Full wwPDB EM Validation Report ⓘ

Aug 15, 2023 – 12:11 PM EDT

PDB ID	:	8FX4
EMDB ID	:	EMD-29523
Title	:	GC-C-Hsp90-Cdc37 regulatory complex
Authors	:	Caveney, N.A.; Garcia, K.C.
Deposited on	:	2023-01-23
Resolution	:	3.90 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:

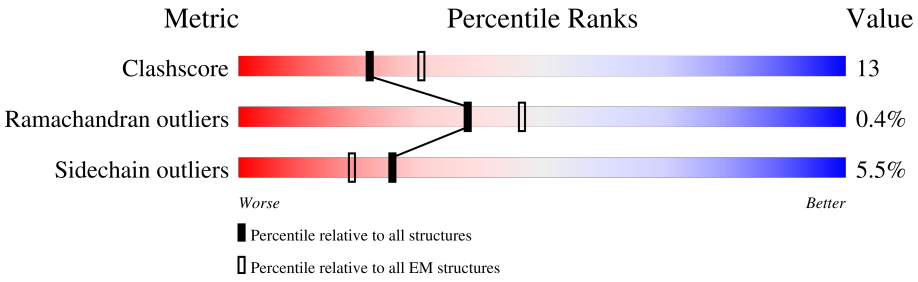
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.90 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	724	7% 63% 21% • 14%
1	B	724	5% 60% 23% • 15%
2	C	379	32% 34% 17% • 47%
3	D	741	11% 14% 12% • 73%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13474 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 Heat shock protein HSP 90-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	623	Total	C	N	O	S	0	0
			5039	3194	847	975	23		
1	B	619	Total	C	N	O	S	0	0
			5011	3182	841	965	23		

- Molecule 2 is a protein called Hsp90 co-chaperone Cdc37.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	200	Total	C	N	O	S	0	0
			1699	1070	297	320	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	48	GLU	ASP	conflict	UNP G3H6C5

- Molecule 3 is a protein called Guanylyl cyclase C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	203	Total	C	N	O	S	0	0
			1663	1064	276	313	10		

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	344	ASP	-	expression tag	UNP P25092
D	345	TYR	-	expression tag	UNP P25092
D	346	LYS	-	expression tag	UNP P25092
D	347	ASP	-	expression tag	UNP P25092
D	348	ASP	-	expression tag	UNP P25092
D	349	ASP	-	expression tag	UNP P25092
D	350	ASP	-	expression tag	UNP P25092
D	351	LYS	-	expression tag	UNP P25092

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Chain	Residue	Modelled	Actual	Comment	Reference
D	352	GLY	-	expression tag	UNP P25092
D	353	SER	-	expression tag	UNP P25092
D	354	LEU	-	expression tag	UNP P25092
D	355	GLU	-	expression tag	UNP P25092
D	356	VAL	-	expression tag	UNP P25092
D	357	LEU	-	expression tag	UNP P25092
D	358	PHE	-	expression tag	UNP P25092
D	359	GLN	-	expression tag	UNP P25092
D	360	GLY	-	expression tag	UNP P25092
D	361	PRO	-	expression tag	UNP P25092
D	362	GLY	-	expression tag	UNP P25092
D	363	ARG	-	expression tag	UNP P25092
D	364	MET	-	expression tag	UNP P25092
D	365	LYS	-	expression tag	UNP P25092
D	366	GLN	-	expression tag	UNP P25092
D	367	LEU	-	expression tag	UNP P25092
D	368	GLU	-	expression tag	UNP P25092
D	369	ASP	-	expression tag	UNP P25092
D	370	LYS	-	expression tag	UNP P25092
D	371	VAL	-	expression tag	UNP P25092
D	372	GLU	-	expression tag	UNP P25092
D	373	GLU	-	expression tag	UNP P25092
D	374	LEU	-	expression tag	UNP P25092
D	375	LEU	-	expression tag	UNP P25092
D	376	SER	-	expression tag	UNP P25092
D	377	LYS	-	expression tag	UNP P25092
D	378	ASN	-	expression tag	UNP P25092
D	379	TYR	-	expression tag	UNP P25092
D	380	HIS	-	expression tag	UNP P25092
D	381	LEU	-	expression tag	UNP P25092
D	382	GLU	-	expression tag	UNP P25092
D	383	ASN	-	expression tag	UNP P25092
D	384	GLU	-	expression tag	UNP P25092
D	385	VAL	-	expression tag	UNP P25092
D	386	ALA	-	expression tag	UNP P25092
D	387	ARG	-	expression tag	UNP P25092
D	388	LEU	-	expression tag	UNP P25092
D	389	LYS	-	expression tag	UNP P25092
D	390	LYS	-	expression tag	UNP P25092
D	391	LEU	-	expression tag	UNP P25092
D	392	VAL	-	expression tag	UNP P25092
D	393	GLY	-	expression tag	UNP P25092

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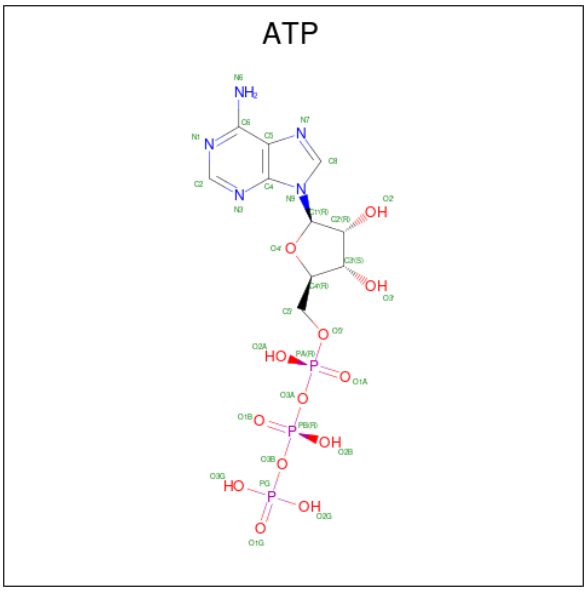
Chain	Residue	Modelled	Actual	Comment	Reference
D	394	GLU	-	expression tag	UNP P25092
D	395	ARG	-	expression tag	UNP P25092
D	1051	ALA	-	expression tag	UNP P25092
D	1052	ALA	-	expression tag	UNP P25092
D	1053	ALA	-	expression tag	UNP P25092
D	1054	LEU	-	expression tag	UNP P25092
D	1055	GLU	-	expression tag	UNP P25092
D	1056	VAL	-	expression tag	UNP P25092
D	1057	LEU	-	expression tag	UNP P25092
D	1058	PHE	-	expression tag	UNP P25092
D	1059	GLN	-	expression tag	UNP P25092
D	1060	GLY	-	expression tag	UNP P25092
D	1061	PRO	-	expression tag	UNP P25092
D	1062	GLY	-	expression tag	UNP P25092
D	1063	ALA	-	expression tag	UNP P25092
D	1064	ALA	-	expression tag	UNP P25092
D	1065	GLU	-	expression tag	UNP P25092
D	1066	ASP	-	expression tag	UNP P25092
D	1067	GLN	-	expression tag	UNP P25092
D	1068	VAL	-	expression tag	UNP P25092
D	1069	ASP	-	expression tag	UNP P25092
D	1070	PRO	-	expression tag	UNP P25092
D	1071	ARG	-	expression tag	UNP P25092
D	1072	LEU	-	expression tag	UNP P25092
D	1073	ILE	-	expression tag	UNP P25092
D	1074	ASP	-	expression tag	UNP P25092
D	1075	GLY	-	expression tag	UNP P25092
D	1076	LYS	-	expression tag	UNP P25092
D	1077	HIS	-	expression tag	UNP P25092
D	1078	HIS	-	expression tag	UNP P25092
D	1079	HIS	-	expression tag	UNP P25092
D	1080	HIS	-	expression tag	UNP P25092
D	1081	HIS	-	expression tag	UNP P25092
D	1082	HIS	-	expression tag	UNP P25092
D	1083	HIS	-	expression tag	UNP P25092
D	1084	HIS	-	expression tag	UNP P25092

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



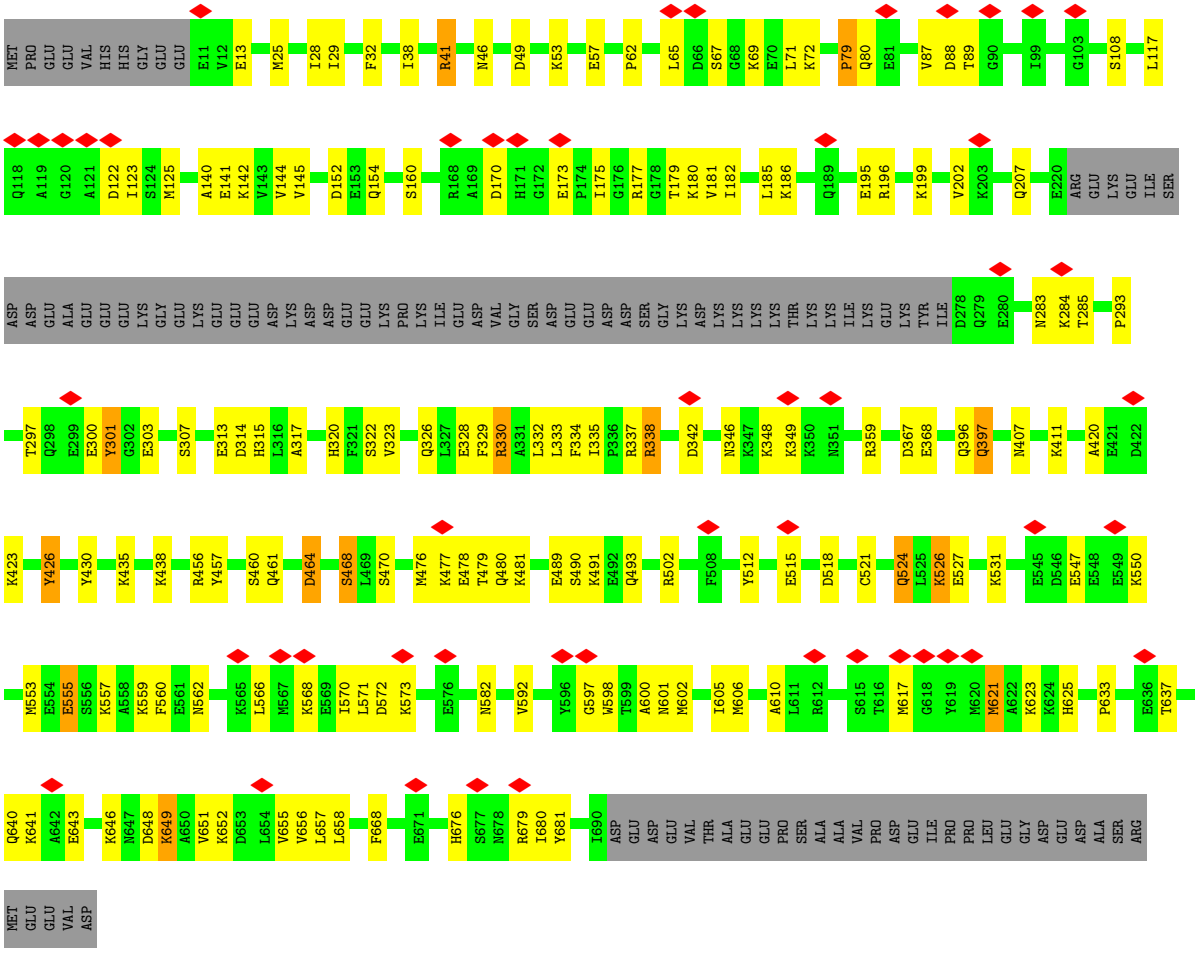
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

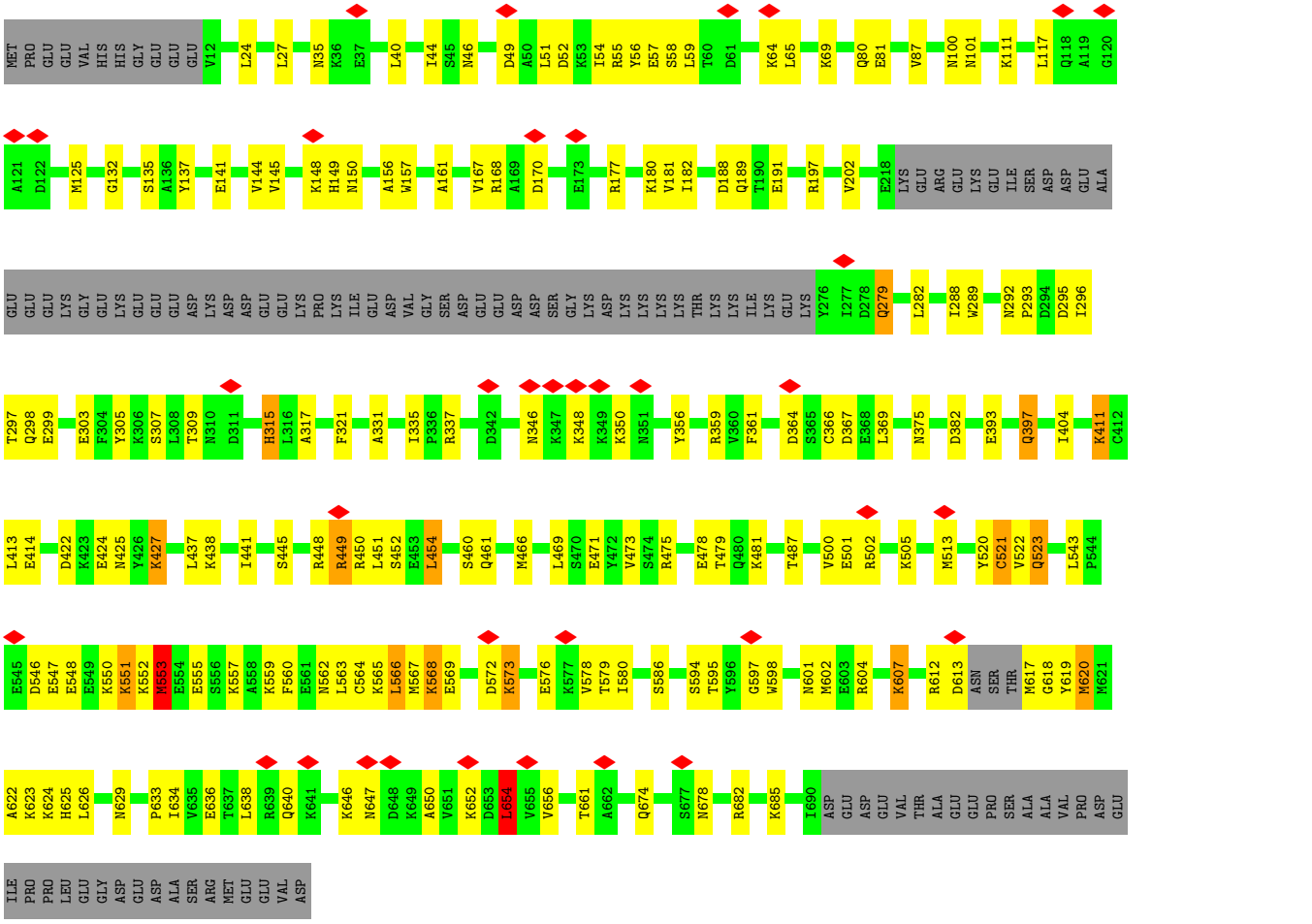
• Molecule 1: Heat shock protein HSP 90-beta

Chain A:



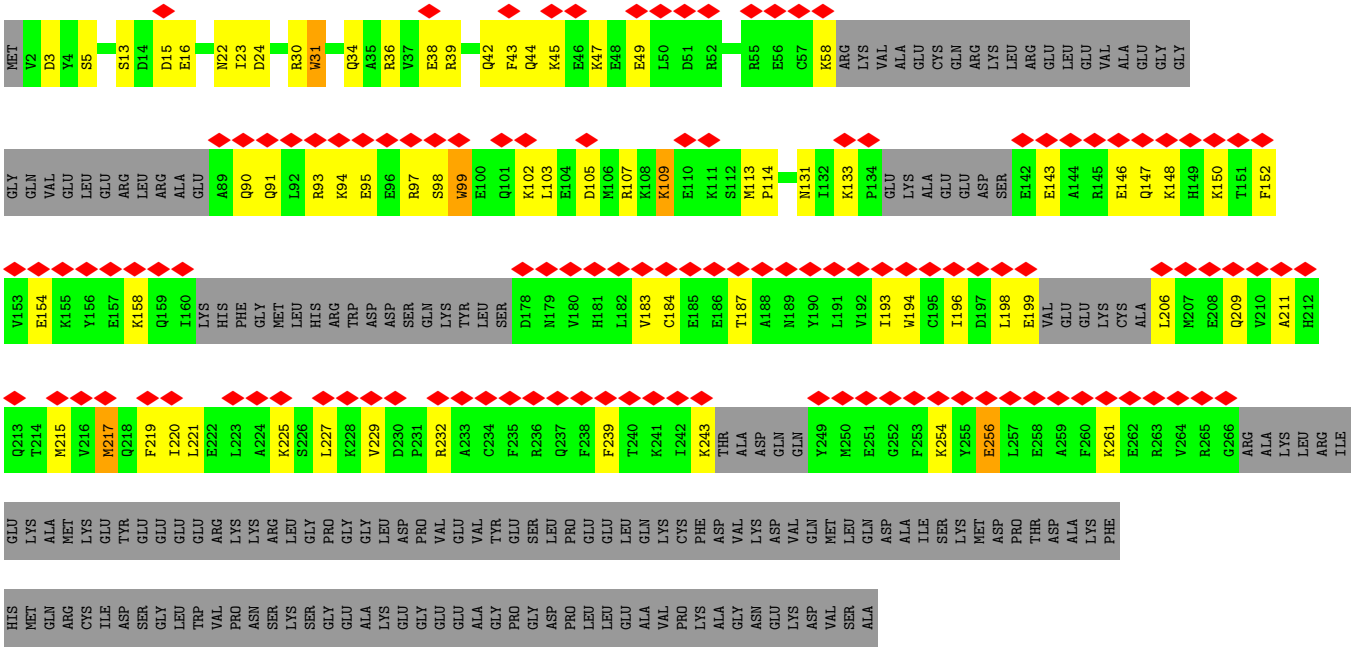
• Molecule 1: Heat shock protein HSP 90-beta

Chain B:



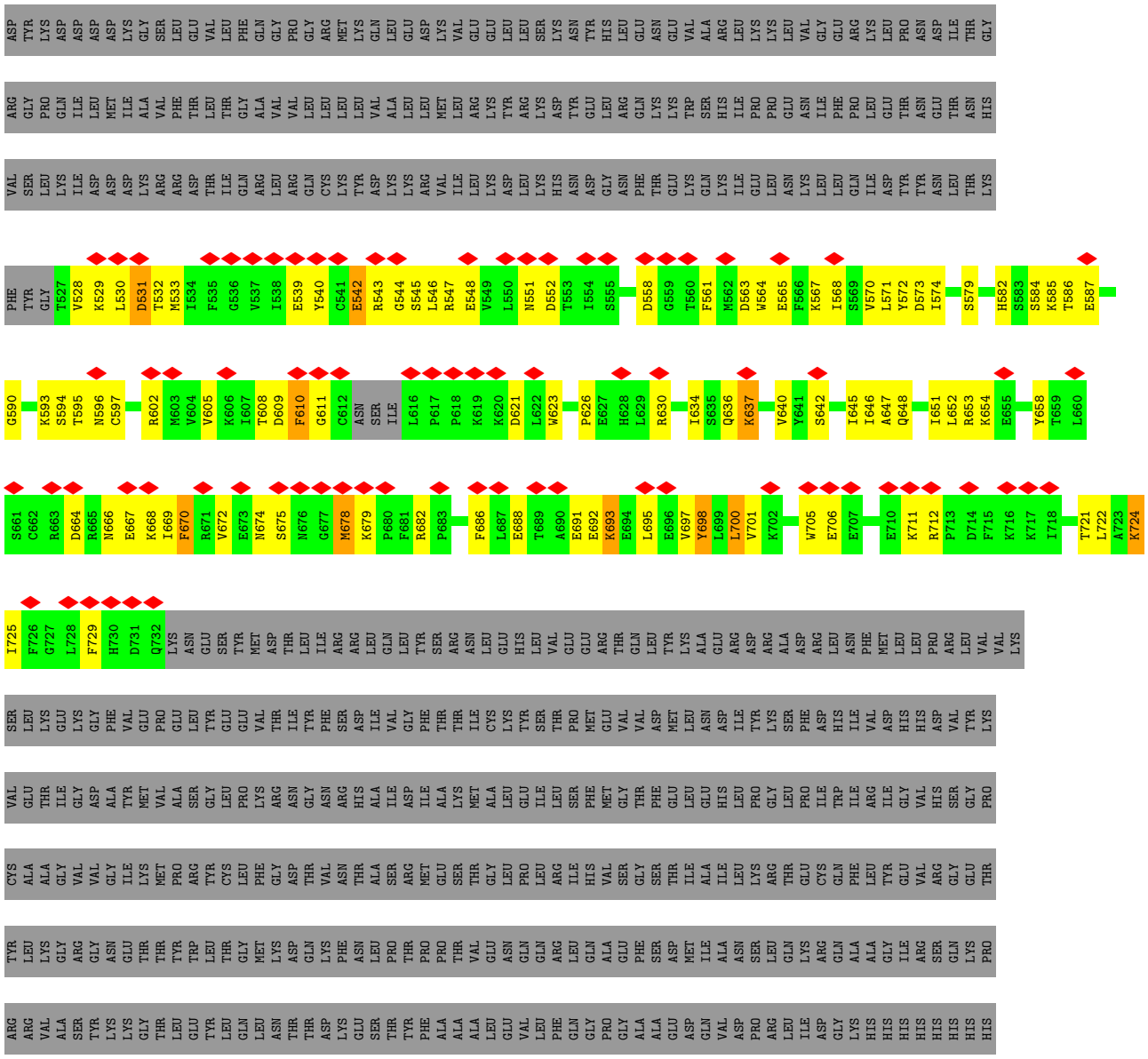
• Molecule 2: Hsp90 co-chaperone Cdc37

Chain C:



• Molecule 3: Guanylyl cyclase C

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	165635, 165635, 165635, 165635	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	58.80	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.349	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.175	Depositor
Map size (Å)	267.0624, 267.0624, 267.0624	wwPDB
Map dimensions	196, 196, 196	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3625633, 1.3625633, 1.3625633	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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	0.29	0/5122	0.61	2/6886 (0.0%)
1	B	0.28	0/5094	0.59	4/6848 (0.1%)
2	C	0.26	0/1728	0.55	0/2307
3	D	0.27	0/1698	0.62	1/2288 (0.0%)
All	All	0.28	0/13642	0.60	7/18329 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	79	PRO	CA-N-CD	-10.08	97.38	111.50
3	D	700	LEU	CA-CB-CG	5.92	128.92	115.30
1	B	654	LEU	CA-CB-CG	5.92	128.91	115.30
1	B	397	GLN	CA-CB-CG	5.37	125.22	113.40
1	B	553	MET	CA-CB-CG	5.20	122.14	113.30
1	B	117	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	621	MET	CA-CB-CG	5.08	121.93	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5039	0	5075	117	0
1	B	5011	0	5051	130	0
2	C	1699	0	1657	45	0
3	D	1663	0	1654	68	0
4	A	31	0	12	1	0
4	B	31	0	12	0	0
All	All	13474	0	13461	351	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 (351) 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:337:ARG:HG3	1:A:338:ARG:HH21	1.44	0.83
3:D:542:GLU:HG3	3:D:543:ARG:H	1.44	0.83
1:B:546:ASP:OD1	1:B:547:GLU:N	2.15	0.78
1:A:476:MET:SD	1:A:480:GLN:NE2	2.60	0.74
1:A:79:PRO:HD2	1:A:80:GLN:H	1.51	0.74
1:B:317:ALA:HB3	1:B:335:ILE:HB	1.69	0.73
1:A:125:MET:SD	1:A:125:MET:N	2.64	0.71
1:B:289:TRP:NE1	1:B:382:ASP:OD2	2.25	0.70
1:B:424:GLU:N	1:B:424:GLU:OE1	2.23	0.69
1:A:79:PRO:HD2	1:A:80:GLN:N	2.08	0.69
2:C:217:MET:HA	2:C:220:ILE:HD12	1.75	0.68
1:A:438:LYS:NZ	1:A:515:GLU:OE2	2.26	0.68
1:B:55:ARG:O	1:B:58:SER:OG	2.12	0.68
1:B:502:ARG:HD3	1:B:543:LEU:HD21	1.77	0.67
1:A:477:LYS:HB3	1:A:480:GLN:HE22	1.58	0.67
3:D:682:ARG:HG3	3:D:705:TRP:HB3	1.76	0.67
1:B:471:GLU:OE1	1:B:475:ARG:NH2	2.27	0.67
2:C:211:ALA:O	2:C:215:MET:HG3	1.95	0.67
1:B:279:GLN:HE21	1:B:279:GLN:HA	1.60	0.66
2:C:22:ASN:ND2	3:D:573:ASP:O	2.27	0.66
1:A:478:GLU:N	1:A:478:GLU:OE1	2.28	0.66
1:B:279:GLN:HE21	1:B:279:GLN:CA	2.06	0.66
2:C:184:CYS:SG	2:C:232:ARG:NH2	2.69	0.66
1:B:478:GLU:HG3	1:B:479:THR:HG23	1.78	0.66
1:B:565:LYS:O	1:B:568:LYS:HB2	1.96	0.65
1:B:141:GLU:N	1:B:141:GLU:OE1	2.31	0.63
1:B:350:LYS:HE3	1:B:375:ASN:HB2	1.79	0.63
1:B:279:GLN:HA	1:B:279:GLN:NE2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:THR:HA	1:B:513:MET:HB2	1.81	0.63
1:A:25:MET:O	1:A:29:ILE:HG22	1.99	0.63
1:A:547:GLU:HA	1:A:550:LYS:HD2	1.79	0.63
1:A:313:GLU:HB3	1:A:337:ARG:HD2	1.81	0.63
1:B:145:VAL:HG22	1:B:181:VAL:HG22	1.81	0.62
1:B:424:GLU:HA	1:B:427:LYS:HG3	1.79	0.62
1:A:49:ASP:O	1:A:53:LYS:HG3	1.99	0.62
1:B:54:ILE:HG12	1:B:177:ARG:HH12	1.65	0.61
1:B:40:LEU:O	1:B:44:ILE:HG13	2.00	0.61
3:D:558:ASP:OD1	3:D:653:ARG:NH1	2.30	0.61
1:A:652:LYS:O	1:A:656:VAL:HG22	2.00	0.61
1:B:346:ASN:O	1:B:348:LYS:N	2.32	0.61
3:D:590:GLY:HA2	3:D:634:ILE:HG12	1.83	0.61
1:B:445:SER:HA	1:B:448:ARG:HH21	1.65	0.61
1:B:144:VAL:HB	1:B:182:ILE:HG23	1.83	0.61
1:B:157:TRP:HD1	1:B:167:VAL:HG12	1.65	0.60
3:D:594:SER:HB3	3:D:646:ILE:HD13	1.82	0.60
1:B:557:LYS:NZ	1:B:580:ILE:HB	2.16	0.60
1:A:464:ASP:N	1:A:464:ASP:OD1	2.34	0.60
3:D:652:LEU:HD22	3:D:654:LYS:HB2	1.82	0.60
1:A:79:PRO:HD2	1:A:80:GLN:OE1	2.02	0.59
2:C:13:SER:OG	2:C:36:ARG:NH1	2.33	0.59
3:D:571:LEU:HG	3:D:722:LEU:HD21	1.84	0.59
1:A:322:SER:HB2	1:A:330:ARG:HD2	1.84	0.58
3:D:626:PRO:HB2	3:D:630:ARG:HH21	1.67	0.58
1:A:601:ASN:O	1:A:605:ILE:HG22	2.02	0.58
1:A:676:HIS:O	1:A:680:ILE:HG12	2.03	0.58
1:B:520:TYR:O	1:B:523:GLN:HB3	2.04	0.58
1:A:87:VAL:HG13	1:A:180:LYS:HD2	1.85	0.58
1:A:435:LYS:NZ	1:B:612:ARG:O	2.31	0.58
1:A:430:TYR:CE2	1:A:456:ARG:HB2	2.39	0.58
1:B:652:LYS:O	1:B:656:VAL:HG13	2.03	0.58
1:B:563:LEU:HA	1:B:566:LEU:HG	1.86	0.58
1:A:637:THR:O	1:A:641:LYS:HG3	2.03	0.58
1:B:501:GLU:OE1	1:B:501:GLU:N	2.37	0.57
1:B:547:GLU:HA	1:B:550:LYS:HE3	1.86	0.57
1:A:195:GLU:O	1:A:199:LYS:NZ	2.37	0.57
1:B:49:ASP:HB2	1:B:125:MET:HE3	1.87	0.57
2:C:103:LEU:O	2:C:107:ARG:HG3	2.05	0.57
1:B:422:ASP:HB3	1:B:425:ASN:HD21	1.70	0.57
3:D:546:LEU:HD23	3:D:594:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ALA:O	1:A:186:LYS:NZ	2.38	0.56
2:C:39:ARG:HG3	2:C:42:GLN:HE21	1.69	0.56
3:D:528:VAL:HG12	3:D:530:LEU:H	1.69	0.56
1:B:569:GLU:N	1:B:569:GLU:OE1	2.35	0.56
1:B:46:ASN:HA	1:B:49:ASP:OD1	2.05	0.56
3:D:672:VAL:O	3:D:675:SER:OG	2.22	0.56
1:B:617:MET:SD	1:B:618:GLY:N	2.79	0.56
3:D:584:SER:OG	3:D:585:LYS:N	2.39	0.56
3:D:698:TYR:HA	3:D:701:VAL:HG22	1.87	0.55
1:A:328:GLU:N	1:A:328:GLU:OE2	2.39	0.55
3:D:609:ASP:O	3:D:611:GLY:N	2.37	0.55
1:B:58:SER:HB3	1:B:65:LEU:HD21	1.88	0.55
1:B:597:GLY:HA3	1:B:622:ALA:HB2	1.89	0.55
1:B:132:GLY:O	1:B:135:SER:OG	2.20	0.55
1:B:552:LYS:O	1:B:555:GLU:HG3	2.07	0.55
1:A:317:ALA:HB3	1:A:335:ILE:HD11	1.89	0.55
3:D:593:LYS:HG2	3:D:595:THR:HG22	1.89	0.55
3:D:697:VAL:HA	3:D:700:LEU:HD13	1.89	0.54
1:B:550:LYS:HA	1:B:553:MET:SD	2.47	0.54
3:D:637:LYS:N	3:D:637:LYS:HD3	2.23	0.54
1:A:397:GLN:O	1:A:397:GLN:HG2	2.08	0.54
1:B:576:GLU:OE1	1:B:576:GLU:N	2.40	0.54
3:D:664:ASP:O	3:D:668:LYS:HG2	2.07	0.54
1:A:199:LYS:HA	1:A:202:VAL:HG22	1.90	0.54
3:D:642:SER:O	3:D:646:ILE:HG22	2.09	0.53
1:A:284:LYS:HG3	1:A:285:THR:HG23	1.91	0.53
1:A:342:ASP:OD1	1:A:342:ASP:N	2.39	0.53
1:B:613:ASP:OD1	1:B:613:ASP:N	2.40	0.53
3:D:539:GLU:HG2	3:D:602:ARG:HG3	1.90	0.53
1:B:52:ASP:OD1	1:B:52:ASP:N	2.41	0.53
1:B:598:TRP:HB3	1:B:602:MET:HB3	1.91	0.52
1:A:154:GLN:NE2	1:A:173:GLU:O	2.34	0.52
1:B:413:LEU:HD11	1:B:451:LEU:HD11	1.91	0.52
1:A:185:LEU:HD23	1:A:186:LYS:N	2.24	0.52
1:A:420:ALA:HA	1:A:426:TYR:CD2	2.44	0.52
1:A:555:GLU:O	1:A:559:LYS:HB3	2.10	0.52
1:A:202:VAL:O	1:A:207:GLN:NE2	2.43	0.52
1:A:570:ILE:HG13	1:A:571:LEU:H	1.73	0.52
1:A:179:THR:HG21	4:A:801:ATP:HN62	1.74	0.52
1:B:148:LYS:NZ	1:B:149:HIS:O	2.36	0.52
1:B:305:TYR:O	1:B:309:THR:OG1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASN:O	1:A:348:LYS:NZ	2.42	0.52
1:A:553:MET:SD	1:A:553:MET:N	2.82	0.52
1:A:557:LYS:HA	1:A:557:LYS:HE3	1.92	0.52
2:C:43:PHE:O	2:C:47:LYS:HG3	2.09	0.52
3:D:542:GLU:HG3	3:D:543:ARG:N	2.18	0.52
3:D:647:ALA:O	3:D:651:ILE:HG12	2.10	0.52
1:A:337:ARG:CG	1:A:338:ARG:HE	2.22	0.52
1:B:297:THR:HG22	1:B:298:GLN:H	1.76	0.51
1:A:152:ASP:OD1	1:A:152:ASP:N	2.44	0.51
1:A:175:ILE:HD13	1:A:180:LYS:NZ	2.25	0.51
1:A:80:GLN:N	1:A:80:GLN:OE1	2.44	0.51
2:C:42:GLN:HA	2:C:45:LYS:HD3	1.93	0.51
2:C:105:ASP:O	2:C:109:LYS:HG3	2.10	0.51
1:A:301:TYR:HE1	1:A:334:PHE:CE1	2.29	0.51
1:A:526:LYS:HD2	1:A:527:GLU:HG3	1.93	0.51
3:D:664:ASP:OD2	3:D:667:GLU:HB3	2.10	0.51
2:C:184:CYS:O	2:C:187:THR:OG1	2.22	0.51
3:D:532:THR:O	3:D:533:MET:HG2	2.11	0.51
3:D:721:THR:HA	3:D:724:LYS:HE3	1.91	0.51
1:A:337:ARG:HG3	1:A:338:ARG:NH2	2.20	0.51
1:A:141:GLU:OE1	1:A:142:LYS:HG3	2.12	0.50
1:A:144:VAL:HG13	1:A:182:ILE:HB	1.92	0.50
1:A:337:ARG:HG2	1:A:338:ARG:HE	1.75	0.50
1:B:650:ALA:O	1:B:654:LEU:HG	2.11	0.50
2:C:183:VAL:O	2:C:232:ARG:NH1	2.44	0.50
3:D:567:LYS:HD2	3:D:567:LYS:N	2.26	0.50
1:A:67:SER:OG	1:A:177:ARG:NH1	2.44	0.50
3:D:637:LYS:HD3	3:D:637:LYS:H	1.76	0.50
3:D:693:LYS:HD2	3:D:729:PHE:HZ	1.77	0.50
1:A:65:LEU:HG	1:A:69:LYS:HE3	1.93	0.50
1:A:559:LYS:HG3	1:A:560:PHE:HD1	1.76	0.50
1:A:348:LYS:O	1:A:349:LYS:HG2	2.11	0.50
1:B:557:LYS:HZ1	1:B:580:ILE:HB	1.76	0.50
1:B:292:ASN:ND2	1:B:293:PRO:O	2.40	0.50
1:B:469:LEU:O	1:B:473:VAL:HG23	2.12	0.50
1:B:586:SER:O	1:B:586:SER:OG	2.29	0.50
2:C:93:ARG:O	2:C:97:ARG:HG2	2.12	0.50
1:B:202:VAL:HG11	1:B:282:LEU:HD13	1.93	0.50
2:C:30:ARG:NH1	3:D:609:ASP:OD1	2.45	0.50
2:C:148:LYS:O	2:C:152:PHE:HB2	2.12	0.50
1:A:460:SER:HB3	1:A:512:TYR:HE1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:VAL:HG13	1:B:180:LYS:HG2	1.94	0.49
1:A:46:ASN:OD1	1:A:46:ASN:O	2.30	0.49
1:A:633:PRO:O	1:A:637:THR:HG23	2.12	0.49
1:B:367:ASP:OD1	1:B:367:ASP:N	2.43	0.49
1:A:605:ILE:HG23	1:A:606:MET:HG2	1.93	0.49
1:B:315:HIS:O	2:C:131:ASN:ND2	2.44	0.49
1:B:411:LYS:O	1:B:414:GLU:HB3	2.13	0.49
1:A:396:GLN:OE1	1:A:396:GLN:N	2.28	0.49
1:B:566:LEU:HD12	1:B:567:MET:H	1.77	0.49
3:D:666:ASN:HA	3:D:669:ILE:HD12	1.94	0.49
3:D:691:GLU:OE1	3:D:698:TYR:OH	2.28	0.49
1:A:175:ILE:HG21	1:A:180:LYS:HZ2	1.77	0.49
1:A:180:LYS:HD3	1:A:180:LYS:N	2.27	0.49
1:A:648:ASP:OD1	1:A:649:LYS:N	2.41	0.49
2:C:15:ASP:OD1	2:C:16:GLU:N	2.38	0.49
3:D:574:ILE:HD11	3:D:605:VAL:HG11	1.94	0.49
1:A:38:ILE:HG23	1:A:41:ARG:HE	1.78	0.49
1:A:477:LYS:NZ	1:A:479:THR:OG1	2.46	0.49
1:B:634:ILE:O	1:B:638:LEU:HG	2.13	0.49
1:B:80:GLN:OE1	1:B:81:GLU:HG3	2.13	0.49
1:B:437:LEU:HD21	1:B:454:LEU:HD13	1.93	0.49
1:B:69:LYS:NZ	1:B:69:LYS:HB3	2.28	0.49
1:B:578:VAL:HG12	1:B:626:LEU:HB3	1.95	0.48
2:C:146:GLU:HG3	2:C:150:LYS:NZ	2.28	0.48
3:D:531:ASP:O	3:D:532:THR:OG1	2.29	0.48
2:C:31:TRP:HB3	3:D:586:THR:HG21	1.95	0.48
1:B:557:LYS:H	1:B:557:LYS:HD2	1.78	0.48
1:B:562:ASN:OD1	1:B:563:LEU:N	2.46	0.48
1:A:460:SER:HB3	1:A:512:TYR:CE1	2.48	0.48
1:A:559:LYS:HG3	1:A:560:PHE:CD1	2.48	0.48
1:B:356:TYR:HB2	1:B:382:ASP:OD1	2.13	0.48
2:C:219:PHE:HZ	2:C:256:GLU:HB3	1.79	0.47
3:D:543:ARG:CZ	3:D:548:GLU:HB2	2.44	0.47
1:A:477:LYS:HB3	1:A:480:GLN:NE2	2.29	0.47
1:B:425:ASN:OD1	1:B:425:ASN:N	2.46	0.47
1:B:559:LYS:HG2	1:B:560:PHE:CD1	2.49	0.47
1:A:57:GLU:OE2	1:A:57:GLU:HA	2.15	0.47
1:B:393:GLU:N	1:B:393:GLU:OE1	2.47	0.47
3:D:593:LYS:HG3	3:D:623:TRP:CZ3	2.48	0.47
1:A:480:GLN:C	1:A:481:LYS:HD3	2.34	0.47
1:B:557:LYS:HD2	1:B:557:LYS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:636:GLN:O	3:D:640:VAL:HG23	2.14	0.47
1:A:293:PRO:HB3	1:A:320:HIS:ND1	2.29	0.47
1:A:314:ASP:OD1	1:A:315:HIS:N	2.47	0.47
1:A:468:SER:OG	1:A:470:SER:OG	2.33	0.47
1:B:288:ILE:HD11	1:B:296:ILE:HD12	1.97	0.47
1:B:337:ARG:HH12	2:C:133:LYS:NZ	2.12	0.47
1:B:502:ARG:CZ	1:B:543:LEU:HD11	2.45	0.47
3:D:570:VAL:O	3:D:574:ILE:HG12	2.14	0.47
3:D:546:LEU:HD22	3:D:597:CYS:HB2	1.96	0.47
3:D:568:ILE:HG12	3:D:725:ILE:HG22	1.96	0.47
1:A:640:GLN:HA	1:A:643:GLU:OE2	2.15	0.46
1:A:88:ASP:OD1	1:A:89:THR:N	2.44	0.46
1:B:548:GLU:OE1	1:B:548:GLU:N	2.43	0.46
1:A:175:ILE:HG21	1:A:180:LYS:NZ	2.31	0.46
1:B:553:MET:O	1:B:557:LYS:HD2	2.15	0.46
2:C:39:ARG:O	2:C:42:GLN:HG3	2.16	0.46
1:B:521:CYS:SG	1:B:522:VAL:N	2.89	0.46
3:D:564:TRP:HA	3:D:567:LYS:HG2	1.98	0.46
3:D:678:MET:SD	3:D:679:LYS:HB2	2.56	0.46
1:B:449:ARG:NH2	1:B:450:ARG:HA	2.30	0.46
1:B:562:ASN:O	1:B:565:LYS:HG2	2.16	0.46
1:A:195:GLU:HG3	1:A:199:LYS:NZ	2.30	0.46
1:B:321:PHE:HB3	1:B:331:ALA:HB3	1.97	0.46
1:B:594:SER:OG	1:B:595:THR:N	2.49	0.46
1:A:681:TYR:HE1	1:B:661:THR:HG21	1.81	0.46
1:B:413:LEU:HD23	1:B:450:ARG:HH11	1.81	0.46
1:B:607:LYS:HA	1:B:607:LYS:HE2	1.98	0.45
3:D:596:ASN:OD1	3:D:610:PHE:HB3	2.16	0.45
1:A:423:LYS:HD3	1:A:423:LYS:N	2.31	0.45
1:B:572:ASP:OD1	1:B:573:LYS:N	2.47	0.45
3:D:724:LYS:HD2	3:D:725:ILE:N	2.32	0.45
1:A:562:ASN:OD1	1:A:562:ASN:N	2.49	0.45
1:B:560:PHE:O	1:B:564:CYS:N	2.44	0.45
1:A:13:GLU:OE2	1:A:13:GLU:N	2.48	0.45
1:A:175:ILE:HD13	1:A:180:LYS:HZ1	1.81	0.45
1:A:320:HIS:CE1	1:A:332:LEU:HD21	2.52	0.45
1:A:323:VAL:O	1:A:328:GLU:HA	2.16	0.45
1:A:368:GLU:OE1	1:A:368:GLU:N	2.49	0.45
1:A:592:VAL:HG12	1:A:625:HIS:HB2	1.98	0.45
1:A:651:VAL:O	1:A:655:VAL:HG12	2.15	0.45
1:B:568:LYS:HD2	1:B:568:LYS:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:542:GLU:CG	3:D:543:ARG:H	2.18	0.45
1:B:438:LYS:HA	1:B:441:ILE:HG22	1.98	0.45
1:B:560:PHE:HB3	1:B:563:LEU:HB3	1.97	0.45
2:C:94:LYS:HA	2:C:94:LYS:HD2	1.72	0.45
1:A:117:LEU:HD12	1:A:117:LEU:O	2.16	0.45
1:A:657:LEU:HD13	1:A:679:ARG:HD3	1.98	0.45
1:B:682:ARG:HH21	1:B:685:LYS:HD3	1.82	0.45
1:B:111:LYS:HD3	1:B:111:LYS:HA	1.75	0.45
3:D:543:ARG:NH1	3:D:544:GLY:H	2.15	0.45
1:A:490:SER:OG	1:A:491:LYS:N	2.50	0.45
1:B:579:THR:OG1	1:B:580:ILE:N	2.50	0.45
3:D:548:GLU:HA	3:D:551:ASN:ND2	2.32	0.45
1:B:674:GLN:O	1:B:678:ASN:ND2	2.35	0.44
1:A:524:GLN:HA	1:A:524:GLN:OE1	2.17	0.44
1:B:24:LEU:HD13	1:B:27:LEU:HD23	1.99	0.44
1:A:179:THR:C	1:A:180:LYS:HD3	2.38	0.44
2:C:221:LEU:O	2:C:225:LYS:HG3	2.18	0.44
1:A:573:LYS:O	1:A:573:LYS:HG2	2.17	0.44
1:B:612:ARG:HE	1:B:613:ASP:H	1.66	0.44
1:B:57:GLU:HG3	1:B:64:LYS:HG3	2.00	0.44
3:D:692:GLU:HB2	3:D:693:LYS:H	1.53	0.44
1:B:633:PRO:O	1:B:636:GLU:HG3	2.16	0.44
1:A:144:VAL:CG1	1:A:182:ILE:HB	2.47	0.44
2:C:239:PHE:O	2:C:243:LYS:HG2	2.17	0.44
1:B:597:GLY:N	3:D:540:TYR:OH	2.45	0.44
1:A:568:LYS:O	1:A:572:ASP:HB3	2.18	0.44
3:D:564:TRP:HB3	3:D:693:LYS:HZ2	1.83	0.44
1:A:145:VAL:HG22	1:A:181:VAL:HG22	1.99	0.43
1:A:333:LEU:HD23	1:A:333:LEU:HA	1.86	0.43
3:D:593:LYS:HG3	3:D:623:TRP:CE3	2.53	0.43
1:B:156:ALA:HB2	1:B:170:ASP:HB2	2.00	0.43
1:B:397:GLN:OE1	1:B:397:GLN:O	2.36	0.43
1:A:570:ILE:HD13	1:A:655:VAL:HG21	2.01	0.43
1:B:623:LYS:HA	1:B:623:LYS:HE3	2.00	0.43
1:B:460:SER:OG	1:B:461:GLN:N	2.51	0.43
2:C:99:TRP:O	2:C:103:LEU:HG	2.19	0.43
3:D:545:SER:C	3:D:547:ARG:H	2.22	0.43
1:B:49:ASP:HA	1:B:52:ASP:OD1	2.18	0.43
1:B:620:MET:SD	1:B:620:MET:N	2.92	0.43
2:C:98:SER:O	2:C:102:LYS:HG2	2.18	0.43
1:A:25:MET:HA	1:A:28:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:ARG:NE	1:B:613:ASP:H	2.17	0.43
2:C:193:ILE:O	2:C:196:ILE:HG22	2.19	0.43
3:D:565:GLU:HA	3:D:568:ILE:HG22	2.01	0.43
1:A:297:THR:HG22	1:A:300:GLU:OE1	2.19	0.42
1:A:598:TRP:HB3	1:A:602:MET:HB3	2.00	0.42
1:B:137:TYR:CD1	1:B:161:ALA:HB2	2.53	0.42
2:C:143:GLU:O	2:C:147:GLN:HG2	2.19	0.42
2:C:194:TRP:CZ3	2:C:198:LEU:HD11	2.53	0.42
1:A:195:GLU:HG3	1:A:199:LYS:HZ1	1.85	0.42
2:C:227:LEU:HB2	2:C:229:VAL:HG22	2.00	0.42
1:B:299:GLU:O	1:B:303:GLU:HG3	2.19	0.42
2:C:91:GLN:O	2:C:95:GLU:HG2	2.20	0.42
1:B:404:ILE:H	1:B:404:ILE:HG13	1.58	0.42
2:C:217:MET:O	2:C:221:LEU:HG	2.19	0.42
3:D:724:LYS:HZ2	3:D:725:ILE:HG13	1.84	0.42
1:A:72:LYS:HE2	1:A:72:LYS:HB2	1.83	0.42
1:A:457:TYR:OH	1:A:518:ASP:OD1	2.28	0.42
1:B:547:GLU:HA	1:B:550:LYS:HG2	2.01	0.42
2:C:261:LYS:HE3	2:C:261:LYS:HB3	1.81	0.42
1:A:502:ARG:HD2	1:A:582:ASN:O	2.19	0.42
1:A:122:ASP:O	1:A:123:ILE:HG23	2.20	0.42
1:A:658:LEU:HD23	1:A:658:LEU:HA	1.91	0.42
1:B:356:TYR:HD1	1:B:361:PHE:HA	1.85	0.42
1:B:500:VAL:HG12	1:B:500:VAL:O	2.20	0.42
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.85	0.42
1:B:350:LYS:HB2	1:B:350:LYS:HE2	1.86	0.42
2:C:24:ASP:HB2	3:D:608:THR:HG22	2.01	0.42
2:C:45:LYS:O	2:C:49:GLU:HG2	2.19	0.42
2:C:194:TRP:O	2:C:198:LEU:HG	2.19	0.42
2:C:254:LYS:HD3	2:C:254:LYS:HA	1.83	0.41
3:D:572:TYR:HA	3:D:722:LEU:HD23	2.02	0.41
1:A:515:GLU:HG2	1:A:518:ASP:HB2	2.02	0.41
1:B:59:LEU:H	1:B:59:LEU:HD12	1.85	0.41
1:A:407:ASN:O	1:A:411:LYS:HG2	2.19	0.41
1:B:479:THR:O	1:B:479:THR:OG1	2.33	0.41
2:C:113:MET:HA	2:C:114:PRO:HD3	1.93	0.41
3:D:667:GLU:HG2	3:D:670:PHE:HD2	1.85	0.41
1:B:356:TYR:CD1	1:B:361:PHE:HA	2.55	0.41
2:C:206:LEU:HA	2:C:209:GLN:NE2	2.34	0.41
3:D:582:HIS:ND1	3:D:587:GLU:HB2	2.35	0.41
1:B:502:ARG:HE	1:B:502:ARG:HB2	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:LEU:HD12	1:B:567:MET:HG2	2.03	0.41
3:D:563:ASP:O	3:D:567:LYS:HD3	2.19	0.41
1:A:489:GLU:HB3	1:A:493:GLN:HG3	2.02	0.41
1:A:566:LEU:HD12	1:A:566:LEU:HA	1.86	0.41
1:B:523:GLN:HA	1:B:523:GLN:HE21	1.86	0.41
1:B:557:LYS:HZ2	1:B:580:ILE:HB	1.84	0.41
1:B:646:LYS:NZ	1:B:647:ASN:OD1	2.45	0.41
1:A:185:LEU:HD23	1:A:186:LYS:H	1.86	0.41
1:A:367:ASP:HB2	1:A:368:GLU:OE1	2.21	0.41
1:B:562:ASN:HA	1:B:565:LYS:HZ3	1.85	0.41
1:B:624:LYS:C	1:B:625:HIS:HD1	2.23	0.41
1:B:361:PHE:CZ	1:B:364:ASP:HB2	2.56	0.41
1:A:597:GLY:HA2	1:A:621:MET:HB3	2.03	0.41
1:B:100:ASN:OD1	1:B:101:ASN:N	2.54	0.41
1:B:547:GLU:OE1	1:B:551:LYS:NZ	2.53	0.41
1:B:566:LEU:HD12	1:B:567:MET:N	2.35	0.41
2:C:34:GLN:O	2:C:38:GLU:HG2	2.20	0.41
3:D:582:HIS:NE2	3:D:636:GLN:OE1	2.53	0.41
3:D:621:ASP:OD2	3:D:623:TRP:HB2	2.21	0.41
1:A:600:ALA:HB2	1:A:668:PHE:CE2	2.55	0.41
1:B:191:GLU:OE1	1:B:197:ARG:NH2	2.44	0.41
3:D:539:GLU:HB2	3:D:602:ARG:NH1	2.35	0.41
3:D:552:ASP:OD1	3:D:552:ASP:N	2.48	0.41
1:A:420:ALA:HA	1:A:426:TYR:CE2	2.56	0.40
1:B:601:ASN:HA	1:B:604:ARG:HG2	2.03	0.40
3:D:695:LEU:HA	3:D:698:TYR:CD2	2.56	0.40
1:A:531:LYS:N	1:A:531:LYS:HD2	2.36	0.40
2:C:23:ILE:HG13	2:C:24:ASP:N	2.35	0.40
1:A:62:PRO:O	1:A:65:LEU:HB2	2.21	0.40
2:C:206:LEU:O	2:C:209:GLN:HG2	2.21	0.40
3:D:706:GLU:O	3:D:712:ARG:NH2	2.54	0.40
1:B:366:CYS:HB3	1:B:369:LEU:HB2	2.04	0.40
2:C:58:LYS:HD2	2:C:58:LYS:HA	1.78	0.40
2:C:154:GLU:O	2:C:158:LYS:HG2	2.21	0.40
3:D:648:GLN:HG3	3:D:705:TRP:CZ2	2.57	0.40
3:D:642:SER:HA	3:D:645:ILE:HG22	2.02	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	619/724 (86%)	568 (92%)	49 (8%)	2 (0%)	41 75
1	B	613/724 (85%)	573 (94%)	40 (6%)	0	100 100
2	C	188/379 (50%)	178 (95%)	10 (5%)	0	100 100
3	D	199/741 (27%)	169 (85%)	25 (13%)	5 (2%)	5 36
All	All	1619/2568 (63%)	1488 (92%)	124 (8%)	7 (0%)	38 71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	610	ALA
3	D	531	ASP
3	D	693	LYS
3	D	688	GLU
3	D	542	GLU
3	D	610	PHE

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	562/653 (86%)	534 (95%)	28 (5%)	24 53
1	B	558/653 (86%)	526 (94%)	32 (6%)	20 50
2	C	187/338 (55%)	177 (95%)	10 (5%)	22 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	187/668 (28%)	175 (94%)	12 (6%)	17 47
All	All	1494/2312 (65%)	1412 (94%)	82 (6%)	25 51

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PHE
1	A	41	ARG
1	A	71	LEU
1	A	108	SER
1	A	160	SER
1	A	170	ASP
1	A	196	ARG
1	A	283	ASN
1	A	301	TYR
1	A	303	GLU
1	A	307	SER
1	A	326	GLN
1	A	329	PHE
1	A	330	ARG
1	A	338	ARG
1	A	359	ARG
1	A	397	GLN
1	A	426	TYR
1	A	464	ASP
1	A	468	SER
1	A	521	CYS
1	A	524	GLN
1	A	526	LYS
1	A	555	GLU
1	A	617	MET
1	A	623	LYS
1	A	646	LYS
1	A	649	LYS
1	B	35	ASN
1	B	56	TYR
1	B	150	ASN
1	B	168	ARG
1	B	188	ASP
1	B	189	GLN
1	B	279	GLN
1	B	295	ASP

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Mol	Chain	Res	Type
1	B	307	SER
1	B	315	HIS
1	B	359	ARG
1	B	411	LYS
1	B	427	LYS
1	B	449	ARG
1	B	452	SER
1	B	454	LEU
1	B	466	MET
1	B	481	LYS
1	B	505	LYS
1	B	521	CYS
1	B	523	GLN
1	B	551	LYS
1	B	553	MET
1	B	566	LEU
1	B	568	LYS
1	B	573	LYS
1	B	607	LYS
1	B	619	TYR
1	B	620	MET
1	B	629	ASN
1	B	640	GLN
1	B	654	LEU
2	C	3	ASP
2	C	5	SER
2	C	31	TRP
2	C	44	GLN
2	C	90	GLN
2	C	99	TRP
2	C	109	LYS
2	C	199	GLU
2	C	217	MET
2	C	256	GLU
3	D	529	LYS
3	D	561	PHE
3	D	579	SER
3	D	637	LYS
3	D	658	TYR
3	D	670	PHE
3	D	674	ASN
3	D	678	MET

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Mol	Chain	Res	Type
3	D	686	PHE
3	D	698	TYR
3	D	711	LYS
3	D	724	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

2 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	ATP	A	801	-	26,33,33	0.61	0	31,52,52	0.74	2 (6%)
4	ATP	B	801	-	26,33,33	0.61	0	31,52,52	0.74	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	ATP	A	801	-	-	10/18/38/38	0/3/3/3
4	ATP	B	801	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	801	ATP	C5-C6-N6	2.30	123.84	120.35
4	A	801	ATP	C5-C6-N6	2.24	123.76	120.35
4	A	801	ATP	PB-O3B-PG	2.06	139.88	132.83
4	B	801	ATP	PB-O3B-PG	2.03	139.81	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	ATP	PB-O3A-PA-O5'
4	A	801	ATP	C5'-O5'-PA-O3A
4	B	801	ATP	C5'-O5'-PA-O3A
4	A	801	ATP	O4'-C4'-C5'-O5'
4	A	801	ATP	C3'-C4'-C5'-O5'
4	A	801	ATP	PG-O3B-PB-O1B
4	B	801	ATP	PB-O3A-PA-O2A
4	A	801	ATP	C5'-O5'-PA-O1A
4	A	801	ATP	PA-O3A-PB-O1B
4	A	801	ATP	PG-O3B-PB-O2B
4	A	801	ATP	PA-O3A-PB-O2B
4	B	801	ATP	PB-O3A-PA-O1A
4	A	801	ATP	C5'-O5'-PA-O2A
4	B	801	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

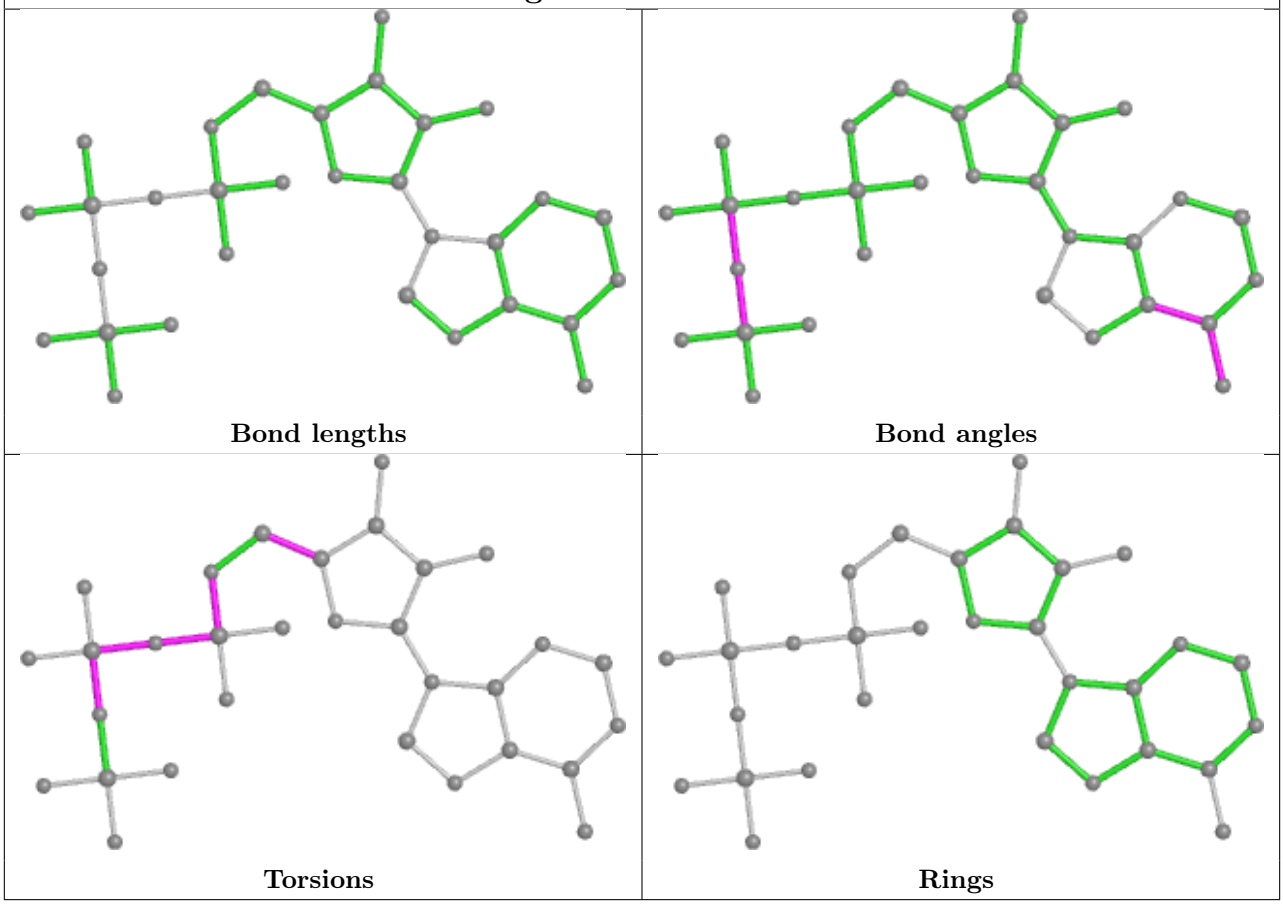
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	ATP	1	0

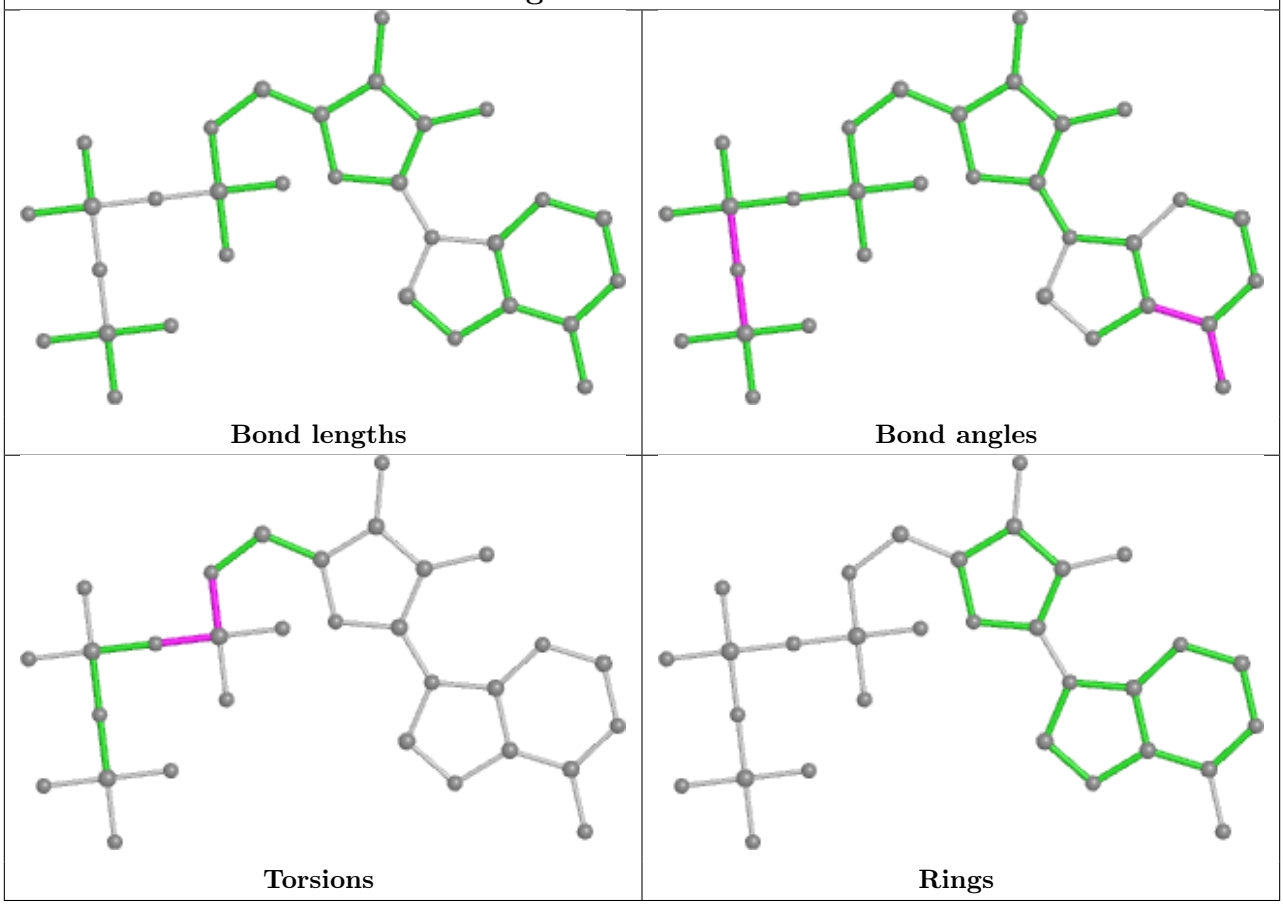
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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 ATP A 801



Ligand ATP B 801



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

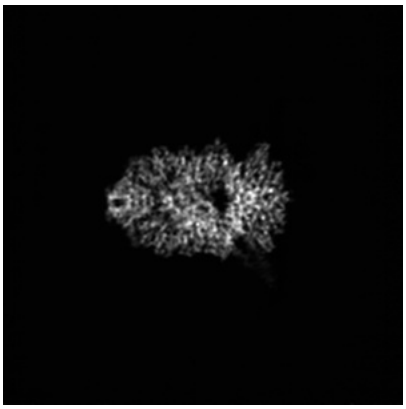
This section contains visualisations of the EMDB entry EMD-29523. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

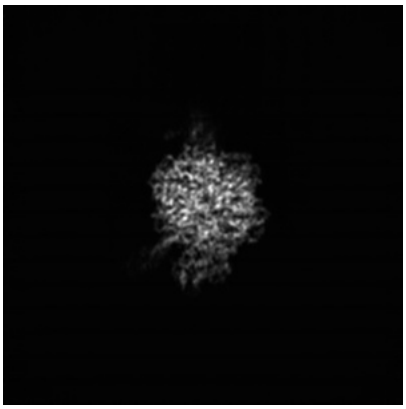
6.1 Orthogonal projections

6.1.1 Primary map

X

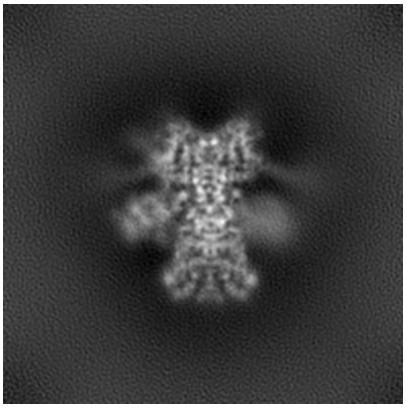


Y

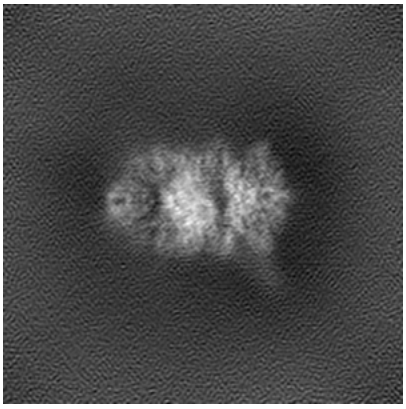


Z

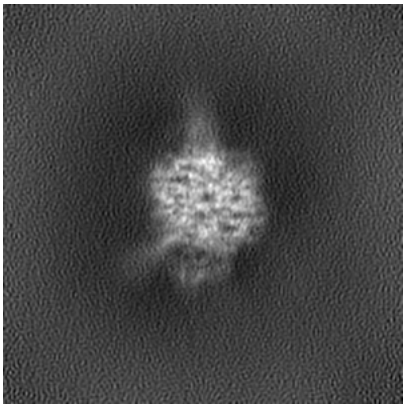
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

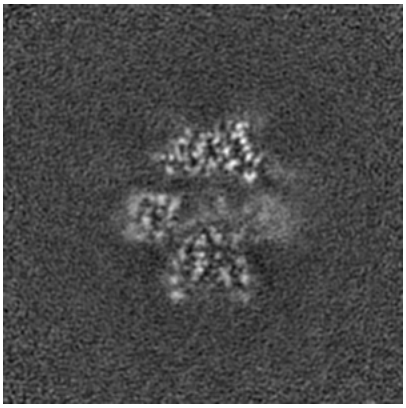
6.2.1 Primary map

X Index: 98

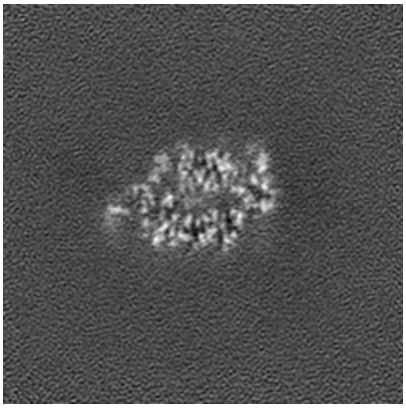
Y Index: 98

Z Index: 98

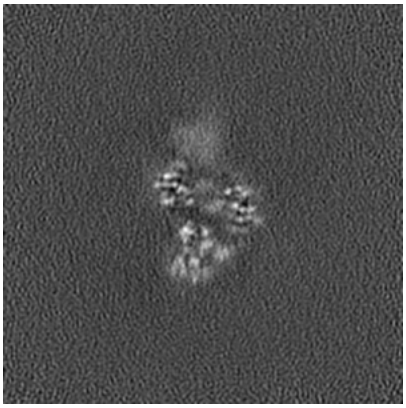
6.2.2 Raw map



X Index: 98



Y Index: 98



Z Index: 98

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

6.3 Largest variance slices (i)

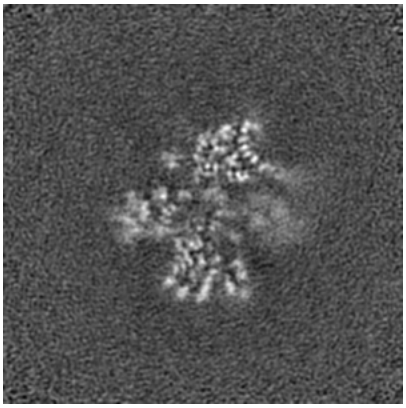
6.3.1 Primary map

X Index: 89

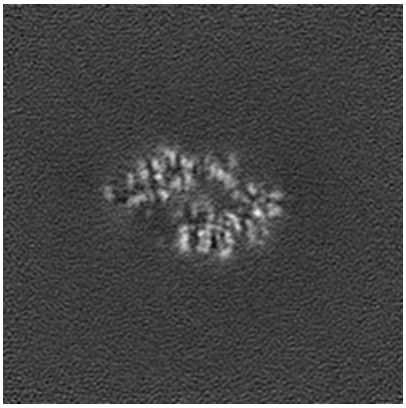
Y Index: 107

Z Index: 115

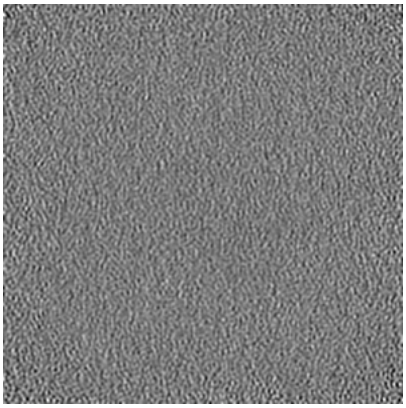
6.3.2 Raw map



X Index: 95



Y Index: 107

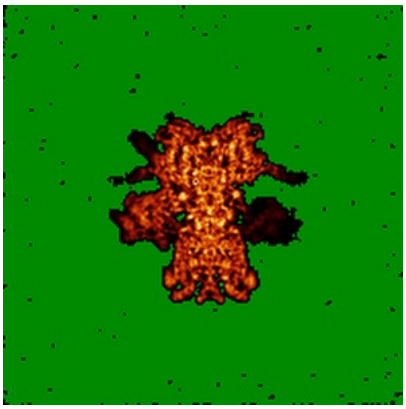


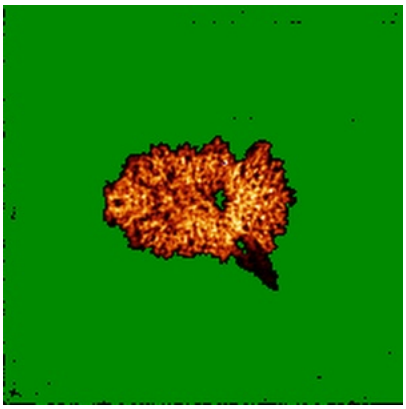
Z Index: 0

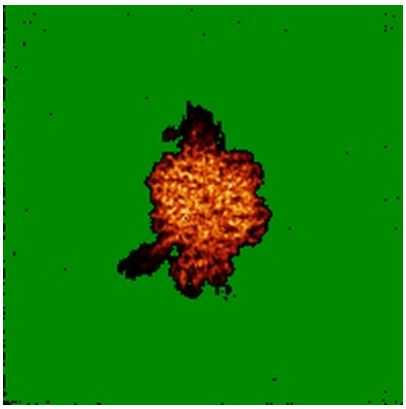
The images above show the largest variance slices of the map in three orthogonal directions.

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

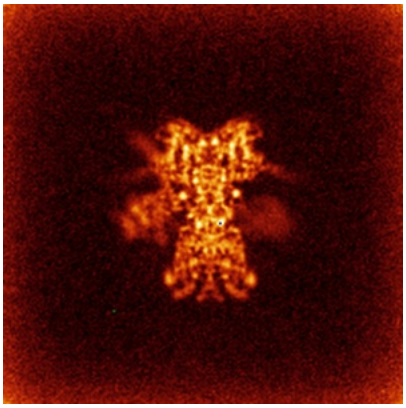
6.4.1 Primary map

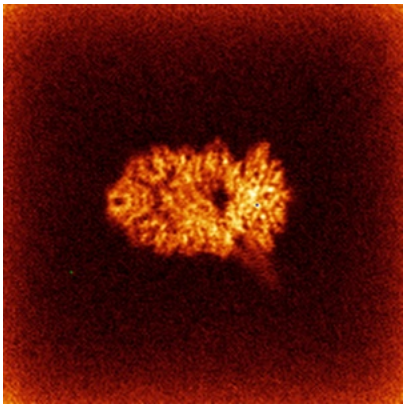

X

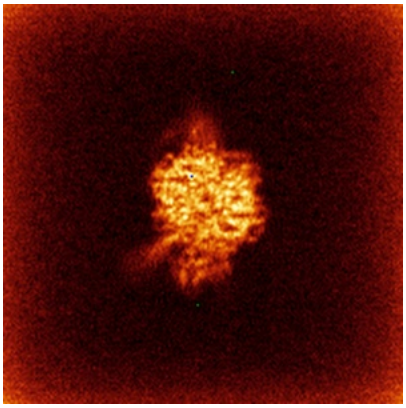

Y


Z

6.4.2 Raw map


X

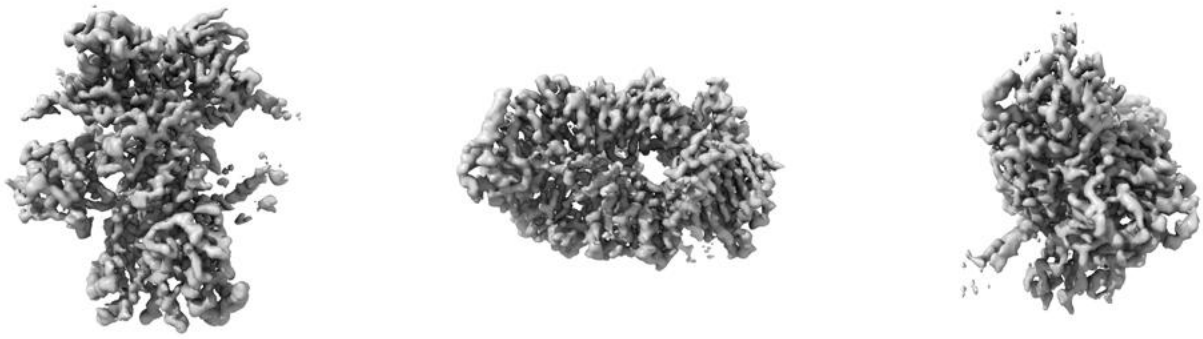

Y


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 0.175. 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.

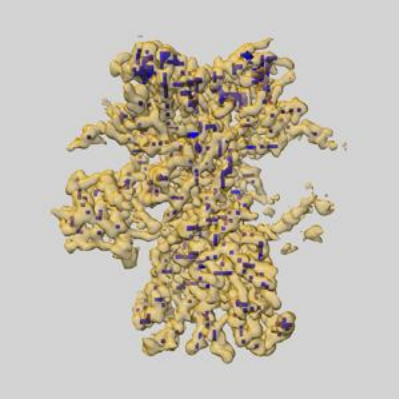
6.6 Mask visualisation

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

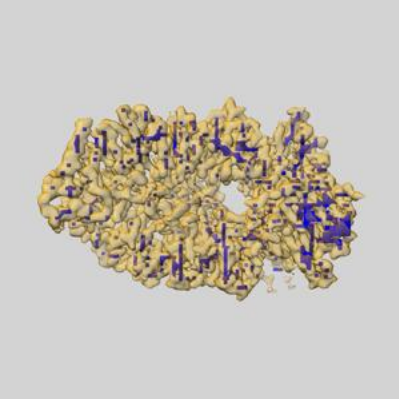
A mask typically either:

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

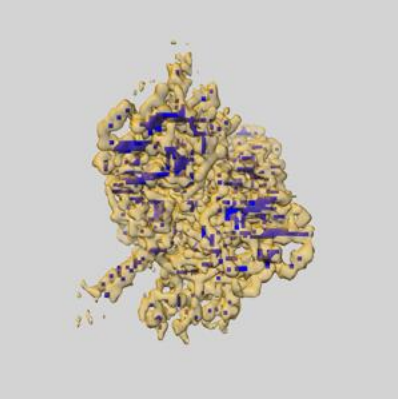
6.6.1 emd_29523_msk_1.map



X



Y

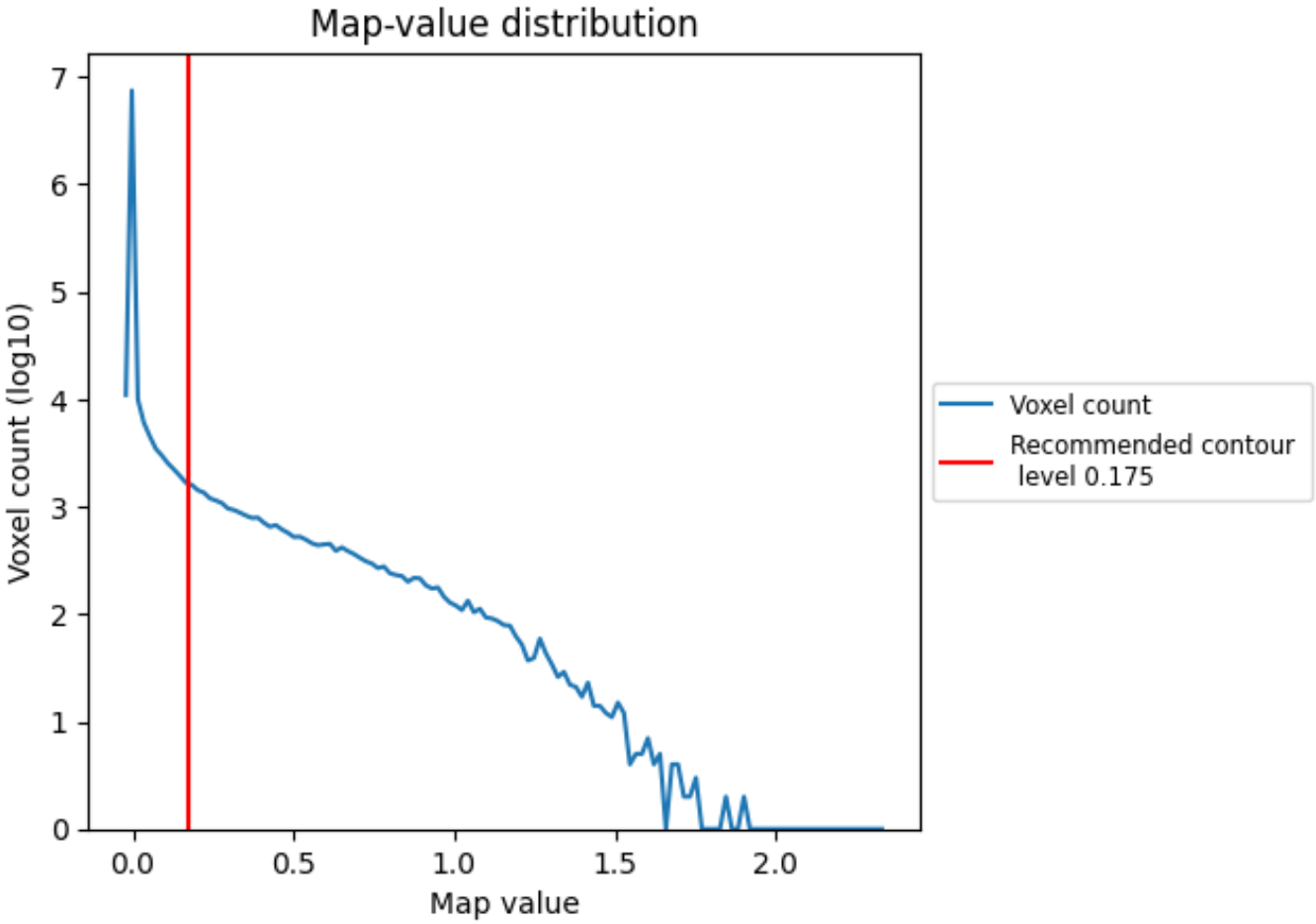


Z

7 Map analysis

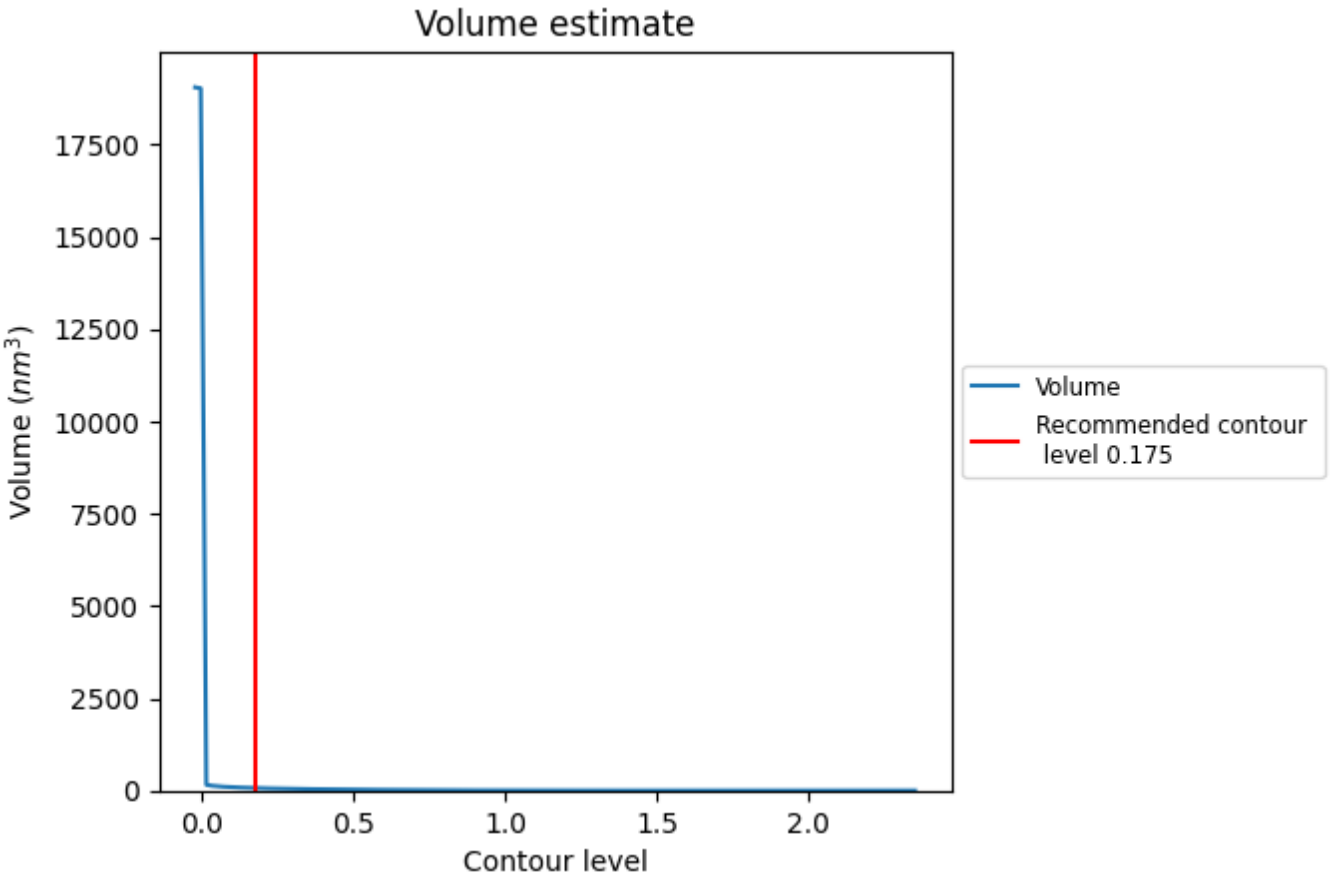
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

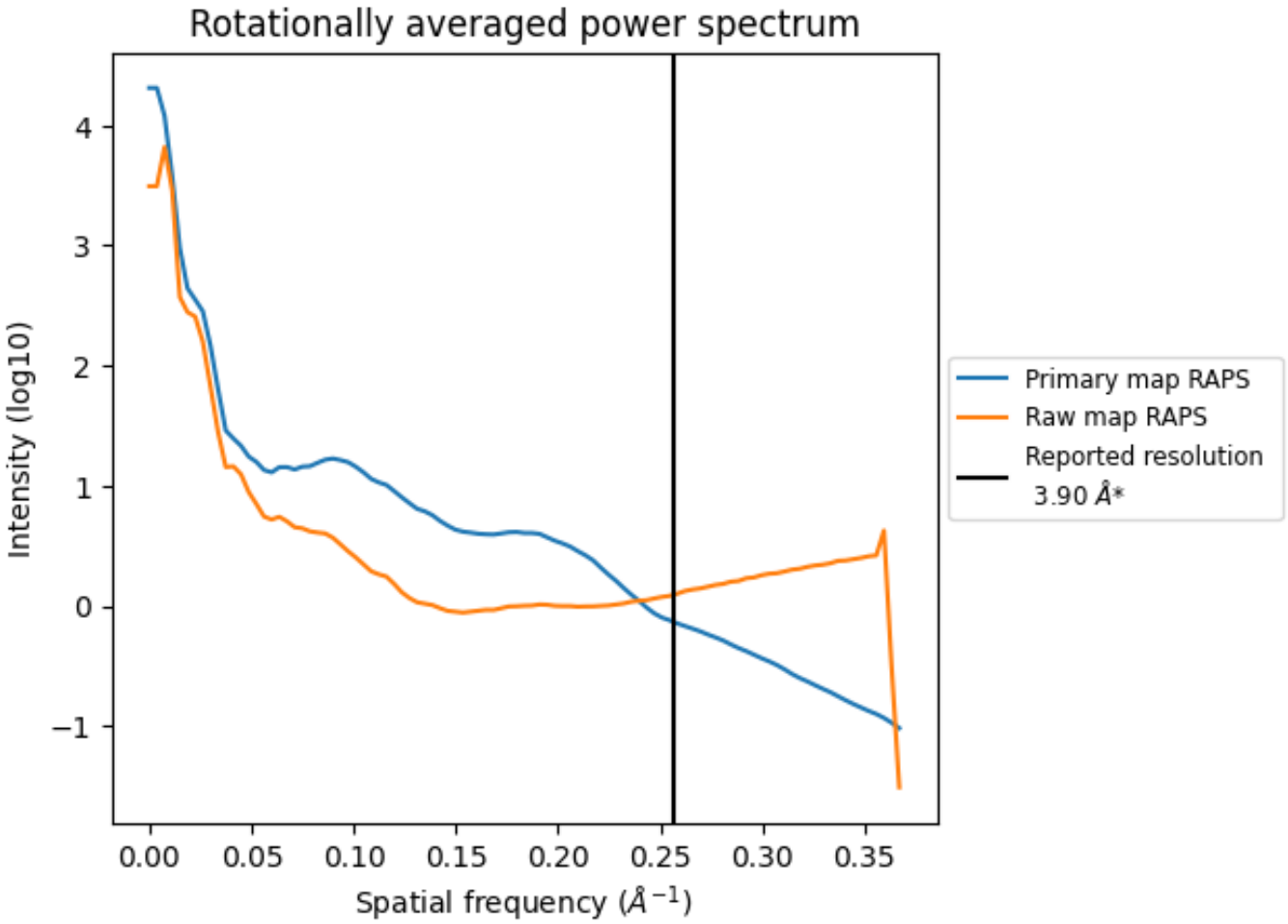
7.2 Volume estimate



The volume at the recommended contour level is 68 nm^3; this corresponds to an approximate mass of 62 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)

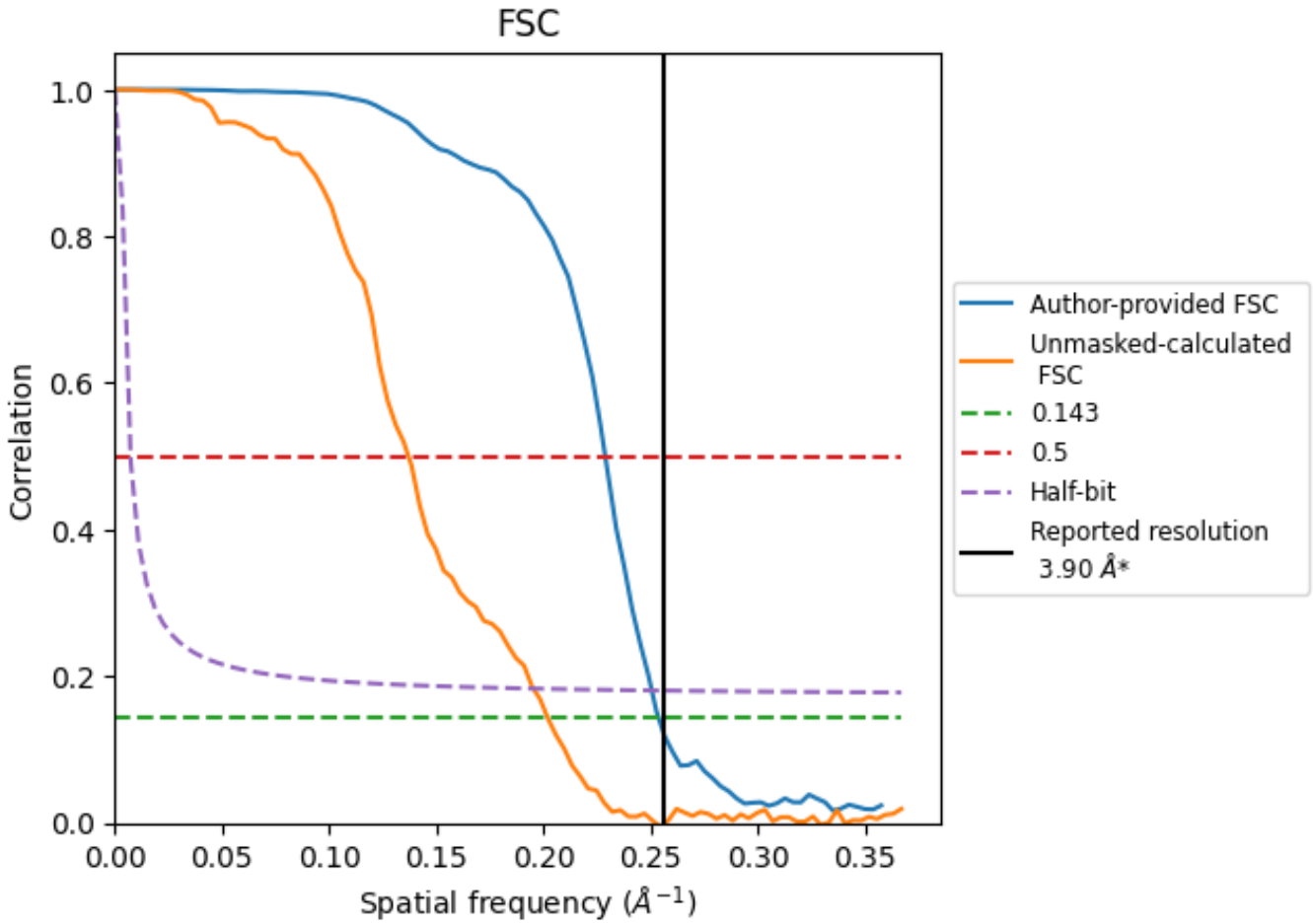


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

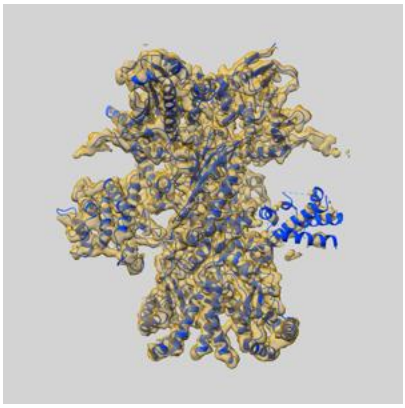
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.94	4.37	3.99
Unmasked-calculated*	4.95	7.30	5.12

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

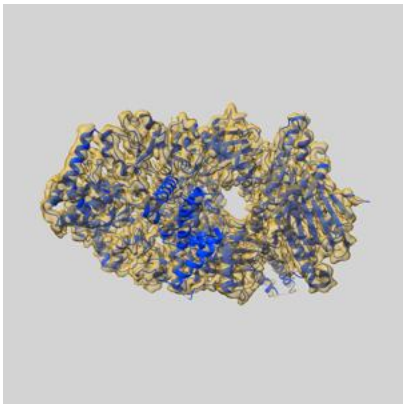
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29523 and PDB model 8FX4. Per-residue inclusion information can be found in section 3 on page 7.

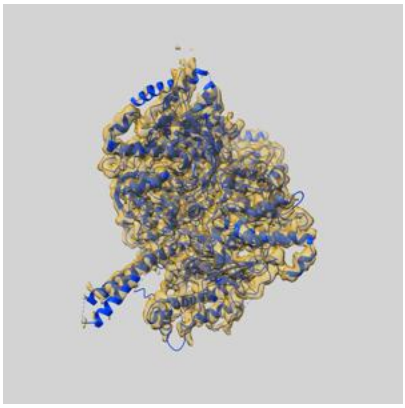
9.1 Map-model overlay



X



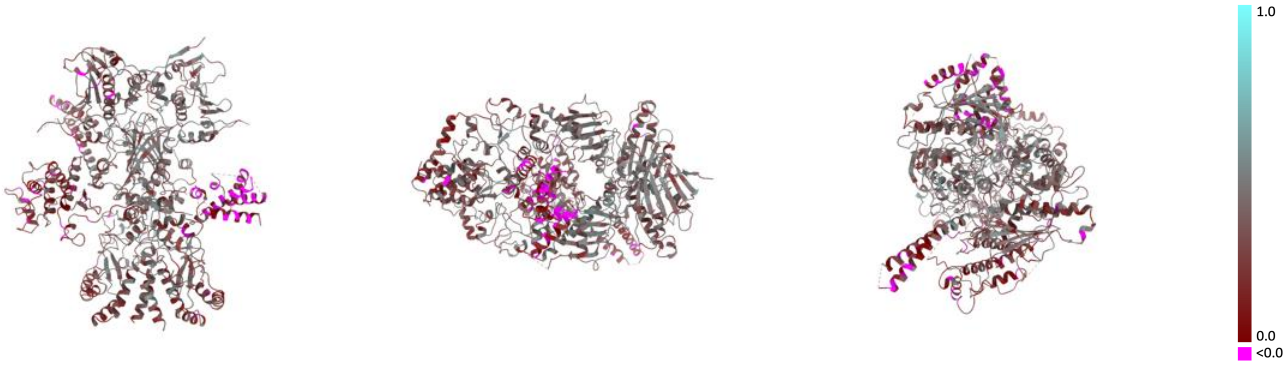
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.175 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.

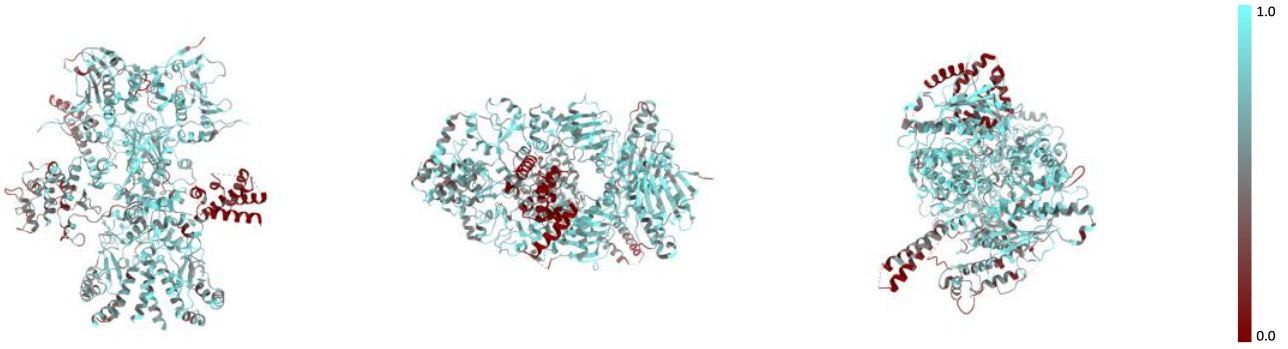
9.2 Q-score mapped to coordinate model (i)



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.

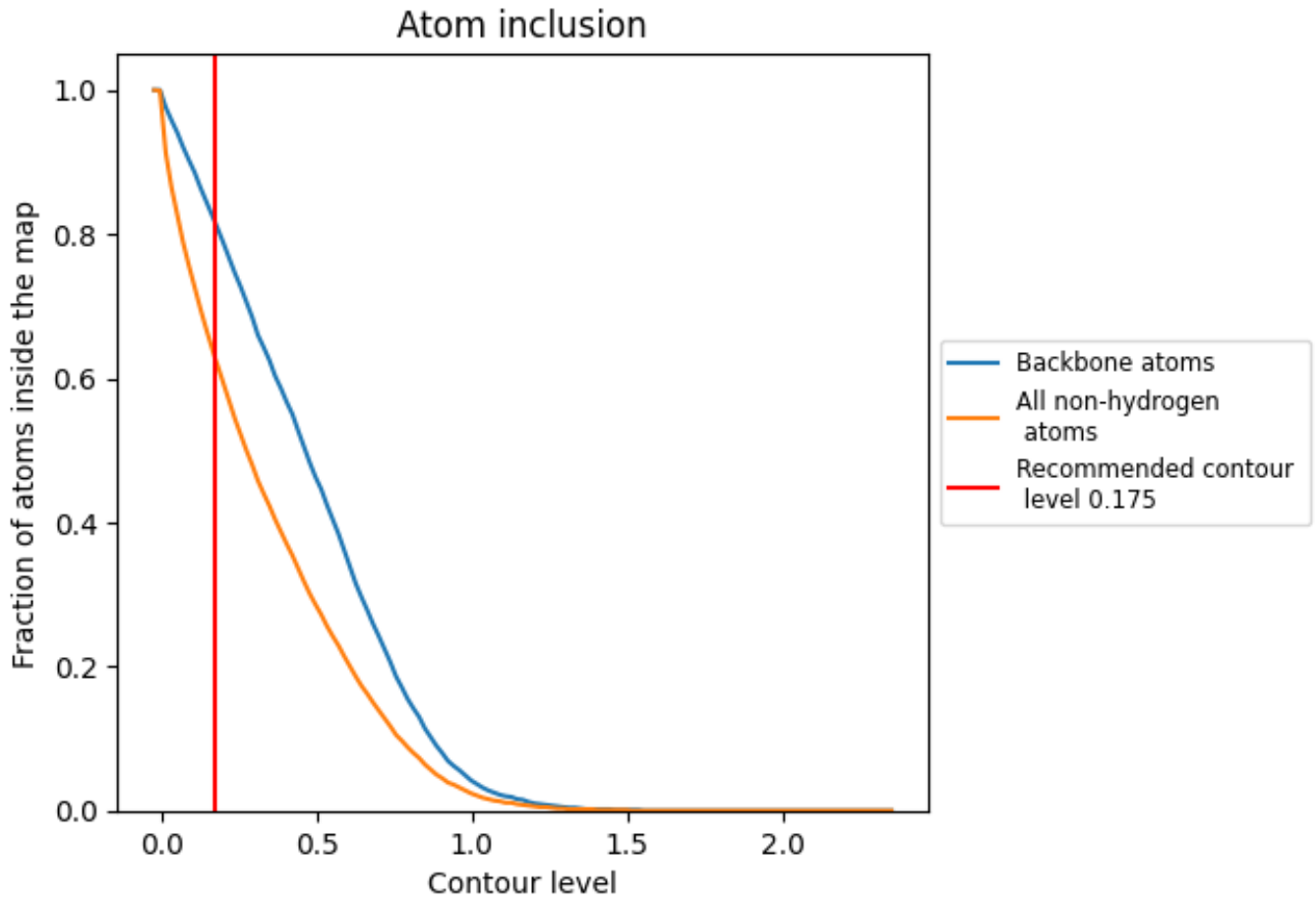
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.175).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 63% 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 (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6260	0.3290
A	0.6920	0.3630
B	0.7200	0.3860
C	0.3030	0.1770
D	0.4720	0.2070