



## Full wwPDB EM Validation Report ⓘ

Jul 16, 2024 – 01:04 PM JST

PDB ID : 8XVV  
EMDB ID : EMD-38720  
Title : The TRRAP module of human NuA4/TIP60 complex  
Authors : Chen, K.; Wang, L.; Yu, Z.; Yu, J.; Ren, Y.; Wang, Q.; Xu, Y.  
Deposited on : 2024-01-15  
Resolution : 3.20 Å (reported)  
Based on initial model : 7KTR

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

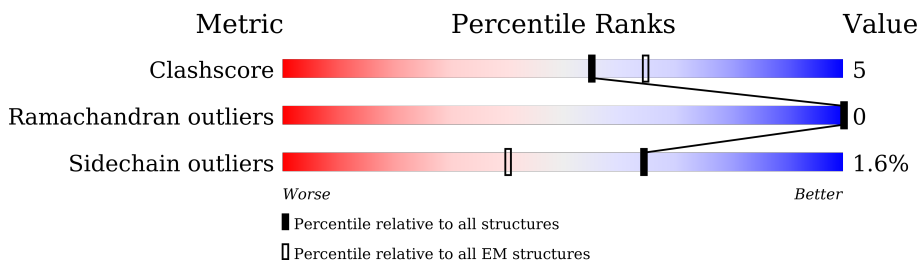
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 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 3.20 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  $\geq 3$ , 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	H	3123	
2	L	3830	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 59257 atoms, of which 29886 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.

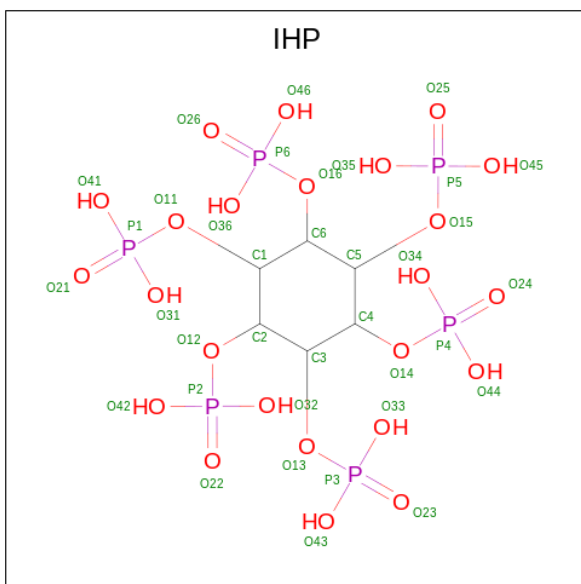
- Molecule 1 is a protein called Isoform 2 of E1A-binding protein p400.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	H	166	2684	844	1352	239	245	4	0	0

- Molecule 2 is a protein called Isoform 2 of Transformation/transcription domain-associated protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	L	3485	56537	17940	28534	4845	5023	195	2	0

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ) (labeled as "Ligand of Interest" by depositor).



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













D3504	D3761
A3505	SER
R3515	PRO
K3529	LJU
R3530	SER
V3545	ALA
V3546	G3768
A3547	Q3769
V3548	P3770
Q3551	E3771
V3555	N3772
N3558	M3773
S3561	D3774
C3572	S3775
G3576	Q3776
R3596	E3803
V3617	N3807
T3629	W3829
F3639	L3830
F3643	
T3644	
F3652	
V3656	
I3669	
V3678	
F3681	
T3689	
G3690	
D3691	
L3710	
T3711	
T3712	
I3713	
D3747	
E3758	
D3759	
T3760	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	190003	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)	1500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.028	Depositor
Map size ( $\text{\AA}$ )	341.504, 341.504, 341.504	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.334, 1.334, 1.334	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: 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	H	0.23	0/1362	0.38	0/1849
2	L	0.24	0/28601	0.38	0/38709
All	All	0.24	0/29963	0.38	0/40558

There are no bond length outliers.

There are no bond angle outliers.

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	H	1332	1352	1349	17	0
2	L	28003	28534	28511	299	0
3	L	36	0	6	0	0
All	All	29371	29886	29866	313	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 5.

All (313) 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:L:663:SER:HB3	2:L:709:LEU:HD13	1.44	0.98
2:L:3305:GLU:HG2	2:L:3483:ALA:CB	1.99	0.93
2:L:2635:SER:OG	2:L:2636:PRO:HD3	1.73	0.88
2:L:924:ILE:HG13	2:L:2592:LEU:HD21	1.59	0.85
2:L:1719:GLU:HA	2:L:1764:LEU:HD13	1.58	0.84
2:L:3305:GLU:HG2	2:L:3483:ALA:HB3	1.64	0.80
2:L:103:ASN:O	2:L:144:ARG:NH2	2.18	0.77
2:L:924:ILE:HG21	2:L:2592:LEU:HD23	1.64	0.76
2:L:3639:PHE:HZ	2:L:3669:ILE:HD11	1.51	0.76
2:L:3515:ARG:NH2	2:L:3747:ASP:OD2	2.19	0.76
2:L:2582:ASP:OD1	2:L:2585:ARG:NH2	2.18	0.76
2:L:1831:ASP:OD1	2:L:1835:ASN:ND2	2.19	0.75
2:L:924:ILE:HG21	2:L:2592:LEU:CD2	2.19	0.73
2:L:3305:GLU:HG2	2:L:3483:ALA:HB2	1.73	0.71
2:L:663:SER:HB3	2:L:709:LEU:CD1	2.19	0.71
1:H:2331:GLU:O	1:H:2377:ARG:NH1	2.24	0.69
2:L:428:ASP:OD1	2:L:429:CYS:N	2.24	0.69
2:L:561:THR:HG21	2:L:638:VAL:HG13	1.76	0.68
2:L:1981:THR:O	2:L:1986:ARG:NH2	2.27	0.67
2:L:2408:ARG:NH1	2:L:2442:GLU:OE2	2.26	0.67
1:H:2370:ASP:OD1	2:L:2680:LYS:NZ	2.17	0.67
2:L:1650:ARG:NH1	2:L:1694:GLU:OE2	2.28	0.67
2:L:2187:ASN:O	2:L:2190:VAL:HG22	1.95	0.67
2:L:1576:HIS:O	2:L:1583:ARG:NH2	2.28	0.67
2:L:663:SER:HA	2:L:709:LEU:HD12	1.77	0.66
2:L:2622:LEU:O	2:L:2627:GLN:NE2	2.29	0.66
2:L:1719:GLU:HA	2:L:1764:LEU:CD1	2.24	0.66
2:L:104:GLU:N	2:L:104:GLU:OE1	2.28	0.66
1:H:2337:ASP:OD2	1:H:2396:ARG:NH2	2.28	0.66
2:L:790:LEU:HD22	2:L:809:LEU:HD11	1.78	0.65
2:L:1211:GLU:OE2	2:L:1266:VAL:HG21	1.97	0.65
2:L:318:SER:O	2:L:365:TYR:OH	2.15	0.65
2:L:856:LEU:HD21	2:L:860:PHE:HD2	1.61	0.65
2:L:3159:ARG:NH2	2:L:3195:ILE:O	2.30	0.65
2:L:2623:SER:OG	2:L:2626:GLN:OE1	2.15	0.64
2:L:2267:TYR:CD1	2:L:2272:ILE:HD11	2.33	0.64
2:L:2747:TRP:O	2:L:2751:CYS:N	2.30	0.63
2:L:622:THR:O	2:L:624:ARG:NH1	2.32	0.63
2:L:1898:ALA:O	2:L:1902:VAL:HG22	1.98	0.63
2:L:793:LEU:HD11	2:L:1198:VAL:CG2	2.27	0.63
2:L:1825:ALA:HB3	2:L:1826:PRO:CD	2.29	0.62
2:L:2454:GLU:N	2:L:2454:GLU:OE1	2.33	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:663:SER:CB	2:L:709:LEU:HD13	2.27	0.62
2:L:3302:ASN:OD1	2:L:3305:GLU:OE1	2.18	0.62
2:L:2249:GLN:O	2:L:2253:THR:HG23	1.98	0.62
1:H:2337:ASP:OD1	1:H:2393:ILE:HD11	2.00	0.61
2:L:699:GLU:N	2:L:699:GLU:OE1	2.33	0.61
2:L:3711:THR:O	2:L:3712:THR:OG1	2.17	0.61
1:H:2343:ALA:HB3	1:H:2368:VAL:HG23	1.82	0.61
2:L:598:GLN:NE2	2:L:657:TYR:OH	2.33	0.61
2:L:3545:VAL:HG22	2:L:3555:VAL:HG23	1.81	0.61
2:L:969:CYS:HB2	2:L:2592:LEU:HD13	1.81	0.61
2:L:1894:HIS:O	2:L:1894:HIS:ND1	2.33	0.61
2:L:2635:SER:OG	2:L:2636:PRO:CD	2.48	0.61
2:L:2348:ALA:O	2:L:2352:ILE:HG23	2.00	0.60
2:L:3105:LYS:O	2:L:3106:SER:OG	2.16	0.59
2:L:291:LEU:HD21	2:L:313:MET:SD	2.42	0.59
2:L:295:ILE:HD11	2:L:337:HIS:CB	2.32	0.59
2:L:357:GLU:OE2	2:L:397:LEU:HD12	2.02	0.59
2:L:1396:SER:N	2:L:1402:GLN:OE1	2.35	0.58
2:L:663:SER:CA	2:L:709:LEU:CD1	2.81	0.58
2:L:1050:THR:HG21	2:L:1121:VAL:HG21	1.85	0.58
2:L:3301:GLU:HG2	2:L:3302:ASN:N	2.19	0.58
2:L:1981:THR:OG1	2:L:1984:GLN:OE1	2.20	0.58
2:L:2804:ASP:OD1	2:L:2805:HIS:N	2.36	0.58
2:L:1815:LEU:O	2:L:1819:THR:HG23	2.04	0.57
2:L:3711:THR:HG23	2:L:3713:ILE:HG12	1.85	0.57
2:L:2626:GLN:OE1	2:L:2626:GLN:N	2.37	0.57
2:L:1961:HIS:O	2:L:1964:VAL:HG22	2.04	0.57
2:L:2677:TYR:O	2:L:2681:THR:OG1	2.23	0.57
1:H:2431:LEU:O	1:H:2435:THR:HG23	2.04	0.57
2:L:2453:TYR:CZ	2:L:2457:LEU:HD11	2.40	0.57
2:L:1381:GLN:OE1	2:L:1381:GLN:N	2.36	0.56
2:L:1474:TRP:O	2:L:1478:VAL:HG23	2.05	0.56
2:L:1659:GLN:OE1	2:L:1706:ARG:NH1	2.35	0.56
2:L:2232:ILE:CG2	2:L:2253:THR:HG22	2.35	0.56
2:L:3242:THR:OG1	2:L:3547:ALA:O	2.21	0.56
2:L:3689:THR:OG1	2:L:3691:ASP:OD1	2.15	0.56
2:L:1819:THR:HG22	2:L:1868:LEU:HA	1.86	0.56
2:L:1825:ALA:HB3	2:L:1826:PRO:HD3	1.88	0.56
1:H:2369:SER:O	1:H:2373:ASN:ND2	2.39	0.56
2:L:1229:GLU:N	2:L:1229:GLU:OE1	2.37	0.56
2:L:2944:ASN:OD1	2:L:2945:SER:N	2.39	0.55

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:663:SER:CB	2:L:709:LEU:CD1	2.85	0.55
2:L:1276:THR:O	2:L:1280:GLU:N	2.40	0.55
2:L:162:TYR:HD2	2:L:241:LEU:HD13	1.72	0.55
2:L:395:LEU:HD22	2:L:426:LEU:HD11	1.89	0.54
2:L:729:GLU:OE2	2:L:772:HIS:ND1	2.39	0.54
2:L:1971:MET:SD	2:L:1992:SER:OG	2.64	0.54
2:L:2340:SER:OG	2:L:2388:ARG:NH1	2.40	0.54
2:L:2453:TYR:CE2	2:L:2457:LEU:HD11	2.42	0.54
2:L:2267:TYR:CE1	2:L:2272:ILE:HD11	2.43	0.54
2:L:2158:PHE:O	2:L:2161:THR:OG1	2.18	0.54
2:L:732:LEU:HD13	2:L:732:LEU:O	2.07	0.54
2:L:3293:VAL:HG22	2:L:3548:VAL:HG21	1.89	0.53
2:L:1005:HIS:CE1	2:L:1143:GLU:HG3	2.42	0.53
2:L:1756:GLN:OE1	2:L:1757:HIS:ND1	2.41	0.53
2:L:1957:TYR:N	2:L:1958:PRO:HD3	2.24	0.53
2:L:561:THR:HG22	2:L:589:TYR:OH	2.09	0.53
2:L:1936:GLY:O	2:L:1938:THR:HG23	2.09	0.53
2:L:295:ILE:HD11	2:L:337:HIS:HB3	1.91	0.53
2:L:295:ILE:HD11	2:L:337:HIS:HB2	1.91	0.53
2:L:3308:LEU:HD21	2:L:3419:LEU:HB3	1.91	0.53
2:L:3311:LEU:HD13	2:L:3416:ILE:HG12	1.90	0.53
2:L:661:ARG:O	2:L:665:ASN:N	2.42	0.52
2:L:2861:GLU:OE1	2:L:2861:GLU:N	2.42	0.52
2:L:1245:LEU:O	2:L:1249:VAL:HG23	2.10	0.52
2:L:2304:GLU:N	2:L:2304:GLU:OE1	2.41	0.52
2:L:3117:VAL:HG21	2:L:3130:TRP:CE3	2.44	0.52
2:L:114:LEU:HD13	2:L:150:GLU:HB3	1.92	0.52
2:L:634:HIS:O	2:L:638:VAL:HG23	2.10	0.52
2:L:1123:SER:O	2:L:1127:GLY:N	2.41	0.52
2:L:25:VAL:HG22	2:L:68:ARG:NH2	2.25	0.52
2:L:294:ILE:HG22	2:L:294:ILE:O	2.08	0.52
2:L:2471:HIS:O	2:L:2646:GLN:NE2	2.42	0.52
2:L:359:ILE:O	2:L:361:ILE:N	2.39	0.52
2:L:3143:GLN:OE1	2:L:3145:HIS:NE2	2.42	0.52
2:L:1538:GLU:OE1	2:L:1538:GLU:N	2.43	0.52
2:L:2145:ASN:O	2:L:2148:ASN:ND2	2.43	0.52
2:L:3774:ASP:OD2	2:L:3776:GLN:NE2	2.43	0.52
2:L:3803:GLU:OE1	2:L:3807:ASN:ND2	2.42	0.52
2:L:1371:ASN:ND2	2:L:1408:CYS:SG	2.83	0.51
2:L:1171:LEU:HD12	2:L:1175:TRP:CZ3	2.45	0.51
2:L:217:ARG:HE	2:L:220:LEU:HD21	1.75	0.51

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:317:LEU:HD22	2:L:331:LEU:HD21	1.93	0.51
2:L:2353:VAL:HG23	2:L:2402:LEU:HD11	1.92	0.51
2:L:2392:ASP:O	2:L:2396:ASN:ND2	2.41	0.51
2:L:630:GLU:OE1	2:L:630:GLU:N	2.43	0.51
2:L:97:ILE:HG23	2:L:135:ILE:HD13	1.93	0.51
2:L:838:SER:O	2:L:842:VAL:HG13	2.10	0.51
2:L:3639:PHE:CZ	2:L:3669:ILE:HD11	2.39	0.51
2:L:2315:THR:HG21	2:L:2352:ILE:HD12	1.92	0.51
2:L:235:MET:SD	2:L:296:ARG:NH2	2.81	0.50
2:L:663:SER:CA	2:L:709:LEU:HD12	2.39	0.50
2:L:101:PRO:O	2:L:102:THR:HG23	2.12	0.50
2:L:3100:LEU:O	2:L:3100:LEU:HD23	2.11	0.50
2:L:3477:VAL:HG21	2:L:3486:ARG:CZ	2.42	0.50
2:L:3710:LEU:O	2:L:3711:THR:HG22	2.11	0.50
1:H:2423:GLN:NE2	2:L:2791:ALA:O	2.45	0.50
2:L:2619:TRP:O	2:L:2627:GLN:NE2	2.45	0.50
2:L:3299:PHE:CE2	2:L:3501:VAL:HG21	2.47	0.50
2:L:1184:LEU:HD22	2:L:1241:VAL:HG13	1.93	0.50
2:L:3643:PHE:HE1	2:L:3669:ILE:HD12	1.76	0.49
2:L:3294:ASP:O	2:L:3297:VAL:HG12	2.12	0.49
2:L:412:PRO:HD2	2:L:415:ILE:HD12	1.94	0.49
2:L:2228:VAL:HA	2:L:2231:VAL:HG12	1.95	0.49
2:L:915:VAL:HG22	2:L:3629:THR:O	2.12	0.49
1:H:2382:SER:OG	1:H:2383:LYS:N	2.45	0.49
1:H:2389:TYR:O	1:H:2393:ILE:HG13	2.13	0.48
2:L:159:LYS:HG2	2:L:241:LEU:HD11	1.95	0.48
2:L:357:GLU:O	2:L:359:ILE:N	2.46	0.48
2:L:1181:GLN:NE2	2:L:1244:ASP:OD2	2.46	0.48
2:L:445:LEU:HB3	2:L:564:ILE:HG22	1.95	0.48
2:L:859:ASP:OD1	2:L:860:PHE:N	2.46	0.48
1:H:2369:SER:HG	1:H:2381:SER:HG	1.60	0.48
2:L:550:VAL:O	2:L:554:VAL:HG23	2.14	0.48
2:L:1193:ASP:O	2:L:3469:ARG:NH1	2.45	0.48
2:L:373:PRO:HB3	2:L:415:ILE:HD11	1.96	0.48
2:L:1797:VAL:HG22	2:L:1798:LEU:HD23	1.96	0.48
2:L:2855:GLU:OE1	2:L:2870:ARG:NH2	2.45	0.48
2:L:2340:SER:O	2:L:2388:ARG:NH1	2.43	0.48
1:H:2369:SER:OG	1:H:2381:SER:OG	2.29	0.48
2:L:1400:GLU:OE1	2:L:1400:GLU:N	2.43	0.48
2:L:2810:SER:OG	2:L:2819:LEU:HD21	2.13	0.48
2:L:3558:ASN:OD1	2:L:3561:SER:OG	2.08	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3617:VAL:HG11	2:L:3829:TRP:CD1	2.49	0.47
1:H:2356:ILE:HG13	1:H:2357:VAL:N	2.28	0.47
2:L:2250:LEU:HD22	2:L:2306:VAL:HG11	1.96	0.47
2:L:2254:LEU:HD23	2:L:2255:MET:N	2.29	0.47
1:H:2336:GLU:OE2	1:H:2380:ARG:NH2	2.48	0.47
2:L:467:ILE:HD12	2:L:605:VAL:HG11	1.97	0.47
2:L:1938:THR:O	2:L:1939:VAL:C	2.53	0.47
2:L:2507:ILE:HG22	2:L:2507:ILE:O	2.13	0.47
1:H:2426:THR:HG21	2:L:2799:TYR:CD2	2.50	0.47
2:L:106:LEU:O	2:L:110:THR:OG1	2.32	0.47
2:L:790:LEU:CD2	2:L:809:LEU:HD11	2.44	0.47
2:L:3311:LEU:HD13	2:L:3416:ILE:CG1	2.44	0.47
2:L:3572:CYS:O	2:L:3576:GLY:N	2.48	0.47
2:L:655:VAL:N	2:L:656:PRO:HD2	2.30	0.47
2:L:1719:GLU:OE1	2:L:1764:LEU:HD21	2.14	0.47
2:L:3222:LEU:HD12	2:L:3274:ILE:HD12	1.97	0.47
2:L:705:GLU:N	2:L:705:GLU:OE1	2.44	0.47
2:L:2666:PRO:N	2:L:2667:PRO:CD	2.77	0.47
2:L:3299:PHE:CD2	2:L:3501:VAL:HG21	2.50	0.47
2:L:1937:HIS:ND1	2:L:1939:VAL:HG13	2.30	0.46
2:L:1347:ASP:OD1	2:L:1366:ARG:NH2	2.46	0.46
2:L:1811:ARG:NH2	2:L:1850:CYS:SG	2.89	0.46
2:L:3251:GLN:NE2	2:L:3263:ARG:O	2.44	0.46
2:L:3774:ASP:OD1	2:L:3775:SER:N	2.47	0.46
2:L:2134:LEU:O	2:L:2137:THR:OG1	2.26	0.46
2:L:850:GLU:HA	2:L:853:VAL:HG12	1.97	0.46
2:L:1253:ASN:HB3	2:L:1256:VAL:HG22	1.98	0.46
2:L:1525:GLU:O	2:L:1529:LEU:N	2.47	0.46
2:L:2850:ALA:O	2:L:2854:VAL:HG23	2.16	0.46
2:L:3311:LEU:HD12	2:L:3312:GLN:N	2.32	0.46
2:L:671:VAL:HG12	2:L:675:PHE:CE2	2.51	0.45
2:L:1313:THR:HG22	2:L:1372:ALA:HA	1.97	0.45
2:L:2121:TRP:N	2:L:2122:PRO:CD	2.79	0.45
2:L:2177:ARG:NH2	2:L:2220:GLU:OE2	2.48	0.45
2:L:709:LEU:HD23	2:L:713:LEU:CD1	2.46	0.45
2:L:930:ASP:OD2	2:L:931:CYS:N	2.49	0.45
2:L:969:CYS:HA	2:L:972:VAL:HG22	1.99	0.45
2:L:3117:VAL:HG21	2:L:3130:TRP:HE3	1.82	0.45
2:L:228:LEU:HG	2:L:229:PRO:HD3	1.98	0.45
2:L:3266:ALA:HB3	2:L:3267:PRO:HD3	1.97	0.45
2:L:2232:ILE:HG21	2:L:2253:THR:HG22	1.98	0.45

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2796:PHE:N	2:L:2797:PRO:HD2	2.31	0.45
2:L:3225:ILE:HA	2:L:3228:VAL:HG12	1.98	0.45
2:L:3348:THR:HG23	2:L:3349:PHE:N	2.31	0.45
2:L:281:ILE:O	2:L:285:ILE:HG23	2.16	0.44
2:L:453:VAL:HG23	2:L:592:LEU:HA	2.00	0.44
2:L:2506:VAL:O	2:L:2515:ARG:NH1	2.50	0.44
2:L:2959:ARG:O	2:L:2960:LEU:HD12	2.17	0.44
2:L:3329:VAL:O	2:L:3330:SER:HB3	2.17	0.44
2:L:3652:PHE:CE1	2:L:3656:VAL:HG21	2.52	0.44
2:L:448:MET:O	2:L:451:VAL:HG22	2.16	0.44
2:L:984:LEU:HD13	2:L:2503:ILE:HG21	1.99	0.44
2:L:1937:HIS:O	2:L:1938:THR:OG1	2.29	0.44
2:L:228:LEU:N	2:L:229:PRO:CD	2.81	0.44
2:L:3432:ILE:N	2:L:3472:PRO:O	2.43	0.44
2:L:1760:ASN:HB2	2:L:1761:PRO:HD3	1.99	0.44
2:L:2887:GLU:OE1	2:L:2887:GLU:N	2.45	0.44
2:L:73:LEU:C	2:L:73:LEU:HD12	2.38	0.44
2:L:1005:HIS:CD2	2:L:3429:PHE:HZ	2.36	0.44
2:L:2159:LEU:HA	2:L:2162:VAL:HG12	2.00	0.44
2:L:679:PRO:O	2:L:680:THR:OG1	2.20	0.44
2:L:1172:PRO:O	2:L:1176:VAL:HG13	2.18	0.44
2:L:475:SER:HG	2:L:614:TYR:HD1	1.64	0.44
2:L:1343:CYS:HB2	2:L:1370:LEU:HD22	1.99	0.44
2:L:3086:LYS:O	2:L:3089:THR:OG1	2.24	0.44
2:L:1117:VAL:O	2:L:1121:VAL:HG22	2.18	0.43
2:L:1050:THR:HG21	2:L:1121:VAL:CG2	2.48	0.43
2:L:295:ILE:HD12	2:L:338:ILE:HG13	1.99	0.43
2:L:427:VAL:HG21	2:L:560:ILE:HG12	2.00	0.43
2:L:348:ILE:N	2:L:349:PRO:HD2	2.33	0.43
2:L:3617:VAL:HG11	2:L:3829:TRP:HD1	1.83	0.43
2:L:663:SER:N	2:L:709:LEU:HD11	2.34	0.43
2:L:824:LEU:N	2:L:825:PRO:CD	2.81	0.43
2:L:1394:LEU:O	2:L:1402:GLN:NE2	2.48	0.43
2:L:3504:ASP:O	2:L:3505:ALA:HB3	2.18	0.43
2:L:125:ASN:ND2	2:L:128:ASN:OD1	2.52	0.43
2:L:390:LEU:HD12	2:L:395:LEU:HD21	1.99	0.43
2:L:1382:SER:O	2:L:1386:ILE:HD13	2.19	0.43
2:L:3134:LEU:HA	2:L:3137:ILE:HG22	2.01	0.43
2:L:1087:MET:SD	2:L:1088:ASP:N	2.92	0.43
2:L:3644:THR:HG22	2:L:3710:LEU:HD22	2.01	0.43
2:L:239:TYR:CZ	2:L:243:ILE:HD11	2.54	0.43

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:561:THR:HG22	2:L:589:TYR:CE1	2.53	0.43
2:L:561:THR:HG21	2:L:638:VAL:CG1	2.45	0.43
2:L:3299:PHE:HD2	2:L:3501:VAL:HG11	1.84	0.43
2:L:663:SER:N	2:L:709:LEU:CD1	2.81	0.42
2:L:1329:VAL:HG13	2:L:1332:HIS:H	1.84	0.42
2:L:2349:VAL:O	2:L:2352:ILE:HG12	2.19	0.42
2:L:423:LEU:O	2:L:427:VAL:HG23	2.19	0.42
2:L:1290:VAL:HB	2:L:1291:PRO:HD3	2.00	0.42
2:L:462:TYR:CZ	2:L:1712:THR:HG21	2.55	0.42
2:L:984:LEU:CD1	2:L:2503:ILE:HG21	2.50	0.42
2:L:1430:LEU:HD21	2:L:1448:LEU:HD12	2.01	0.42
2:L:3301:GLU:HG2	2:L:3302:ASN:H	1.83	0.42
2:L:106:LEU:HD11	2:L:139:LEU:HG	2.00	0.42
2:L:336:LYS:O	2:L:340:THR:OG1	2.33	0.42
2:L:2381:MET:O	2:L:2385:ILE:HG22	2.19	0.42
2:L:1309:MET:SD	2:L:1339:LEU:HD21	2.60	0.42
2:L:1309:MET:O	2:L:1313:THR:HG23	2.20	0.42
2:L:238:LEU:HD13	2:L:241:LEU:HD12	2.01	0.42
2:L:1552:VAL:HG11	2:L:1585:VAL:CG2	2.50	0.42
2:L:2650:GLN:HB3	2:L:2651:PRO:HD3	2.02	0.42
2:L:2479:GLU:OE2	2:L:2601:HIS:NE2	2.53	0.42
1:H:2356:ILE:HG13	1:H:2357:VAL:H	1.85	0.41
2:L:2863:ALA:HB1	2:L:2896:LEU:HD13	2.01	0.41
2:L:3643:PHE:CE1	2:L:3669:ILE:HD12	2.55	0.41
2:L:719:GLY:O	2:L:722:SER:OG	2.33	0.41
2:L:1243:HIS:O	2:L:1246:VAL:HG22	2.19	0.41
2:L:1386:ILE:N	2:L:1386:ILE:HD12	2.35	0.41
2:L:2400:LEU:HD13	2:L:2436:ILE:HG21	2.02	0.41
2:L:1194:LEU:HD12	2:L:1199:SER:HB2	2.02	0.41
2:L:2928:ALA:HB1	2:L:2980:HIS:NE2	2.35	0.41
2:L:3678:VAL:HG21	2:L:3681:PHE:CD2	2.56	0.41
2:L:558:LYS:HA	2:L:638:VAL:HG22	2.01	0.41
2:L:986:GLN:NE2	2:L:2519:ALA:O	2.52	0.41
2:L:2214:VAL:HG12	2:L:2214:VAL:O	2.20	0.41
2:L:3132:ASP:O	2:L:3136:ASN:ND2	2.46	0.41
2:L:2239:TYR:O	2:L:2281:LYS:NZ	2.45	0.41
2:L:3113:PHE:O	2:L:3117:VAL:HG23	2.20	0.41
2:L:935:LEU:HD11	2:L:2618:LEU:HD23	2.02	0.41
2:L:340:THR:HG22	2:L:340:THR:O	2.19	0.41
2:L:793:LEU:HD11	2:L:1198:VAL:HG21	2.02	0.41
2:L:1887:PHE:CE2	2:L:1891:LEU:HD11	2.55	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:216:PRO:HD3	2:L:286:LYS:HG2	2.03	0.41
2:L:294:ILE:O	2:L:294:ILE:CG2	2.69	0.41
2:L:1145:LEU:HD13	2:L:1163:SER:HB2	2.03	0.41
2:L:1184:LEU:HG	2:L:1188:LEU:HD23	2.03	0.41
2:L:1303:ASN:OD1	2:L:1304:ALA:N	2.54	0.41
2:L:1366:ARG:O	2:L:1370:LEU:HD23	2.21	0.41
2:L:2173:LYS:N	2:L:2174:PRO:CD	2.84	0.41
2:L:3344:LYS:O	2:L:3348:THR:HG22	2.20	0.41
2:L:3759:ASP:OD1	2:L:3760:THR:HG23	2.20	0.41
1:H:2357:VAL:O	1:H:2358:SER:HB2	2.21	0.41
2:L:678:ASN:OD1	2:L:681:THR:OG1	2.26	0.41
2:L:877:TRP:CD2	2:L:2908:VAL:HG21	2.56	0.41
2:L:1082:ASN:OD1	2:L:1083:GLY:N	2.46	0.41
2:L:1803:GLN:HA	2:L:1803:GLN:OE1	2.21	0.41
2:L:2436:ILE:HA	2:L:2439:LYS:HG2	2.03	0.41
2:L:2634:ILE:O	2:L:2638:LEU:N	2.44	0.40
2:L:324:THR:HG21	2:L:327:LEU:HD12	2.04	0.40
2:L:2472:PHE:CE2	2:L:2474:ILE:HD11	2.56	0.40
2:L:137:ILE:HD11	2:L:220:LEU:HD12	2.04	0.40
2:L:1171:LEU:HB3	2:L:1172:PRO:HD2	2.03	0.40
2:L:1825:ALA:CB	2:L:1826:PRO:CD	2.96	0.40
2:L:2393:LEU:HD12	2:L:2394:GLU:N	2.36	0.40
2:L:2449:LYS:O	2:L:2455:ARG:NE	2.51	0.40
2:L:3194:CYS:O	2:L:3197:VAL:HG22	2.22	0.40
2:L:3504:ASP:N	2:L:3551:GLN:O	2.54	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	H	158/3123 (5%)	145 (92%)	13 (8%)	0	100 100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	3453/3830 (90%)	3333 (96%)	120 (4%)	0	100	100
All	All	3611/6953 (52%)	3478 (96%)	133 (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	H	151/2634 (6%)	148 (98%)	3 (2%)	55	80
2	L	3112/3396 (92%)	3064 (98%)	48 (2%)	65	85
All	All	3263/6030 (54%)	3212 (98%)	51 (2%)	64	84

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2279	ARG
1	H	2389	TYR
1	H	2396	ARG
2	L	85	PRO
2	L	119	ARG
2	L	290	PHE
2	L	320	CYS
2	L	358	SER
2	L	368	ARG
2	L	371	LEU
2	L	402	PHE
2	L	456	PHE
2	L	535	LYS
2	L	624	ARG
2	L	645	LEU
2	L	778	GLU
2	L	897	LYS
2	L	904	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	L	912	LEU
2	L	927	GLU
2	L	939	MET
2	L	1146	CYS
2	L	1343	CYS
2	L	1526	ARG
2	L	1537	ARG
2	L	1650	ARG
2	L	1701	ARG
2	L	1707	PHE
2	L	1742	ASN
2	L	1763	PHE
2	L	1769	LYS
2	L	1785	ASN
2	L	1811	ARG
2	L	1879	HIS
2	L	1885	GLN
2	L	1986	ARG
2	L	2121	TRP
2	L	2158	PHE
2	L	2373	GLU
2	L	2393	LEU
2	L	2571	HIS
2	L	2676	LYS
2	L	2691	MET
2	L	3069	CYS
2	L	3127	TRP
2	L	3166	SER
2	L	3220	LEU
2	L	3300	ARG
2	L	3529	LYS
2	L	3530	ARG
2	L	3596	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	2373	ASN
1	H	2384	GLN
1	H	2387	ASN
1	H	2428	HIS
2	L	64	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	L	245	ASN
2	L	463	GLN
2	L	598	GLN
2	L	619	ASN
2	L	621	GLN
2	L	1269	GLN
2	L	1287	GLN
2	L	1371	ASN
2	L	2470	ASN
2	L	2513	HIS
2	L	2650	GLN
2	L	2695	GLN
2	L	2828	HIS
2	L	2906	HIS
2	L	3295	GLN
2	L	3302	ASN
2	L	3406	HIS
2	L	3480	HIS
2	L	3492	HIS

### 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](#)

1 ligand is 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	$\# Z  > 2$
3	IHP	L	3901	-	36,36,36	0.74	0	54,60,60	1.41	7 (12%)

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
3	IHP	L	3901	-	-	6/30/54/54	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	L	3901	IHP	O14-C4-C3	3.07	115.94	108.69
3	L	3901	IHP	O14-C4-C5	2.84	115.37	108.69
3	L	3901	IHP	C6-C5-C4	2.79	116.51	110.41
3	L	3901	IHP	C5-C4-C3	-2.72	104.45	110.41
3	L	3901	IHP	C6-C1-C2	2.54	115.97	110.41
3	L	3901	IHP	C5-C6-C1	2.34	115.53	110.41
3	L	3901	IHP	O15-P5-O25	-2.19	100.94	109.39

There are no chirality outliers.

All (6) torsion outliers are listed below:

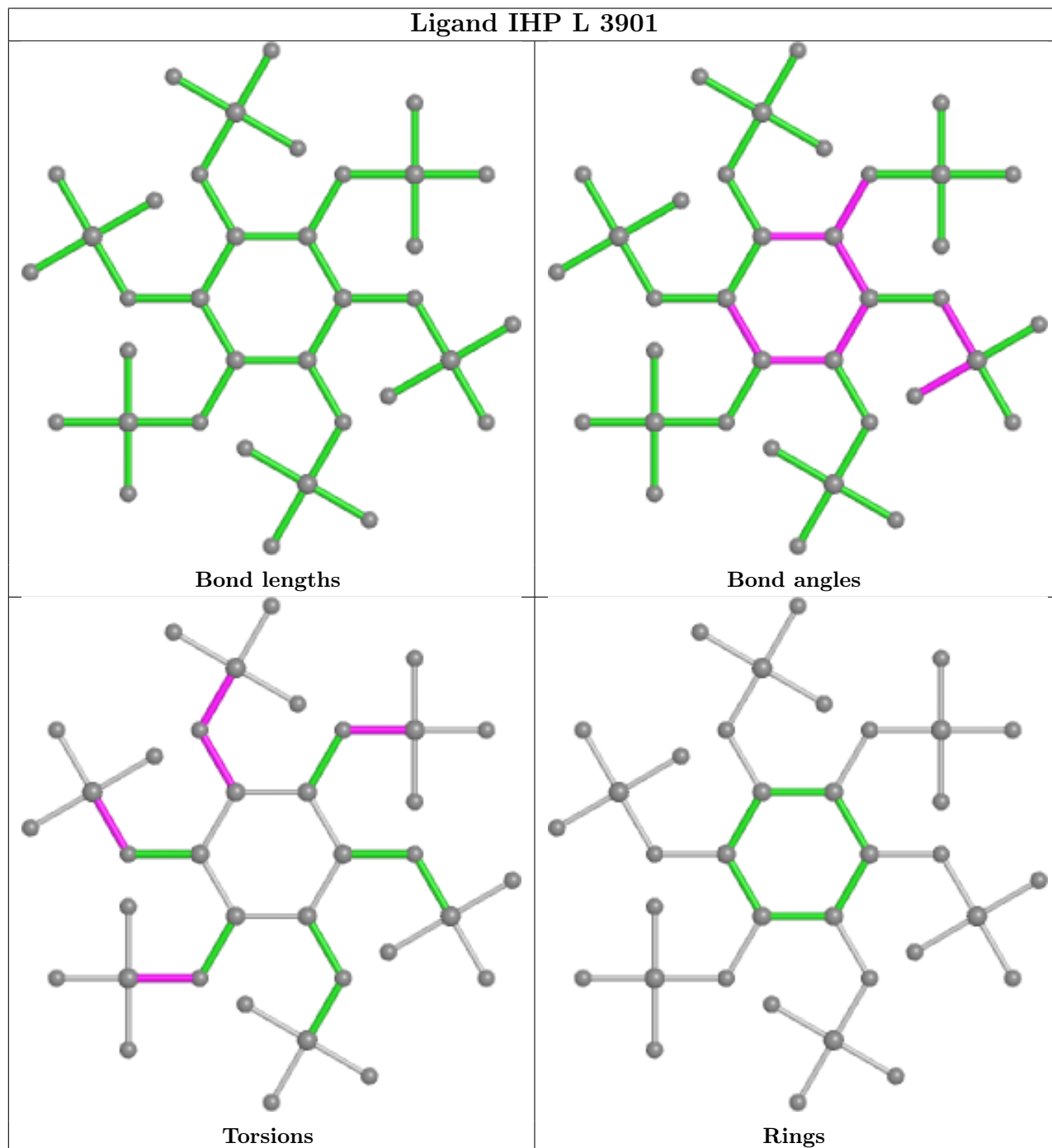
Mol	Chain	Res	Type	Atoms
3	L	3901	IHP	C4-C3-O13-P3
3	L	3901	IHP	C1-O11-P1-O41
3	L	3901	IHP	C4-O14-P4-O24
3	L	3901	IHP	C1-O11-P1-O31
3	L	3901	IHP	C2-O12-P2-O42
3	L	3901	IHP	C3-O13-P3-O33

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

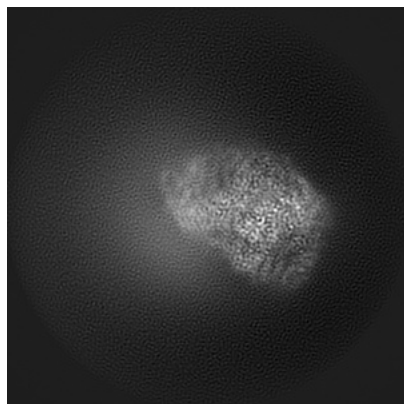
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38720. These allow visual inspection of the internal detail of the map and identification of artifacts.

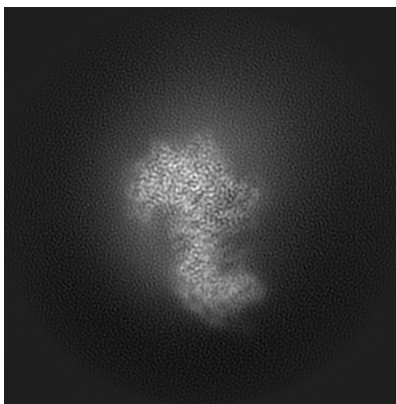
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

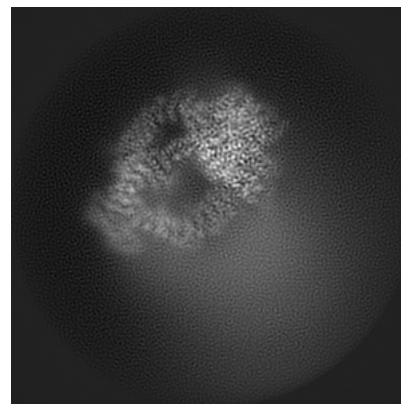
#### 6.1.1 Primary map



X

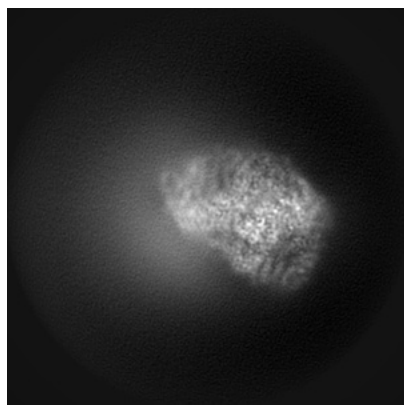


Y

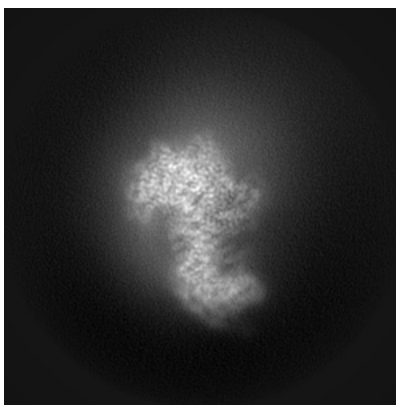


Z

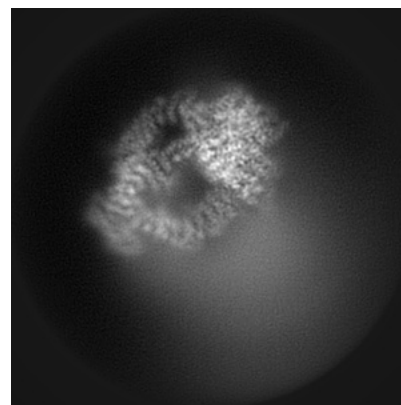
#### 6.1.2 Raw map



X



Y

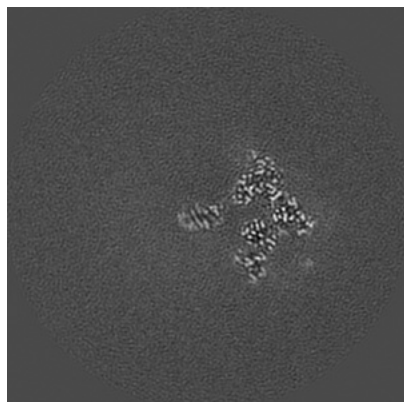


Z

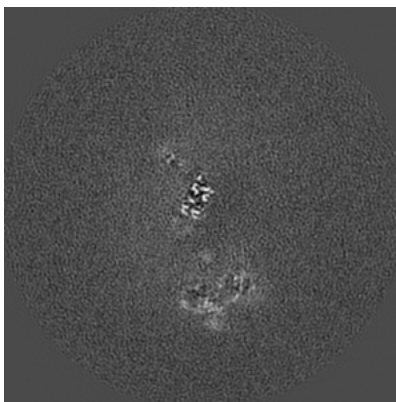
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

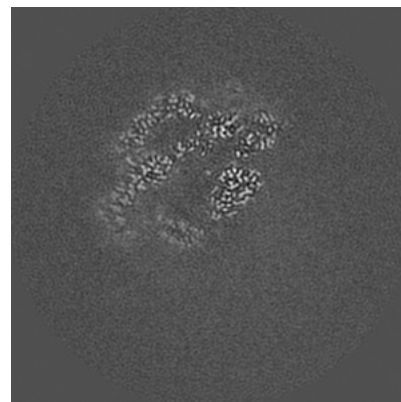
### 6.2.1 Primary map



X Index: 128

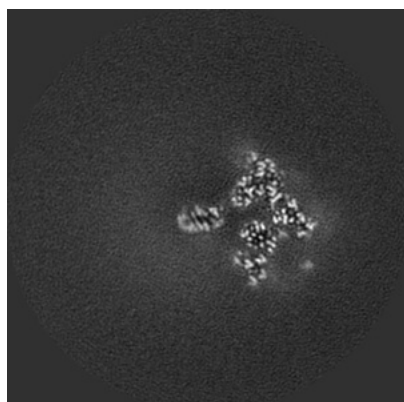


Y Index: 128

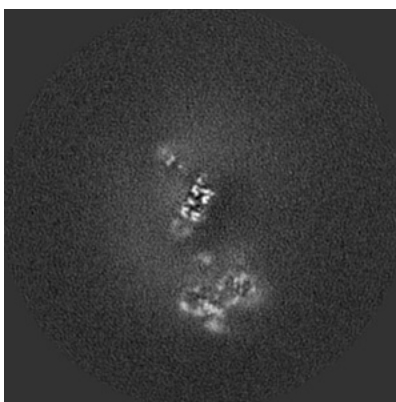


Z Index: 128

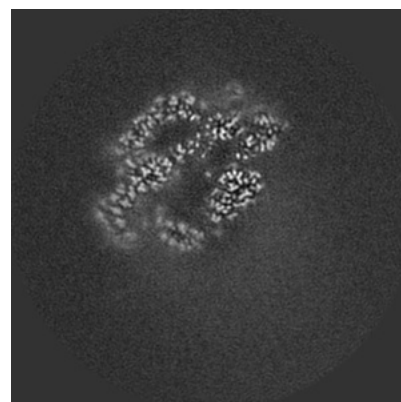
### 6.2.2 Raw map



X Index: 128



Y Index: 128

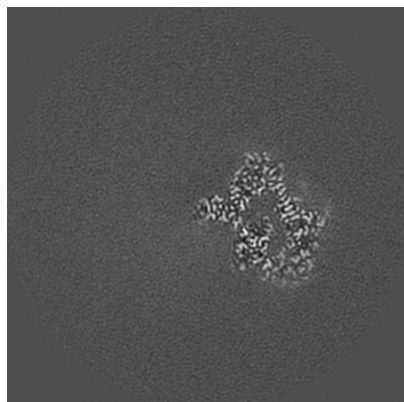


Z Index: 128

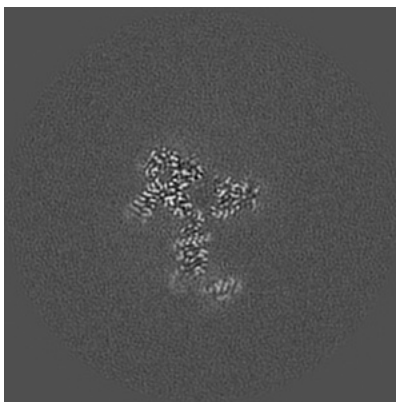
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

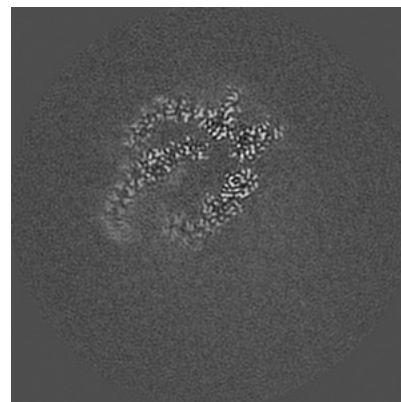
### 6.3.1 Primary map



X Index: 139

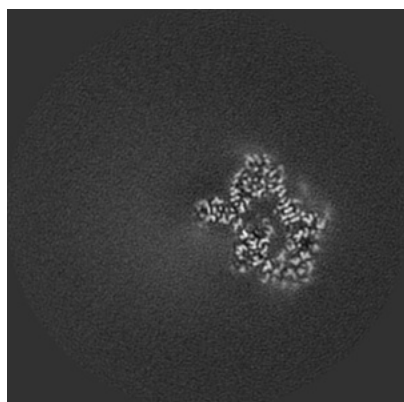


Y Index: 159

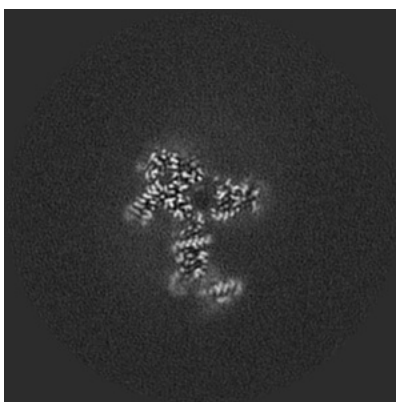


Z Index: 124

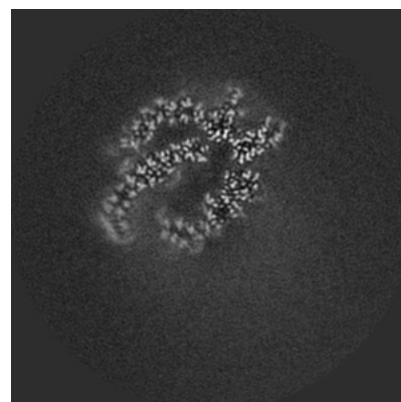
### 6.3.2 Raw map



X Index: 139



Y Index: 159

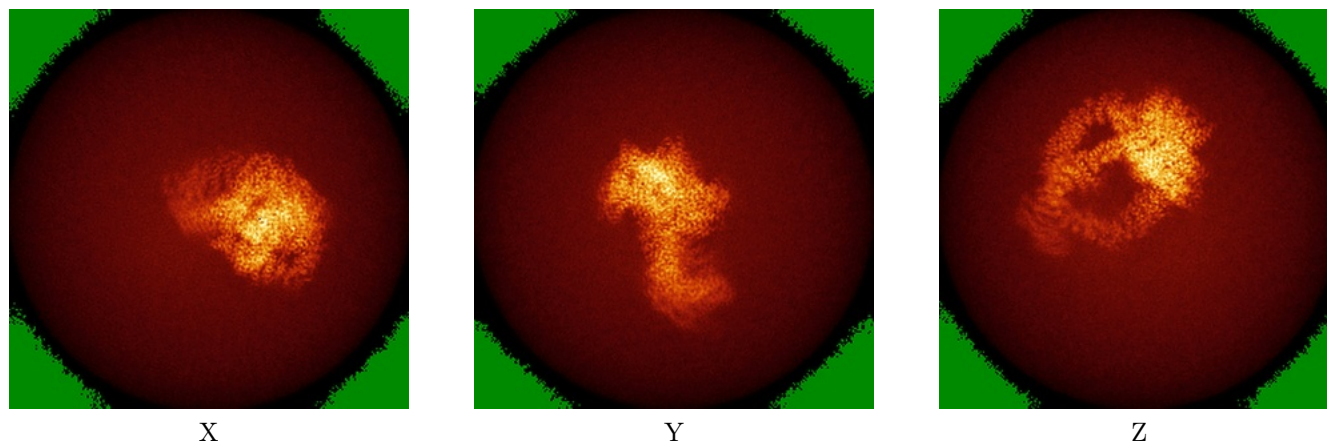


Z Index: 125

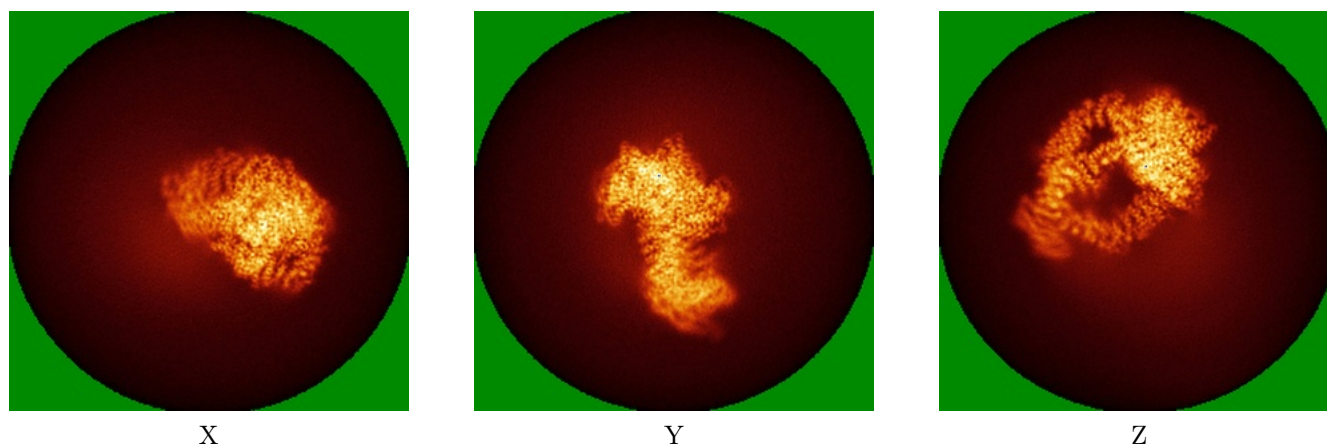
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



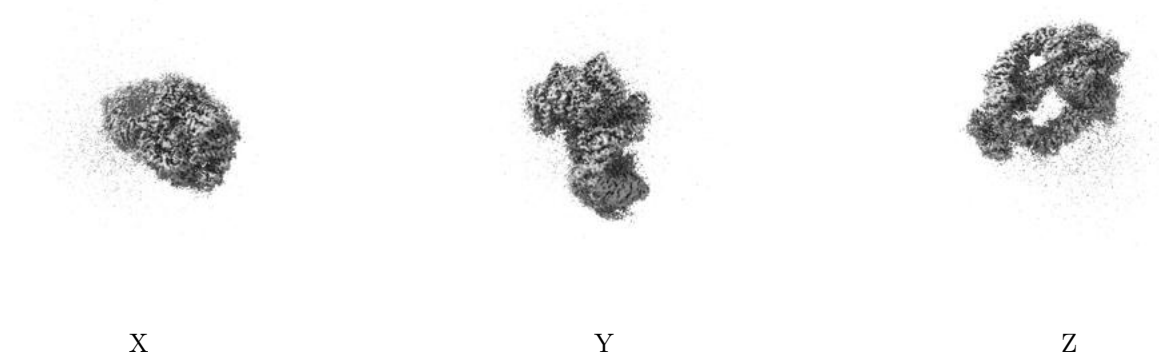
### 6.4.2 Raw map



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.

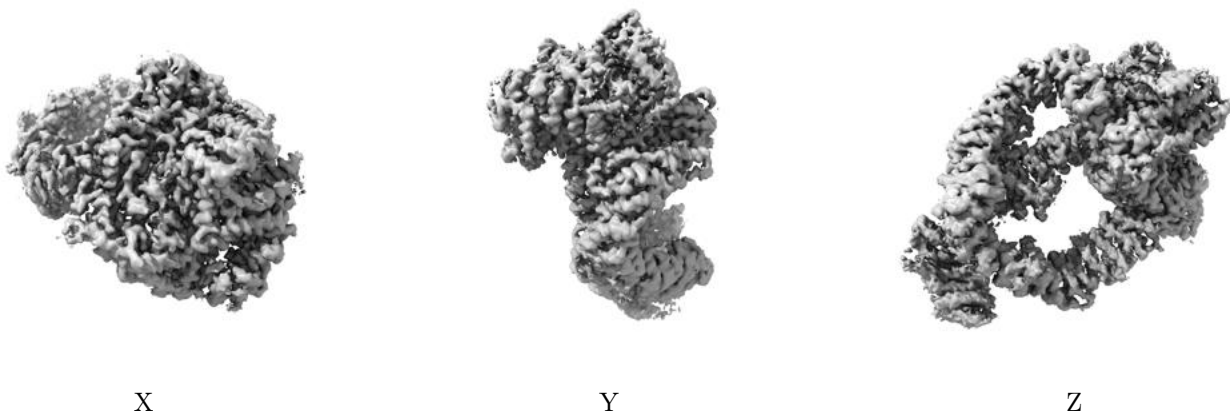
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. 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.

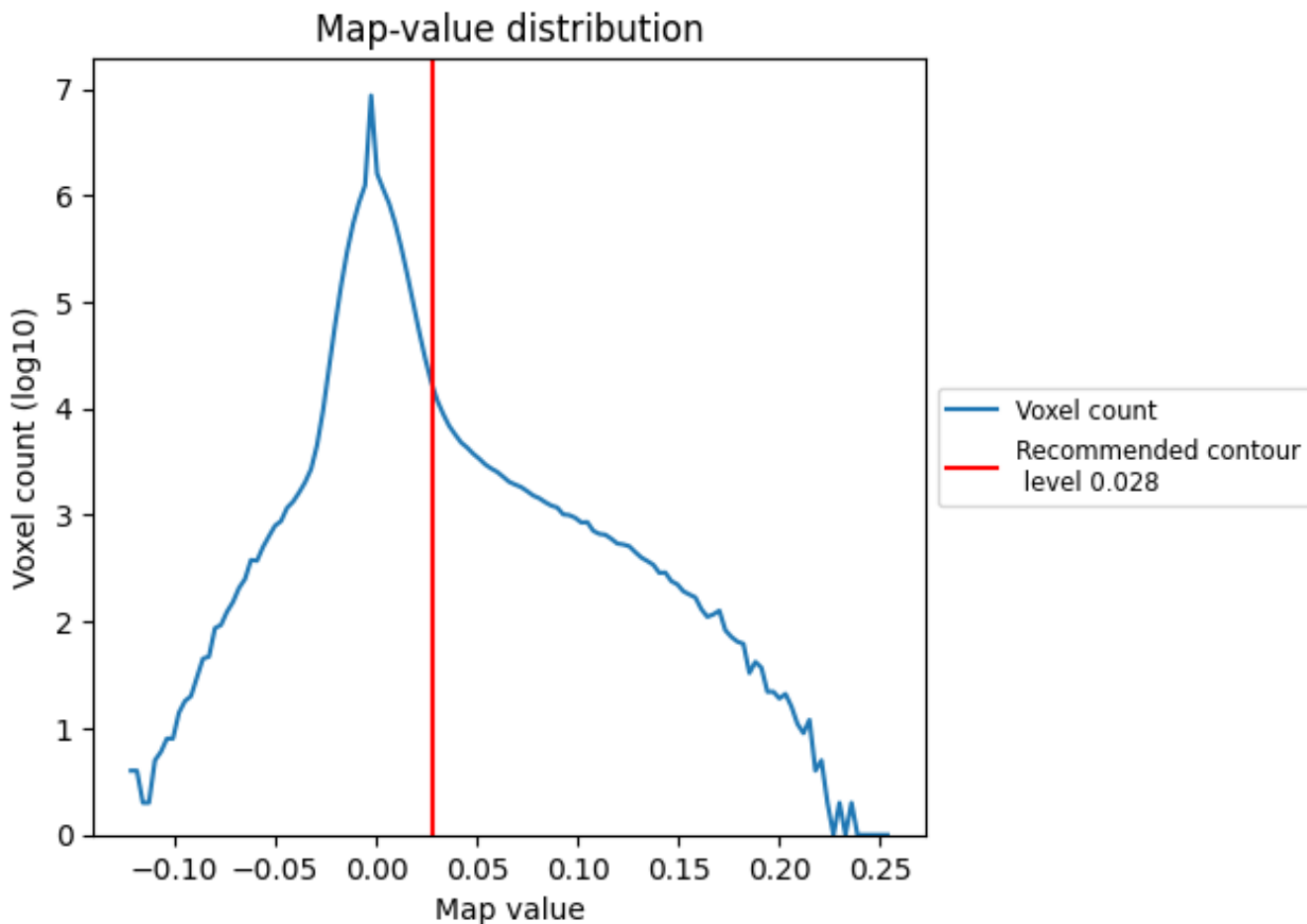
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

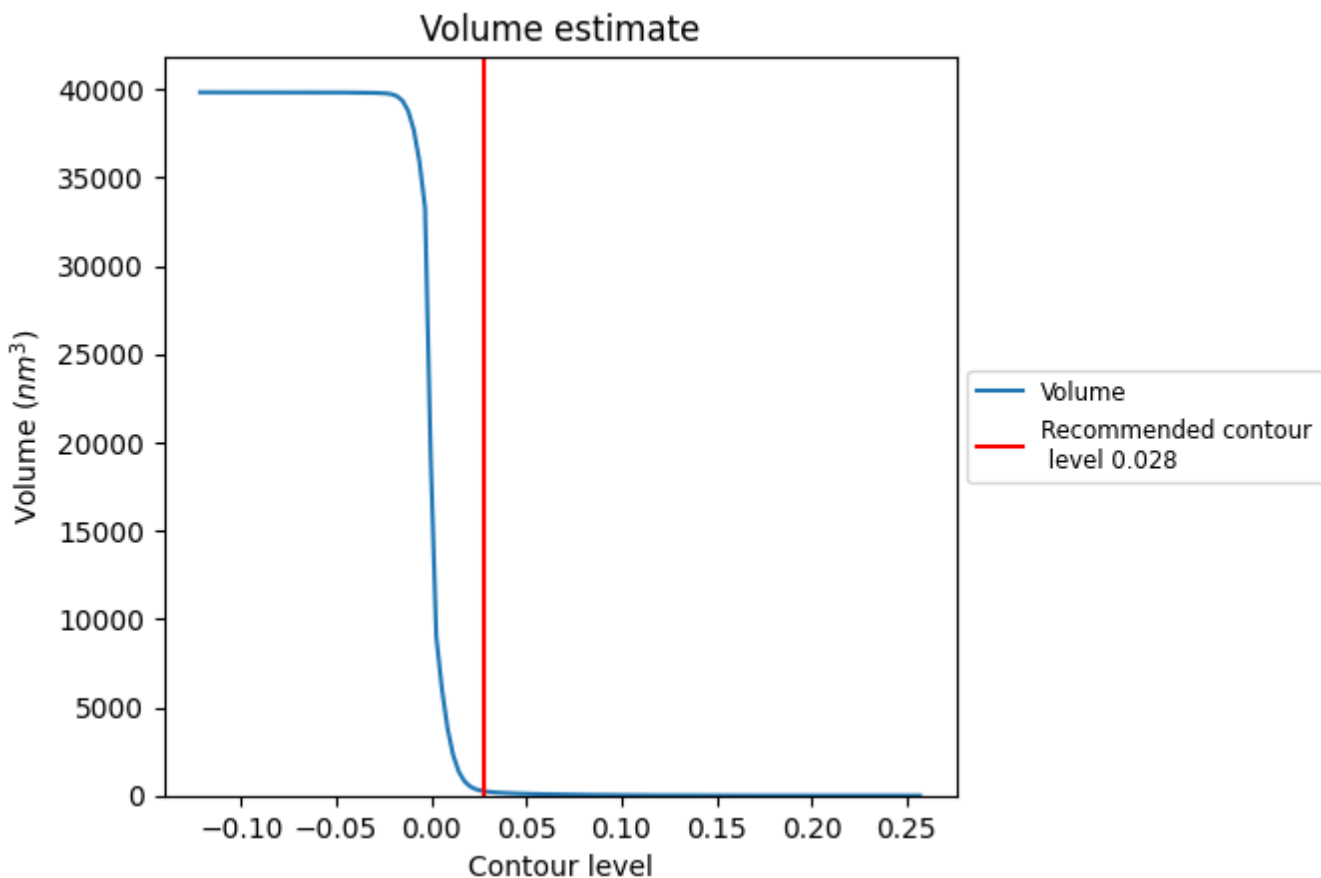
This section contains the results of statistical analysis of the map.

### 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](#)

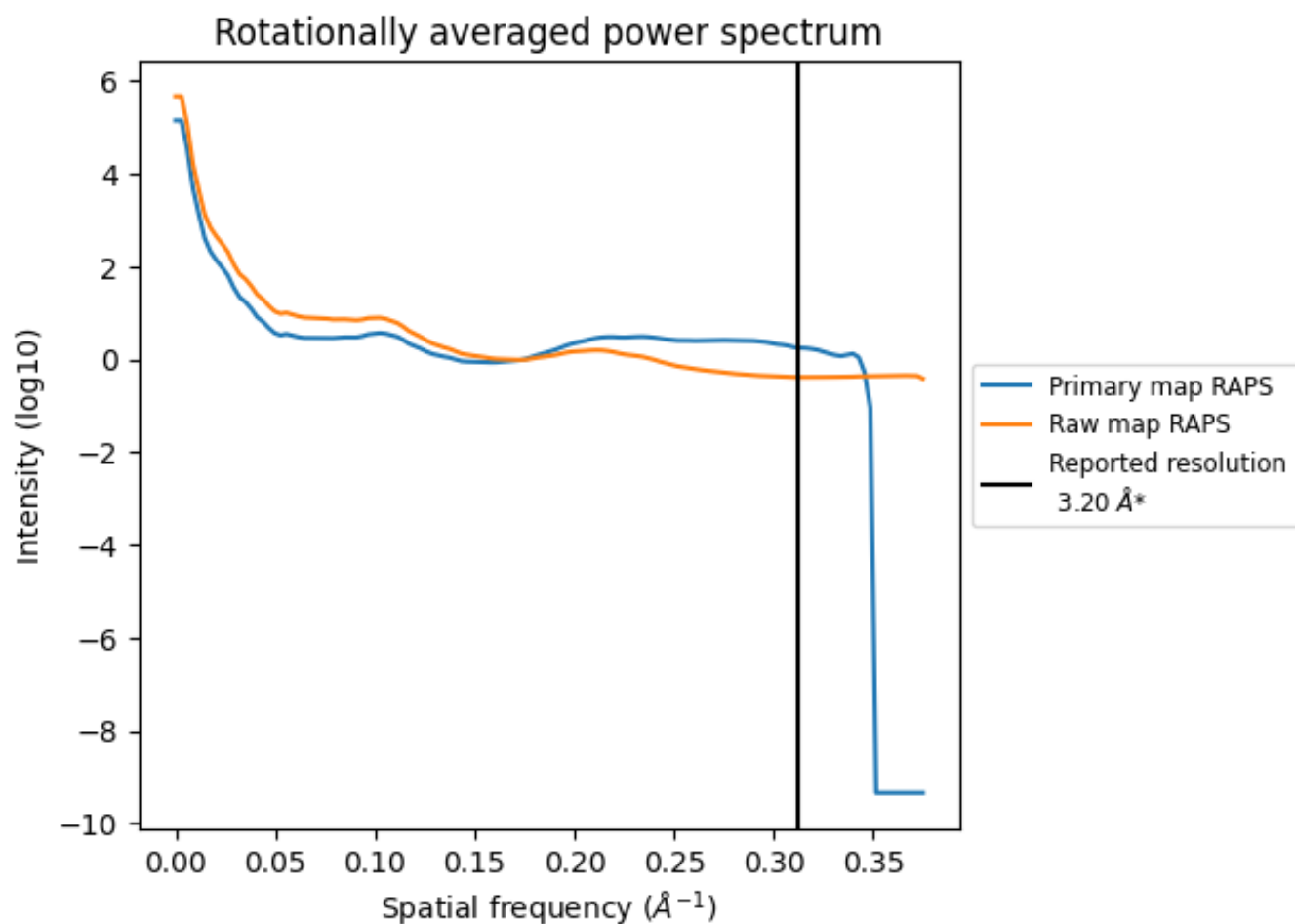


The volume at the recommended contour level is 243 nm<sup>3</sup>; this corresponds to an approximate mass of 219 kDa.

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

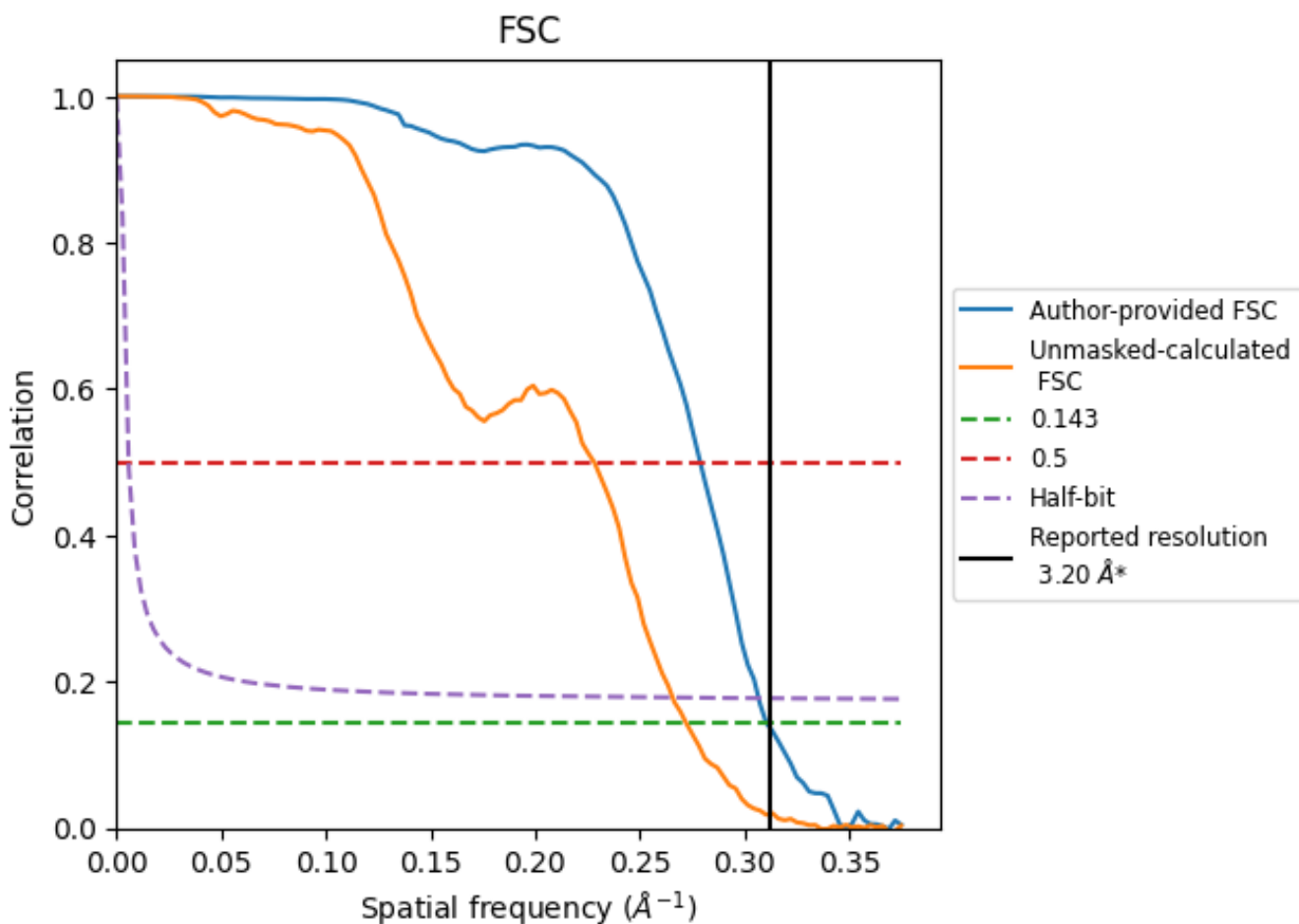


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

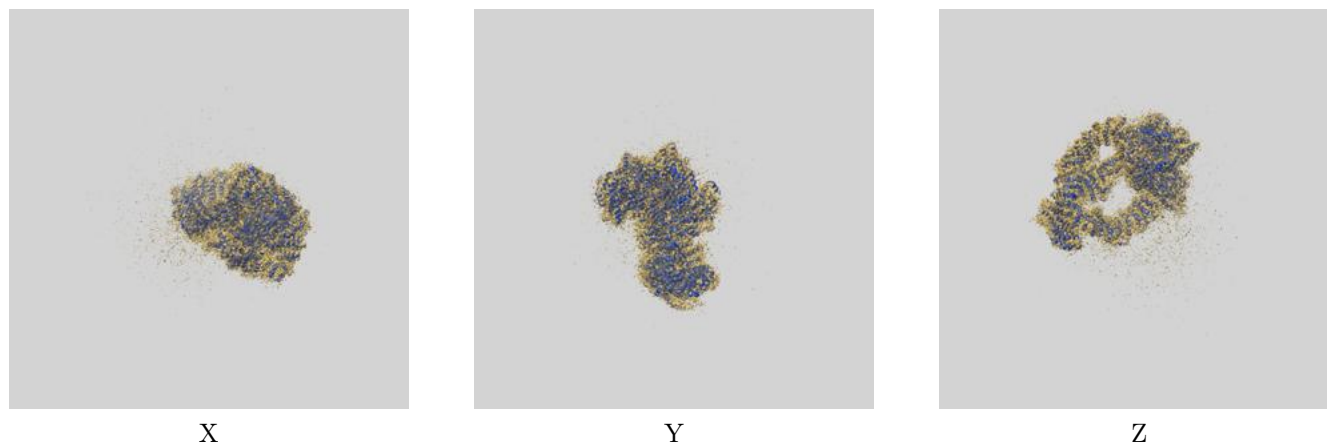
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.59	3.26
Unmasked-calculated*	3.67	4.38	3.76

\*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 3.67 differs from the reported value 3.2 by more than 10 %

## 9 Map-model fit [i](#)

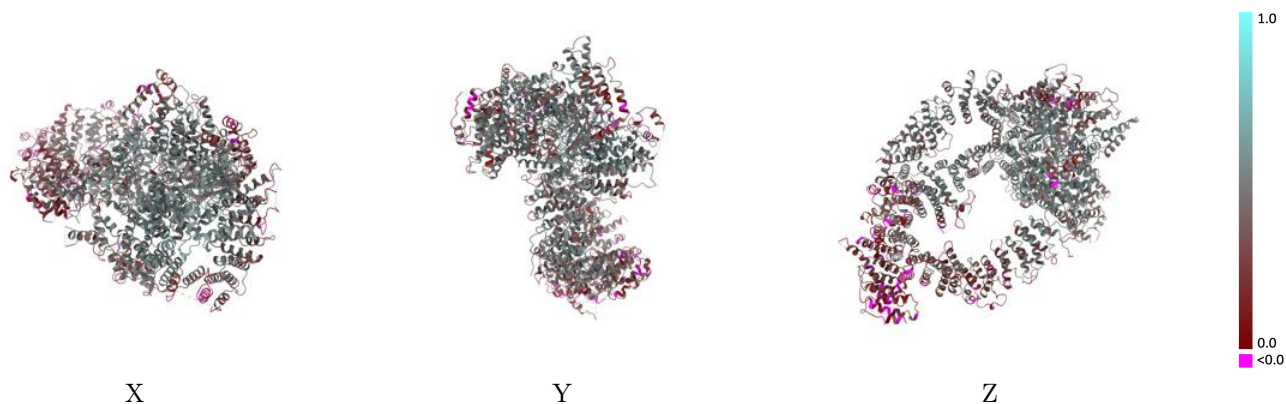
This section contains information regarding the fit between EMDB map EMD-38720 and PDB model 8XVV. Per-residue inclusion information can be found in section [3](#) on page [4](#).

### 9.1 Map-model overlay [i](#)



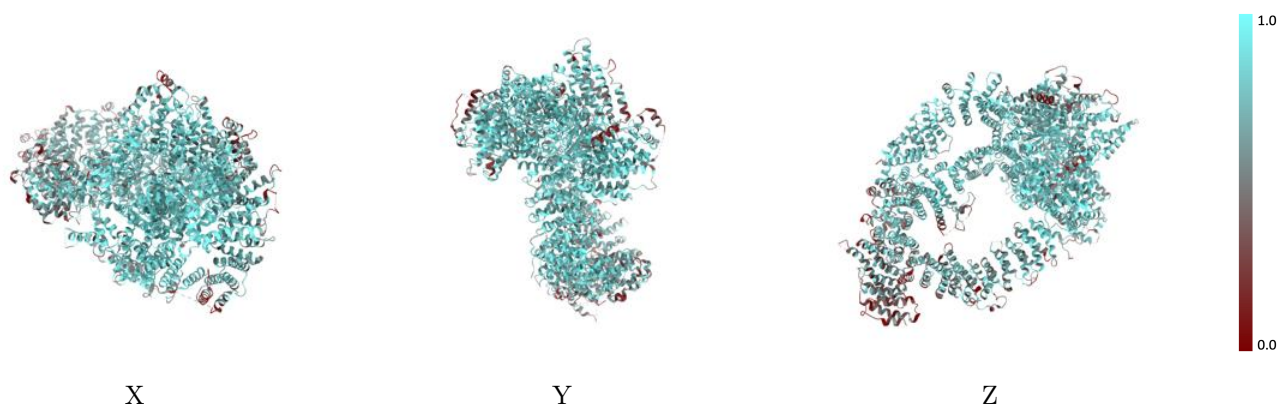
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



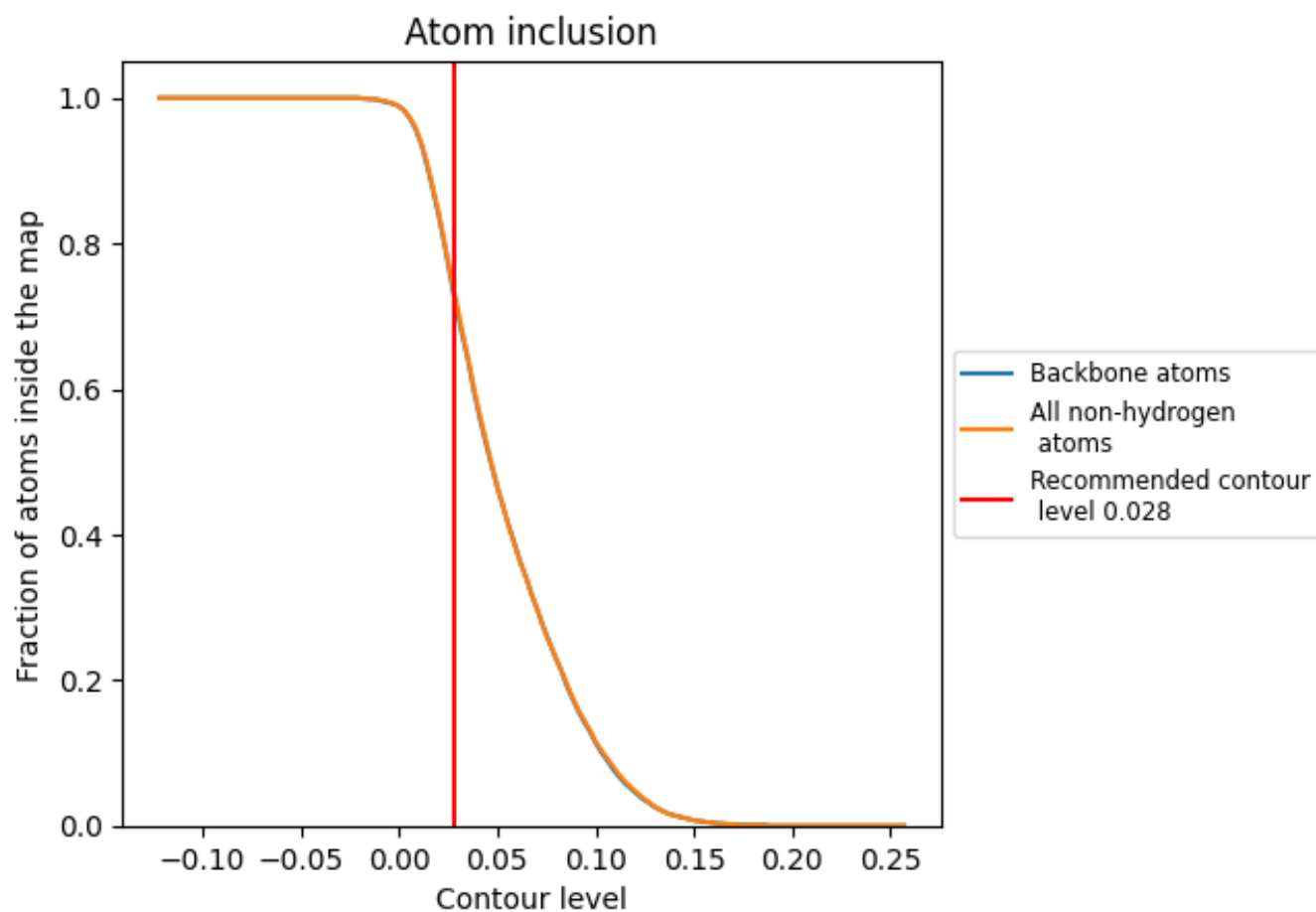
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.028).







## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7340	 0.3960
H	 0.6620	 0.3720
L	 0.7460	 0.3970

