Full wwPDB EM Validation Report (i)

May 18, 2024 – 09:18 pm BST

PDB ID	:	6Z3R
EMDB ID	:	EMD-11063
Title	:	Structure of SMG1-8-9 kinase complex bound to UPF1-LSQ
Authors	:	Langer, L.M.; Gat, Y.; Conti, E.
Deposited on	:	2020-05-21
Resolution	:	2.97 Å(reported)
Based on initial model	:	6SYT

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

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

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

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

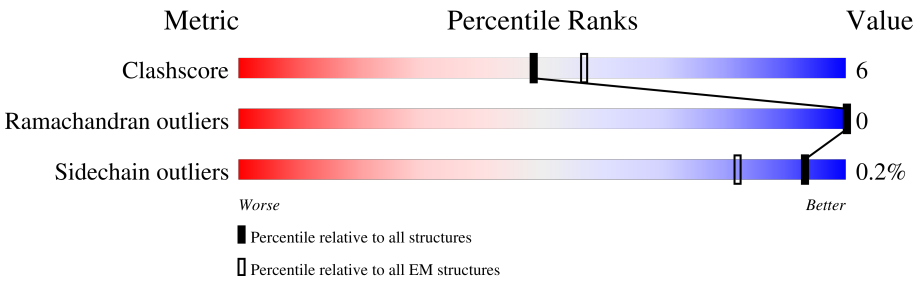
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.97 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	3411	7% 50% 7% 43%
2	B	991	6% 34% • 62%
3	C	520	50% 10% 40%
4	E	11	9% 55% 9% 36%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 36011 atoms, of which 17024 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 Serine/threonine-protein kinase SMG1,Serine/threonine-protein kinase SMG1,SMG1,Serine/threonine-protein kinase SMG1,Serine/threonine-protein kinase SMG1,Serine/threonine-protein kinase SMG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1943	25901	8798	12197	2443	2400	63	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	743	ARG	LYS	conflict	UNP Q96Q15
A	834	LYS	ASN	conflict	UNP Q96Q15
A	1209	SER	ALA	conflict	UNP Q96Q15

- Molecule 2 is a protein called Protein SMG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	376	5218	1770	2500	486	449	13	0	0

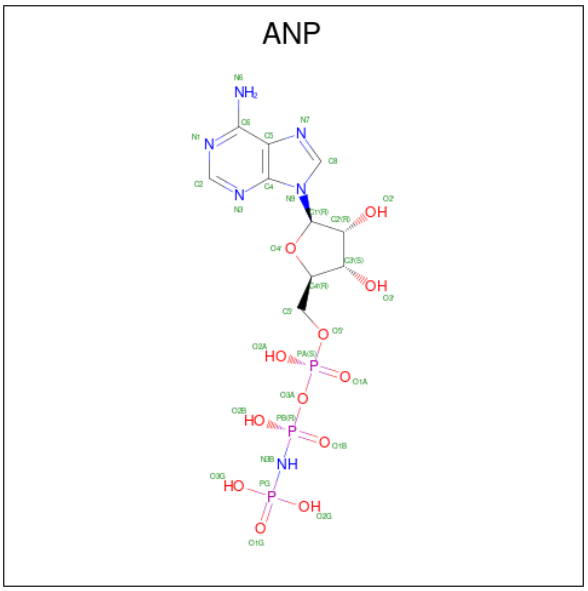
- Molecule 3 is a protein called Protein SMG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	310	4719	1575	2296	417	414	17	0	0

- Molecule 4 is a protein called Regulator of nonsense transcripts 1.

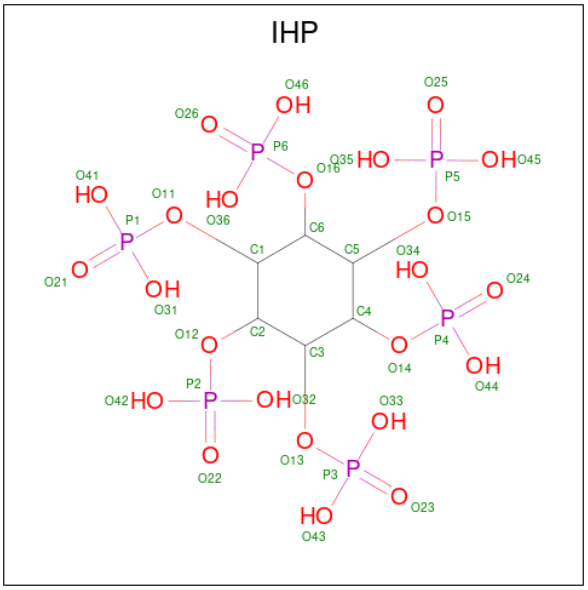
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	7	43	26	8	9	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



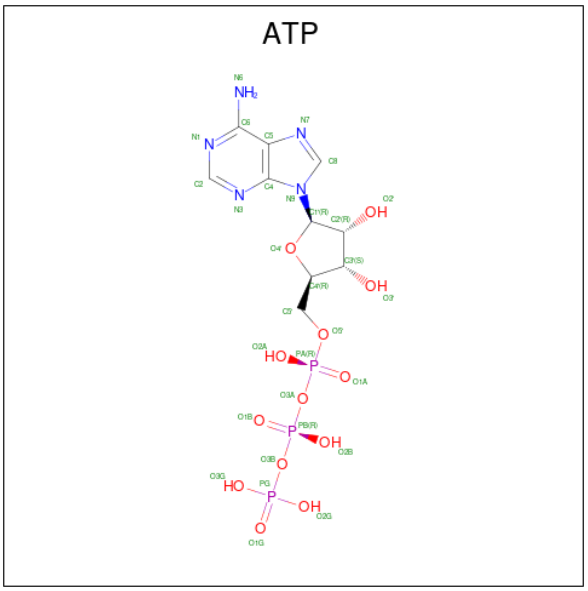
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
5	A	1	44	10	13	6	12	3	0

- Molecule 6 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
6	A	1	42	6	6	24	6	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
7	C	1	43	10	12	5	13	3	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

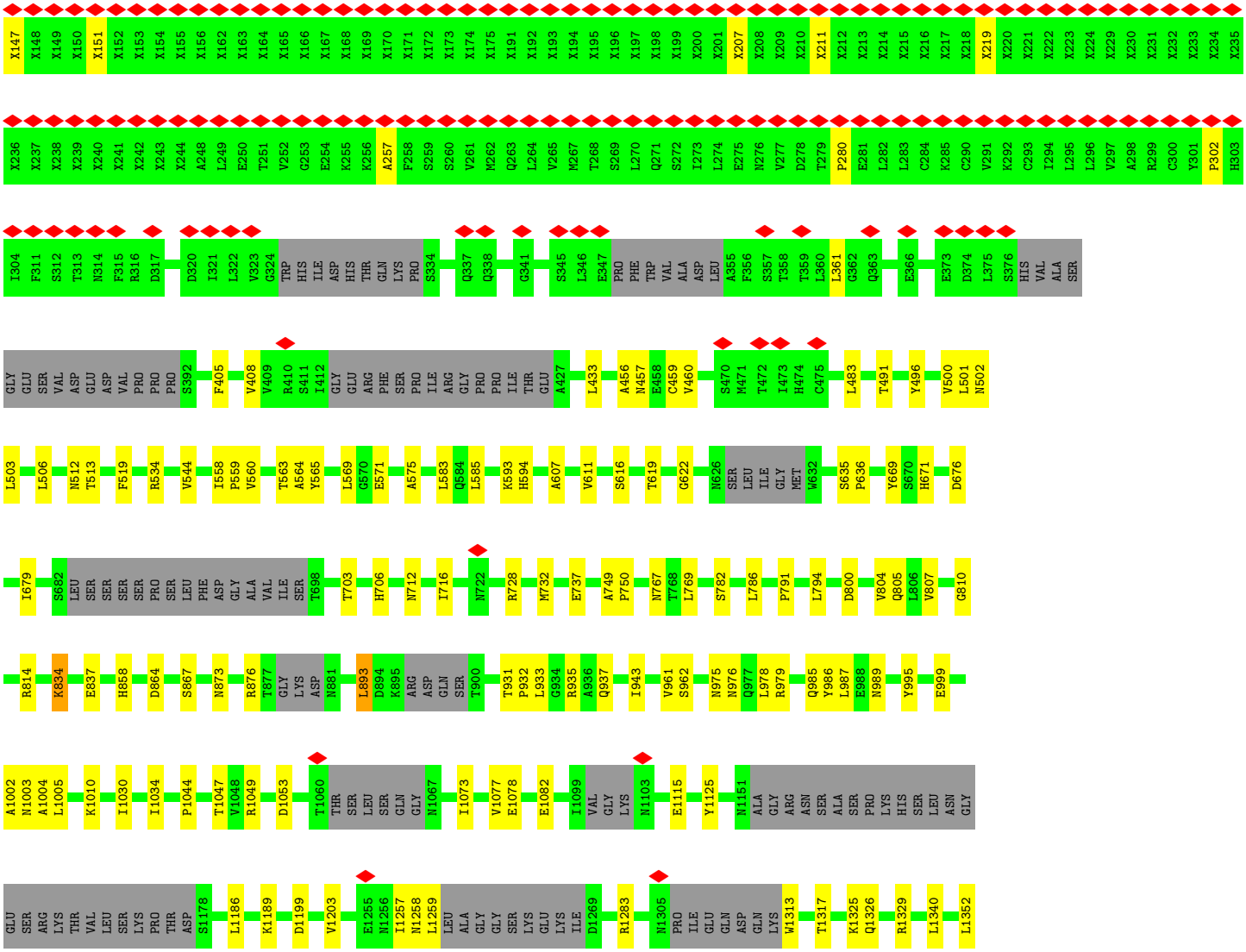
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	C	1	1	1	0

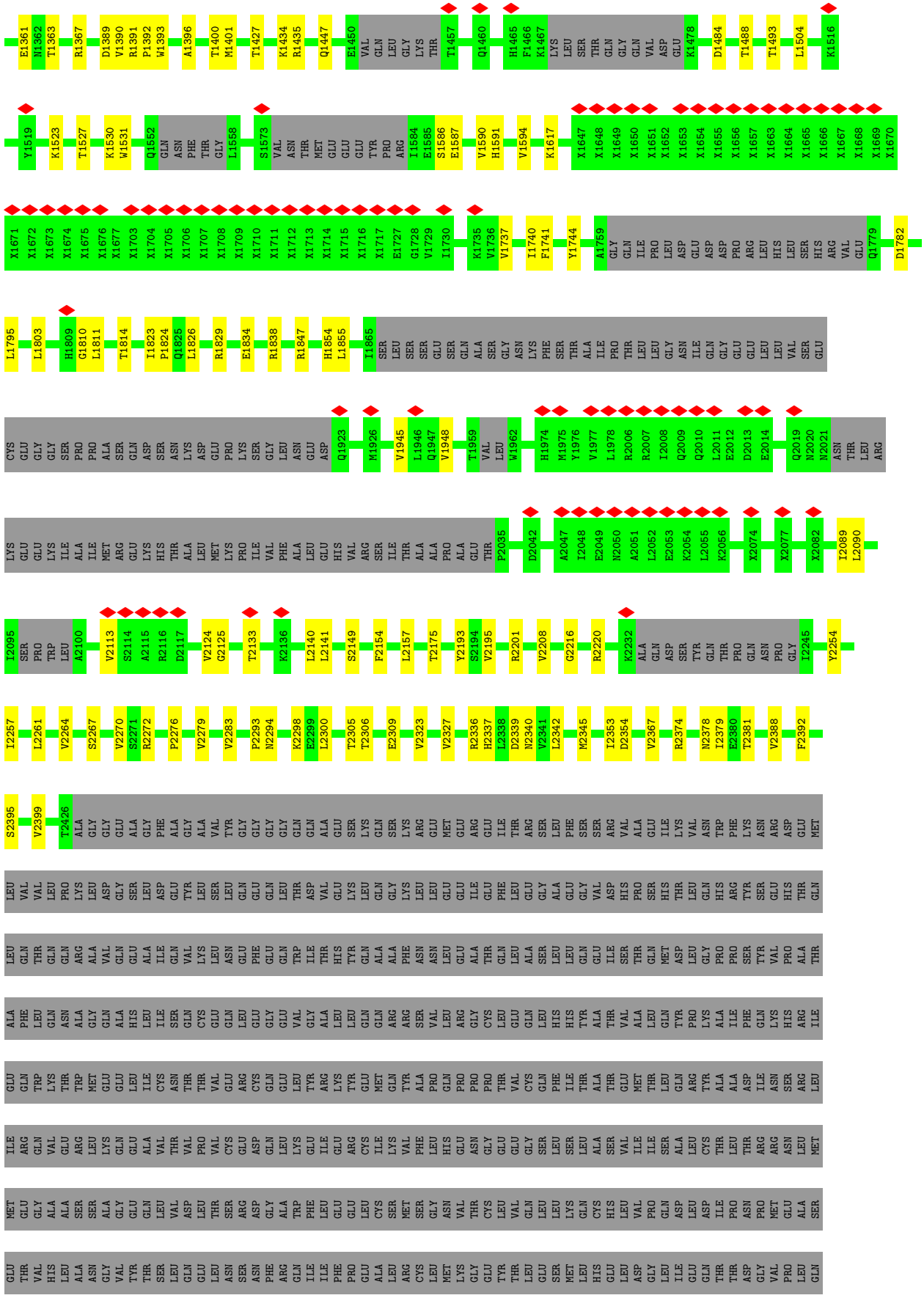
3 Residue-property plots (i)

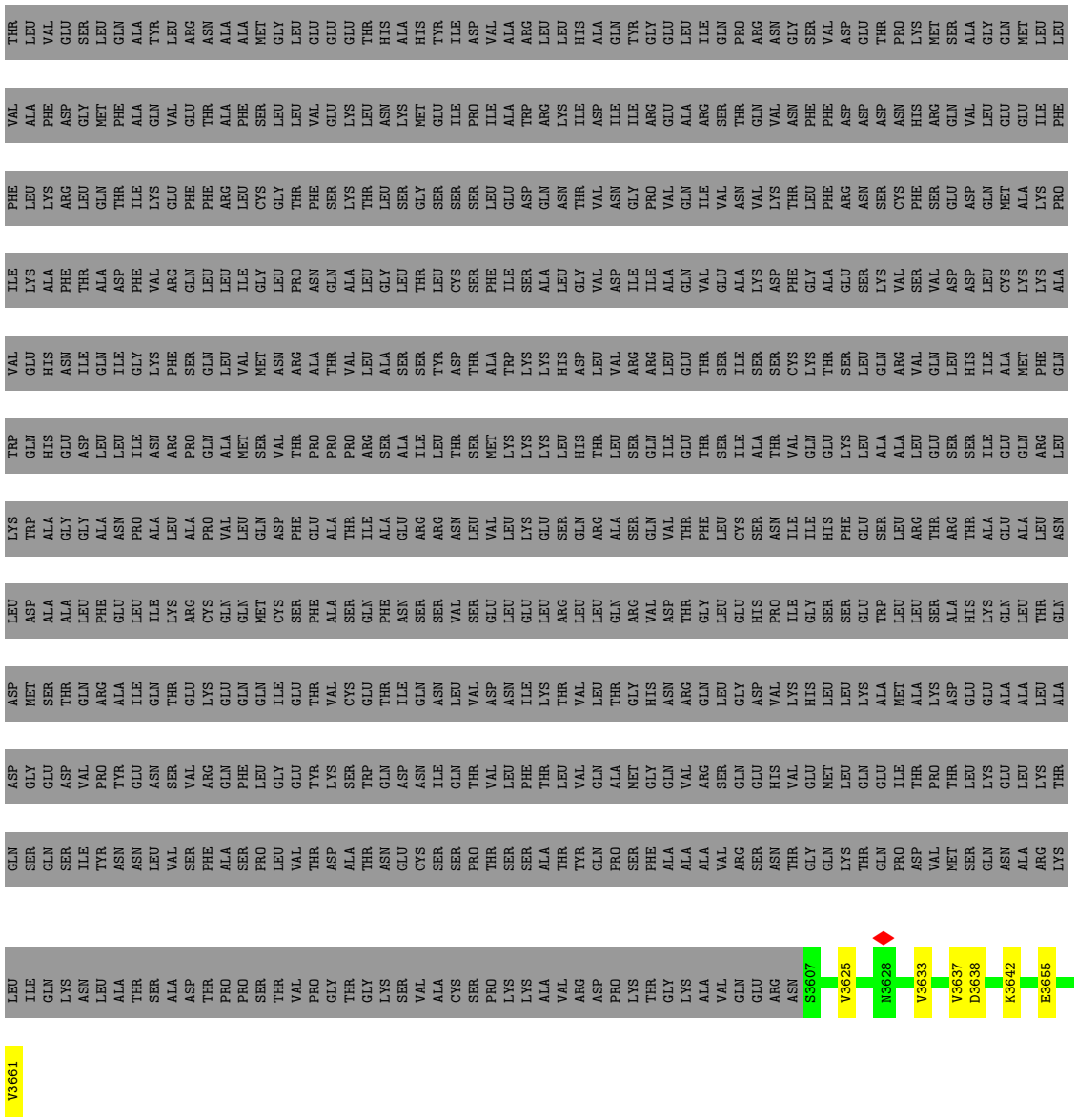
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Serine/threonine-protein kinase SMG1,Serine/threonine-protein kinase SMG1,SMG1,Serine/threonine-protein kinase SMG1,Serine/threonine-protein kinase SMG1,Serine/threonine-protein kinase SMG1

Chain A: 7% 50% 7% 43%

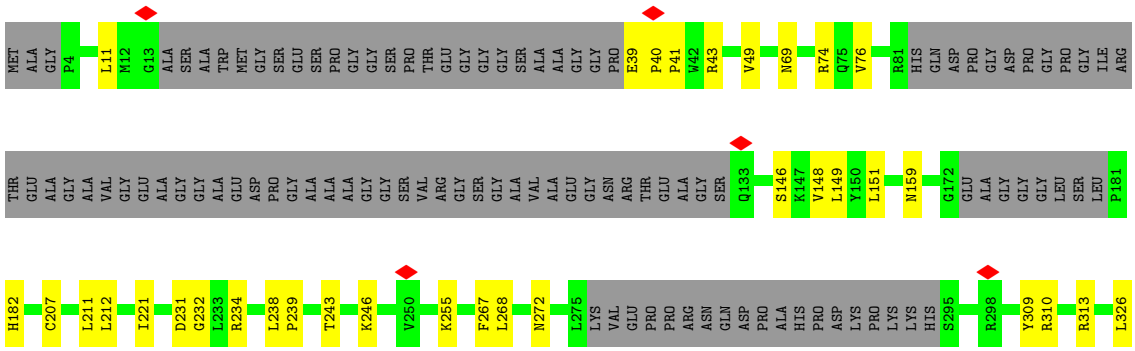


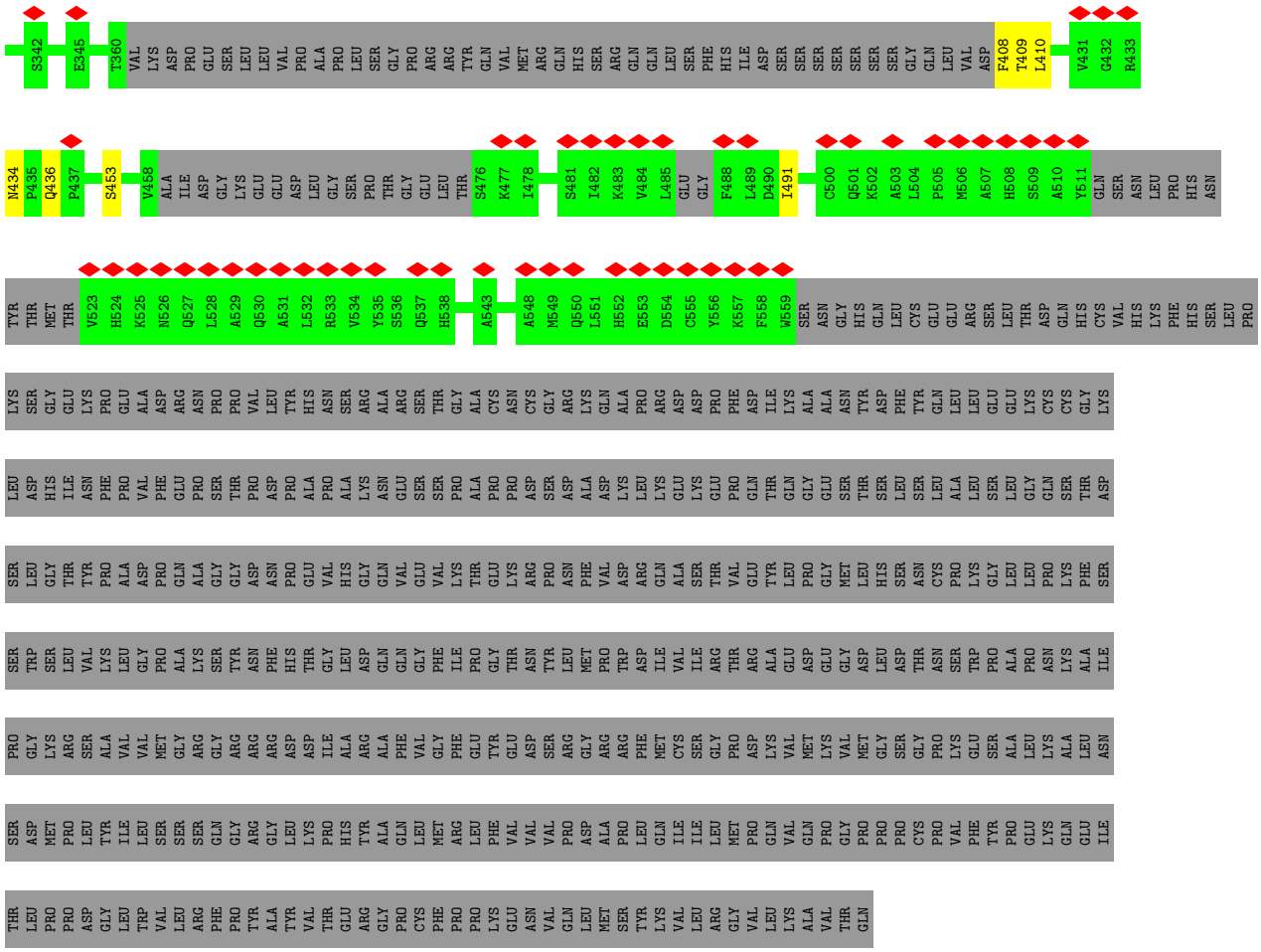

E1361 N1362 T1363 R1367 D1389 V1390 R1391 P1392 W1393 A1396 T1400 M1401 T1427 K1434 R1435 Q1447 E1450 VAL GLN LEU GLY LYS THR T1457 Q1460 H1465 F1466 K1467 LYS LEU SER THR GLN GLY GLN VAL ASP GLU K1478 D1484 T1488 T1493 L1504 K1516
Y1519 K1523 T1527 K1530 W1531 Q1552 GLN ASN PHE THR GLY L1558 S1573 VAL ASN THR MET GLU GLU TYR PRO ARG I1584 E1585 S1586 E1587 V1590 H1591 V1594 K1617 X1647 X1648 X1649 X1650 X1651 X1652 X1653 X1654 X1655 X1656 X1657 X1663 X1664 X1665 X1666 X1667 X1668 X1669 X1670
X1671 X1672 X1673 X1674 X1675 X1676 X1677 X1703 X1704 X1705 X1706 X1707 X1708 X1709 X1710 X1711 X1712 X1713 X1714 X1715 X1716 X1717 E1727 G1728 V1729 I1730 K1735 V1736 V1737 I1740 F1741 Y1744 A1759 GLY GLN ILE PRO LEU ASP GLU ASP ASP PRO ARG LEU HIS LEU SER HIS ARG VAL GLU Q1779 D1782
L1795 L1803 H1809 G1810 L1811 T1814 I1823 P1824 Q1825 L1826 R1829 E1834 R1838 R1847 H1854 L1855 I1865 SER LEU SER SER GLU SER GLN ALA SER GLY ASN LYS PHE SER THR ALA ILE PRO THR LEU LEU LEU GLY ASN ILE GLN GLY GLU GLU LEU LEU VAL SER GLU
CYS GLU GLY GLY SER PRO PRO ALA SER GLN ASP SER ASN LYS ASP GLU PRO LYS SER GLY LEU ASN GLU ASP Q1923 M1926 V1945 L1946 Q1947 V1948 T1959 VAL LEU W1962 H1974 M1975 Y1976 V1977 L1978 R2006 R2007 I2008 Q2009 Q2010 L2011 E2012 D2013 E2014 Q2019 N2020 N2021 ASN THR LEU ARG
LYS GLU GLU LYS ILE ALA ILE MET ARG GLU LYS HIS THR ALA LEU MET LYS PRO ILE VAL PHE ALA LEU GLU HIS VAL ARG SER ILE THR ALA ALA PRO ALA GLU THR P2035 D2042 A2047 I2048 E2049 N2050 A2051 L2052 E2053 K2054 L2055 K2056 X2074 X2077 X2082 I2089 L2090
I2095 SER PRO TRP LEU A2100 V2113 S2114 A2115 R2116 D2117 V2124 G2125 T2133 K2136 L2140 L2141 S2149 F2154 L2157 T2175 Y2193 S2194 V2195 R2201 V2208 G2216 R2220 K2232 ALA GLN ASP SER TYR GLN THR PRO GLN ASN PRO GLY I2245 Y2254
I2257 L2261 V2264 S2267 V2270 S2271 R2272 P2276 V2279 V2283 P2293 N2294 K2298 E2299 L2300 T2305 T2306 E2309 V2323 V2327 R2336 H2337 L2338 D2339 N2340 V2341 L2342 M2345 I2353 D2354 V2367 R2374 N2378 I2379 E2380 T2381 V2388 F2392
S2395 V2399 T2426 ALA GLY GLY GLU ALA GLY PHE ALA GLY ALA VAL TYR GLY GLY GLY GLN GLN ALA GLU SER LYS GLN SER LYS ARG GLU MET GLU ARG GLU ILE THR ARG SER LEU PHE SER SER ARG VAL ALA GLU ILE LYS VAL ASN TRP PHE LYS ASN ARG ASP GLU MET
LEU VAL VAL LEU PRO LYS LEU ASP GLY SER LEU ASP GLU TYR LEU THR ASP VAL GLU LYS LEU GLN GLY LYS LEU LEU GLU GLU ILE GLU PHE LEU GLU GLY VAL ASP HIS PRO SER HIS THR LEU GLN HIS ARG TYR SER GLU HIS THR GLN
LEU GLN THR GLN GLN ARG ALA VAL GLN GLU ALA ILE SER GLN VAL LYS LEU ASN GLU PHE GLU GLN GLN TRP ILE THR HIS TYR GLN ALA ARG PHE ASN ASN LEU GLU ALA THR GLN LEU LEU ALA SER LEU LEU LEU GLN GLU ILE SER THR GLN MET GLU LEU GLN TYR PRO PRO SER TYR VAL PRO ALA THR
ALA PHE LEU GLN ASN ALA GLY GLN ALA HIS LEU ILE SER GLN CYS GLU GLN LEU GLU GLU GLU VAL ALA LEU LEU LEU GLN GLN ARG ARG SER VAL LEU ARG GLY CYS LEU GLU GLN LEU HIS HIS TYR ALA THR VAL ALA LEU GLN TYR PRO LYS ALA ILE PHE GLN LYS HIS ARG ILE
GLU GLN TRP LYS TYR TRP MET GLU GLU LEU ILE CYS ASN THR THR VAL GLU ARG CYS GLN GLU LEU LYS ILE GLU ARG GLY TYR ALA PRO GLN PRO PRO PRO THR VAL CYS GLU GLN PHE ILE THR ALA THR GLU MET THR LEU GLN TYR ARG TYR SER VAL ILE
ILE ARG GLN VAL GLU ARG LEU LYS GLN VAL ALA ASP GLU ALA VAL THR VAL PRO VAL CYS GLU ASP GLN LEU LYS ILE GLU ARG CYS ILE LYS VAL PHE LEU HIS GLU ASN ASN GLY GLU GLU GLY SER LEU SER LEU SER ALA LEU CYS TYR ARG ARG ILE
MET GLU GLY ALA ALA SER SER ALA GLY GLU GLU GLU LEU CYS SER MET SER GLY ASN VAL THR CYS LEU VAL GLN LEU LEU LYS GLN CYS HIS LEU VAL PRO GLN ASP ASP PRO MET GLU ALA SER
GLU THR VAL HIS LEU ALA ASN GLY VAL TYR THR SER LEU GLN GLU LEU ASN SER ASN PHE ARG GLN PHE ILE ILE PHE PRO GLU ALA LEU ARG CYS LEU MET LYS GLY GLU TYR THR LEU GLU SER MET LEU HIS GLU LEU ASP GLY LEU ILE GLU GLN THR THR ASP GLY VAL PRO LEU LEU



• Molecule 2: Protein SMG8

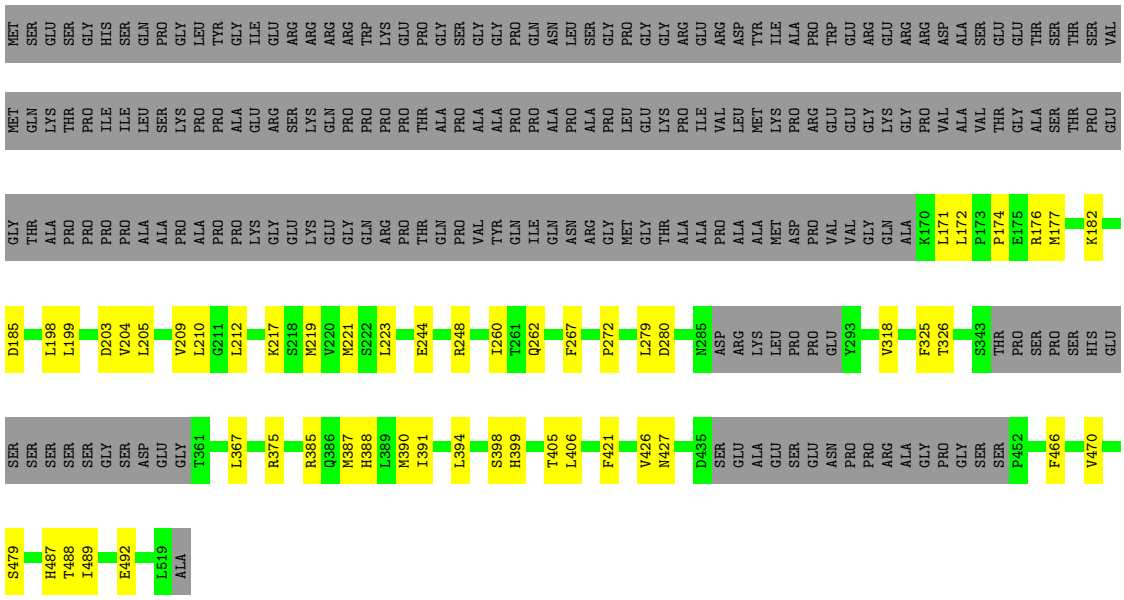
Chain B: 6% 34% • 62%





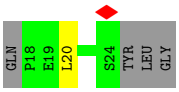
- Molecule 3: Protein SMG9

Chain C: 50% 10% 40%



- Molecule 4: Regulator of nonsense transcripts 1

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	481754	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 ($e^-/Å^2$)	68.75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0312	Depositor
Map size (Å)	350.71997, 350.71997, 350.71997	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.096, 1.096, 1.096	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: ANP, ATP, MG, IHP

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	0.32	0/13304	0.47	2/18167 (0.0%)
2	B	0.30	0/2776	0.46	0/3781
3	C	0.36	0/2481	0.51	0/3368
4	E	0.22	0/42	0.38	0/56
All	All	0.32	0/18603	0.47	2/25372 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	PRO	N-CA-CB	5.60	110.02	103.30
1	A	302	PRO	N-CA-CB	5.55	109.96	103.30

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	13704	12197	12423	160	0
2	B	2718	2500	2505	29	0
3	C	2423	2296	2378	44	0
4	E	43	0	31	1	0
5	A	31	13	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	36	6	6	4	0
7	C	31	12	12	2	0
8	C	1	0	0	0	0
All	All	18987	17024	17368	225	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 6.

All (225) 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:616:SER:O	1:A:619:THR:OG1	1.86	0.91
2:B:434:ASN:O	2:B:436:GLN:NE2	2.06	0.88
1:A:732:MET:SD	1:A:767:ASN:ND2	2.48	0.87
2:B:159:ASN:ND2	3:C:326:THR:OG1	2.08	0.87
3:C:176:ARG:NH1	3:C:262:GLN:OE1	2.09	0.86
1:A:1078:GLU:OE1	1:A:1189:LYS:NZ	2.15	0.79
1:A:1199:ASP:O	1:A:1203:VAL:HG23	1.83	0.78
1:A:1811:LEU:O	1:A:1847:ARG:NH1	2.18	0.75
3:C:198:LEU:HD13	3:C:492:GLU:O	1.87	0.75
1:A:2272:ARG:NH2	1:A:3655:GLU:OE2	2.21	0.74
2:B:69:ASN:OD1	2:B:76:VAL:N	2.21	0.73
1:A:867:SER:OG	1:A:873:ASN:O	2.03	0.73
2:B:272:ASN:OD1	3:C:375:ARG:NH2	2.22	0.72
1:A:361:LEU:HD22	1:A:405:PHE:CE1	2.23	0.72
1:A:669:TYR:OH	1:A:737:GLU:OE1	2.07	0.71
1:A:405:PHE:HZ	1:A:433:LEU:HD21	1.53	0.71
2:B:246:LYS:O	2:B:255:LYS:NZ	2.15	0.71
2:B:231:ASP:OD1	2:B:232:GLY:N	2.23	0.70
1:A:1401:MET:SD	1:A:1447:GLN:NE2	2.65	0.70
1:A:2141:LEU:HD11	1:A:2149:SER:OG	1.92	0.68
1:A:1326:GLN:OE1	1:A:1329:ARG:NH1	2.27	0.68
3:C:367:LEU:O	3:C:427:ASN:ND2	2.27	0.68
1:A:2388:VAL:HG22	1:A:2388:VAL:O	1.94	0.67
1:A:1587:GLU:O	1:A:1591:HIS:N	2.29	0.66
1:A:1782:ASP:HB2	1:A:2175:THR:CG2	2.26	0.64
3:C:487:HIS:O	3:C:488:THR:OG1	2.15	0.64
1:A:2388:VAL:HG23	1:A:2392:PHE:CD2	2.33	0.64
3:C:325:PHE:CE2	3:C:326:THR:HG23	2.34	0.63
3:C:209:VAL:C	3:C:210:LEU:HD12	2.20	0.62
1:A:512:ASN:O	1:A:513:THR:OG1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1325:LYS:NZ	1:A:1361:GLU:OE1	2.34	0.61
1:A:491:THR:O	2:B:74:ARG:NH1	2.33	0.61
1:A:807:VAL:HG13	1:A:807:VAL:O	2.00	0.61
3:C:209:VAL:O	3:C:210:LEU:HD12	2.01	0.60
3:C:212:LEU:O	3:C:217:LYS:NZ	2.34	0.60
1:A:2279:VAL:O	1:A:2283:VAL:HG23	2.02	0.59
3:C:406:LEU:O	3:C:406:LEU:HD23	2.03	0.59
1:A:703:THR:HG22	1:A:706:HIS:CE1	2.38	0.58
1:A:501:LEU:HD13	1:A:544:VAL:HG23	1.84	0.58
1:A:2276:PRO:HB2	1:A:2279:VAL:HG23	1.85	0.58
1:A:583:LEU:HD11	1:A:585:LEU:HD12	1.84	0.58
1:A:1352:LEU:HD11	1:A:1392:PRO:HB3	1.86	0.58
2:B:39:GLU:O	2:B:43:ARG:N	2.37	0.57
3:C:326:THR:HG21	3:C:390:MET:CE	2.35	0.57
1:A:1073:ILE:O	1:A:1077:VAL:HG23	2.04	0.57
1:A:2157:LEU:HA	1:A:2201:ARG:HB3	1.86	0.57
1:A:1782:ASP:HB2	1:A:2175:THR:HG23	1.87	0.56
2:B:211:LEU:HD12	2:B:268:LEU:HD13	1.87	0.56
3:C:466:PHE:O	3:C:470:VAL:HG23	2.05	0.56
1:A:1810:GLY:O	1:A:1814:THR:HG23	2.06	0.56
1:A:2340:ASN:ND2	1:A:2354:ASP:HB2	2.19	0.56
1:A:728:ARG:NH1	1:A:767:ASN:OD1	2.39	0.56
1:A:1834:GLU:O	1:A:1838:ARG:NH1	2.39	0.56
1:A:3633:VAL:O	1:A:3637:VAL:HG23	2.06	0.55
2:B:146:SER:OG	2:B:148:VAL:HG12	2.06	0.55
1:A:1617:LYS:NZ	6:A:3702:IHP:O34	2.29	0.55
1:A:1393:TRP:CH2	1:A:1427:THR:HG21	2.42	0.54
1:A:1493:THR:O	1:A:1493:THR:HG22	2.07	0.54
1:A:1740:ILE:HG23	1:A:1741:PHE:CD1	2.43	0.54
1:A:769:LEU:HD23	1:A:769:LEU:O	2.07	0.54
2:B:408:PHE:O	2:B:409:THR:OG1	2.25	0.54
1:A:2293:PRO:HB2	1:A:2381:THR:HG21	1.90	0.54
1:A:1044:PRO:O	1:A:1047:THR:HG22	2.07	0.54
2:B:234:ARG:O	2:B:238:LEU:N	2.41	0.54
1:A:361:LEU:HD22	1:A:405:PHE:CD1	2.43	0.54
1:A:2339:ASP:OD2	4:E:20:LEU:HD12	2.08	0.53
1:A:2089:ILE:C	1:A:2090:LEU:HD12	2.27	0.53
1:A:2254:TYR:HA	1:A:2257:ILE:HG22	1.90	0.53
1:A:405:PHE:HD2	1:A:459:CYS:HG	1.55	0.53
1:A:1257:ILE:HD12	1:A:1257:ILE:H	1.74	0.53
1:A:1737:VAL:HA	1:A:1740:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1744:TYR:HD1	1:A:1795:LEU:HD21	1.72	0.52
1:A:1803:LEU:HD12	1:A:1803:LEU:O	2.09	0.52
3:C:388:HIS:HD2	3:C:426:VAL:HG22	1.74	0.52
1:A:2305:THR:OG1	1:A:2309:GLU:OE1	2.19	0.52
2:B:326:LEU:HD23	2:B:326:LEU:H	1.73	0.52
1:A:1363:THR:O	1:A:1367:ARG:N	2.42	0.52
1:A:1258:ASN:O	1:A:1259:LEU:HD22	2.09	0.52
2:B:310:ARG:NH1	3:C:280:ASP:OD1	2.42	0.52
3:C:326:THR:HG21	3:C:390:MET:HE1	1.91	0.52
1:A:995:TYR:CZ	1:A:999:GLU:HG2	2.45	0.52
1:A:1389:ASP:OD2	1:A:1391:ARG:NE	2.36	0.52
1:A:2089:ILE:O	1:A:2090:LEU:HD12	2.10	0.52
1:A:2367:VAL:HG13	1:A:2367:VAL:O	2.10	0.52
1:A:496:TYR:O	1:A:500:VAL:HG23	2.09	0.51
1:A:995:TYR:CE2	1:A:2298:LYS:HG2	2.45	0.51
1:A:834:LYS:O	1:A:834:LYS:HG3	2.09	0.51
1:A:2379:ILE:O	1:A:2379:ILE:HG22	2.11	0.51
6:A:3702:IHP:H5	6:A:3702:IHP:O26	2.11	0.51
1:A:2342:LEU:HD11	1:A:2353:ILE:HD11	1.91	0.51
1:A:534:ARG:NH2	1:A:571:GLU:OE2	2.44	0.50
1:A:2261:LEU:O	1:A:2264:VAL:HG12	2.12	0.50
1:A:3625:VAL:HG13	1:A:3625:VAL:O	2.12	0.50
1:A:3638:ASP:OD2	1:A:3642:LYS:NZ	2.23	0.50
1:A:502:ASN:O	1:A:506:LEU:HD23	2.12	0.49
2:B:40:PRO:N	2:B:41:PRO:HD2	2.27	0.49
1:A:893:LEU:HD13	3:C:479:SER:HB2	1.95	0.49
1:A:1002:ALA:O	1:A:1003:ASN:HB2	2.12	0.49
1:A:2300:LEU:HD23	1:A:2345:MET:SD	2.52	0.49
2:B:221:ILE:HD11	3:C:279:LEU:CD2	2.42	0.49
3:C:209:VAL:HG12	3:C:210:LEU:N	2.26	0.49
1:A:2140:LEU:HD21	1:A:2154:PHE:CE1	2.48	0.49
1:A:1049:ARG:NH1	1:A:1053:ASP:OD2	2.46	0.49
1:A:1258:ASN:C	1:A:1259:LEU:HD22	2.33	0.48
1:A:864:ASP:OD2	1:A:876:ARG:NE	2.47	0.48
1:A:1389:ASP:OD1	1:A:1389:ASP:N	2.46	0.48
1:A:219:UNK:HA	1:A:257:ALA:HB1	1.95	0.48
3:C:171:LEU:HD12	3:C:171:LEU:O	2.14	0.48
1:A:2337:HIS:ND1	1:A:2339:ASP:HB2	2.29	0.48
1:A:943:ILE:HG21	1:A:987:LEU:HD21	1.96	0.48
1:A:2276:PRO:HB2	1:A:2279:VAL:CG2	2.45	0.47
1:A:935:ARG:NH2	1:A:937:GLN:OE1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:TRP:O	1:A:1317:THR:OG1	2.33	0.47
1:A:1504:LEU:HD12	1:A:1531:TRP:CZ3	2.49	0.47
1:A:1586:SER:O	1:A:1590:VAL:HG22	2.14	0.47
1:A:676:ASP:O	1:A:679:ILE:HG12	2.14	0.47
3:C:204:VAL:HG22	3:C:205:LEU:N	2.30	0.47
1:A:207:UNK:O	1:A:211:UNK:N	2.48	0.47
1:A:560:VAL:O	1:A:560:VAL:HG22	2.14	0.47
3:C:174:PRO:HG3	3:C:199:LEU:HD11	1.97	0.47
1:A:405:PHE:O	1:A:408:VAL:HG12	2.15	0.47
1:A:1115:GLU:O	1:A:1435:ARG:NE	2.42	0.47
1:A:1078:GLU:O	1:A:1082:GLU:HG3	2.15	0.46
3:C:210:LEU:HD13	3:C:318:VAL:CG1	2.46	0.46
2:B:49:VAL:CG2	2:B:207:CYS:HA	2.45	0.46
3:C:177:MET:SD	3:C:260:ILE:HG22	2.55	0.46
2:B:211:LEU:N	2:B:211:LEU:HD23	2.30	0.46
1:A:1823:ILE:HA	1:A:1826:LEU:HD12	1.97	0.46
1:A:805:GLN:OE1	1:A:805:GLN:HA	2.16	0.46
1:A:995:TYR:OH	1:A:999:GLU:HG2	2.15	0.46
1:A:810:GLY:O	1:A:814:ARG:NH1	2.49	0.45
1:A:1434:LYS:NZ	6:A:3702:IHP:O11	2.49	0.45
1:A:457:ASN:OD1	1:A:503:LEU:HD22	2.17	0.45
1:A:622:GLY:O	1:A:671:HIS:ND1	2.41	0.45
1:A:867:SER:HB2	3:C:171:LEU:HD11	1.98	0.45
2:B:409:THR:HG22	2:B:410:LEU:N	2.30	0.45
3:C:390:MET:O	3:C:394:LEU:HD12	2.16	0.45
1:A:782:SER:O	1:A:786:LEU:HD23	2.16	0.45
1:A:858:HIS:NE2	3:C:203:ASP:OD1	2.49	0.45
2:B:491:ILE:HD12	2:B:491:ILE:H	1.82	0.45
1:A:976:ASN:OD1	1:A:979:ARG:NH2	2.37	0.45
1:A:2378:ASN:HD22	1:A:3661:VAL:HG23	1.80	0.45
1:A:483:LEU:HD21	1:A:519:PHE:HE1	1.82	0.45
1:A:563:THR:HG23	1:A:564:ALA:N	2.31	0.45
1:A:1484:ASP:O	1:A:1488:THR:HG23	2.16	0.45
1:A:786:LEU:HG	1:A:786:LEU:O	2.18	0.44
1:A:1829:ARG:O	1:A:1829:ARG:HG3	2.18	0.44
1:A:2378:ASN:ND2	1:A:3661:VAL:HG23	2.31	0.44
1:A:749:ALA:N	1:A:750:PRO:HD2	2.32	0.44
1:A:1945:VAL:O	1:A:1948:VAL:HG12	2.17	0.44
3:C:221:MET:HE3	3:C:267:PHE:HD1	1.82	0.44
1:A:1010:LYS:HB3	1:A:1010:LYS:HE3	1.74	0.44
2:B:309:TYR:OH	2:B:313:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:LYS:NZ	6:A:3702:IHP:O25	2.49	0.44
1:A:1030:ILE:O	1:A:1034:ILE:HG12	2.18	0.44
3:C:272:PRO:HD3	7:C:601:ATP:O3G	2.18	0.44
1:A:712:ASN:OD1	1:A:716:ILE:HD11	2.17	0.44
1:A:933:LEU:O	1:A:933:LEU:HD23	2.17	0.44
2:B:211:LEU:HD23	2:B:211:LEU:H	1.83	0.44
1:A:995:TYR:CZ	1:A:2298:LYS:HG2	2.53	0.44
3:C:244:GLU:O	3:C:248:ARG:NE	2.51	0.44
1:A:2323:VAL:O	1:A:2327:VAL:HG23	2.18	0.43
1:A:405:PHE:CZ	1:A:433:LEU:HD21	2.43	0.43
1:A:593:LYS:HG2	1:A:594:HIS:H	1.83	0.43
2:B:212:LEU:HD11	2:B:267:PHE:HD1	1.82	0.43
2:B:212:LEU:HD12	2:B:212:LEU:O	2.19	0.43
3:C:388:HIS:CD2	3:C:426:VAL:HG22	2.53	0.43
3:C:398:SER:O	3:C:399:HIS:HB2	2.18	0.43
1:A:985:GLN:HE22	1:A:2306:THR:HA	1.84	0.43
1:A:2195:VAL:HG23	1:A:2195:VAL:O	2.18	0.43
1:A:2374:ARG:NH2	1:A:3661:VAL:O	2.49	0.43
1:A:593:LYS:HG2	1:A:594:HIS:N	2.33	0.43
3:C:219:MET:O	3:C:223:LEU:HD13	2.18	0.43
1:A:1396:ALA:O	1:A:1400:THR:OG1	2.30	0.43
1:A:931:THR:HB	1:A:932:PRO:HD2	2.00	0.43
1:A:2208:VAL:HG23	1:A:2208:VAL:O	2.18	0.43
2:B:221:ILE:HD11	3:C:279:LEU:HD22	1.99	0.43
3:C:387:MET:O	3:C:391:ILE:HG12	2.19	0.43
3:C:182:LYS:HD3	3:C:185:ASP:HA	2.01	0.43
3:C:405:THR:HG22	3:C:406:LEU:N	2.34	0.42
1:A:147:UNK:O	1:A:151:UNK:N	2.51	0.42
1:A:1854:HIS:CD2	1:A:1855:LEU:HD22	2.53	0.42
1:A:2124:VAL:HG12	1:A:2125:GLY:N	2.33	0.42
1:A:2133:THR:O	5:A:3701:ANP:O2A	2.37	0.42
2:B:11:LEU:HD13	2:B:453:SER:HA	2.01	0.42
3:C:172:LEU:HD23	3:C:172:LEU:H	1.84	0.42
1:A:1855:LEU:HD11	1:A:2113:VAL:HA	2.01	0.42
1:A:558:ILE:N	1:A:559:PRO:CD	2.82	0.42
1:A:1523:LYS:O	1:A:1527:THR:HG23	2.20	0.42
1:A:2193:TYR:OH	1:A:2353:ILE:O	2.37	0.42
1:A:2395:SER:O	1:A:2399:VAL:HG23	2.18	0.42
3:C:385:ARG:NH1	3:C:421:PHE:O	2.53	0.42
1:A:975:ASN:O	1:A:979:ARG:HG3	2.18	0.42
1:A:1590:VAL:O	1:A:1594:VAL:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:209:VAL:HG21	3:C:221:MET:SD	2.60	0.42
1:A:575:ALA:HB1	1:A:607:ALA:HB1	2.02	0.42
1:A:635:SER:CB	1:A:636:PRO:CD	2.97	0.42
1:A:2294:ASN:O	1:A:2298:LYS:HB3	2.18	0.42
2:B:182:HIS:CG	2:B:182:HIS:O	2.72	0.42
3:C:325:PHE:CD2	3:C:326:THR:HG23	2.55	0.42
1:A:2216:GLY:O	1:A:2220:ARG:HG2	2.20	0.41
1:A:607:ALA:O	1:A:611:VAL:HG23	2.20	0.41
1:A:800:ASP:O	1:A:804:VAL:HG23	2.21	0.41
1:A:565:TYR:O	1:A:569:LEU:HG	2.20	0.41
1:A:2264:VAL:HG22	1:A:2264:VAL:O	2.20	0.41
1:A:456:ALA:O	1:A:460:VAL:HG23	2.21	0.41
1:A:893:LEU:HD12	1:A:893:LEU:HA	1.91	0.41
2:B:149:LEU:HD21	2:B:151:LEU:CD2	2.50	0.41
3:C:405:THR:O	3:C:427:ASN:HB3	2.20	0.41
3:C:488:THR:HG22	3:C:489:ILE:N	2.36	0.41
1:A:961:VAL:HG12	1:A:962:SER:N	2.36	0.41
1:A:1125:TYR:CD1	1:A:1186:LEU:HD22	2.55	0.41
1:A:2337:HIS:CE1	1:A:2339:ASP:HB2	2.56	0.41
1:A:978:LEU:HD12	1:A:1340:LEU:HD22	2.03	0.41
1:A:1390:VAL:O	1:A:1390:VAL:HG22	2.20	0.41
1:A:1823:ILE:HB	1:A:1824:PRO:HD3	2.03	0.40
1:A:804:VAL:HG21	1:A:837:GLU:HB3	2.03	0.40
1:A:1004:ALA:O	1:A:1005:LEU:HD12	2.20	0.40
1:A:2267:SER:O	1:A:2270:VAL:HG23	2.21	0.40
1:A:2336:ARG:NH2	1:A:2354:ASP:O	2.54	0.40
1:A:1125:TYR:HD1	1:A:1186:LEU:HD22	1.87	0.40
1:A:791:PRO:HD2	1:A:794:LEU:HD12	2.04	0.40
1:A:986:TYR:O	1:A:989:ASN:OD1	2.39	0.40
2:B:239:PRO:O	2:B:243:THR:HG23	2.22	0.40
3:C:219:MET:HB2	7:C:601:ATP:O2A	2.21	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	1754/3411 (51%)	1660 (95%)	94 (5%)	0	100	100
2	B	358/991 (36%)	335 (94%)	23 (6%)	0	100	100
3	C	302/520 (58%)	274 (91%)	28 (9%)	0	100	100
4	E	5/11 (46%)	5 (100%)	0	0	100	100
All	All	2419/4933 (49%)	2274 (94%)	145 (6%)	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	1200/2895 (42%)	1197 (100%)	3 (0%)	92	97
2	B	240/847 (28%)	240 (100%)	0	100	100
3	C	254/450 (56%)	254 (100%)	0	100	100
4	E	3/10 (30%)	3 (100%)	0	100	100
All	All	1697/4202 (40%)	1694 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	834	LYS
1	A	893	LEU
1	A	1283	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	600	HIS
1	A	706	HIS

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Mol	Chain	Res	Type
1	A	815	GLN
1	A	881	ASN
1	A	985	GLN
1	A	1050	HIS
1	A	1314	GLN
1	A	1758	ASN
1	A	2189	HIS
1	A	2192	HIS
1	A	3628	ASN
2	B	159	ASN
2	B	208	HIS
3	C	213	GLN
3	C	297	HIS
3	C	393	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\|Z\| > 2$
7	ATP	C	601	8	26,33,33	0.72	0	31,52,52	0.81	1 (3%)
6	IHP	A	3702	-	36,36,36	1.49	6 (16%)	54,60,60	1.98	10 (18%)
5	ANP	A	3701	-	29,33,33	1.20	5 (17%)	31,52,52	1.10	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
7	ATP	C	601	8	-	7/18/38/38	0/3/3/3
6	IHP	A	3702	-	-	8/30/54/54	0/1/1/1
5	ANP	A	3701	-	-	7/14/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3701	ANP	PG-O1G	3.27	1.51	1.46
6	A	3702	IHP	P5-O15	3.17	1.65	1.59
6	A	3702	IHP	P3-O13	3.14	1.65	1.59
6	A	3702	IHP	P4-O14	3.12	1.65	1.59
6	A	3702	IHP	P2-O12	3.10	1.65	1.59
6	A	3702	IHP	P6-O16	3.04	1.65	1.59
6	A	3702	IHP	P1-O11	2.97	1.64	1.59
5	A	3701	ANP	PB-O1B	2.92	1.50	1.46
5	A	3701	ANP	PB-O2B	-2.19	1.50	1.56
5	A	3701	ANP	PG-O3G	-2.04	1.51	1.56
5	A	3701	ANP	PG-O2G	-2.01	1.51	1.56

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	3702	IHP	O14-C4-C3	5.47	121.58	108.69
6	A	3702	IHP	O14-C4-C5	5.41	121.44	108.69
6	A	3702	IHP	O15-C5-C6	5.25	121.06	108.69
6	A	3702	IHP	O13-C3-C4	5.12	120.75	108.69
6	A	3702	IHP	O15-C5-C4	4.99	120.45	108.69
6	A	3702	IHP	O13-C3-C2	4.45	119.17	108.69
5	A	3701	ANP	O2B-PB-O1B	4.11	118.54	109.92
6	A	3702	IHP	C4-C3-C2	3.85	118.84	110.41
6	A	3702	IHP	C6-C5-C4	3.17	117.35	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	3702	IHP	C6-C1-C2	2.92	116.81	110.41
5	A	3701	ANP	C5-C6-N6	2.36	123.94	120.35
7	C	601	ATP	C5-C6-N6	2.35	123.92	120.35
6	A	3702	IHP	C5-C4-C3	2.17	115.16	110.41

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3701	ANP	PG-N3B-PB-O1B
5	A	3701	ANP	PB-O3A-PA-O5'
5	A	3701	ANP	C5'-O5'-PA-O1A
5	A	3701	ANP	C5'-O5'-PA-O2A
6	A	3702	IHP	C4-C3-O13-P3
6	A	3702	IHP	C5-C4-O14-P4
6	A	3702	IHP	C6-C5-O15-P5
7	C	601	ATP	C5'-O5'-PA-O1A
7	C	601	ATP	C5'-O5'-PA-O2A
5	A	3701	ANP	O4'-C4'-C5'-O5'
6	A	3702	IHP	C5-C6-O16-P6
7	C	601	ATP	PB-O3A-PA-O5'
6	A	3702	IHP	C4-O14-P4-O24
5	A	3701	ANP	C5'-O5'-PA-O3A
6	A	3702	IHP	C1-C6-O16-P6
6	A	3702	IHP	C2-O12-P2-O32
6	A	3702	IHP	C3-O13-P3-O43
5	A	3701	ANP	C4'-C5'-O5'-PA
7	C	601	ATP	O4'-C4'-C5'-O5'
7	C	601	ATP	C5'-O5'-PA-O3A
7	C	601	ATP	C4'-C5'-O5'-PA
7	C	601	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

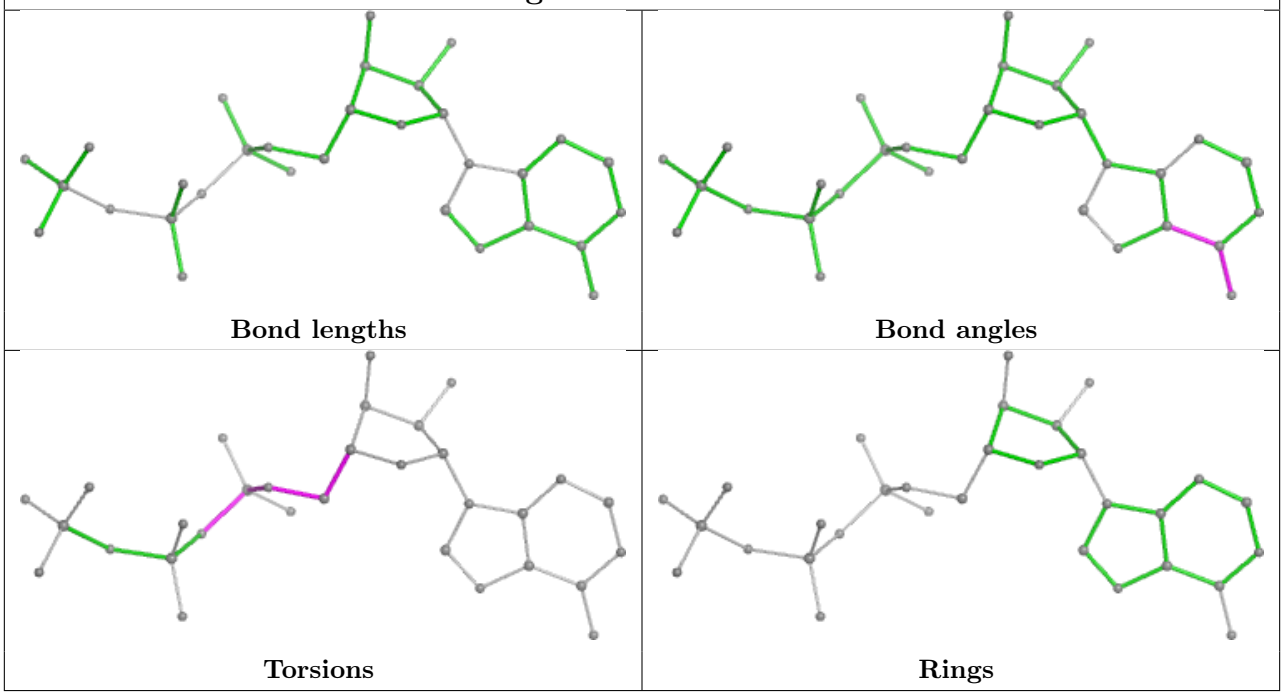
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	601	ATP	2	0
6	A	3702	IHP	4	0
5	A	3701	ANP	1	0

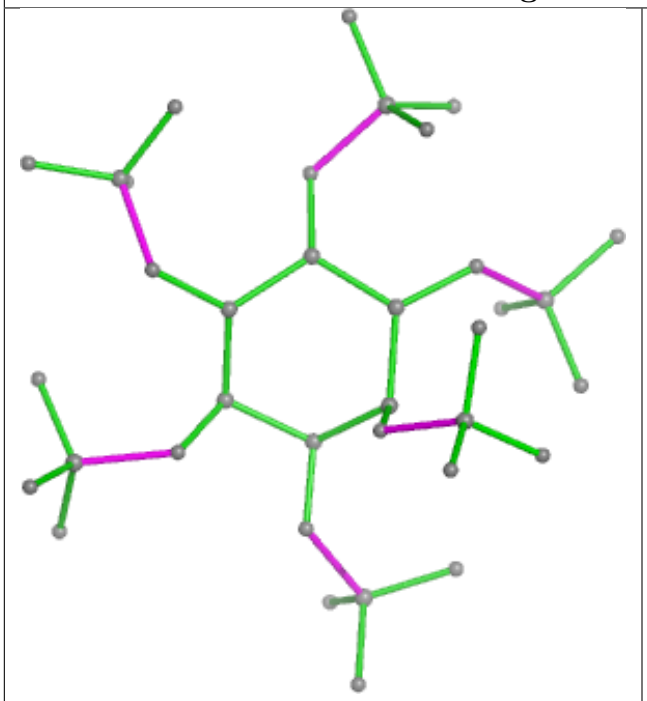
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

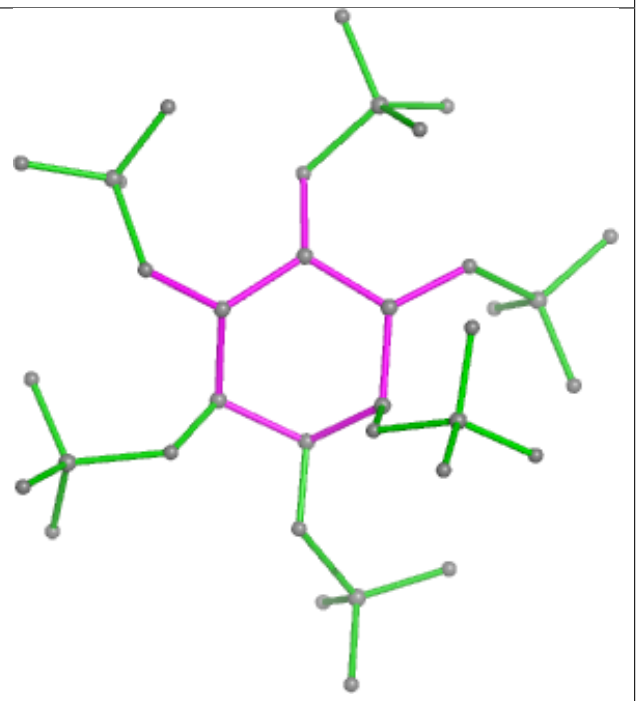
Ligand ATP C 601



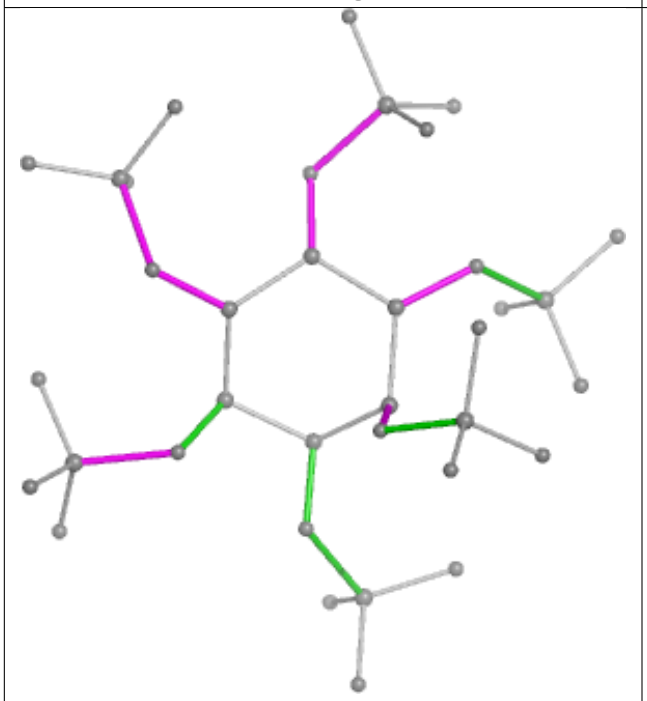
Ligand IHP A 3702



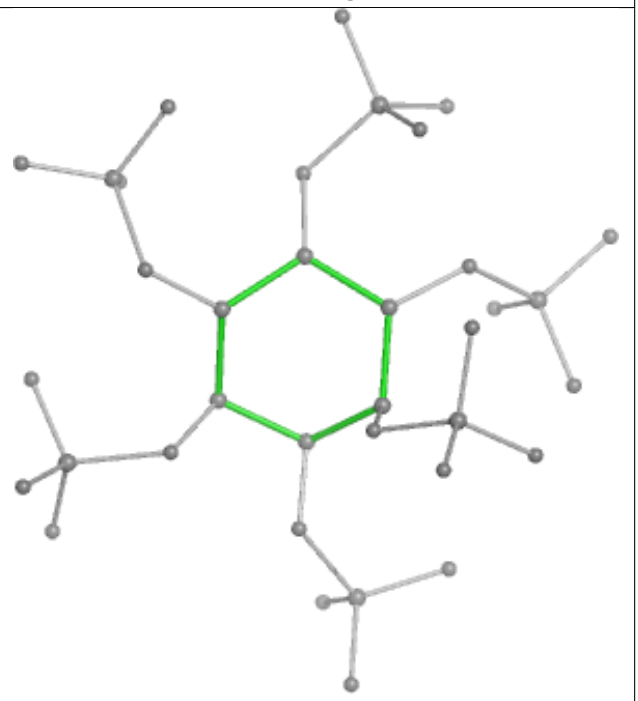
Bond lengths



Bond angles

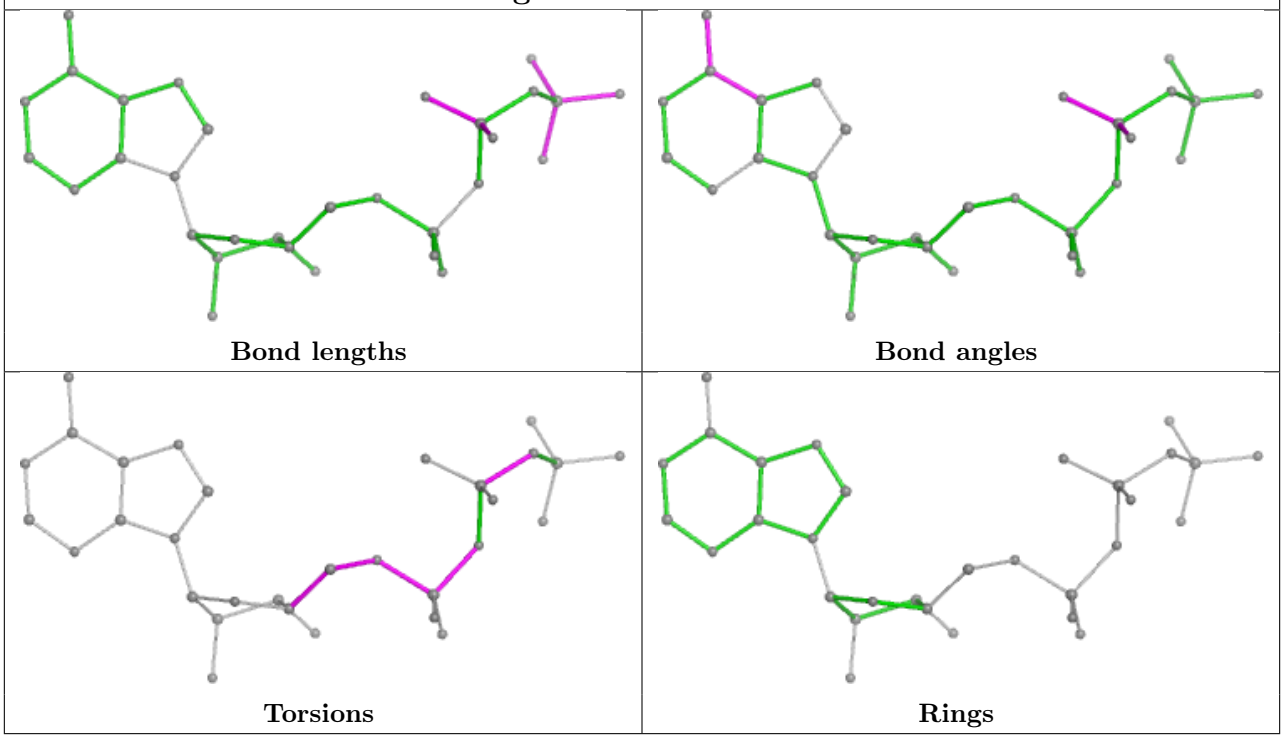


Torsions



Rings

Ligand ANP A 3701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	15

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1638:SER	C	1646:UNK	N	21.20
1	A	175:UNK	C	191:UNK	N	15.48
1	A	1717:UNK	C	1727:GLU	N	14.50
1	A	1657:UNK	C	1663:UNK	N	12.67
1	A	1677:UNK	C	1703:UNK	N	12.15
1	A	304:ILE	C	311:PHE	N	11.52
1	A	265:VAL	C	267:MET	N	11.51
1	A	156:UNK	C	162:UNK	N	10.02
1	A	244:UNK	C	248:ALA	N	9.98

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1978:LEU	C	2006:ARG	N	9.49
1	A	224:UNK	C	229:UNK	N	8.21
1	A	2056:LYS	C	2068:UNK	N	7.91
1	A	2083:UNK	C	2088:TYR	N	6.46
1	A	285:LYS	C	290:CYS	N	4.88
1	A	201:UNK	C	207:UNK	N	4.74

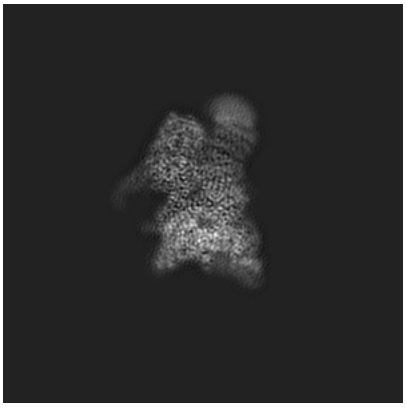
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11063. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

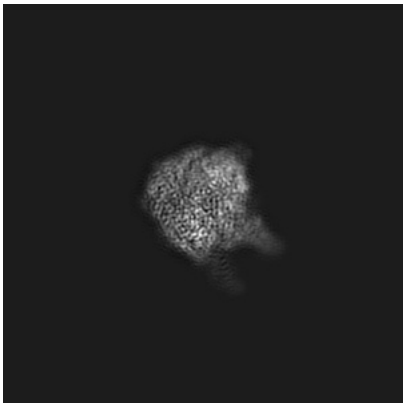
6.1 Orthogonal projections (i)

6.1.1 Primary map



X

Y

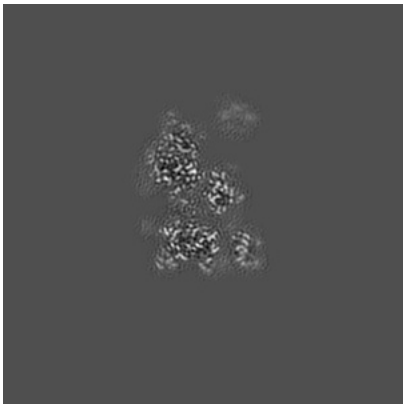


Z

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

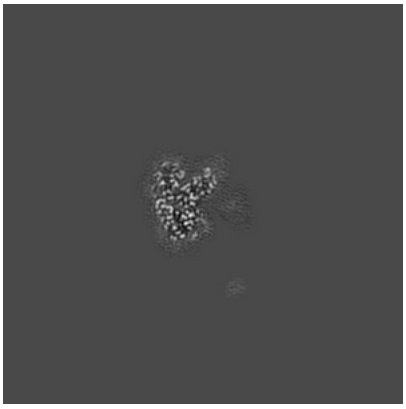
6.2 Central slices (i)

6.2.1 Primary map



X Index: 160

Y Index: 160

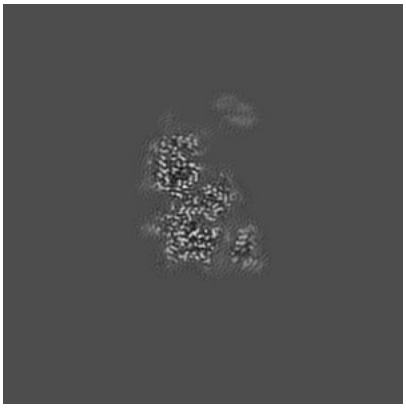


Z Index: 160

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

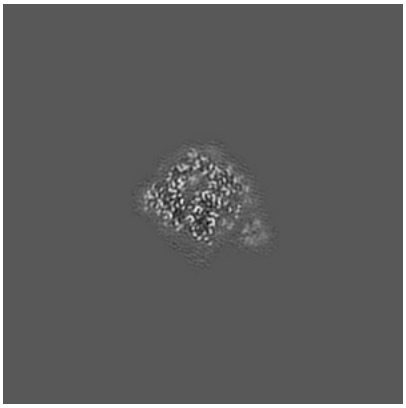
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 155

Y Index: 145

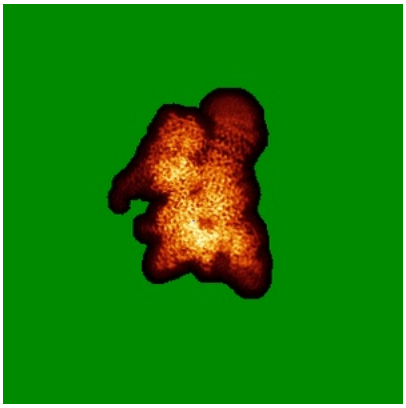


Z Index: 133

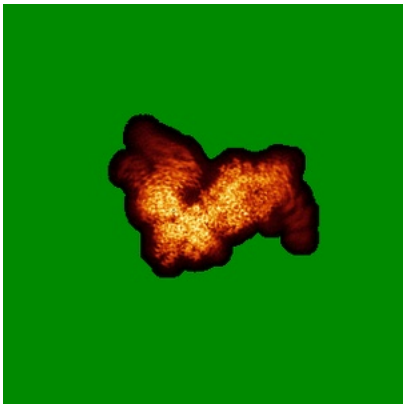
The images above show the largest variance slices of the map in three orthogonal directions.

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

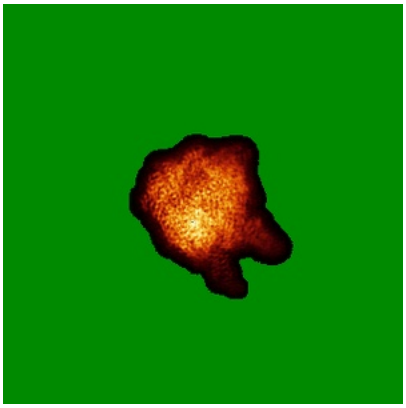
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

The images above show the 3D surface view of the map at the recommended contour level 0.0312. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

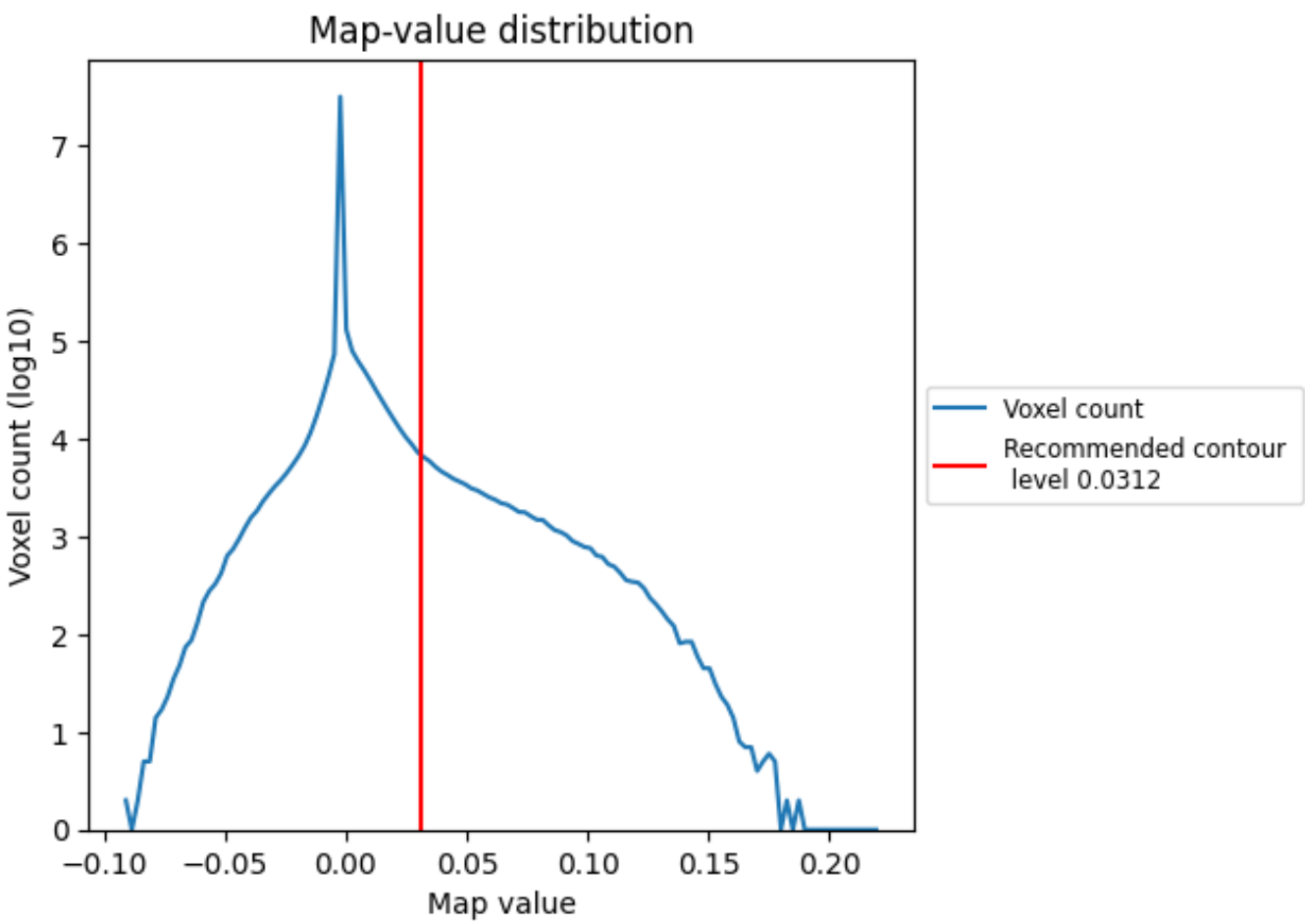
6.6 Mask visualisation (i)

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

7 Map analysis (i)

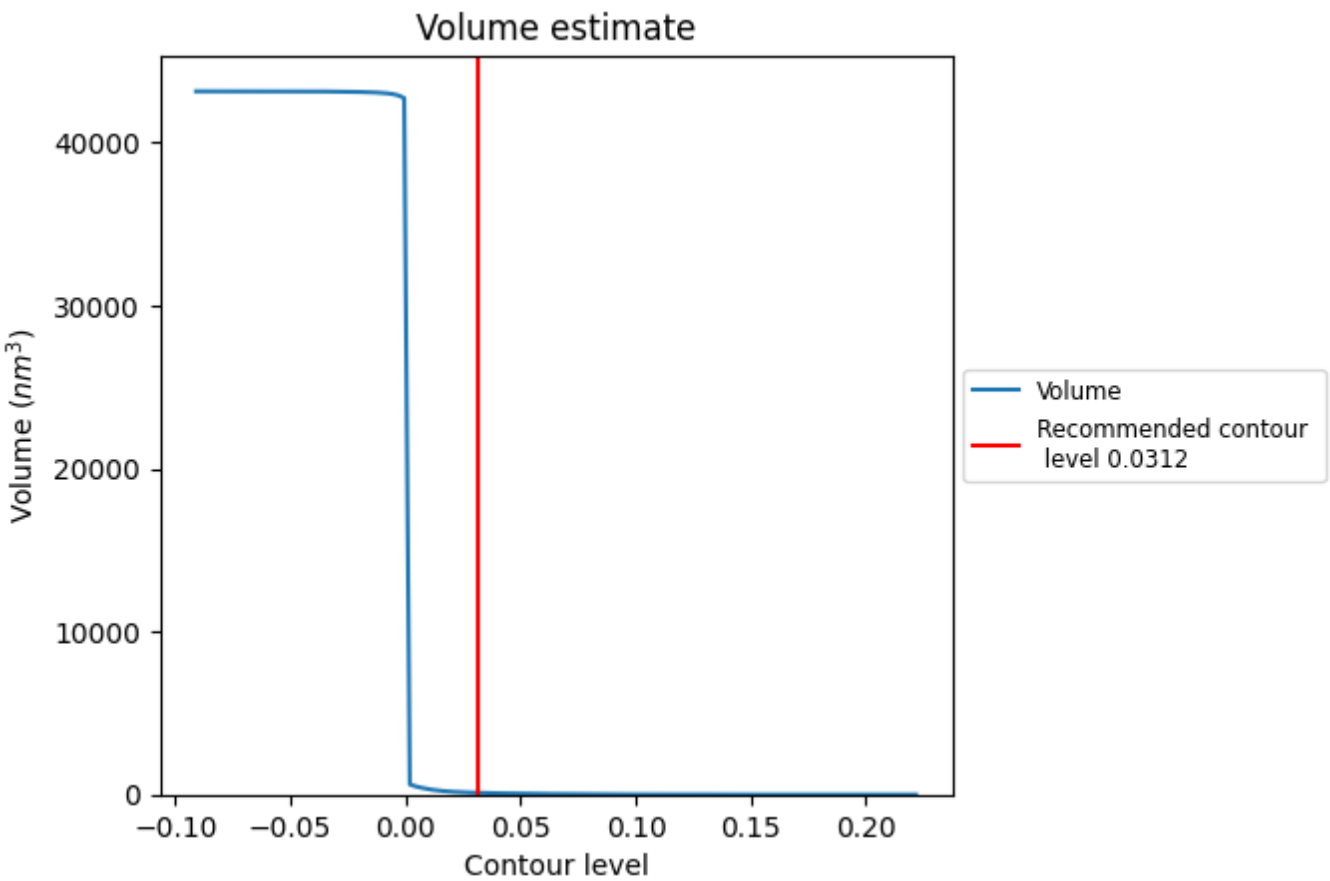
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

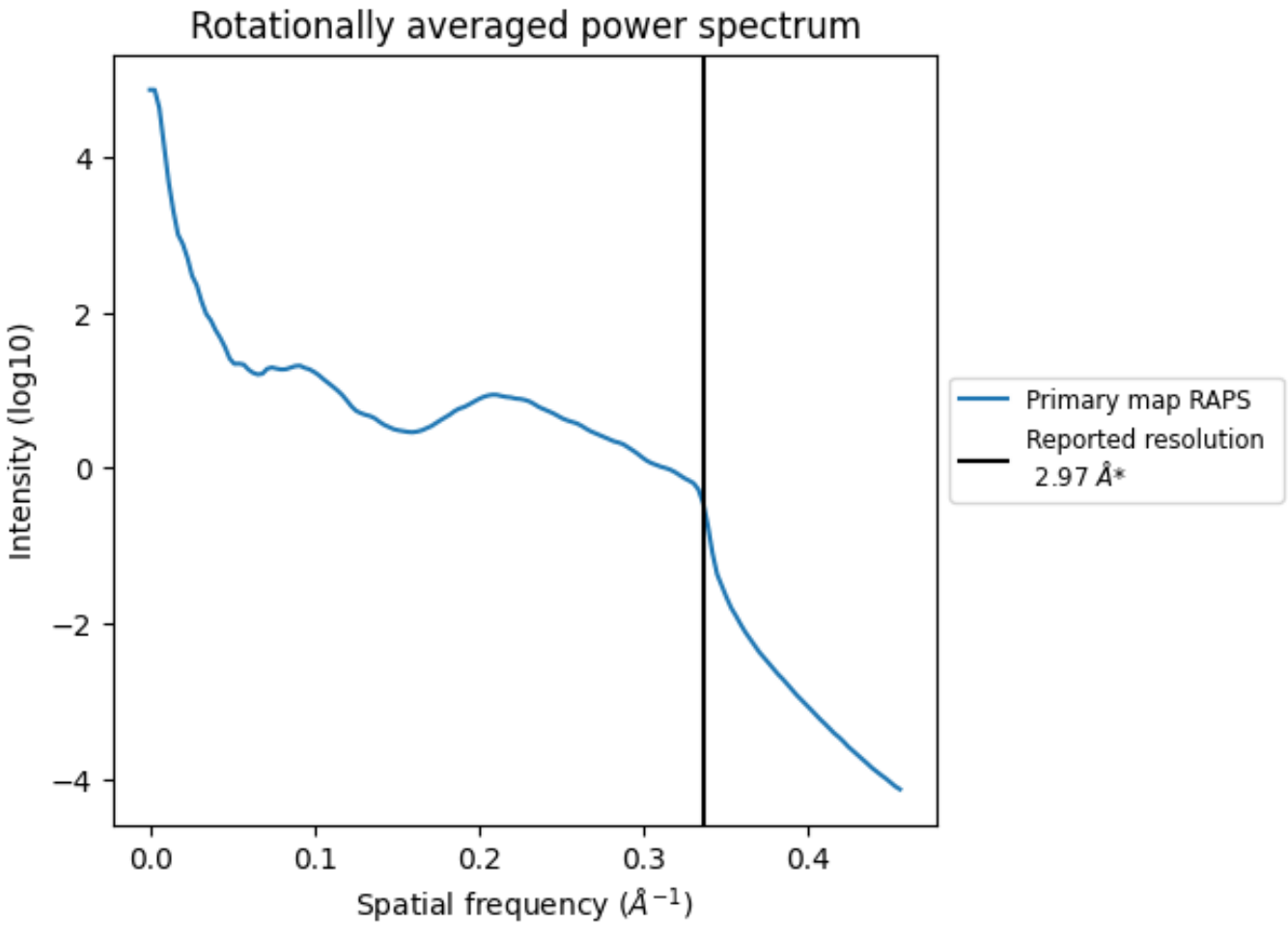
7.2 Volume estimate (i)



The volume at the recommended contour level is 108 nm^3; this corresponds to an approximate mass of 98 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)

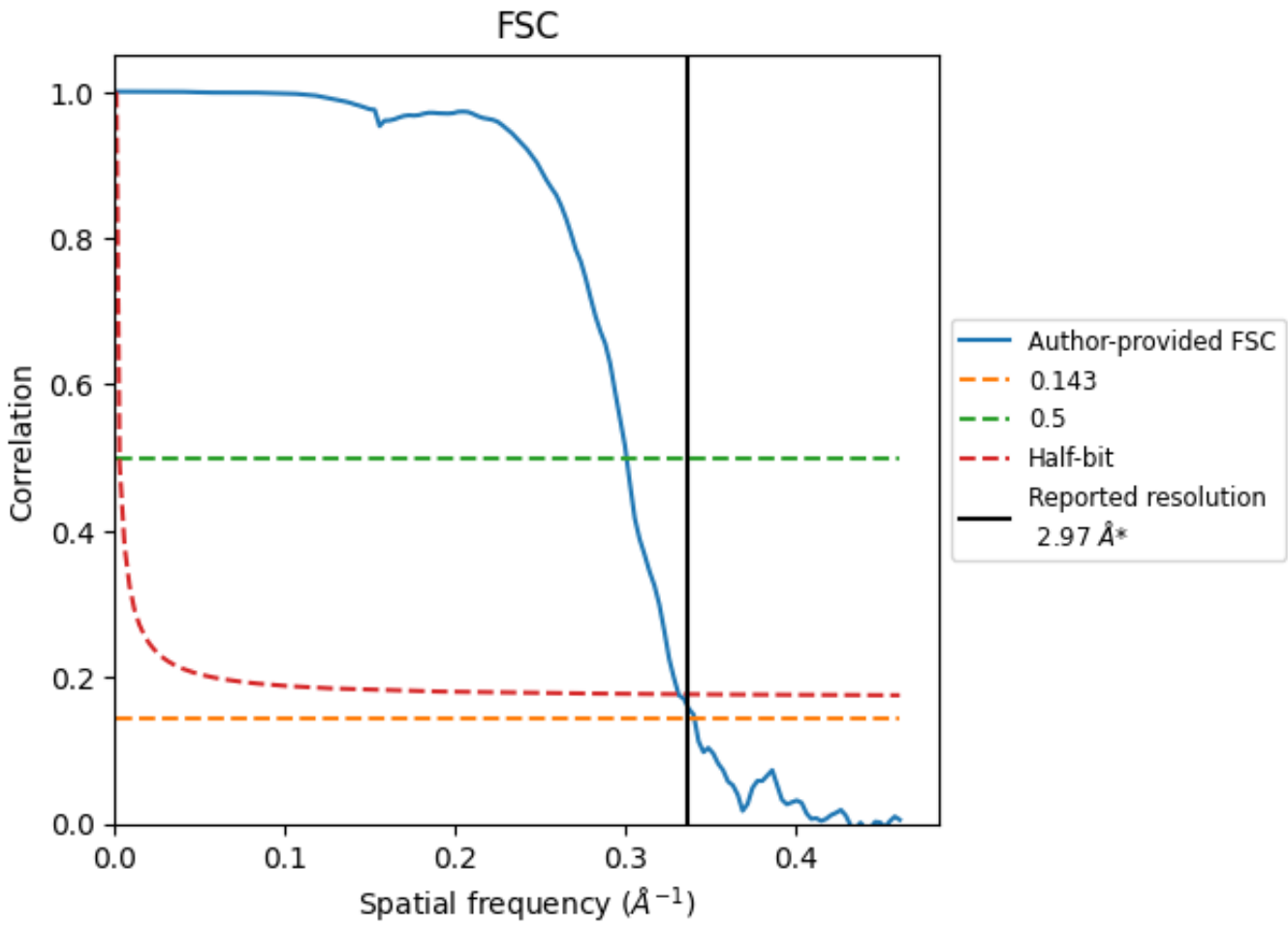


*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

8.2 Resolution estimates (i)

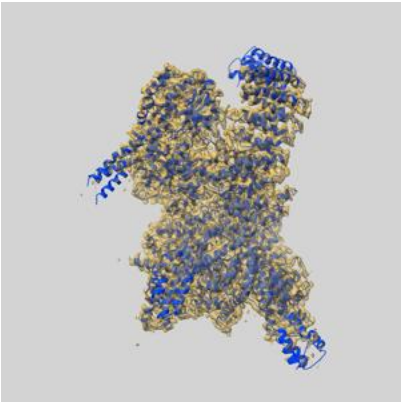
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.93	3.32	3.01
Unmasked-calculated*	-	-	-

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

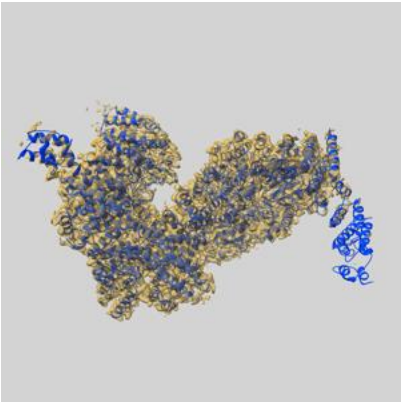
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11063 and PDB model 6Z3R. Per-residue inclusion information can be found in section 3 on page 6.

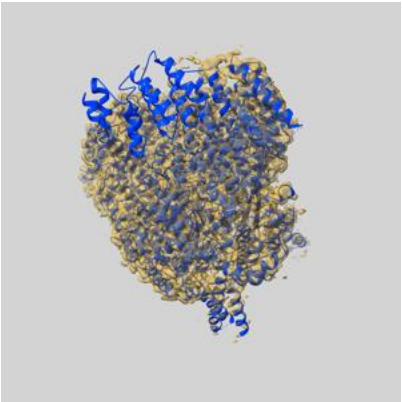
9.1 Map-model overlay (i)



X



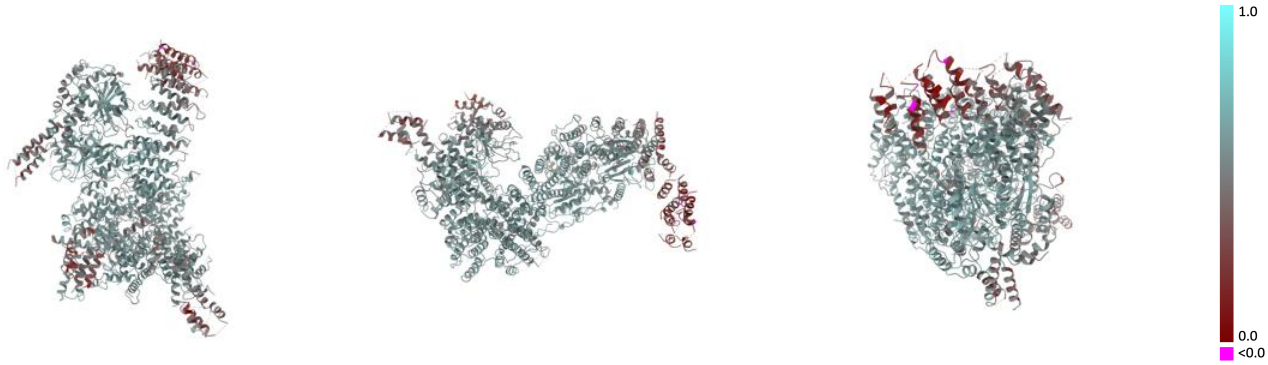
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0312 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.

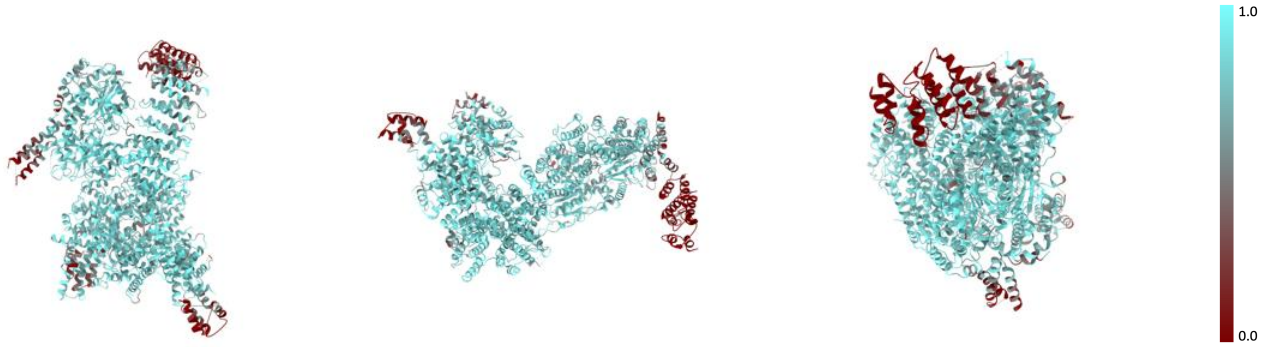
9.2 Q-score mapped to coordinate model (i)



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.

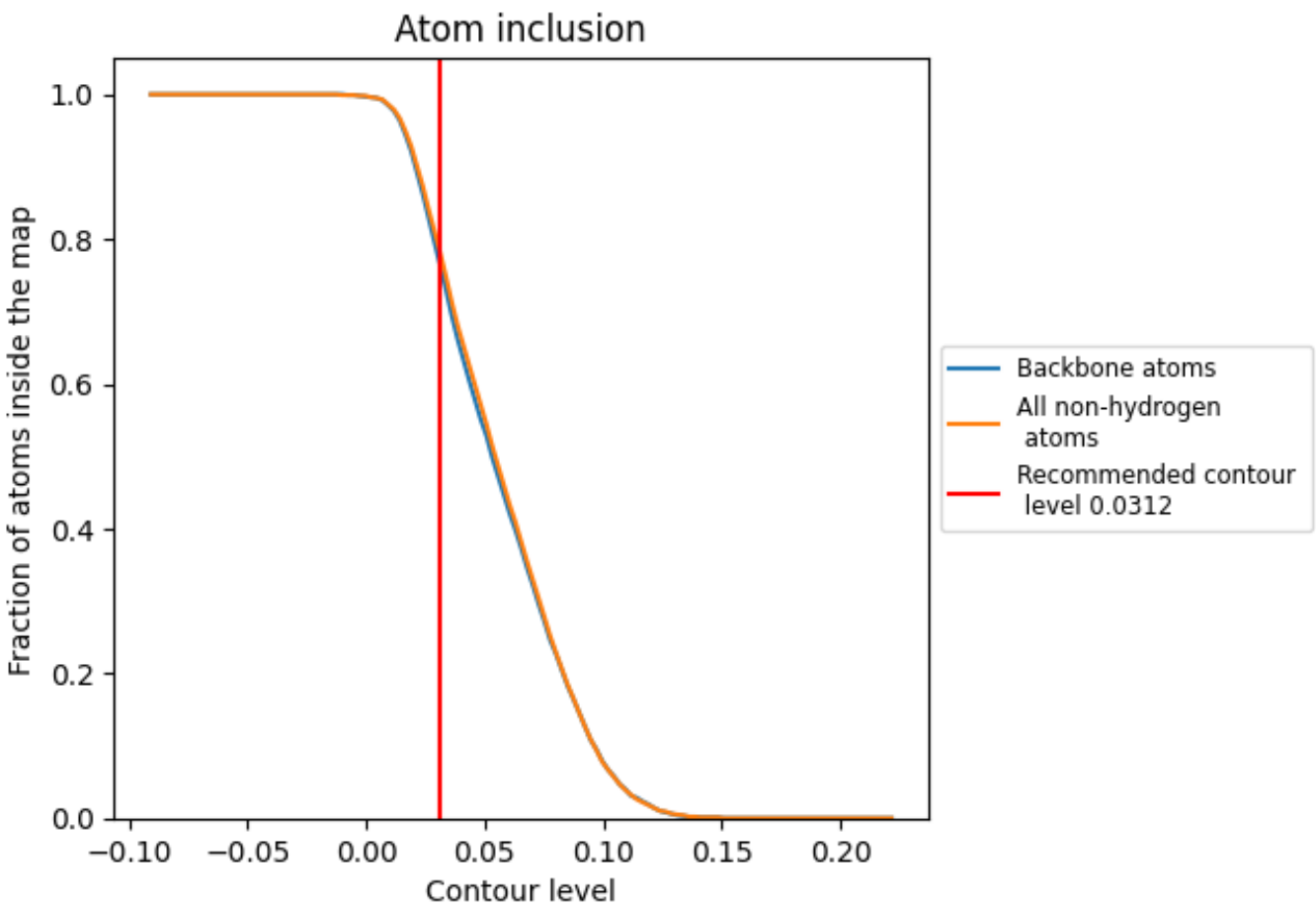
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0312).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0312) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.5450
A	0.7860	0.5390
B	0.7320	0.5420
C	0.8740	0.5870
E	0.7440	0.5880