



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:50 PM UTC

PDB ID : 6WSL / pdb_00006wsl
EMDB ID : EMD-21893
Title : Cryo-EM structure of VASH1-SVBP bound to microtubules
Authors : Li, F.; Li, Y.; Yu, H.
Deposited on : 2020-05-01
Resolution : 3.10 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:

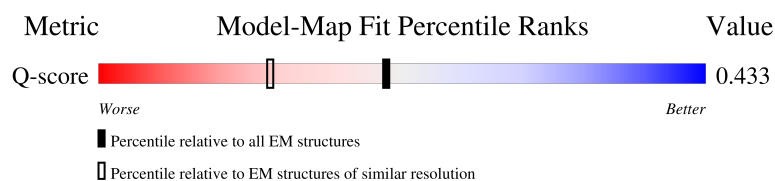
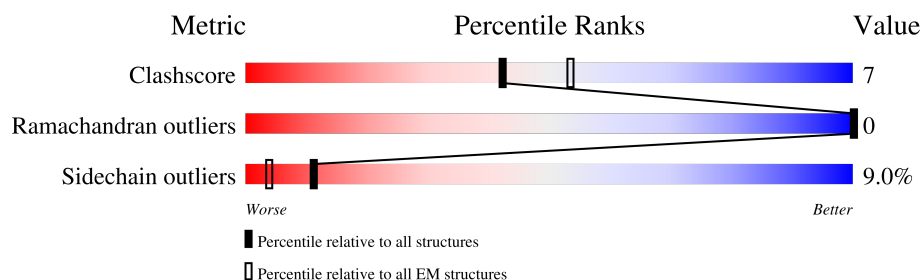
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	451	
1	E	451	
2	B	450	
2	F	450	

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Mol	Chain	Length	Quality of chain
3	C	259	25% 77% 18%
3	G	259	27% 79% 16%
4	D	66	12% 41% 6% 53%
4	H	66	14% 36% 11% 53%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18204 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 Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3378	2142	574	640	22		
1	E	431	Total	C	N	O	S	0	0
			3378	2142	574	640	22		

- Molecule 2 is a protein called Tubulin beta-3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	429	Total	C	N	O	S	0	0
			3370	2119	577	648	26		
2	F	429	Total	C	N	O	S	0	0
			3370	2119	577	648	26		

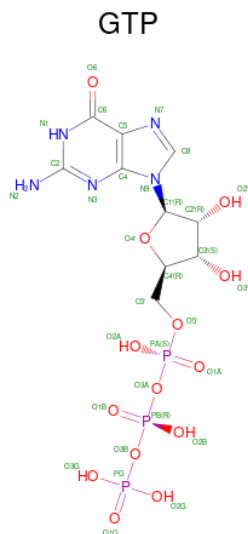
- Molecule 3 is a protein called Tubuliny1-Tyr carboxypeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	248	Total	C	N	O	S	0	0
			2026	1303	362	352	9		
3	G	248	Total	C	N	O	S	0	0
			2026	1303	362	352	9		

- Molecule 4 is a protein called Small vasohibin-binding protein.

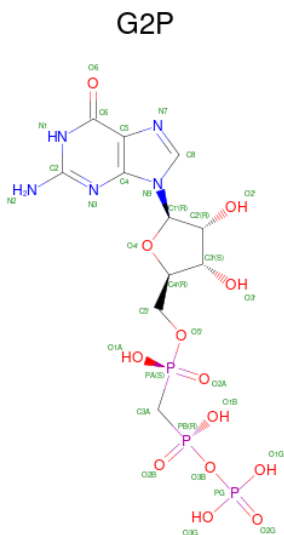
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	31	Total	C	N	O	S	0	0
			264	160	49	54	1		
4	H	31	Total	C	N	O	S	0	0
			264	160	49	54	1		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 32	C 10	N 5	O 14	P 3	0
5	E	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 6 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total 32	C 11	N 5	O 13	P 3	0

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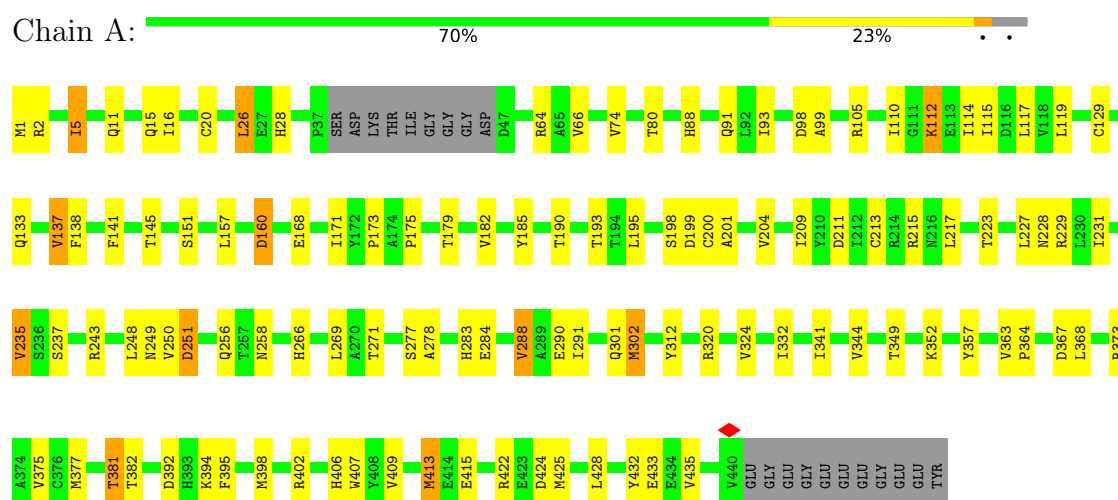
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	F	1	32	11	5	13	3	0

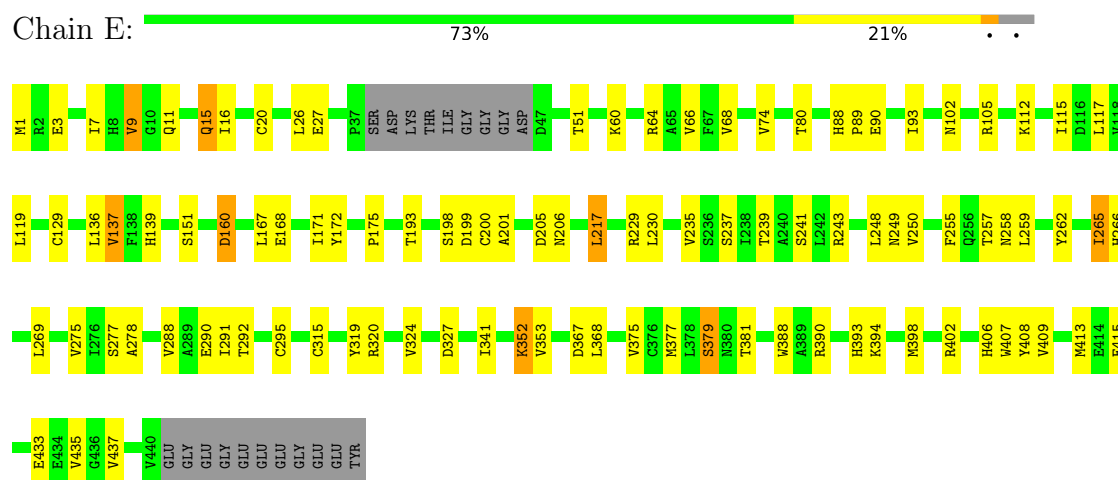
3 Residue-property plots

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

• Molecule 1: Tubulin alpha-1A chain

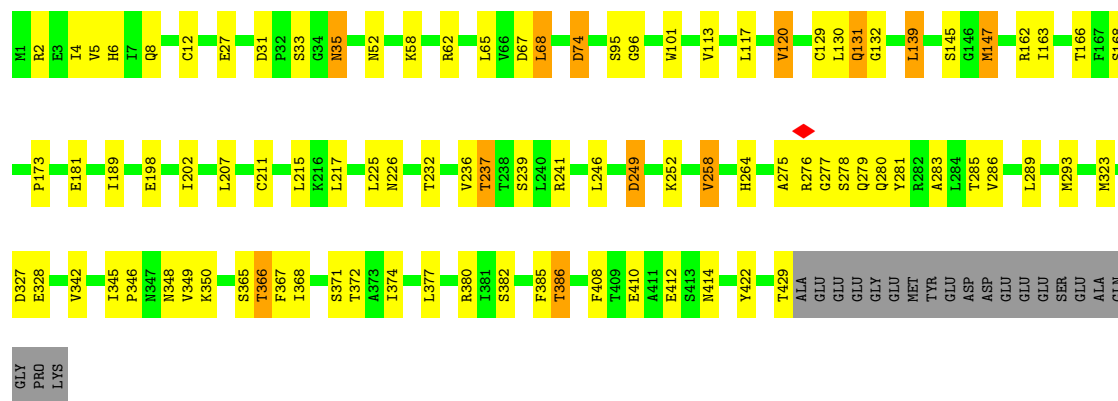


• Molecule 1: Tubulin alpha-1A chain



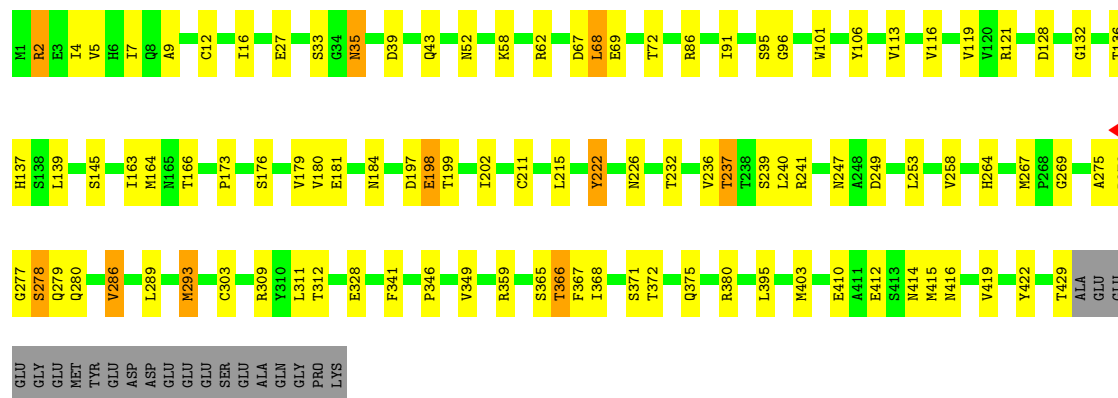
• Molecule 2: Tubulin beta-3 chain





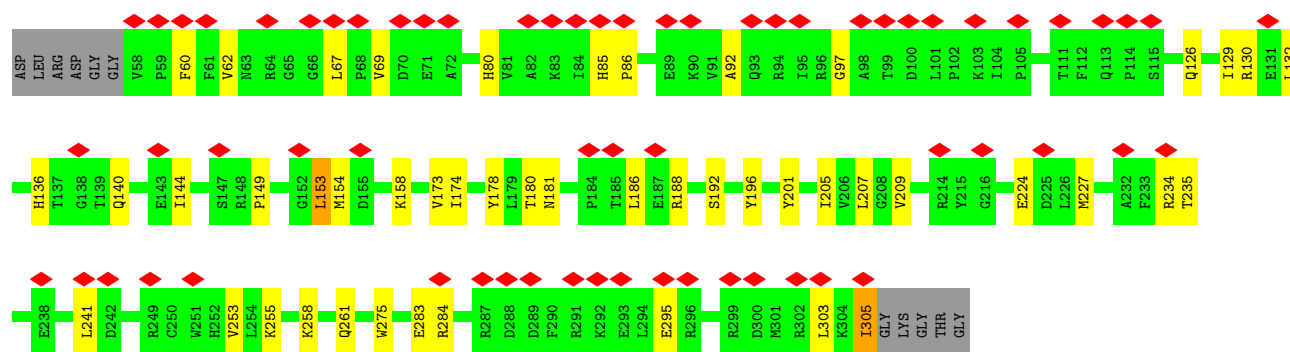
• Molecule 2: Tubulin beta-3 chain

Chain F: 73% 20% 5%



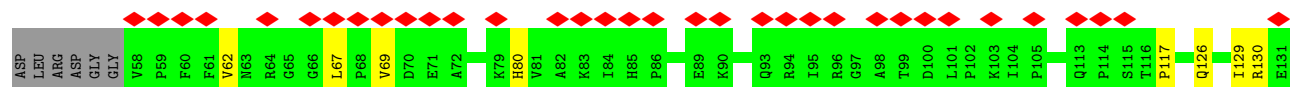
• Molecule 3: Tubuliny-Tyr carboxypeptidase 1

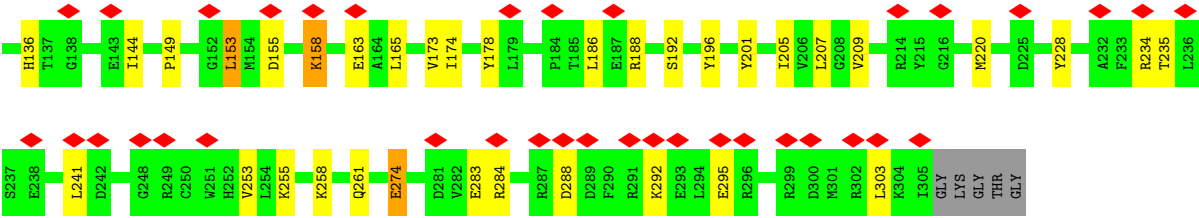
Chain C: 25% 77% 18%



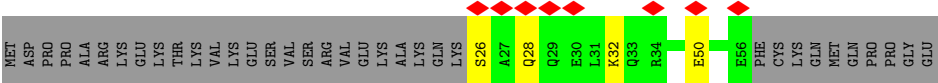
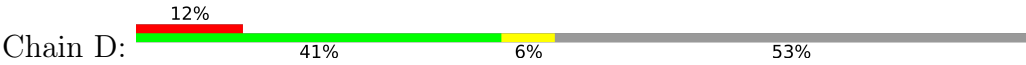
• Molecule 3: Tubuliny-Tyr carboxypeptidase 1

Chain G: 27% 79% 16%

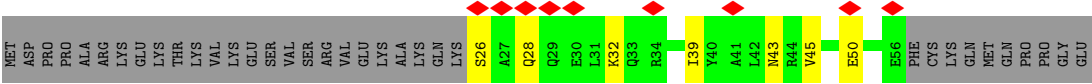
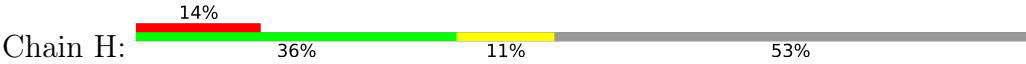




• Molecule 4: Small vasohibin-binding protein



• Molecule 4: Small vasohibin-binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46999	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.132	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	217.45999, 387.61, 180.94	wwPDB
Map dimensions	262, 467, 218	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, G2P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/3455	0.44	0/4691
1	E	0.29	0/3455	0.45	0/4691
2	B	0.28	0/3445	0.44	0/4666
2	F	0.28	0/3445	0.43	0/4666
3	C	0.15	0/2080	0.40	0/2811
3	G	0.15	0/2080	0.41	2/2811 (0.1%)
4	D	0.14	0/265	0.37	0/353
4	H	0.13	0/265	0.38	0/353
All	All	0.26	0/18490	0.43	2/25042 (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
2	B	0	1
2	F	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	117	PRO	CA-C-N	5.04	124.36	120.33
3	G	117	PRO	C-N-CA	5.04	124.36	120.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	286	VAL	Peptide
2	F	286	VAL	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	3378	0	3295	56	0
1	E	3378	0	3294	48	0
2	B	3370	0	3258	51	0
2	F	3370	0	3258	47	0
3	C	2026	0	2049	24	0
3	G	2026	0	2049	23	0
4	D	264	0	254	3	0
4	H	264	0	254	4	0
5	A	32	0	12	1	0
5	E	32	0	12	1	0
6	B	32	0	14	1	0
6	F	32	0	13	0	0
All	All	18204	0	17762	242	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 7.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:43:GLN:HE22	2:F:359:ARG:HH21	1.43	0.67
1:E:88:HIS:HD2	1:E:90:GLU:H	1.45	0.63
3:C:153:LEU:HD11	3:C:174:ILE:HD12	1.81	0.62
2:B:2:ARG:H	2:B:2:ARG:HE	1.48	0.61
3:C:186:LEU:HD11	3:C:209:VAL:HB	1.83	0.61
3:G:153:LEU:HD11	3:G:174:ILE:HD12	1.83	0.60
1:A:99:ALA:HB2	1:A:110:ILE:HD12	1.83	0.60
2:F:132:GLY:HA3	2:F:163:ILE:HG22	1.82	0.59
2:F:52:ASN:OD1	2:F:62:ARG:NH1	2.36	0.59
2:F:293:MET:SD	2:F:365:SER:OG	2.61	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:173:VAL:HG13	3:G:207:LEU:HB2	1.84	0.59
1:A:64:ARG:NH2	1:A:129:CYS:SG	2.76	0.59
1:E:172:TYR:HH	1:E:388:TRP:CD1	2.20	0.58
2:F:366:THR:OG1	2:F:367:PHE:N	2.35	0.58
1:A:284:GLU:HB2	1:E:88:HIS:HE1	1.69	0.58
1:A:398:MET:HE2	2:B:346:PRO:HD2	1.86	0.58
1:E:11:GLN:HB3	5:E:501:GTP:H5"	1.87	0.57
2:F:198:GLU:HA	2:F:264:HIS:HB2	1.86	0.56
3:G:192:SER:HB2	3:G:258:LYS:HD2	1.87	0.56
3:C:283:GLU:HG3	3:C:284:ARG:HG3	1.88	0.56
2:B:2:ARG:HB3	2:B:131:GLN:HB2	1.88	0.56
2:B:207:LEU:HB3	2:B:225:LEU:HD22	1.87	0.56
1:A:93:ILE:HD12	1:A:117:LEU:HG	1.88	0.56
2:B:276:ARG:O	2:B:280:GLN:NE2	2.39	0.55
3:G:188:ARG:HB3	3:G:207:LEU:HD11	1.88	0.55
1:A:151:SER:HA	1:A:193:THR:HG21	1.88	0.55
2:B:67:ASP:OD1	2:B:67:ASP:N	2.37	0.55
2:F:275:ALA:HB3	2:F:279:GLN:H	1.71	0.55
3:C:173:VAL:HG13	3:C:207:LEU:HB2	1.88	0.55
1:E:239:THR:O	1:E:243:ARG:NH1	2.40	0.55
2:F:277:GLY:HA2	2:F:280:GLN:HE21	1.72	0.55
2:F:101:TRP:NE1	2:F:145:SER:O	2.40	0.55
2:B:198:GLU:HA	2:B:264:HIS:HB2	1.89	0.55
2:F:164:MET:HB3	2:F:197:ASP:H	1.71	0.55
1:E:11:GLN:NE2	1:E:15:GLN:OE1	2.38	0.55
3:G:126:GLN:HE21	3:G:130:ARG:HG3	1.72	0.55
2:F:35:ASN:OD1	2:F:35:ASN:N	2.40	0.55
2:B:35:ASN:N	2:B:35:ASN:OD1	2.40	0.54
3:C:196:TYR:HB3	3:C:253:VAL:HB	1.88	0.54
1:A:160:ASP:OD1	1:A:160:ASP:N	2.38	0.54
2:B:237:THR:O	2:B:241:ARG:NH1	2.41	0.54
1:A:16:ILE:O	1:A:20:CYS:N	2.40	0.54
2:B:293:MET:SD	2:B:365:SER:OG	2.65	0.54
3:G:186:LEU:HD11	3:G:209:VAL:HB	1.90	0.54
3:G:136:HIS:ND1	4:H:50:GLU:OE1	2.38	0.54
2:B:117:LEU:HA	2:B:120:VAL:HG12	1.90	0.54
2:B:278:SER:OG	2:B:279:GLN:OE1	2.26	0.54
4:H:39:ILE:O	4:H:43:ASN:ND2	2.39	0.54
2:B:101:TRP:NE1	2:B:145:SER:O	2.40	0.53
1:A:433:GLU:HB2	3:C:149:PRO:HG3	1.89	0.53
1:E:1:MET:SD	1:E:1:MET:N	2.78	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:SD	1:A:1:MET:N	2.78	0.53
4:D:26:SER:O	4:D:28:GLN:NE2	2.41	0.53
3:G:173:VAL:HG21	3:G:205:ILE:HG12	1.90	0.53
2:F:2:ARG:HD3	2:F:240:LEU:HD22	1.91	0.53
2:B:52:ASN:OD1	2:B:62:ARG:NH1	2.42	0.53
3:C:192:SER:HB2	3:C:258:LYS:HD2	1.90	0.53
2:B:279:GLN:HG3	2:B:283:ALA:HB3	1.91	0.53
1:E:198:SER:OG	1:E:199:ASP:N	2.42	0.53
1:E:160:ASP:OD1	1:E:160:ASP:N	2.41	0.52
1:E:151:SER:HA	1:E:193:THR:HG21	1.91	0.52
2:F:276:ARG:O	2:F:280:GLN:NE2	2.42	0.52
3:G:283:GLU:HG3	3:G:284:ARG:HG3	1.89	0.52
1:E:295:CYS:HB3	1:E:377:MET:HG2	1.90	0.52
2:B:249:ASP:OD1	2:B:249:ASP:N	2.43	0.52
1:E:9:VAL:HG13	1:E:139:HIS:HB3	1.91	0.52
1:E:398:MET:HE2	2:F:346:PRO:HD2	1.91	0.52
2:B:366:THR:OG1	2:B:367:PHE:N	2.40	0.52
1:E:377:MET:SD	1:E:379:SER:OG	2.68	0.52
2:F:278:SER:OG	2:F:279:GLN:N	2.43	0.52
2:B:278:SER:OG	2:B:279:GLN:N	2.42	0.52
2:F:67:ASP:N	2:F:67:ASP:OD1	2.40	0.52
2:B:211:CYS:HA	2:B:215:LEU:HB3	1.92	0.51
3:G:126:GLN:NE2	3:G:220:MET:SD	2.83	0.51
2:F:412:GLU:OE2	2:F:416:ASN:ND2	2.44	0.51
2:F:371:SER:OG	2:F:372:THR:N	2.44	0.51
2:B:74:ASP:N	2:B:74:ASP:OD1	2.43	0.51
2:F:237:THR:O	2:F:241:ARG:NH1	2.44	0.51
3:G:196:TYR:HB3	3:G:253:VAL:HB	1.92	0.51
3:C:126:GLN:HE21	3:C:130:ARG:HG3	1.76	0.51
2:B:27:GLU:OE1	2:B:241:ARG:NH2	2.42	0.51
4:H:26:SER:O	4:H:28:GLN:NE2	2.42	0.51
1:A:406:HIS:HA	1:A:409:VAL:HG12	1.92	0.50
2:B:226:ASN:OD1	6:B:501:G2P:N1	2.34	0.50
1:E:237:SER:OG	1:E:320:ARG:NE	2.44	0.50
3:C:305:ILE:HD13	1:E:112:LYS:HD3	1.91	0.50
1:E:93:ILE:HD12	1:E:117:LEU:HG	1.92	0.50
3:C:201:TYR:HE1	3:C:255:LYS:HE2	1.76	0.50
2:B:132:GLY:HA3	2:B:163:ILE:HG22	1.93	0.50
2:F:410:GLU:O	2:F:414:ASN:ND2	2.45	0.50
1:A:137:VAL:HG22	1:A:168:GLU:HA	1.94	0.50
1:A:175:PRO:O	1:A:394:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ALA:HA	1:A:105:ARG:HH21	1.77	0.49
2:F:2:ARG:NH1	2:F:249:ASP:OD2	2.44	0.49
1:E:175:PRO:O	1:E:394:LYS:NZ	2.45	0.49
3:C:173:VAL:HG21	3:C:205:ILE:HG12	1.95	0.49
1:E:229:ARG:NH2	1:E:367:ASP:OD2	2.45	0.49
1:E:402:ARG:NH1	1:E:415:GLU:OE2	2.46	0.49
1:A:271:THR:HB	1:A:377:MET:HG3	1.95	0.49
2:B:33:SER:O	2:B:58:LYS:NZ	2.44	0.49
2:B:130:LEU:O	2:B:162:ARG:NH1	2.43	0.49
3:C:192:SER:HA	3:C:205:ILE:HA	1.95	0.49
1:E:277:SER:OG	1:E:278:ALA:N	2.45	0.49
2:F:211:CYS:HA	2:F:215:LEU:HB3	1.95	0.49
3:C:60:PHE:HB2	3:C:140:GLN:HB2	1.94	0.48
1:E:239:THR:OG1	1:E:243:ARG:NH1	2.45	0.48
1:E:433:GLU:HB2	3:G:149:PRO:HG3	1.94	0.48
2:B:237:THR:OG1	2:B:241:ARG:NH1	2.45	0.48
3:C:67:LEU:HD13	4:D:32:LYS:HE3	1.94	0.48
3:G:192:SER:HA	3:G:205:ILE:HA	1.95	0.48
1:A:28:HIS:HE1	1:A:243:ARG:HH11	1.60	0.48
1:A:145:THR:N	5:A:501:GTP:O2B	2.40	0.48
1:E:64:ARG:NH2	1:E:129:CYS:SG	2.75	0.48
2:B:252:LYS:HE2	2:B:350:LYS:HZ1	1.78	0.48
1:E:137:VAL:HG22	1:E:168:GLU:HA	1.95	0.47
2:F:106:TYR:HE2	2:F:403:MET:HE3	1.78	0.47
3:G:67:LEU:HD13	4:H:32:LYS:HE3	1.96	0.47
1:A:237:SER:OG	1:A:320:ARG:NE	2.47	0.47
3:C:234:ARG:HG3	3:C:235:THR:HG23	1.96	0.47
1:E:406:HIS:HA	1:E:409:VAL:HG12	1.96	0.47
1:E:16:ILE:O	1:E:20:CYS:N	2.43	0.47
1:A:213:CYS:HA	1:A:217:LEU:HB3	1.97	0.47
2:B:236:VAL:HG22	2:B:368:ILE:HD11	1.96	0.47
1:E:3:GLU:HA	1:E:51:THR:HA	1.95	0.47
2:B:173:PRO:HG3	2:B:380:ARG:HD3	1.97	0.47
1:E:27:GLU:OE1	1:E:243:ARG:NH2	2.38	0.47
1:A:182:VAL:HG22	1:A:185:TYR:HB2	1.97	0.47
1:A:312:TYR:HD1	1:A:381:THR:HB	1.80	0.47
1:E:217:LEU:HD23	1:E:277:SER:HB2	1.97	0.47
1:A:395:PHE:HE2	1:A:422:ARG:HB2	1.78	0.47
1:E:292:THR:HG1	1:E:319:TYR:HH	1.56	0.47
1:E:7:ILE:HG22	1:E:66:VAL:HB	1.96	0.46
1:A:277:SER:OG	1:A:278:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:GLY:HA2	2:B:280:GLN:HE21	1.79	0.46
3:C:224:GLU:HA	3:C:227:MET:HG3	1.98	0.46
1:A:5:ILE:HG22	1:A:64:ARG:HH12	1.80	0.46
1:A:16:ILE:HD11	1:A:171:ILE:HD11	1.97	0.46
2:B:215:LEU:HG	2:B:217:LEU:HG	1.98	0.46
2:F:278:SER:OG	2:F:279:GLN:OE1	2.34	0.45
2:F:375:GLN:HB2	2:F:419:VAL:HG13	1.97	0.45
3:C:188:ARG:HB3	3:C:207:LEU:HD11	1.99	0.45
1:A:2:ARG:HA	1:A:133:GLN:HE21	1.81	0.45
1:A:283:HIS:HD2	1:E:89:PRO:HD3	1.81	0.45
1:A:402:ARG:NH1	1:A:415:GLU:OE2	2.49	0.45
2:F:222:TYR:O	2:F:226:ASN:ND2	2.37	0.45
3:G:261:GLN:H	3:G:274:GLU:HG2	1.81	0.45
3:C:92:ALA:O	3:C:97:GLY:N	2.46	0.45
1:A:198:SER:OG	1:A:199:ASP:N	2.50	0.45
1:A:229:ARG:NH1	1:A:367:ASP:OD2	2.46	0.45
1:A:179:THR:HG21	2:B:246:LEU:HD21	1.99	0.45
1:A:271:THR:OG1	1:A:301:GLN:OE1	2.35	0.45
1:A:377:MET:HE2	1:A:377:MET:HB2	1.85	0.45
2:F:267:MET:HE1	2:F:303:CYS:HB2	1.98	0.45
1:A:11:GLN:NE2	1:A:15:GLN:OE1	2.49	0.44
2:F:33:SER:O	2:F:58:LYS:NZ	2.49	0.44
1:A:112:LYS:HE2	1:A:112:LYS:HB3	1.85	0.44
2:B:429:THR:O	2:B:429:THR:OG1	2.35	0.44
2:B:232:THR:O	2:B:232:THR:OG1	2.35	0.44
2:B:385:PHE:HE2	2:B:412:GLU:HB2	1.82	0.44
2:F:69:GLU:HB2	2:F:96:GLY:HA3	1.99	0.44
3:C:136:HIS:ND1	4:D:50:GLU:OE1	2.39	0.44
1:E:168:GLU:HB3	1:E:201:ALA:HA	1.99	0.44
1:E:205:ASP:OD1	1:E:206:ASN:N	2.48	0.44
3:G:201:TYR:HE1	3:G:255:LYS:HE2	1.83	0.44
2:F:27:GLU:OE2	2:F:241:ARG:NH2	2.50	0.44
2:F:67:ASP:OD2	2:F:72:THR:OG1	2.35	0.44
3:G:158:LYS:NZ	3:G:178:TYR:OH	2.43	0.44
1:E:102:ASN:HA	1:E:408:TYR:HE1	1.83	0.44
1:E:315:CYS:HA	1:E:379:SER:HA	1.99	0.43
3:G:288:ASP:OD1	3:G:292:LYS:NZ	2.43	0.43
1:E:102:ASN:HB3	1:E:105:ARG:HB2	2.01	0.43
1:E:258:ASN:OD1	1:E:352:LYS:NZ	2.42	0.43
2:F:173:PRO:HG3	2:F:380:ARG:HD3	2.00	0.43
1:A:302:MET:HE3	1:A:302:MET:HB3	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:ALA:HB3	2:F:137:HIS:HB3	2.00	0.43
1:E:3:GLU:OE1	1:E:64:ARG:NH2	2.50	0.43
2:B:139:LEU:HD13	2:B:168:SER:HB2	2.00	0.43
2:B:275:ALA:H	2:B:279:GLN:HB2	1.83	0.43
2:F:39:ASP:OD1	2:F:39:ASP:N	2.40	0.43
2:F:68:LEU:HB3	2:F:96:GLY:HA2	2.00	0.43
2:F:236:VAL:HG22	2:F:368:ILE:HD11	2.00	0.43
1:A:195:LEU:HD11	1:A:428:LEU:HD22	2.00	0.43
3:C:129:ILE:HG23	3:C:132:LEU:HD12	2.00	0.43
1:E:377:MET:HB2	1:E:377:MET:HE2	1.80	0.43
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.37	0.43
2:B:68:LEU:HD13	2:B:68:LEU:HA	1.88	0.43
2:B:147:MET:HE2	2:B:147:MET:HB2	1.92	0.43
1:E:262:TYR:HB2	1:E:265:ILE:HG13	2.00	0.43
1:A:251:ASP:N	1:A:251:ASP:OD1	2.52	0.42
1:A:99:ALA:HB1	1:A:105:ARG:HB3	2.00	0.42
3:G:129:ILE:HG23	3:G:132:LEU:HD12	2.01	0.42
1:A:168:GLU:HB3	1:A:201:ALA:HA	2.00	0.42
2:B:283:ALA:HB1	2:F:86:ARG:HE	1.84	0.42
2:B:345:ILE:HG22	2:B:348:ASN:HB3	2.01	0.42
1:A:88:HIS:H	1:A:91:GLN:NE2	2.17	0.42
1:A:141:PHE:HB2	1:A:173:PRO:HD3	2.00	0.42
1:A:288:VAL:HG22	1:A:373:ARG:HD3	2.01	0.42
1:A:98:ASP:OD1	1:A:98:ASP:N	2.52	0.42
1:A:228:ASN:HA	1:A:231:ILE:HG22	2.00	0.42
3:G:234:ARG:HG3	3:G:235:THR:HG23	2.01	0.42
1:E:200:CYS:H	1:E:266:HIS:HB2	1.83	0.42
1:A:290:GLU:H	1:A:290:GLU:HG2	1.68	0.42
3:G:155:ASP:HA	3:G:158:LYS:HB2	2.02	0.42
2:F:16:ILE:HD11	2:F:136:THR:HB	2.01	0.42
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.68	0.42
2:B:323:MET:HE3	2:B:323:MET:HB3	1.93	0.42
1:E:175:PRO:HG3	1:E:390:ARG:HD3	2.01	0.42
2:F:365:SER:OG	2:F:365:SER:O	2.38	0.41
3:G:165:LEU:HD23	3:G:165:LEU:HA	1.92	0.41
1:A:200:CYS:H	1:A:266:HIS:HB2	1.85	0.41
1:A:407:TRP:HE1	2:B:258:VAL:HG23	1.84	0.41
2:F:309:ARG:NH1	2:F:341:PHE:O	2.53	0.41
1:A:363:VAL:HA	1:A:364:PRO:HD3	1.92	0.41
1:E:102:ASN:ND2	1:E:407:TRP:O	2.46	0.41
2:F:95:SER:OG	2:F:96:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:429:THR:O	2:F:429:THR:OG1	2.35	0.41
1:A:211:ASP:HB3	1:A:215:ARG:HH11	1.86	0.41
1:E:136:LEU:HD12	1:E:167:LEU:HB2	2.02	0.41
1:A:26:LEU:HD13	1:A:26:LEU:HA	1.92	0.41
1:A:138:PHE:HZ	1:A:235:VAL:HG11	1.86	0.41
1:A:413:MET:HE3	1:A:413:MET:HB2	1.91	0.41
2:B:410:GLU:O	2:B:414:ASN:ND2	2.53	0.41
2:F:269:GLY:O	2:F:367:PHE:N	2.53	0.41
3:C:154:MET:HE1	3:C:178:TYR:HA	2.01	0.41
2:B:371:SER:OG	2:B:372:THR:N	2.51	0.41
2:B:385:PHE:HZ	2:B:408:PHE:HB3	1.86	0.41
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.89	0.41
3:C:85:HIS:HA	3:C:86:PRO:HD3	1.96	0.41
2:B:95:SER:OG	2:B:96:GLY:N	2.54	0.41
3:C:158:LYS:NZ	3:C:178:TYR:OH	2.40	0.41
2:B:382:SER:O	2:B:386:THR:OG1	2.28	0.40
2:F:91:ILE:HD13	2:F:116:VAL:HA	2.03	0.40
2:F:415:MET:HB2	2:F:415:MET:HE3	1.81	0.40
1:E:292:THR:OG1	1:E:319:TYR:OH	2.31	0.40
2:B:374:ILE:HD12	2:B:374:ILE:HA	1.94	0.40
2:F:128:ASP:OD1	2:F:128:ASP:N	2.52	0.40
1:A:114:ILE:HD12	1:A:114:ILE:HA	1.89	0.40
3:C:178:TYR:O	3:C:181:ASN:ND2	2.55	0.40
3:G:163:GLU:HG2	3:G:165:LEU:HG	2.02	0.40
1:A:381:THR:OG1	1:A:382:THR:N	2.54	0.40
1:E:327:ASP:OD1	1:E:327:ASP:N	2.54	0.40
2:F:184:ASN:OD1	2:F:184:ASN:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/451 (95%)	399 (93%)	28 (7%)	0	100	100
1	E	427/451 (95%)	397 (93%)	30 (7%)	0	100	100
2	B	427/450 (95%)	395 (92%)	32 (8%)	0	100	100
2	F	427/450 (95%)	398 (93%)	29 (7%)	0	100	100
3	C	246/259 (95%)	231 (94%)	15 (6%)	0	100	100
3	G	246/259 (95%)	231 (94%)	15 (6%)	0	100	100
4	D	29/66 (44%)	27 (93%)	2 (7%)	0	100	100
4	H	29/66 (44%)	27 (93%)	2 (7%)	0	100	100
All	All	2258/2452 (92%)	2105 (93%)	153 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	364/378 (96%)	322 (88%)	42 (12%)	5	23
1	E	364/378 (96%)	324 (89%)	40 (11%)	6	24
2	B	369/386 (96%)	336 (91%)	33 (9%)	9	33
2	F	369/386 (96%)	332 (90%)	37 (10%)	7	29
3	C	219/225 (97%)	207 (94%)	12 (6%)	19	50
3	G	219/225 (97%)	208 (95%)	11 (5%)	22	53
4	D	28/60 (47%)	28 (100%)	0	100	100
4	H	28/60 (47%)	27 (96%)	1 (4%)	31	62
All	All	1960/2098 (93%)	1784 (91%)	176 (9%)	11	33

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	26	LEU

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Mol	Chain	Res	Type
1	A	66	VAL
1	A	74	VAL
1	A	80	THR
1	A	112	LYS
1	A	115	ILE
1	A	119	LEU
1	A	137	VAL
1	A	160	ASP
1	A	190	THR
1	A	204	VAL
1	A	209	ILE
1	A	223	THR
1	A	227	LEU
1	A	235	VAL
1	A	248	LEU
1	A	249	ASN
1	A	250	VAL
1	A	251	ASP
1	A	256	GLN
1	A	258	ASN
1	A	269	LEU
1	A	288	VAL
1	A	291	ILE
1	A	302	MET
1	A	324	VAL
1	A	332	ILE
1	A	341	ILE
1	A	344	VAL
1	A	349	THR
1	A	352	LYS
1	A	357	TYR
1	A	368	LEU
1	A	375	VAL
1	A	381	THR
1	A	392	ASP
1	A	413	MET
1	A	424	ASP
1	A	425	MET
1	A	432	TYR
1	A	435	VAL
2	B	4	ILE
2	B	5	VAL

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Mol	Chain	Res	Type
2	B	12	CYS
2	B	31	ASP
2	B	35	ASN
2	B	65	LEU
2	B	68	LEU
2	B	74	ASP
2	B	113	VAL
2	B	120	VAL
2	B	129	CYS
2	B	131	GLN
2	B	139	LEU
2	B	147	MET
2	B	166	THR
2	B	181	GLU
2	B	189	ILE
2	B	202	ILE
2	B	237	THR
2	B	239	SER
2	B	249	ASP
2	B	258	VAL
2	B	281	TYR
2	B	285	THR
2	B	289	LEU
2	B	327	ASP
2	B	328	GLU
2	B	342	VAL
2	B	349	VAL
2	B	366	THR
2	B	377	LEU
2	B	386	THR
2	B	422	TYR
3	C	62	VAL
3	C	69	VAL
3	C	80	HIS
3	C	144	ILE
3	C	153	LEU
3	C	180	THR
3	C	241	LEU
3	C	261	GLN
3	C	275	TRP
3	C	295	GLU
3	C	303	LEU

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Mol	Chain	Res	Type
3	C	305	ILE
1	E	9	VAL
1	E	15	GLN
1	E	26	LEU
1	E	60	LYS
1	E	68	VAL
1	E	74	VAL
1	E	80	THR
1	E	115	ILE
1	E	119	LEU
1	E	137	VAL
1	E	160	ASP
1	E	171	ILE
1	E	217	LEU
1	E	230	LEU
1	E	235	VAL
1	E	241	SER
1	E	248	LEU
1	E	249	ASN
1	E	250	VAL
1	E	255	PHE
1	E	257	THR
1	E	259	LEU
1	E	265	ILE
1	E	269	LEU
1	E	275	VAL
1	E	288	VAL
1	E	290	GLU
1	E	291	ILE
1	E	324	VAL
1	E	341	ILE
1	E	352	LYS
1	E	353	VAL
1	E	368	LEU
1	E	375	VAL
1	E	379	SER
1	E	381	THR
1	E	393	HIS
1	E	413	MET
1	E	435	VAL
1	E	437	VAL
2	F	2	ARG

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Mol	Chain	Res	Type
2	F	4	ILE
2	F	5	VAL
2	F	7	ILE
2	F	12	CYS
2	F	35	ASN
2	F	68	LEU
2	F	113	VAL
2	F	119	VAL
2	F	121	ARG
2	F	139	LEU
2	F	166	THR
2	F	176	SER
2	F	179	VAL
2	F	180	VAL
2	F	181	GLU
2	F	198	GLU
2	F	199	THR
2	F	202	ILE
2	F	222	TYR
2	F	232	THR
2	F	237	THR
2	F	239	SER
2	F	247	ASN
2	F	253	LEU
2	F	258	VAL
2	F	278	SER
2	F	286	VAL
2	F	289	LEU
2	F	293	MET
2	F	311	LEU
2	F	312	THR
2	F	328	GLU
2	F	349	VAL
2	F	366	THR
2	F	395	LEU
2	F	422	TYR
3	G	62	VAL
3	G	69	VAL
3	G	80	HIS
3	G	144	ILE
3	G	153	LEU
3	G	158	LYS

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Mol	Chain	Res	Type
3	G	228	TYR
3	G	241	LEU
3	G	274	GLU
3	G	295	GLU
3	G	303	LEU
4	H	45	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	15	GLN
1	A	28	HIS
1	A	133	GLN
1	A	186	ASN
1	A	197	HIS
1	A	256	GLN
1	A	283	HIS
1	A	309	HIS
1	A	358	GLN
2	B	8	GLN
2	B	94	GLN
2	B	131	GLN
2	B	165	ASN
2	B	280	GLN
2	B	334	GLN
2	B	426	GLN
3	C	80	HIS
3	C	126	GLN
3	C	133	GLN
3	C	181	ASN
3	C	200	ASN
3	C	204	HIS
3	C	210	ASN
3	C	261	GLN
3	C	277	HIS
1	E	101	ASN
1	E	186	ASN
1	E	256	GLN
1	E	372	GLN
1	E	393	HIS
2	F	6	HIS

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Mol	Chain	Res	Type
2	F	43	GLN
2	F	89	ASN
2	F	94	GLN
2	F	256	ASN
2	F	280	GLN
2	F	334	GLN
2	F	414	ASN
3	G	80	HIS
3	G	126	GLN
3	G	181	ASN
3	G	200	ASN
3	G	210	ASN
3	G	277	HIS
4	H	35	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	G2P	B	501	-	30,34,34	3.42	15 (50%)	46,54,54	2.23	13 (28%)
5	GTP	E	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.71	10 (20%)
5	GTP	A	501	-	33,34,34	0.94	2 (6%)	50,54,54	1.64	9 (18%)
6	G2P	F	501	-	30,34,34	3.36	15 (50%)	46,54,54	2.26	12 (26%)

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
6	G2P	B	501	-	-	4/19/38/38	0/3/3/3
5	GTP	E	501	-	-	8/22/38/38	0/3/3/3
5	GTP	A	501	-	-	4/22/38/38	0/3/3/3
6	G2P	F	501	-	-	7/19/38/38	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	501	G2P	C2'-C3'	-10.96	1.23	1.53
6	B	501	G2P	C2'-C3'	-10.95	1.23	1.53
6	B	501	G2P	PB-O3B	7.73	1.67	1.58
6	F	501	G2P	PB-O3B	7.02	1.66	1.58
6	B	501	G2P	C2-N2	5.12	1.46	1.34
6	F	501	G2P	C2-N2	5.08	1.46	1.34
6	F	501	G2P	O4'-C1'	-5.05	1.30	1.42
6	B	501	G2P	O4'-C1'	-4.96	1.30	1.42
6	B	501	G2P	C5'-C4'	-4.08	1.39	1.51
6	F	501	G2P	C5'-C4'	-4.07	1.39	1.51
6	F	501	G2P	C2'-C1'	3.99	1.66	1.53
6	B	501	G2P	C2'-C1'	3.98	1.66	1.53
6	B	501	G2P	C6-N1	-3.33	1.32	1.38
6	B	501	G2P	O3'-C3'	3.07	1.50	1.43
6	F	501	G2P	O3'-C3'	3.04	1.50	1.43
6	B	501	G2P	C3'-C4'	2.89	1.60	1.53
6	F	501	G2P	C3'-C4'	2.89	1.60	1.53
6	F	501	G2P	C6-N1	-2.86	1.33	1.38
6	F	501	G2P	C5-N7	-2.85	1.33	1.39
6	B	501	G2P	C5-N7	-2.80	1.33	1.39
6	B	501	G2P	O6-C6	-2.78	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	501	G2P	O6-C6	-2.71	1.18	1.23
6	B	501	G2P	PA-O1A	-2.58	1.50	1.56
6	F	501	G2P	O4'-C4'	2.58	1.50	1.45
6	B	501	G2P	O4'-C4'	2.49	1.50	1.45
6	F	501	G2P	PA-O1A	-2.41	1.50	1.56
6	F	501	G2P	PB-O1B	-2.30	1.50	1.56
5	E	501	GTP	C5-N7	-2.23	1.34	1.39
6	B	501	G2P	PB-O1B	-2.23	1.50	1.56
5	A	501	GTP	C5-N7	-2.17	1.34	1.39
6	F	501	G2P	C8-N9	-2.14	1.32	1.37
6	B	501	G2P	C8-N9	-2.11	1.32	1.37
5	A	501	GTP	C2-N3	2.06	1.38	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	G2P	C1'-N9-C4	-6.77	106.50	126.49
6	B	501	G2P	C1'-N9-C8	6.40	144.90	126.73
6	F	501	G2P	C1'-N9-C4	-6.24	108.06	126.49
6	F	501	G2P	C5-C4-N3	-5.90	119.00	128.39
6	F	501	G2P	C1'-N9-C8	5.87	143.41	126.73
6	B	501	G2P	C5-C4-N3	-5.29	119.98	128.39
5	A	501	GTP	C5-C4-N3	-5.23	120.07	128.39
5	E	501	GTP	C5-C4-N3	-5.17	120.15	128.39
5	A	501	GTP	C2-N3-C4	4.73	120.45	112.30
5	E	501	GTP	C2-N3-C4	4.71	120.42	112.30
6	F	501	G2P	C2-N3-C4	4.71	120.41	112.30
6	B	501	G2P	C2-N3-C4	4.47	120.00	112.30
6	F	501	G2P	C2-N1-C6	-3.83	118.17	125.11
6	F	501	G2P	N9-C4-N3	3.78	133.51	125.95
5	A	501	GTP	C2-N1-C6	-3.31	119.10	125.11
5	A	501	GTP	N9-C4-N3	3.27	132.49	125.95
6	B	501	G2P	N9-C8-N7	-3.22	107.44	113.40
5	E	501	GTP	C2-N1-C6	-3.19	119.32	125.11
6	F	501	G2P	PB-O3B-PG	-3.17	121.10	132.45
6	F	501	G2P	N9-C8-N7	-3.15	107.56	113.40
5	E	501	GTP	N9-C4-N3	3.15	132.24	125.95
6	B	501	G2P	N9-C4-N3	3.10	132.15	125.95
6	F	501	G2P	C5-C6-N1	3.10	121.14	113.25
6	B	501	G2P	PB-O3B-PG	-3.04	121.55	132.45
6	F	501	G2P	O6-C6-C5	-2.96	118.72	126.53
6	B	501	G2P	C2-N1-C6	-2.91	119.83	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	G2P	C5-C6-N1	2.76	120.29	113.25
5	A	501	GTP	N9-C8-N7	-2.76	108.28	113.40
5	A	501	GTP	C5-C6-N1	2.75	120.26	113.25
5	E	501	GTP	C5-C6-N1	2.65	119.99	113.25
5	A	501	GTP	O6-C6-C5	-2.63	119.58	126.53
5	E	501	GTP	N9-C8-N7	-2.57	108.64	113.40
5	A	501	GTP	C8-N7-C5	2.51	108.72	104.26
5	E	501	GTP	O6-C6-C5	-2.47	120.02	126.53
6	B	501	G2P	O6-C6-C5	-2.45	120.06	126.53
5	A	501	GTP	O2A-PA-O3A	2.45	113.89	107.27
5	E	501	GTP	C8-N7-C5	2.45	108.62	104.26
6	B	501	G2P	C3'-C2'-C1'	2.37	105.95	101.46
5	E	501	GTP	C2'-C3'-C4'	2.32	107.08	102.61
6	F	501	G2P	C3'-C2'-C1'	2.30	105.82	101.46
5	E	501	GTP	O2A-PA-O5'	2.22	117.62	107.57
6	F	501	G2P	C8-N7-C5	2.20	108.17	104.26
6	B	501	G2P	C8-N7-C5	2.16	108.11	104.26
6	B	501	G2P	O3G-PG-O3B	2.11	111.72	104.64

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	E	501	GTP	PB-O3A-PA-O5'
6	F	501	G2P	PB-C3A-PA-O1A
6	F	501	G2P	PB-C3A-PA-O2A
6	F	501	G2P	PB-C3A-PA-O5'
6	F	501	G2P	C3'-C4'-C5'-O5'
5	E	501	GTP	C3'-C4'-C5'-O5'
6	B	501	G2P	O4'-C4'-C5'-O5'
6	B	501	G2P	C3'-C4'-C5'-O5'
5	E	501	GTP	O4'-C4'-C5'-O5'
6	F	501	G2P	O4'-C4'-C5'-O5'
5	E	501	GTP	PA-O3A-PB-O1B
5	E	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O2A
5	E	501	GTP	PG-O3B-PB-O1B
5	E	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
6	B	501	G2P	C4'-C5'-O5'-PA
6	B	501	G2P	PA-C3A-PB-O2B

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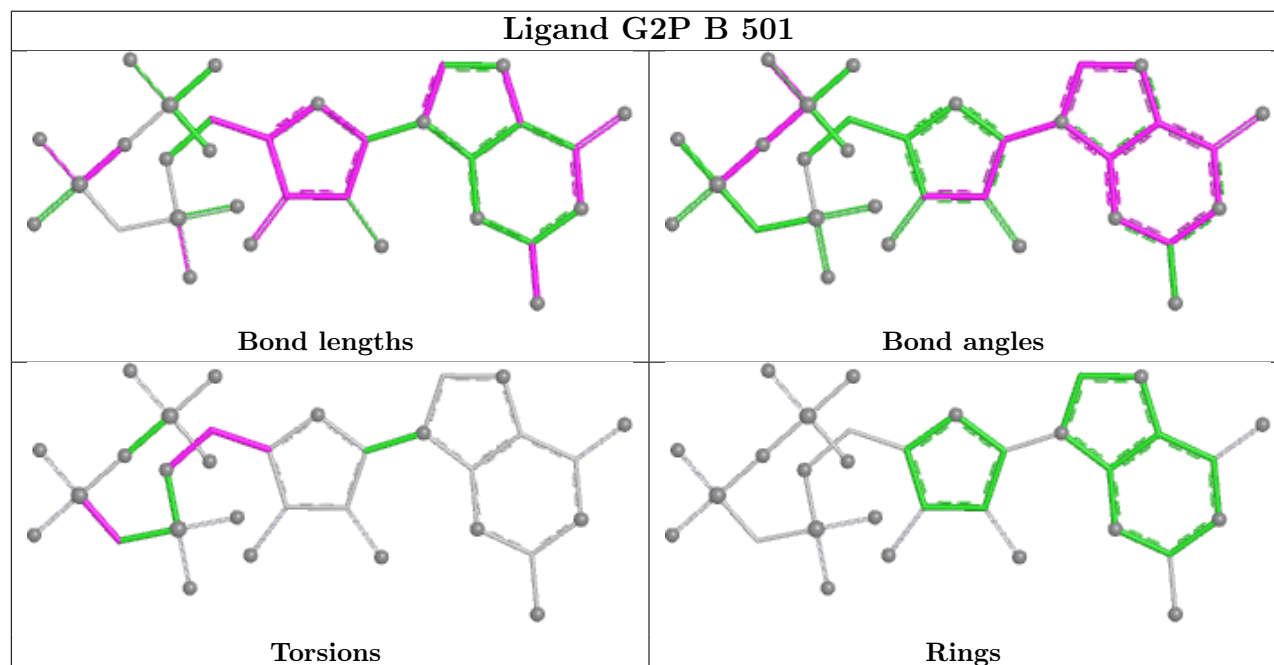
Mol	Chain	Res	Type	Atoms
6	F	501	G2P	C5'-O5'-PA-O1A
5	A	501	GTP	PB-O3A-PA-O1A
6	F	501	G2P	C4'-C5'-O5'-PA
5	E	501	GTP	PG-O3B-PB-O2B

There are no ring outliers.

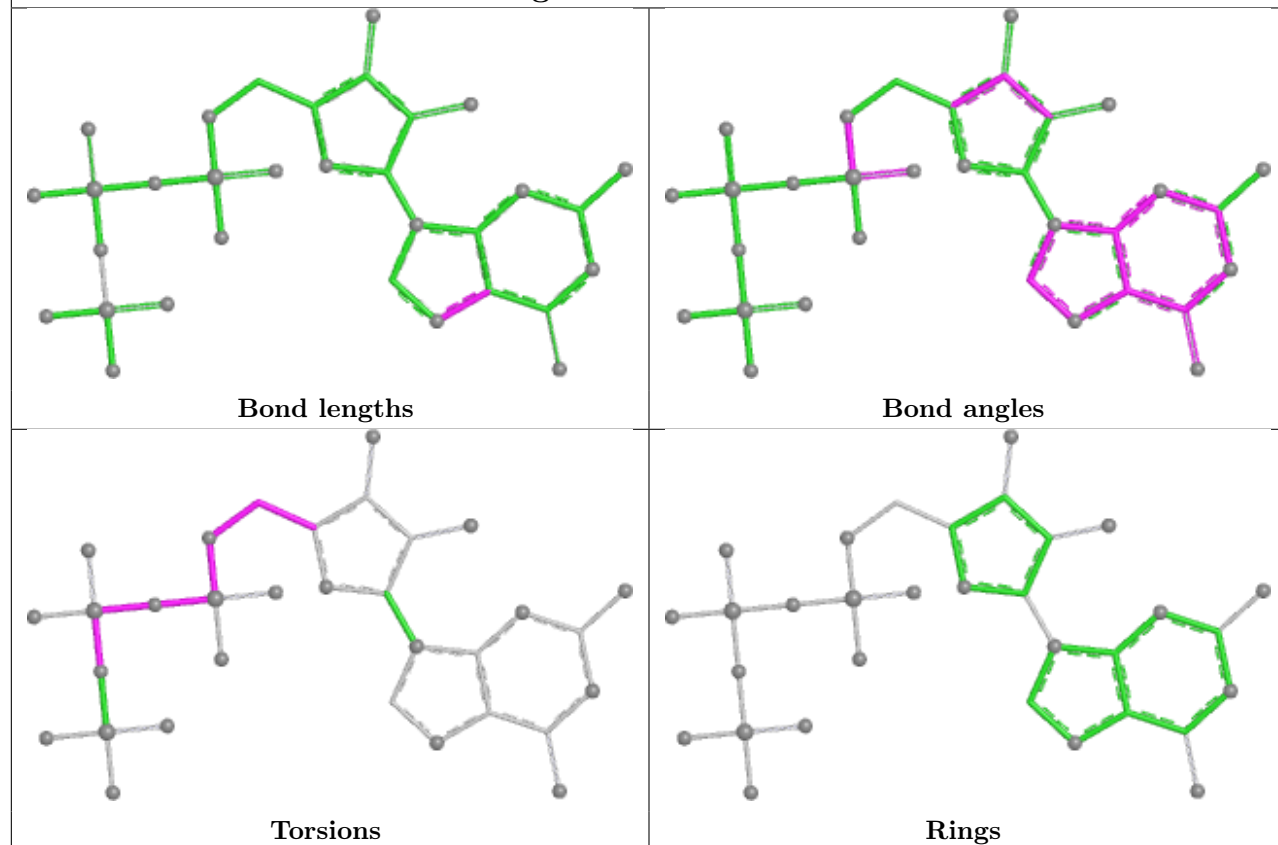
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	G2P	1	0
5	E	501	GTP	1	0
5	A	501	GTP	1	0

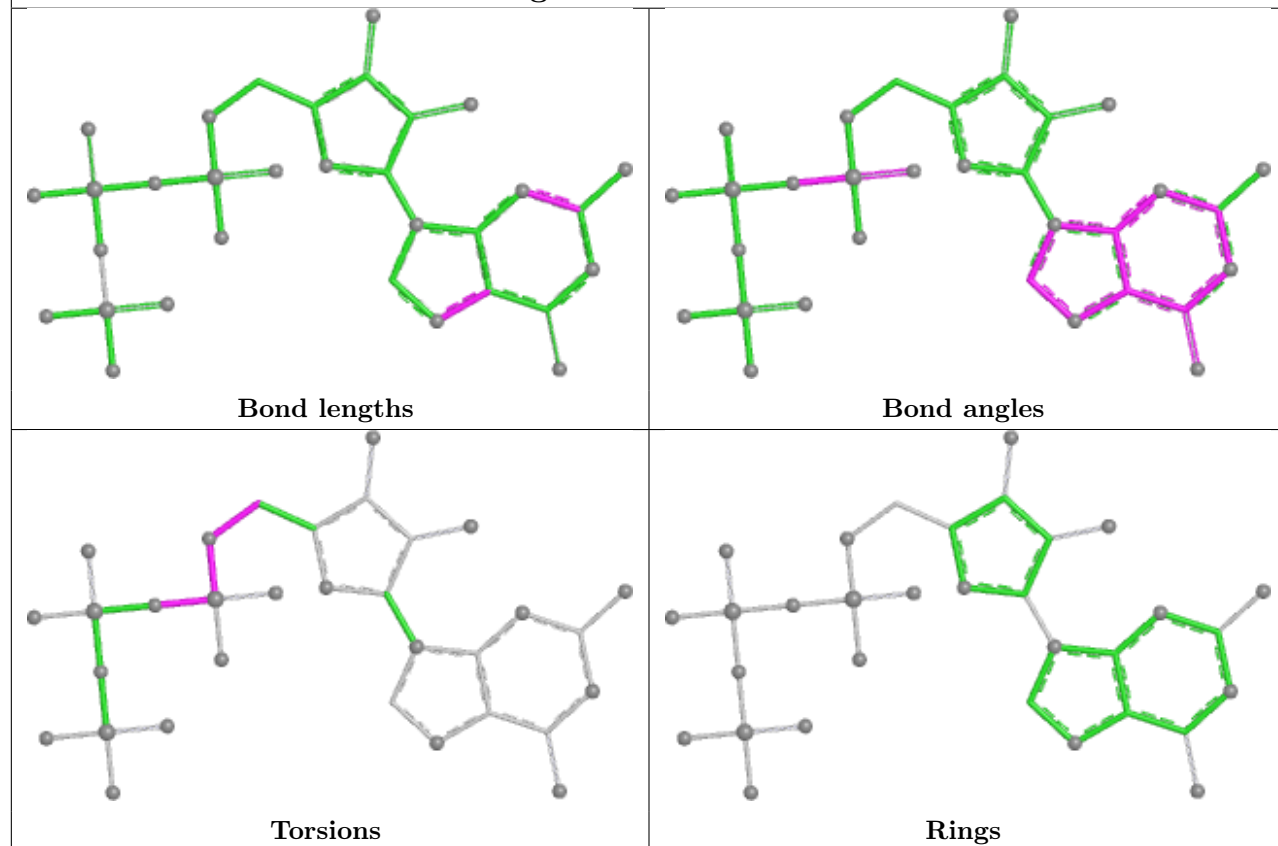
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

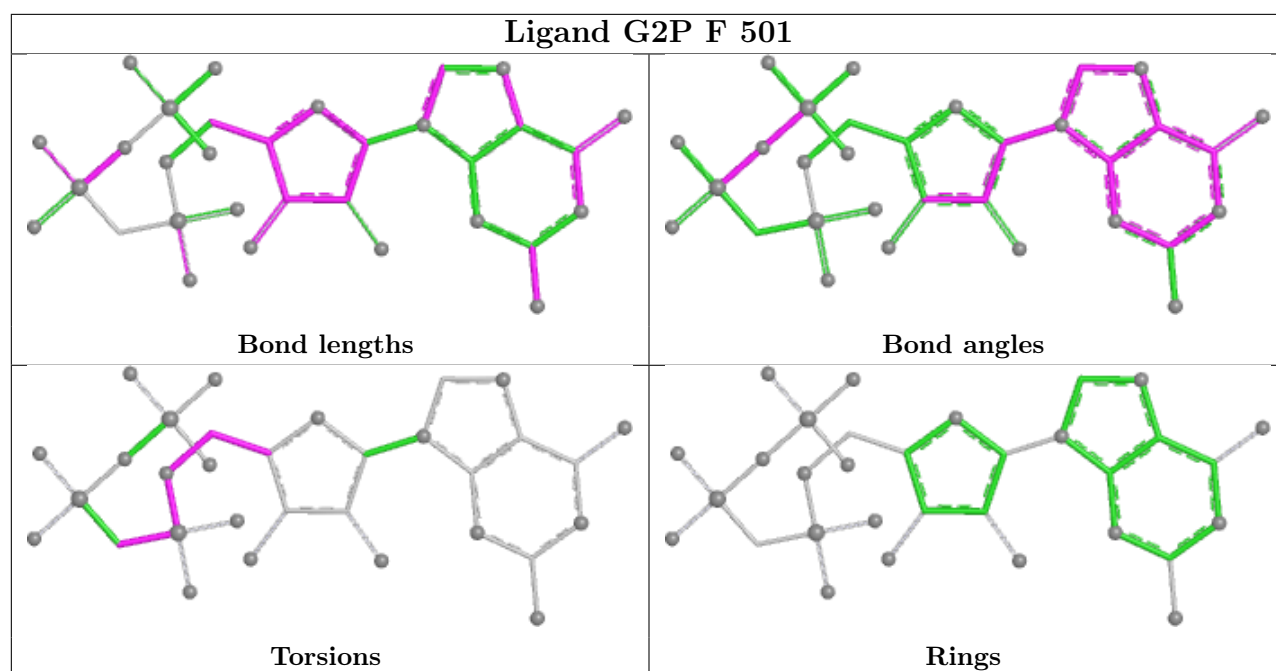


Ligand GTP E 501



Ligand GTP A 501





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.

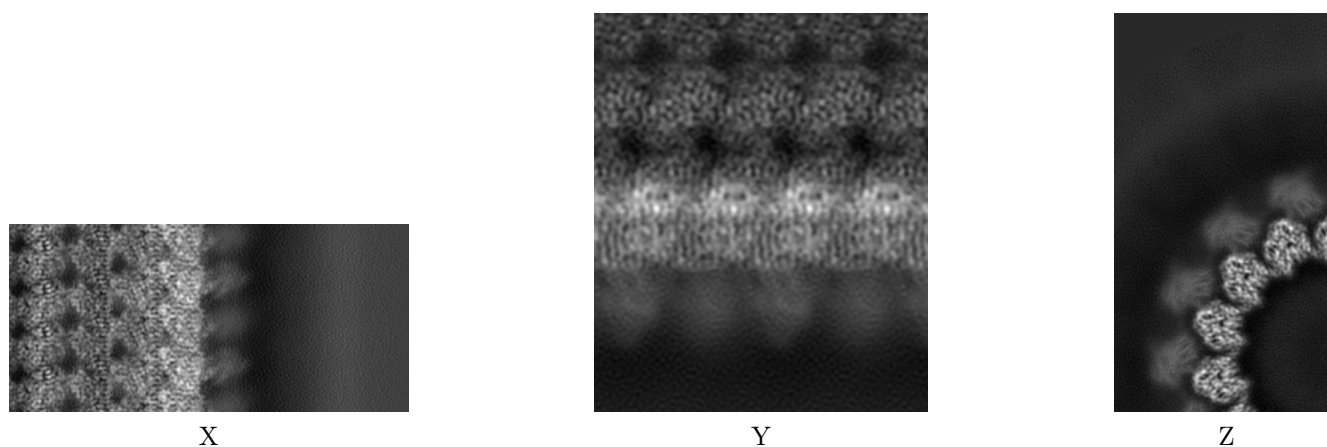
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21893. 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](#)

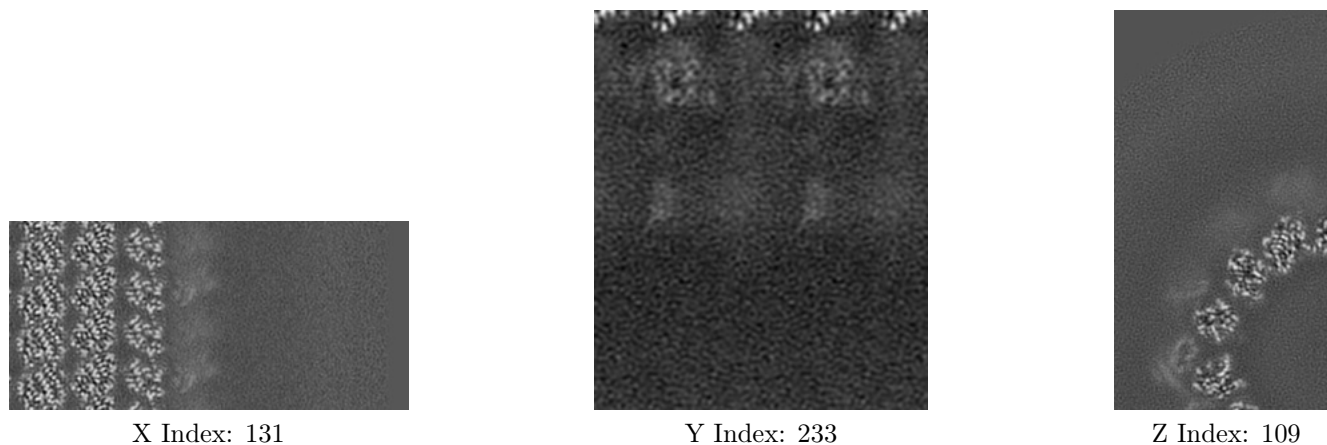
6.1.1 Primary map



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

6.2 Central slices [i](#)

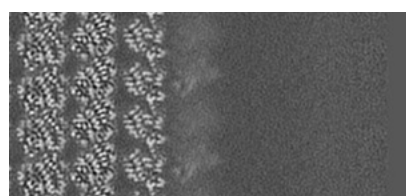
6.2.1 Primary map



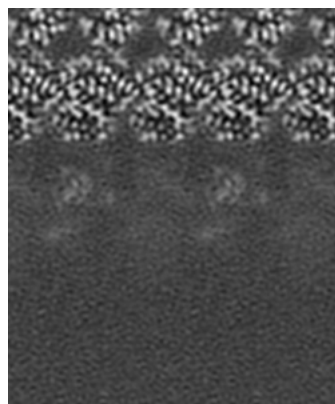
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

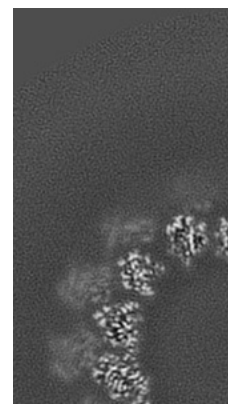
6.3.1 Primary map



X Index: 132



Y Index: 191

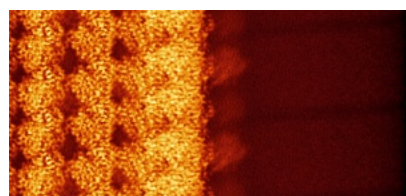


Z Index: 28

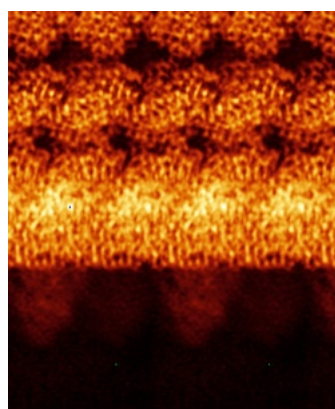
The images above show the largest variance slices of the map in three orthogonal directions.

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

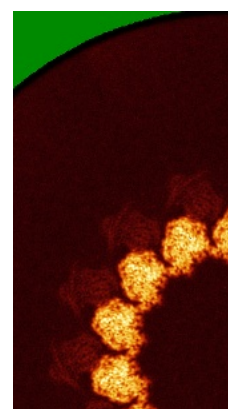
6.4.1 Primary map



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

This section was not generated.

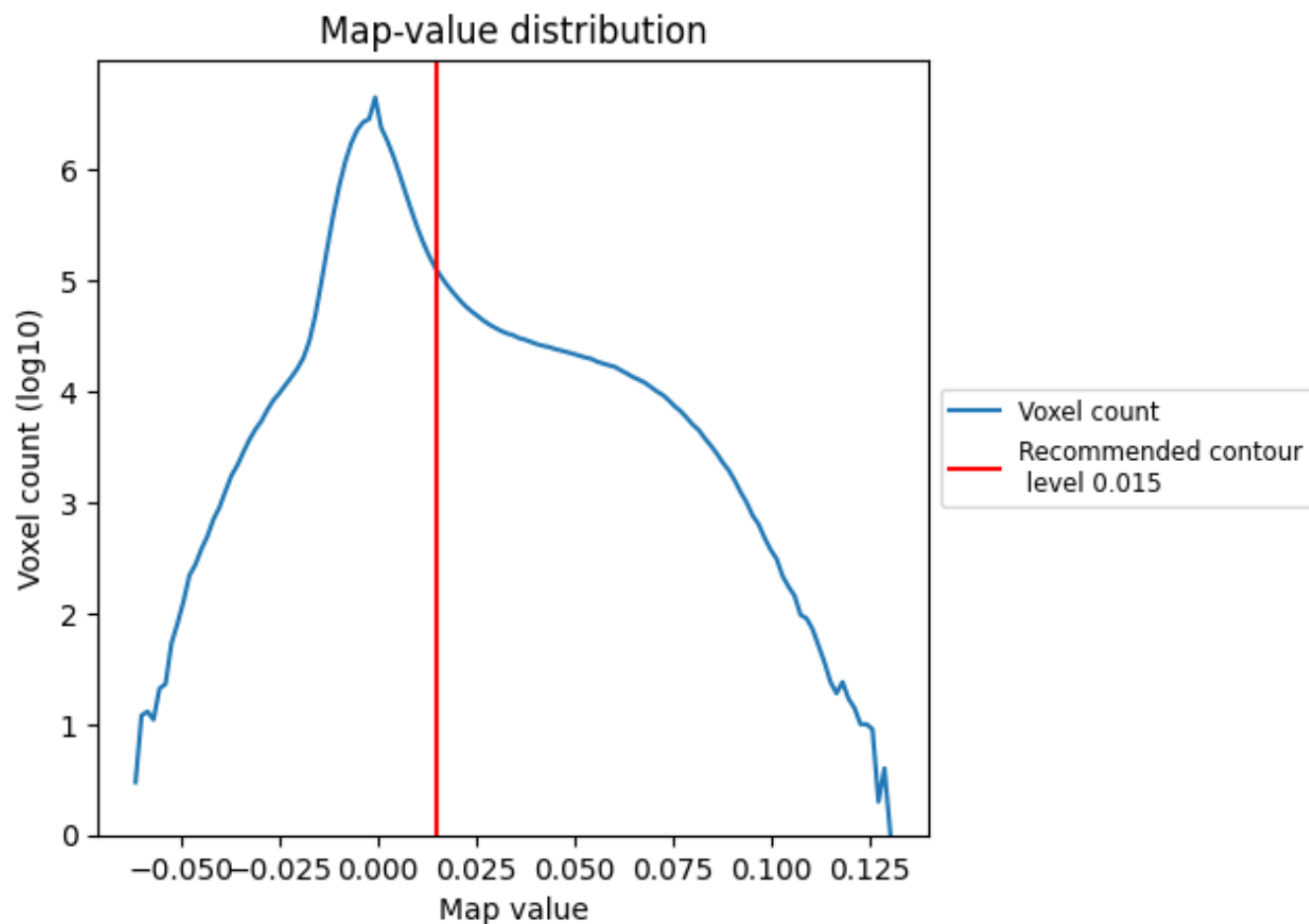
6.6 Mask visualisation

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

7 Map analysis [i](#)

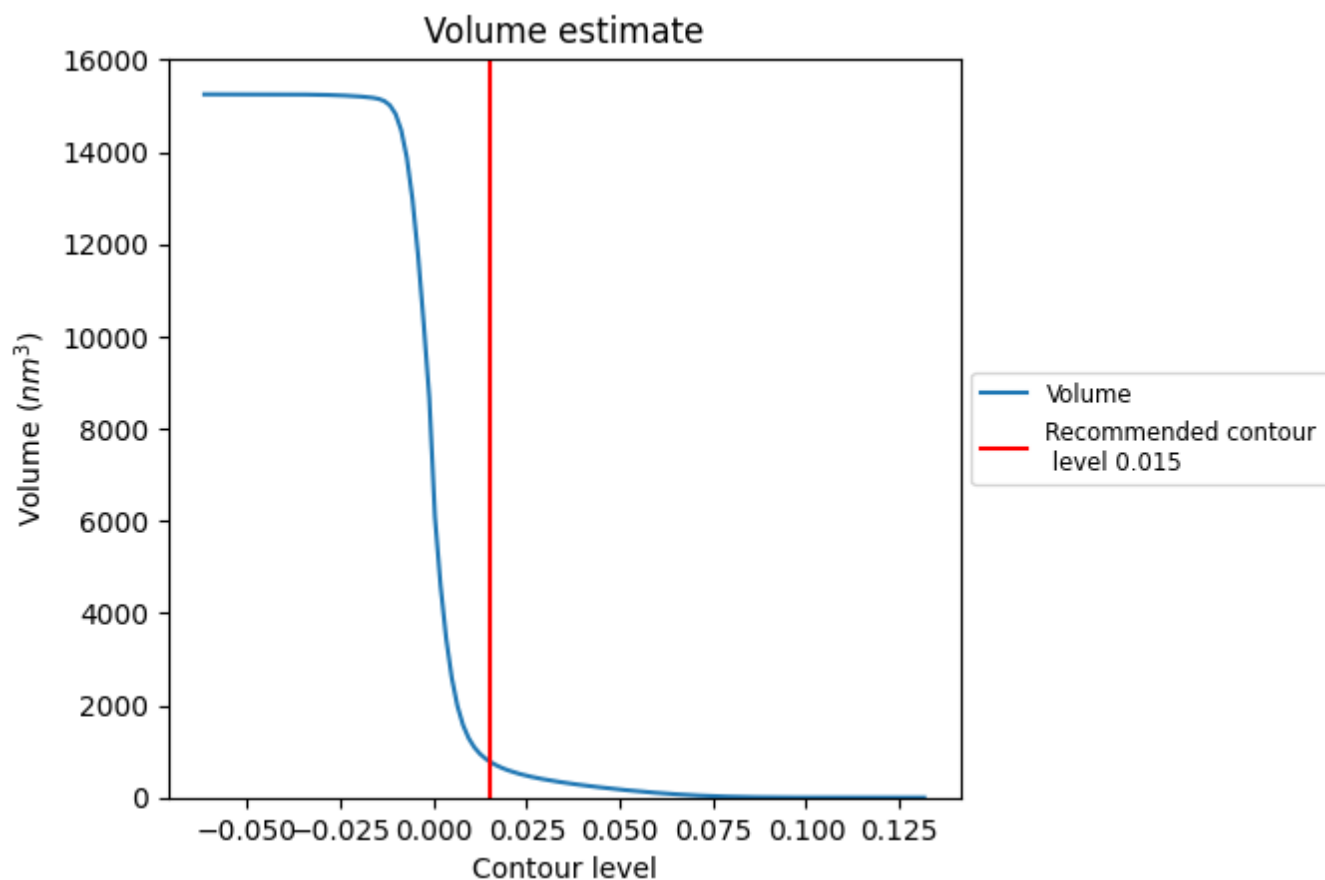
This section contains the results of statistical analysis of the map.

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 787 nm³; this corresponds to an approximate mass of 711 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

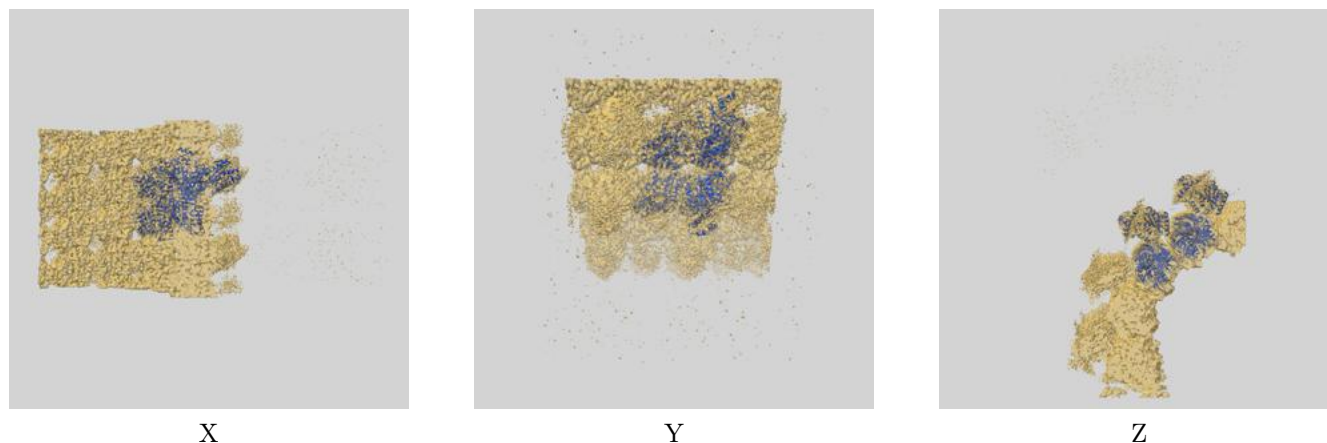
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

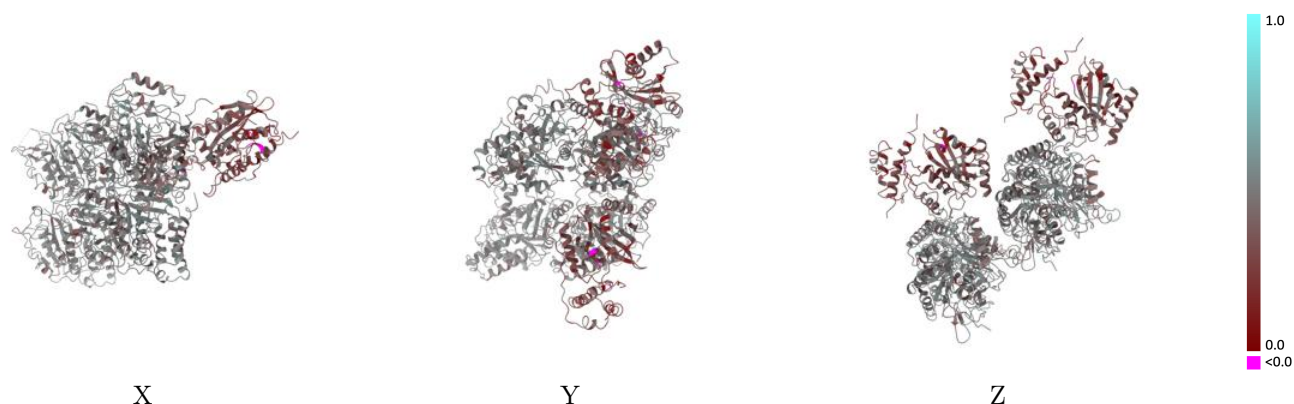
This section contains information regarding the fit between EMDB map EMD-21893 and PDB model 6WSL. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.015 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](#)

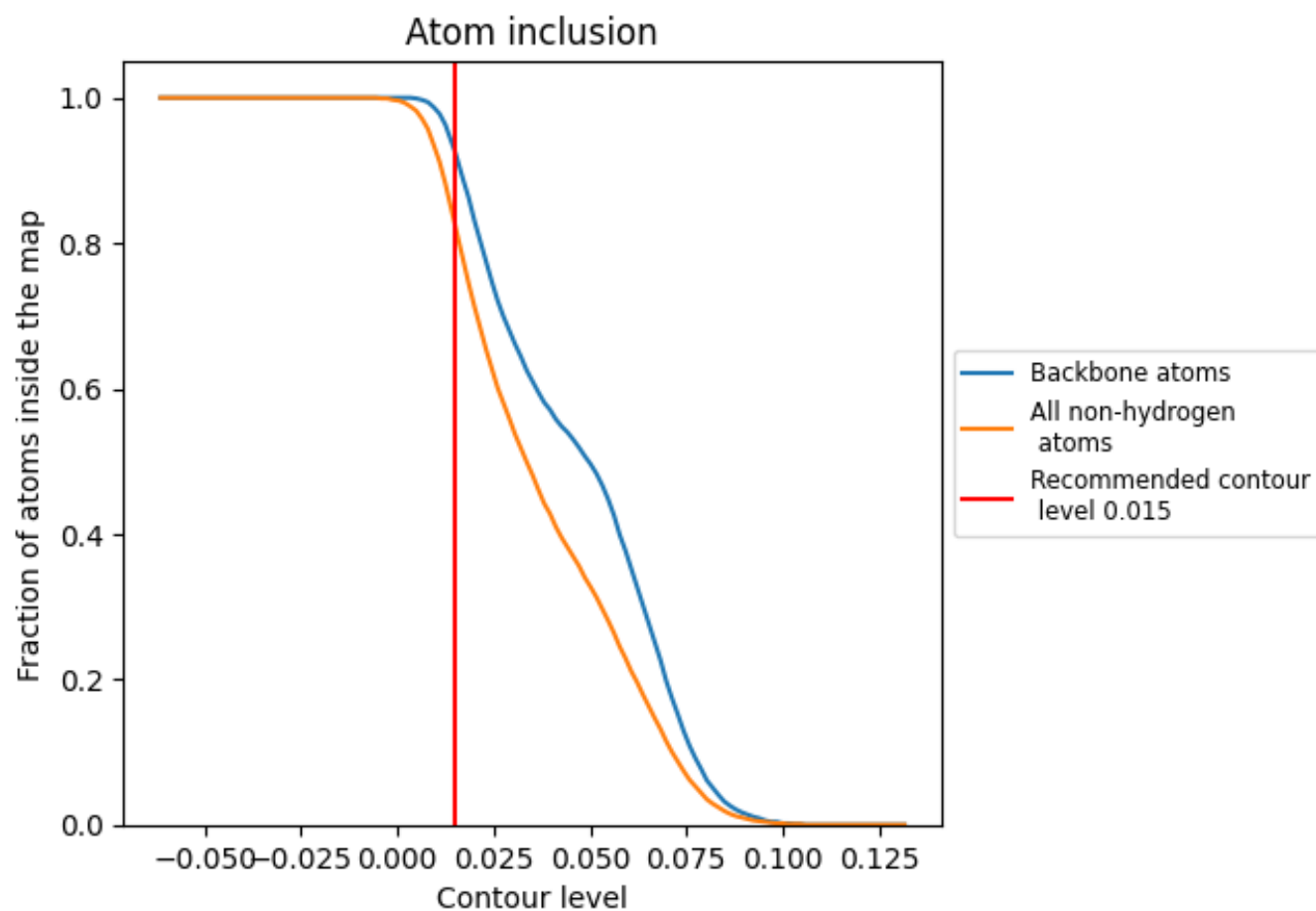


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.4330
A	0.9120	0.4720
B	0.9130	0.4710
C	0.5590	0.3240
D	0.5490	0.2960
E	0.9120	0.4720
F	0.9160	0.4710
G	0.5540	0.3220
H	0.5370	0.2970

1.0

0.0

<0.0