



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 11:44 PM JST

PDB ID : 7CTG  
EMDB ID : EMD-30464  
Title : Human Origin Recognition Complex, ORC1-5 State I  
Authors : Cheng, J.; Li, N.; Wang, X.; Hu, J.; Zhai, Y.; Gao, N.  
Deposited on : 2020-08-18  
Resolution : 5.00 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](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>.

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

EMDB validation analysis : 0.0.1.dev43  
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 : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

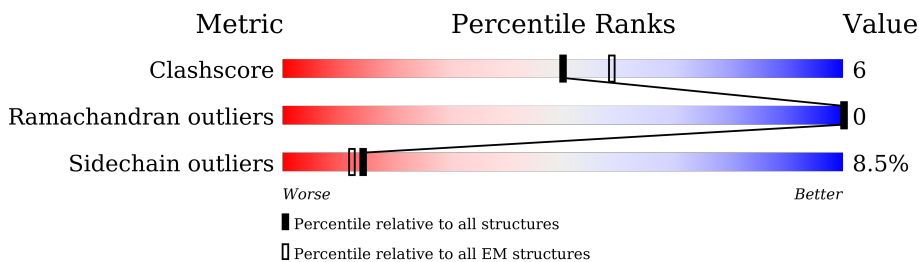
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	A	861	
2	B	577	
3	C	711	
4	D	436	
5	E	435	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14504 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 Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	102	Total	C	N	O	S	0	0
			805	504	140	155	6		

- Molecule 2 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	302	Total	C	N	O	S	1	0
			2460	1581	411	462	6		

- Molecule 3 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	592	Total	C	N	O	S	0	0
			4828	3109	811	881	27		

- Molecule 4 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	406	Total	C	N	O	S	0	0
			3305	2115	570	599	21		

There is a discrepancy between the modelled and reference sequences:

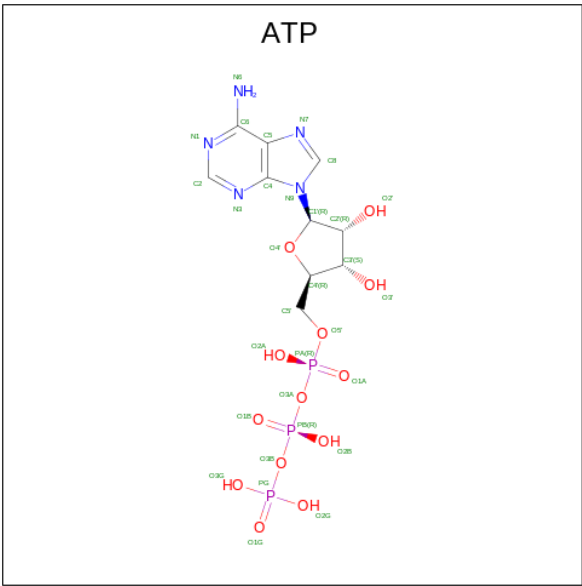
Chain	Residue	Modelled	Actual	Comment	Reference
D	396	GLU	GLN	conflict	UNP O43929

- Molecule 5 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	373	Total	C	N	O	S	0	0
			3044	1985	504	545	10		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

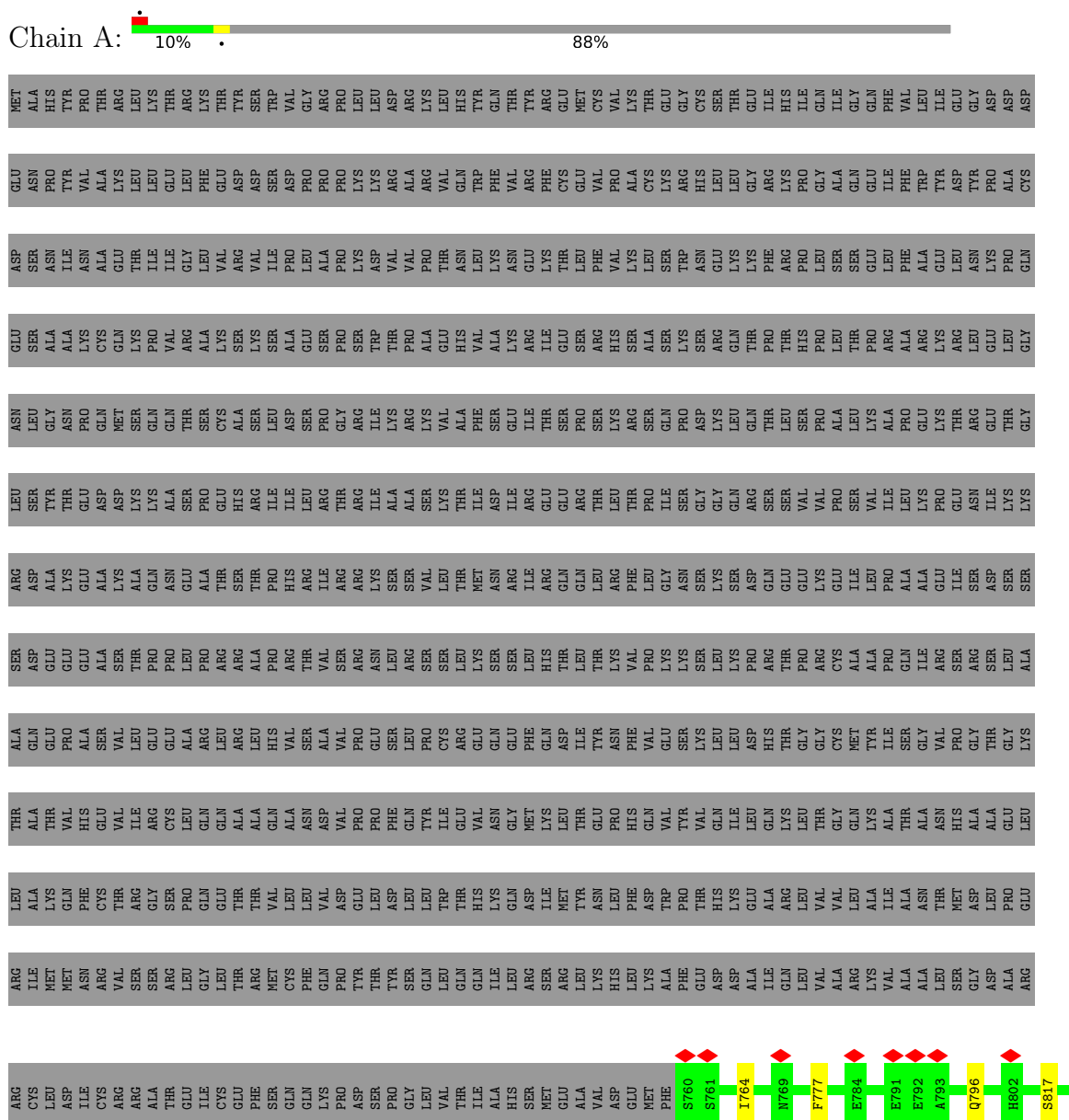
C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

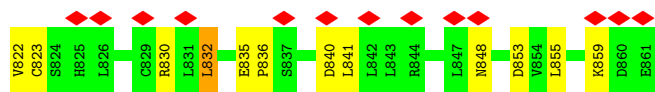


### 3 Residue-property plots

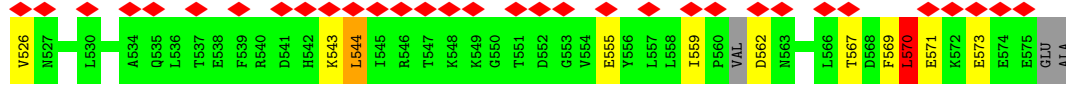
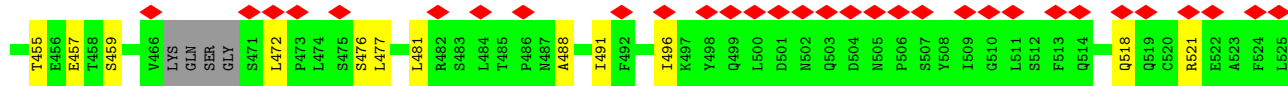
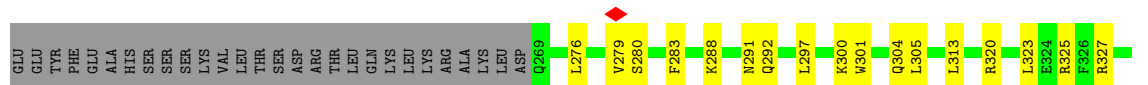
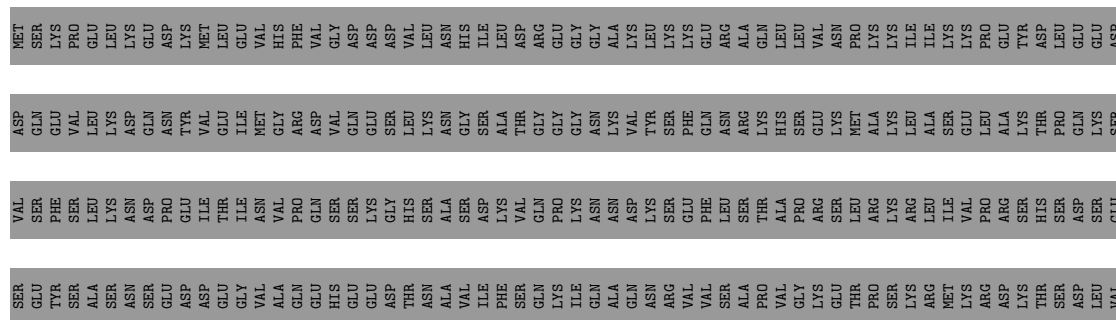
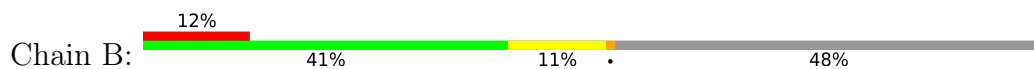
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Origin recognition complex subunit 1

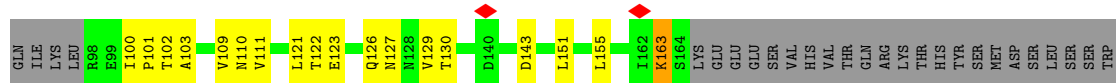
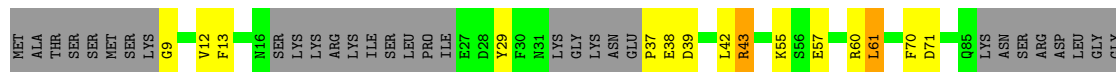


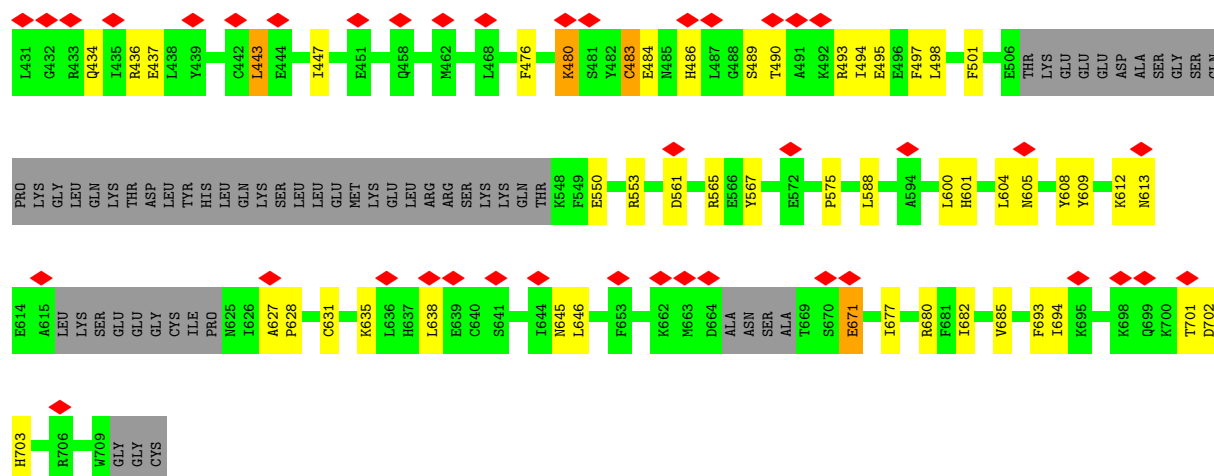


• Molecule 2: Origin recognition complex subunit 2

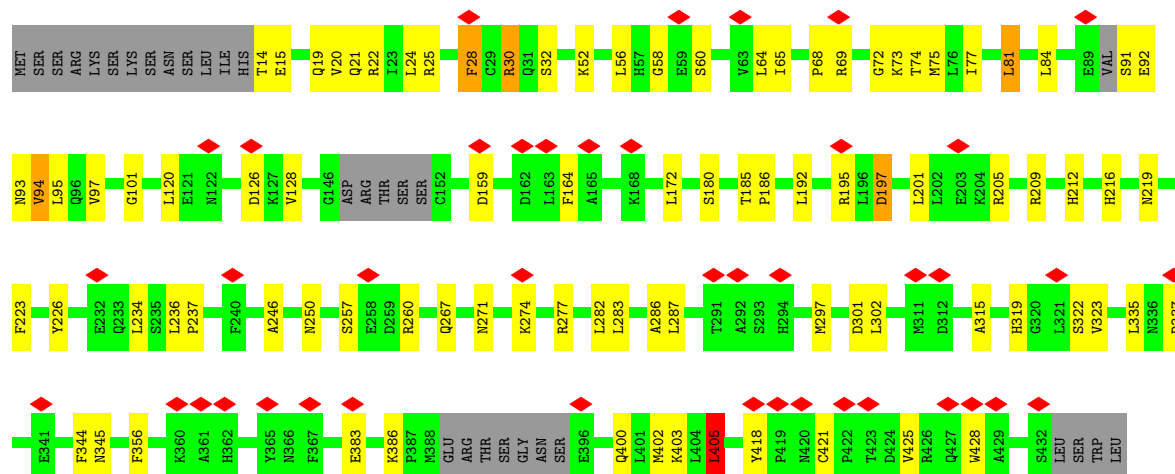
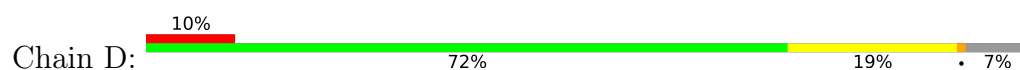


• Molecule 3: Origin recognition complex subunit 3

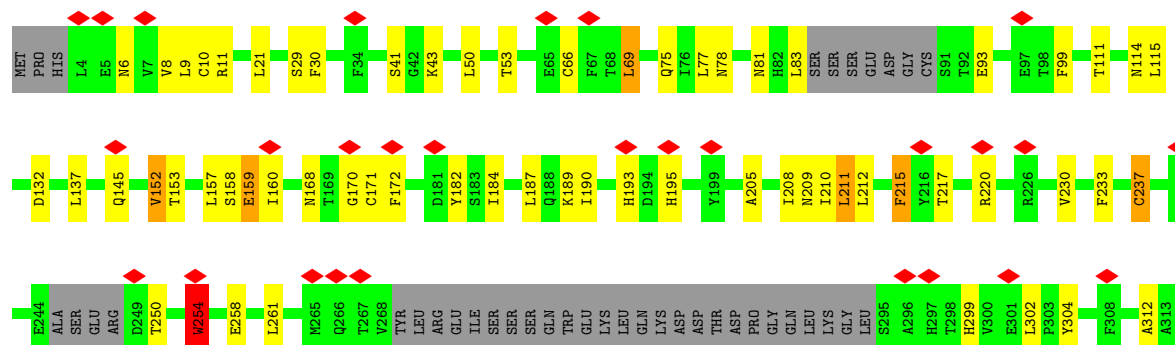


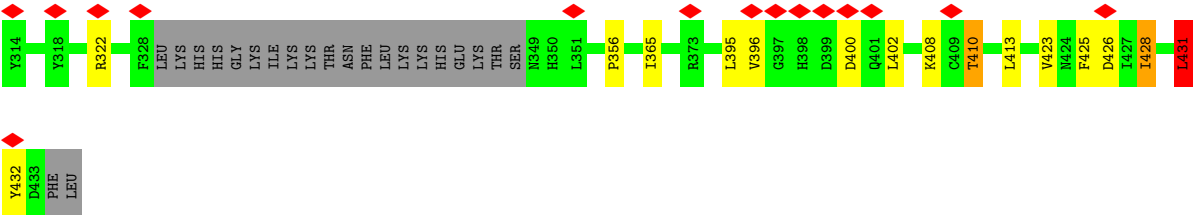


• Molecule 4: Origin recognition complex subunit 4



• Molecule 5: Origin recognition complex subunit 5





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49000	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 ( $e^-/\text{\AA}^2$ )	65.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	248.58, 248.58, 248.58	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6572, 1.6572, 1.6572	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.40	0/816	0.66	0/1102
2	B	0.41	0/2512	0.63	1/3402 (0.0%)
3	C	0.41	1/4927 (0.0%)	0.69	2/6663 (0.0%)
4	D	0.40	0/3366	0.66	1/4534 (0.0%)
5	E	0.44	0/3117	0.69	3/4233 (0.1%)
All	All	0.41	1/14738 (0.0%)	0.67	7/19934 (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	2
3	C	0	9
4	D	0	4
5	E	0	2
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	13	PHE	C-N	-5.91	1.20	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	369	LEU	CA-CB-CG	9.02	136.05	115.30
5	E	431	LEU	CA-CB-CG	6.63	130.56	115.30
5	E	254	TRP	CA-CB-CG	6.58	126.20	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	405	LEU	CA-CB-CG	6.47	130.18	115.30
5	E	395	LEU	CA-CB-CG	6.06	129.24	115.30
2	B	570	LEU	CA-CB-CG	-6.00	101.50	115.30
3	C	369	LEU	CB-CG-CD2	-5.76	101.20	111.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	280	SER	Peptide
2	B	570	LEU	Peptide
3	C	143	ASP	Peptide
3	C	242	HIS	Peptide
3	C	280	SER	Peptide
3	C	39	ASP	Peptide
3	C	609	TYR	Peptide
3	C	627	ALA	Peptide
3	C	628	PRO	Peptide
3	C	693	PHE	Peptide
3	C	701	THR	Peptide
4	D	212	HIS	Peptide
4	D	337	ASP	Peptide
4	D	400	GLN	Peptide
4	D	72	GLY	Peptide
5	E	195	HIS	Peptide
5	E	400	ASP	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	805	0	811	8	0
2	B	2460	0	2423	33	0
3	C	4828	0	4848	68	0
4	D	3305	0	3350	41	0
5	E	3044	0	3058	34	0
6	D	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	31	0	12	1	0
All	All	14504	0	14514	175	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 (175) 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:C:561:ASP:O	3:C:565:ARG:HB2	1.71	0.89
4:D:21:GLN:O	4:D:25:ARG:HB2	1.90	0.72
3:C:408:TYR:O	3:C:412:TYR:HB2	1.92	0.70
3:C:383:LYS:O	3:C:387:LEU:HB2	1.93	0.69
3:C:288:VAL:O	3:C:292:LEU:HB2	1.93	0.67
4:D:205:ARG:O	4:D:209:ARG:HB2	1.96	0.65
3:C:365:ASN:HA	3:C:368:ARG:HG2	1.82	0.62
3:C:402:LEU:HA	3:C:405:LEU:HD12	1.81	0.61
2:B:288:LYS:O	2:B:292:GLN:HB2	2.01	0.61
3:C:600:LEU:O	3:C:604:LEU:HB2	2.03	0.59
2:B:339:ILE:HB	2:B:392:ILE:HG12	1.84	0.58
5:E:211:LEU:O	5:E:215:PHE:HB2	2.03	0.58
5:E:171:CYS:SG	5:E:172:PHE:N	2.77	0.58
5:E:208:ILE:HG13	5:E:211:LEU:HD23	1.85	0.58
4:D:77:ILE:O	4:D:81:LEU:HB2	2.04	0.58
3:C:38:GLU:OE2	3:C:43:ARG:NH1	2.37	0.58
3:C:200:LEU:HD11	3:C:243:GLU:HB3	1.86	0.58
2:B:300:LYS:O	2:B:304:GLN:HB2	2.04	0.57
2:B:472:LEU:HD22	2:B:544:LEU:HD21	1.85	0.57
3:C:483:CYS:SG	3:C:484:GLU:N	2.77	0.57
3:C:401:LEU:HD21	3:C:575:PRO:HB2	1.87	0.57
4:D:58:GLY:HA2	4:D:186:PRO:HG3	1.87	0.57
2:B:320:ARG:HA	2:B:323:LEU:HD12	1.86	0.56
3:C:61:LEU:HD21	3:C:288:VAL:HG23	1.86	0.56
4:D:159:ASP:HA	4:D:192:LEU:HB2	1.87	0.56
2:B:570:LEU:HA	2:B:573[A]:GLU:HB2	1.87	0.55
4:D:267:GLN:O	4:D:271:ASN:ND2	2.40	0.55
5:E:182:TYR:O	5:E:220:ARG:NH2	2.39	0.55
2:B:355:ILE:HD11	2:B:388:LEU:HD21	1.90	0.54
3:C:346:CYS:HB3	3:C:350:GLU:HB2	1.88	0.54
3:C:646:LEU:HD13	3:C:702:ASP:HB3	1.89	0.54
2:B:340:ASN:ND2	3:C:9:GLY:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:498:LEU:HA	3:C:501:PHE:HB2	1.90	0.54
2:B:477:LEU:O	2:B:481:LEU:HB2	2.08	0.53
2:B:291:ASN:OD1	2:B:325:ARG:NH1	2.42	0.53
2:B:496:ILE:HG21	2:B:570:LEU:HD13	1.89	0.53
3:C:601:HIS:O	3:C:605:ASN:ND2	2.41	0.53
5:E:189:LYS:O	5:E:193:HIS:ND1	2.38	0.53
1:A:764:ILE:HD11	1:A:853:ASP:HB3	1.90	0.53
4:D:30:ARG:NH1	4:D:30:ARG:O	2.41	0.52
3:C:285:LEU:HA	3:C:288:VAL:HG12	1.91	0.52
3:C:434:GLN:OE1	3:C:436:ARG:NH2	2.42	0.52
5:E:145:GLN:NE2	5:E:152:VAL:O	2.43	0.52
5:E:77:LEU:O	5:E:81:ASN:ND2	2.42	0.52
3:C:368:ARG:O	3:C:373:ARG:NH2	2.43	0.52
3:C:101:PRO:HG2	3:C:247:ILE:HG12	1.92	0.51
4:D:68:PRO:O	4:D:73:LYS:NZ	2.38	0.51
3:C:110:ASN:OD1	3:C:110:ASN:N	2.43	0.51
3:C:436:ARG:NH1	3:C:437:GLU:OE2	2.44	0.51
2:B:337:VAL:HG13	3:C:12:VAL:HG22	1.92	0.51
2:B:342:PHE:HB3	2:B:457:GLU:HG3	1.91	0.51
4:D:386:LYS:HB3	4:D:403:LYS:HB3	1.93	0.51
4:D:277:ARG:NH2	6:D:901:ATP:O2B	2.44	0.51
4:D:14:THR:OG1	4:D:15:GLU:N	2.44	0.50
3:C:227:THR:HG23	3:C:228:LYS:HD2	1.92	0.50
1:A:855:LEU:O	1:A:859:LYS:CB	2.60	0.50
5:E:205:ALA:O	5:E:209:ASN:HB2	2.11	0.50
3:C:645:ASN:HA	3:C:703:HIS:HA	1.93	0.50
3:C:355:ILE:HD11	3:C:402:LEU:HD22	1.93	0.49
5:E:43:LYS:NZ	6:E:901:ATP:O2G	2.45	0.49
3:C:411:ASN:ND2	3:C:490:THR:OG1	2.44	0.49
5:E:312:ALA:HB1	5:E:365:ILE:HG23	1.93	0.49
3:C:480:LYS:HA	3:C:483:CYS:HB3	1.94	0.49
5:E:66:CYS:SG	5:E:75:GLN:NE2	2.81	0.48
5:E:428:ILE:HA	5:E:431:LEU:HD23	1.95	0.48
2:B:397:SER:O	2:B:401:ARG:NE	2.46	0.48
4:D:223:PHE:HA	4:D:226:TYR:HB3	1.95	0.48
4:D:246:ALA:O	4:D:250:ASN:ND2	2.40	0.48
4:D:92:GLU:HB3	4:D:94:VAL:HG12	1.95	0.48
2:B:279:VAL:O	3:C:680:ARG:NH2	2.46	0.48
4:D:315:ALA:O	4:D:319:HIS:HB3	2.13	0.48
2:B:359:VAL:HG11	2:B:388:LEU:HD22	1.95	0.48
3:C:57:GLU:OE2	3:C:60:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:65:ILE:HA	4:D:216:HIS:HB2	1.94	0.48
3:C:447:ILE:HG12	3:C:567:TYR:HE1	1.78	0.48
4:D:101:GLY:N	4:D:159:ASP:O	2.47	0.47
1:A:855:LEU:O	1:A:859:LYS:HB2	2.14	0.47
2:B:407:GLN:HG3	2:B:437:LYS:HD2	1.96	0.47
5:E:11:ARG:NH1	5:E:41:SER:O	2.47	0.47
3:C:202:LYS:HE3	3:C:202:LYS:HB3	1.74	0.47
3:C:550:GLU:OE2	3:C:553:ARG:NH2	2.48	0.47
4:D:345:ASN:OD1	4:D:345:ASN:N	2.44	0.47
1:A:832:LEU:HA	1:A:848:ASN:H	1.79	0.47
4:D:69:ARG:NH1	5:E:170:GLY:O	2.48	0.47
3:C:495:GLU:HA	3:C:498:LEU:HB3	1.97	0.46
5:E:258:GLU:HA	5:E:261:LEU:HB2	1.98	0.46
3:C:101:PRO:HA	3:C:272:CYS:HB3	1.97	0.46
5:E:187:LEU:HB3	5:E:212:LEU:HD21	1.98	0.46
1:A:836:PRO:HG3	2:B:518:GLN:HE22	1.80	0.46
5:E:69:LEU:HD12	5:E:137:LEU:HD22	1.98	0.46
5:E:233:PHE:O	5:E:237:CYS:HB3	2.16	0.46
3:C:415:VAL:HA	3:C:418:CYS:HB3	1.98	0.46
4:D:91:SER:O	4:D:91:SER:OG	2.34	0.45
5:E:304:TYR:HE2	5:E:423:VAL:HG11	1.81	0.45
2:B:300:LYS:HE3	2:B:300:LYS:HB2	1.82	0.45
3:C:216:VAL:HG12	3:C:247:ILE:HB	1.97	0.45
3:C:103:ALA:HB3	3:C:249:ILE:HG22	1.98	0.45
3:C:677:ILE:HD13	3:C:677:ILE:HA	1.84	0.45
3:C:476:PHE:O	3:C:480:LYS:HB2	2.16	0.44
3:C:682:ILE:HA	3:C:685:VAL:HG12	1.98	0.44
5:E:356:PRO:HB3	5:E:396:VAL:HG21	1.99	0.44
3:C:219:LEU:HB2	3:C:250:PHE:HB3	1.99	0.44
2:B:369:ILE:HA	2:B:372:GLN:HE21	1.82	0.44
2:B:543:LYS:HD2	2:B:543:LYS:HA	1.77	0.44
5:E:50:LEU:O	5:E:53:THR:OG1	2.36	0.44
3:C:55:LYS:HB3	3:C:55:LYS:HE2	1.77	0.44
4:D:20:VAL:HG23	4:D:236:LEU:HD21	2.00	0.44
5:E:9:LEU:HD23	5:E:9:LEU:HA	1.91	0.44
5:E:410:THR:O	5:E:410:THR:OG1	2.33	0.44
4:D:15:GLU:O	4:D:19:GLN:HB2	2.18	0.44
1:A:830:ARG:HD3	1:A:830:ARG:HA	1.76	0.44
3:C:122:THR:O	3:C:126:GLN:HB2	2.18	0.43
3:C:638:LEU:HD12	3:C:638:LEU:HA	1.86	0.43
3:C:671:GLU:H	3:C:671:GLU:HG3	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:521:ARG:NH2	5:E:132:ASP:OD2	2.52	0.43
2:B:305:LEU:HG	2:B:419:TYR:HB3	2.00	0.43
2:B:555:GLU:H	2:B:555:GLU:HG2	1.48	0.43
4:D:195:ARG:NH1	4:D:197:ASP:OD1	2.52	0.43
5:E:187:LEU:HD23	5:E:212:LEU:HD11	2.01	0.43
3:C:37:PRO:HB2	3:C:38:GLU:H	1.63	0.43
4:D:52:LYS:O	4:D:56:LEU:HB2	2.18	0.43
3:C:631:CYS:O	3:C:635:LYS:HB2	2.19	0.43
4:D:418:TYR:HB3	4:D:421:CYS:HB2	1.99	0.43
3:C:163:LYS:HE3	3:C:163:LYS:HB3	1.73	0.43
4:D:60:SER:OG	4:D:180:SER:O	2.35	0.43
4:D:344:PHE:O	4:D:402:MET:N	2.42	0.43
3:C:608:TYR:HA	3:C:613:ASN:HB2	2.00	0.42
2:B:567:THR:O	2:B:571:GLU:HB2	2.19	0.42
3:C:304:GLU:HB2	3:C:443:LEU:HD22	2.01	0.42
3:C:280:SER:OG	3:C:283:GLU:OE2	2.36	0.42
3:C:483:CYS:HA	3:C:494:ILE:HD12	2.02	0.42
3:C:494:ILE:HD13	3:C:494:ILE:HA	1.90	0.42
3:C:100:ILE:HG23	3:C:271:LEU:HB3	2.00	0.42
5:E:83:LEU:O	5:E:114:ASN:ND2	2.52	0.42
3:C:355:ILE:HG21	3:C:399:GLN:HG3	2.00	0.42
1:A:840:ASP:HB3	4:D:405:LEU:HD12	2.01	0.42
2:B:488:ALA:HA	2:B:491:ILE:HD12	2.02	0.42
4:D:95:LEU:HD13	4:D:95:LEU:HA	1.90	0.42
5:E:29:SER:HG	5:E:153:THR:HG1	1.67	0.42
3:C:123:GLU:OE2	3:C:127:ASN:ND2	2.53	0.42
4:D:356:PHE:CZ	4:D:428:TRP:HB2	2.55	0.42
4:D:205:ARG:O	4:D:209:ARG:CB	2.65	0.41
4:D:315:ALA:O	4:D:319:HIS:CB	2.68	0.41
2:B:562:ASP:N	2:B:562:ASP:OD1	2.52	0.41
4:D:126:ASP:OD1	4:D:126:ASP:N	2.53	0.41
3:C:354:ARG:HE	3:C:354:ARG:HB2	1.66	0.41
3:C:494:ILE:O	3:C:498:LEU:HB2	2.20	0.41
4:D:286:ALA:HB1	4:D:297:MET:HE1	2.02	0.41
5:E:6:ASN:OD1	5:E:9:LEU:N	2.54	0.41
3:C:109:VAL:HG21	5:E:302:LEU:HD23	2.03	0.41
4:D:19:GLN:OE1	4:D:22:ARG:NH2	2.53	0.41
4:D:28:PHE:CZ	4:D:283:LEU:HB3	2.55	0.41
4:D:236:LEU:HD23	4:D:237:PRO:HD2	2.03	0.41
2:B:472:LEU:HD21	2:B:476:SER:HB3	2.02	0.41
3:C:155:LEU:HD22	3:C:202:LYS:HZ3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:158:SER:OG	5:E:159:GLU:N	2.53	0.41
3:C:493:ARG:O	3:C:497:PHE:HB2	2.21	0.41
1:A:796:GLN:H	1:A:796:GLN:HG3	1.72	0.41
2:B:455:THR:O	2:B:459:SER:HB3	2.20	0.41
3:C:259:ILE:HD12	3:C:259:ILE:HA	1.96	0.41
3:C:302:ILE:HD12	3:C:302:ILE:HA	1.88	0.41
3:C:367:ARG:HE	3:C:388:LEU:HD12	1.84	0.41
4:D:383:GLU:HB2	5:E:160:ILE:HD11	2.02	0.41
2:B:337:VAL:H	2:B:390:LEU:HA	1.86	0.41
3:C:155:LEU:HD23	3:C:155:LEU:HA	1.93	0.40
4:D:73:LYS:HB3	4:D:192:LEU:HD22	2.03	0.40
5:E:210:ILE:HD13	5:E:254:TRP:HB2	2.03	0.40
5:E:431:LEU:HD12	5:E:432:TYR:HB3	2.03	0.40
2:B:301:TRP:O	2:B:305:LEU:HB2	2.21	0.40
5:E:78:ASN:HD21	5:E:93:GLU:HA	1.85	0.40
2:B:430:PRO:HB3	2:B:445:TRP:HH2	1.87	0.40
3:C:286:THR:O	3:C:290:ASP:CB	2.69	0.40
4:D:195:ARG:HE	4:D:195:ARG:HB3	1.66	0.40
4:D:386:LYS:HB2	4:D:405:LEU:HD22	2.04	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	100/861 (12%)	97 (97%)	3 (3%)	0	100	100
2	B	296/577 (51%)	284 (96%)	12 (4%)	0	100	100
3	C	576/711 (81%)	529 (92%)	47 (8%)	0	100	100
4	D	398/436 (91%)	370 (93%)	28 (7%)	0	100	100
5	E	363/435 (83%)	331 (91%)	32 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1733/3020 (57%)	1611 (93%)	122 (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	92/766 (12%)	85 (92%)	7 (8%)	13	39
2	B	276/529 (52%)	253 (92%)	23 (8%)	11	36
3	C	546/659 (83%)	502 (92%)	44 (8%)	11	37
4	D	374/403 (93%)	341 (91%)	33 (9%)	10	33
5	E	341/399 (86%)	310 (91%)	31 (9%)	9	31
All	All	1629/2756 (59%)	1491 (92%)	138 (8%)	14	36

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	777	PHE
1	A	817	SER
1	A	822	VAL
1	A	823	CYS
1	A	832	LEU
1	A	835	GLU
1	A	841	LEU
2	B	276	LEU
2	B	283	PHE
2	B	297	LEU
2	B	313	LEU
2	B	327	ARG
2	B	335	ILE
2	B	342	PHE
2	B	350	SER
2	B	369	ILE

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Mol	Chain	Res	Type
2	B	388	LEU
2	B	390	LEU
2	B	391	LEU
2	B	420	LEU
2	B	426	HIS
2	B	434	ASP
2	B	437	LYS
2	B	441	PHE
2	B	443	TRP
2	B	448	THR
2	B	449	THR
2	B	526	VAL
2	B	544	LEU
2	B	559	ILE
3	C	29	TYR
3	C	42	LEU
3	C	43	ARG
3	C	61	LEU
3	C	70	PHE
3	C	71	ASP
3	C	102	THR
3	C	111	VAL
3	C	121	LEU
3	C	129	VAL
3	C	130	THR
3	C	151	LEU
3	C	163	LYS
3	C	202	LYS
3	C	211	GLN
3	C	215	VAL
3	C	228	LYS
3	C	248	LEU
3	C	250	PHE
3	C	262	LEU
3	C	269	SER
3	C	271	LEU
3	C	275	LEU
3	C	281	CYS
3	C	293	LEU
3	C	307	LEU
3	C	319	PHE
3	C	331	SER

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Mol	Chain	Res	Type
3	C	342	SER
3	C	358	LEU
3	C	363	CYS
3	C	369	LEU
3	C	374	ARG
3	C	383	LYS
3	C	418	CYS
3	C	443	LEU
3	C	480	LYS
3	C	483	CYS
3	C	486	HIS
3	C	489	SER
3	C	588	LEU
3	C	612	LYS
3	C	671	GLU
3	C	694	ILE
4	D	24	LEU
4	D	28	PHE
4	D	30	ARG
4	D	32	SER
4	D	64	LEU
4	D	74	THR
4	D	75	MET
4	D	81	LEU
4	D	84	LEU
4	D	93	ASN
4	D	94	VAL
4	D	97	VAL
4	D	120	LEU
4	D	128	VAL
4	D	164	PHE
4	D	172	LEU
4	D	185	THR
4	D	197	ASP
4	D	201	LEU
4	D	219	ASN
4	D	234	LEU
4	D	257	SER
4	D	260	ARG
4	D	274	LYS
4	D	282	LEU
4	D	287	LEU

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Mol	Chain	Res	Type
4	D	301	ASP
4	D	302	LEU
4	D	322	SER
4	D	323	VAL
4	D	335	LEU
4	D	405	LEU
4	D	425	VAL
5	E	8	VAL
5	E	10	CYS
5	E	21	LEU
5	E	30	PHE
5	E	69	LEU
5	E	99	PHE
5	E	111	THR
5	E	115	LEU
5	E	152	VAL
5	E	157	LEU
5	E	159	GLU
5	E	168	ASN
5	E	184	ILE
5	E	190	ILE
5	E	211	LEU
5	E	215	PHE
5	E	217	THR
5	E	230	VAL
5	E	237	CYS
5	E	250	THR
5	E	254	TRP
5	E	299	HIS
5	E	322	ARG
5	E	402	LEU
5	E	408	LYS
5	E	410	THR
5	E	413	LEU
5	E	425	PHE
5	E	426	ASP
5	E	428	ILE
5	E	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	802	HIS
2	B	270	GLN
2	B	336	HIS
2	B	372	GLN
2	B	411	GLN
2	B	563	ASN
3	C	211	GLN
3	C	347	ASN
3	C	399	GLN
3	C	613	ASN
3	C	637	HIS
4	D	98	HIS
4	D	119	ASN
4	D	271	ASN
4	D	347	GLN
5	E	81	ASN
5	E	168	ASN
5	E	299	HIS
5	E	383	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	ATP	E	901	-	26,33,33	0.95	1 (3%)	31,52,52	1.67	7 (22%)
6	ATP	D	901	-	26,33,33	0.97	1 (3%)	31,52,52	1.65	5 (16%)

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	ATP	E	901	-	-	3/18/38/38	0/3/3/3
6	ATP	D	901	-	-	1/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	901	ATP	C5-C4	2.39	1.47	1.40
6	D	901	ATP	C5-C4	2.26	1.46	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	901	ATP	PB-O3B-PG	-4.50	117.37	132.83
6	D	901	ATP	PA-O3A-PB	-4.43	117.64	132.83
6	E	901	ATP	PB-O3B-PG	-3.56	120.60	132.83
6	E	901	ATP	C3'-C2'-C1'	3.43	106.15	100.98
6	E	901	ATP	N3-C2-N1	-3.41	123.34	128.68
6	E	901	ATP	PA-O3A-PB	-3.39	121.21	132.83
6	D	901	ATP	N3-C2-N1	-3.16	123.73	128.68
6	D	901	ATP	C4-C5-N7	-2.16	107.14	109.40
6	D	901	ATP	O3G-PG-O2G	2.08	115.58	107.64
6	E	901	ATP	O2A-PA-O1A	2.07	122.45	112.24
6	E	901	ATP	C4-C5-N7	-2.02	107.29	109.40
6	E	901	ATP	O3G-PG-O2G	2.00	115.28	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

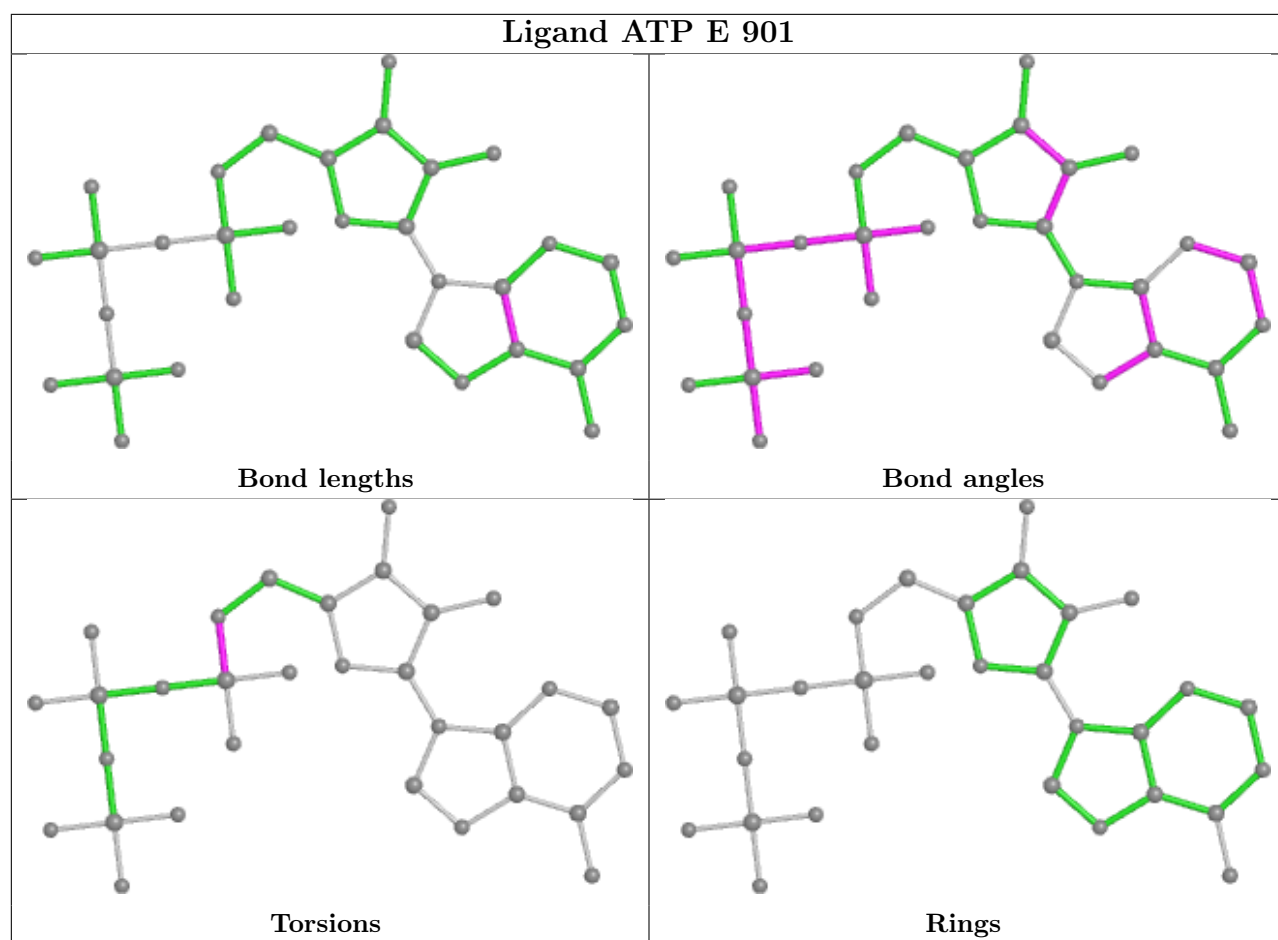
Mol	Chain	Res	Type	Atoms
6	E	901	ATP	C5'-O5'-PA-O1A
6	E	901	ATP	C5'-O5'-PA-O2A
6	E	901	ATP	C5'-O5'-PA-O3A
6	D	901	ATP	O4'-C4'-C5'-O5'

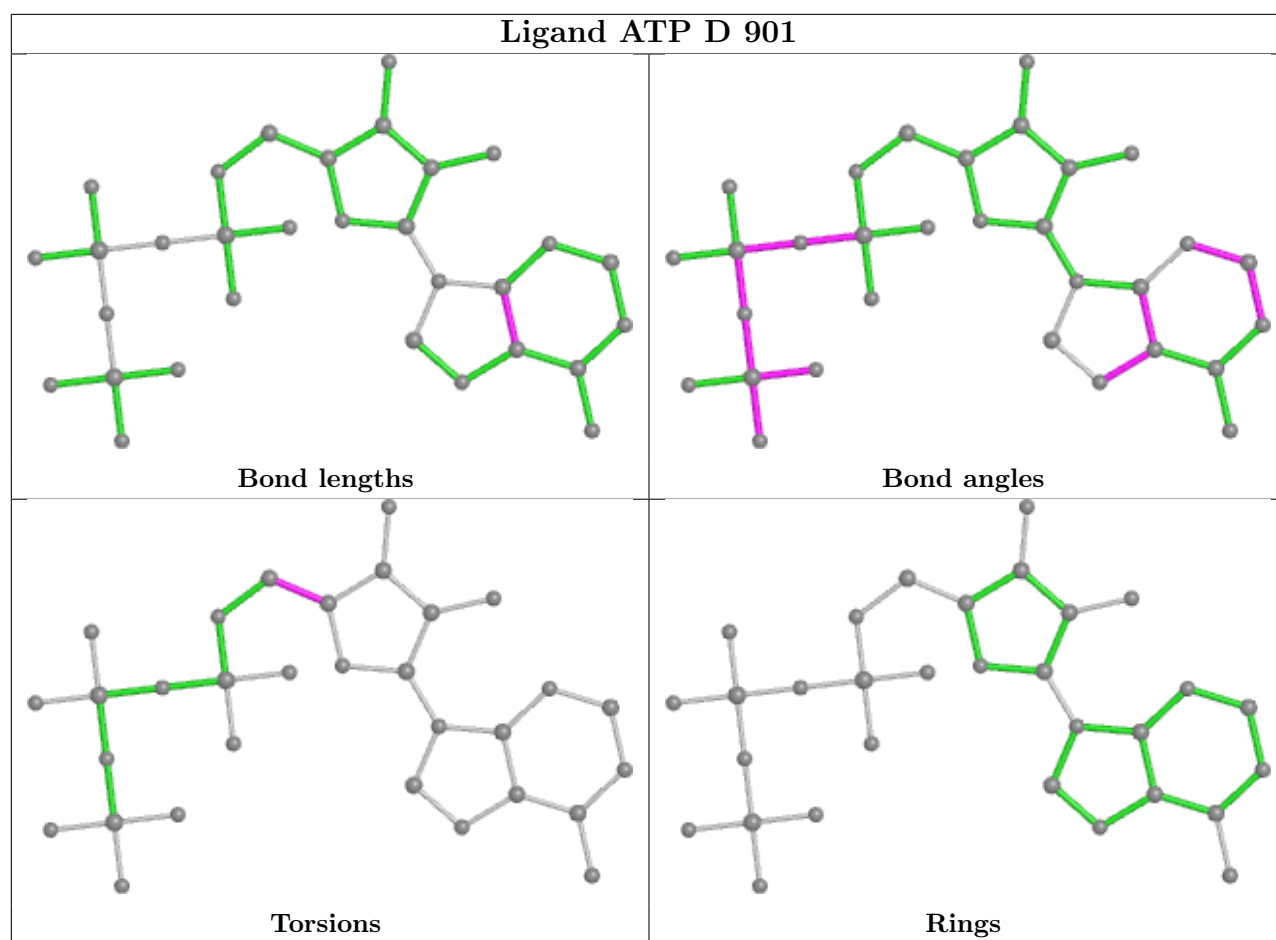
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	901	ATP	1	0
6	D	901	ATP	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.

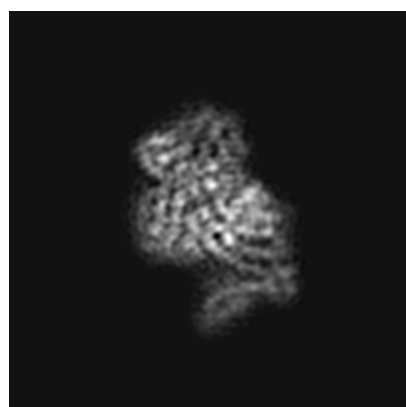
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30464. These allow visual inspection of the internal detail of the map and identification of artifacts.

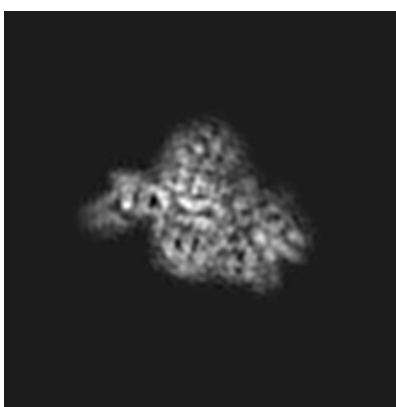
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

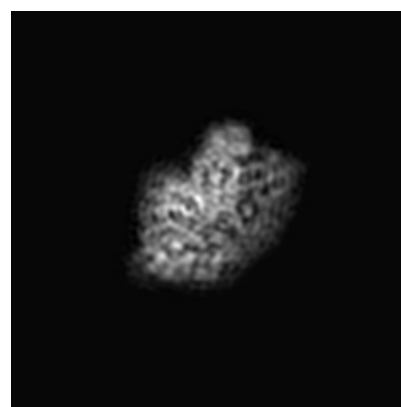
#### 6.1.1 Primary map



X



Y

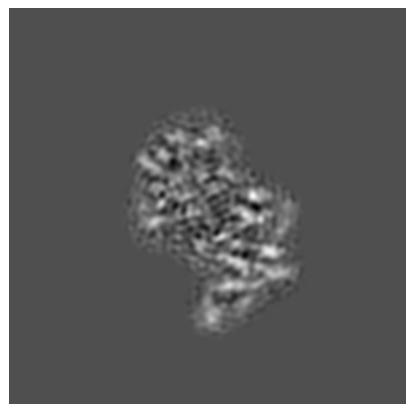


Z

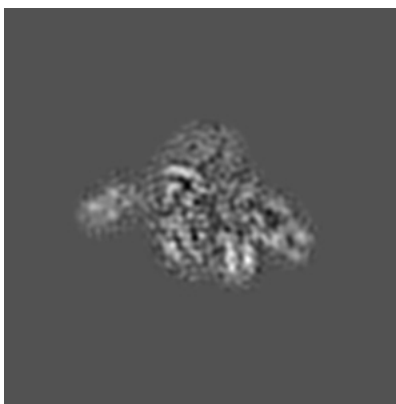
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

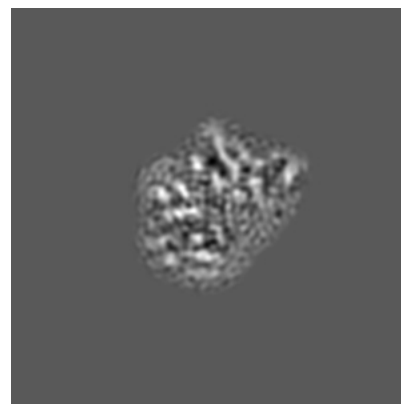
#### 6.2.1 Primary map



X Index: 75



Y Index: 75



Z Index: 75

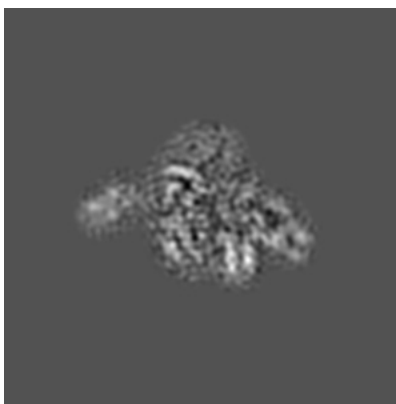
The images above show central slices of the map in three orthogonal directions.

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

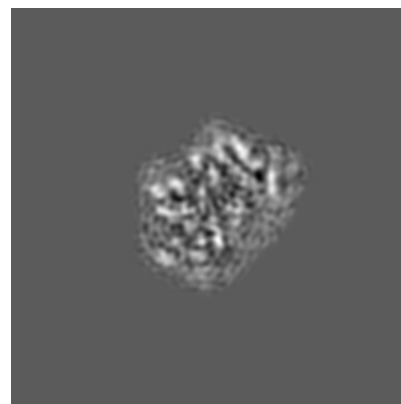
### 6.3.1 Primary map



X Index: 77



Y Index: 75

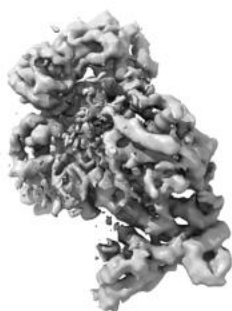


Z Index: 73

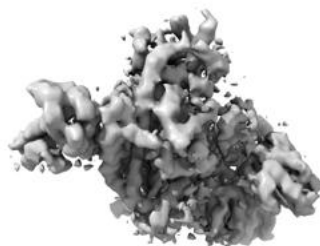
The images above show the largest variance slices of the map in three orthogonal directions.

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

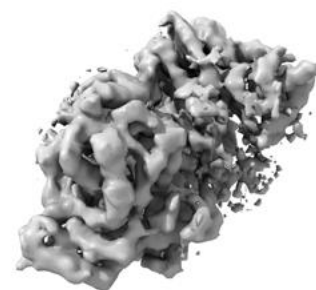
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

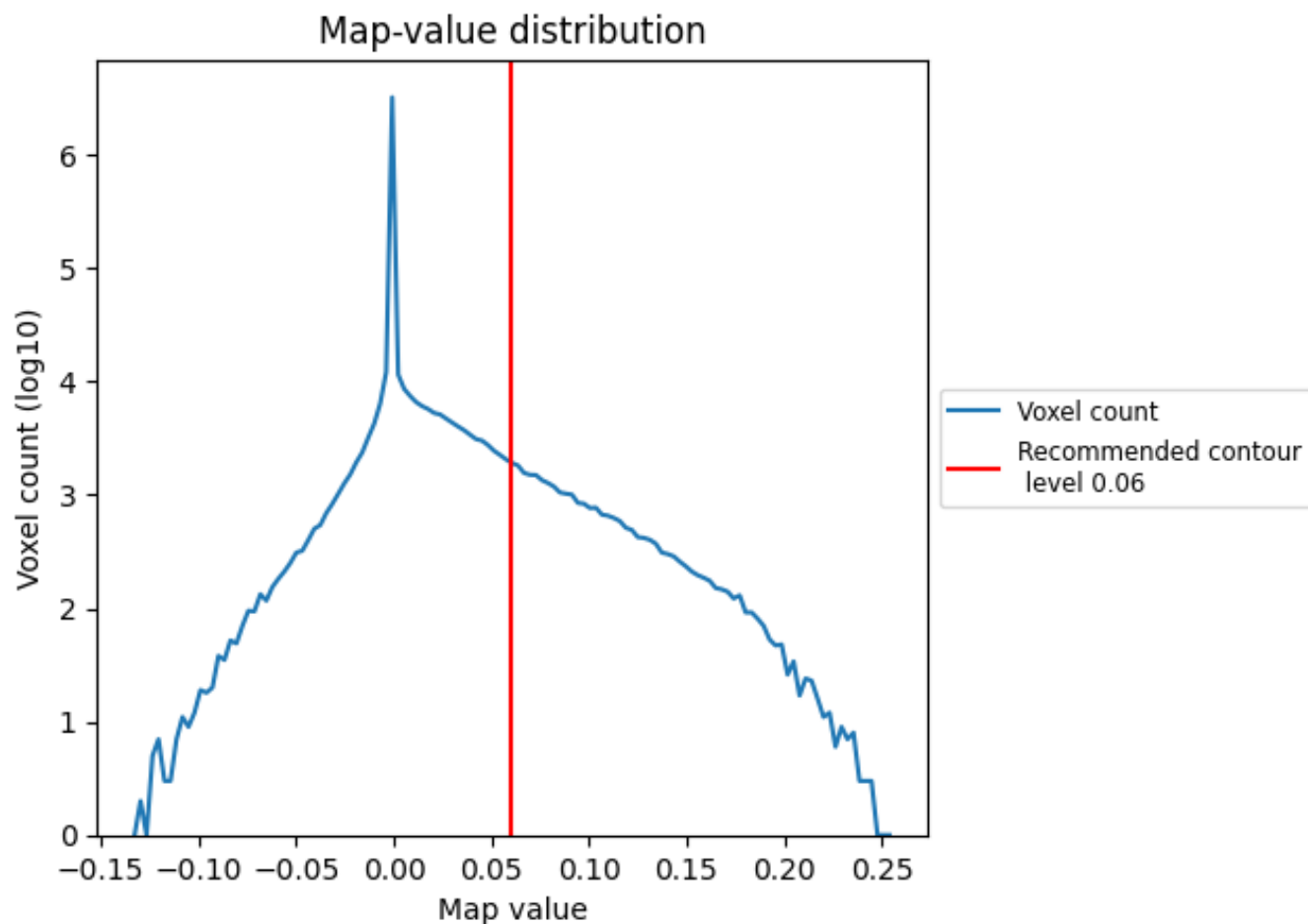
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

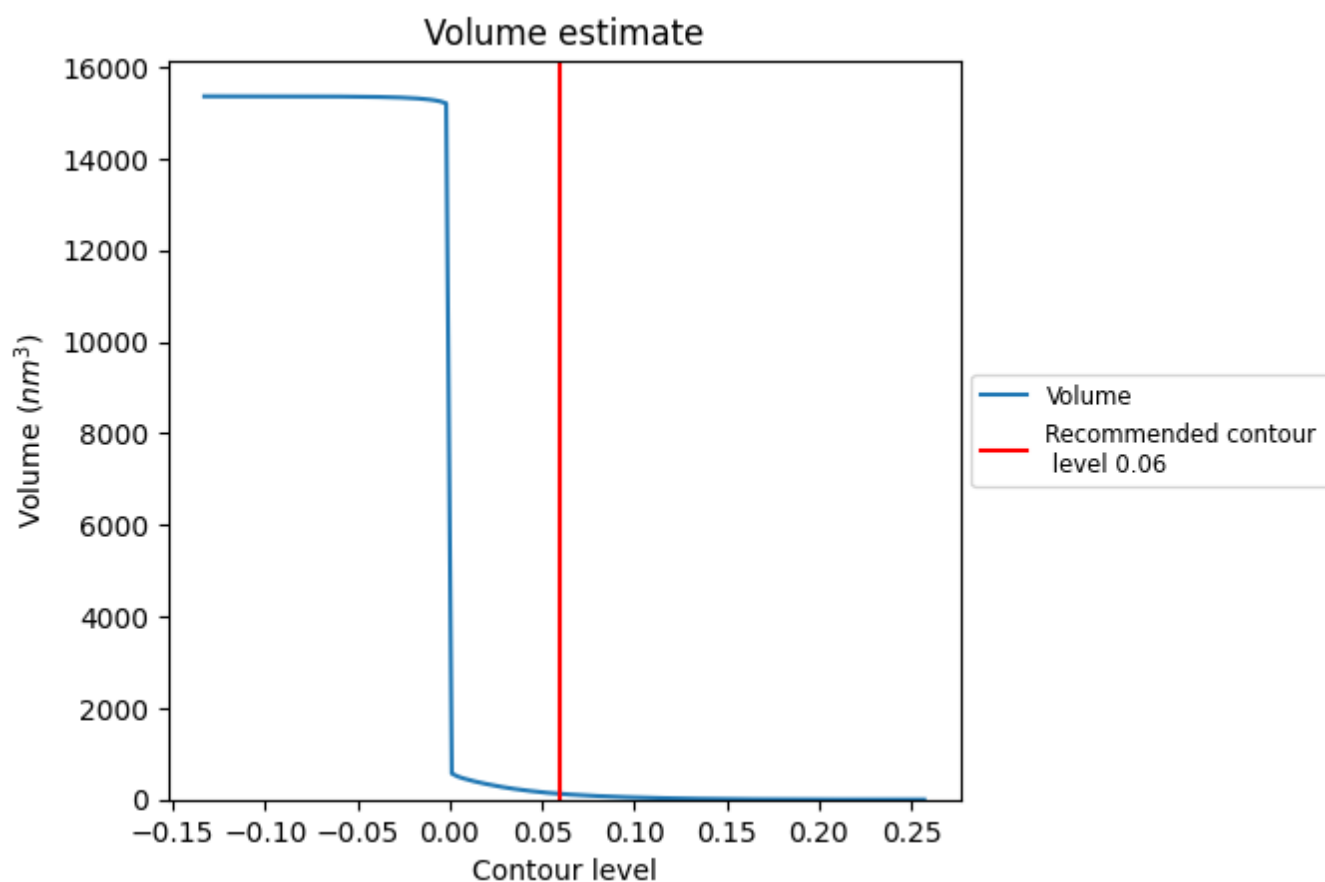
This section contains the results of statistical analysis of the map.

### 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.

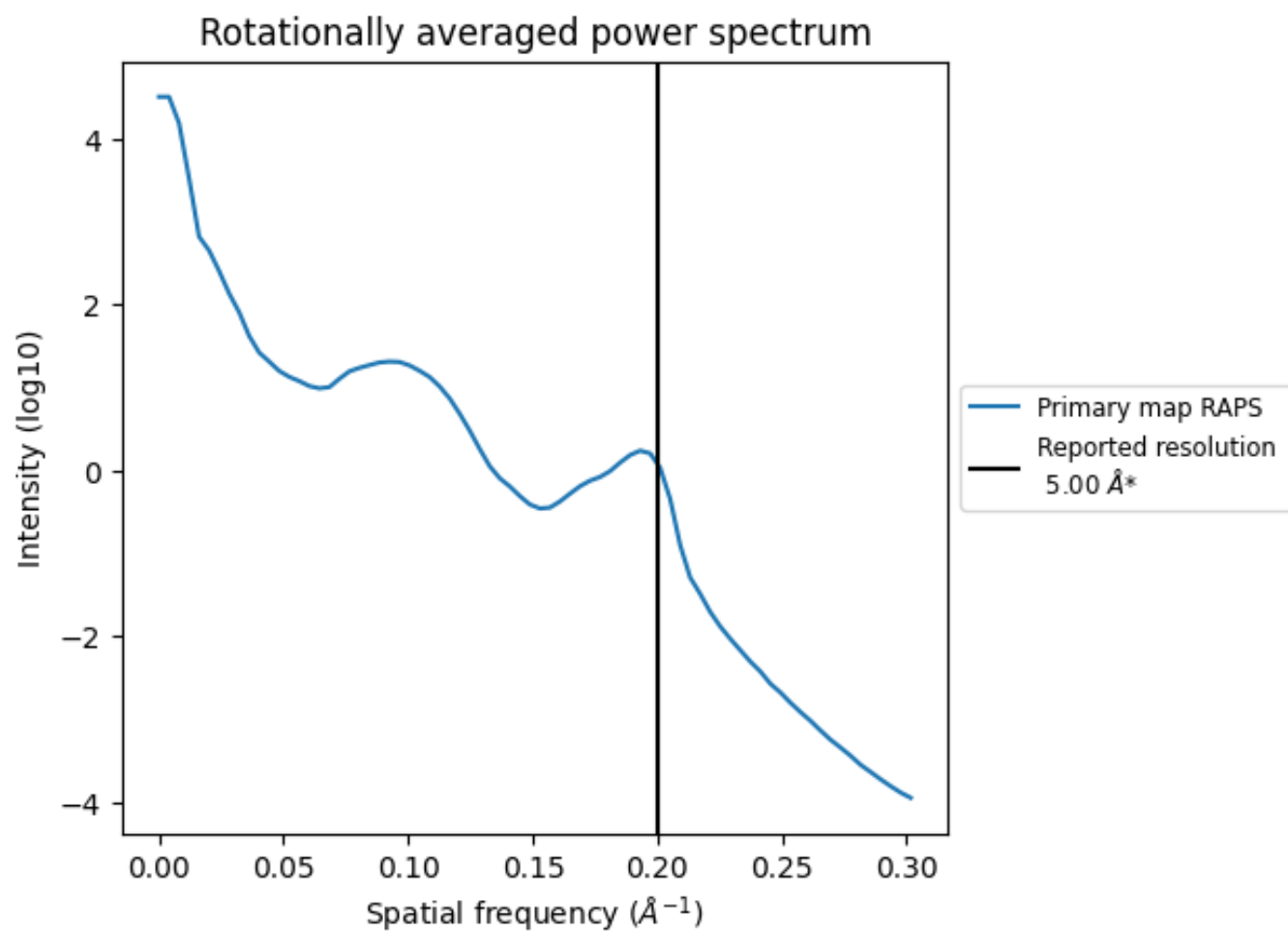
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm<sup>3</sup>; this corresponds to an approximate mass of 113 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 0.200 Å<sup>-1</sup>

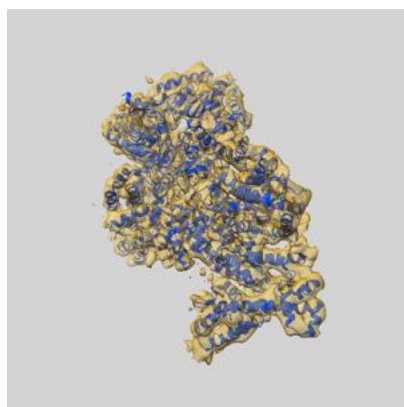
## 8 Fourier-Shell correlation

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

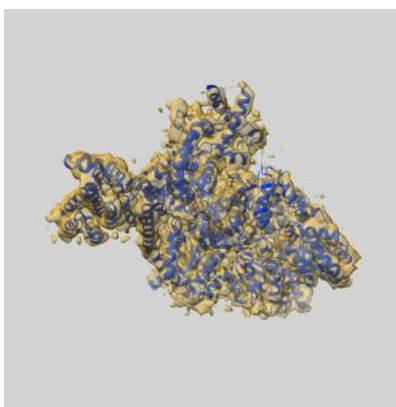
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30464 and PDB model 7CTG. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

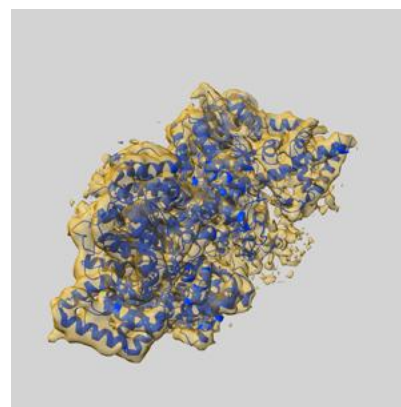
### 9.1 Map-model overlay [i](#)



X



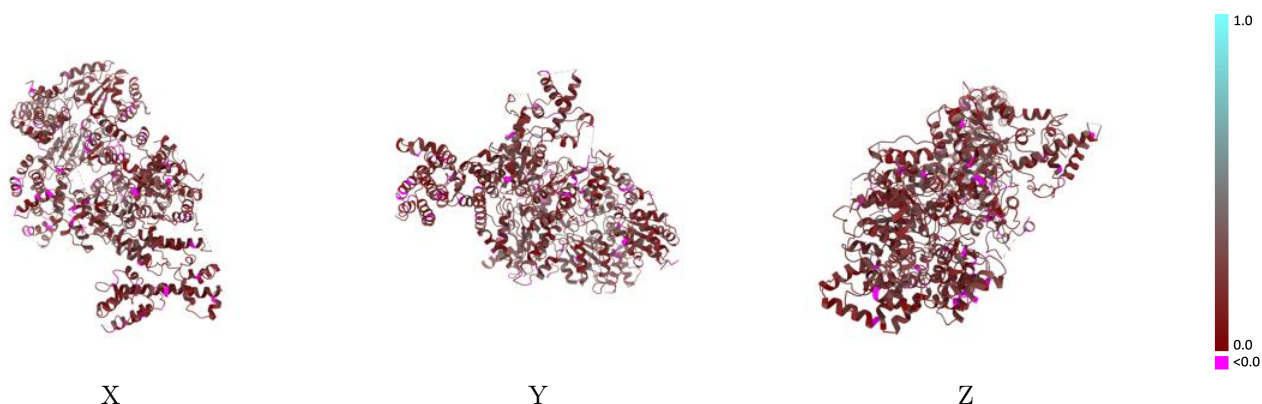
Y



Z

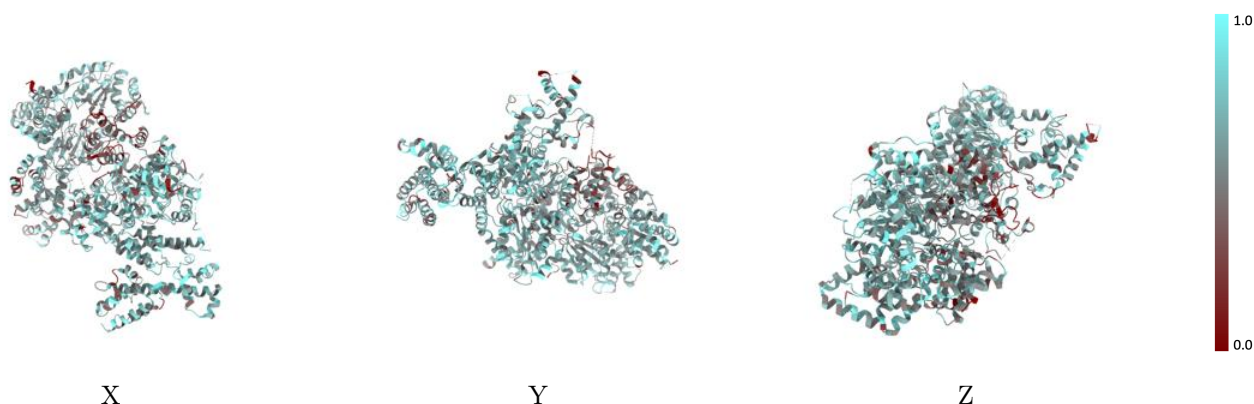
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



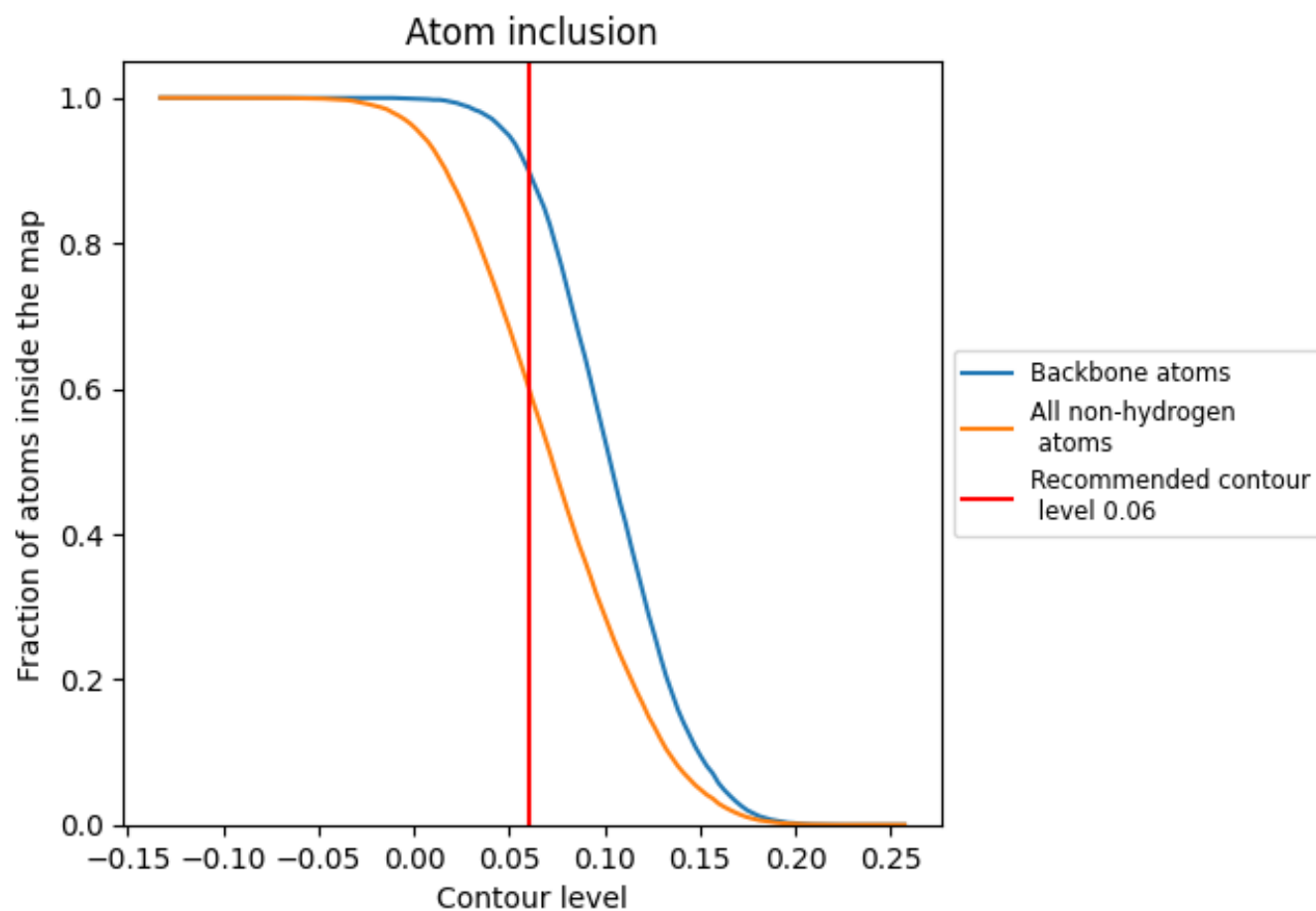
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 60% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6025	<div></div> 0.1990
A	<div></div> 0.5465	<div></div> 0.2060
B	<div></div> 0.5455	<div></div> 0.1990
C	<div></div> 0.6327	<div></div> 0.1940
D	<div></div> 0.6013	<div></div> 0.1890
E	<div></div> 0.6166	<div></div> 0.2160

