1%)	12	40
1	D	317/328 (97%)	290 (92%)	25 (8%)	2 (1%)	21	52
1	E	318/328 (97%)	296 (93%)	22 (7%)	0	100	100
1	F	317/328 (97%)	293 (92%)	24 (8%)	0	100	100
2	G	302/637 (47%)	273 (90%)	29 (10%)	0	100	100
2	a	199/637 (31%)	187 (94%)	12 (6%)	0	100	100
2	c	201/637 (32%)	179 (89%)	22 (11%)	0	100	100
All	All	2553/3879 (66%)	2355 (92%)	192 (8%)	6 (0%)	44	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	320	GLU
1	A	321	SER
1	D	321	SER
1	C	190	LEU
1	D	319	PRO
1	C	319	PRO

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	257/278 (92%)	253 (98%)	4 (2%)	55	72
1	B	254/278 (91%)	253 (100%)	1 (0%)	84	84
1	C	264/278 (95%)	256 (97%)	8 (3%)	36	61
1	D	270/278 (97%)	264 (98%)	6 (2%)	45	66
1	E	270/278 (97%)	270 (100%)	0	100	100
1	F	270/278 (97%)	266 (98%)	4 (2%)	57	72
2	G	256/517 (50%)	253 (99%)	3 (1%)	63	75
2	a	138/517 (27%)	137 (99%)	1 (1%)	76	80
2	c	139/517 (27%)	138 (99%)	1 (1%)	76	80
All	All	2118/3219 (66%)	2090 (99%)	28 (1%)	59	74

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	155	GLN
1	F	324	ASN
1	F	325	ILE
1	F	327	LEU
2	G	351	LEU
2	G	440	ASP
2	G	447	GLU
2	a	141	ARG
2	c	42	MET
1	A	27	ASP
1	A	69	VAL
1	A	316	VAL
1	A	318	LEU
1	B	227	ASN
1	C	184	THR
1	C	186	ASN
1	C	188	VAL
1	C	190	LEU
1	C	267	VAL
1	C	316	VAL
1	C	317	GLU
1	C	320	GLU
1	D	109	LYS
1	D	174	ARG
1	D	301	LEU
1	D	317	GLU

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Mol	Chain	Res	Type
1	D	318	LEU
1	D	320	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	96	ASN
1	E	119	GLN
1	E	133	GLN
1	E	155	GLN
1	E	227	ASN
1	F	222	HIS
1	F	257	GLN
1	F	324	ASN
2	G	406	GLN
2	c	130	ASN
1	A	52	GLN
1	A	133	GLN
1	A	205	GLN
1	A	207	GLN
1	A	218	ASN
1	A	261	ASN
1	A	279	ASN
1	A	284	ASN
1	A	296	ASN
1	A	311	GLN
1	A	324	ASN
1	B	237	GLN
1	B	238	ASN
1	B	311	GLN
1	C	119	GLN
1	C	169	GLN
1	C	204	ASN
1	C	237	GLN
1	C	324	ASN
1	D	96	ASN
1	D	324	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\# Z > 2$
3	ATP	F	401	4	29,33,33	0.32	0	44,52,52	0.47	1 (2%)
3	ATP	D	401	4	29,33,33	0.31	0	44,52,52	0.52	1 (2%)
3	ATP	A	401	4	29,33,33	0.29	0	44,52,52	0.46	1 (2%)
3	ATP	B	401	-	29,33,33	0.32	0	44,52,52	0.56	1 (2%)
3	ATP	E	401	4	29,33,33	0.32	0	44,52,52	0.47	1 (2%)
3	ATP	C	401	4	29,33,33	0.30	0	44,52,52	0.47	1 (2%)

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
3	ATP	F	401	4	-	9/22/38/38	0/3/3/3
3	ATP	D	401	4	-	7/22/38/38	0/3/3/3
3	ATP	A	401	4	-	7/22/38/38	0/3/3/3
3	ATP	B	401	-	-	6/22/38/38	0/3/3/3
3	ATP	E	401	4	-	8/22/38/38	0/3/3/3
3	ATP	C	401	4	-	5/22/38/38	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	ATP	PB-O3B-PG	2.07	139.92	132.83
3	D	401	ATP	PB-O3B-PG	2.07	139.91	132.83
3	C	401	ATP	PB-O3B-PG	2.05	139.86	132.83
3	A	401	ATP	PB-O3B-PG	2.02	139.76	132.83
3	B	401	ATP	PB-O3B-PG	2.01	139.73	132.83
3	E	401	ATP	PB-O3B-PG	2.00	139.69	132.83

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	401	ATP	O4'-C4'-C5'-O5'
3	E	401	ATP	C3'-C4'-C5'-O5'
3	F	401	ATP	PB-O3B-PG-O3G
3	F	401	ATP	C5'-O5'-PA-O1A
3	A	401	ATP	PB-O3B-PG-O2G
3	A	401	ATP	C5'-O5'-PA-O1A
3	A	401	ATP	O4'-C4'-C5'-O5'
3	B	401	ATP	C5'-O5'-PA-O2A
3	C	401	ATP	C5'-O5'-PA-O3A
3	D	401	ATP	C5'-O5'-PA-O1A
3	D	401	ATP	C5'-O5'-PA-O2A
3	D	401	ATP	C5'-O5'-PA-O3A
3	D	401	ATP	O4'-C1'-N9-C8
3	D	401	ATP	O4'-C1'-N9-C4
3	D	401	ATP	O4'-C4'-C5'-O5'
3	F	401	ATP	O4'-C4'-C5'-O5'
3	F	401	ATP	C3'-C4'-C5'-O5'
3	A	401	ATP	C3'-C4'-C5'-O5'
3	E	401	ATP	O4'-C1'-N9-C4
3	E	401	ATP	PB-O3B-PG-O1G
3	E	401	ATP	O4'-C1'-N9-C8
3	D	401	ATP	C3'-C4'-C5'-O5'
3	B	401	ATP	C4'-C5'-O5'-PA
3	F	401	ATP	PB-O3A-PA-O5'
3	E	401	ATP	PB-O3B-PG-O3G
3	F	401	ATP	C5'-O5'-PA-O3A
3	A	401	ATP	C5'-O5'-PA-O3A
3	B	401	ATP	C5'-O5'-PA-O3A
3	E	401	ATP	PG-O3B-PB-O1B

Continued on next page...

Continued from previous page...

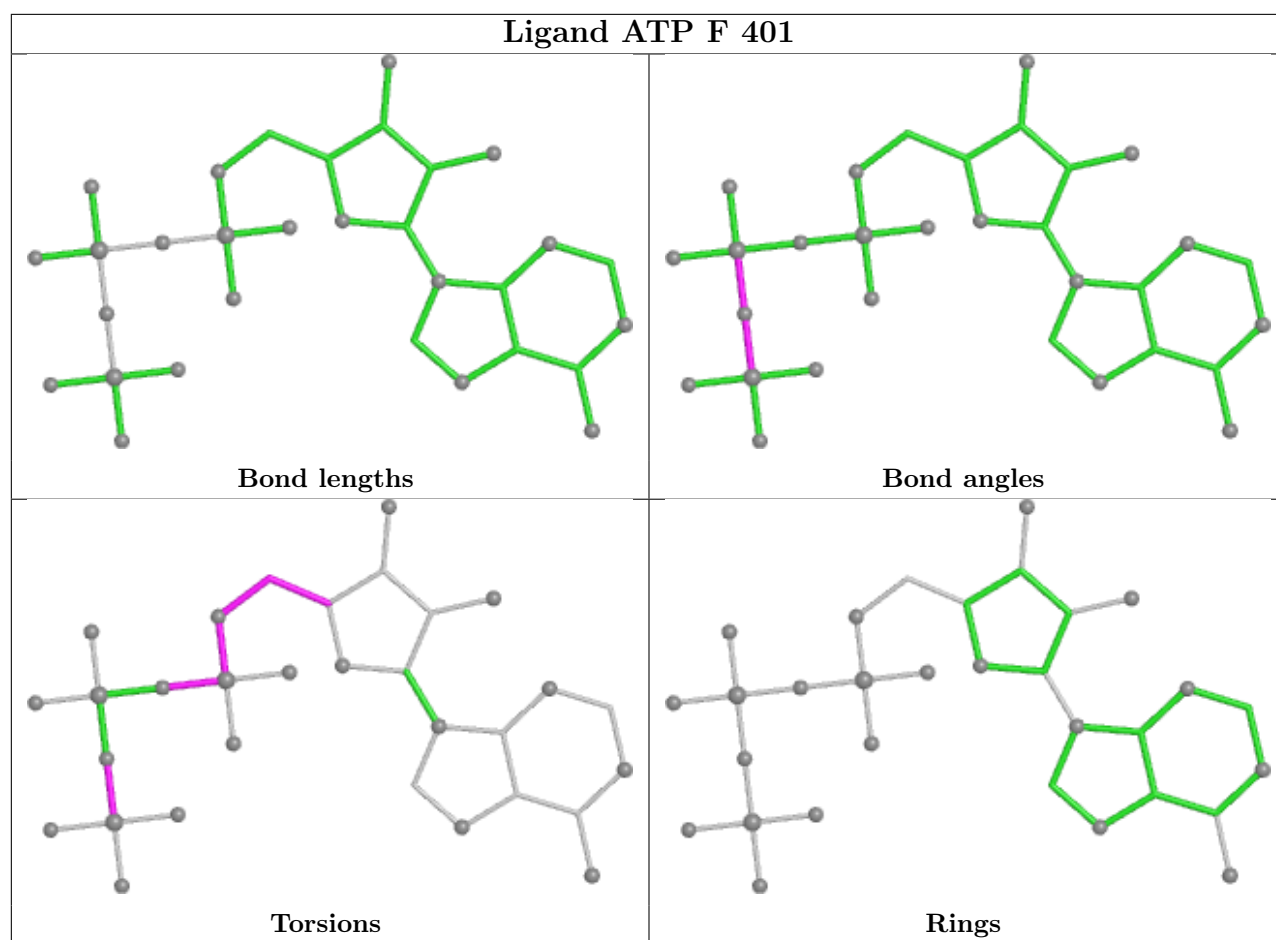
Mol	Chain	Res	Type	Atoms
3	F	401	ATP	C5'-O5'-PA-O2A
3	A	401	ATP	C5'-O5'-PA-O2A
3	B	401	ATP	C5'-O5'-PA-O1A
3	C	401	ATP	C5'-O5'-PA-O1A
3	C	401	ATP	C4'-C5'-O5'-PA
3	C	401	ATP	PA-O3A-PB-O3B
3	F	401	ATP	C4'-C5'-O5'-PA
3	A	401	ATP	PB-O3B-PG-O1G
3	E	401	ATP	C2'-C1'-N9-C8
3	F	401	ATP	PB-O3B-PG-O2G
3	B	401	ATP	PB-O3B-PG-O2G
3	C	401	ATP	PA-O3A-PB-O1B
3	B	401	ATP	O4'-C4'-C5'-O5'

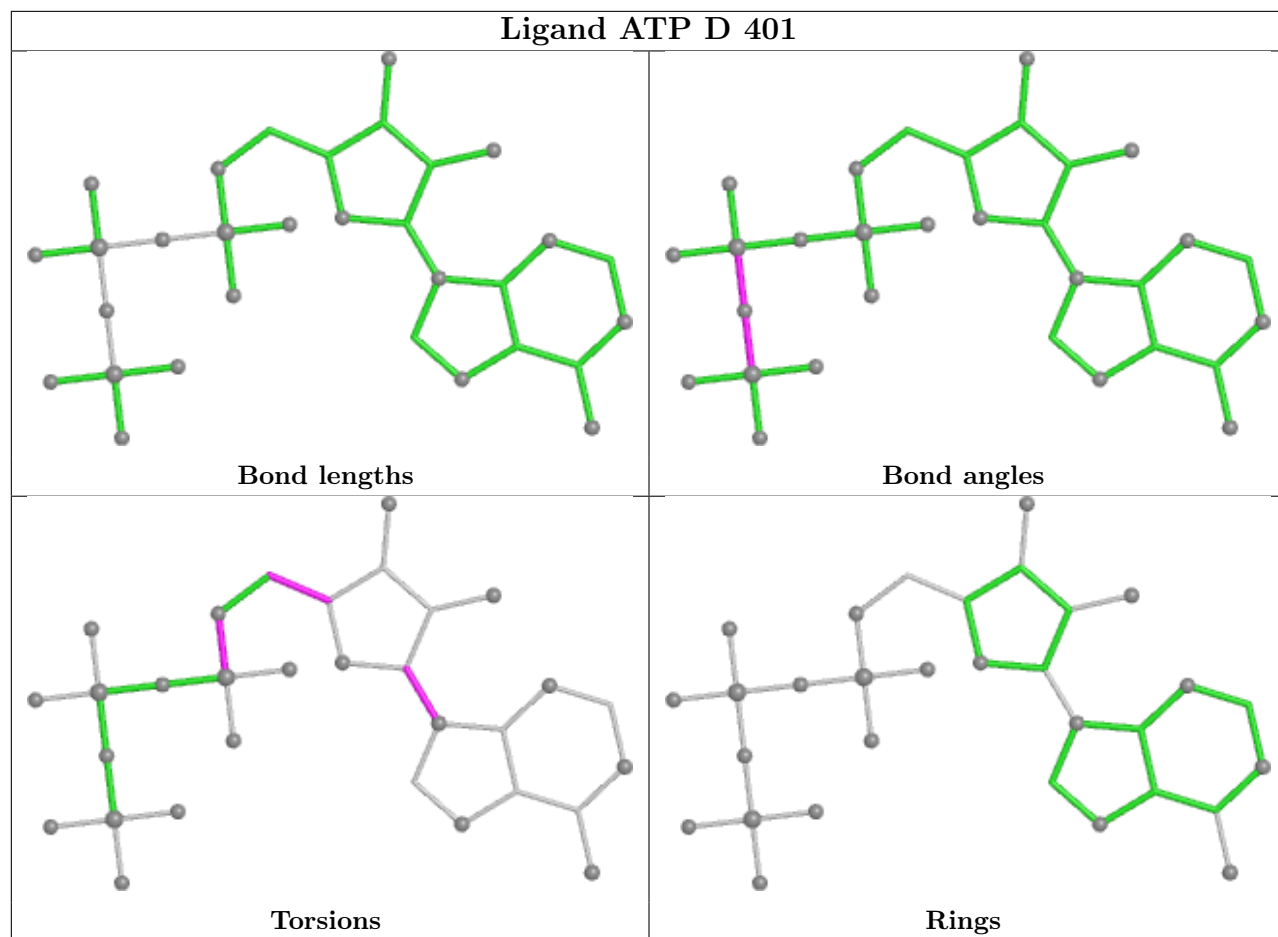
There are no ring outliers.

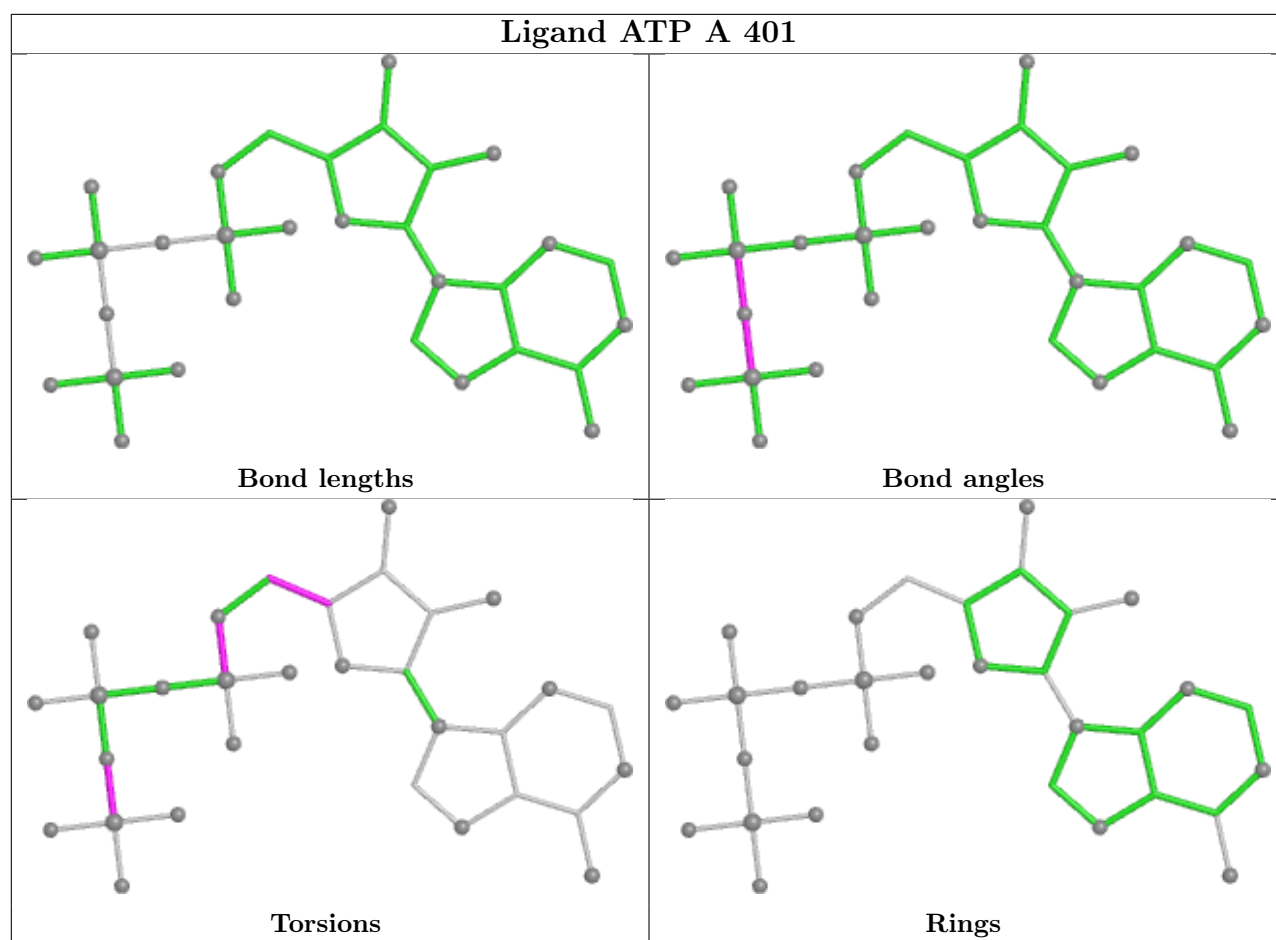
6 monomers are involved in 12 short contacts:

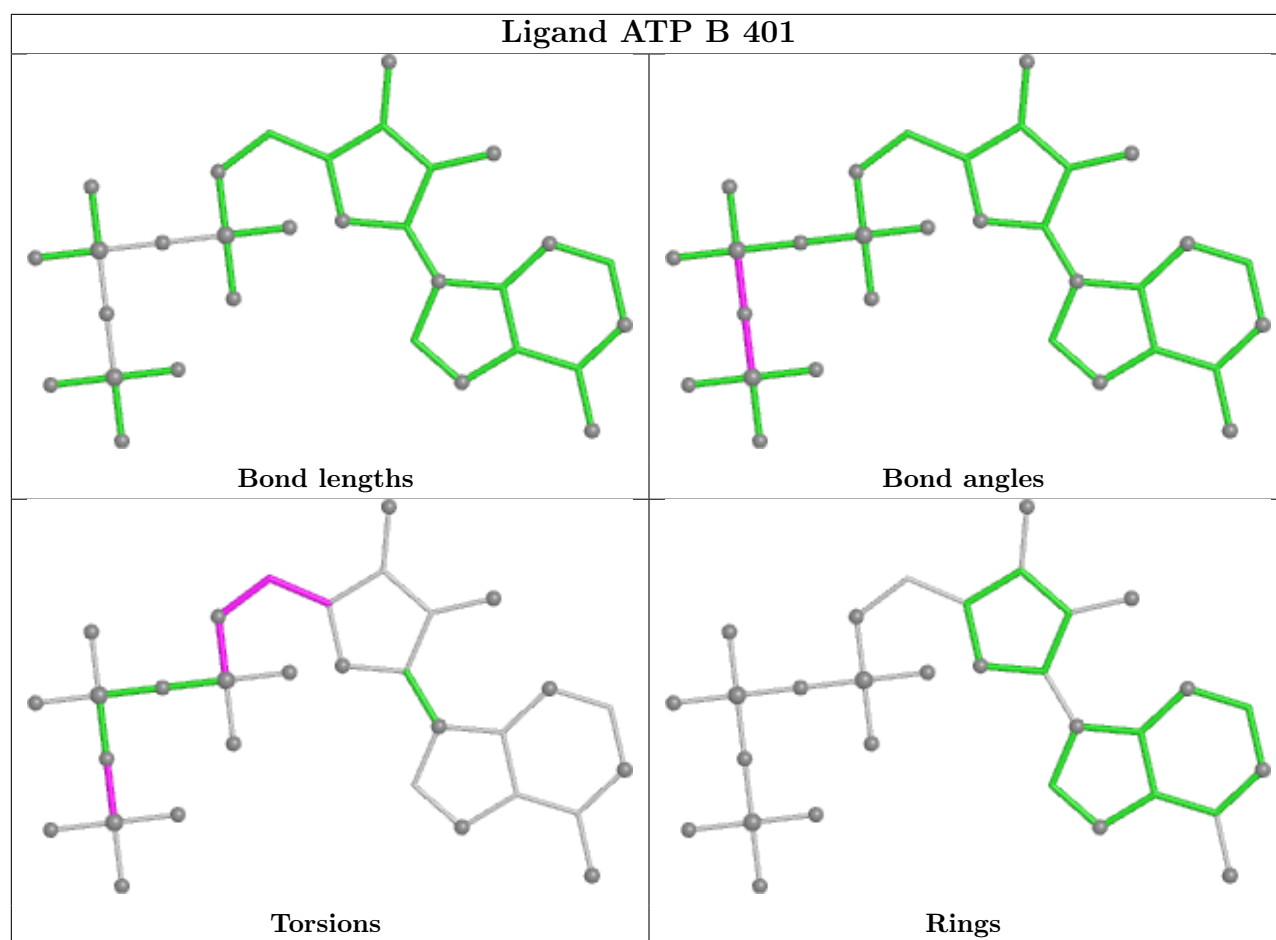
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	ATP	2	0
3	D	401	ATP	2	0
3	A	401	ATP	1	0
3	B	401	ATP	2	0
3	E	401	ATP	2	0
3	C	401	ATP	3	0

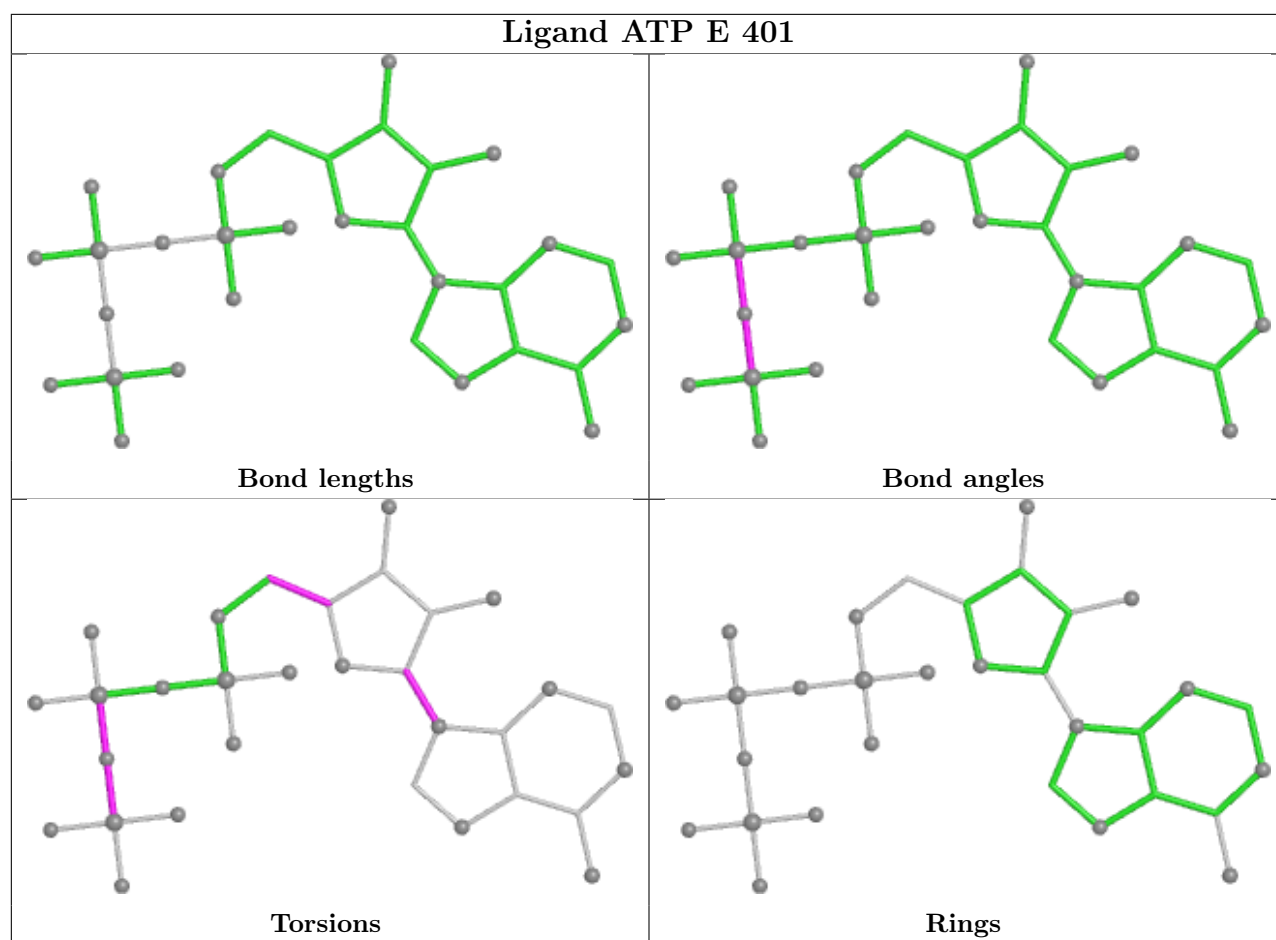
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

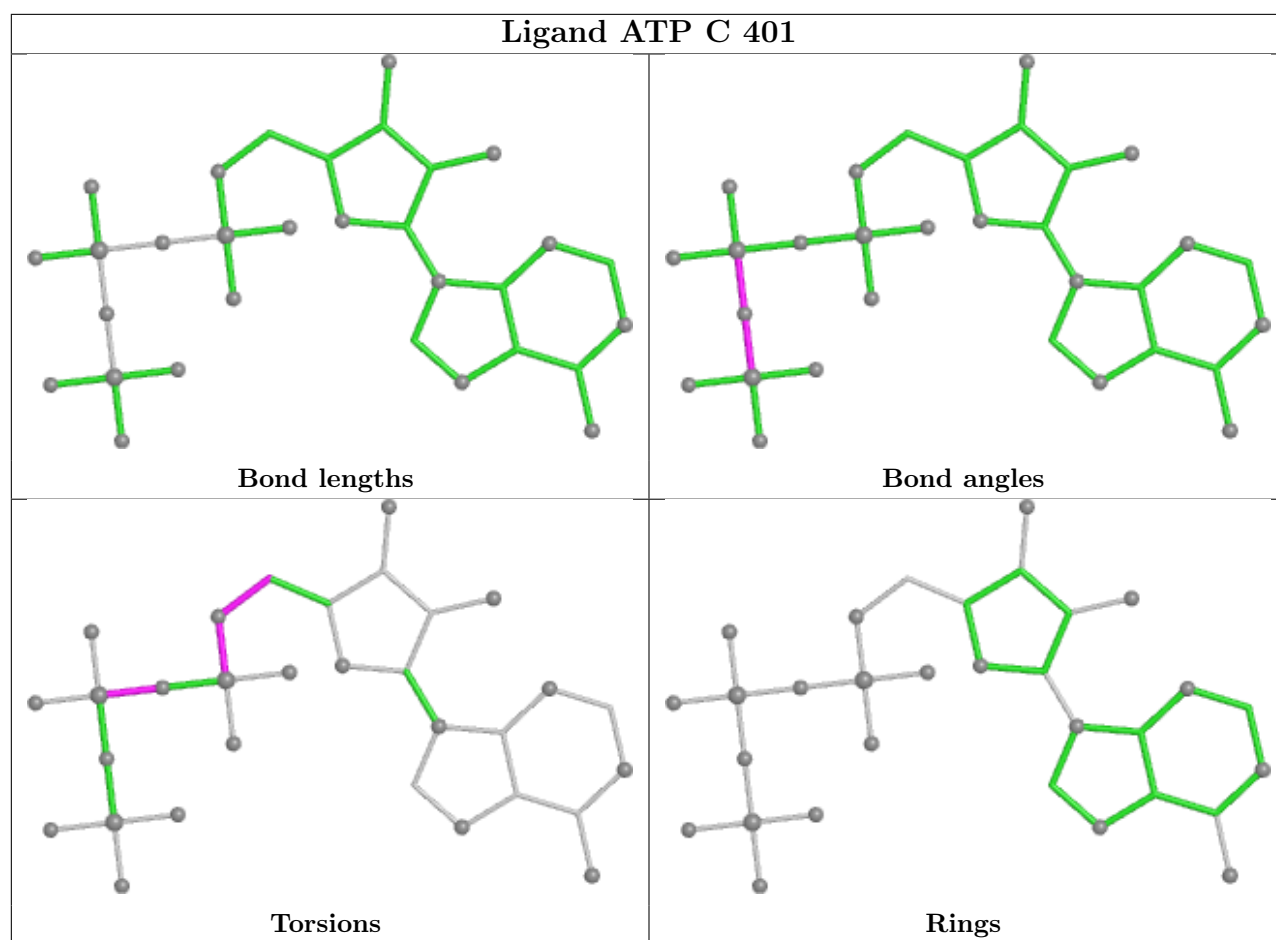












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

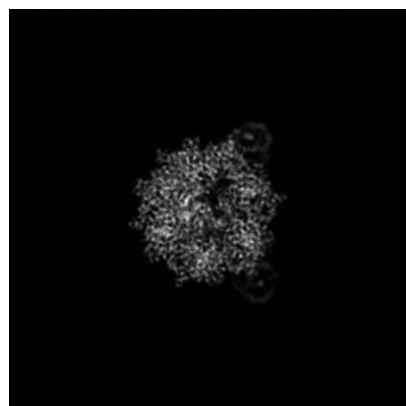
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64237. These allow visual inspection of the internal detail of the map and identification of artifacts.

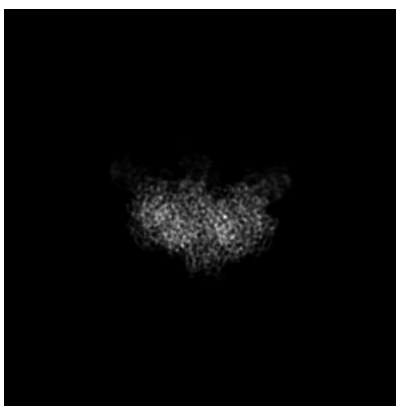
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

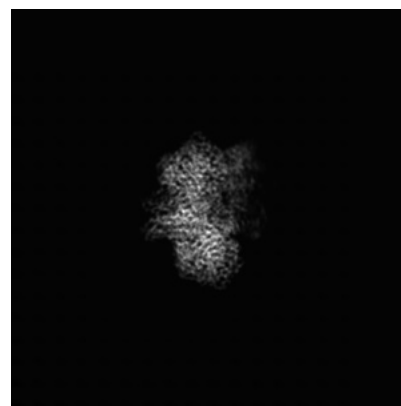
6.1.1 Primary map



X

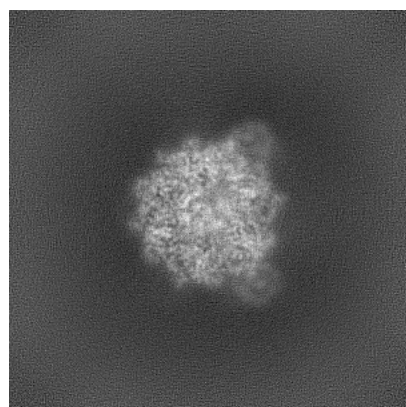


Y

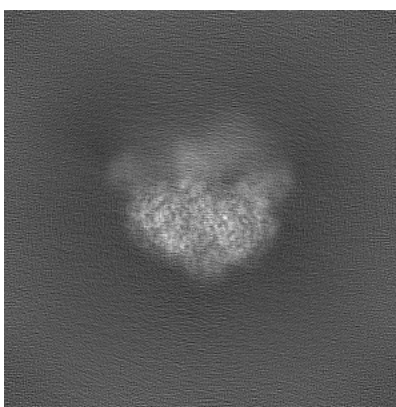


Z

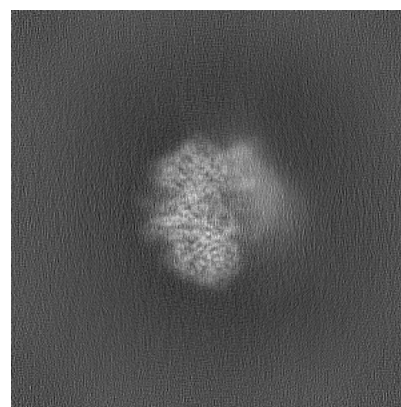
6.1.2 Raw map



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: 210

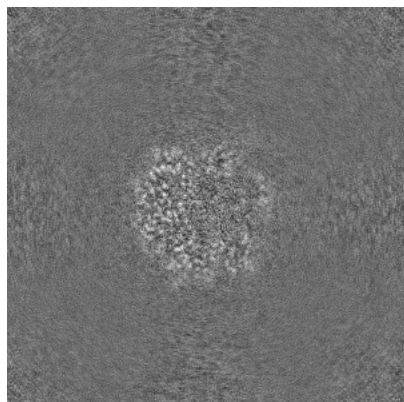


Y Index: 210

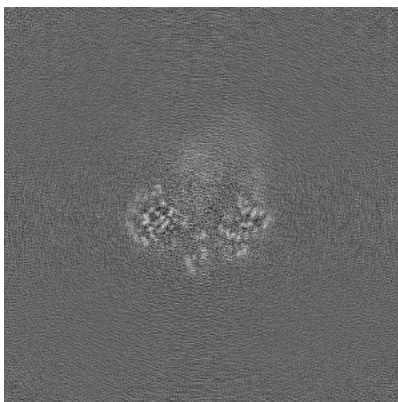


Z Index: 210

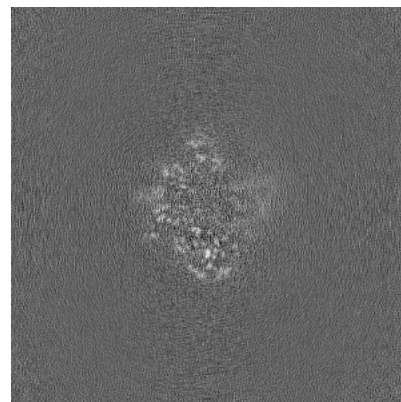
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

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

6.3 Largest variance slices [i](#)

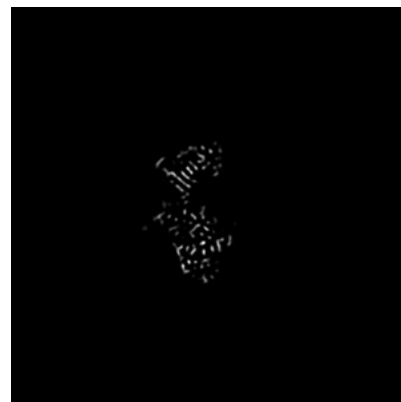
6.3.1 Primary map



X Index: 197

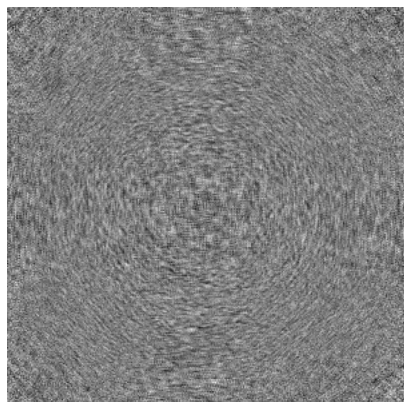


Y Index: 187

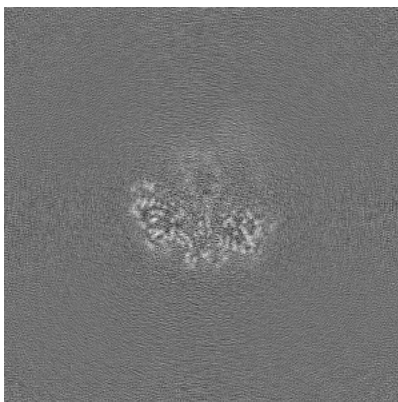


Z Index: 231

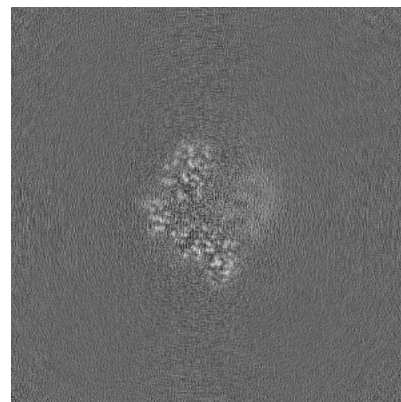
6.3.2 Raw map



X Index: 0



Y Index: 200

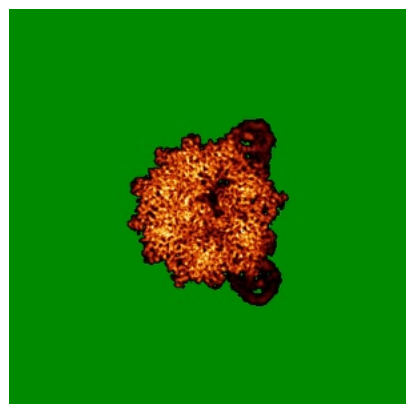


Z Index: 198

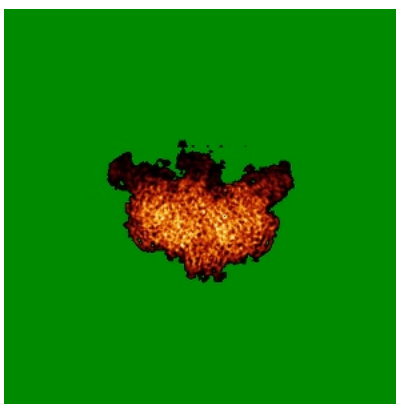
The images above show the largest variance slices of the map in three orthogonal directions.

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

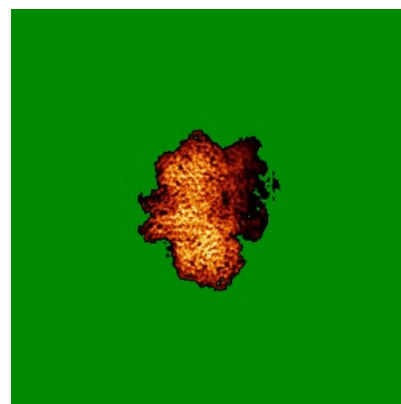
6.4.1 Primary map



X

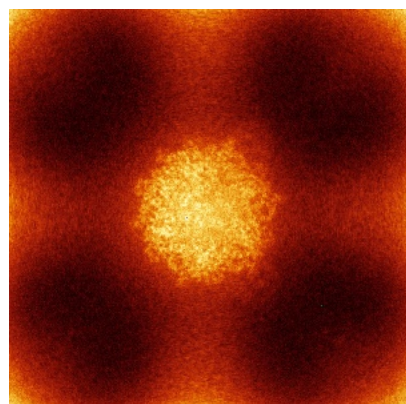


Y

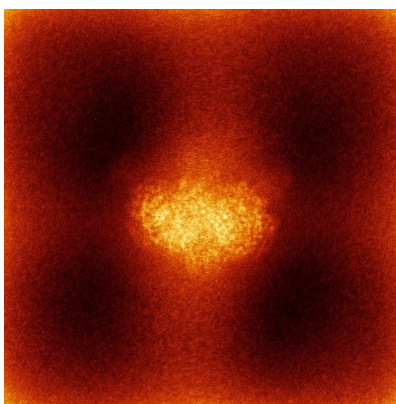


Z

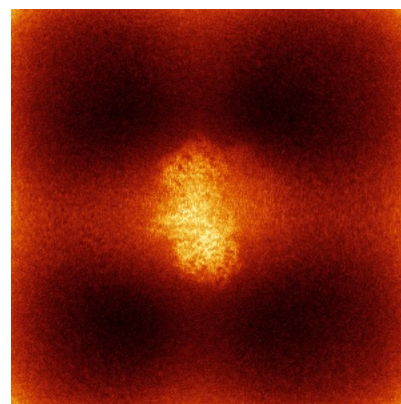
6.4.2 Raw map



X



Y

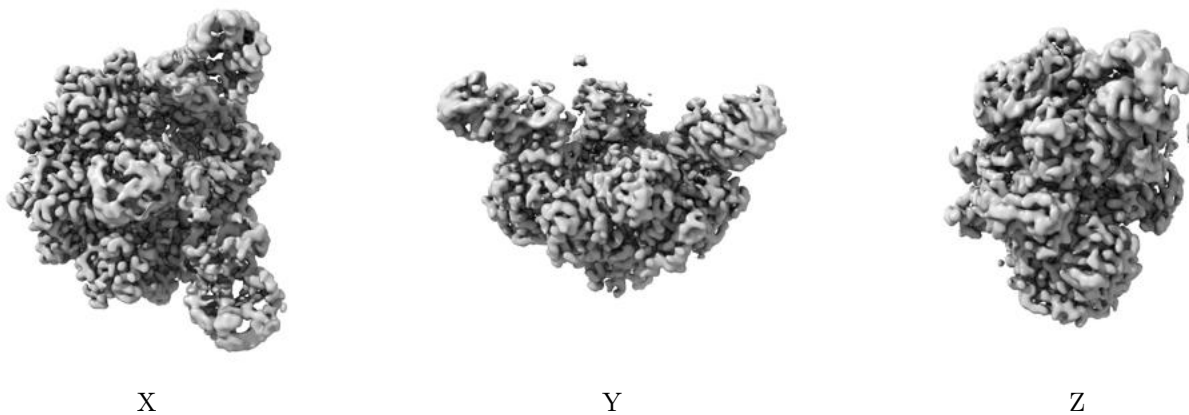


Z

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

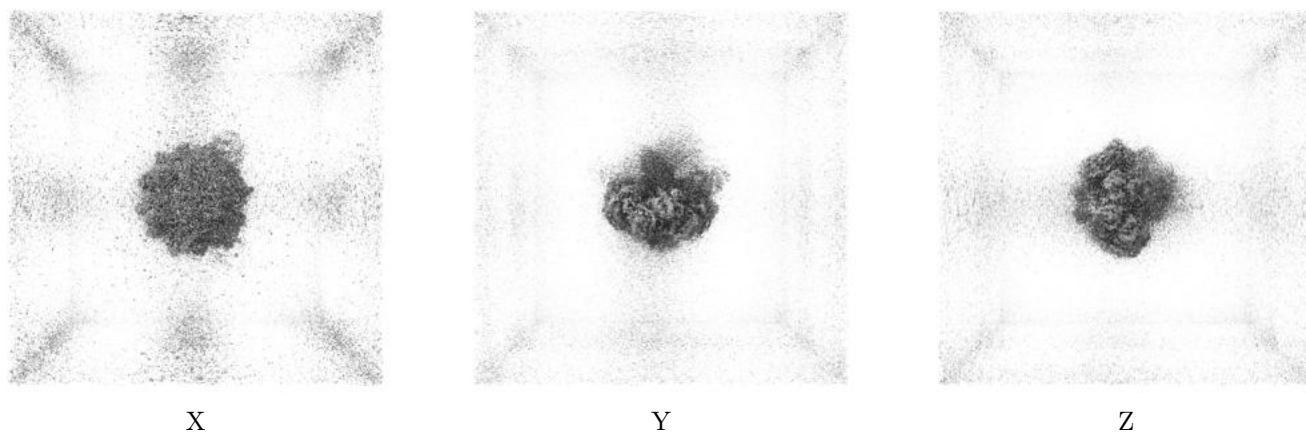
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

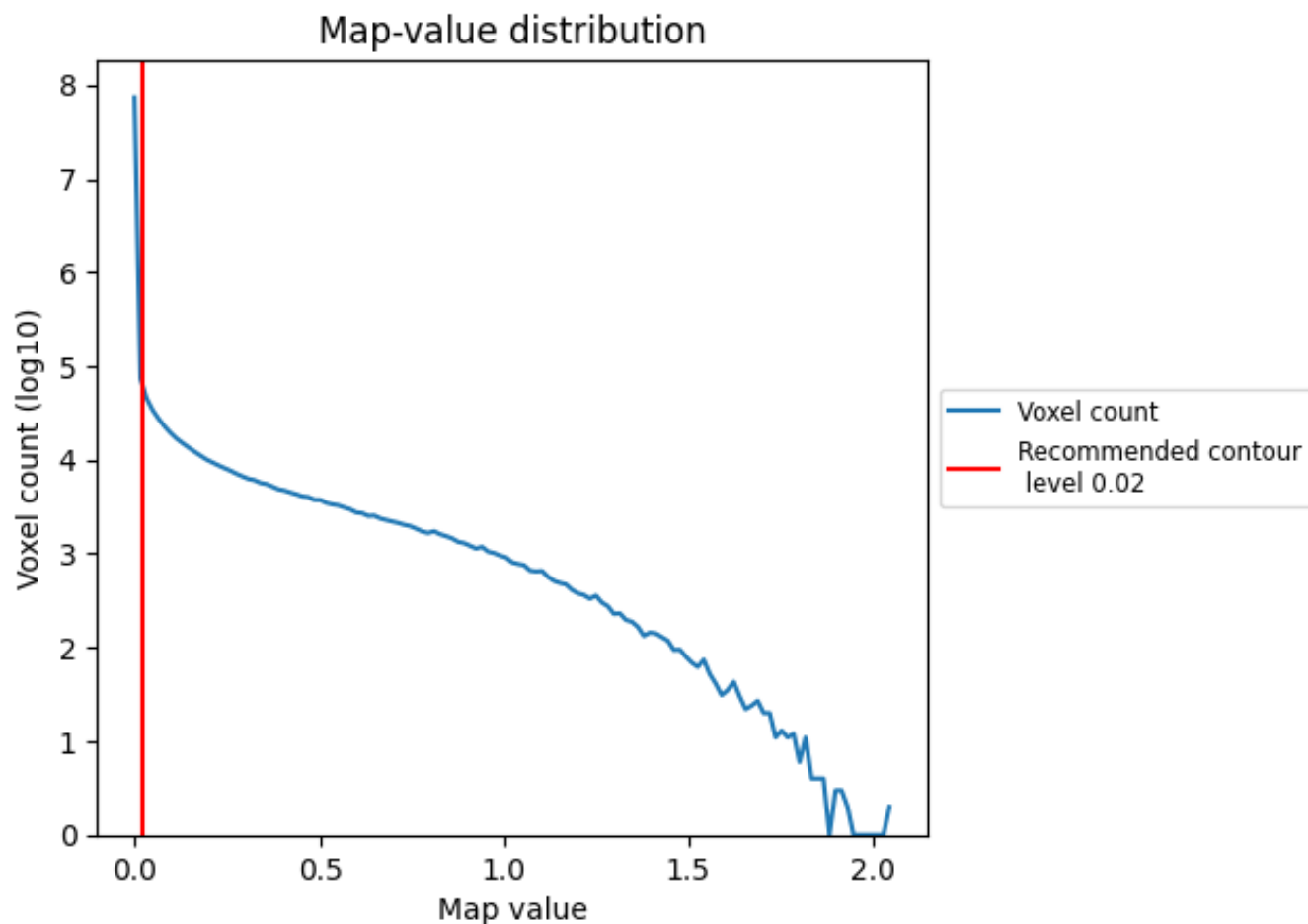
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

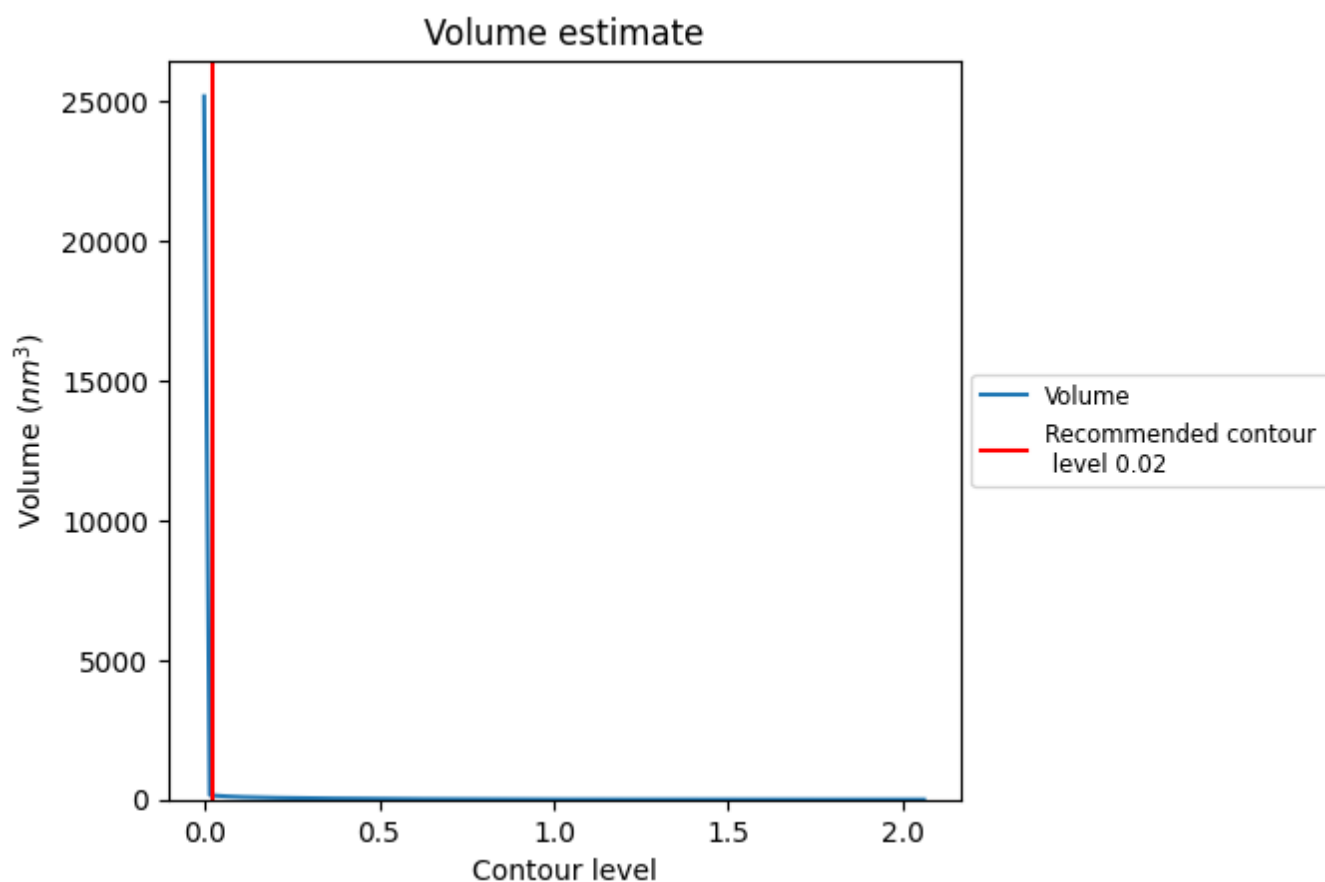
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

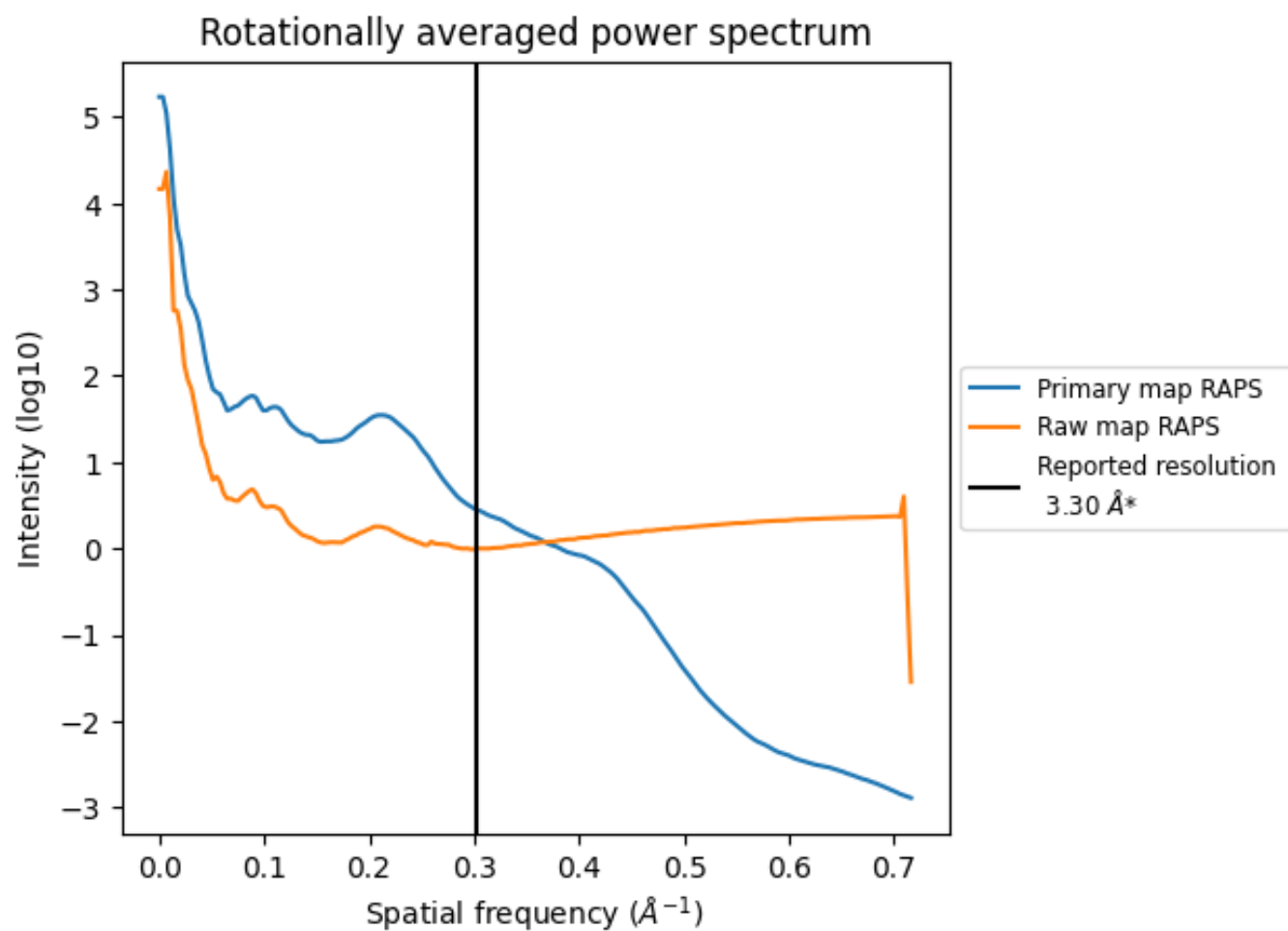
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm^3 ; this corresponds to an approximate mass of 141 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 ⓘ

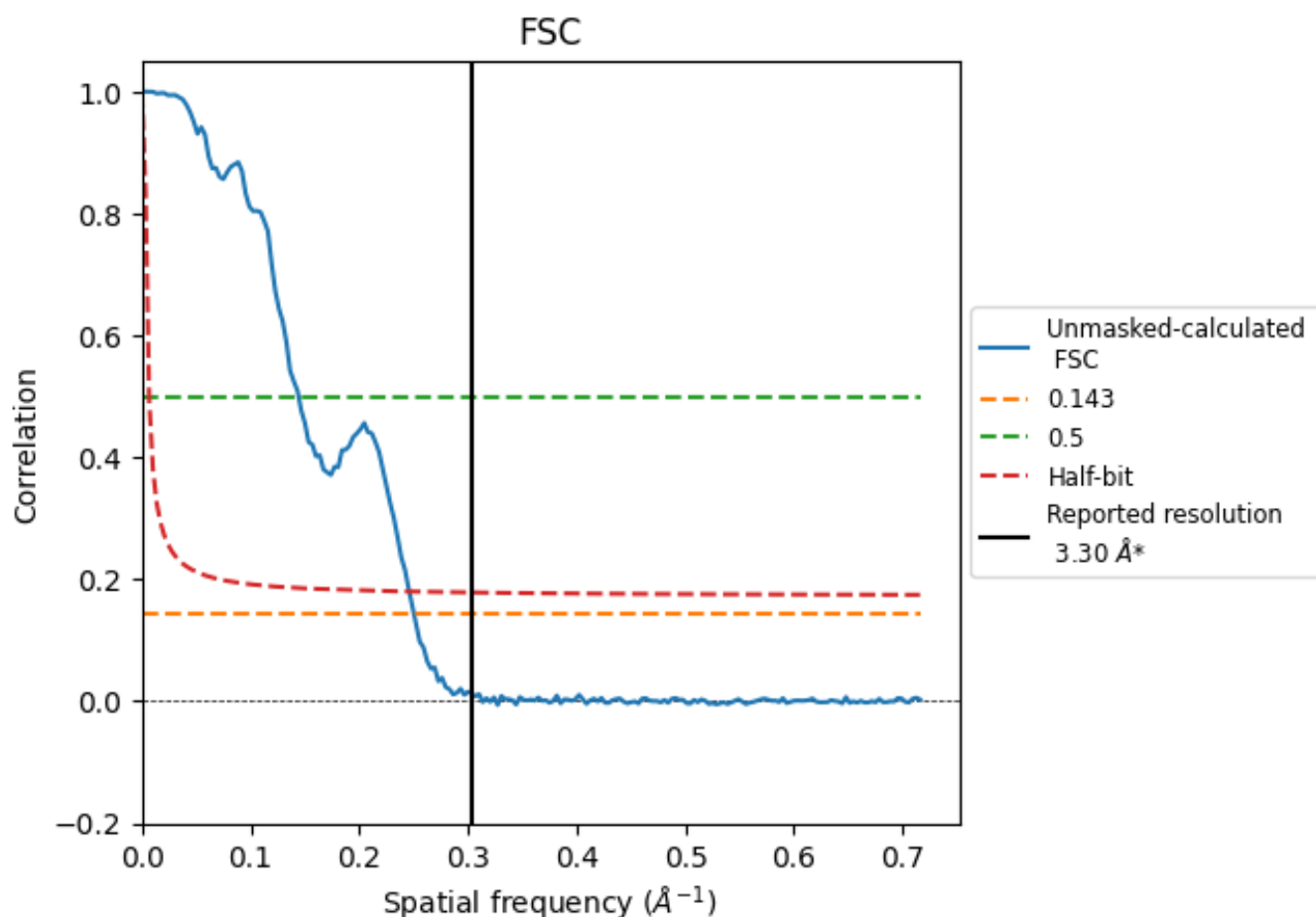


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

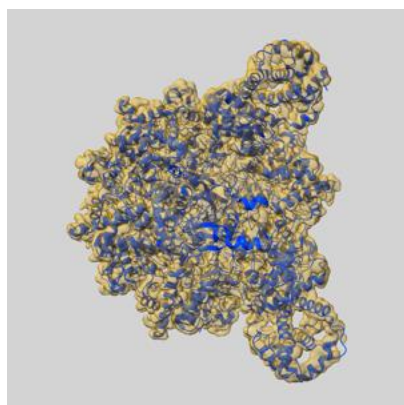
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	6.93	4.06

*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 3.99 differs from the reported value 3.3 by more than 10 %

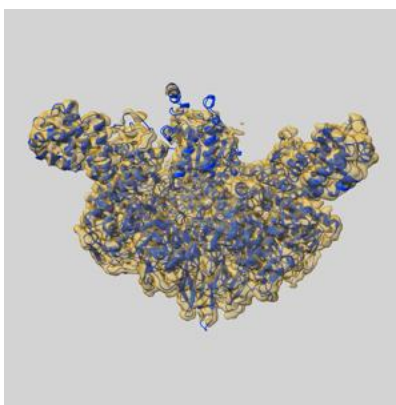
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64237 and PDB model 9UKF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

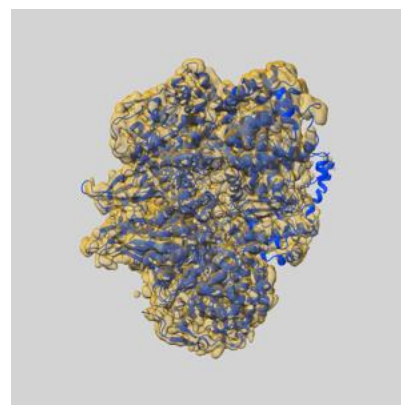
9.1 Map-model overlay [i](#)



X



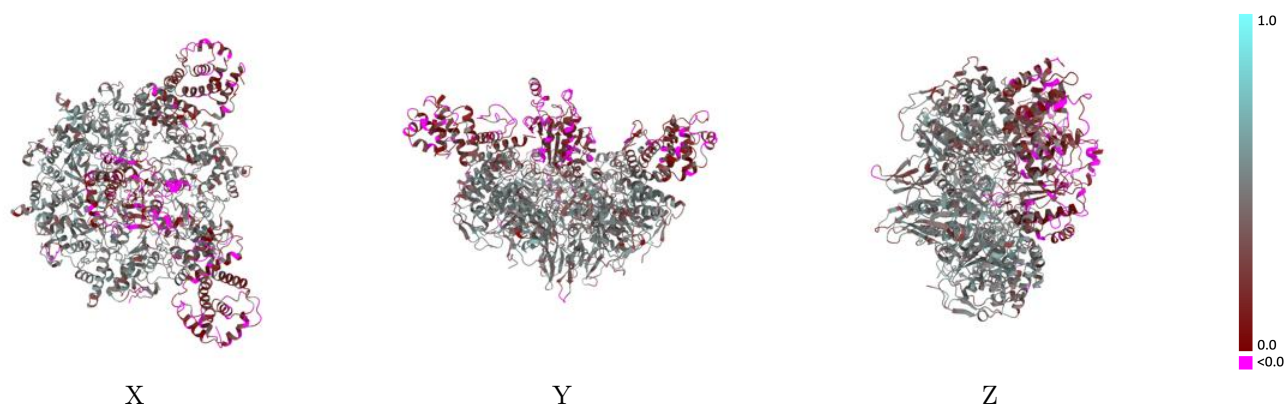
Y



Z

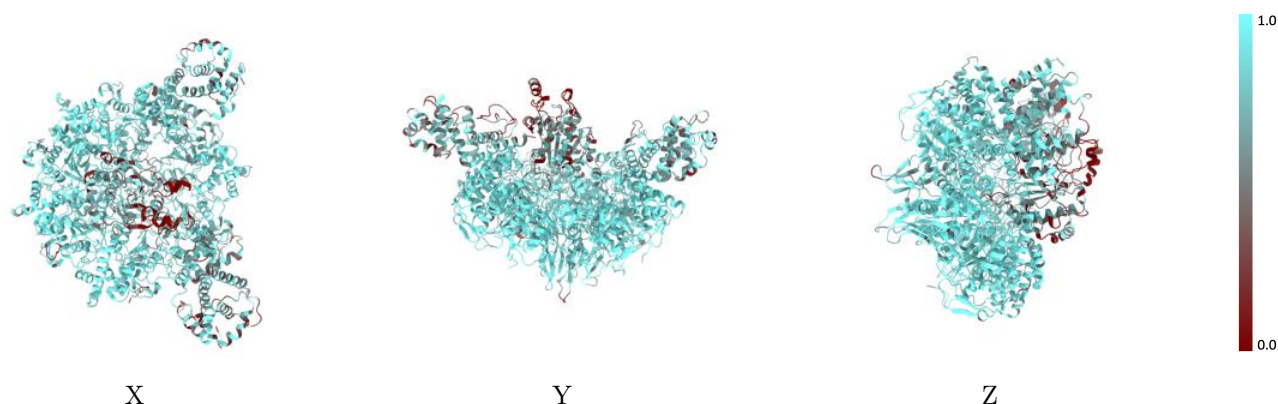
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



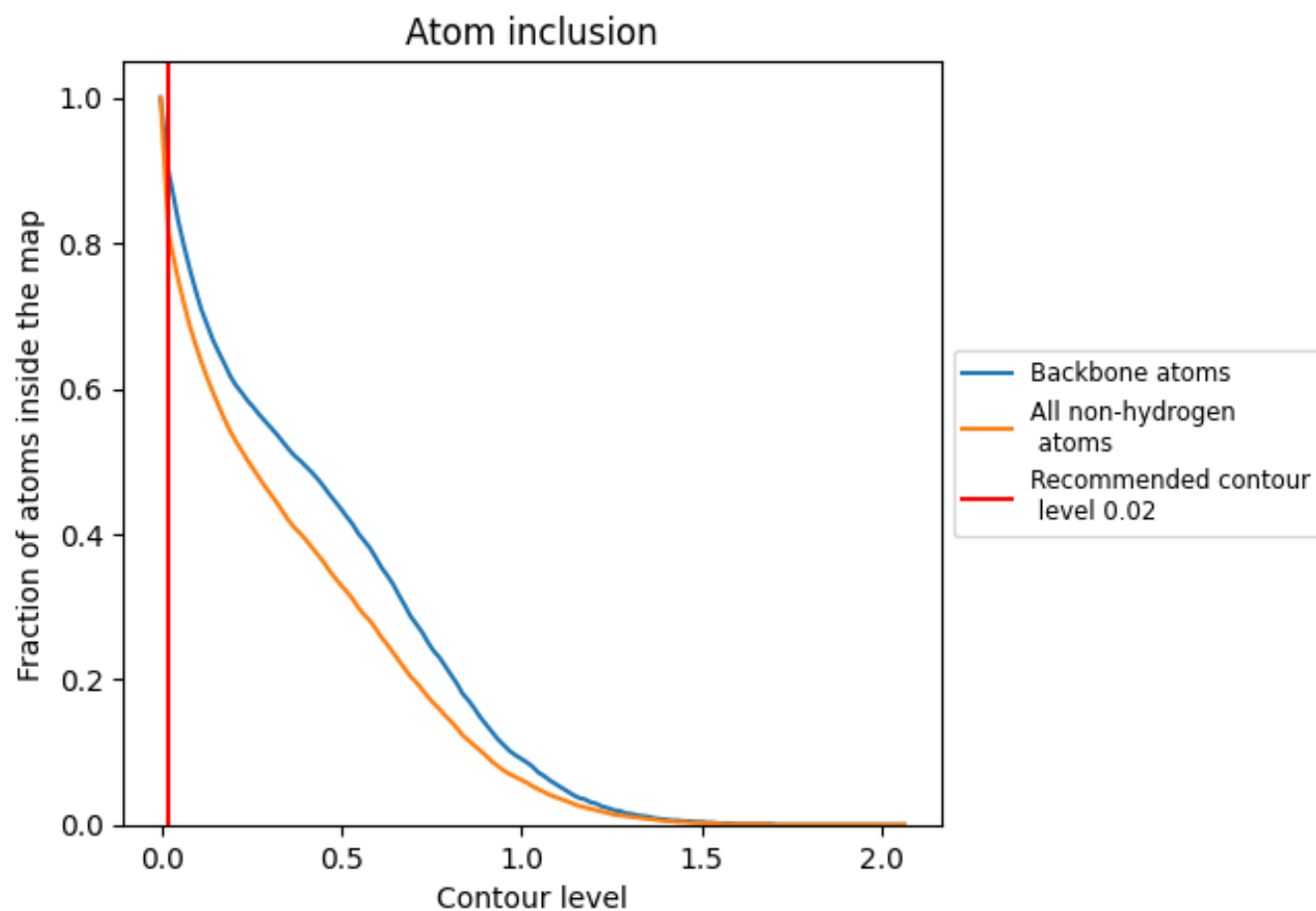
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 82% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.3810
A	0.8850	0.4340
B	0.9020	0.4510
C	0.9020	0.4620
D	0.9180	0.4780
E	0.9110	0.4760
F	0.9000	0.4620
G	0.4810	0.1400
a	0.7110	0.2040
c	0.5770	0.1460

1.0

0.0

<0.0