



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 02:23 PM UTC

PDB ID : 6ZWO / pdb_00006zwo
EMDB ID : EMD-11492
Title : cryo-EM structure of human mTOR complex 2, focused on one half
Authors : Scaiola, A.; Mangia, F.; Inseng, S.; Boehringer, D.; Ban, N.; Maier, T.
Deposited on : 2020-07-28
Resolution : 3.00 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

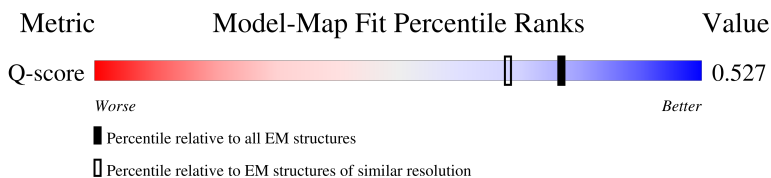
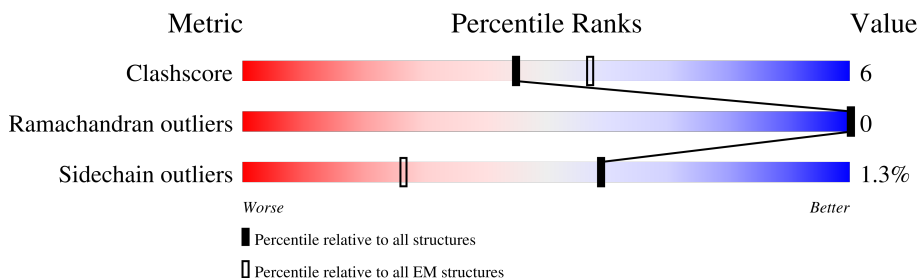
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	B	2549	
2	D	326	
3	F	1708	
4	H	521	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24994 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1592	Total	C	N	O	S	0	0
			12841	8209	2240	2304	88		

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	319	Total	C	N	O	S	0	0
			2465	1533	437	477	18		

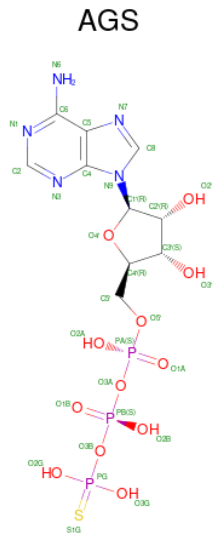
- Molecule 3 is a protein called Rapamycin-insensitive companion of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	1117	Total	C	N	O	S	0	0
			8931	5689	1584	1611	47		

- Molecule 4 is a protein called Target of rapamycin complex 2 subunit MAPKAP1.

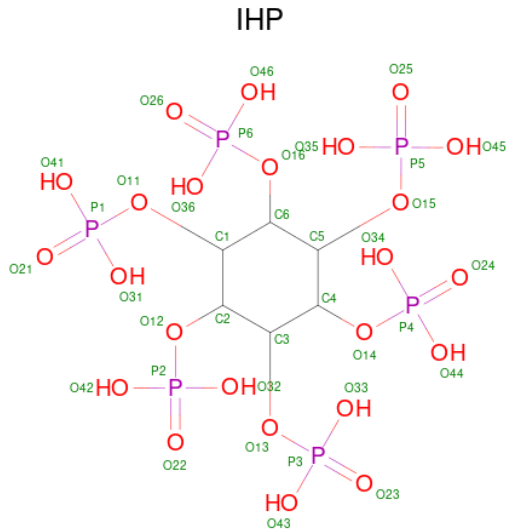
Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	98	Total	C	N	O	S	0	0
			655	399	125	127	4		

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
5	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
5	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

- Molecule 6 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $\text{C}_6\text{H}_{18}\text{O}_{24}\text{P}_6$) (labeled as "Ligand of Interest" by depositor).

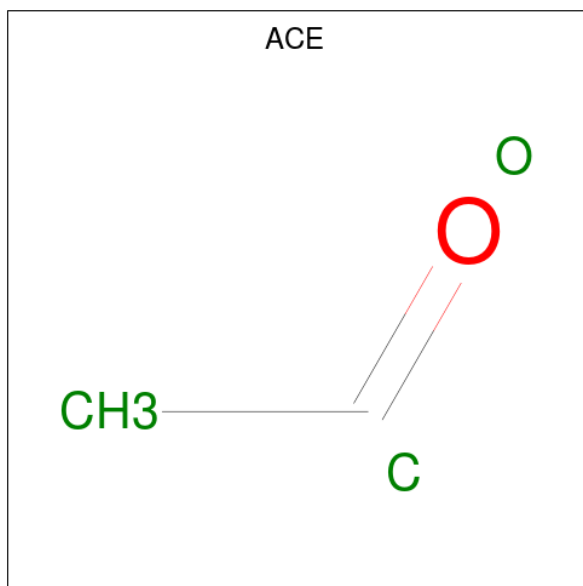


Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

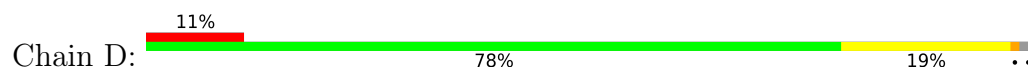
Mol	Chain	Residues	Atoms		AltConf
7	F	1	Total	Zn	0
			1	1	

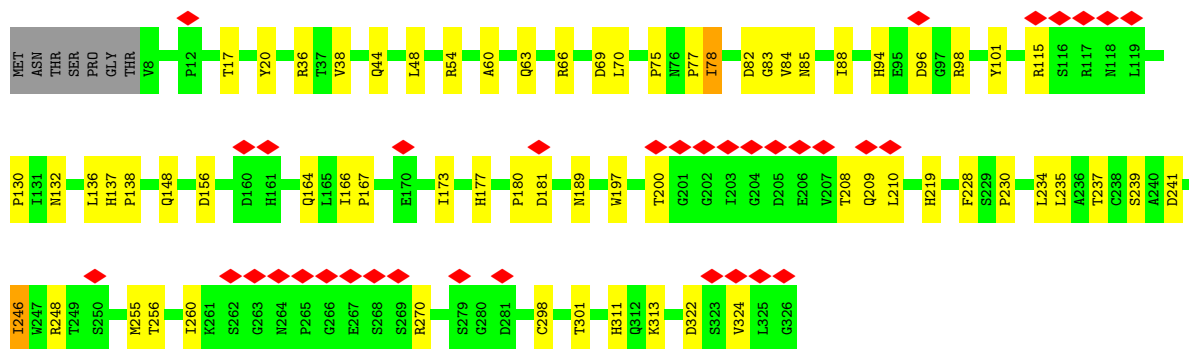
- Molecule 8 is ACETYL GROUP (CCD ID: ACE) (formula: C₂H₄O).



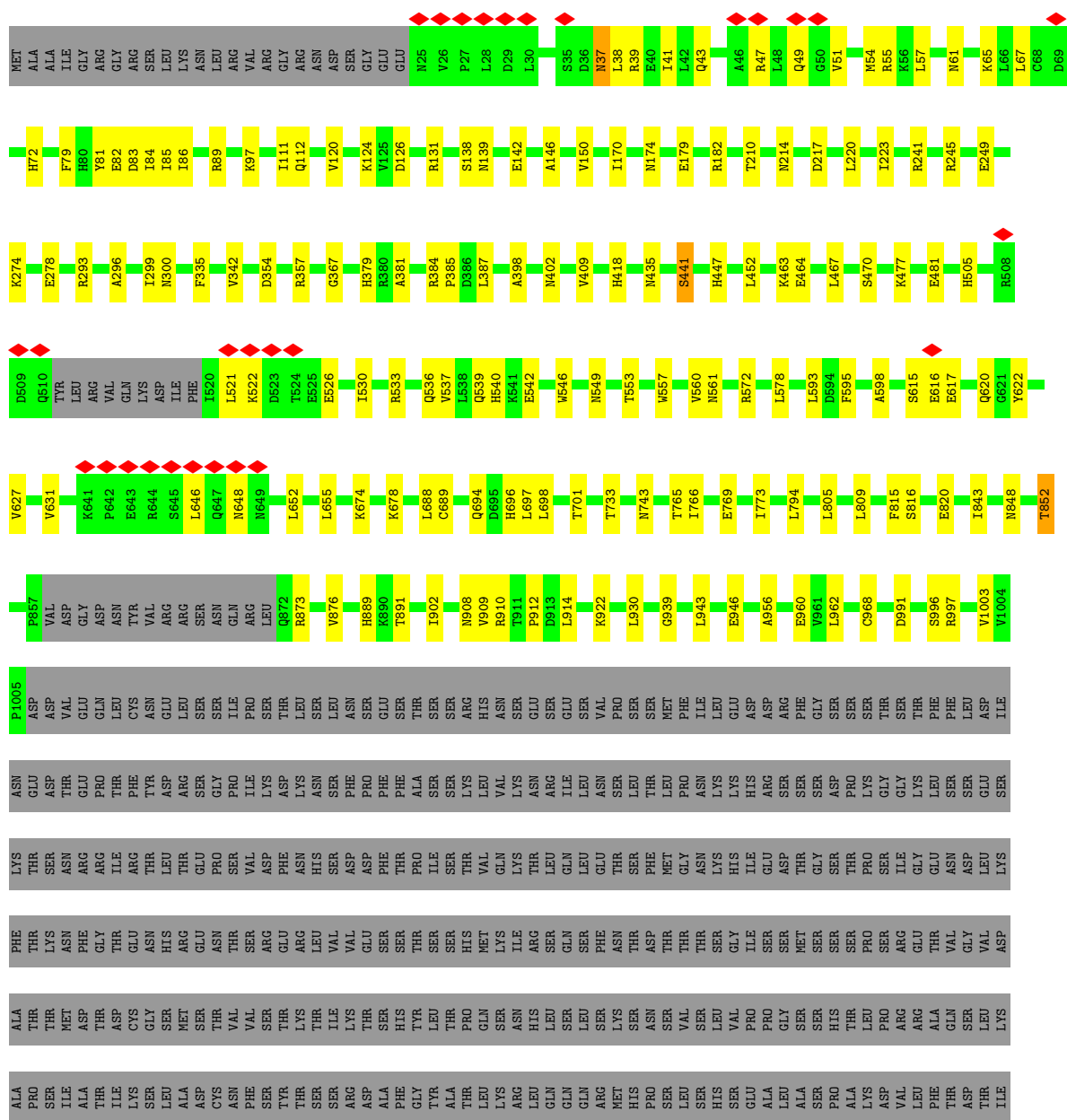
Mol	Chain	Residues	Atoms			AltConf
8	H	1	Total	C	O	0
			3	2	1	

- Molecule 2: Target of rapamycin complex subunit LST8

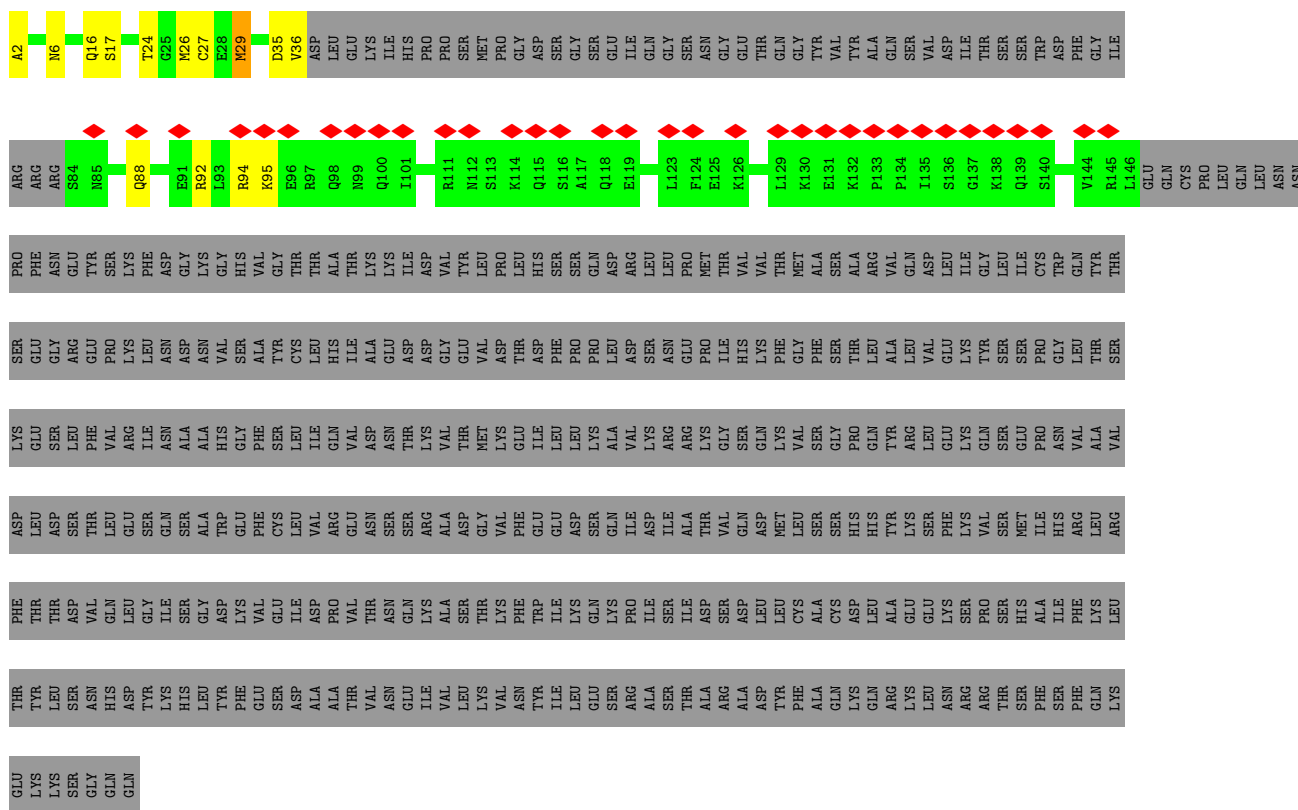




• Molecule 3: Rapamycin-insensitive companion of mTOR



- Molecule 4: Target of rapamycin complex 2 subunit MAPKAP1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	293038	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	46300	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.739	Depositor
Minimum map value	-2.097	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	430.08, 430.08, 430.08	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.344, 1.344, 1.344	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: ZN, IHP, ACE, AGS

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	B	0.11	0/13126	0.29	0/17791
2	D	0.11	0/2523	0.33	0/3438
3	F	0.12	0/9092	0.30	0/12300
4	H	0.13	0/660	0.40	0/900
All	All	0.11	0/25401	0.30	0/34429

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
3	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	367	GLY	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	B	12841	0	12892	158	0
2	D	2465	0	2351	35	0
3	F	8931	0	9080	124	0
4	H	655	0	519	9	0
5	B	31	0	12	1	0
5	F	31	0	12	1	0
6	B	36	0	6	1	0
7	F	1	0	0	0	0
8	H	3	0	3	0	0
All	All	24994	0	24875	314	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 (314) 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)
3:F:124:LYS:HE2	3:F:1519:ASN:HA	1.70	0.74
1:B:2278:LEU:HB2	1:B:2283:LYS:HG3	1.74	0.70
3:F:1535:ASN:HD21	3:F:1684:GLN:HG3	1.56	0.69
2:D:173:ILE:HA	2:D:189:ASN:HA	1.75	0.69
1:B:1031:MET:HE1	1:B:1059:ILE:HD13	1.75	0.68
1:B:2025:GLU:OE2	1:B:2170:ARG:NH2	2.27	0.67
3:F:910:ARG:NH2	3:F:946:GLU:O	2.28	0.67
3:F:733:THR:HG21	3:F:766:ILE:HG23	1.78	0.66
3:F:688:LEU:HD11	3:F:697:LEU:HD23	1.79	0.65
3:F:384:ARG:O	3:F:997:ARG:NH2	2.30	0.64
3:F:616:GLU:O	3:F:620:GLN:NE2	2.30	0.64
2:D:298:CYS:HB3	2:D:301:THR:HG22	1.79	0.64
1:B:1702:LYS:NZ	6:B:2602:IHP:O22	2.30	0.64
3:F:595:PHE:HB3	3:F:598:ALA:HB2	1.78	0.64
2:D:84:VAL:HG21	2:D:88:ILE:HD11	1.80	0.64
2:D:54:ARG:NH2	2:D:322:ASP:O	2.31	0.63
1:B:2270:ARG:O	2:D:313:LYS:NZ	2.30	0.63
3:F:648:ASN:HD21	3:F:694:GLN:HG2	1.64	0.63
1:B:1724:MET:HE3	1:B:1747:MET:HG2	1.81	0.63
1:B:850:SER:HA	1:B:1611:ARG:HH12	1.63	0.63
1:B:1501:TRP:O	1:B:1509:GLN:NE2	2.31	0.63
1:B:894:LEU:O	1:B:1583:TYR:OH	2.17	0.62
1:B:1069:LEU:HD22	3:F:463:LYS:HG3	1.82	0.62
1:B:1509:GLN:HA	1:B:1512:MET:HG2	1.81	0.62
3:F:1510:THR:HG22	3:F:1511:GLY:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:PRO:HG2	2:D:230:PRO:HA	1.82	0.61
1:B:2260:LEU:H	1:B:2260:LEU:HD23	1.66	0.61
1:B:1211:VAL:HA	3:F:553:THR:HG21	1.81	0.60
1:B:2009:ALA:HA	1:B:2138:LEU:HD11	1.83	0.60
3:F:47:ARG:HB2	3:F:49:GLN:HE21	1.66	0.60
2:D:200:THR:HG23	2:D:208:THR:H	1.67	0.59
1:B:1878:LEU:HD11	1:B:1918:ASP:HB2	1.83	0.59
1:B:2194:GLN:HG3	1:B:2421:PHE:HZ	1.67	0.59
1:B:1878:LEU:HA	1:B:1881:THR:HG22	1.84	0.59
3:F:39:ARG:HH22	3:F:43:GLN:HB2	1.68	0.59
3:F:794:LEU:HB2	3:F:805:LEU:HD12	1.85	0.58
1:B:2249:LEU:HB3	1:B:2302:LEU:HD21	1.85	0.58
3:F:912:PRO:HB2	3:F:914:LEU:HD13	1.86	0.58
1:B:1615:ILE:HA	1:B:1618:ILE:HG12	1.86	0.58
3:F:41:ILE:HG13	3:F:1693:LEU:HD21	1.85	0.58
1:B:824:ILE:HD13	1:B:844:LEU:HB2	1.86	0.57
1:B:1097:LEU:HD22	1:B:1138:THR:HG21	1.85	0.57
1:B:1069:LEU:HD23	3:F:467:LEU:HD12	1.86	0.57
3:F:86:ILE:HA	3:F:89:ARG:HD3	1.86	0.57
3:F:81:TYR:O	3:F:85:ILE:HG13	2.05	0.57
1:B:2252:ASP:HA	1:B:2255:GLU:HG2	1.87	0.57
3:F:441:SER:HB3	3:F:991:ASP:OD2	2.05	0.56
2:D:82:ASP:OD1	2:D:83:GLY:N	2.38	0.56
1:B:2276:ASP:OD1	1:B:2276:ASP:N	2.33	0.56
3:F:533:ARG:HG2	3:F:533:ARG:HH11	1.70	0.56
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	1.88	0.56
1:B:2503:ARG:HH21	1:B:2512:ASP:HB2	1.70	0.56
1:B:2192:LEU:HD21	1:B:2237:ILE:HG13	1.89	0.55
3:F:593:LEU:HD23	3:F:655:LEU:HD12	1.87	0.55
3:F:616:GLU:HG2	3:F:617:GLU:HG2	1.87	0.55
3:F:1628:SER:O	3:F:1632:HIS:ND1	2.39	0.55
1:B:1400:LYS:HE2	1:B:1415:SER:HB2	1.89	0.55
2:D:36:ARG:HH22	2:D:70:LEU:HA	1.72	0.55
1:B:1129:LEU:HD21	1:B:1168:GLU:HG3	1.90	0.54
1:B:1307:ALA:HB1	1:B:1314:ALA:HB2	1.90	0.54
1:B:2192:LEU:HD22	1:B:2235:GLY:HA3	1.89	0.54
2:D:98:ARG:HA	2:D:115:ARG:HH22	1.73	0.54
3:F:299:ILE:HD12	3:F:962:LEU:HB3	1.90	0.54
4:H:94:ARG:HE	4:H:95:LYS:HD2	1.72	0.54
1:B:1044:MET:O	1:B:1049:GLN:NE2	2.41	0.53
3:F:956:ALA:HB2	3:F:968:CYS:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2011:MET:O	1:B:2015:GLU:HB2	2.08	0.53
3:F:182:ARG:HH22	4:H:26:MET:HE3	1.73	0.53
3:F:572:ARG:NH1	5:F:4802:AGS:O2B	2.41	0.53
3:F:1649:ASP:OD1	3:F:1649:ASP:N	2.40	0.53
1:B:1540:THR:HG23	1:B:1543:GLY:H	1.73	0.53
3:F:769:GLU:O	3:F:773:ILE:HG12	2.08	0.53
1:B:1595:MET:HG3	1:B:1639:VAL:HG11	1.89	0.53
2:D:164:GLN:HE22	2:D:166:ILE:HD11	1.72	0.53
3:F:37:ASN:O	3:F:41:ILE:HG12	2.09	0.53
1:B:2055:HIS:O	1:B:2059:GLU:HG3	2.08	0.53
1:B:825:MET:HE1	1:B:861:TYR:HB3	1.89	0.52
3:F:335:PHE:O	3:F:873:ARG:NH2	2.40	0.52
2:D:260:ILE:O	2:D:270:ARG:NH2	2.39	0.52
2:D:94:HIS:CD2	2:D:96:ASP:H	2.27	0.52
3:F:379:HIS:HD2	3:F:381:ALA:H	1.56	0.52
1:B:1566:LYS:HE2	1:B:1570:LEU:HD11	1.92	0.52
1:B:823:ILE:O	1:B:827:MET:HG3	2.10	0.52
1:B:1066:GLU:HG2	1:B:1069:LEU:HD12	1.92	0.52
3:F:1488:SER:OG	3:F:1489:LEU:N	2.43	0.52
3:F:387:LEU:HD22	3:F:843:ILE:HD11	1.92	0.52
1:B:1044:MET:HE2	1:B:1044:MET:HA	1.93	0.51
1:B:1211:VAL:HG22	3:F:553:THR:HG21	1.92	0.51
1:B:1601:GLU:OE1	1:B:1619:TRP:NE1	2.43	0.51
1:B:2332:TYR:OH	1:B:2512:ASP:OD2	2.25	0.51
3:F:1527:GLU:HG2	3:F:1528:ILE:N	2.25	0.51
2:D:66:ARG:HB3	2:D:77:PRO:HB3	1.92	0.51
3:F:220:LEU:HD12	3:F:223:ILE:HD12	1.92	0.51
3:F:138:SER:O	3:F:138:SER:OG	2.29	0.50
1:B:1797:ASN:O	1:B:1801:VAL:HG23	2.10	0.50
3:F:296:ALA:O	3:F:300:ASN:ND2	2.41	0.50
3:F:1535:ASN:ND2	3:F:1684:GLN:HG3	2.25	0.50
3:F:398:ALA:O	3:F:402:ASN:ND2	2.43	0.50
3:F:561:ASN:O	3:F:615:SER:HB3	2.11	0.50
1:B:1425:GLN:HG3	1:B:2314:PHE:HZ	1.77	0.50
3:F:521:LEU:HD12	3:F:522:LYS:H	1.77	0.50
3:F:1613:ARG:NH2	3:F:1649:ASP:OD2	2.37	0.50
1:B:1902:ASP:O	1:B:1906:VAL:HG13	2.12	0.49
2:D:130:PRO:HB2	2:D:148:GLN:HG3	1.94	0.49
1:B:1707:SER:OG	1:B:1708:ALA:N	2.45	0.49
4:H:35:ASP:OD2	4:H:35:ASP:N	2.36	0.49
1:B:1733:ALA:HB3	1:B:1740:LYS:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2231:SER:OG	1:B:2232:THR:N	2.44	0.49
3:F:170:ILE:O	3:F:174:ASN:HB2	2.12	0.49
1:B:2185:LEU:HD23	1:B:2187:LYS:HD3	1.95	0.49
2:D:248:ARG:HD3	2:D:255:MET:HE2	1.94	0.49
2:D:69:ASP:HB2	2:D:78:ILE:HD13	1.95	0.48
3:F:67:LEU:HD11	3:F:72:HIS:HB3	1.95	0.48
1:B:1416:LEU:O	1:B:1420:ASN:ND2	2.43	0.48
3:F:617:GLU:HA	3:F:620:GLN:HE22	1.78	0.48
1:B:1793:TRP:O	1:B:1797:ASN:ND2	2.47	0.48
1:B:2161:GLN:HG3	1:B:2171:LYS:HB3	1.95	0.48
2:D:137:HIS:CG	2:D:138:PRO:HD2	2.47	0.48
1:B:2254:ARG:NH1	1:B:2261:LEU:O	2.46	0.48
2:D:167:PRO:HB3	2:D:197:TRP:HZ2	1.79	0.48
3:F:996:SER:OG	3:F:997:ARG:N	2.46	0.48
1:B:2203:GLY:O	1:B:2207:THR:HG23	2.13	0.48
3:F:97:LYS:NZ	3:F:138:SER:O	2.44	0.48
3:F:889:HIS:CD2	3:F:891:THR:HB	2.49	0.48
1:B:797:ASN:O	1:B:801:THR:HG23	2.14	0.47
1:B:1954:GLY:O	1:B:1958:HIS:ND1	2.45	0.47
3:F:540:HIS:HD2	3:F:542:GLU:HB3	1.79	0.47
3:F:1623:LEU:HD23	3:F:1673:ILE:HD11	1.96	0.47
3:F:82:GLU:HB3	3:F:1529:LEU:HD21	1.97	0.47
3:F:505:HIS:CE1	3:F:743:ASN:HB3	2.50	0.47
1:B:1342:GLU:O	1:B:1346:THR:HG22	2.15	0.47
1:B:1898:ASN:OD1	1:B:1898:ASN:N	2.46	0.47
3:F:549:ASN:O	3:F:553:THR:HG23	2.13	0.47
1:B:1499:GLU:HG3	1:B:1500:LYS:HG3	1.95	0.47
1:B:1487:LEU:O	1:B:1665:ARG:NH1	2.47	0.47
1:B:1971:ALA:HB2	1:B:2144:TYR:HE2	1.79	0.47
1:B:2145:ASP:OD1	1:B:2145:ASP:N	2.47	0.47
2:D:17:THR:OG1	2:D:311:HIS:NE2	2.41	0.47
2:D:38:VAL:HG13	2:D:75:PRO:HA	1.97	0.47
1:B:1777:SER:O	1:B:1781:GLU:HG3	2.14	0.47
3:F:296:ALA:HA	3:F:962:LEU:HD12	1.96	0.47
3:F:1653:TYR:HA	3:F:1656:VAL:HG12	1.97	0.47
1:B:1590:MET:HE3	1:B:1590:MET:HB2	1.88	0.47
1:B:959:PHE:HB2	1:B:971:VAL:HG11	1.95	0.46
3:F:354:ASP:O	3:F:357:ARG:NH2	2.44	0.46
3:F:1526:ILE:HA	3:F:1531:PHE:HB2	1.96	0.46
1:B:1413:LEU:HD13	1:B:1436:ALA:HB2	1.97	0.46
1:B:1422:LYS:HE2	1:B:1422:LYS:HB3	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:698:LEU:HA	3:F:701:THR:HG22	1.96	0.46
1:B:2370:LYS:HE3	1:B:2370:LYS:HB2	1.70	0.46
3:F:111:ILE:HD11	3:F:120:VAL:HG21	1.97	0.46
3:F:126:ASP:OD1	3:F:126:ASP:N	2.47	0.46
3:F:241:ARG:NH2	3:F:960:GLU:O	2.48	0.46
3:F:1487:MET:HG2	3:F:1492:ILE:HD13	1.96	0.46
3:F:39:ARG:NH2	3:F:43:GLN:HB2	2.31	0.46
1:B:958:ILE:HD11	1:B:1313:MET:HB2	1.96	0.46
1:B:1771:LYS:O	1:B:1774:GLN:HG2	2.15	0.46
1:B:2047:MET:O	1:B:2051:LEU:HG	2.15	0.46
3:F:274:LYS:O	3:F:278:GLU:HG2	2.16	0.46
1:B:974:ALA:O	1:B:978:ILE:HG12	2.16	0.46
1:B:1973:ILE:O	1:B:1977:THR:HG23	2.15	0.46
1:B:1004:CYS:O	1:B:1009:ARG:NH2	2.49	0.46
1:B:2121:LEU:HD22	1:B:2126:VAL:HG21	1.98	0.46
1:B:2137:GLU:O	1:B:2152:ARG:NH1	2.49	0.46
1:B:2246:LEU:HD11	1:B:2383:LEU:HD21	1.98	0.46
3:F:61:ASN:O	3:F:65:LYS:HG3	2.15	0.46
1:B:1085:ASP:OD2	1:B:1093:SER:OG	2.32	0.46
1:B:1930:ILE:HD11	1:B:1935:TRP:CZ2	2.51	0.46
1:B:1614:ILE:O	1:B:1618:ILE:HG23	2.16	0.45
1:B:818:ASP:O	1:B:822:ILE:HG13	2.15	0.45
1:B:885:ILE:HD11	1:B:1568:ARG:HB3	1.98	0.45
1:B:1214:CYS:HB2	3:F:557:TRP:HZ3	1.81	0.45
1:B:1503:LEU:H	1:B:1503:LEU:HD23	1.81	0.45
2:D:234:LEU:HD22	2:D:246:ILE:HG13	1.96	0.45
3:F:146:ALA:O	3:F:150:VAL:HG13	2.17	0.45
3:F:688:LEU:HD21	3:F:697:LEU:HB3	1.98	0.45
4:H:29:MET:H	4:H:29:MET:HG2	1.57	0.45
1:B:1276:SER:OG	1:B:1277:LYS:N	2.49	0.45
3:F:182:ARG:NH2	4:H:26:MET:HE3	2.31	0.45
3:F:557:TRP:HB3	3:F:560:VAL:HG22	1.99	0.45
3:F:1623:LEU:HD13	3:F:1632:HIS:HB2	1.98	0.45
1:B:2012:VAL:O	1:B:2016:LEU:HG	2.17	0.45
3:F:816:SER:O	3:F:820:GLU:HG2	2.16	0.45
1:B:845:GLY:HA3	1:B:887:VAL:HG22	1.98	0.45
1:B:2212:ASP:HB3	1:B:2215:SER:HB2	1.98	0.45
3:F:1520:CYS:HB3	3:F:1523:CYS:HB2	1.99	0.45
4:H:88:GLN:O	4:H:92:ARG:HG3	2.17	0.45
1:B:1220:TYR:CD2	1:B:1221:THR:HG23	2.52	0.45
1:B:1227:GLU:OE2	1:B:1235:ARG:NH2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2250:ILE:HD13	1:B:2382:MET:HE3	1.98	0.45
1:B:994:MET:HE1	1:B:1019:LEU:HD23	1.99	0.45
1:B:2336:LEU:HD21	1:B:2358:PHE:HD1	1.82	0.45
1:B:2379:LEU:HD21	1:B:2392:LEU:HD13	1.99	0.45
1:B:1971:ALA:HB2	1:B:2144:TYR:CE2	2.52	0.44
1:B:2204:LEU:HD22	1:B:2417:VAL:HG21	1.99	0.44
2:D:60:ALA:HB1	2:D:88:ILE:HB	1.98	0.44
2:D:239:SER:HB3	2:D:241:ASP:OD1	2.17	0.44
3:F:627:VAL:O	3:F:631:VAL:HG23	2.17	0.44
3:F:536:GLN:HA	3:F:539:GLN:HE21	1.82	0.44
1:B:1278:ASP:O	1:B:1282:GLU:HG2	2.17	0.44
3:F:1518:ASP:HA	3:F:1524:VAL:HG12	1.99	0.44
1:B:2210:ALA:HA	1:B:2216:LEU:HD13	1.99	0.44
3:F:245:ARG:HB2	3:F:249:GLU:HG3	2.00	0.44
3:F:540:HIS:CD2	3:F:542:GLU:HB3	2.52	0.44
5:B:2601:AGS:O2B	5:B:2601:AGS:S1G	2.76	0.44
1:B:1028:ARG:NH2	3:F:464:GLU:OE2	2.50	0.44
1:B:1163:LEU:O	1:B:1170:ARG:NE	2.50	0.44
1:B:1910:TRP:NE1	1:B:1953:VAL:HG23	2.33	0.44
1:B:2022:LEU:HD12	1:B:2024:HIS:HE1	1.82	0.44
1:B:1034:ILE:HG22	1:B:1038:MET:HE2	1.99	0.44
1:B:1214:CYS:HB2	3:F:557:TRP:CZ3	2.52	0.44
3:F:435:ASN:HB3	3:F:447:HIS:CE1	2.52	0.44
3:F:533:ARG:HG2	3:F:533:ARG:NH1	2.32	0.44
3:F:848:ASN:O	3:F:852:THR:HG22	2.18	0.44
3:F:81:TYR:HA	3:F:84:ILE:HD12	2.00	0.43
3:F:1516:THR:HG22	3:F:1517:ASP:H	1.81	0.43
1:B:942:PRO:HG2	1:B:945:GLU:HG2	2.01	0.43
3:F:674:LYS:O	3:F:678:LYS:HG2	2.17	0.43
1:B:2392:LEU:HD23	1:B:2392:LEU:H	1.83	0.43
1:B:888:LEU:HD12	1:B:888:LEU:HA	1.88	0.43
1:B:1704:MET:HG3	1:B:1709:ARG:HH21	1.83	0.43
1:B:1972:LEU:O	1:B:1976:LEU:HB2	2.18	0.43
2:D:94:HIS:HB3	2:D:98:ARG:H	1.82	0.43
1:B:1109:ASP:OD2	3:F:470:SER:OG	2.34	0.43
1:B:1177:LEU:O	1:B:1181:VAL:HG13	2.19	0.43
3:F:384:ARG:HG3	3:F:385:PRO:HD2	2.00	0.43
3:F:1512:LEU:HG	3:F:1613:ARG:HD3	2.00	0.43
1:B:1787:TYR:HB2	1:B:1894:LEU:HB3	1.99	0.43
2:D:132:ASN:OD1	2:D:148:GLN:NE2	2.51	0.43
3:F:139:ASN:ND2	3:F:142:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:342:VAL:HG12	3:F:418:HIS:HD2	1.83	0.43
3:F:578:LEU:HD22	3:F:622:TYR:HB3	2.01	0.43
1:B:1572:ASP:O	1:B:1576:THR:HG22	2.19	0.43
1:B:1115:LEU:O	1:B:1119:VAL:HG23	2.19	0.42
1:B:1269:TRP:CZ2	1:B:1287:LEU:HD21	2.53	0.42
1:B:1423:LEU:HD12	1:B:1423:LEU:HA	1.89	0.42
1:B:2340:HIS:CD2	1:B:2342:SER:HB2	2.54	0.42
3:F:51:VAL:HG13	3:F:55:ARG:HD2	2.00	0.42
3:F:293:ARG:O	4:H:2:ALA:N	2.52	0.42
1:B:1372:LEU:HA	1:B:1373:PRO:HD3	1.94	0.42
1:B:1548:ALA:HB2	1:B:1563:CYS:HB2	2.00	0.42
1:B:1701:MET:HE1	1:B:1720:PHE:CD2	2.54	0.42
2:D:20:TYR:HB2	2:D:313:LYS:HB3	2.01	0.42
1:B:1680:ASP:H	1:B:1683:ARG:HH11	1.66	0.42
1:B:1728:ALA:HB2	1:B:1743:LEU:HD23	2.00	0.42
1:B:883:GLU:O	1:B:887:VAL:HG23	2.19	0.42
1:B:957:ARG:NH1	1:B:1316:ASP:OD2	2.50	0.42
1:B:1456:TRP:HB2	1:B:1487:LEU:HD13	2.01	0.42
1:B:1888:PHE:HB3	1:B:1906:VAL:HG12	2.00	0.42
3:F:652:LEU:HD21	3:F:696:HIS:CE1	2.54	0.42
3:F:939:GLY:O	3:F:943:LEU:HB2	2.19	0.42
4:H:6:ASN:OD1	4:H:6:ASN:N	2.52	0.42
3:F:409:VAL:HG13	3:F:452:LEU:HD13	2.02	0.42
1:B:1338:ILE:HA	1:B:1341:ILE:HG22	2.02	0.42
3:F:83:ASP:HA	3:F:86:ILE:HG12	2.01	0.42
1:B:2019:VAL:HG13	1:B:2126:VAL:HG11	2.02	0.42
3:F:72:HIS:NE2	3:F:112:GLN:HG3	2.35	0.42
3:F:1634:THR:O	3:F:1638:THR:HG23	2.19	0.42
1:B:886:ARG:HG3	1:B:1568:ARG:NH2	2.35	0.42
2:D:177:HIS:HD1	2:D:228:PHE:HB2	1.84	0.42
4:H:16:GLN:HG3	4:H:17:SER:N	2.35	0.42
1:B:2195:ASP:HA	1:B:2198:VAL:HG22	2.01	0.42
2:D:246:ILE:HG23	2:D:256:THR:HB	2.02	0.42
1:B:1072:PRO:HA	1:B:1075:ILE:HD12	2.01	0.41
3:F:467:LEU:HA	3:F:467:LEU:HD23	1.74	0.41
3:F:909:VAL:HG21	3:F:930:LEU:HD12	2.02	0.41
3:F:139:ASN:OD1	3:F:139:ASN:N	2.52	0.41
1:B:1920:ASN:O	1:B:1924:VAL:HG13	2.21	0.41
3:F:217:ASP:OD1	3:F:217:ASP:N	2.51	0.41
3:F:689:CYS:HA	3:F:698:LEU:HD21	2.02	0.41
1:B:1719:HIS:O	1:B:1723:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:505:HIS:NE2	3:F:743:ASN:O	2.54	0.41
1:B:856:GLU:OE1	1:B:859:ARG:NH2	2.52	0.41
1:B:947:TYR:CZ	1:B:1324:SER:HB3	2.55	0.41
1:B:950:VAL:HA	1:B:953:VAL:HG22	2.02	0.41
1:B:2134:ARG:HD3	1:B:2134:ARG:HA	1.81	0.41
2:D:219:HIS:CG	2:D:239:SER:HB2	2.55	0.41
1:B:2123:LEU:HD23	1:B:2123:LEU:HA	1.91	0.41
3:F:38:LEU:HB2	3:F:79:PHE:CE2	2.55	0.41
3:F:477:LYS:O	3:F:481:GLU:HG3	2.21	0.41
1:B:870:ASN:O	1:B:874:THR:HG23	2.21	0.41
1:B:1119:VAL:HA	1:B:1122:PHE:CE2	2.55	0.41
1:B:1785:SER:O	1:B:1785:SER:OG	2.34	0.41
1:B:2156:ILE:HG12	1:B:2174:LEU:HD22	2.01	0.41
2:D:173:ILE:HG22	2:D:189:ASN:HB3	2.02	0.41
3:F:210:THR:O	3:F:214:ASN:HB2	2.21	0.41
3:F:809:LEU:HG	3:F:815:PHE:HD2	1.86	0.41
1:B:1422:LYS:H	1:B:1422:LYS:HG2	1.74	0.41
1:B:1607:LEU:HD23	1:B:1607:LEU:HA	1.93	0.41
1:B:1673:LEU:HD13	1:B:1700:TYR:HA	2.03	0.41
1:B:1993:LYS:O	1:B:1996:LYS:HG3	2.20	0.41
1:B:2496:LYS:O	1:B:2499:GLN:HG2	2.21	0.41
3:F:54:MET:O	3:F:57:LEU:HG	2.21	0.41
1:B:949:ALA:O	1:B:953:VAL:HG13	2.21	0.41
1:B:999:ASN:O	1:B:1003:VAL:HG23	2.20	0.41
3:F:505:HIS:HE1	3:F:743:ASN:HB3	1.84	0.41
1:B:1063:LEU:HD23	1:B:1063:LEU:HA	1.87	0.40
2:D:63:GLN:HG2	2:D:85:ASN:C	2.46	0.40
2:D:209:GLN:O	2:D:210:LEU:HD23	2.21	0.40
3:F:179:GLU:OE1	3:F:1671:ARG:NH1	2.54	0.40
3:F:537:VAL:HA	3:F:546:TRP:NE1	2.36	0.40
3:F:1492:ILE:HG23	3:F:1611:LEU:HD21	2.02	0.40
1:B:872:LEU:O	1:B:881:ARG:NH1	2.47	0.40
3:F:131:ARG:HH22	3:F:1678:GLN:HA	1.86	0.40
3:F:646:LEU:HD23	3:F:646:LEU:HA	1.95	0.40
1:B:1533:THR:HG21	1:B:1550:LEU:HD22	2.04	0.40
1:B:2202:PHE:CZ	1:B:2327:MET:HE1	2.57	0.40
2:D:101:TYR:CE1	2:D:136:LEU:HD22	2.56	0.40
3:F:908:ASN:HD21	3:F:922:LYS:HE3	1.86	0.40
1:B:1031:MET:O	1:B:1034:ILE:HB	2.22	0.40
1:B:1759:LEU:HD23	1:B:1759:LEU:HA	1.91	0.40
3:F:526:GLU:O	3:F:530:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1609:ARG:HH22	3:F:1646:THR:HA	1.85	0.40
1:B:2054:LEU:O	1:B:2057:MET:HG3	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	B	1582/2549 (62%)	1533 (97%)	49 (3%)	0	100	100
2	D	317/326 (97%)	296 (93%)	21 (7%)	0	100	100
3	F	1103/1708 (65%)	1065 (97%)	38 (3%)	0	100	100
4	H	94/521 (18%)	87 (93%)	7 (7%)	0	100	100
All	All	3096/5104 (61%)	2981 (96%)	115 (4%)	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	B	1393/2220 (63%)	1379 (99%)	14 (1%)	68	84
2	D	269/276 (98%)	261 (97%)	8 (3%)	36	69
3	F	987/1539 (64%)	979 (99%)	8 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	50/470 (11%)	46 (92%)	4 (8%)	11	38
All	All	2699/4505 (60%)	2665 (99%)	34 (1%)	59	81

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	890	LEU
1	B	936	VAL
1	B	1113	LEU
1	B	1172	THR
1	B	1504	VAL
1	B	1593	CYS
1	B	1639	VAL
1	B	1679	VAL
1	B	1768	THR
1	B	1988	HIS
1	B	2173	THR
1	B	2214	THR
1	B	2261	LEU
1	B	2326	VAL
2	D	48	LEU
2	D	78	ILE
2	D	156	ASP
2	D	181	ASP
2	D	235	LEU
2	D	237	THR
2	D	246	ILE
2	D	324	VAL
3	F	37	ASN
3	F	441	SER
3	F	765	THR
3	F	852	THR
3	F	876	VAL
3	F	902	ILE
3	F	1003	VAL
3	F	1521	LEU
4	H	24	THR
4	H	27	CYS
4	H	29	MET
4	H	36	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59)

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	797	ASN
1	B	838	GLN
1	B	967	HIS
1	B	968	HIS
1	B	1014	GLN
1	B	1045	ASN
1	B	1202	HIS
1	B	1421	ASN
1	B	1494	HIS
1	B	1525	GLN
1	B	1617	GLN
1	B	1715	GLN
1	B	1716	HIS
1	B	1719	HIS
1	B	1722	GLN
1	B	1744	HIS
1	B	1809	GLN
1	B	1968	HIS
1	B	1997	ASN
1	B	2024	HIS
1	B	2106	HIS
1	B	2117	GLN
1	B	2154	GLN
1	B	2189	HIS
1	B	2265	HIS
1	B	2385	ASN
1	B	2401	HIS
2	D	41	GLN
2	D	71	ASN
2	D	128	ASN
2	D	153	HIS
2	D	198	ASN
2	D	264	ASN
3	F	49	GLN
3	F	94	ASN
3	F	112	GLN
3	F	145	GLN
3	F	219	GLN
3	F	264	HIS
3	F	359	GLN
3	F	379	HIS
3	F	390	ASN

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Mol	Chain	Res	Type
3	F	418	HIS
3	F	447	HIS
3	F	496	HIS
3	F	539	GLN
3	F	540	HIS
3	F	549	ASN
3	F	559	ASN
3	F	647	GLN
3	F	648	ASN
3	F	748	ASN
3	F	848	ASN
3	F	894	HIS
3	F	908	ASN
3	F	958	GLN
3	F	1532	GLN
3	F	1535	ASN
4	H	85	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
5	AGS	B	2601	-	32,33,33	1.69	8 (25%)	45,52,52	2.10	14 (31%)
5	AGS	F	4802	-	32,33,33	1.71	8 (25%)	45,52,52	2.17	16 (35%)
6	IHP	B	2602	-	36,36,36	1.49	3 (8%)	60,60,60	1.07	5 (8%)
8	ACE	H	601	4	1,2,2	0.74	0	0,1,1	-	-

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
5	AGS	B	2601	-	-	5/21/38/38	0/3/3/3
5	AGS	F	4802	-	-	3/21/38/38	0/3/3/3
6	IHP	B	2602	-	-	7/30/54/54	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2602	IHP	P4-O24	3.81	1.62	1.50
5	F	4802	AGS	C2-N3	3.49	1.40	1.33
5	F	4802	AGS	C2-N1	3.42	1.40	1.33
6	B	2602	IHP	P3-O23	3.37	1.60	1.50
5	B	2601	AGS	C2-N3	3.34	1.39	1.33
6	B	2602	IHP	P6-O26	3.33	1.60	1.50
5	B	2601	AGS	C2-N1	3.27	1.39	1.33
5	B	2601	AGS	C5-N7	-3.18	1.33	1.39
5	F	4802	AGS	C5-N7	-3.17	1.33	1.39
5	B	2601	AGS	C5-C4	-3.08	1.33	1.39
5	F	4802	AGS	C5-C4	-2.90	1.33	1.39
5	B	2601	AGS	C5-C6	-2.73	1.33	1.41
5	F	4802	AGS	C5-C6	-2.66	1.33	1.41
5	F	4802	AGS	C8-N9	-2.43	1.33	1.37
5	B	2601	AGS	C8-N9	-2.35	1.33	1.37
5	B	2601	AGS	PG-O2G	2.33	1.62	1.54
5	F	4802	AGS	PG-O2G	2.33	1.62	1.54
5	B	2601	AGS	C4-N9	-2.14	1.33	1.37
5	F	4802	AGS	O4'-C1'	2.03	1.46	1.42

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	4802	AGS	N3-C2-N1	-6.91	118.12	128.58
5	B	2601	AGS	N3-C2-N1	-6.85	118.21	128.58
5	F	4802	AGS	C5-C4-N3	-4.58	120.41	126.72
5	B	2601	AGS	C5-C4-N3	-4.48	120.55	126.72
5	F	4802	AGS	N9-C8-N7	-4.03	108.22	113.94
5	B	2601	AGS	N9-C8-N7	-4.00	108.26	113.94
5	F	4802	AGS	C2'-C3'-C4'	-3.97	94.94	102.61
5	B	2601	AGS	C2'-C3'-C4'	-3.73	95.40	102.61
5	F	4802	AGS	PB-O3B-PG	-3.59	120.05	133.17
5	B	2601	AGS	PB-O3B-PG	-3.50	120.34	133.17
5	F	4802	AGS	C2-N3-C4	3.33	119.95	111.83
5	B	2601	AGS	C2-N3-C4	3.27	119.81	111.83
6	B	2602	IHP	O43-P3-O33	3.10	119.43	107.80
6	B	2602	IHP	O46-P6-O36	3.05	119.22	107.80
5	F	4802	AGS	C5-N7-C8	2.93	108.06	103.45
5	F	4802	AGS	C5-C6-N6	-2.88	116.16	123.29
5	B	2601	AGS	C5-N7-C8	2.88	107.97	103.45
5	B	2601	AGS	C5-C6-N6	-2.84	116.25	123.29
5	F	4802	AGS	N3-C4-N9	2.70	131.77	127.17
5	B	2601	AGS	C6-C5-C4	2.69	120.85	117.18
5	F	4802	AGS	O4'-C4'-C3'	-2.67	99.84	105.15
5	F	4802	AGS	C6-C5-C4	2.67	120.82	117.18
5	B	2601	AGS	N3-C4-N9	2.41	131.27	127.17
5	B	2601	AGS	C4-C5-N7	-2.34	107.90	110.58
5	F	4802	AGS	C4'-O4'-C1'	-2.30	104.40	109.47
5	F	4802	AGS	C4-C5-N7	-2.25	108.01	110.58
6	B	2602	IHP	O41-P1-O21	2.20	119.42	110.83
6	B	2602	IHP	O32-P2-O22	2.19	119.37	110.83
5	B	2601	AGS	C5-C4-N9	2.18	108.18	105.81
5	F	4802	AGS	O3G-PG-O3B	2.17	111.89	104.64
5	F	4802	AGS	C1'-N9-C8	-2.16	122.30	127.09
6	B	2602	IHP	O45-P5-O25	2.16	119.25	110.83
5	B	2601	AGS	O3G-PG-O3B	2.12	111.73	104.64
5	B	2601	AGS	O4'-C4'-C3'	-2.07	101.04	105.15
5	F	4802	AGS	C4-N9-C8	2.05	107.89	105.74

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2601	AGS	PB-O3B-PG-O3G
5	B	2601	AGS	C5'-O5'-PA-O1A
5	F	4802	AGS	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

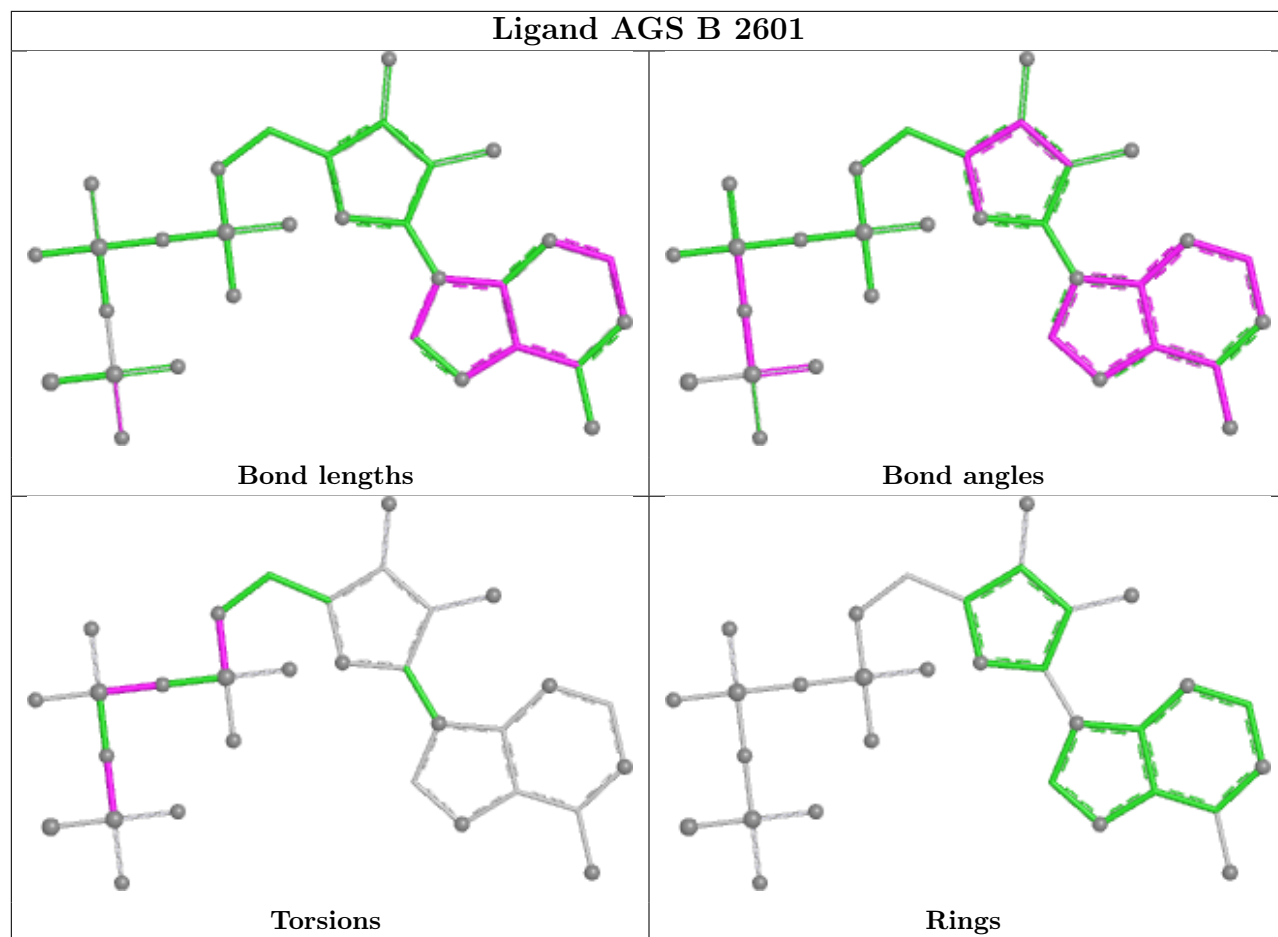
Mol	Chain	Res	Type	Atoms
5	F	4802	AGS	O4'-C1'-N9-C4
5	F	4802	AGS	O4'-C1'-N9-C8
5	B	2601	AGS	PA-O3A-PB-O3B
6	B	2602	IHP	C2-C3-O13-P3
6	B	2602	IHP	C4-C3-O13-P3
6	B	2602	IHP	C4-O14-P4-O24
6	B	2602	IHP	C6-O16-P6-O26
6	B	2602	IHP	C2-O12-P2-O42
6	B	2602	IHP	C2-O12-P2-O22
6	B	2602	IHP	C1-C2-O12-P2
5	B	2601	AGS	PA-O3A-PB-O1B
5	B	2601	AGS	PA-O3A-PB-O2B

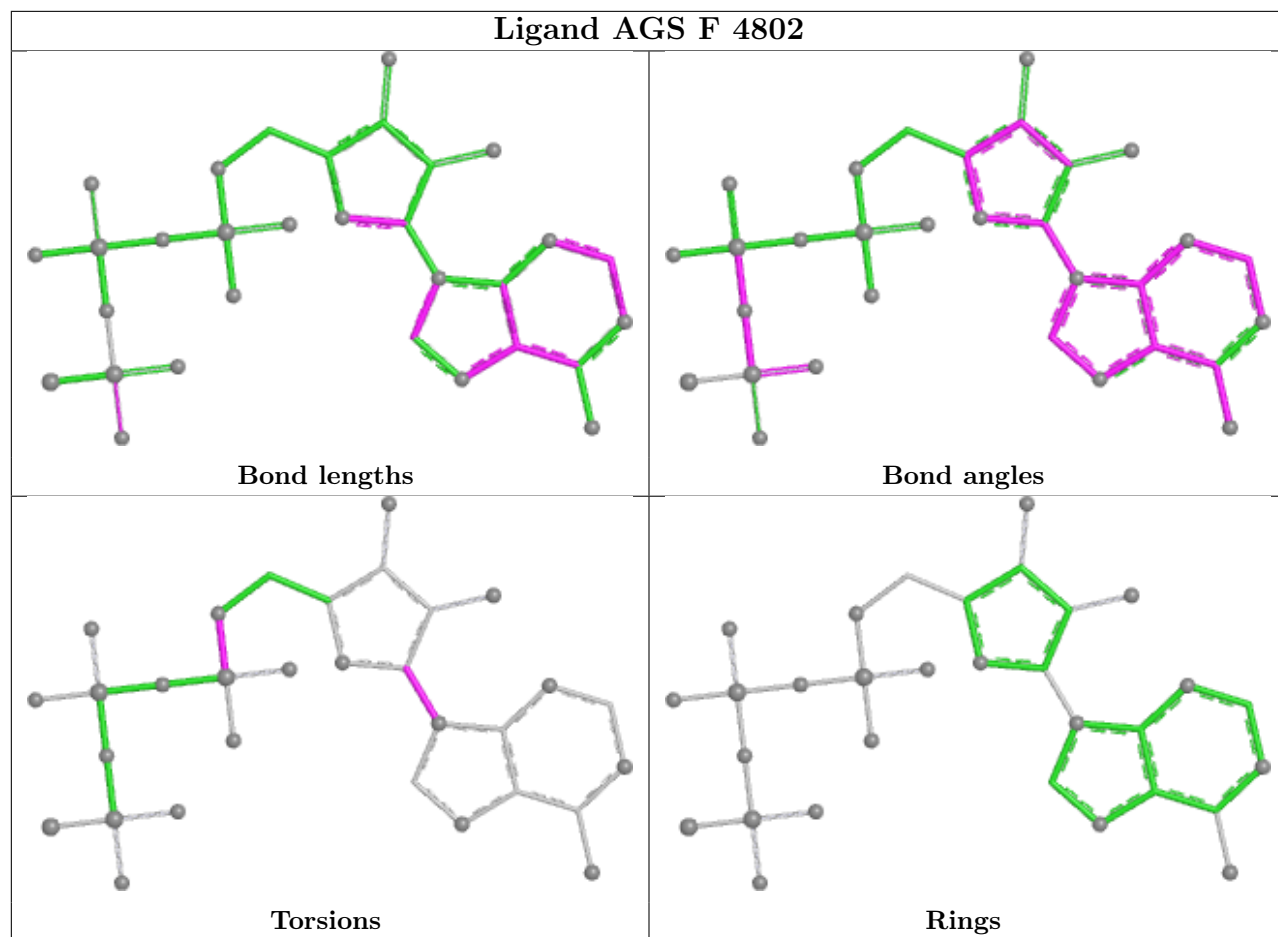
There are no ring outliers.

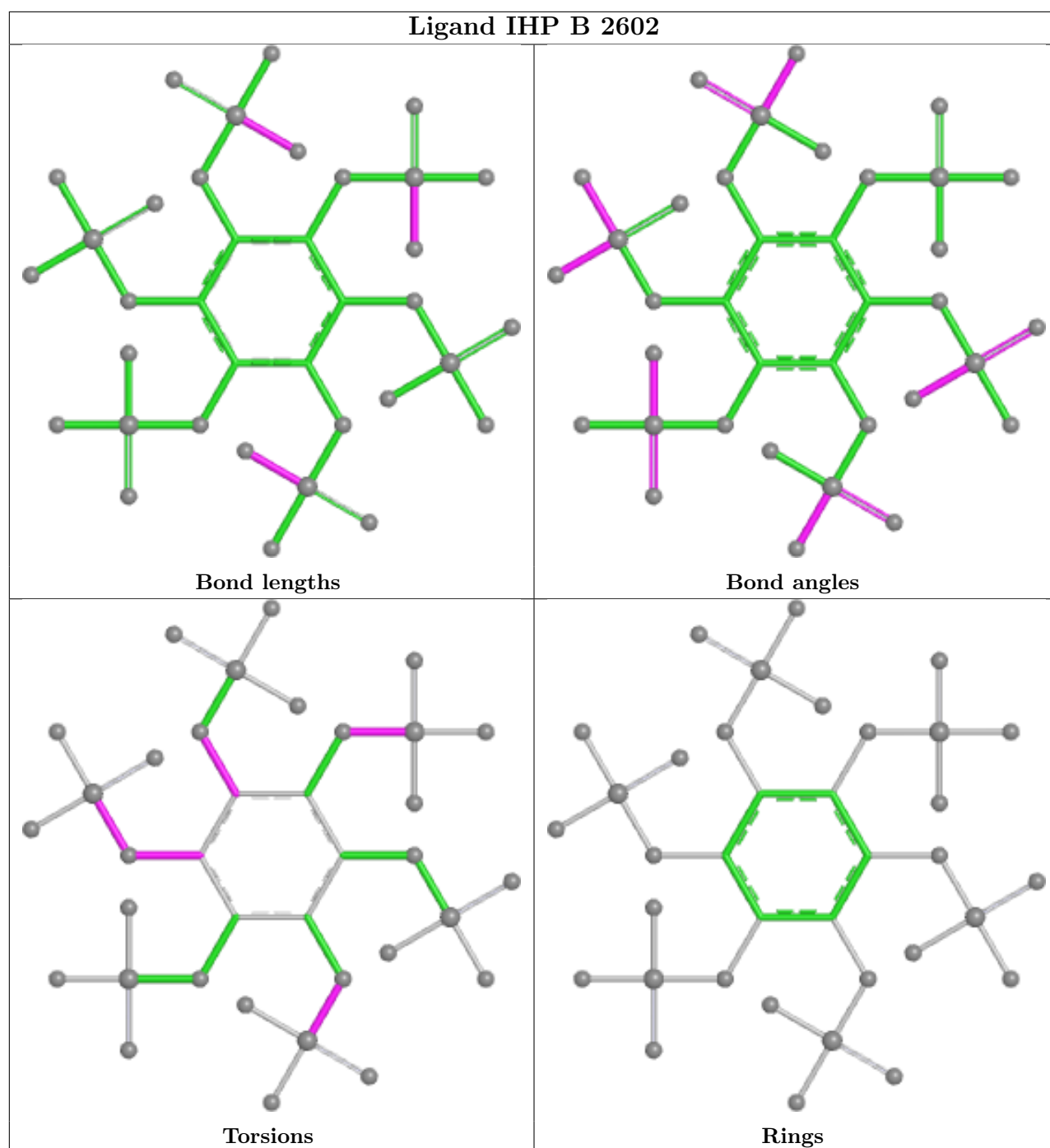
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2601	AGS	1	0
5	F	4802	AGS	1	0
6	B	2602	IHP	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

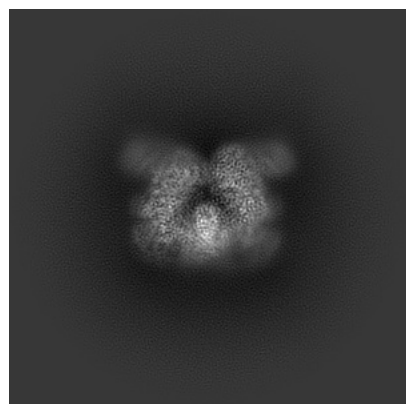
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11492. These allow visual inspection of the internal detail of the map and identification of artifacts.

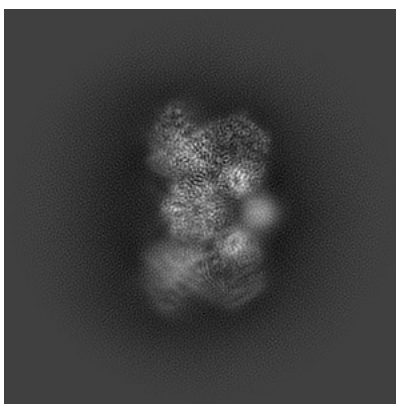
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

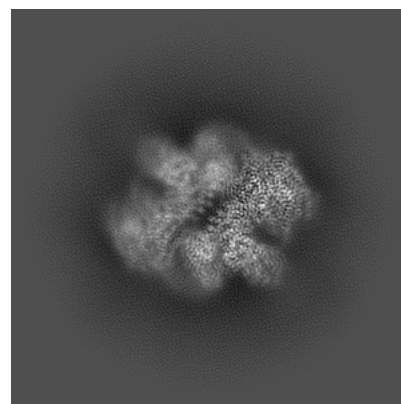
6.1.1 Primary map



X

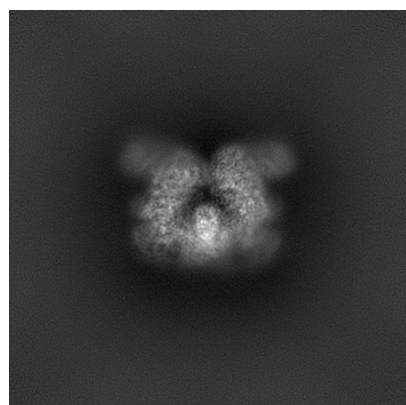


Y

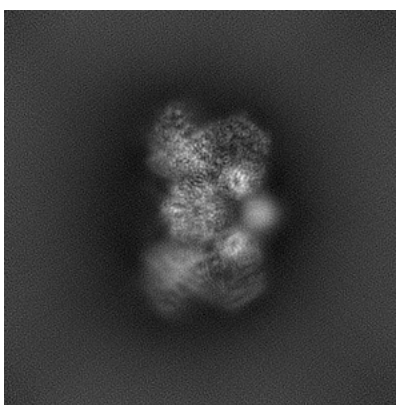


Z

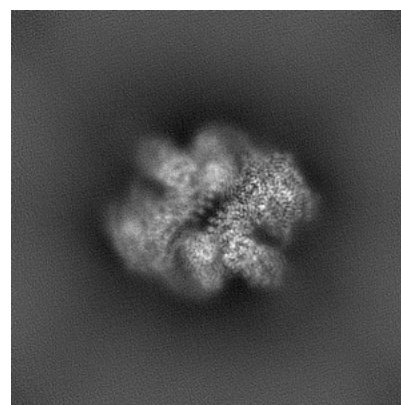
6.1.2 Raw map



X



Y



Z

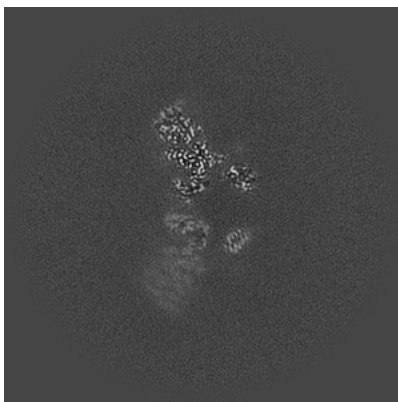
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

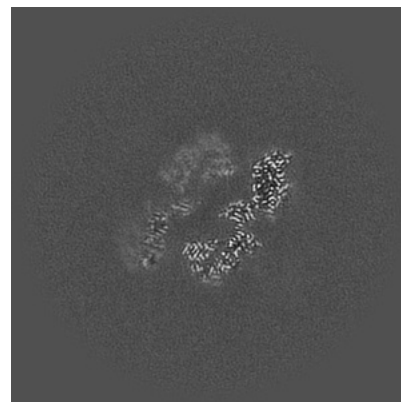
6.2.1 Primary map



X Index: 160

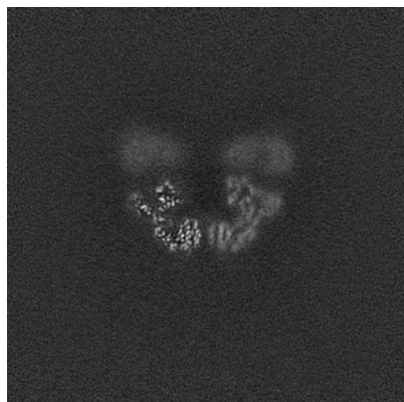


Y Index: 160



Z Index: 160

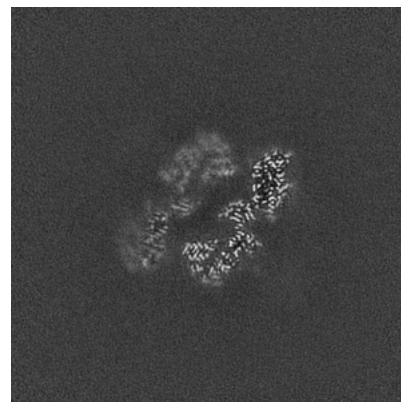
6.2.2 Raw map



X Index: 160



Y Index: 160

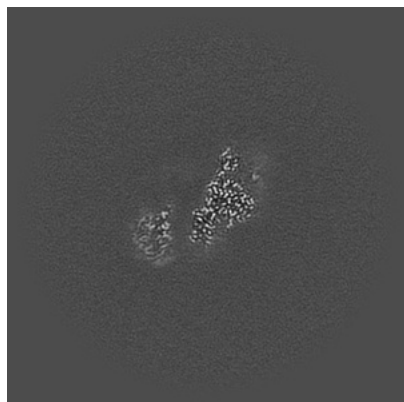


Z Index: 160

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

6.3 Largest variance slices [i](#)

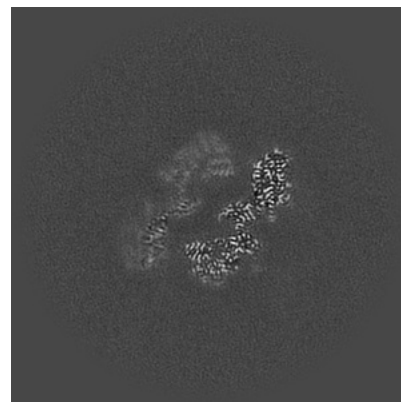
6.3.1 Primary map



X Index: 199

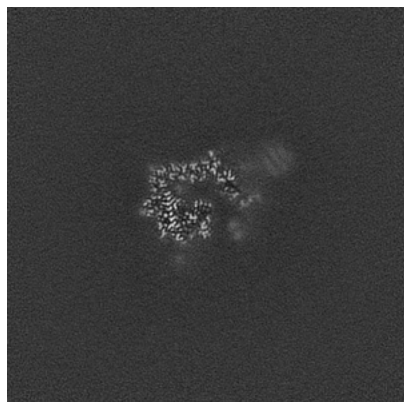


Y Index: 174



Z Index: 159

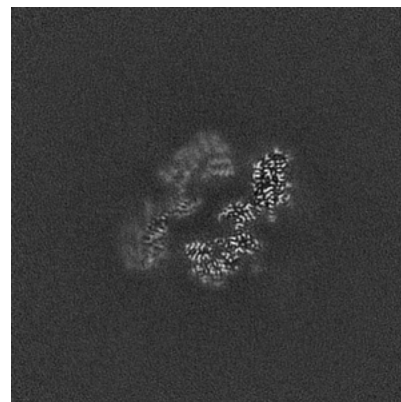
6.3.2 Raw map



X Index: 178



Y Index: 174

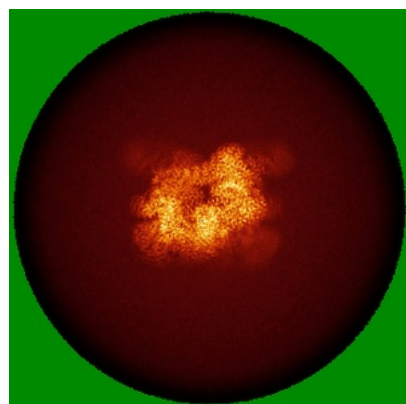


Z Index: 159

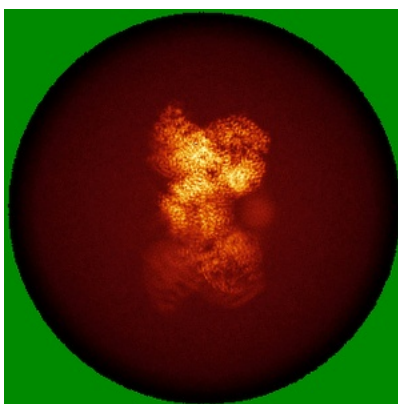
The images above show the largest variance slices of the map in three orthogonal directions.

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

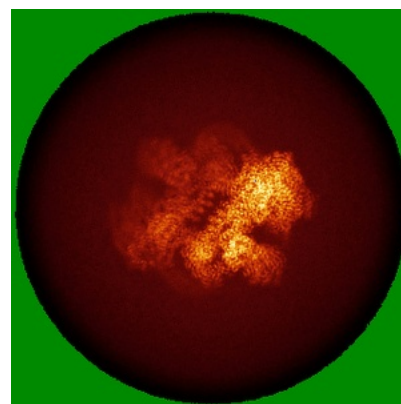
6.4.1 Primary map



X

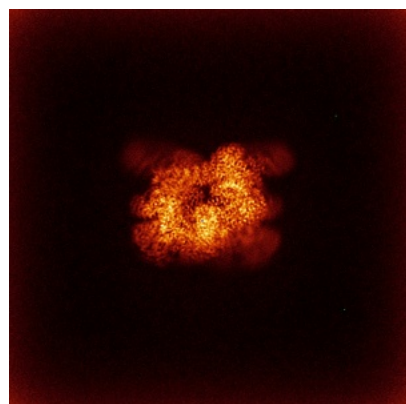


Y

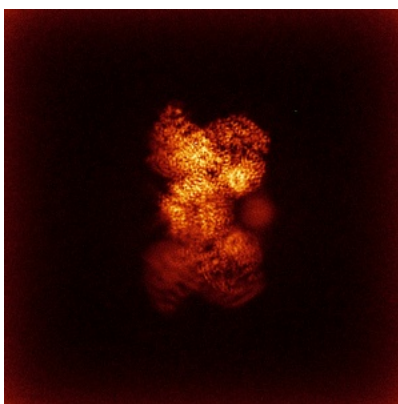


Z

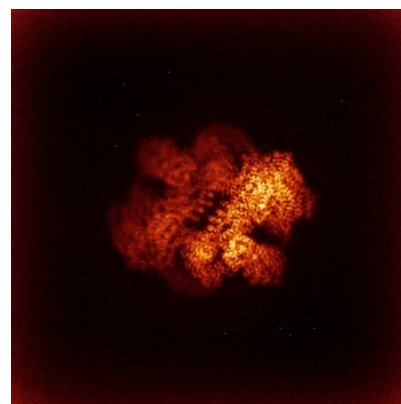
6.4.2 Raw map



X



Y

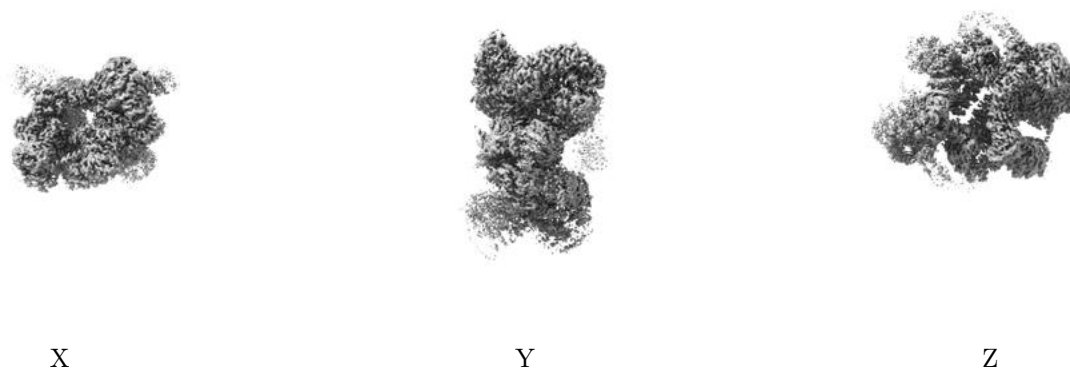


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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

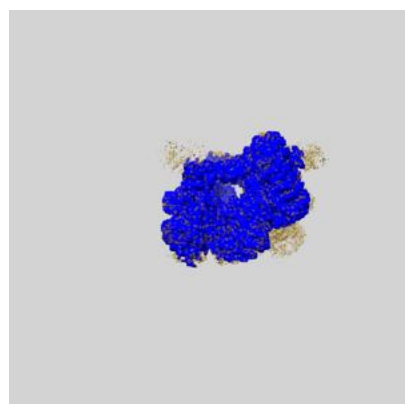
6.6 Mask visualisation [i](#)

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

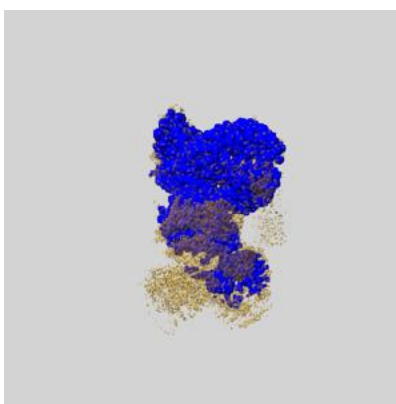
A mask typically either:

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

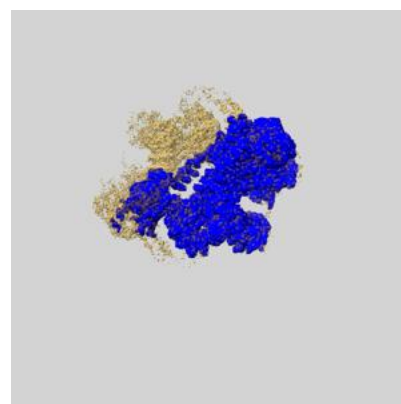
6.6.1 emd_11492_msk_2.map [i](#)



X

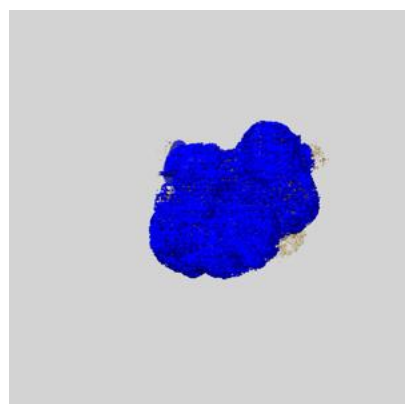


Y

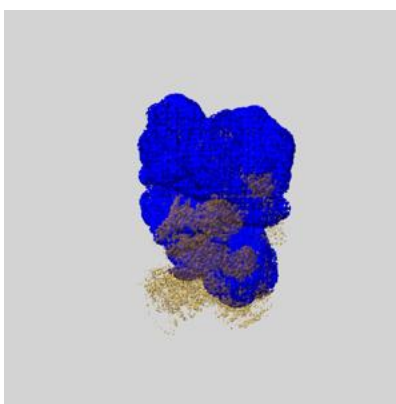


Z

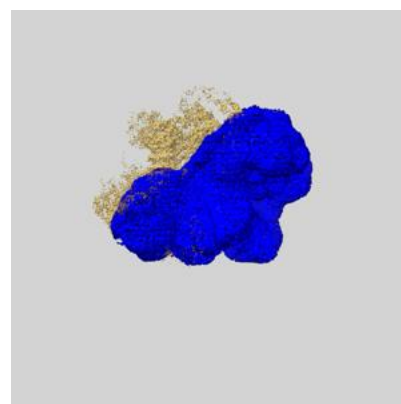
6.6.2 emd_11492_msk_1.map [i](#)



X



Y

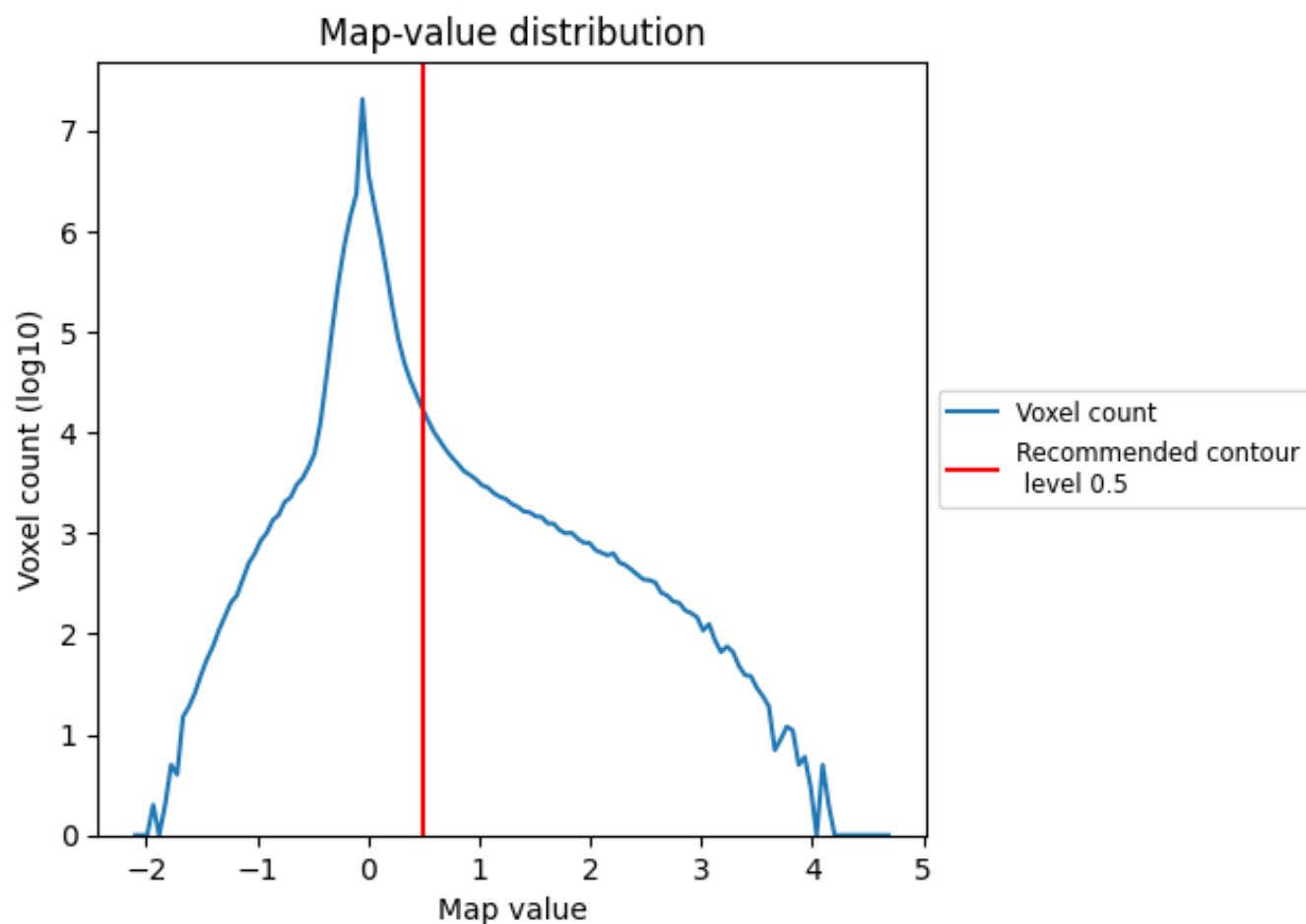


Z

7 Map analysis [i](#)

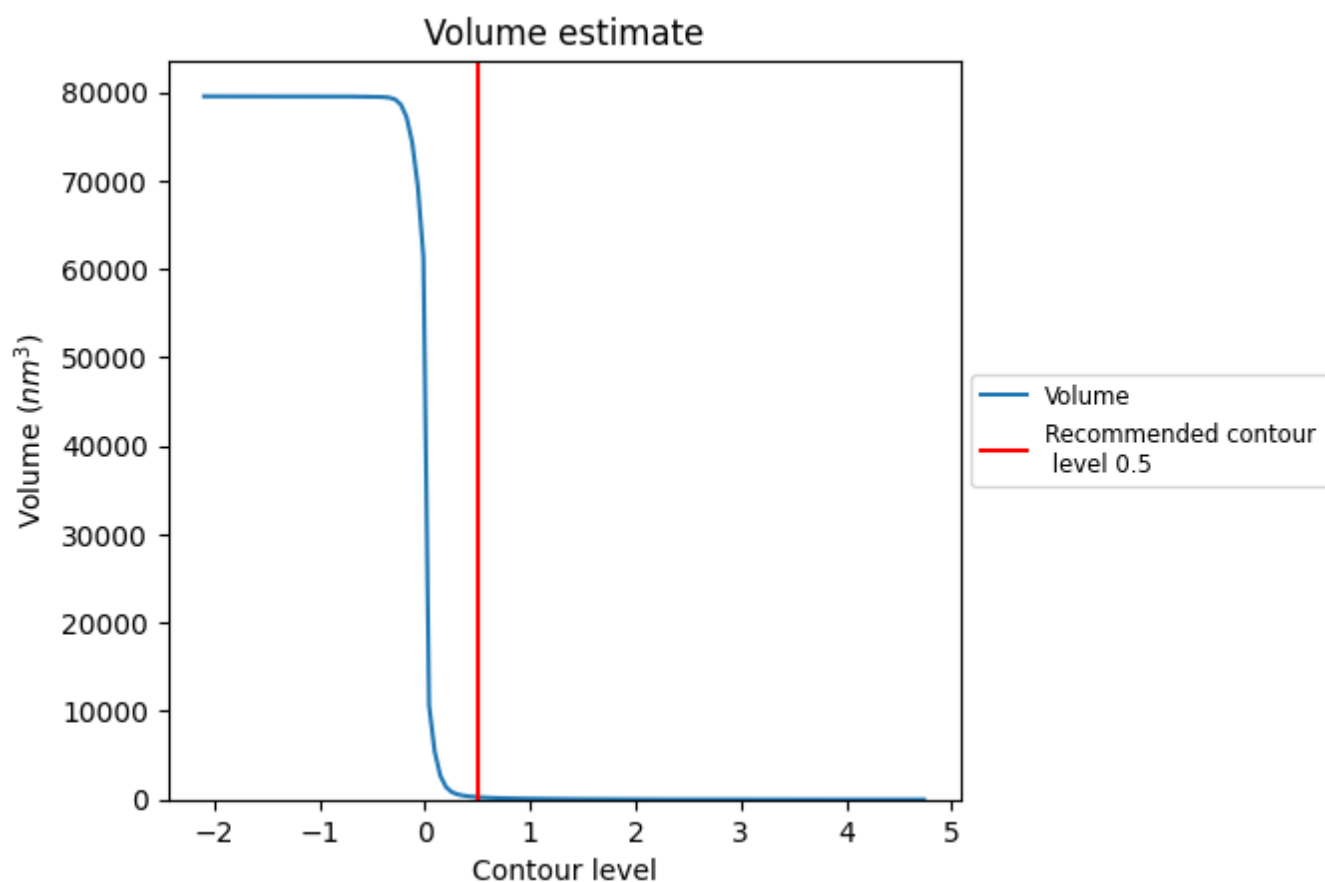
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

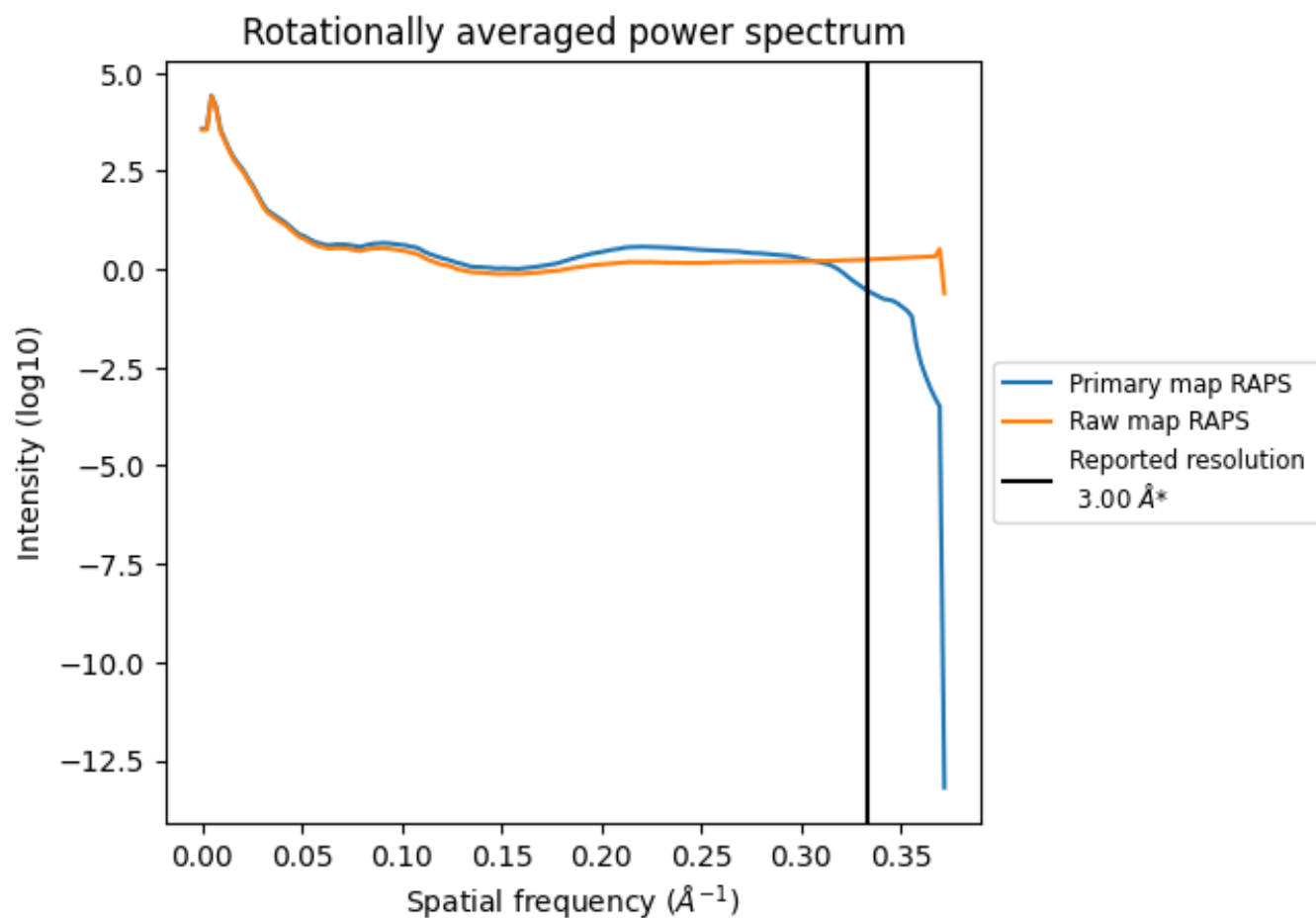
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 271 nm³; this corresponds to an approximate mass of 245 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

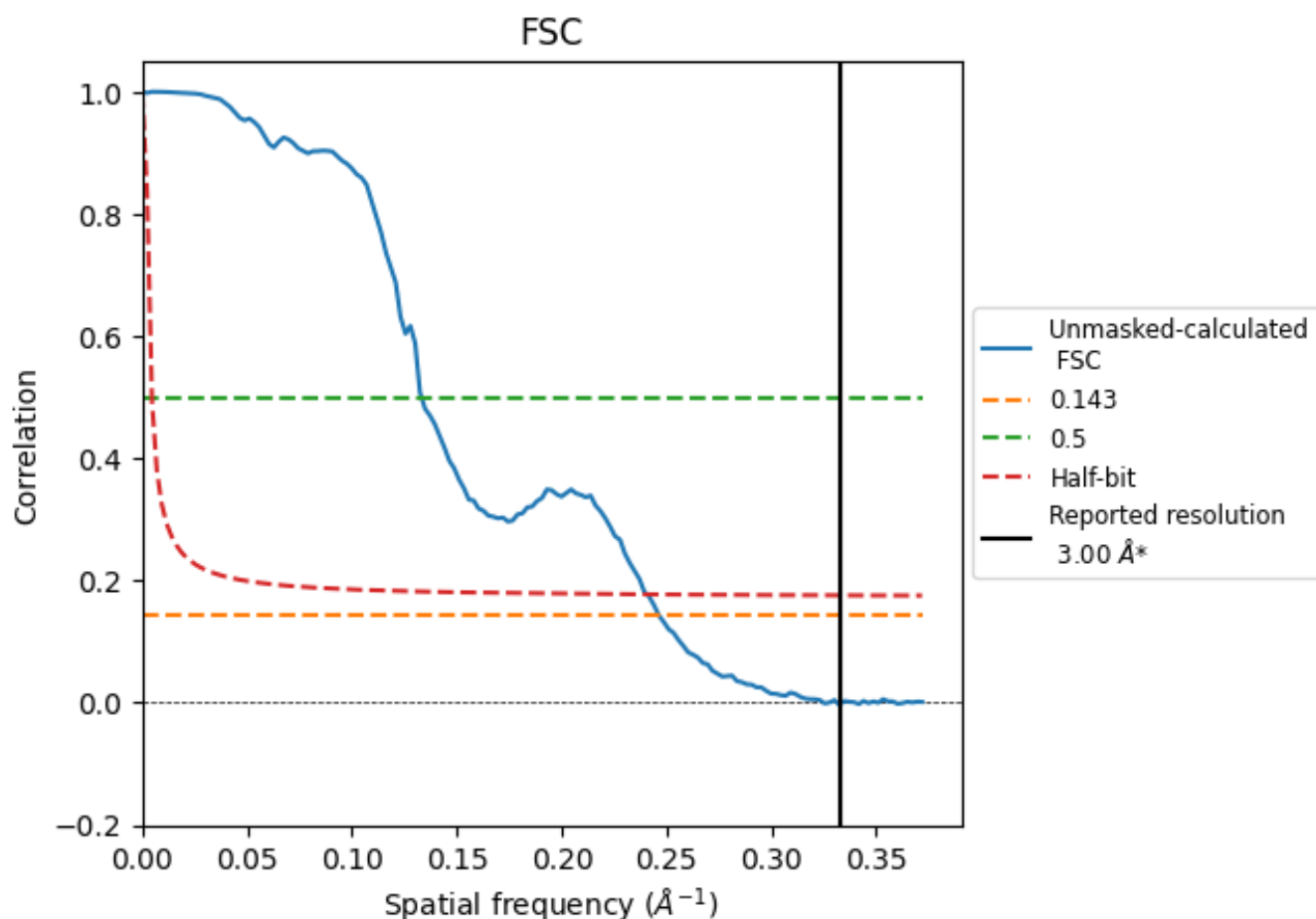


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

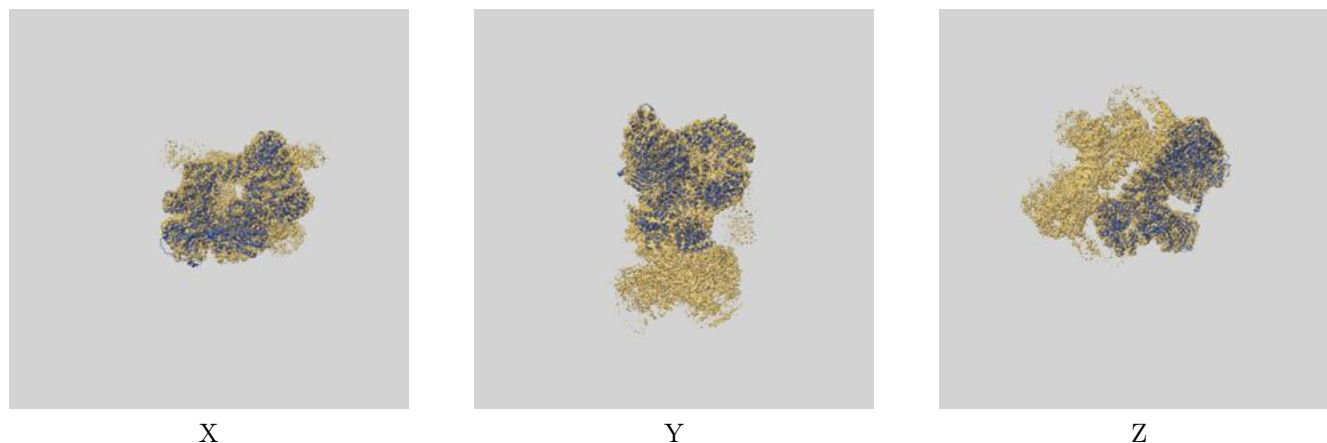
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	7.51	4.15

*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 4.06 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

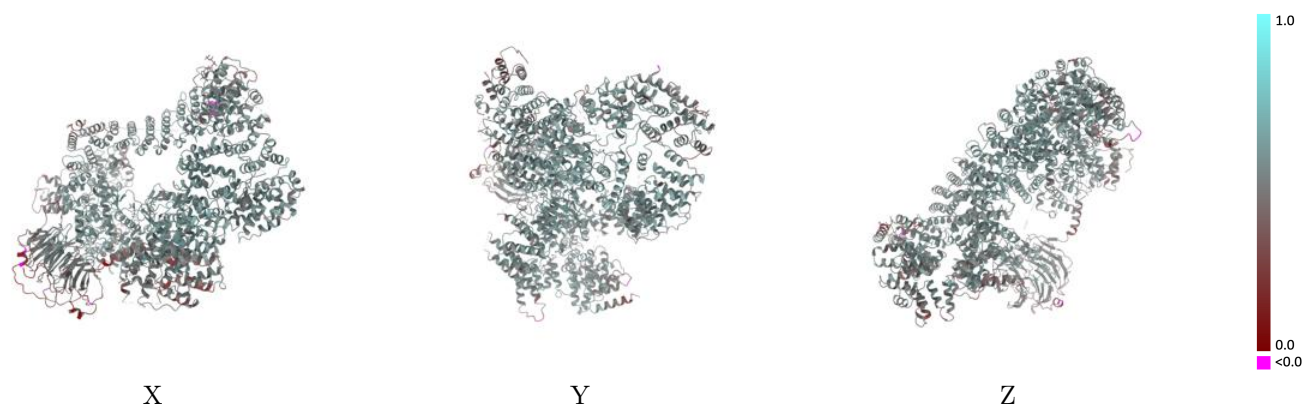
This section contains information regarding the fit between EMDB map EMD-11492 and PDB model 6ZWO. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



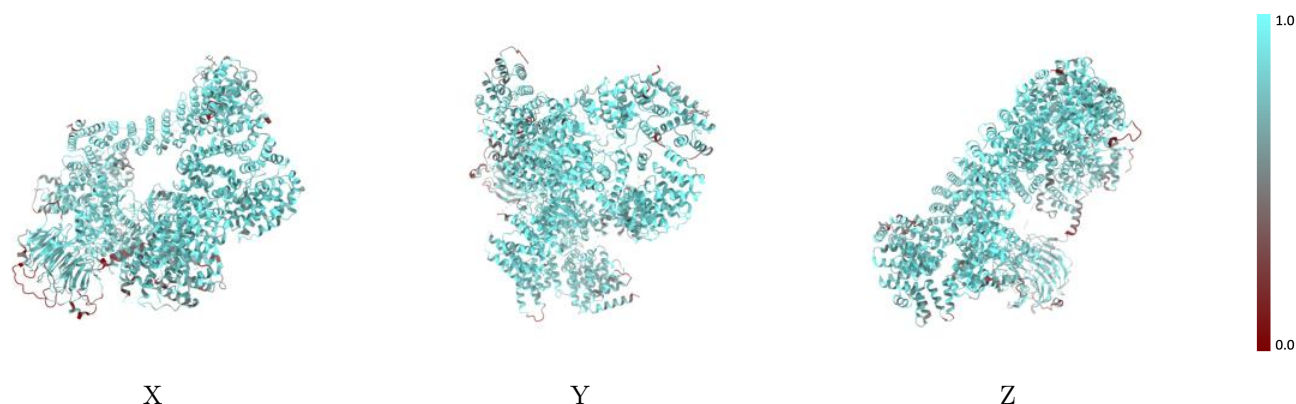
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



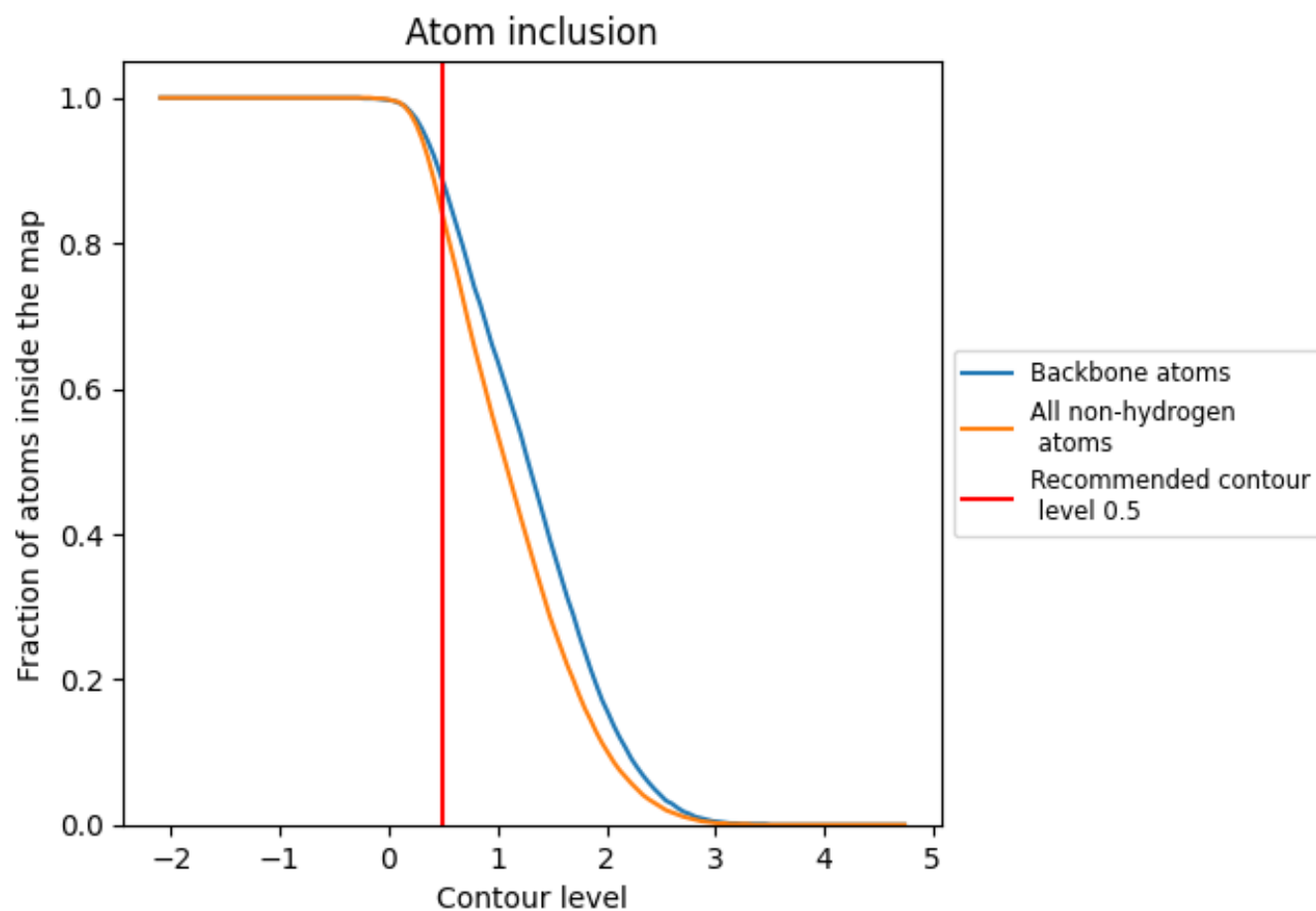
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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	0.8360	0.5270
B	0.8660	0.5390
D	0.7280	0.4530
F	0.8410	0.5370
H	0.6050	0.4240

