wwPDB EM Validation Summary Report (i)

Oct 1, 2024 – 10:24 AM EDT

PDB ID	:	8VH5
EMDB ID	:	EMD-43235
Title	:	Cryo-EM structure of Rab12-LRRK2 complex in the LRRK2 dimer state
Authors	:	Zhu, H.; Sun, J.
Deposited on	:	2023-12-30
Resolution	:	4.00 Å(reported)

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

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

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

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

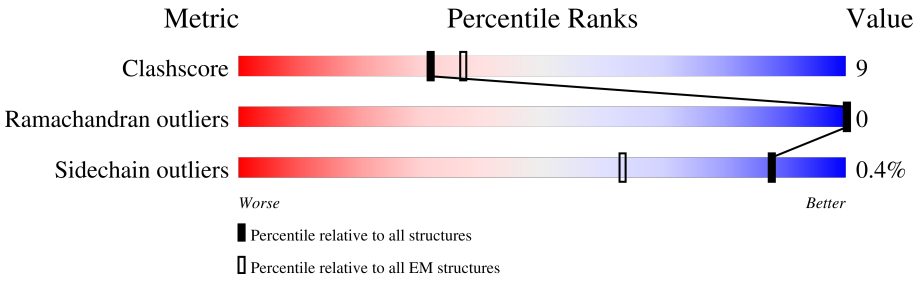
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2527	9% 72% 16% 12%
1	C	2527	8% 72% 16% 12%
2	B	176	60% 75% 22% .
2	D	176	64% 75% 22% .

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 33744 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 Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2221	Total	C	N	O	S	0	0
			15573	10054	2651	2783	85		
1	C	2221	Total	C	N	O	S	0	0
			15587	10060	2655	2787	85		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	HIS	ARG	conflict	UNP Q5S007
A	1647	THR	SER	conflict	UNP Q5S007
A	2397	THR	MET	conflict	UNP Q5S007
C	50	HIS	ARG	conflict	UNP Q5S007
C	1647	THR	SER	conflict	UNP Q5S007
C	2397	THR	MET	conflict	UNP Q5S007

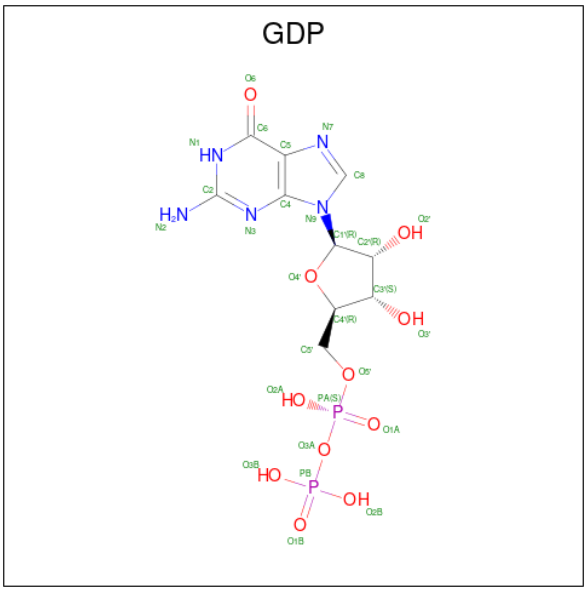
- Molecule 2 is a protein called Ras-related protein Rab-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	171	Total	C	N	O	S	0	0
			1200	775	199	220	6		
2	D	171	Total	C	N	O	S	0	0
			1200	775	199	220	6		

There are 2 discrepancies between the modelled and reference sequences:

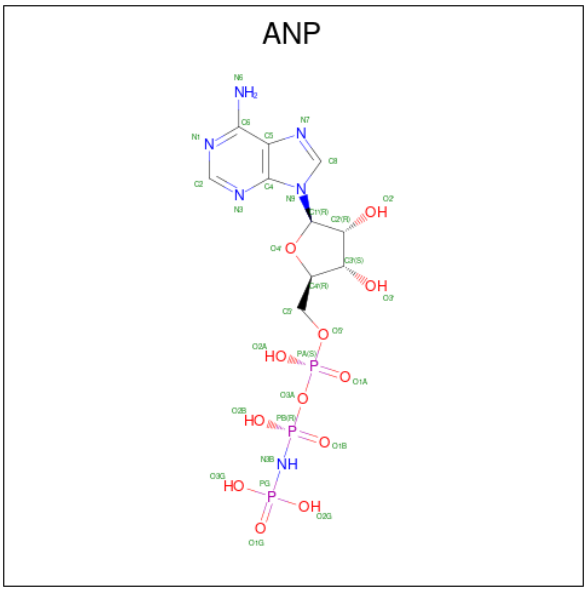
Chain	Residue	Modelled	Actual	Comment	Reference
B	101	LEU	GLN	conflict	UNP Q6IQ22
D	101	LEU	GLN	conflict	UNP Q6IQ22

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	C	1	Total	C	N	O	P	0
			28	10	5	11	2	

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



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

Continued on next page...

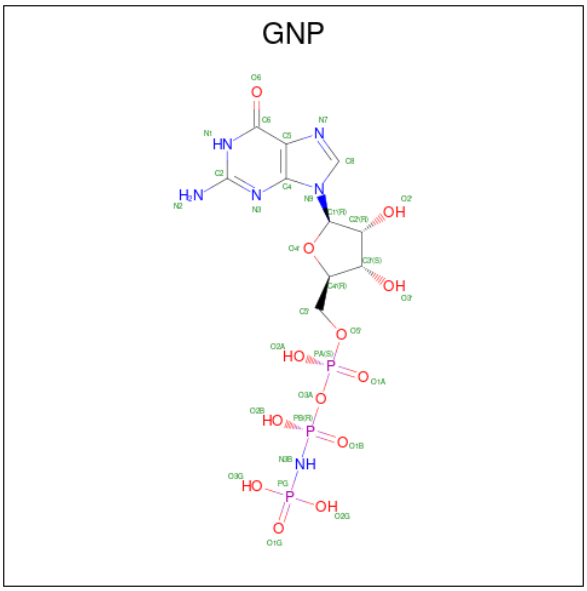
Continued from previous page...

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



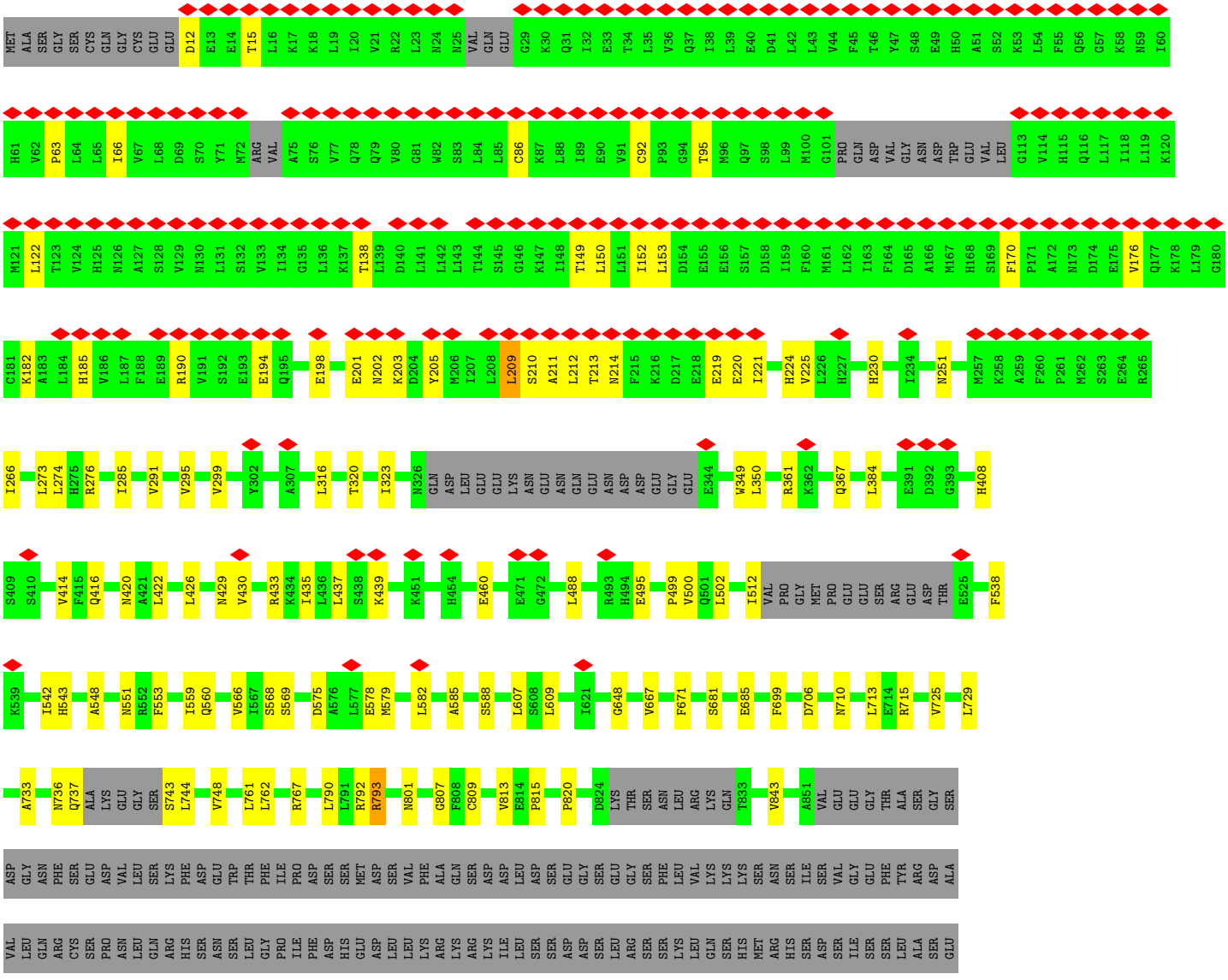
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			32	10	6	13	3	
6	D	1	Total	C	N	O	P	0
			32	10	6	13	3	

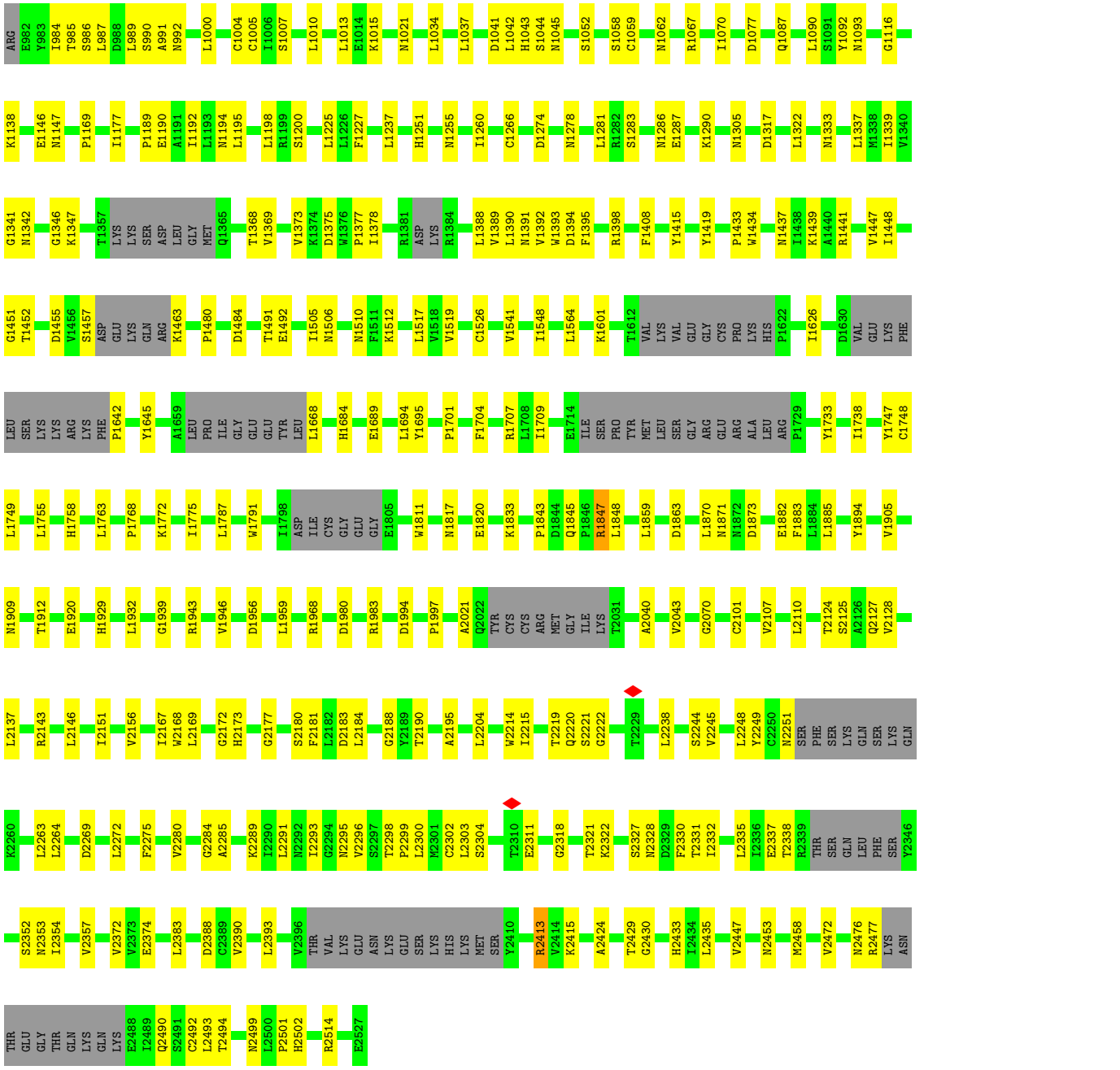
3 Residue-property plots (i)

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: Leucine-rich repeat serine/threonine-protein kinase 2

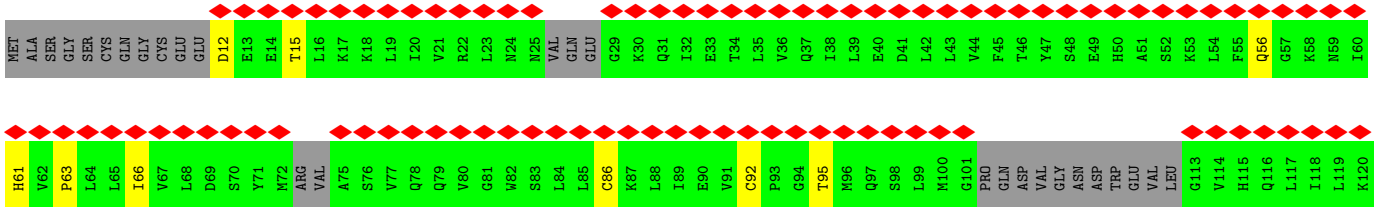
Chain A:

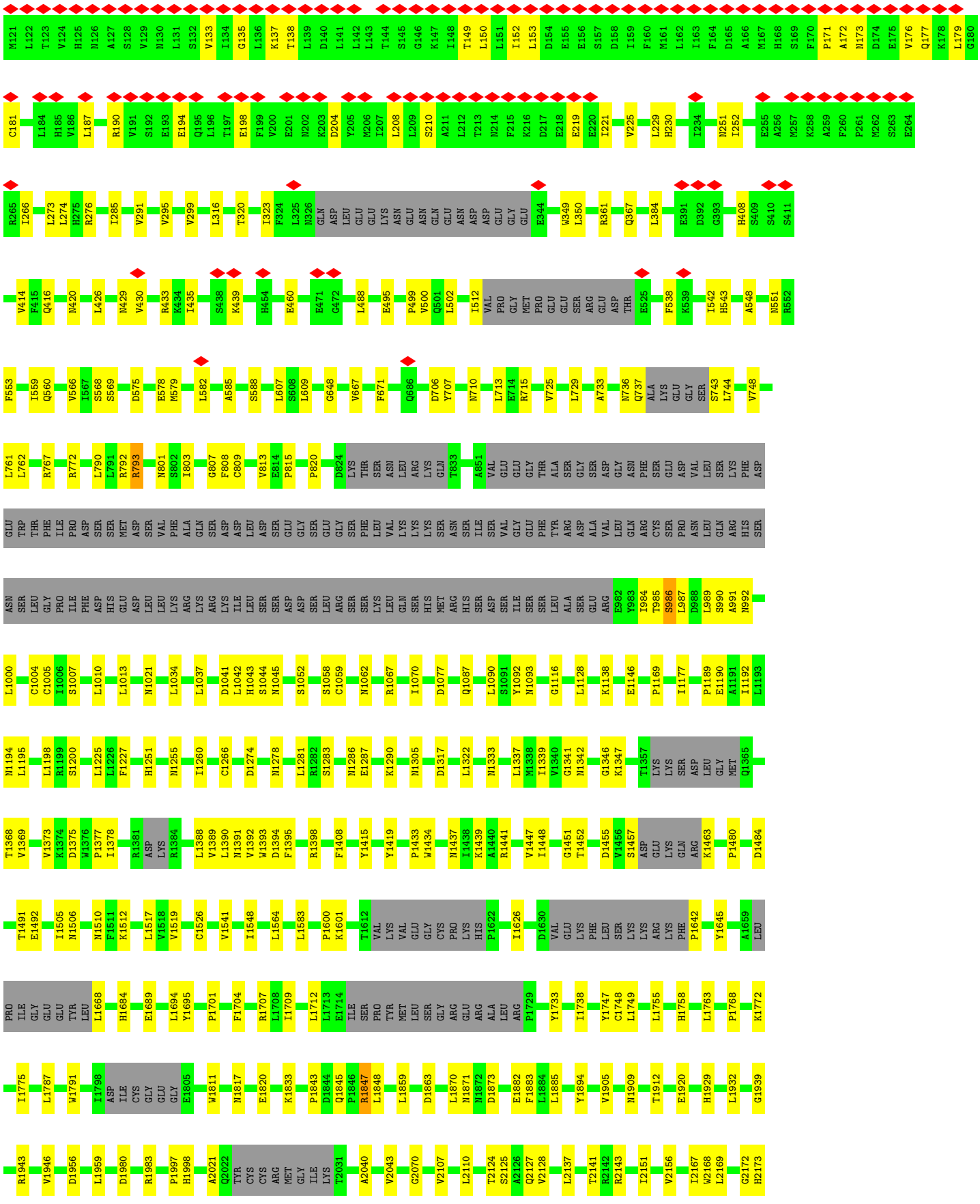


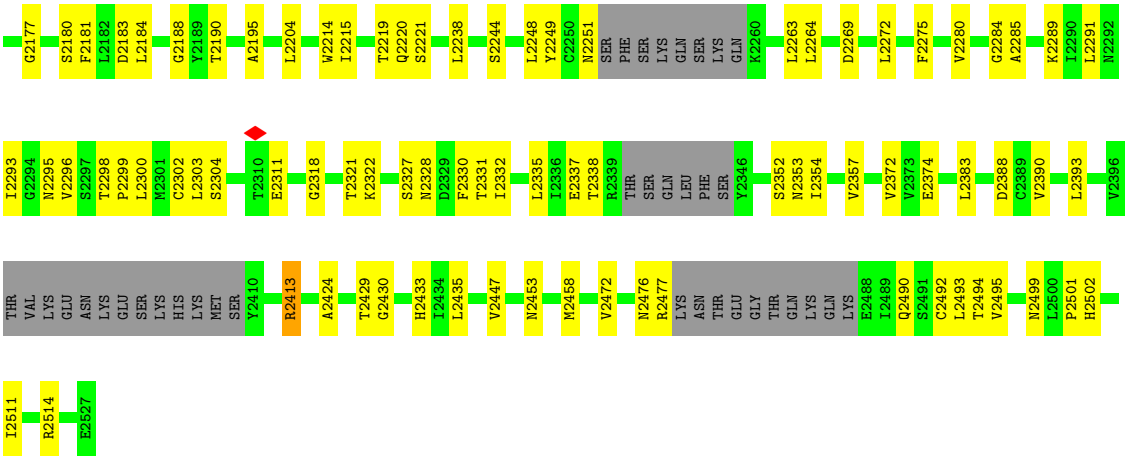


• Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2

Chain C:

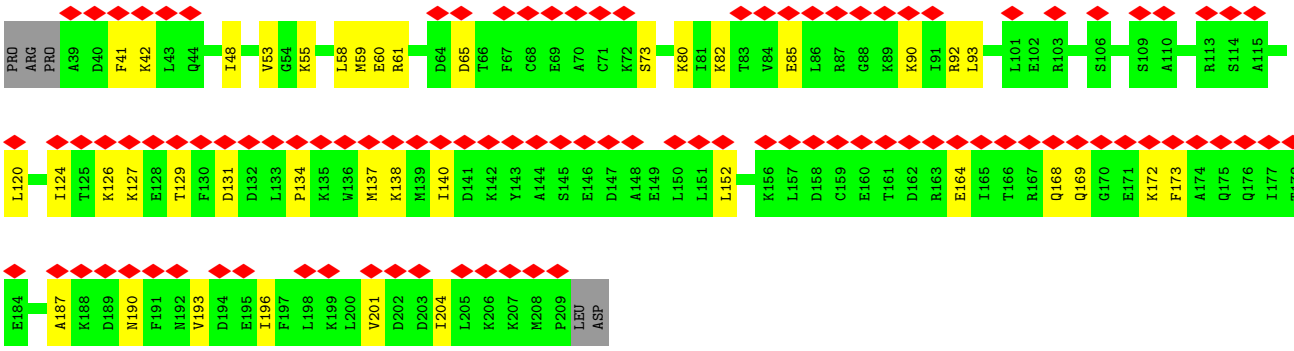



M121 L122 T123 V124 H125 N126 A127 S128 V129 N130 L131 S132 V133 I134 G135 L136 K137 T138 L139 D140 L141 L142 L143 T144 S145 G146 K147 I148 T149 L150 L151 I152 L153 D154 E155 E156 S157 D158 I159 F160 M161 L162 I163 F164 D165 A166 M167 H168 S169 F170 P171 A172 N173 D174 E175 V176 Q177 K178 L179 G180
C181 L184 H185 V186 L187 R190 V191 S192 E193 E194 Q195 L196 T197 E198 F199 V200 E201 N202 K203 D204 Y205 M206 I207 L208 L209 S210 A211 L212 T213 N214 F215 K216 D217 E218 E219 E220 I221 V225 L229 H230 I234 N251 I252 E255 A256 M257 K258 A259 F260 P261 M262 S263 E264
R265 I266 L273 L274 H275 R276 I285 V291 V295 V299 L316 T320 I323 F324 L325 N326 GLN ASP LEU GLU GLU LYS ASN GLU ASN GLN GLU ASN ASP ASP GLU GLY GLU E344 W349 L350 R361 Q367 L384 E391 D392 G393 H408 S409 S410 S411
V414 F415 Q416 N420 L426 N429 V430 R433 K434 I435 S438 K439 H454 E460 E471 G472 L488 E495 P499 V500 Q501 L502 I512 VAL PRO GLY MET PRO GLU GLU SER ARG GLU ASP THR E525 F538 K539 I542 H543 A548 N551 R552
F553 I559 Q560 V566 I567 S568 S569 D575 E578 M579 L582 A585 S588 L607 S608 L609 G648 V667 F671 Q686 D706 Y707 N710 L713 E714 R715 V725 L729 A733 N736 Q737 ALA LYS GLU GLY SER S743 L744 V748
L761 L762 R767 R772 L790 L791 R792 R793 N801 S802 I803 G807 F808 C809 V813 E814 P815 P820 D824 LYS THR SER ASN LEU ARG LYS GLN T833 A851 VAL GLU GLU GLY THR ALA SER GLY SER ASP GLY ASN PHE SER GLU ASP VAL LEU SER LYS PHE ASP
GLU TRP THR PHE ILE PRO ASP SER SER MET ASP SER VAL PHE ALA GLN SER ASP ASP LEU ASP SER GLU GLY SER GLU GLY SER PHE LEU VAL LYS LYS LYS SER SER ASN SER ILE SER VAL GLY GLU PHE TYR ARG ASP ALA VAL LEU GLN ARG CYS SER PRO ASN LEU GLN LEU GLN ARG HIS SER
ASN SER LEU GLY PRO ILE PHE ASP HIS GLU ASP LEU LEU LYS ARG LYS ARG LYS ILE LEU LEU SER SER ASP ASP SER LEU ARG SER SER LYS LEU GLN SER HIS MET ARG HIS SER ASP SER ILE SER SER LEU ALA SER GLU ARG E982 Y983 I984 T985 S986 L987 D988 L989 S990 A991 N992
L1000 C1004 C1005 I1006 S1007 L1010 L1013 N1021 L1034 L1037 D1041 L1042 H1043 S1044 N1045 S1052 S1058 C1059 N1062 R1067 I1070 D1077 Q1087 L1090 S1091 Y1092 N1093 G1116 L1128 K1138 E1146 P1169 I1177 P1189 E1190 A1191 I1192 L1193
N1194 L1195 L1198 R1199 S1200 L1225 L1226 F1227 H1251 N1255 I1260 C1266 D1274 N1278 L1281 R1282 S1283 N1286 E1287 K1290 N1305 D1317 L1322 N1333 L1337 M1338 I1339 V1340 G1341 N1342 G1346 K1347 T1357 LYS LYS SER ASP LEU GLY MET Q1365
T1368 V1369 V1373 K1374 D1375 W1376 P1377 I1378 R1381 ASP LYS R1384 L1388 V1389 L1390 N1391 V1392 W1393 D1394 F1395 R1398 F1408 Y1415 Y1419 P1433 W1434 N1437 I1438 K1439 A1440 R1441 V1447 I1448 G1451 T1452 D1455 V1456 S1457 ASP GLU LYS GLN ARG K1463 P1480 D1484
T1491 E1492 I1505 N1506 N1510 F1511 K1512 L1517 V1518 V1519 C1526 V1541 I1548 L1564 L1583 P1600 K1601 T1612 VAL LYS VAL GLU GLY CYS PRO LYS HIS P1622 I1626 D1630 VAL GLU LYS PHE LEU SER LYS LYS ARG LYS PHE P1642 Y1645 A1659 LEU
PRO ILE GLY GLU GLU TYR LEU L1668 H1684 E1689 L1694 Y1695 P1701 F1704 R1707 L1708 I1709 L1712 L1713 E1714 ILE SER PRO TYR MET LEU SER GLY ARG GLU ARG ALA LEU ARG P1729 Y1733 I1738 Y1747 C1748 L1749 L1755 H1758 L1763 P1768 K1772
I1775 L1787 W1791 I1798 ASP ILE CYS GLY GLU GLY E1805 W1811 N1817 E1820 K1833 P1843 D1844 Q1845 P1846 R1847 L1848 L1859 D1863 L1870 N1871 N1872 D1873 E1882 F1883 L1884 L1885 Y1894 V1905 N1909 T1912 E1920 H1929 L1932 G1939
R1943 V1946 D1956 L1959 D1980 R1983 P1997 H1998 A2021 Q2022 TYR CYS CYS ARG MET GLY ILE LYS T2031 A2040 V2043 G2070 V2107 L2110 T2124 S2125 A2126 Q2127 V2128 L2137 T2141 R2142 R2143 I2151 V2156 I2167 W2168 L2169 G2172 H2173



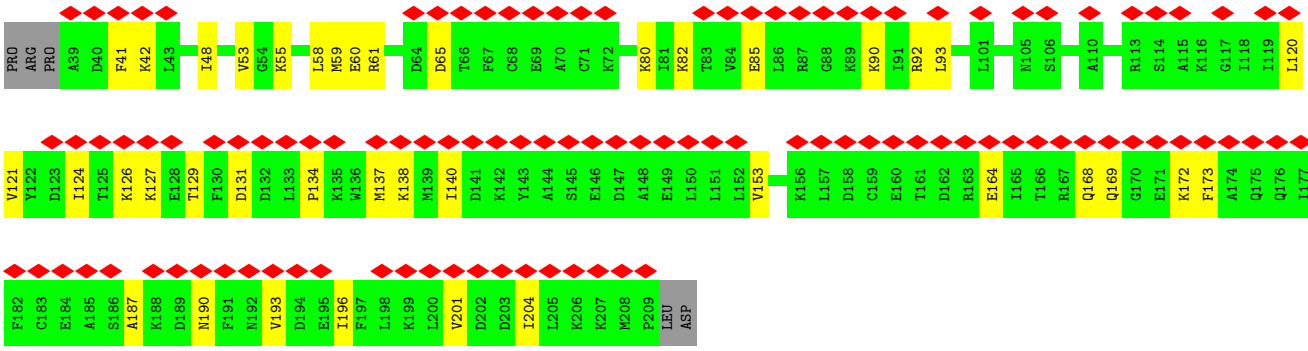
• Molecule 2: Ras-related protein Rab-12

Chain B:



• Molecule 2: Ras-related protein Rab-12

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	77265	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	77.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.547	Depositor
Minimum map value	-1.169	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	508.288, 508.288, 508.288	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.444, 1.444, 1.444	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, GNP, MG, GDP

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	0.34	0/15858	0.51	2/21732 (0.0%)
1	C	0.34	0/15871	0.51	2/21745 (0.0%)
2	B	0.32	0/1219	0.49	0/1662
2	D	0.32	0/1219	0.49	0/1662
All	All	0.34	0/34167	0.51	4/46801 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	213	THR	C-N-CA	-6.61	105.17	121.70
1	A	1042	LEU	CA-CB-CG	5.82	128.67	115.30
1	C	1042	LEU	CA-CB-CG	5.79	128.63	115.30
1	C	210	SER	C-N-CA	-5.39	108.22	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	LEU	Mainchain
1	A	986	SER	Peptide
1	C	172	ALA	Mainchain
1	C	986	SER	Peptide

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	15573	0	14262	245	0
1	C	15587	0	14299	255	0
2	B	1200	0	1080	25	0
2	D	1200	0	1080	24	0
3	A	28	0	12	0	0
3	C	28	0	12	0	0
4	A	31	0	13	1	0
4	C	31	0	13	2	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	32	0	13	3	0
6	D	32	0	13	2	0
All	All	33744	0	30797	551	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 9.

The worst 5 of 551 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:C:173:ASN:ND2	1:C:176:VAL:HG23	1.25	1.48
1:C:173:ASN:ND2	1:C:176:VAL:CG2	1.92	1.32
1:C:173:ASN:HD22	1:C:176:VAL:CG2	1.61	1.05
1:C:133:VAL:HG12	1:C:176:VAL:HG22	1.52	0.89
1:A:813:VAL:HG21	1:A:989:LEU:HD21	1.55	0.87

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	2177/2527 (86%)	1966 (90%)	211 (10%)	0	100	100
1	C	2177/2527 (86%)	1968 (90%)	209 (10%)	0	100	100
2	B	169/176 (96%)	154 (91%)	15 (9%)	0	100	100
2	D	169/176 (96%)	154 (91%)	15 (9%)	0	100	100
All	All	4692/5406 (87%)	4242 (90%)	450 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1423/2281 (62%)	1418 (100%)	5 (0%)	89	91
1	C	1428/2281 (63%)	1422 (100%)	6 (0%)	89	91
2	B	104/156 (67%)	104 (100%)	0	100	100
2	D	104/156 (67%)	104 (100%)	0	100	100
All	All	3059/4874 (63%)	3048 (100%)	11 (0%)	88	91

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	793	ARG
1	C	1266	CYS
1	C	2413	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1847	ARG
1	A	2413	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1758	HIS
1	C	1871	ASN
1	C	2353	ASN
1	A	1872	ASN
1	A	1871	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
4	ANP	C	2602	-	29,33,33	1.15	4 (13%)	31,52,52	0.81	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GDP	A	2601	-	25,30,30	0.98	1 (4%)	30,47,47	1.17	3 (10%)
6	GNP	B	302	5	29,34,34	1.50	7 (24%)	33,54,54	2.20	6 (18%)
3	GDP	C	2601	-	25,30,30	0.99	1 (4%)	30,47,47	1.17	3 (10%)
6	GNP	D	302	5	29,34,34	1.50	7 (24%)	33,54,54	2.19	5 (15%)
4	ANP	A	2602	-	29,33,33	1.16	4 (13%)	31,52,52	0.81	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	C	2602	-	-	8/14/38/38	0/3/3/3
3	GDP	A	2601	-	-	4/12/32/32	0/3/3/3
6	GNP	B	302	5	-	7/14/38/38	0/3/3/3
3	GDP	C	2601	-	-	4/12/32/32	0/3/3/3
6	GNP	D	302	5	-	7/14/38/38	0/3/3/3
4	ANP	A	2602	-	-	8/14/38/38	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	302	GNP	PB-O3A	3.49	1.63	1.59
6	B	302	GNP	PB-O3A	3.44	1.63	1.59
6	D	302	GNP	C6-N1	3.06	1.38	1.33
6	B	302	GNP	C6-N1	3.02	1.38	1.33
3	C	2601	GDP	C6-N1	-2.93	1.33	1.37

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	302	GNP	C5-C6-N1	-8.63	111.88	123.42
6	D	302	GNP	C5-C6-N1	-8.63	111.88	123.42
6	B	302	GNP	C2-N1-C6	6.64	125.19	115.96
6	D	302	GNP	C2-N1-C6	6.62	125.17	115.96
3	C	2601	GDP	C8-N7-C5	2.93	107.53	102.55

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2601	GDP	C5'-O5'-PA-O3A
3	A	2601	GDP	C5'-O5'-PA-O1A
3	A	2601	GDP	C5'-O5'-PA-O2A
3	C	2601	GDP	C5'-O5'-PA-O3A
3	C	2601	GDP	C5'-O5'-PA-O1A

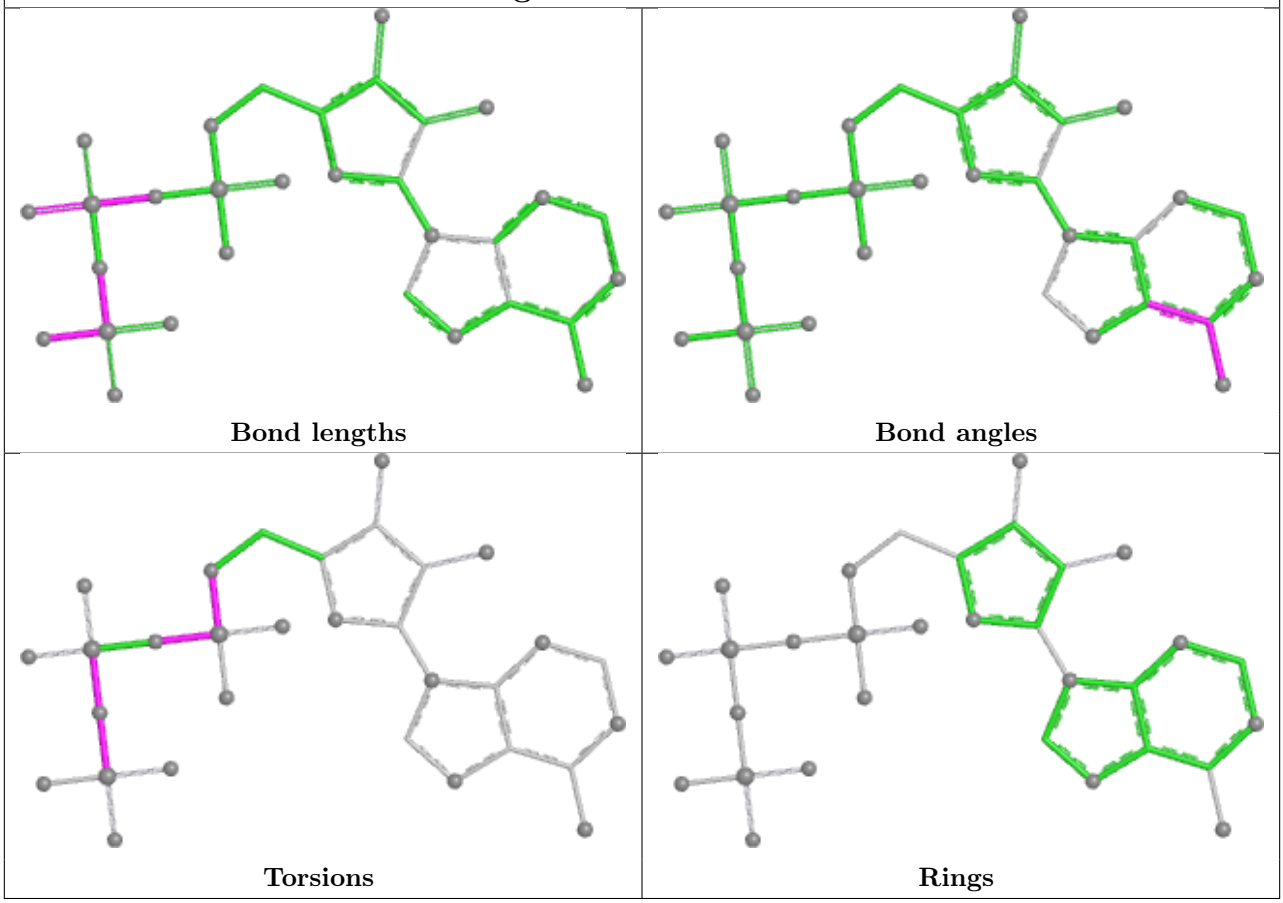
There are no ring outliers.

4 monomers are involved in 8 short contacts:

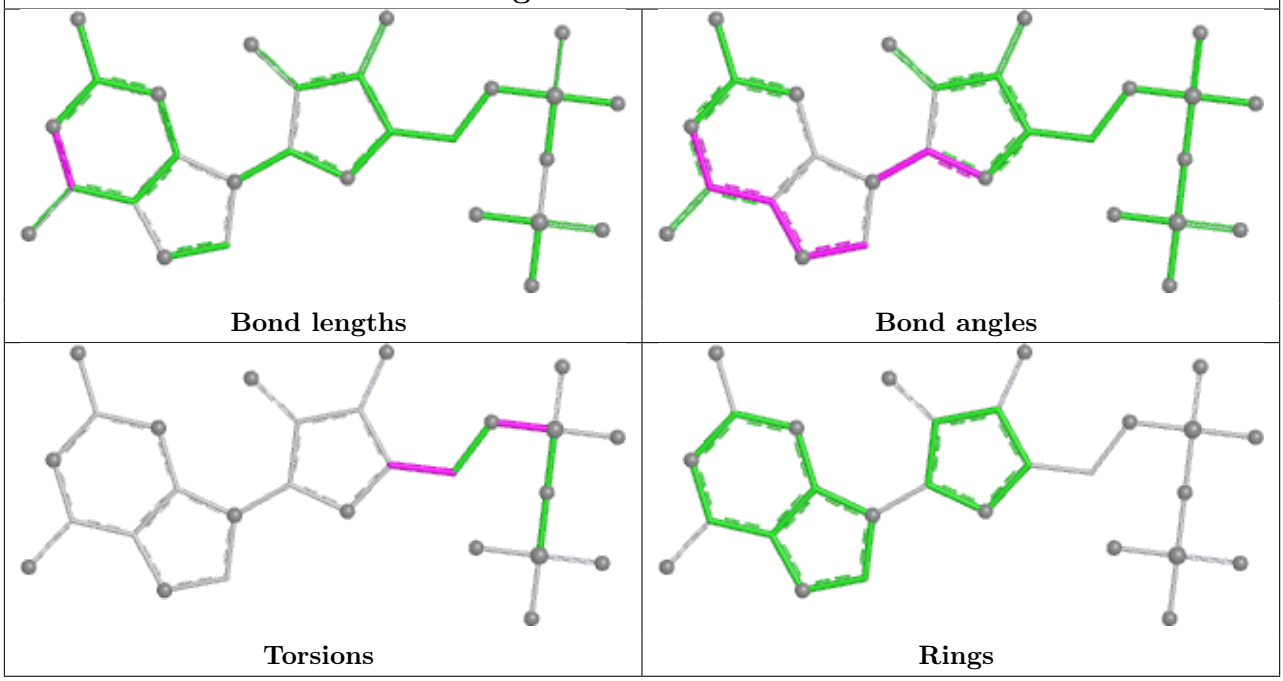
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2602	ANP	2	0
6	B	302	GNP	3	0
6	D	302	GNP	2	0
4	A	2602	ANP	1	0

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.

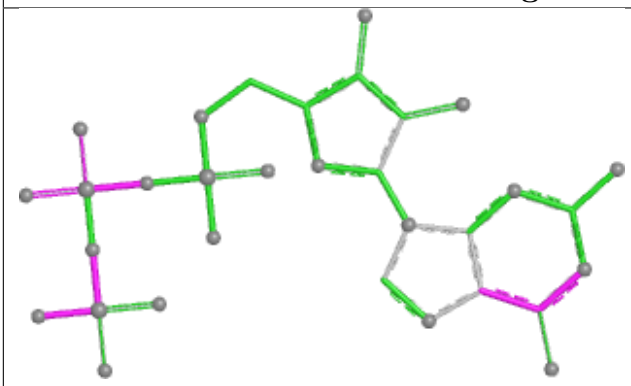
Ligand ANP C 2602



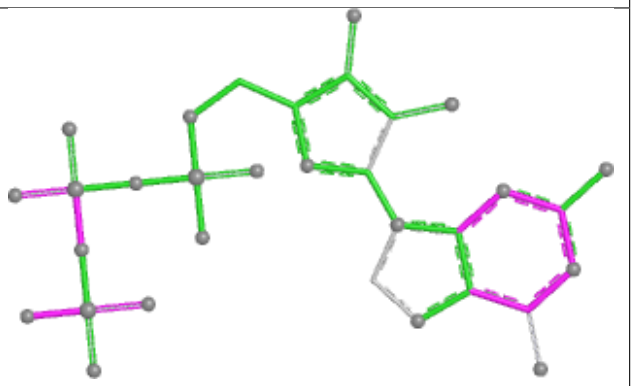
Ligand GDP A 2601



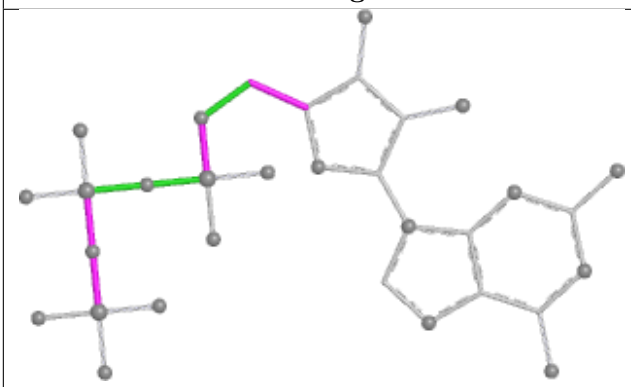
Ligand GNP B 302



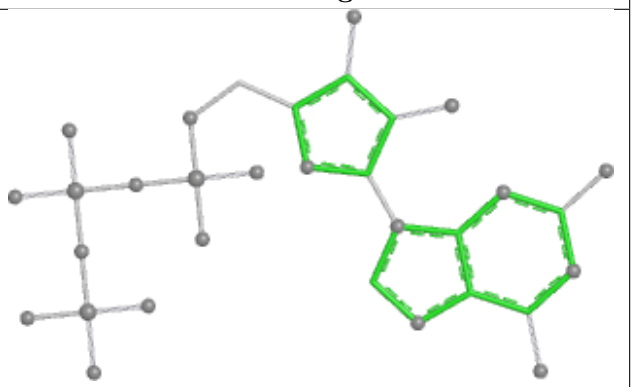
Bond lengths



Bond angles

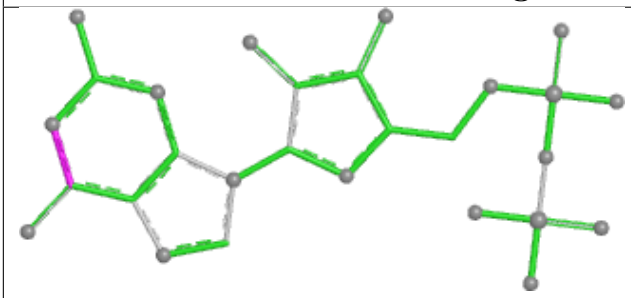


Torsions

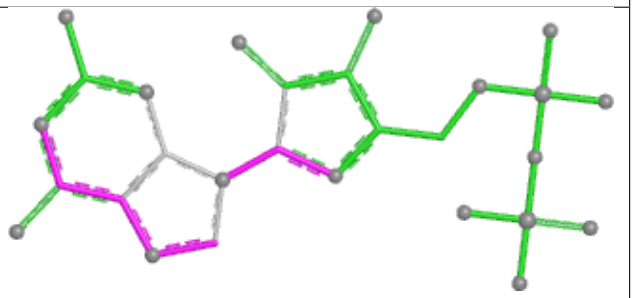


Rings

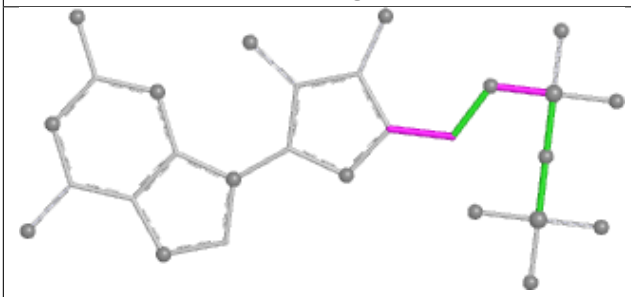
Ligand GDP C 2601



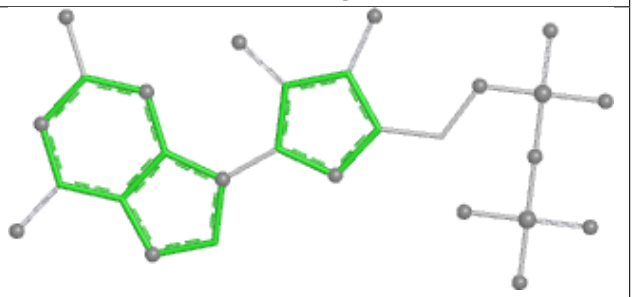
Bond lengths



Bond angles

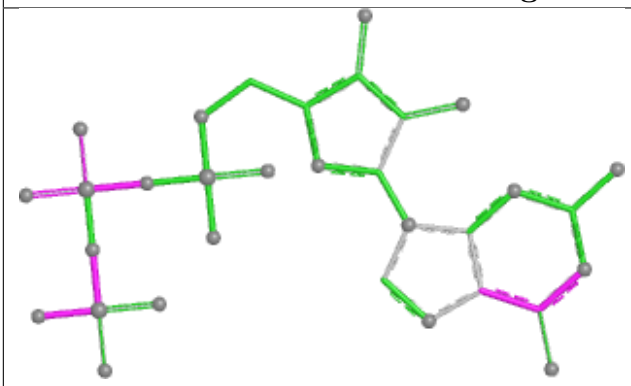


Torsions

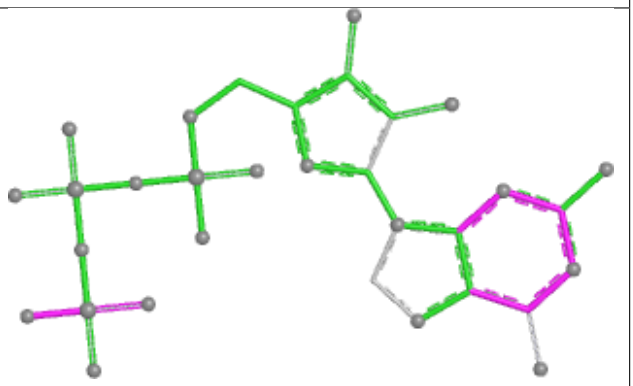


Rings

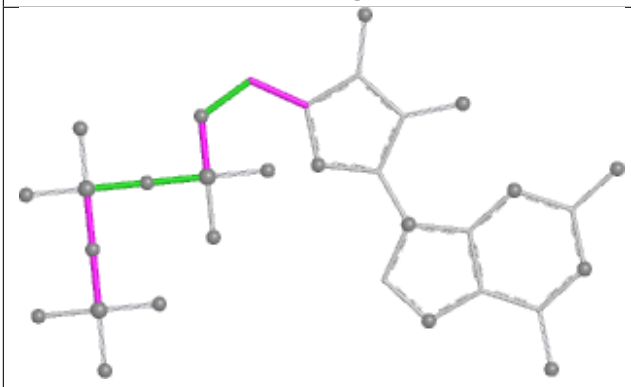
Ligand GNP D 302



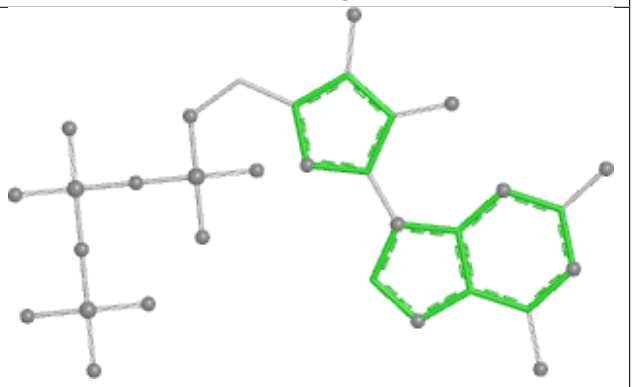
Bond lengths



Bond angles

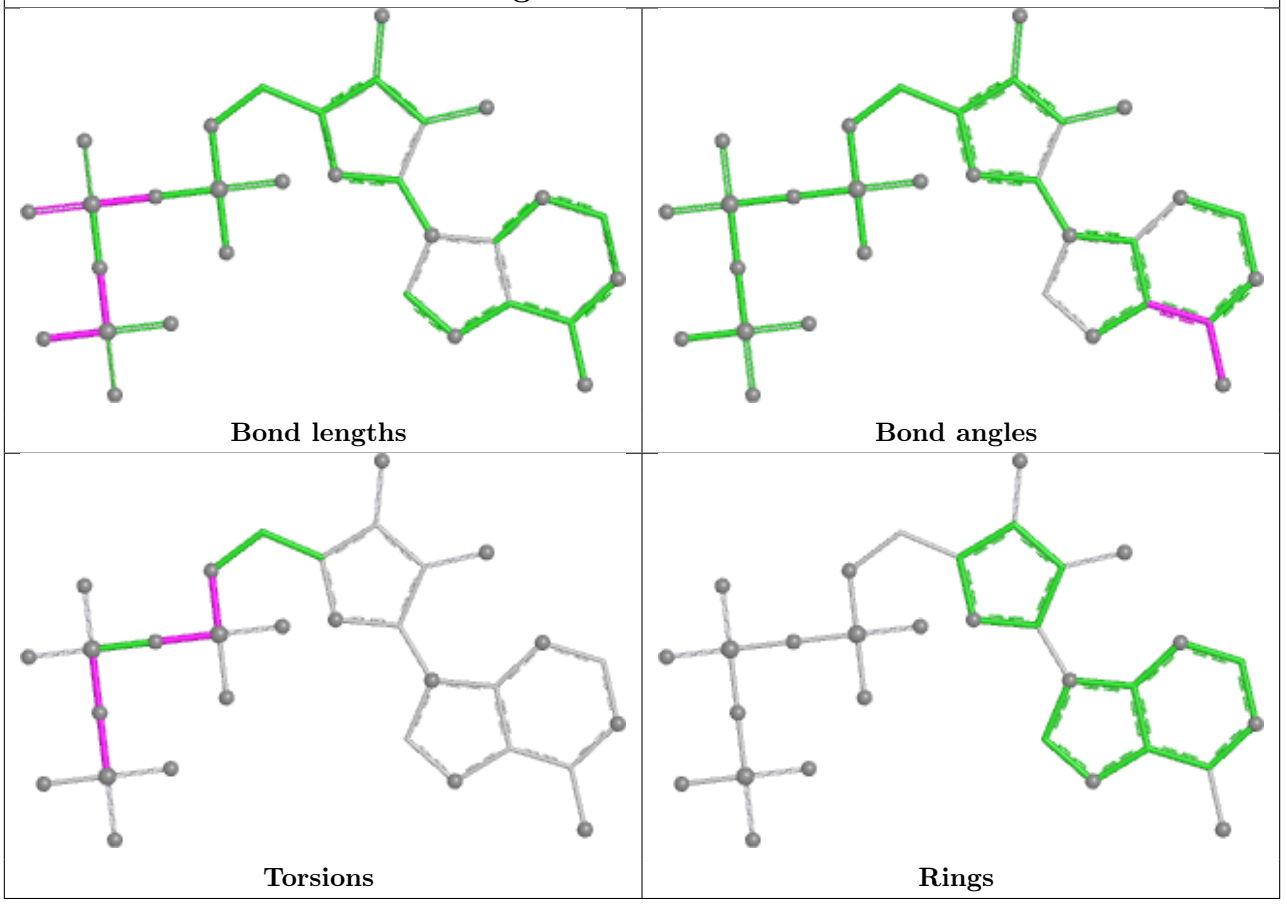


Torsions



Rings

Ligand ANP A 2602



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.

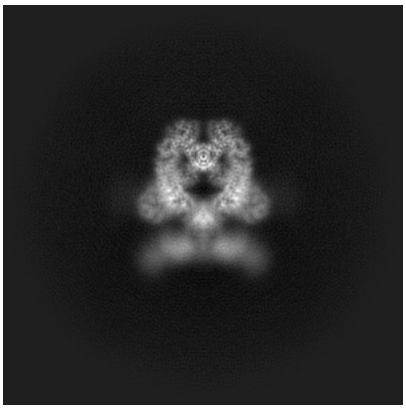
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43235. These allow visual inspection of the internal detail of the map and identification of artifacts.

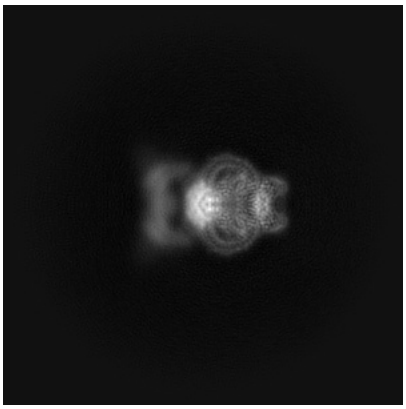
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

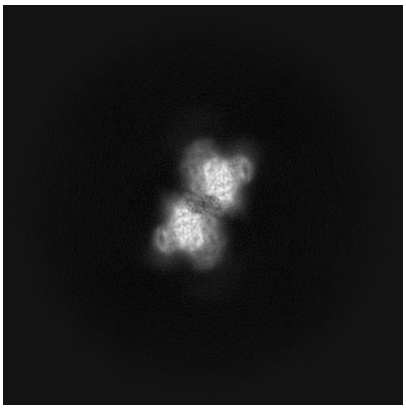
6.1.1 Primary map



X

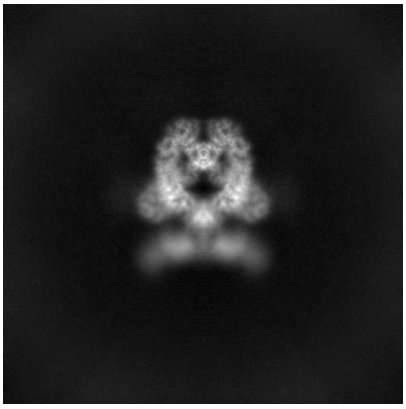


Y

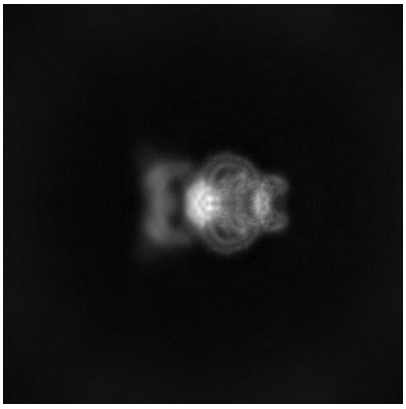


Z

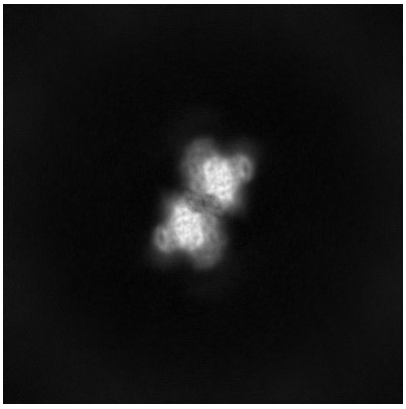
6.1.2 Raw map



X



Y

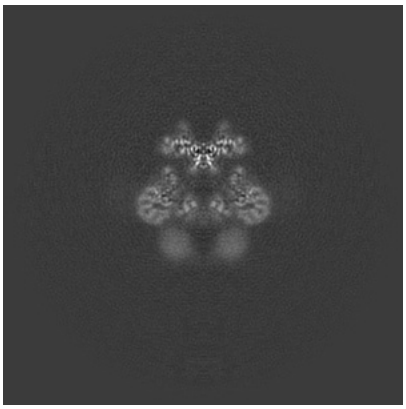


Z

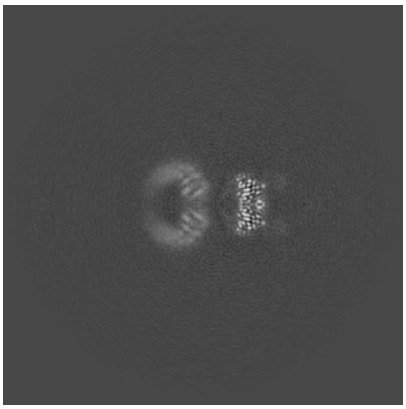
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

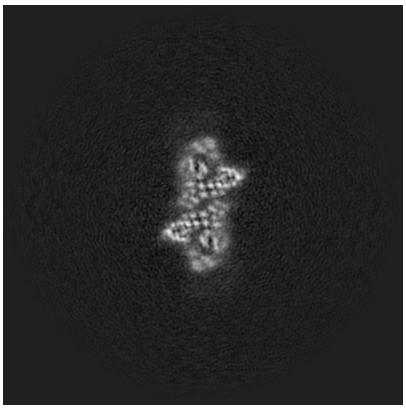
6.2.1 Primary map



X Index: 176

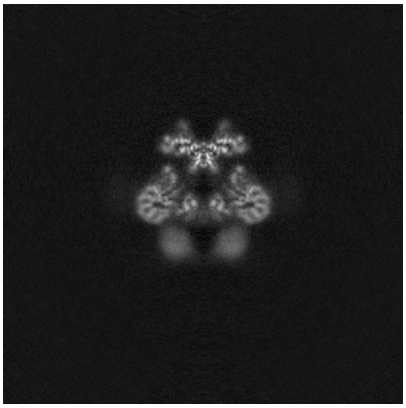


Y Index: 176

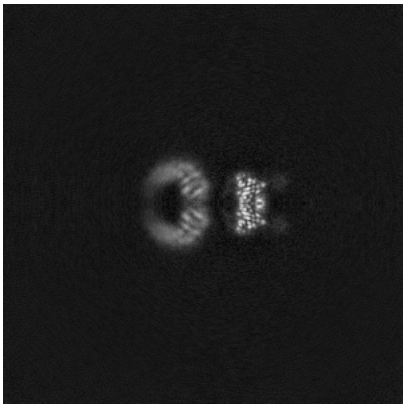


Z Index: 176

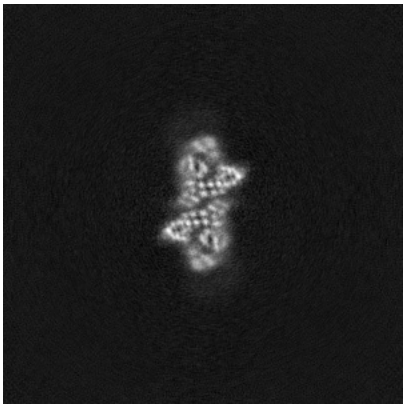
6.2.2 Raw map



X Index: 176



Y Index: 176

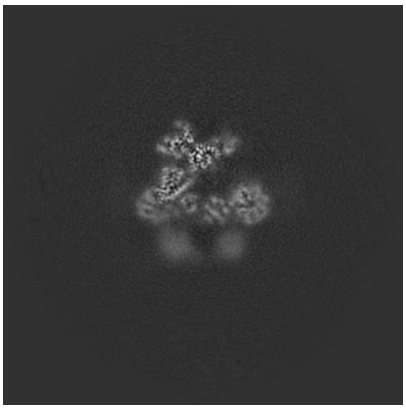


Z Index: 176

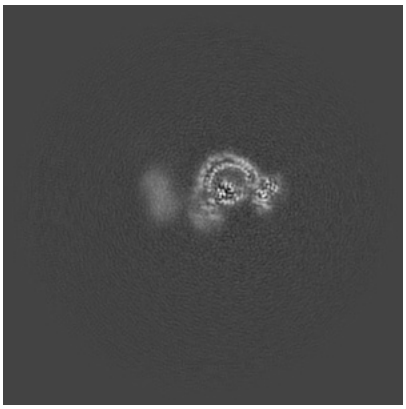
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

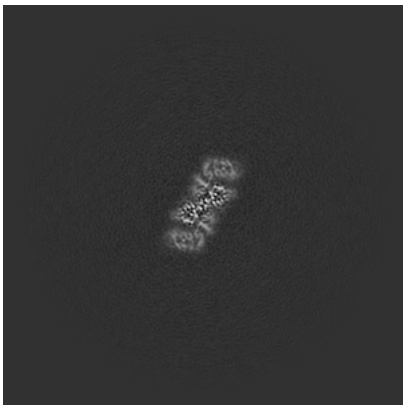
6.3.1 Primary map



X Index: 172

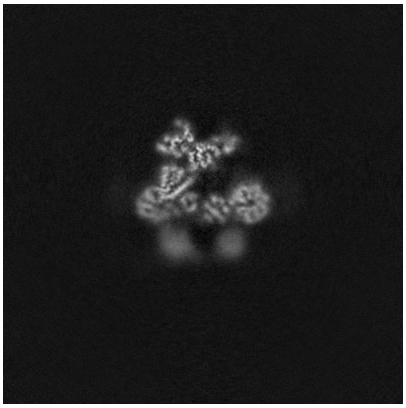


Y Index: 203

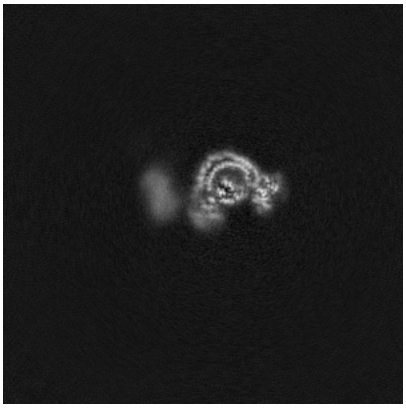


Z Index: 223

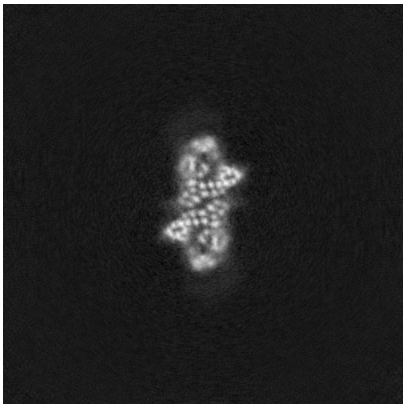
6.3.2 Raw map



X Index: 172



Y Index: 203

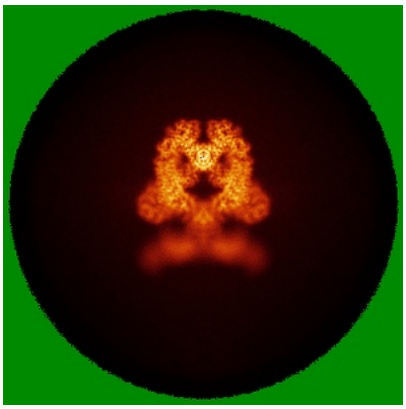


Z Index: 175

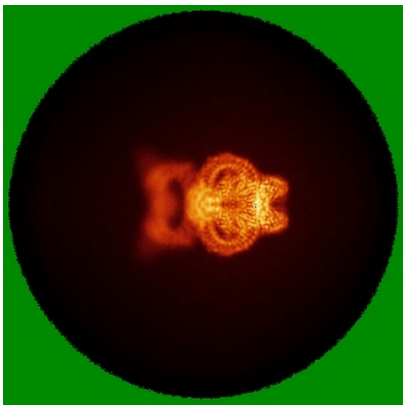
The images above show the largest variance slices of the map in three orthogonal directions.

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

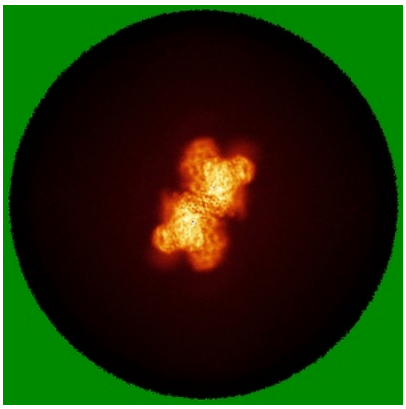
6.4.1 Primary map



X

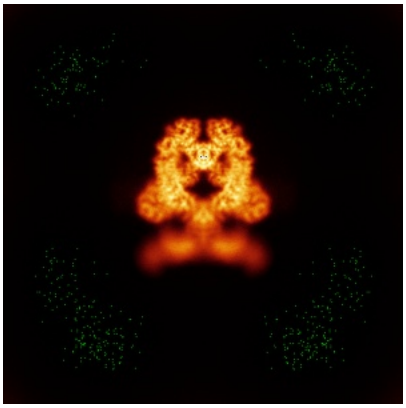


Y

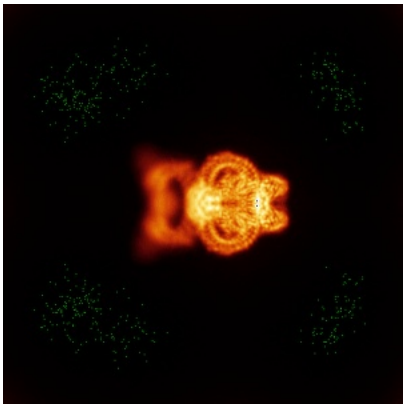


Z

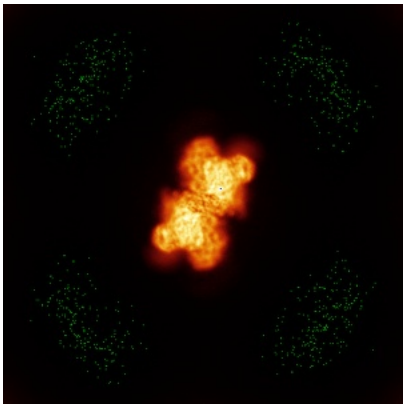
6.4.2 Raw map



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.

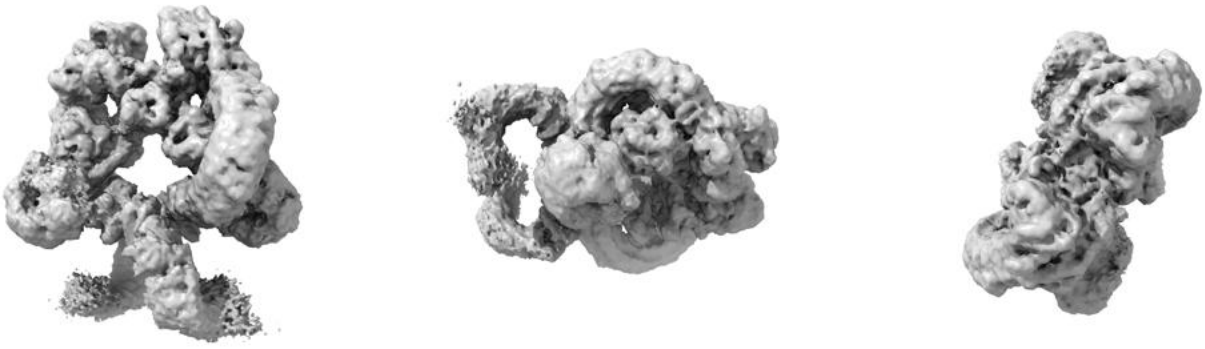
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

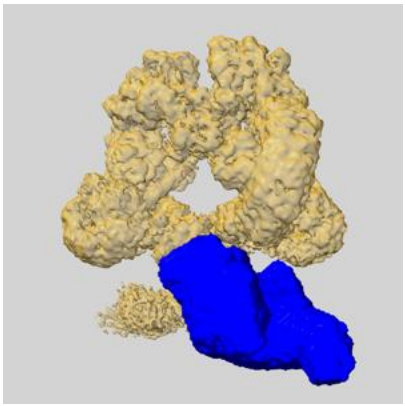
6.6 Mask visualisation

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

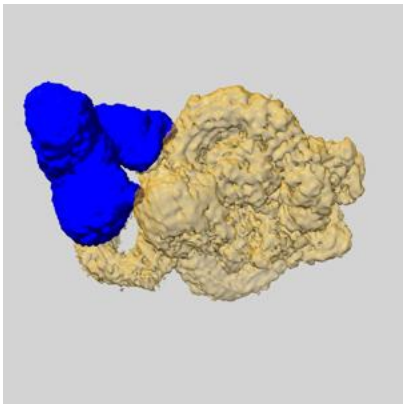
A mask typically either:

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

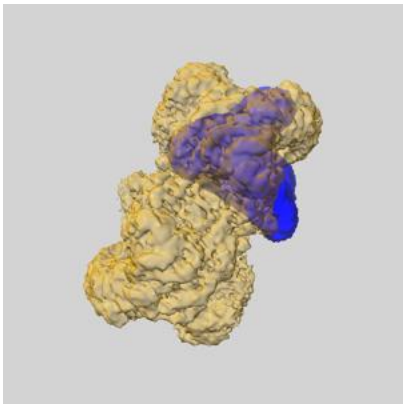
6.6.1 emd_43235_msk_1.map



X

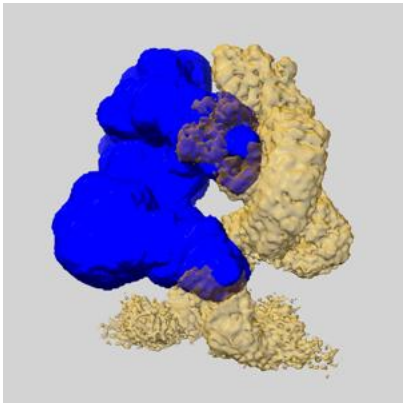


Y

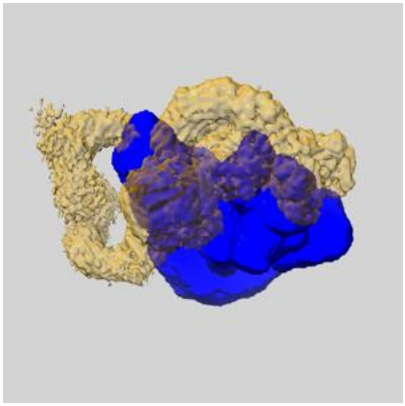


Z

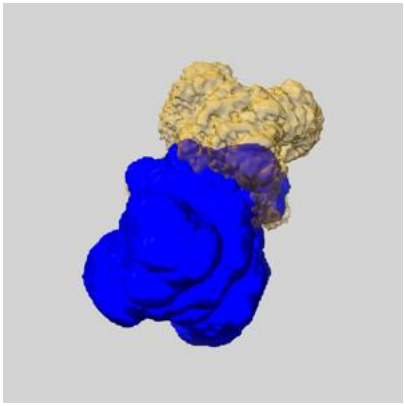
6.6.2 emd_43235_msk_2.map



X



Y

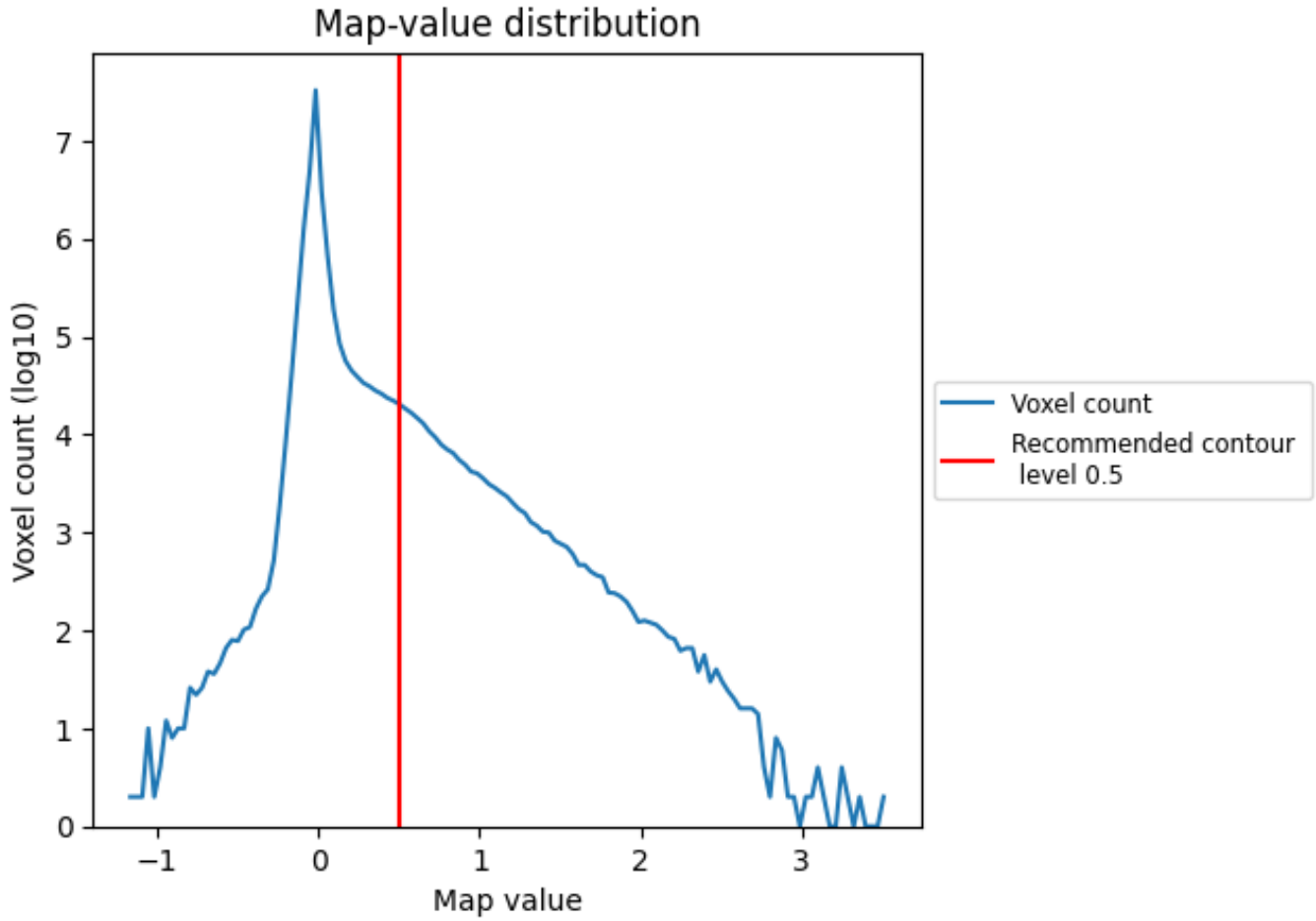


Z

7 Map analysis

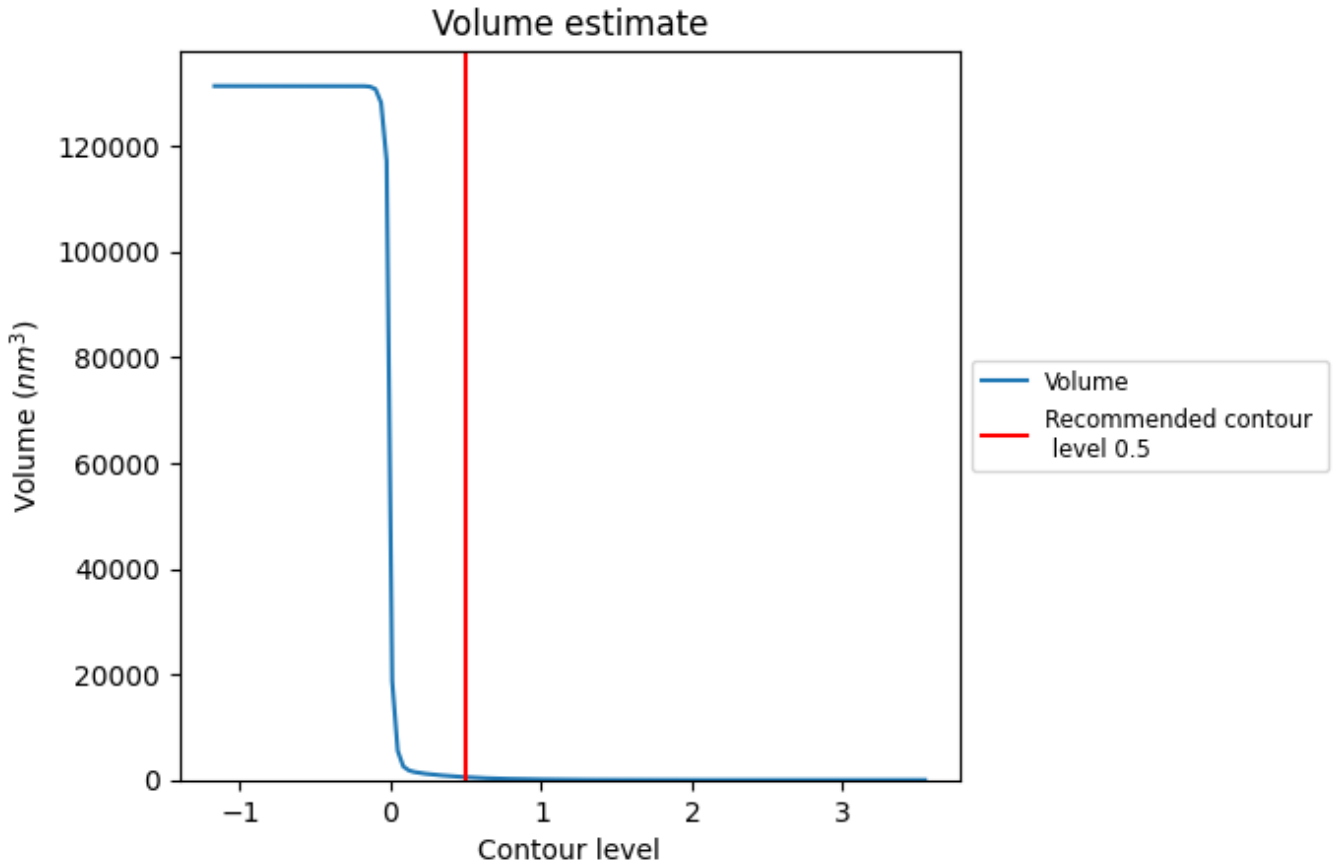
This section contains the results of statistical analysis of the map.

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.

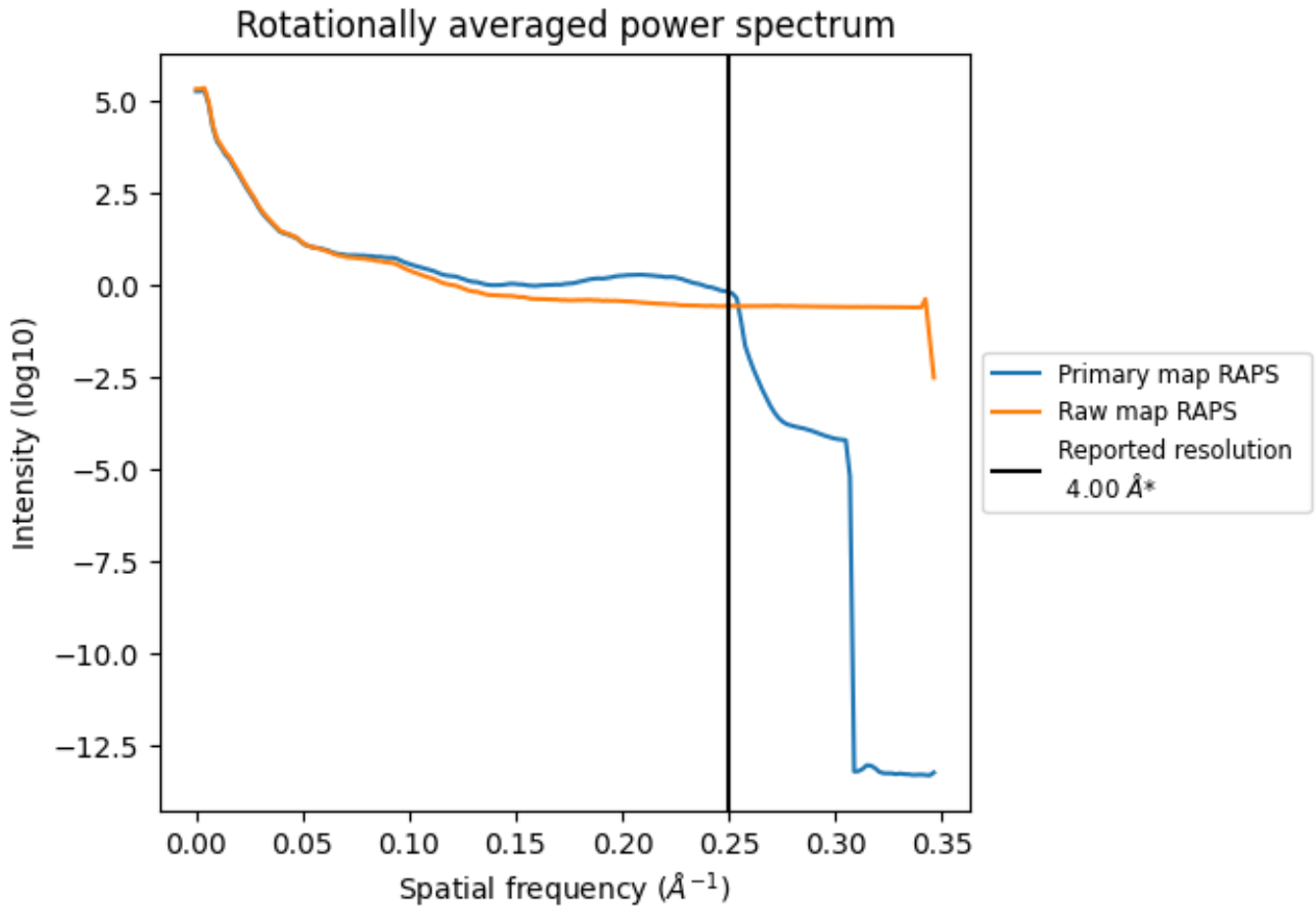
7.2 Volume estimate (i)



The volume at the recommended contour level is 530 nm^3; this corresponds to an approximate mass of 479 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)

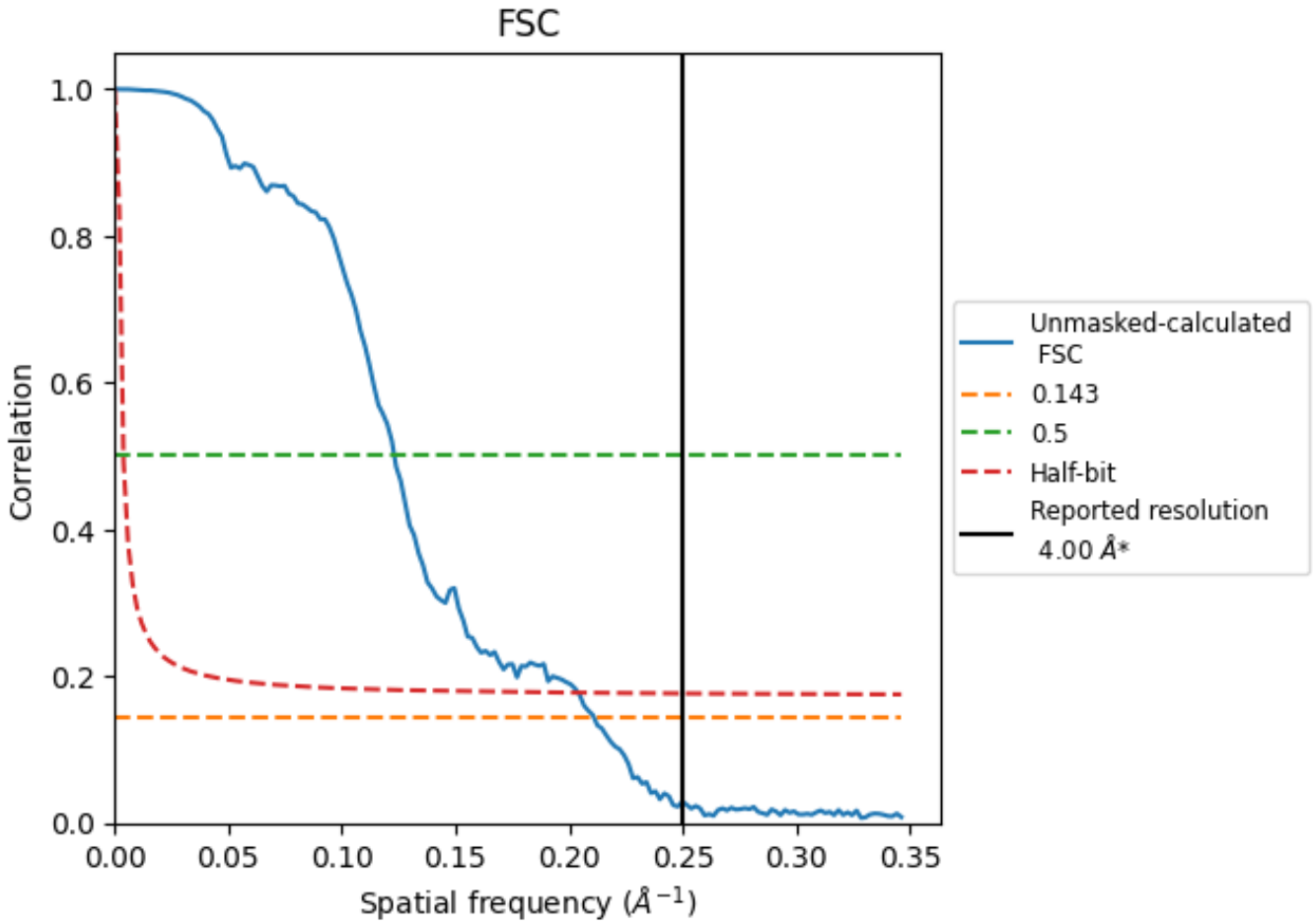


*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

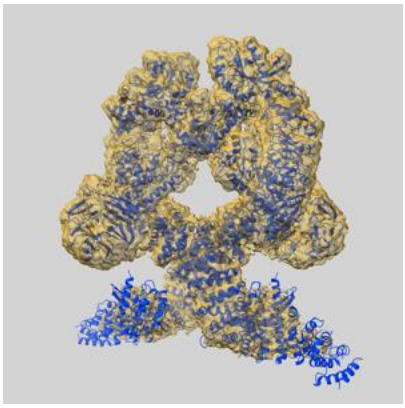
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.74	8.12	4.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.74 differs from the reported value 4.0 by more than 10 %

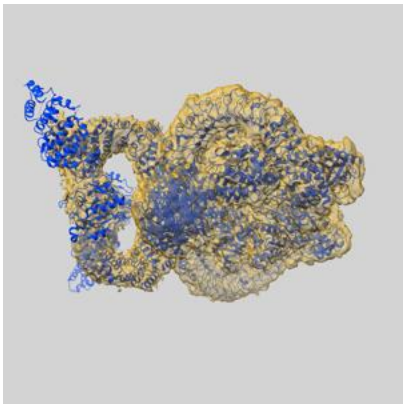
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43235 and PDB model 8VH5. Per-residue inclusion information can be found in section 3 on page 6.

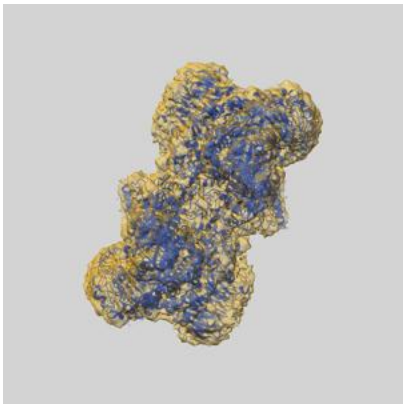
9.1 Map-model overlay



X



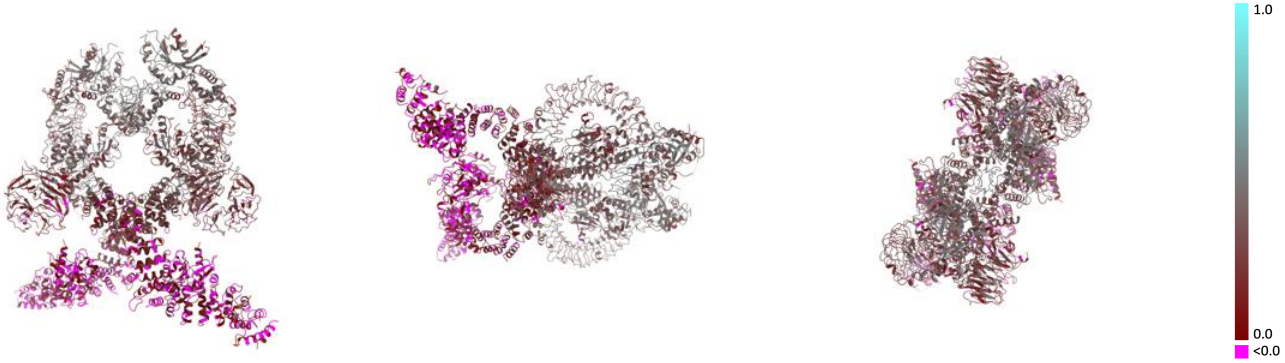
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

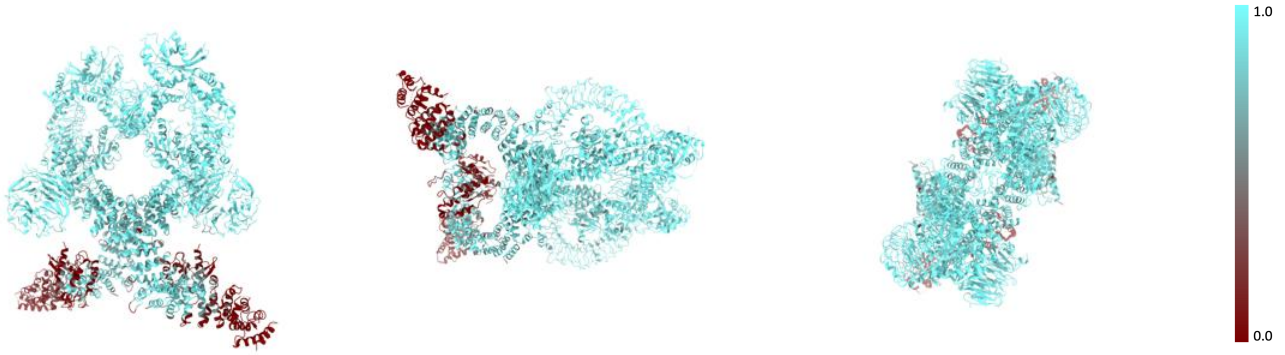
9.2 Q-score mapped to coordinate model



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.

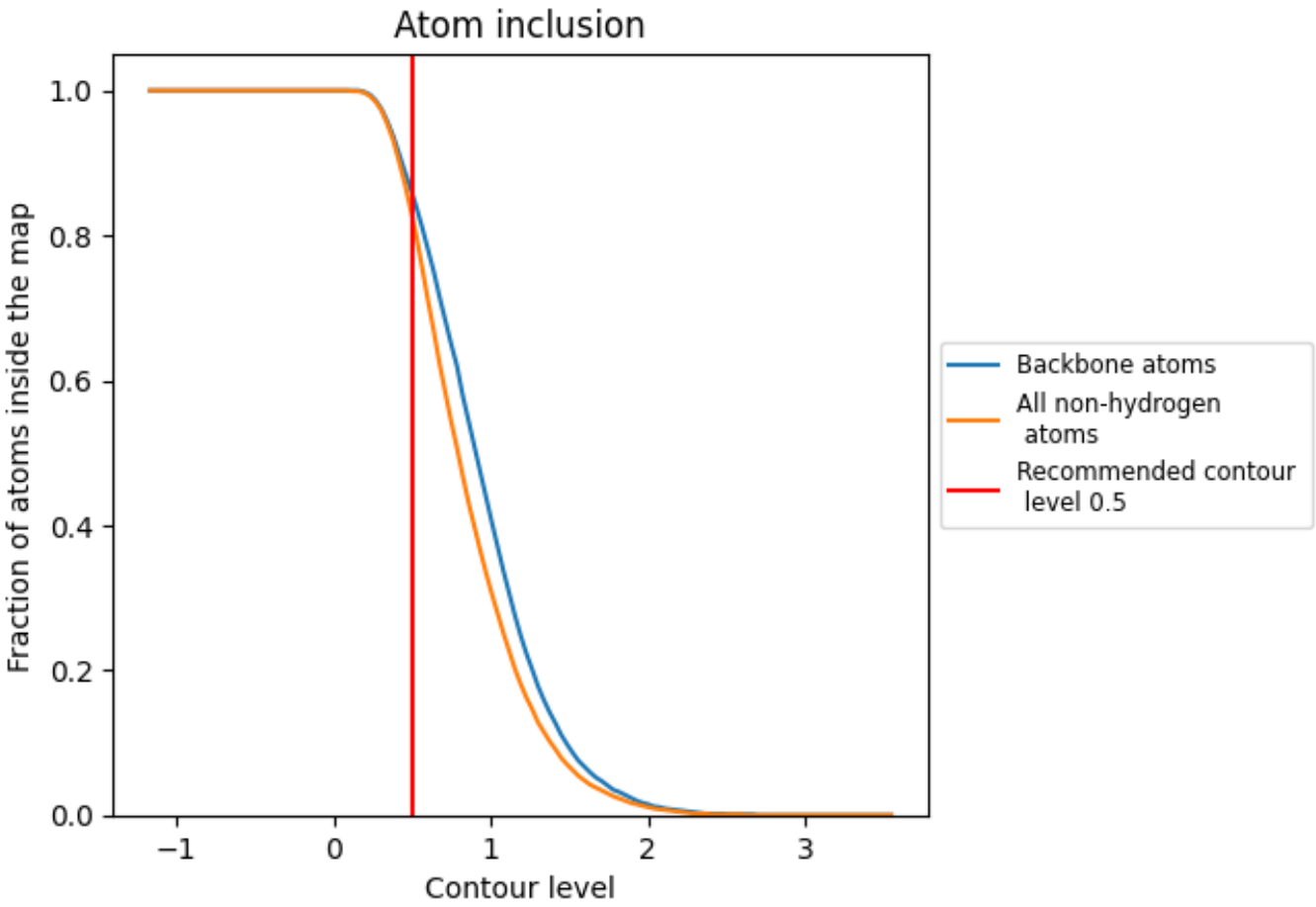
9.3 Atom inclusion mapped to coordinate model



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 86% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.2480
A	0.8600	0.2600
B	0.3670	0.0350
C	0.8650	0.2690
D	0.3400	0.0440