



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:16 PM UTC

PDB ID : 9LXD / pdb\_00009lxd  
EMDB ID : EMD-63474  
Title : Structure of DNA-free MCM SH at 3.2 Angstroms resolution  
Authors : Liu, Y.; Lu, P.; Yang, M.; Gao, H.; Yu, H.  
Deposited on : 2025-02-18  
Resolution : 3.27 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>.

---

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

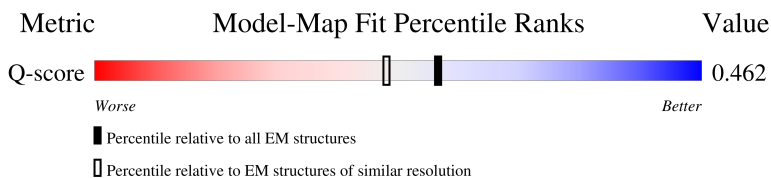
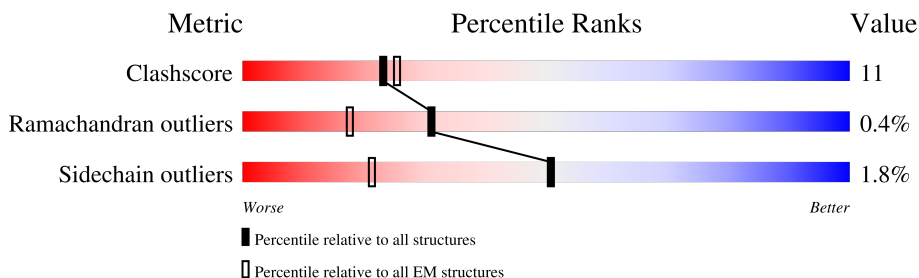
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.27 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.




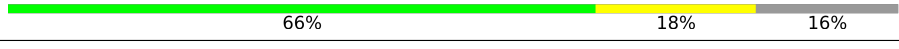

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14508 ( 2.77 - 3.77 )

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	2	904	
2	3	853	
2	B	853	
3	4	863	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	5	734	
5	6	821	
6	7	719	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ATP	2	1001	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32927 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	709	Total	C	N	O	S	0	0
			5628	3537	1005	1054	32		

- Molecule 2 is a protein called Isoform 2 of DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	629	Total	C	N	O	S	0	0
			4922	3077	863	956	26		
2	B	73	Total	C	N	O	S	0	0
			575	359	98	115	3		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	724	Total	C	N	O	S	0	0
			5753	3620	1013	1092	28		

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	659	Total	C	N	O	S	0	0
			5183	3258	929	959	37		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	601	ALA	ASP	conflict	UNP P33992
5	602	LEU	ARG	conflict	UNP P33992
5	603	LEU	ARG	conflict	UNP P33992
5	604	ALA	SER	conflict	UNP P33992
5	652	THR	ALA	conflict	UNP P33992

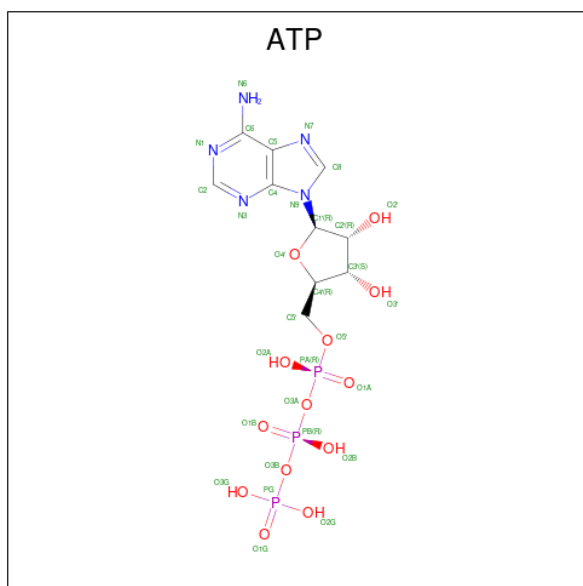
- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	693	Total	C	N	O	S	0	0
			5586	3516	985	1058	27		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	649	Total	C	N	O	S	0	0
			5141	3212	918	979	32		

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



Mol	Chain	Residues	Atoms					AltConf
7	2	1	Total	C	N	O	P	0
			31	10	5	13	3	

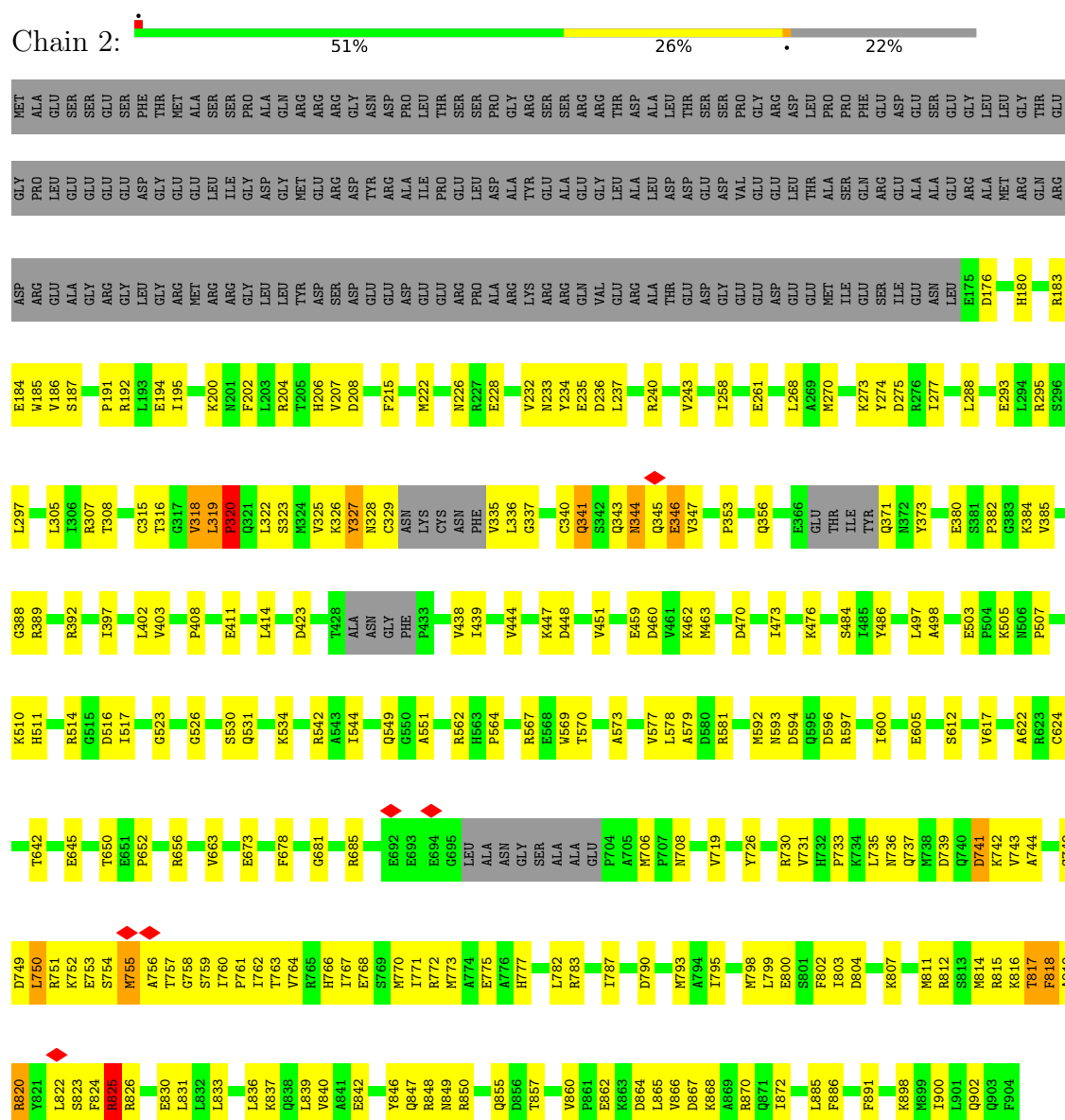
- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



### 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.

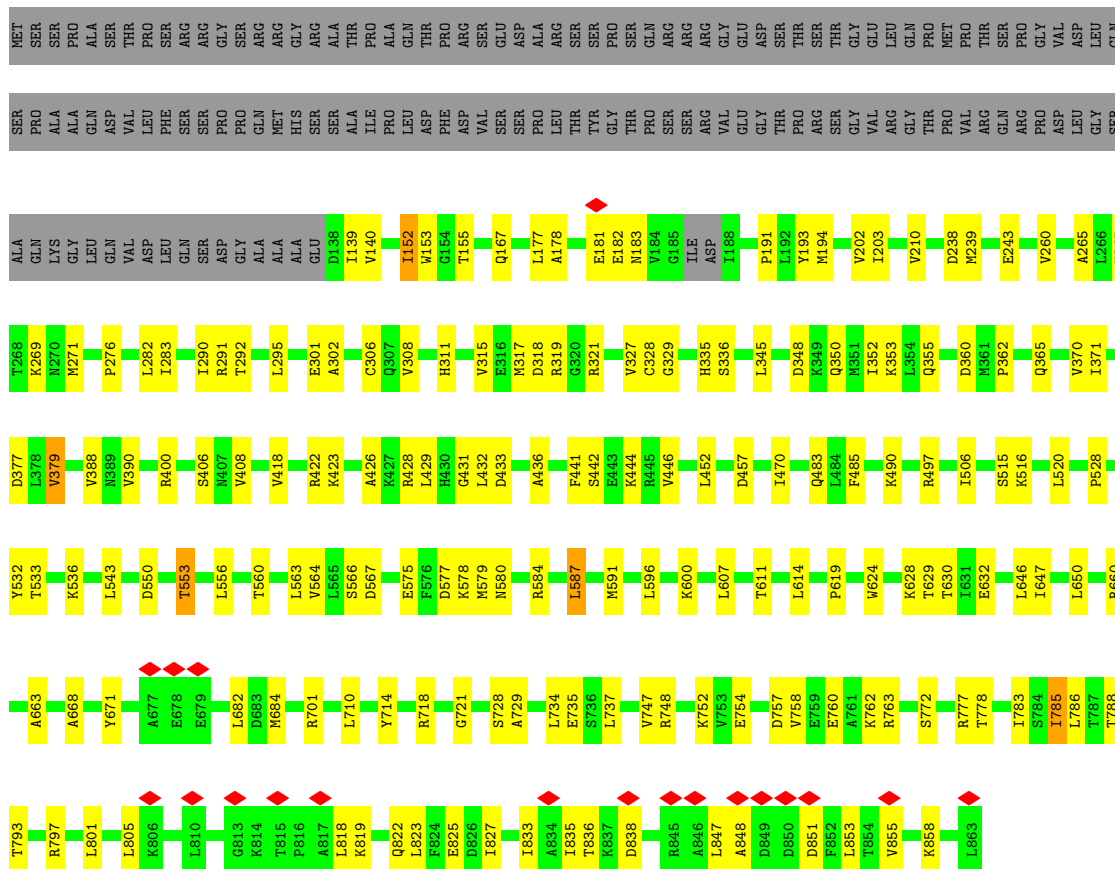
- Molecule 1: DNA replication licensing factor MCM2



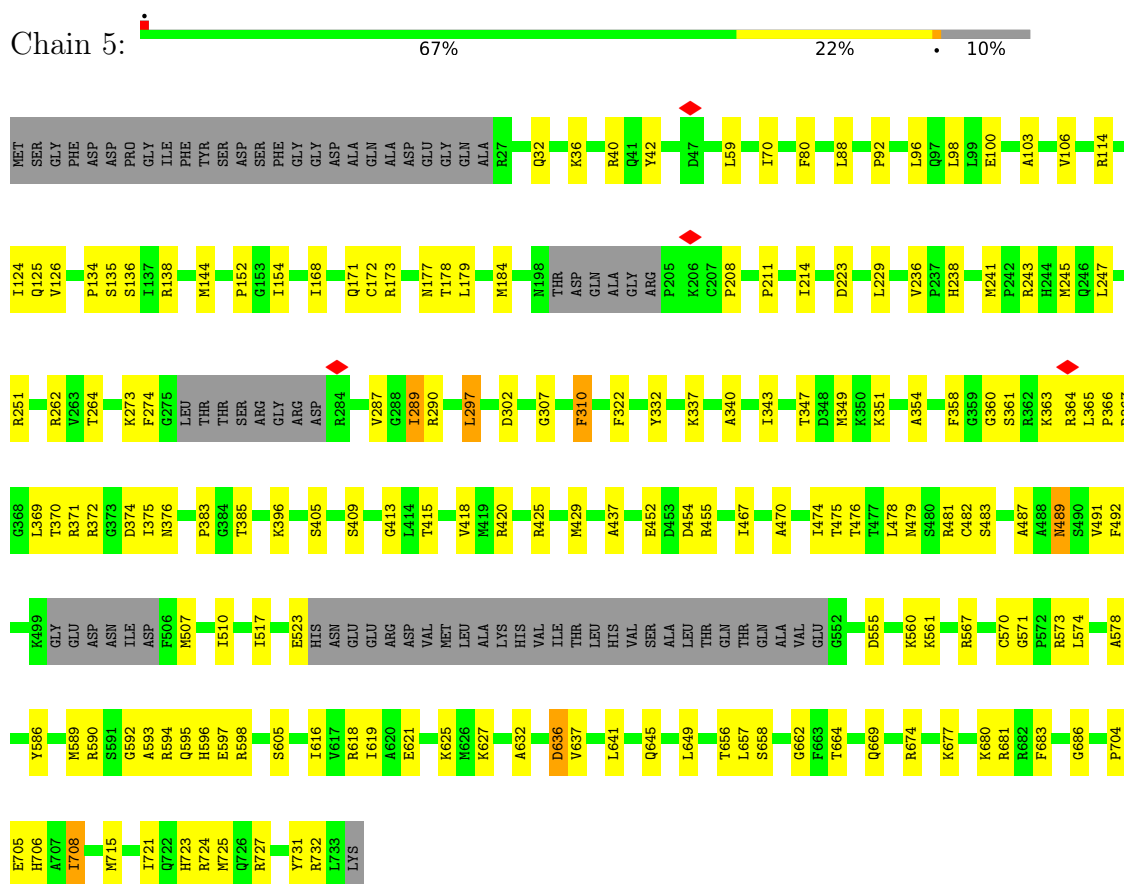
- Molecule 2: Isoform 2 of DNA replication licensing factor MCM3



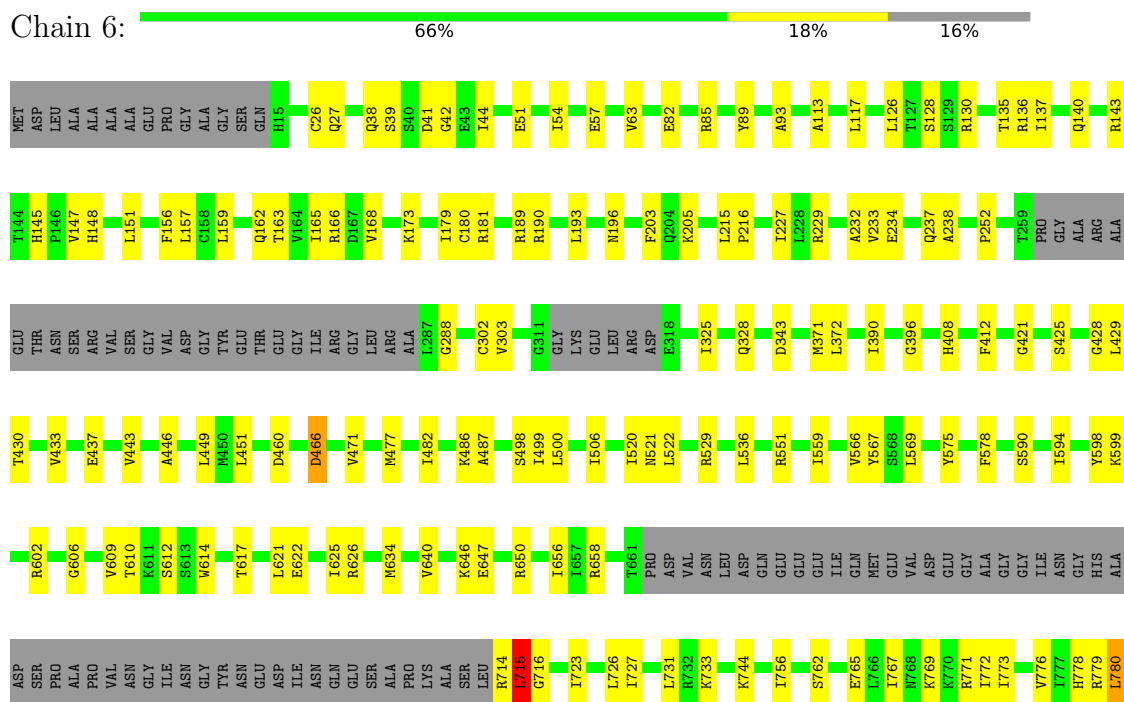


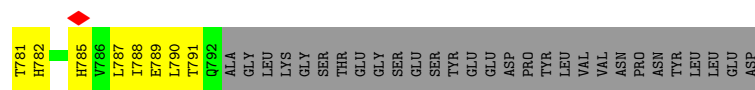


• Molecule 4: DNA replication licensing factor MCM5

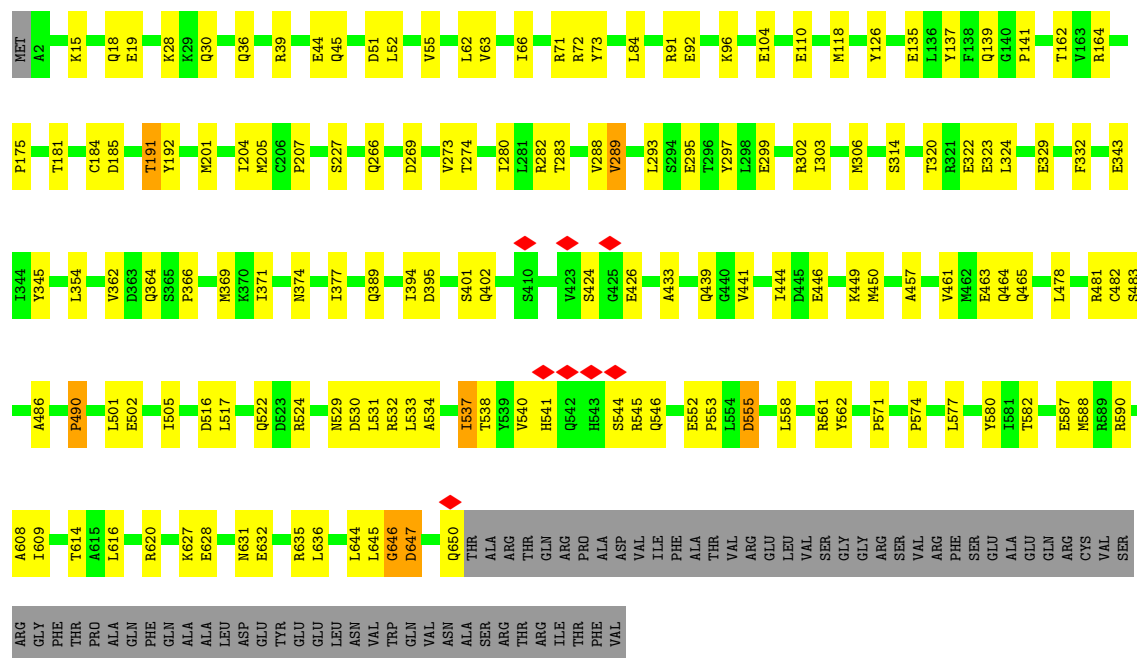


• Molecule 5: DNA replication licensing factor MCM6





• Molecule 6: DNA replication licensing factor MCM7



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	242055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.455	Depositor
Minimum map value	-1.888	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.218	Depositor
Map size ( $\text{\AA}$ )	430.91998, 430.91998, 430.91998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0773, 1.0773, 1.0773	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, ADP

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	2	0.29	0/5730	0.59	4/7731 (0.1%)
2	3	0.15	0/4997	0.34	0/6750
2	B	0.15	0/580	0.47	0/776
3	4	0.14	0/5848	0.34	0/7898
4	5	0.10	0/5263	0.30	0/7066
5	6	0.12	0/5676	0.30	0/7654
6	7	0.13	0/5222	0.30	0/7049
All	All	0.17	0/33316	0.38	4/44924 (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
1	2	0	1
2	3	0	3
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	320	PRO	N-CA-CB	-7.35	95.53	103.25
1	2	825	ARG	CA-C-O	-5.88	115.05	121.87
1	2	741	ASP	N-CA-C	-5.86	105.62	112.89
1	2	344	ASN	N-CA-C	-5.39	105.52	113.61

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	825	ARG	Sidechain
2	3	531	ASP	Peptide
2	3	69	ALA	Peptide
2	3	83	PHE	Peptide

## 5.2 Too-close contacts

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	2	5628	0	5638	218	0
2	3	4922	0	4954	120	0
2	B	575	0	579	12	0
3	4	5753	0	5820	109	0
4	5	5183	0	5296	113	0
5	6	5586	0	5619	109	0
6	7	5141	0	5180	93	0
7	2	31	0	12	9	0
8	3	27	0	12	0	0
8	4	27	0	12	0	0
8	6	27	0	12	1	0
8	7	27	0	12	2	0
All	All	32927	0	33146	733	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 11.

All (733) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:726:TYR:OH	1:2:730:ARG:CD	2.08	1.02
1:2:726:TYR:CZ	1:2:730:ARG:HD3	1.96	1.00
1:2:322:LEU:HD22	1:2:343:GLN:HA	1.43	0.98
1:2:486:TYR:H	7:2:1001:ATP:HN61	1.09	0.95
1:2:726:TYR:CZ	1:2:730:ARG:CD	2.53	0.92
2:3:220:ILE:HD11	6:7:289:VAL:HG11	1.53	0.90
1:2:514:ARG:HG3	1:2:772:ARG:HH12	1.42	0.84
6:7:463:GLU:HG3	6:7:464:GLN:HG3	1.60	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:345:TYR:HB2	6:7:532:ARG:HD2	1.61	0.80
2:B:761:GLN:HE21	2:B:807:LEU:HD22	1.48	0.79
5:6:714:ARG:C	5:6:716:GLY:H	1.89	0.78
1:2:819:ALA:HA	1:2:824:PHE:HD1	1.47	0.78
6:7:364:GLN:HB2	6:7:371:ILE:HB	1.64	0.78
3:4:301:GLU:HB2	3:4:345:LEU:HB2	1.66	0.78
1:2:592:MET:HE3	1:2:597:ARG:HG2	1.67	0.76
1:2:848:ARG:HH22	5:6:606:GLY:HA3	1.48	0.76
4:5:680:LYS:HG2	4:5:732:ARG:HH22	1.49	0.76
2:3:327:ARG:NH1	6:7:537:ILE:O	2.19	0.75
2:3:83:PHE:O	2:3:85:ALA:N	2.19	0.75
1:2:486:TYR:N	7:2:1001:ATP:HN61	1.81	0.74
1:2:328:ASN:HD21	1:2:353:PRO:HB3	1.52	0.74
5:6:714:ARG:HB3	5:6:779:ARG:CD	2.16	0.74
1:2:207:VAL:H	1:2:240:ARG:HH22	1.37	0.73
1:2:726:TYR:OH	1:2:730:ARG:NE	2.19	0.73
5:6:714:ARG:HB3	5:6:779:ARG:HD2	1.69	0.73
4:5:172:CYS:HB3	4:5:177:ASN:H	1.52	0.73
1:2:486:TYR:H	7:2:1001:ATP:N6	1.86	0.72
1:2:807:LYS:HE3	5:6:790:LEU:HD11	1.71	0.71
1:2:819:ALA:HA	1:2:824:PHE:CD1	2.24	0.71
2:3:82:ASP:O	2:3:86:SER:CB	2.38	0.71
4:5:686:GLY:H	4:5:732:ARG:HB3	1.56	0.71
3:4:178:ALA:HB3	3:4:181:GLU:HG2	1.72	0.70
1:2:731:VAL:HG21	1:2:782:LEU:HD22	1.74	0.70
1:2:526:GLY:N	7:2:1001:ATP:O1B	2.24	0.70
4:5:365:LEU:HD22	4:5:370:THR:HG23	1.73	0.70
1:2:768:GLU:OE2	1:2:772:ARG:NH2	2.23	0.69
1:2:341:GLN:O	1:2:344:ASN:HB2	1.92	0.68
2:3:102:LEU:HD12	2:3:124:VAL:HG11	1.75	0.68
1:2:320:PRO:HA	1:2:371:GLN:O	1.94	0.68
1:2:486:TYR:N	7:2:1001:ATP:N6	2.41	0.68
3:4:777:ARG:HG3	3:4:778:THR:HG23	1.74	0.68
2:B:754:VAL:HG21	2:B:771:SER:HB3	1.74	0.68
1:2:750:LEU:HD22	1:2:761:PRO:HA	1.76	0.68
3:4:701:ARG:HH12	5:6:559:ILE:HG12	1.59	0.68
4:5:637:VAL:O	4:5:641:LEU:HD12	1.93	0.68
1:2:337:GLY:O	5:6:190:ARG:NH2	2.26	0.67
5:6:113:ALA:HB1	5:6:302:CYS:HB2	1.75	0.67
2:3:82:ASP:O	2:3:86:SER:HB3	1.94	0.67
4:5:208:PRO:HG2	4:5:211:PRO:HB3	1.75	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:345:GLN:NE2	1:2:423:ASP:OD1	2.27	0.67
1:2:531:GLN:HG2	7:2:1001:ATP:O2A	1.95	0.67
1:2:233:ASN:OD1	1:2:234:TYR:N	2.28	0.67
1:2:328:ASN:ND2	1:2:353:PRO:HB3	2.10	0.67
1:2:510:LYS:NZ	2:B:794:ASP:OD1	2.28	0.66
5:6:714:ARG:C	5:6:716:GLY:N	2.53	0.66
3:4:202:VAL:HG23	3:4:203:ILE:HG23	1.76	0.66
2:3:82:ASP:O	2:3:86:SER:OG	2.14	0.66
1:2:726:TYR:CZ	1:2:730:ARG:HD2	2.30	0.66
1:2:526:GLY:CA	7:2:1001:ATP:O1B	2.44	0.65
4:5:491:VAL:HG12	4:5:492:PHE:CD1	2.31	0.65
1:2:323:SER:HA	1:2:346:GLU:O	1.95	0.65
6:7:164:ARG:NH1	6:7:306:MET:SD	2.69	0.65
1:2:650:THR:HG22	1:2:652:PRO:HD2	1.78	0.65
2:3:69:ALA:O	2:3:71:GLU:N	2.30	0.65
5:6:788:ILE:HG22	5:6:789:GLU:H	1.62	0.65
1:2:766:HIS:O	1:2:770:MET:HG2	1.96	0.65
5:6:130:ARG:HH21	5:6:135:THR:HG22	1.62	0.65
1:2:818:PHE:O	1:2:819:ALA:C	2.39	0.64
1:2:763:THR:HG22	1:2:764:VAL:H	1.61	0.64
2:3:507:TYR:O	4:5:573:ARG:NH1	2.30	0.64
4:5:287:VAL:HG13	4:5:289:ILE:H	1.61	0.64
6:7:529:ASN:O	6:7:531:LEU:N	2.31	0.64
4:5:396:LYS:O	4:5:560:LYS:NZ	2.31	0.64
6:7:545:ARG:NH1	6:7:546:GLN:O	2.30	0.64
1:2:731:VAL:HG11	1:2:782:LEU:HA	1.79	0.64
1:2:726:TYR:OH	1:2:730:ARG:HD3	1.85	0.63
4:5:429:MET:HE1	4:5:476:THR:HG21	1.79	0.63
1:2:514:ARG:O	1:2:772:ARG:NH1	2.31	0.63
2:3:84:VAL:HA	2:3:87:ILE:HG12	1.81	0.63
2:3:378:LEU:HD12	2:3:418:ASP:HB3	1.80	0.63
4:5:724:ARG:HH12	4:5:731:TYR:HB2	1.62	0.63
5:6:343:ASP:OD2	5:6:567:TYR:OH	2.15	0.63
1:2:183:ARG:HD2	1:2:184:GLU:H	1.64	0.63
1:2:770:MET:HE1	1:2:795:ILE:HA	1.81	0.63
2:3:419:ARG:NH2	2:3:470:GLY:O	2.31	0.63
4:5:491:VAL:HG12	4:5:492:PHE:HD1	1.62	0.63
6:7:184:CYS:SG	6:7:185:ASP:N	2.71	0.63
1:2:517:ILE:HD11	1:2:772:ARG:HB3	1.81	0.63
1:2:526:GLY:HA2	7:2:1001:ATP:O1B	1.98	0.63
2:3:132:THR:HG22	2:3:400:LEU:HD21	1.81	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:82:GLU:HB3	5:6:85:ARG:HB3	1.81	0.62
1:2:503:GLU:HG2	1:2:733:PRO:HD2	1.81	0.62
2:3:464:THR:HG23	2:3:467:GLU:H	1.64	0.62
1:2:183:ARG:HD2	1:2:184:GLU:N	2.14	0.62
1:2:831:LEU:HD13	1:2:872:ILE:HD11	1.81	0.62
4:5:627:LYS:NZ	4:5:636:ASP:OD1	2.32	0.62
1:2:295:ARG:HG3	1:2:392:ARG:HG3	1.81	0.62
1:2:463:MET:HE3	1:2:719:VAL:HG23	1.79	0.62
1:2:726:TYR:OH	1:2:730:ARG:HD2	2.00	0.62
4:5:32:GLN:HB2	4:5:98:LEU:HD12	1.81	0.62
1:2:316:THR:HG22	1:2:570:THR:HG22	1.82	0.62
5:6:769:LYS:HA	5:6:772:ILE:HG12	1.81	0.62
6:7:329:GLU:HB2	6:7:332:PHE:HB2	1.82	0.61
2:3:58:ASN:HD21	2:3:60:LYS:HB2	1.64	0.61
1:2:750:LEU:CD1	1:2:762:ILE:HG23	2.30	0.61
4:5:236:VAL:HG12	4:5:238:HIS:H	1.66	0.61
1:2:726:TYR:CE2	1:2:730:ARG:HD3	2.35	0.61
1:2:470:ASP:OD2	1:2:476:LYS:NZ	2.33	0.61
5:6:233:VAL:HG13	5:6:234:GLU:HG2	1.82	0.61
6:7:545:ARG:NH2	6:7:552:GLU:OE1	2.33	0.61
1:2:497:LEU:HD23	1:2:773:MET:HG2	1.83	0.61
4:5:36:LYS:HB3	4:5:40:ARG:HH22	1.65	0.61
2:3:164:THR:HG22	2:3:166:VAL:H	1.65	0.60
6:7:343:GLU:O	6:7:532:ARG:NH1	2.34	0.60
1:2:833:LEU:HD11	1:2:885:LEU:HG	1.83	0.60
1:2:498:ALA:HA	1:2:517:ILE:HB	1.83	0.60
2:3:616:ARG:O	2:3:620:THR:HG23	2.01	0.60
2:3:564:SER:HB3	2:3:567:PHE:HB3	1.83	0.60
3:4:718:ARG:NH1	3:4:729:ALA:O	2.34	0.60
4:5:570:CYS:HB3	4:5:625:LYS:HG3	1.83	0.60
5:6:156:PHE:HA	5:6:193:LEU:HA	1.83	0.60
2:3:471:LEU:HD22	2:3:475:LEU:HD23	1.85	0.59
4:5:134:PRO:HB2	4:5:152:PRO:HD3	1.84	0.59
6:7:439:GLN:OE1	6:7:481:ARG:NH1	2.34	0.59
1:2:226:ASN:HB3	1:2:277:ILE:HG21	1.85	0.59
6:7:55:VAL:HG13	6:7:63:VAL:HG22	1.85	0.59
1:2:804:ASP:HA	1:2:811:MET:HE2	1.84	0.58
3:4:167:GLN:NE2	3:4:243:GLU:OE1	2.35	0.58
4:5:168:ILE:HD11	4:5:214:ILE:HD12	1.86	0.58
4:5:723:HIS:HB3	4:5:727:ARG:HE	1.67	0.58
2:B:751:LEU:HD12	2:B:768:LEU:HD21	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:271:ASP:OD1	2:3:364:ARG:NH2	2.36	0.58
3:4:271:MET:HE3	3:4:370:VAL:HG23	1.84	0.58
5:6:27:GLN:HG3	5:6:93:ALA:HB2	1.84	0.58
4:5:452:GLU:HA	4:5:455:ARG:HG2	1.86	0.58
5:6:27:GLN:HB2	5:6:89:TYR:HB3	1.86	0.58
5:6:778:HIS:O	5:6:781:THR:OG1	2.21	0.58
1:2:356:GLN:HE21	5:6:189:ARG:HE	1.50	0.58
4:5:223:ASP:N	4:5:223:ASP:OD1	2.36	0.58
2:3:270:LYS:O	2:3:364:ARG:NH1	2.36	0.58
2:3:597:LEU:HD22	2:3:654:PHE:HE2	1.67	0.58
5:6:506:ILE:HD11	5:6:521:ASN:HB3	1.85	0.58
6:7:580:TYR:OH	6:7:631:ASN:OD1	2.21	0.58
5:6:714:ARG:HH21	5:6:716:GLY:HA2	1.69	0.58
2:3:344:ILE:HD12	2:3:482:LEU:HD21	1.85	0.58
4:5:360:GLY:O	4:5:625:LYS:NZ	2.32	0.57
3:4:748:ARG:HH22	3:4:754:GLU:HG2	1.70	0.57
4:5:645:GLN:HA	4:5:649:LEU:HB2	1.85	0.57
2:3:311:ASP:N	2:3:311:ASP:OD1	2.36	0.57
3:4:328:CYS:SG	3:4:329:GLY:N	2.78	0.57
3:4:533:THR:HG21	3:4:543:LEU:HD13	1.86	0.57
2:3:270:LYS:NZ	2:3:402:ASP:OD2	2.36	0.57
6:7:540:VAL:O	6:7:544:SER:N	2.35	0.57
4:5:366:PRO:HG2	4:5:371:ARG:HE	1.69	0.57
1:2:382:PRO:HB3	1:2:544:ILE:HD11	1.87	0.57
4:5:125:GLN:HB2	4:5:251:ARG:HE	1.69	0.57
4:5:375:ILE:HA	4:5:618:ARG:HD3	1.87	0.57
6:7:91:ARG:NH1	6:7:92:GLU:O	2.37	0.57
1:2:176:ASP:HB2	1:2:243:VAL:HG11	1.86	0.57
3:4:318:ASP:OD1	3:4:319:ARG:N	2.36	0.57
6:7:139:GLN:HG2	6:7:302:ARG:HD2	1.86	0.57
1:2:800:GLU:HG2	1:2:824:PHE:HE2	1.69	0.56
1:2:293:GLU:OE2	1:2:295:ARG:NH1	2.38	0.56
3:4:350:GLN:HB2	3:4:379:VAL:HG23	1.87	0.56
3:4:579:MET:O	3:4:584:ARG:NH2	2.38	0.56
6:7:110:GLU:HB2	6:7:126:TYR:HE2	1.68	0.56
1:2:750:LEU:HB2	1:2:818:PHE:HZ	1.70	0.56
1:2:799:LEU:HD12	1:2:823:SER:HB3	1.87	0.56
2:3:371:ARG:NH1	2:3:410:GLU:OE1	2.37	0.56
4:5:241:MET:SD	4:5:241:MET:N	2.78	0.56
6:7:36:GLN:OE1	6:7:45:GLN:NE2	2.37	0.56
6:7:441:VAL:HG12	6:7:483:SER:HB2	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:348:ASP:OD1	5:6:128:SER:OG	2.21	0.56
6:7:620:ARG:NH1	6:7:628:GLU:OE2	2.39	0.56
1:2:749:ASP:HA	1:2:752:LYS:NZ	2.21	0.56
2:3:600:GLN:HA	2:3:603:MET:HE3	1.87	0.56
5:6:412:PHE:HD1	5:6:569:LEU:HD22	1.71	0.56
1:2:388:GLY:O	1:2:389:ARG:NE	2.38	0.56
1:2:438:VAL:HG22	1:2:439:ILE:H	1.71	0.56
3:4:550:ASP:OD2	3:4:553:THR:N	2.33	0.56
1:2:191:PRO:HA	1:2:194:GLU:HB3	1.88	0.56
1:2:322:LEU:CD2	1:2:343:GLN:HA	2.26	0.56
1:2:549:GLN:OE1	5:6:471:VAL:HG12	2.06	0.55
1:2:860:VAL:HG23	1:2:900:ILE:HB	1.88	0.55
2:3:185:GLU:OE2	6:7:72:ARG:NH1	2.38	0.55
2:3:508:ARG:HD2	2:3:514:ASP:HA	1.88	0.55
3:4:426:ALA:HB2	3:4:431:GLY:O	2.07	0.55
6:7:374:ASN:ND2	6:7:465:GLN:OE1	2.39	0.55
6:7:389:GLN:HE22	8:7:801:ADP:H3'	1.71	0.55
3:4:483:GLN:HE22	3:4:614:LEU:HB2	1.71	0.55
5:6:767:ILE:O	5:6:771:ARG:HG3	2.06	0.55
6:7:632:GLU:OE2	6:7:635:ARG:NH2	2.27	0.55
1:2:773:MET:HE1	1:2:798:MET:HE2	1.88	0.55
4:5:680:LYS:HA	4:5:732:ARG:HH12	1.70	0.55
5:6:594:ILE:HD13	5:6:625:ILE:HG22	1.87	0.55
1:2:459:GLU:O	1:2:462:LYS:HG2	2.06	0.55
4:5:349:MET:HE3	4:5:349:MET:HA	1.89	0.55
1:2:750:LEU:HD12	1:2:762:ILE:HG23	1.88	0.55
5:6:430:THR:HB	5:6:482:ILE:HD13	1.89	0.55
1:2:542:ARG:NH2	1:2:578:LEU:O	2.39	0.55
1:2:226:ASN:HD22	1:2:274:TYR:HE1	1.54	0.55
3:4:619:PRO:HG3	3:4:624:TRP:HE3	1.71	0.55
4:5:322:PHE:HZ	4:5:561:LYS:HB3	1.72	0.55
1:2:847:GLN:NE2	1:2:855:GLN:OE1	2.35	0.55
5:6:647:GLU:OE2	5:6:650:ARG:NH2	2.39	0.55
1:2:514:ARG:NH2	1:2:516:ASP:OD1	2.38	0.54
1:2:731:VAL:HG12	1:2:731:VAL:O	2.08	0.54
1:2:757:THR:O	1:2:759:SER:N	2.36	0.54
2:3:307:ILE:HD12	2:3:350:ALA:HB1	1.89	0.54
2:3:487:ASP:OD1	4:5:590:ARG:NH2	2.40	0.54
2:3:655:LYS:HE2	2:3:658:LEU:HD12	1.88	0.54
6:7:71:ARG:NH1	6:7:299:GLU:OE1	2.40	0.54
1:2:800:GLU:CG	1:2:824:PHE:HE2	2.20	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:822:GLN:NE2	3:4:823:LEU:HG	2.22	0.54
5:6:477:MET:HE3	5:6:529:ARG:HB2	1.88	0.54
2:3:465:PRO:HG3	2:3:610:THR:HA	1.89	0.54
3:4:663:ALA:HB3	6:7:582:THR:HG23	1.88	0.54
1:2:473:ILE:HA	1:2:476:LYS:HB3	1.89	0.54
1:2:484:SER:HA	1:2:678:PHE:HZ	1.73	0.54
4:5:479:ASN:HD21	4:5:481:ARG:CZ	2.21	0.54
6:7:191:THR:HG21	6:7:207:PRO:HD2	1.89	0.54
1:2:612:SER:HA	1:2:617:VAL:HG22	1.90	0.54
5:6:425:SER:HB2	5:6:428:GLY:HA2	1.90	0.54
1:2:328:ASN:O	1:2:329:CYS:HB2	2.07	0.54
3:4:406:SER:OG	6:7:201:MET:SD	2.66	0.54
2:3:416:ASP:HA	2:3:419:ARG:HD3	1.90	0.54
4:5:363:LYS:NZ	4:5:621:GLU:OE2	2.40	0.54
6:7:96:LYS:NZ	6:7:104:GLU:OE1	2.37	0.53
1:2:812:ARG:O	1:2:816:LYS:HG2	2.09	0.53
3:4:819:LYS:HB2	3:4:858:LYS:HG2	1.90	0.53
5:6:466:ASP:OD1	5:6:466:ASP:N	2.34	0.53
6:7:51:ASP:HA	6:7:139:GLN:HB2	1.90	0.53
6:7:204:ILE:HG22	6:7:205:MET:HE2	1.90	0.53
5:6:610:THR:OG1	5:6:658:ARG:NH1	2.41	0.53
6:7:571:PRO:HG2	6:7:614:THR:HG23	1.91	0.53
1:2:448:ASP:O	1:2:581:ARG:NH2	2.41	0.53
3:4:177:LEU:CD2	3:4:182:GLU:HB2	2.37	0.53
6:7:282:ARG:NH1	6:7:295:GLU:OE1	2.39	0.53
6:7:574:PRO:HD2	6:7:577:LEU:HD12	1.90	0.53
4:5:374:ASP:C	4:5:375:ILE:HD13	2.33	0.53
5:6:598:TYR:HB2	5:6:621:LEU:HD13	1.91	0.53
3:4:335:HIS:HB3	5:6:179:ILE:HG13	1.89	0.53
5:6:126:LEU:HD11	5:6:137:ILE:HG21	1.91	0.53
1:2:850:ARG:NH1	5:6:756:ILE:HG12	2.23	0.53
3:4:276:PRO:HB3	6:7:175:PRO:HB3	1.89	0.53
6:7:66:ILE:HD13	6:7:73:TYR:HB3	1.89	0.53
6:7:343:GLU:HA	6:7:532:ARG:HH22	1.74	0.53
1:2:755:MET:O	1:2:756:ALA:C	2.51	0.52
2:3:582:LEU:HA	2:3:637:VAL:HG13	1.90	0.52
3:4:506:ILE:HG12	3:4:646:LEU:HB2	1.90	0.52
3:4:777:ARG:HD2	3:4:793:THR:HG21	1.90	0.52
6:7:52:LEU:HD12	6:7:141:PRO:HD3	1.92	0.52
1:2:866:VAL:O	1:2:870:ARG:HG2	2.10	0.52
3:4:629:THR:OG1	3:4:630:THR:N	2.42	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:144:MET:HE2	4:5:144:MET:HA	1.91	0.52
6:7:534:ALA:O	6:7:538:THR:HG23	2.09	0.52
6:7:588:MET:HE1	6:7:609:ILE:HD11	1.89	0.52
6:7:18:GLN:HG3	6:7:84:LEU:HD21	1.90	0.52
1:2:206:HIS:HA	1:2:240:ARG:HH12	1.75	0.52
2:3:593:GLU:OE2	2:3:596:ARG:NH2	2.42	0.52
4:5:361:SER:H	4:5:375:ILE:HG21	1.74	0.52
6:7:540:VAL:HG13	6:7:541:HIS:H	1.73	0.52
1:2:202:PHE:CE2	1:2:237:LEU:HA	2.44	0.52
1:2:751:ARG:O	1:2:754:SER:HB2	2.09	0.52
2:3:101:GLY:HA2	2:3:263:CYS:HB2	1.92	0.52
2:3:443:ASN:OD1	2:3:445:ARG:NE	2.43	0.52
3:4:321:ARG:HH21	5:6:288:GLY:HA3	1.75	0.52
4:5:152:PRO:HA	4:5:264:THR:HA	1.91	0.52
1:2:402:LEU:HD22	1:2:444:VAL:HG12	1.92	0.52
2:3:106:PHE:HB3	2:3:109:LYS:HB2	1.92	0.52
2:3:321:LEU:HD22	2:3:362:ALA:HB2	1.91	0.52
3:4:267:LYS:NZ	3:4:360:ASP:OD2	2.43	0.52
3:4:710:LEU:HD23	3:4:737:LEU:HD22	1.91	0.52
6:7:555:ASP:OD2	6:7:558:LEU:N	2.43	0.52
2:3:618:LEU:HD23	6:7:533:LEU:HD12	1.93	0.51
3:4:317:MET:HA	3:4:317:MET:HE2	1.92	0.51
1:2:783:ARG:HH11	1:2:787:ILE:HD12	1.73	0.51
6:7:587:GLU:OE1	6:7:590:ARG:NH1	2.44	0.51
1:2:836:LEU:HB2	1:2:865:LEU:HD11	1.92	0.51
2:3:36:VAL:HA	2:3:39:LEU:HD23	1.93	0.51
3:4:177:LEU:HD21	3:4:182:GLU:HB2	1.93	0.51
2:3:53:ASP:O	2:3:57:LYS:HG2	2.11	0.51
5:6:726:LEU:HD11	5:6:780:LEU:HD12	1.93	0.51
1:2:328:ASN:OD1	1:2:353:PRO:HD3	2.10	0.51
1:2:236:ASP:OD1	1:2:237:LEU:N	2.42	0.51
1:2:380:GLU:OE1	1:2:392:ARG:N	2.42	0.51
1:2:750:LEU:HG	1:2:818:PHE:CE2	2.46	0.51
1:2:770:MET:HE1	1:2:795:ILE:CA	2.41	0.51
1:2:817:THR:O	1:2:818:PHE:C	2.54	0.51
4:5:385:THR:HG22	4:5:523:GLU:HG2	1.92	0.51
1:2:839:LEU:O	1:2:842:GLU:HG3	2.11	0.50
3:4:516:LYS:HG2	3:4:650:LEU:HD22	1.92	0.50
2:3:137:VAL:HG13	2:3:226:VAL:HG11	1.94	0.50
2:3:351:LYS:NZ	2:3:453:ASN:OD1	2.35	0.50
3:4:400:ARG:HG3	3:4:408:VAL:HG12	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:420:ARG:HH21	4:5:425:ARG:HD3	1.76	0.50
5:6:51:GLU:O	5:6:54:ILE:HG22	2.12	0.50
2:3:24:ASP:OD1	2:3:25:ASP:N	2.40	0.50
5:6:723:ILE:O	5:6:727:ILE:HG12	2.11	0.50
3:4:596:LEU:N	3:4:607:LEU:O	2.42	0.50
1:2:183:ARG:NH2	5:6:166:ARG:HH12	2.10	0.50
5:6:41:ASP:OD1	5:6:41:ASP:N	2.43	0.50
5:6:612:SER:HA	5:6:658:ARG:HA	1.93	0.50
6:7:345:TYR:H	8:7:801:ADP:HN61	1.60	0.50
1:2:318:VAL:HB	1:2:403:VAL:HG21	1.93	0.50
1:2:815:ARG:O	1:2:819:ALA:HB2	2.10	0.50
3:4:441:PHE:HA	3:4:446:VAL:HG23	1.93	0.50
3:4:566:SER:OG	3:4:567:ASP:N	2.45	0.50
3:4:838:ASP:N	3:4:838:ASP:OD1	2.45	0.50
4:5:96:LEU:HD13	4:5:297:LEU:HD22	1.94	0.50
5:6:215:LEU:HD12	5:6:216:PRO:HD2	1.92	0.50
1:2:297:LEU:HD11	1:2:308:THR:HG21	1.93	0.50
2:3:402:ASP:OD1	2:3:402:ASP:N	2.44	0.50
4:5:586:TYR:OH	4:5:590:ARG:NH1	2.45	0.50
5:6:429:LEU:O	5:6:449:LEU:N	2.32	0.50
1:2:833:LEU:HD21	1:2:886:PHE:HB3	1.94	0.49
5:6:590:SER:OG	5:6:640:VAL:O	2.25	0.49
6:7:490:PRO:HB3	6:7:505:ILE:HD13	1.93	0.49
1:2:322:LEU:HB3	1:2:345:GLN:H	1.77	0.49
1:2:411:GLU:HG3	1:2:447:LYS:HE3	1.95	0.49
5:6:421:GLY:N	5:6:460:ASP:O	2.42	0.49
6:7:320:THR:O	6:7:324:LEU:N	2.37	0.49
1:2:195:ILE:HD11	1:2:258:ILE:HD13	1.95	0.49
1:2:739:ASP:OD2	2:B:767:ARG:NH1	2.45	0.49
6:7:118:MET:HA	6:7:118:MET:HE2	1.95	0.49
2:3:575:ALA:HB2	2:3:633:MET:HE3	1.95	0.49
6:7:283:THR:O	6:7:283:THR:OG1	2.30	0.49
6:7:646:GLY:O	6:7:647:ASP:HB2	2.13	0.49
1:2:864:ASP:HA	1:2:867:ASP:HB3	1.94	0.49
4:5:455:ARG:NH2	4:5:507:MET:HG2	2.27	0.49
5:6:785:HIS:O	5:6:785:HIS:ND1	2.46	0.49
1:2:202:PHE:CE1	1:2:215:PHE:HE2	2.31	0.49
1:2:268:LEU:HD21	1:2:275:ASP:OD1	2.13	0.49
2:3:622:ILE:HD13	6:7:537:ILE:HD12	1.94	0.49
4:5:597:GLU:O	4:5:598:ARG:HG2	2.13	0.49
1:2:343:GLN:HE21	1:2:371:GLN:N	2.10	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:138:ARG:HA	4:5:243:ARG:HH22	1.78	0.49
2:3:305:PRO:HG2	4:5:369:LEU:HD11	1.94	0.48
3:4:587:LEU:O	3:4:591:MET:HG3	2.13	0.48
3:4:191:PRO:HB2	3:4:194:MET:HG2	1.95	0.48
3:4:291:ARG:NH1	3:4:550:ASP:OD1	2.46	0.48
1:2:750:LEU:HB2	1:2:818:PHE:CZ	2.47	0.48
2:3:181:ASN:OD1	2:3:182:ASN:N	2.47	0.48
3:4:560:THR:HB	3:4:564:VAL:HB	1.94	0.48
1:2:344:ASN:C	1:2:345:GLN:CD	2.81	0.48
2:3:366:ILE:HD12	2:3:401:ALA:HB2	1.96	0.48
3:4:388:VAL:HA	3:4:423:LYS:HA	1.94	0.48
1:2:460:ASP:HB3	1:2:463:MET:HE2	1.96	0.48
1:2:767:ILE:HG21	2:B:806:PHE:CE2	2.48	0.48
4:5:574:LEU:HA	4:5:632:ALA:HB3	1.94	0.48
5:6:159:LEU:HD12	5:6:190:ARG:HB3	1.96	0.48
1:2:408:PRO:HB3	1:2:573:ALA:HB2	1.94	0.48
1:2:579:ALA:O	1:2:624:CYS:HB3	2.13	0.48
5:6:238:ALA:HB1	5:6:446:ALA:HB2	1.95	0.48
5:6:486:LYS:HG3	5:6:487:ALA:H	1.77	0.48
1:2:192:ARG:NH2	1:2:261:GLU:OE1	2.41	0.48
1:2:288:LEU:HD21	1:2:305:LEU:HD23	1.95	0.48
1:2:820:ARG:H	1:2:820:ARG:HE	1.60	0.48
3:4:302:ALA:HB3	3:4:315:VAL:HG12	1.95	0.48
1:2:451:VAL:HG12	1:2:542:ARG:HG3	1.96	0.48
1:2:757:THR:C	1:2:759:SER:H	2.21	0.48
3:4:490:LYS:HD3	5:6:559:ILE:HG21	1.95	0.48
1:2:448:ASP:OD1	1:2:448:ASP:N	2.41	0.47
2:3:134:CYS:HA	2:3:199:ILE:HG22	1.95	0.47
5:6:371:MET:HE1	5:6:500:LEU:HB2	1.96	0.47
6:7:15:LYS:O	6:7:19:GLU:HG2	2.13	0.47
2:3:110:HIS:HA	2:3:126:CYS:HB3	1.96	0.47
4:5:683:PHE:O	4:5:732:ARG:NH1	2.46	0.47
1:2:642:THR:HG22	1:2:645:GLU:HG2	1.96	0.47
4:5:680:LYS:HG2	4:5:732:ARG:NH2	2.25	0.47
2:3:242:ARG:HE	2:3:261:ILE:HD13	1.78	0.47
5:6:232:ALA:HB1	5:6:303:VAL:HG12	1.96	0.47
2:3:131:VAL:HG23	2:3:231:PRO:HA	1.96	0.47
3:4:836:THR:OG1	3:4:838:ASP:OD1	2.30	0.47
4:5:367:ASP:HB3	4:5:369:LEU:HG	1.96	0.47
5:6:372:LEU:HD21	5:6:412:PHE:CE2	2.50	0.47
2:3:202:GLN:HG3	2:3:203:GLU:H	1.79	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:593:GLU:HG2	2:3:646:VAL:HG11	1.96	0.47
2:3:600:GLN:O	2:3:604:SER:N	2.47	0.47
4:5:168:ILE:HD11	4:5:214:ILE:HG23	1.96	0.47
1:2:748:SER:O	1:2:749:ASP:C	2.58	0.47
2:3:600:GLN:HG2	2:3:613:VAL:HG12	1.96	0.47
3:4:452:LEU:HD21	3:4:682:LEU:HD21	1.95	0.47
4:5:555:ASP:OD1	4:5:555:ASP:N	2.38	0.47
5:6:38:GLN:HA	5:6:44:ILE:HG13	1.97	0.47
5:6:39:SER:OG	5:6:42:GLY:O	2.17	0.47
5:6:151:LEU:H	5:6:151:LEU:HD23	1.79	0.47
6:7:354:LEU:HD13	6:7:394:ILE:HG13	1.95	0.47
6:7:362:VAL:HG12	6:7:614:THR:HG21	1.97	0.47
4:5:154:ILE:HG12	4:5:262:ARG:HD3	1.95	0.47
4:5:578:ALA:HB1	4:5:637:VAL:HG21	1.97	0.47
2:B:741:GLU:O	2:B:745:LYS:HG3	2.14	0.47
1:2:270:MET:HA	1:2:270:MET:HE2	1.96	0.47
5:6:173:LYS:HG3	5:6:252:PRO:HG2	1.97	0.47
5:6:437:GLU:OE1	5:6:437:GLU:N	2.48	0.47
6:7:39:ARG:HG3	6:7:44:GLU:HB2	1.97	0.47
3:4:308:VAL:HG22	5:6:181:ARG:HH22	1.80	0.47
5:6:390:ILE:O	5:6:498:SER:OG	2.31	0.47
1:2:307:ARG:HA	1:2:414:LEU:O	2.15	0.46
1:2:340:CYS:SG	1:2:341:GLN:N	2.76	0.46
1:2:605:GLU:HB3	1:2:656:ARG:HD2	1.97	0.46
1:2:741:ASP:O	1:2:742:LYS:C	2.58	0.46
1:2:750:LEU:HD13	1:2:761:PRO:HA	1.96	0.46
2:3:64:ARG:NH2	2:3:72:GLU:OE2	2.48	0.46
2:3:460:ASP:OD1	2:3:468:ASN:ND2	2.33	0.46
2:3:564:SER:OG	2:3:565:ALA:N	2.44	0.46
3:4:752:LYS:HE2	3:4:752:LYS:HB3	1.72	0.46
4:5:100:GLU:HG2	4:5:126:VAL:HG12	1.96	0.46
6:7:332:PHE:CE1	6:7:562:TYR:HE2	2.33	0.46
2:3:16:GLN:OE1	2:3:78:ARG:NH1	2.47	0.46
2:3:220:ILE:CG2	2:3:261:ILE:HA	2.45	0.46
2:3:220:ILE:HG22	2:3:261:ILE:HA	1.98	0.46
4:5:492:PHE:HZ	4:5:658:SER:HA	1.79	0.46
5:6:449:LEU:HD11	5:6:499:ILE:HD11	1.97	0.46
6:7:273:VAL:HG12	6:7:303:ILE:HG12	1.96	0.46
6:7:395:ASP:OD1	6:7:401:SER:OG	2.29	0.46
1:2:503:GLU:CG	1:2:733:PRO:HD2	2.45	0.46
1:2:862:GLU:HB2	1:2:898:LYS:HG3	1.98	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:522:GLN:HB2	6:7:524:ARG:HH21	1.79	0.46
4:5:415:THR:OG1	4:5:454:ASP:OD1	2.24	0.46
4:5:592:GLY:HA2	4:5:595:GLN:HB2	1.96	0.46
1:2:384:LYS:HG2	1:2:385:VAL:HG23	1.98	0.46
1:2:868:LYS:O	1:2:872:ILE:HG22	2.15	0.46
2:3:563:VAL:HG23	2:3:564:SER:H	1.80	0.46
2:3:614:THR:OG1	2:3:615:ALA:N	2.48	0.46
3:4:577:ASP:OD1	3:4:577:ASP:N	2.48	0.46
3:4:785:ILE:O	3:4:786:LEU:HD23	2.16	0.46
5:6:325:ILE:HD11	5:6:578:PHE:HA	1.97	0.46
6:7:627:LYS:O	6:7:631:ASN:ND2	2.48	0.46
1:2:768:GLU:O	1:2:771:ILE:HG12	2.16	0.46
3:4:265:ALA:O	3:4:422:ARG:NH1	2.48	0.46
4:5:171:GLN:HG3	4:5:178:THR:HG22	1.98	0.46
1:2:268:LEU:HD21	1:2:275:ASP:CG	2.41	0.46
2:3:414:MET:HG2	2:3:418:ASP:HB2	1.96	0.46
3:4:295:LEU:HD12	3:4:379:VAL:HG21	1.98	0.46
5:6:622:GLU:HA	5:6:625:ILE:HG12	1.98	0.46
1:2:802:PHE:HE2	1:2:814:MET:HE1	1.81	0.46
2:3:219:VAL:HG22	2:3:220:ILE:H	1.80	0.46
3:4:735:GLU:OE2	8:6:901:ADP:O3'	2.33	0.46
4:5:662:GLY:C	4:5:664:THR:H	2.24	0.46
1:2:208:ASP:OD1	1:2:208:ASP:N	2.46	0.45
4:5:59:LEU:HD13	4:5:70:ILE:HD12	1.98	0.45
1:2:505:LYS:O	1:2:507:PRO:HD3	2.16	0.45
2:3:598:ARG:HH12	2:3:614:THR:HA	1.81	0.45
5:6:575:TYR:OH	5:6:634:MET:O	2.22	0.45
4:5:467:ILE:O	4:5:478:LEU:N	2.36	0.45
1:2:438:VAL:HG22	1:2:439:ILE:N	2.30	0.45
2:3:425:VAL:HG22	2:3:431:VAL:HG22	1.98	0.45
3:4:183:ASN:OD1	3:4:183:ASN:N	2.49	0.45
3:4:292:THR:HG22	3:4:352:ILE:HG12	1.97	0.45
3:4:818:LEU:HB3	3:4:822:GLN:NE2	2.32	0.45
4:5:184:MET:HE3	4:5:184:MET:HB3	1.79	0.45
2:3:474:SER:O	2:3:477:SER:OG	2.34	0.45
1:2:673:GLU:OE2	5:6:599:LYS:HB2	2.17	0.45
2:3:594:TYR:OH	2:3:598:ARG:NH1	2.50	0.45
4:5:674:ARG:HD2	4:5:677:LYS:HD3	1.98	0.45
6:7:162:THR:HG23	6:7:274:THR:HG22	1.99	0.45
6:7:446:GLU:HG2	6:7:449:LYS:HG3	1.98	0.45
1:2:186:VAL:HG12	1:2:186:VAL:O	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:658:LEU:HD23	2:3:659:GLU:HB2	1.99	0.45
3:4:847:LEU:O	3:4:851:ASP:N	2.50	0.45
4:5:674:ARG:NH1	4:5:681:ARG:HH12	2.15	0.45
5:6:325:ILE:HA	5:6:328:GLN:HG2	1.99	0.45
1:2:564:PRO:HB2	5:6:487:ALA:HB1	1.99	0.45
1:2:855:GLN:NE2	1:2:857:THR:O	2.50	0.45
3:4:432:LEU:HD11	3:4:528:PRO:HG3	1.99	0.45
4:5:337:LYS:HZ1	4:5:340:ALA:H	1.63	0.45
1:2:315:CYS:SG	1:2:316:THR:N	2.90	0.45
3:4:563:LEU:HD11	3:4:587:LEU:HD22	1.99	0.45
4:5:229:LEU:HB2	4:5:247:LEU:HD11	1.99	0.45
6:7:377:ILE:HA	6:7:517:LEU:O	2.17	0.45
6:7:457:ALA:O	6:7:461:VAL:HG12	2.17	0.45
2:B:751:LEU:HD13	2:B:792:MET:HE1	1.99	0.45
2:3:113:PRO:HG3	2:3:127:VAL:HG13	1.99	0.44
3:4:628:LYS:HE2	3:4:632:GLU:HB3	1.99	0.44
4:5:114:ARG:HA	4:5:114:ARG:HD3	1.73	0.44
5:6:614:TRP:CZ2	5:6:656:ILE:HA	2.52	0.44
1:2:176:ASP:OD1	1:2:176:ASP:N	2.49	0.44
3:4:647:ILE:O	3:4:772:SER:OG	2.28	0.44
3:4:801:LEU:HD21	3:4:835:ILE:HD13	1.99	0.44
1:2:326:LYS:O	1:2:327:TYR:O	2.34	0.44
1:2:592:MET:HE1	1:2:600:ILE:HD11	1.97	0.44
2:3:197:GLN:HG2	2:3:199:ILE:HG23	2.00	0.44
2:3:515:GLY:O	4:5:571:GLY:N	2.50	0.44
3:4:377:ASP:OD1	3:4:377:ASP:O	2.35	0.44
4:5:517:ILE:HD12	4:5:517:ILE:N	2.32	0.44
5:6:733:LYS:HZ2	5:6:787:LEU:HD22	1.82	0.44
6:7:516:ASP:OD1	6:7:608:ALA:HB1	2.17	0.44
2:3:203:GLU:HG3	2:3:215:ARG:H	1.83	0.44
3:4:580:ASN:OD1	3:4:580:ASN:N	2.49	0.44
5:6:520:ILE:HG22	5:6:522:LEU:H	1.82	0.44
6:7:62:LEU:O	6:7:66:ILE:HG12	2.17	0.44
2:3:241:TYR:CZ	2:3:256:PHE:HE2	2.36	0.44
4:5:664:THR:HG22	4:5:669:GLN:HB2	1.98	0.44
1:2:706:MET:HE2	1:2:708:ASN:OD1	2.17	0.44
2:3:273:GLN:HG2	2:3:275:SER:H	1.83	0.44
4:5:567:ARG:HA	4:5:567:ARG:HD2	1.71	0.44
5:6:159:LEU:O	5:6:162:GLN:NE2	2.44	0.44
1:2:507:PRO:HG2	1:2:511:HIS:HB2	1.99	0.44
1:2:849:ASN:HD22	5:6:727:ILE:HB	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:497:ARG:HA	5:6:408:HIS:HE2	1.83	0.44
4:5:715:MET:HG3	4:5:721:ILE:HG12	2.00	0.44
5:6:773:ILE:HA	5:6:776:VAL:HG12	2.00	0.44
6:7:546:GLN:HE22	6:7:553:PRO:HG3	1.83	0.44
1:2:326:LYS:O	1:2:327:TYR:C	2.61	0.44
1:2:830:GLU:HA	1:2:833:LEU:HD12	2.00	0.44
1:2:846:TYR:O	1:2:850:ARG:HB2	2.18	0.44
4:5:383:PRO:HD3	4:5:487:ALA:HB1	2.00	0.44
4:5:409:SER:HB3	4:5:413:GLY:HA3	2.00	0.44
1:2:741:ASP:O	1:2:744:ALA:N	2.51	0.43
1:2:743:VAL:HG11	2:B:806:PHE:HE2	1.82	0.43
2:3:526:ILE:HB	4:5:372:ARG:NH2	2.33	0.43
3:4:520:LEU:HB3	3:4:532:TYR:HE1	1.81	0.43
4:5:437:ALA:O	4:5:482:CYS:HB3	2.18	0.43
6:7:280:ILE:HB	6:7:297:TYR:CD1	2.53	0.43
1:2:523:GLY:HA3	1:2:663:VAL:HG23	2.00	0.43
1:2:777:HIS:CE1	1:2:793:MET:HG2	2.53	0.43
2:3:316:ALA:HB2	2:3:648:LEU:HD21	2.00	0.43
3:4:282:LEU:HD23	3:4:282:LEU:HA	1.88	0.43
3:4:848:ALA:HB2	3:4:853:LEU:HD11	2.00	0.43
4:5:674:ARG:HH12	4:5:681:ARG:HH12	1.65	0.43
3:4:721:GLY:HA3	3:4:728:SER:HB2	2.01	0.43
4:5:418:VAL:HG21	4:5:474:ILE:HD12	2.01	0.43
6:7:646:GLY:N	6:7:650:GLN:HA	2.33	0.43
2:B:736:LYS:O	2:B:739:LEU:HD22	2.19	0.43
1:2:750:LEU:CD2	1:2:761:PRO:HA	2.46	0.43
2:3:271:ASP:HB2	2:3:364:ARG:HH12	1.84	0.43
4:5:405:SER:O	4:5:409:SER:OG	2.33	0.43
4:5:704:PRO:HB2	4:5:706:HIS:CD2	2.53	0.43
5:6:147:VAL:O	5:6:148:HIS:ND1	2.51	0.43
5:6:787:LEU:O	5:6:788:ILE:HD13	2.17	0.43
2:3:230:LYS:O	2:3:232:GLY:N	2.48	0.43
3:4:788:THR:O	3:4:788:THR:OG1	2.35	0.43
1:2:759:SER:O	1:2:760:ILE:C	2.61	0.43
2:3:614:THR:H	2:3:617:THR:HG23	1.83	0.43
3:4:428:ARG:HH22	3:4:432:LEU:HD22	1.83	0.43
4:5:42:TYR:HE2	4:5:80:PHE:HB2	1.84	0.43
4:5:88:LEU:HD12	4:5:92:PRO:HA	2.00	0.43
4:5:179:LEU:HD12	4:5:179:LEU:HA	1.90	0.43
5:6:646:LYS:HB3	5:6:646:LYS:HE3	1.85	0.43
6:7:288:VAL:HG11	6:7:293:LEU:HD13	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:307:GLY:HA2	4:5:310:PHE:HB2	2.00	0.43
6:7:366:PRO:HD2	6:7:369:MET:O	2.17	0.43
1:2:819:ALA:CA	1:2:824:PHE:HD1	2.26	0.43
1:2:836:LEU:HD11	1:2:860:VAL:HG21	2.00	0.43
2:3:219:VAL:HG23	2:3:260:LEU:HB3	2.00	0.43
3:4:668:ALA:HA	3:4:671:TYR:CD2	2.53	0.43
5:6:551:ARG:HE	5:6:551:ARG:HB2	1.67	0.43
1:2:273:LYS:O	1:2:273:LYS:HG2	2.19	0.43
2:3:224:ASP:OD1	2:3:224:ASP:O	2.37	0.43
2:3:257:ARG:C	2:3:259:VAL:HG13	2.44	0.43
3:4:660:ARG:HG3	6:7:582:THR:HG21	2.00	0.43
4:5:616:ILE:HA	4:5:619:ILE:HD12	2.01	0.43
5:6:396:GLY:HA2	5:6:536:LEU:O	2.19	0.43
5:6:744:LYS:HD2	5:6:744:LYS:HA	1.75	0.43
1:2:335:VAL:C	1:2:336:LEU:HD12	2.43	0.43
2:3:68:ASN:O	2:3:72:GLU:HB2	2.19	0.43
5:6:196:ASN:OD1	5:6:196:ASN:N	2.52	0.43
5:6:205:LYS:HG2	5:6:227:ILE:HG12	2.01	0.43
2:B:768:LEU:O	2:B:772:ILE:HG12	2.19	0.43
1:2:345:GLN:CD	1:2:373:TYR:HH	2.27	0.42
1:2:750:LEU:O	1:2:754:SER:N	2.50	0.42
2:3:260:LEU:HD23	2:3:260:LEU:HA	1.86	0.42
3:4:429:LEU:HD12	3:4:429:LEU:HA	1.88	0.42
1:2:202:PHE:HE1	1:2:215:PHE:HE2	1.66	0.42
2:3:435:LYS:HG3	2:3:436:ALA:H	1.84	0.42
3:4:362:PRO:HB2	3:4:365:GLN:HG3	2.00	0.42
5:6:145:HIS:ND1	5:6:205:LYS:O	2.52	0.42
2:3:54:LEU:HD12	2:3:54:LEU:HA	1.84	0.42
2:3:91:TYR:CG	2:3:92:ALA:N	2.88	0.42
2:3:223:ASP:O	2:3:224:ASP:HB3	2.19	0.42
2:3:480:ASP:HB2	2:3:620:THR:CG2	2.50	0.42
2:3:598:ARG:HA	2:3:613:VAL:HG11	2.00	0.42
3:4:353:LYS:HE2	3:4:353:LYS:HB3	1.73	0.42
4:5:135:SER:OG	4:5:136:SER:N	2.47	0.42
1:2:837:LYS:HA	1:2:840:VAL:HG12	2.02	0.42
2:3:382:VAL:HA	2:3:393:LEU:HA	2.01	0.42
5:6:203:PHE:CE1	5:6:229:ARG:HB3	2.55	0.42
5:6:477:MET:HG3	5:6:499:ILE:HD12	2.01	0.42
2:B:743:ARG:HE	2:B:784:GLU:HG2	1.84	0.42
1:2:233:ASN:OD1	1:2:235:GLU:N	2.51	0.42
1:2:397:ILE:HG12	1:2:438:VAL:HG21	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:46:ARG:HB3	2:3:99:TYR:HB2	2.01	0.42
3:4:457:ASP:N	3:4:457:ASP:OD1	2.50	0.42
4:5:262:ARG:HB2	4:5:302:ASP:OD1	2.19	0.42
5:6:477:MET:CE	5:6:529:ARG:HB2	2.50	0.42
1:2:593:ASN:OD1	1:2:594:ASP:N	2.53	0.42
1:2:847:GLN:NE2	1:2:855:GLN:H	2.17	0.42
3:4:193:TYR:CZ	3:4:210:VAL:HG23	2.55	0.42
3:4:760:GLU:OE2	3:4:763:ARG:NH2	2.53	0.42
2:3:308:HIS:HB2	2:3:500:HIS:CD2	2.55	0.42
3:4:485:PHE:CE2	3:4:747:VAL:HA	2.54	0.42
3:4:536:LYS:NZ	3:4:575:GLU:OE1	2.39	0.42
4:5:376:ASN:HD22	4:5:483:SER:N	2.18	0.42
5:6:165:ILE:HG23	5:6:181:ARG:HD3	2.01	0.42
6:7:181:THR:HG23	6:7:227:SER:HA	2.01	0.42
6:7:306:MET:HE3	6:7:306:MET:HB2	1.98	0.42
6:7:314:SER:HB3	6:7:561:ARG:HG3	2.01	0.42
1:2:356:GLN:HE21	5:6:189:ARG:NE	2.16	0.42
1:2:681:GLY:O	1:2:685:ARG:HG2	2.20	0.42
3:4:600:LYS:HD3	3:4:600:LYS:HA	1.84	0.42
6:7:424:SER:OG	6:7:426:GLU:OE1	2.29	0.42
6:7:616:LEU:HD13	6:7:632:GLU:HB3	2.02	0.42
1:2:531:GLN:CG	7:2:1001:ATP:O2A	2.67	0.42
1:2:799:LEU:O	1:2:803:ILE:HG12	2.20	0.42
3:4:306:CYS:HB3	3:4:311:HIS:H	1.84	0.42
3:4:353:LYS:HG2	3:4:371:ILE:HD13	2.02	0.42
3:4:758:VAL:O	3:4:762:LYS:HG3	2.19	0.42
4:5:103:ALA:HA	4:5:106:VAL:HG12	2.02	0.42
4:5:470:ALA:HA	4:5:474:ILE:O	2.20	0.42
5:6:140:GLN:NE2	5:6:451:LEU:HB2	2.35	0.42
6:7:181:THR:HG22	6:7:192:TYR:HD1	1.85	0.42
1:2:202:PHE:CE2	1:2:240:ARG:HB2	2.55	0.41
1:2:389:ARG:NE	1:2:389:ARG:HA	2.35	0.41
1:2:577:VAL:HG12	1:2:622:ALA:HB2	2.02	0.41
1:2:750:LEU:O	1:2:751:ARG:C	2.62	0.41
2:3:390:GLU:OE2	2:3:392:ARG:NH2	2.38	0.41
3:4:556:LEU:HD23	3:4:556:LEU:HA	1.89	0.41
4:5:125:GLN:HG3	4:5:251:ARG:HH21	1.85	0.41
4:5:347:THR:HA	4:5:351:LYS:HB2	2.02	0.41
4:5:455:ARG:HH21	4:5:510:ILE:HD12	1.84	0.41
4:5:478:LEU:HD23	4:5:478:LEU:HA	1.86	0.41
4:5:589:MET:HE2	4:5:589:MET:HB2	1.88	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:157:LEU:HD23	5:6:157:LEU:HA	1.83	0.41
5:6:788:ILE:HG22	5:6:789:GLU:N	2.33	0.41
1:2:319:LEU:HG	1:2:373:TYR:HB3	2.02	0.41
2:3:500:HIS:O	2:3:504:MET:HG2	2.20	0.41
2:3:518:MET:HB3	4:5:364:ARG:HG2	2.01	0.41
4:5:274:PHE:HE1	4:5:290:ARG:HD2	1.85	0.41
5:6:602:ARG:HA	5:6:602:ARG:HD2	1.73	0.41
6:7:28:LYS:HE3	6:7:30:GLN:HG2	2.02	0.41
2:3:177:LYS:HB3	2:3:179:GLU:O	2.21	0.41
2:3:393:LEU:HD22	2:3:438:ILE:HG21	2.01	0.41
2:3:568:MET:HE2	2:3:568:MET:HB3	1.98	0.41
3:4:306:CYS:SG	3:4:336:SER:OG	2.68	0.41
3:4:822:GLN:HE22	3:4:823:LEU:HG	1.84	0.41
4:5:593:ALA:HA	4:5:596:HIS:CD2	2.55	0.41
1:2:200:LYS:O	1:2:204:ARG:HG2	2.20	0.41
1:2:322:LEU:HD21	1:2:373:TYR:CG	2.56	0.41
1:2:846:TYR:HB2	5:6:731:LEU:HD23	2.01	0.41
2:3:208:ALA:N	2:3:209:PRO:HD3	2.36	0.41
2:3:641:ASP:OD1	2:3:641:ASP:N	2.51	0.41
3:4:238:ASP:OD1	3:4:260:VAL:HG12	2.20	0.41
3:4:290:ILE:HG13	3:4:355:GLN:HB2	2.02	0.41
5:6:163:THR:HG1	5:6:180:CYS:HG	1.65	0.41
6:7:529:ASN:OD1	6:7:529:ASN:N	2.53	0.41
6:7:636:LEU:HD23	6:7:636:LEU:HA	1.93	0.41
1:2:753:GLU:OE1	1:2:817:THR:HG21	2.20	0.41
1:2:757:THR:C	1:2:759:SER:N	2.78	0.41
1:2:770:MET:HE3	1:2:770:MET:HB3	1.77	0.41
3:4:152:ILE:O	3:4:153:TRP:HD1	2.03	0.41
3:4:793:THR:O	3:4:797:ARG:HG2	2.21	0.41
4:5:596:HIS:HE1	4:5:605:SER:HA	1.86	0.41
5:6:117:LEU:O	5:6:136:ARG:NH1	2.53	0.41
5:6:715:LEU:HA	5:6:715:LEU:HD22	1.71	0.41
5:6:779:ARG:HA	5:6:782:HIS:CD2	2.56	0.41
6:7:644:LEU:HD23	6:7:644:LEU:HA	1.81	0.41
1:2:753:GLU:C	1:2:755:MET:N	2.77	0.41
1:2:783:ARG:NH1	1:2:787:ILE:HD12	2.35	0.41
2:3:116:LEU:HD23	2:3:116:LEU:HA	1.89	0.41
2:3:241:TYR:CE1	2:3:259:VAL:HG21	2.56	0.41
3:4:470:ILE:HD12	3:4:515:SER:OG	2.20	0.41
3:4:556:LEU:HD11	5:6:437:GLU:HG3	2.03	0.41
3:4:853:LEU:HD13	3:4:855:VAL:HG23	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:762:SER:O	5:6:765:GLU:N	2.53	0.41
6:7:501:LEU:HG	6:7:502:GLU:H	1.86	0.41
1:2:549:GLN:O	1:2:551:ALA:N	2.54	0.41
1:2:726:TYR:CE1	1:2:730:ARG:HD2	2.55	0.41
1:2:735:LEU:HD12	1:2:736:ASN:H	1.86	0.41
2:3:373:SER:HB2	2:3:377:GLY:HA3	2.03	0.41
4:5:489:ASN:OD1	4:5:489:ASN:N	2.53	0.41
6:7:266:GLN:O	6:7:269:ASP:HB2	2.20	0.41
1:2:180:HIS:CG	1:2:185:TRP:HZ3	2.39	0.41
1:2:185:TRP:C	1:2:187:SER:H	2.28	0.41
1:2:202:PHE:HE2	1:2:240:ARG:HB2	1.85	0.41
1:2:596:ASP:O	1:2:600:ILE:HG12	2.21	0.41
1:2:737:GLN:OE1	1:2:737:GLN:N	2.34	0.41
1:2:799:LEU:CD1	1:2:823:SER:HB3	2.50	0.41
4:5:332:TYR:HE2	4:5:351:LYS:HE3	1.85	0.41
4:5:596:HIS:CE1	4:5:605:SER:HA	2.56	0.41
5:6:622:GLU:H	5:6:622:GLU:HG2	1.70	0.41
6:7:646:GLY:O	6:7:647:ASP:O	2.39	0.41
1:2:325:VAL:H	1:2:347:VAL:HG21	1.86	0.41
1:2:530:SER:O	1:2:534:LYS:HG2	2.21	0.41
1:2:564:PRO:HG2	5:6:487:ALA:HA	2.02	0.41
1:2:750:LEU:HD13	1:2:762:ILE:N	2.36	0.41
1:2:753:GLU:OE2	1:2:817:THR:HB	2.21	0.41
1:2:783:ARG:NE	1:2:790:ASP:OD2	2.54	0.41
1:2:891:PHE:CE1	1:2:902:GLN:HB2	2.55	0.41
2:3:252:THR:HG22	2:3:253:SER:H	1.85	0.41
2:3:383:THR:OG1	2:3:394:GLU:OE2	2.38	0.41
2:3:655:LYS:O	2:3:657:VAL:N	2.53	0.41
3:4:578:LYS:HB3	3:4:578:LYS:HE3	1.86	0.41
3:4:714:TYR:HB2	3:4:734:LEU:HD13	2.03	0.41
3:4:748:ARG:HH21	3:4:757:ASP:CG	2.29	0.41
4:5:273:LYS:HA	4:5:273:LYS:HD3	1.67	0.41
4:5:354:ALA:O	4:5:358:PHE:HB2	2.21	0.41
4:5:683:PHE:CE2	4:5:732:ARG:HB2	2.56	0.41
6:7:135:GLU:HG3	6:7:137:TYR:CZ	2.56	0.41
6:7:402:GLN:HG3	6:7:433:ALA:O	2.21	0.41
2:3:376:VAL:HG22	2:3:376:VAL:O	2.21	0.41
2:3:435:LYS:HD3	2:3:435:LYS:HA	1.87	0.41
2:3:489:MET:HB3	4:5:594:ARG:HH11	1.86	0.41
4:5:656:THR:OG1	4:5:657:LEU:N	2.54	0.41
5:6:433:VAL:HB	5:6:486:LYS:HG2	2.03	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:222:MET:SD	1:2:228:GLU:N	2.94	0.40
2:3:327:ARG:HD3	2:3:327:ARG:HA	1.88	0.40
2:3:376:VAL:HG22	2:3:396:GLY:HA2	2.03	0.40
3:4:433:ASP:O	3:4:436:ALA:N	2.50	0.40
3:4:442:SER:C	3:4:444:LYS:H	2.30	0.40
5:6:163:THR:OG1	5:6:180:CYS:SG	2.72	0.40
1:2:215:PHE:HZ	1:2:232:VAL:HG13	1.85	0.40
1:2:562:ARG:HH11	1:2:569:TRP:CD1	2.40	0.40
1:2:771:ILE:O	1:2:775:GLU:OE1	2.38	0.40
3:4:684:MET:HE2	3:4:684:MET:HB3	1.92	0.40
6:7:364:GLN:OE1	6:7:364:GLN:N	2.53	0.40
2:3:632:ARG:NH1	2:3:641:ASP:OD2	2.53	0.40
3:4:783:ILE:HD12	3:4:783:ILE:HA	1.97	0.40
4:5:724:ARG:HG2	4:5:725:MET:HG2	2.03	0.40
1:2:562:ARG:HE	1:2:567:ARG:NH2	2.20	0.40
3:4:269:LYS:HD2	3:4:283:ILE:HD11	2.04	0.40
4:5:173:ARG:N	4:5:211:PRO:O	2.40	0.40
6:7:322:GLU:HG2	6:7:323:GLU:N	2.36	0.40
6:7:444:ILE:O	6:7:486:ALA:HA	2.22	0.40
1:2:820:ARG:C	1:2:822:LEU:H	2.29	0.40
3:4:428:ARG:HG3	3:4:429:LEU:H	1.87	0.40
3:4:805:LEU:HD21	3:4:827:ILE:HD11	2.03	0.40
3:4:822:GLN:O	3:4:825:GLU:HG3	2.22	0.40
4:5:59:LEU:HD11	4:5:124:ILE:HG21	2.04	0.40
4:5:705:GLU:O	4:5:708:ILE:HG12	2.22	0.40
5:6:143:ARG:HD3	5:6:443:VAL:HG21	2.03	0.40
5:6:203:PHE:HE1	5:6:229:ARG:HB3	1.86	0.40
5:6:390:ILE:HG23	5:6:626:ARG:HD2	2.04	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	2	699/904 (77%)	600 (86%)	91 (13%)	8 (1%)	11	39
2	3	625/853 (73%)	537 (86%)	83 (13%)	5 (1%)	16	44
2	B	71/853 (8%)	68 (96%)	3 (4%)	0	100	100
3	4	720/863 (83%)	656 (91%)	64 (9%)	0	100	100
4	5	649/734 (88%)	593 (91%)	56 (9%)	0	100	100
5	6	685/821 (83%)	639 (93%)	45 (7%)	1 (0%)	48	76
6	7	647/719 (90%)	608 (94%)	35 (5%)	4 (1%)	21	51
All	All	4096/5747 (71%)	3701 (90%)	377 (9%)	18 (0%)	31	60

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	327	TYR
2	3	70	PHE
2	3	84	VAL
1	2	320	PRO
1	2	755	MET
1	2	818	PHE
1	2	826	ARG
6	7	646	GLY
1	2	817	THR
1	2	341	GLN
2	3	69	ALA
2	3	118	SER
6	7	490	PRO
6	7	530	ASP
6	7	647	ASP
2	3	162	LEU
5	6	715	LEU
1	2	758	GLY

### 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	2	622/781 (80%)	615 (99%)	7 (1%)	65	76
2	3	542/742 (73%)	528 (97%)	14 (3%)	40	64
2	B	65/742 (9%)	65 (100%)	0	100	100
3	4	636/753 (84%)	622 (98%)	14 (2%)	45	66
4	5	563/624 (90%)	554 (98%)	9 (2%)	55	72
5	6	627/724 (87%)	615 (98%)	12 (2%)	50	69
6	7	560/619 (90%)	552 (99%)	8 (1%)	59	74
All	All	3615/4985 (72%)	3551 (98%)	64 (2%)	51	70

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	318	VAL
1	2	319	LEU
1	2	320	PRO
1	2	346	GLU
1	2	750	LEU
1	2	820	ARG
1	2	825	ARG
2	3	39	LEU
2	3	47	LEU
2	3	70	PHE
2	3	115	THR
2	3	125	VAL
2	3	141	VAL
2	3	198	THR
2	3	252	THR
2	3	382	VAL
2	3	406	VAL
2	3	498	SER
2	3	508	ARG
2	3	637	VAL
2	3	648	LEU
3	4	139	ILE
3	4	140	VAL
3	4	152	ILE
3	4	155	THR
3	4	239	MET
3	4	327	VAL
3	4	379	VAL
3	4	390	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	4	418	VAL
3	4	553	THR
3	4	587	LEU
3	4	611	THR
3	4	785	ILE
3	4	833	ILE
4	5	245	MET
4	5	289	ILE
4	5	297	LEU
4	5	310	PHE
4	5	343	ILE
4	5	475	THR
4	5	489	ASN
4	5	636	ASP
4	5	708	ILE
5	6	26	CYS
5	6	57	GLU
5	6	63	VAL
5	6	168	VAL
5	6	237	GLN
5	6	466	ASP
5	6	566	VAL
5	6	609	VAL
5	6	617	THR
5	6	715	LEU
5	6	780	LEU
5	6	791	THR
6	7	191	THR
6	7	289	VAL
6	7	450	MET
6	7	478	LEU
6	7	482	CYS
6	7	537	ILE
6	7	555	ASP
6	7	645	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	257	GLN
1	2	356	GLN
1	2	506	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2	849	ASN
2	3	33	GLN
2	3	50	ASN
2	3	58	ASN
3	4	167	GLN
3	4	415	HIS
3	4	483	GLN
3	4	618	ASN
3	4	765	HIS
3	4	771	GLN
3	4	822	GLN
4	5	64	ASN
4	5	376	ASN
4	5	479	ASN
4	5	678	GLN
4	5	701	GLN
4	5	706	HIS
4	5	723	HIS
5	6	212	GLN
5	6	359	HIS
5	6	644	HIS
6	7	389	GLN
6	7	546	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](#)

5 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	$\# Z  > 2$
7	ATP	2	1001	-	32,33,33	0.54	0	48,52,52	0.59	0
8	ADP	6	901	-	28,29,29	1.39	4 (14%)	43,45,45	1.92	8 (18%)
8	ADP	7	801	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
8	ADP	3	901	-	28,29,29	1.38	4 (14%)	43,45,45	1.86	8 (18%)
8	ADP	4	901	-	28,29,29	1.40	4 (14%)	43,45,45	1.93	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	2	1001	-	-	4/22/38/38	0/3/3/3
8	ADP	6	901	-	-	4/16/32/32	0/3/3/3
8	ADP	7	801	-	-	3/16/32/32	0/3/3/3
8	ADP	3	901	-	-	2/16/32/32	0/3/3/3
8	ADP	4	901	-	-	3/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	4	901	ADP	C5-C4	4.76	1.47	1.39
8	6	901	ADP	C5-C4	4.68	1.47	1.39
8	7	801	ADP	C5-C4	4.62	1.47	1.39
8	3	901	ADP	C5-C4	4.57	1.47	1.39
8	3	901	ADP	C5-C6	2.71	1.48	1.41
8	4	901	ADP	C5-C6	2.69	1.48	1.41
8	7	801	ADP	C5-C6	2.65	1.48	1.41
8	6	901	ADP	C5-C6	2.64	1.48	1.41
8	4	901	ADP	C5-N7	-2.42	1.34	1.39
8	6	901	ADP	C5-N7	-2.41	1.34	1.39
8	3	901	ADP	C5-N7	-2.39	1.34	1.39
8	7	801	ADP	C5-N7	-2.33	1.34	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	801	ADP	C8-N7	2.29	1.36	1.31
8	3	901	ADP	C8-N7	2.26	1.36	1.31
8	6	901	ADP	C8-N7	2.20	1.35	1.31
8	4	901	ADP	C8-N7	2.19	1.35	1.31

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	4	901	ADP	C5-C4-N3	-6.68	117.52	126.72
8	6	901	ADP	C5-C4-N3	-6.53	117.72	126.72
8	3	901	ADP	C5-C4-N3	-6.13	118.28	126.72
8	7	801	ADP	C5-C4-N3	-5.77	118.77	126.72
8	4	901	ADP	N3-C4-N9	5.37	136.31	127.17
8	6	901	ADP	N3-C4-N9	5.21	136.02	127.17
8	3	901	ADP	N3-C4-N9	4.83	135.38	127.17
8	7	801	ADP	N3-C4-N9	4.52	134.85	127.17
8	6	901	ADP	C2-N3-C4	3.99	121.57	111.83
8	4	901	ADP	C2-N3-C4	3.98	121.55	111.83
8	3	901	ADP	C2-N3-C4	3.83	121.18	111.83
8	7	801	ADP	C2-N3-C4	3.68	120.81	111.83
8	7	801	ADP	C4-C5-N7	-3.43	106.66	110.58
8	3	901	ADP	C4-C5-N7	-3.41	106.68	110.58
8	6	901	ADP	C4-C5-N7	-3.30	106.81	110.58
8	4	901	ADP	C4-C5-N7	-3.29	106.82	110.58
8	6	901	ADP	N3-C2-N1	-3.29	123.61	128.58
8	7	801	ADP	N3-C2-N1	-3.23	123.69	128.58
8	3	901	ADP	N3-C2-N1	-3.21	123.72	128.58
8	4	901	ADP	N3-C2-N1	-3.16	123.80	128.58
8	6	901	ADP	C3'-C2'-C1'	2.54	106.27	101.46
8	7	801	ADP	C4-N9-C8	2.53	108.39	105.74
8	3	901	ADP	C5-N7-C8	2.50	107.38	103.45
8	4	901	ADP	C5-N7-C8	2.46	107.31	103.45
8	7	801	ADP	C5-N7-C8	2.44	107.28	103.45
8	6	901	ADP	C5-N7-C8	2.43	107.27	103.45
8	3	901	ADP	C4-N9-C8	2.38	108.23	105.74
8	4	901	ADP	C3'-C2'-C1'	2.36	105.93	101.46
8	6	901	ADP	C4-N9-C8	2.16	108.00	105.74
8	4	901	ADP	C4-N9-C8	2.14	107.99	105.74
8	7	801	ADP	O4'-C1'-N9	2.10	112.13	108.09
8	7	801	ADP	C6-C5-N7	2.07	136.07	132.09
8	3	901	ADP	C3'-C2'-C1'	2.02	105.29	101.46

There are no chirality outliers.

All (16) torsion outliers are listed below:

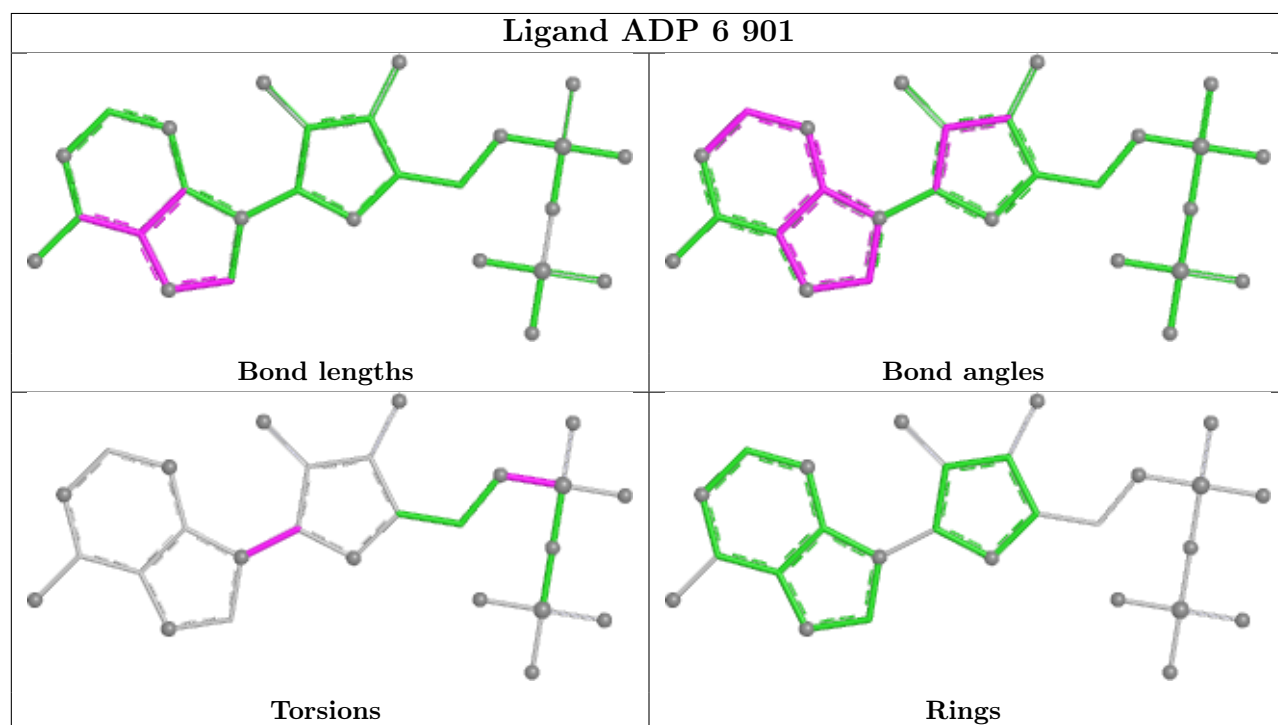
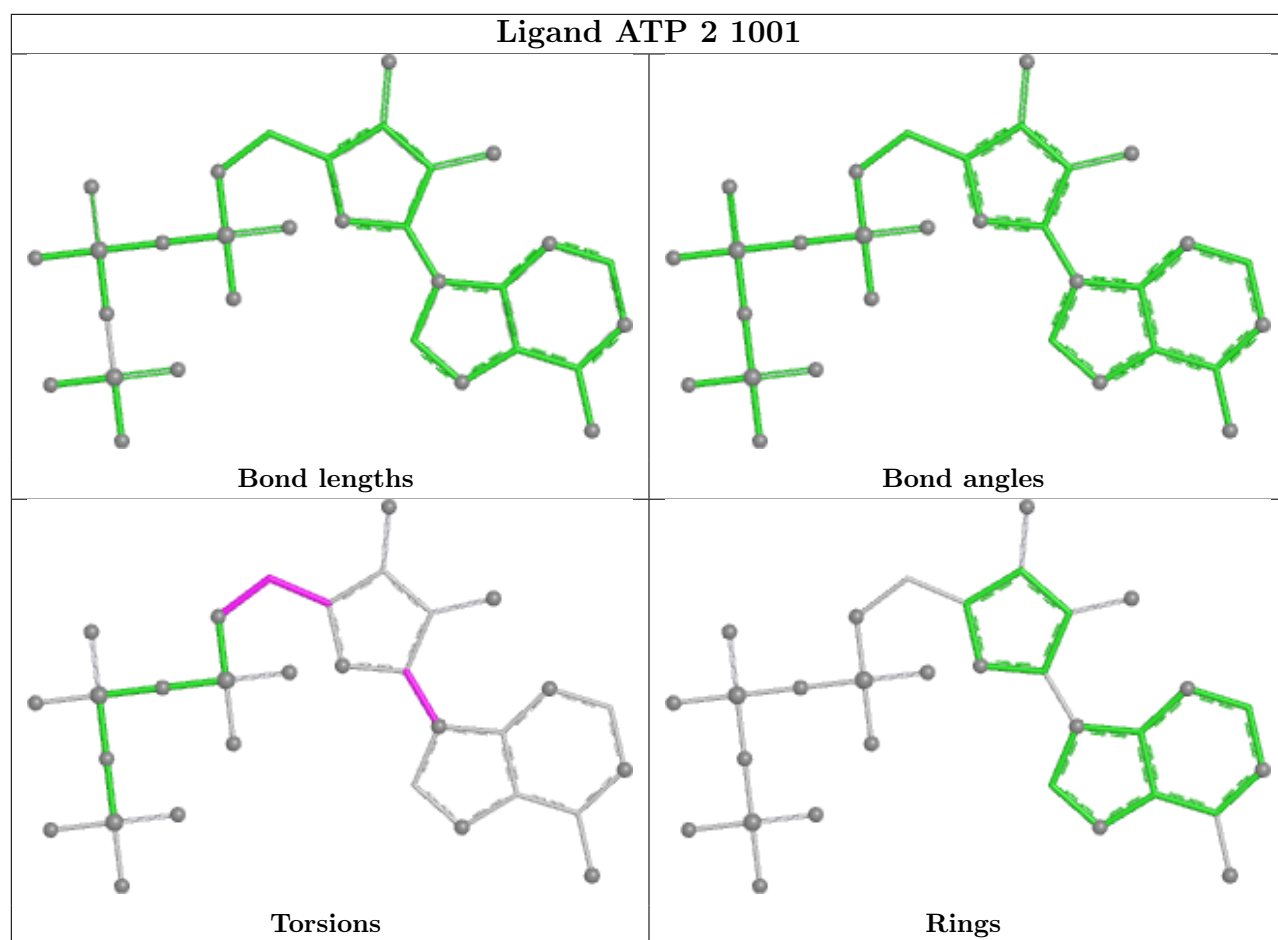
Mol	Chain	Res	Type	Atoms
7	2	1001	ATP	O4'-C1'-N9-C8
7	2	1001	ATP	O4'-C1'-N9-C4
8	4	901	ADP	C5'-O5'-PA-O1A
8	6	901	ADP	C5'-O5'-PA-O1A
8	7	801	ADP	C2'-C1'-N9-C4
8	3	901	ADP	O4'-C4'-C5'-O5'
8	3	901	ADP	C3'-C4'-C5'-O5'
8	7	801	ADP	C2'-C1'-N9-C8
8	4	901	ADP	C2'-C1'-N9-C8
8	6	901	ADP	C5'-O5'-PA-O3A
8	7	801	ADP	C5'-O5'-PA-O1A
7	2	1001	ATP	O4'-C4'-C5'-O5'
8	4	901	ADP	C2'-C1'-N9-C4
8	6	901	ADP	C2'-C1'-N9-C8
8	6	901	ADP	C2'-C1'-N9-C4
7	2	1001	ATP	C4'-C5'-O5'-PA

There are no ring outliers.

3 monomers are involved in 12 short contacts:

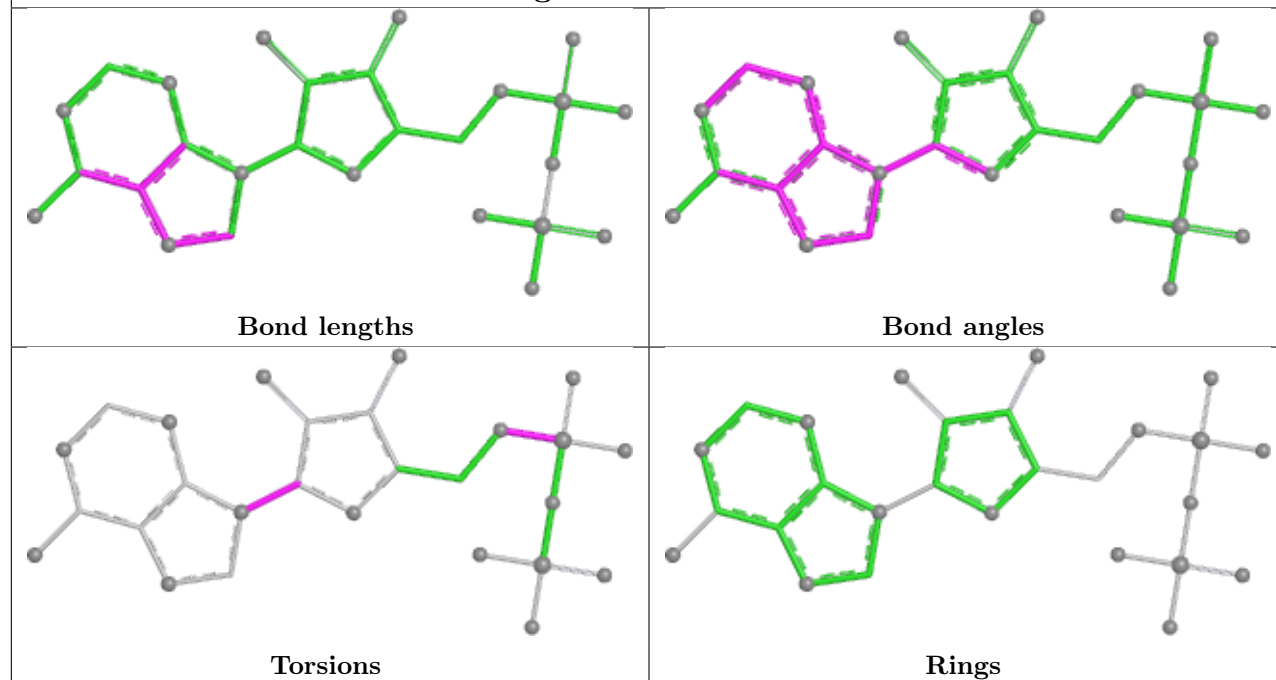
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	2	1001	ATP	9	0
8	6	901	ADP	1	0
8	7	801	ADP	2	0

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.

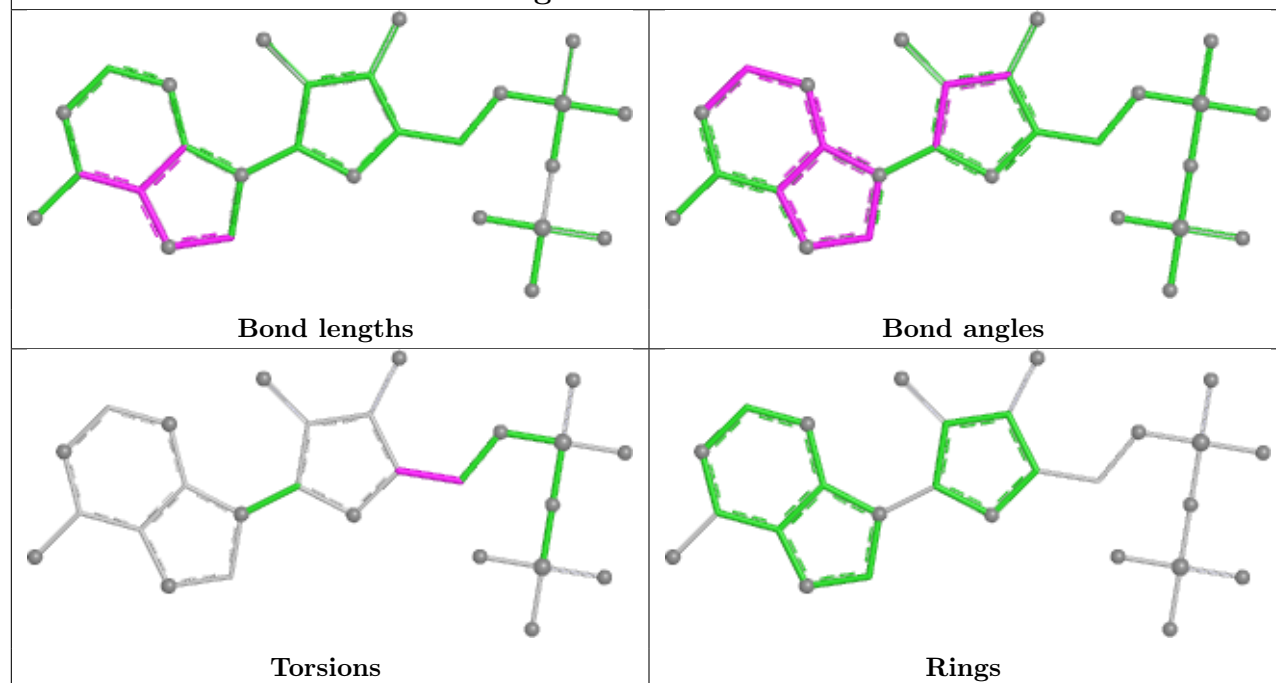


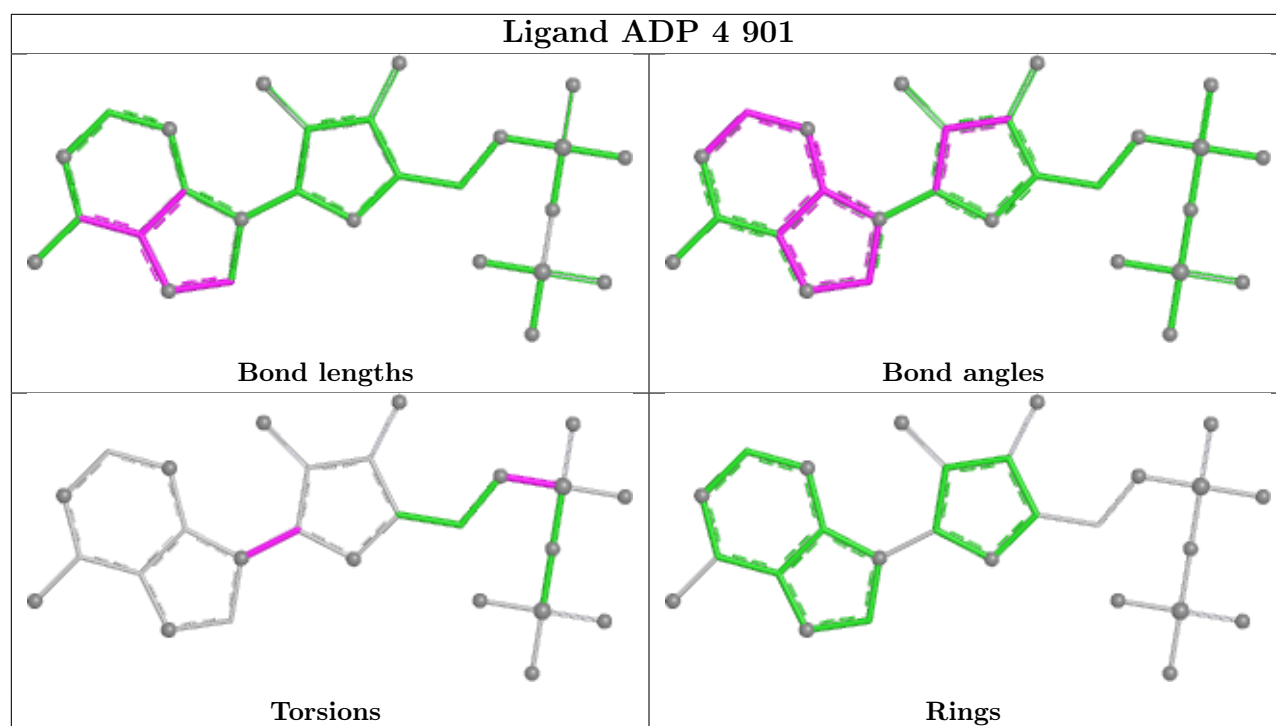


## Ligand ADP 7 801



## Ligand ADP 3 901





## 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.

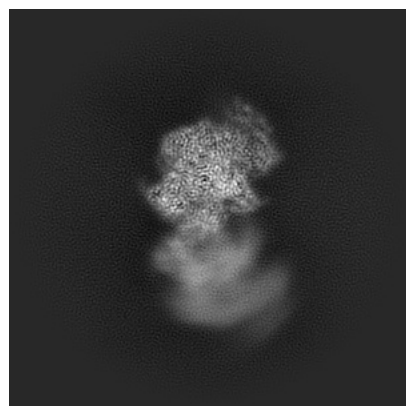
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63474. These allow visual inspection of the internal detail of the map and identification of artifacts.

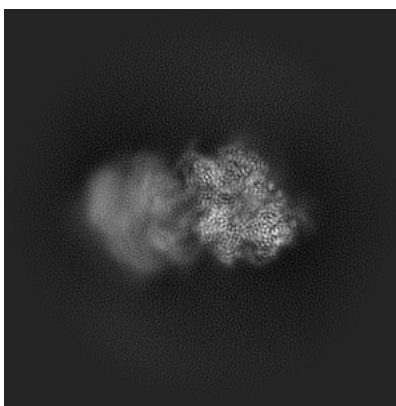
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

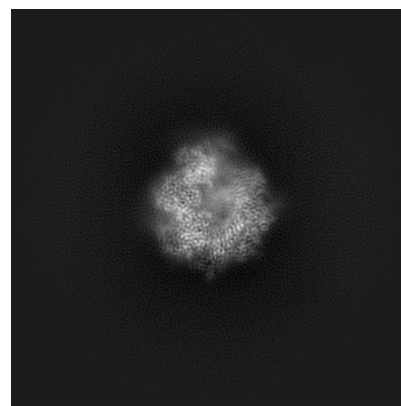
#### 6.1.1 Primary map



X

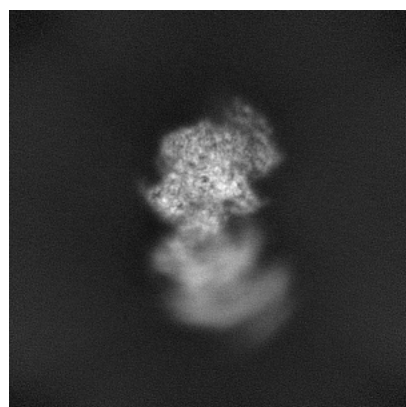


Y

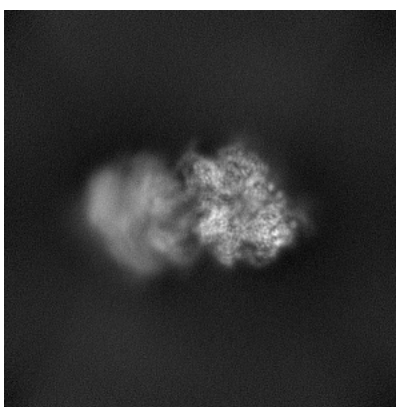


Z

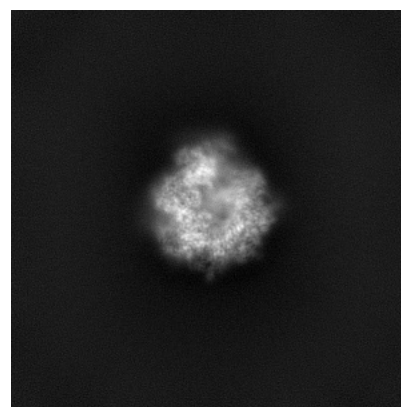
#### 6.1.2 Raw map



X



Y

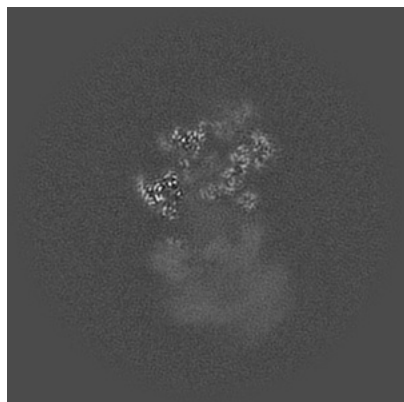


Z

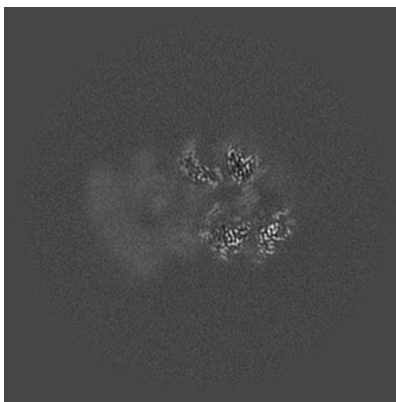
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

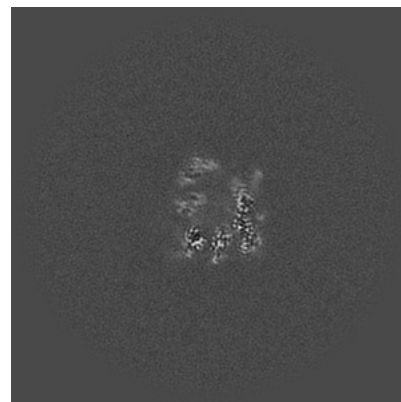
### 6.2.1 Primary map



X Index: 200

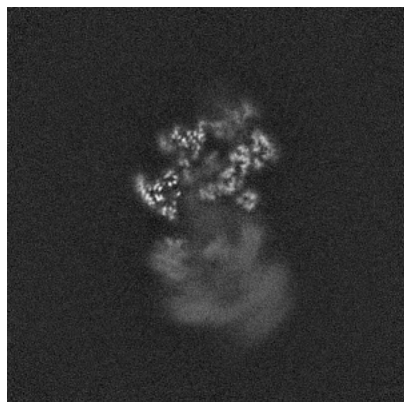


Y Index: 200

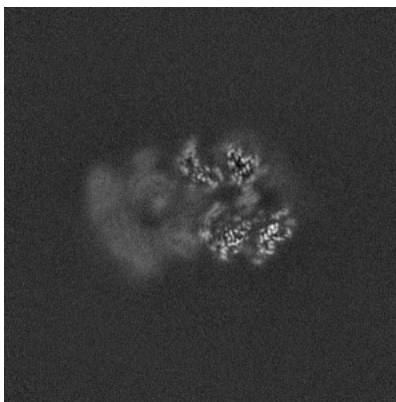


Z Index: 200

### 6.2.2 Raw map



X Index: 200



Y Index: 200

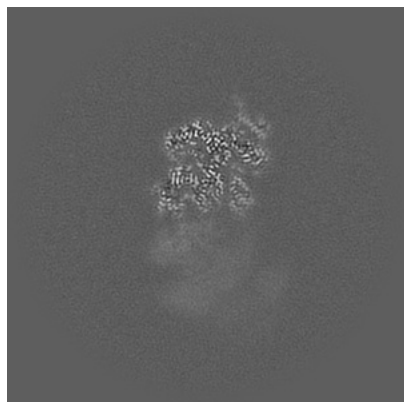


Z Index: 200

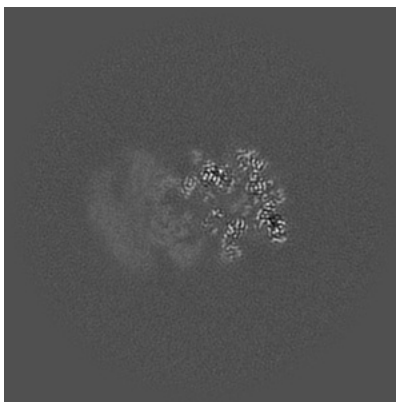
The images above show central slices of the map in three orthogonal directions.

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

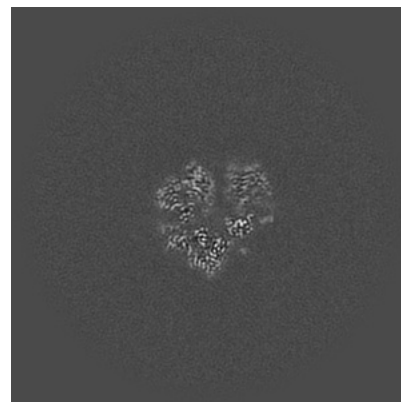
### 6.3.1 Primary map



X Index: 176

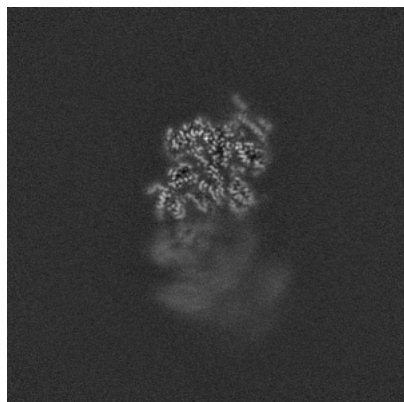


Y Index: 179

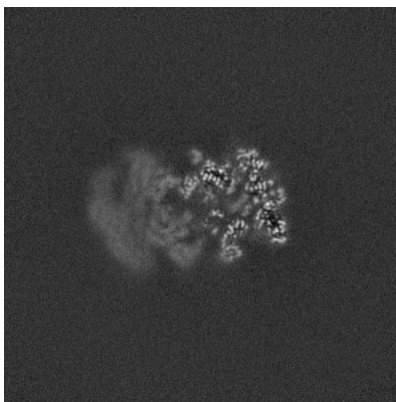


Z Index: 218

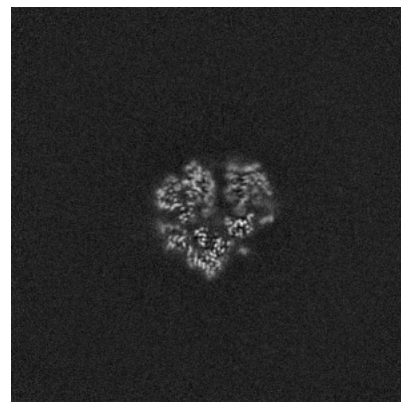
### 6.3.2 Raw map



X Index: 178



Y Index: 179



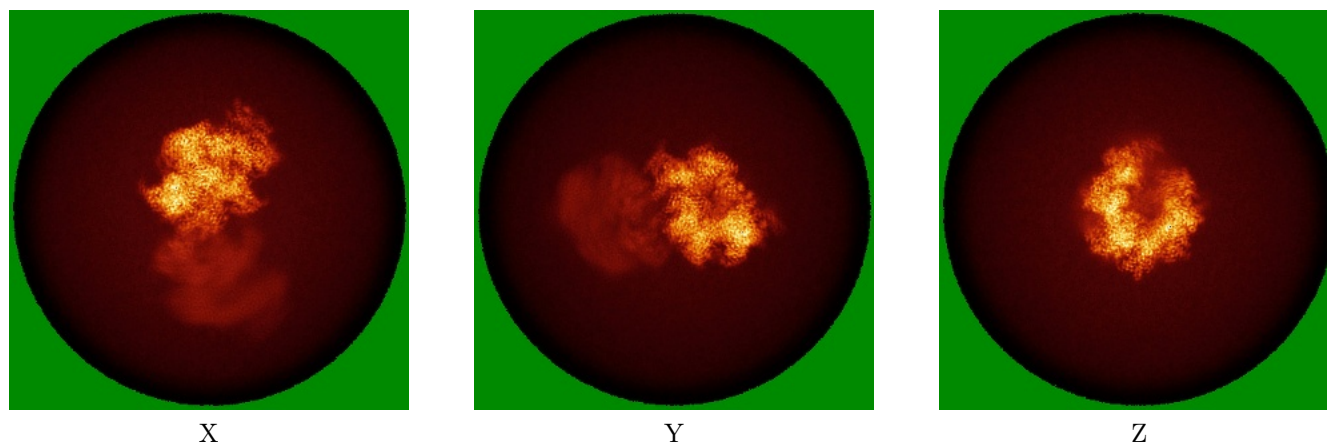
Z Index: 218

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

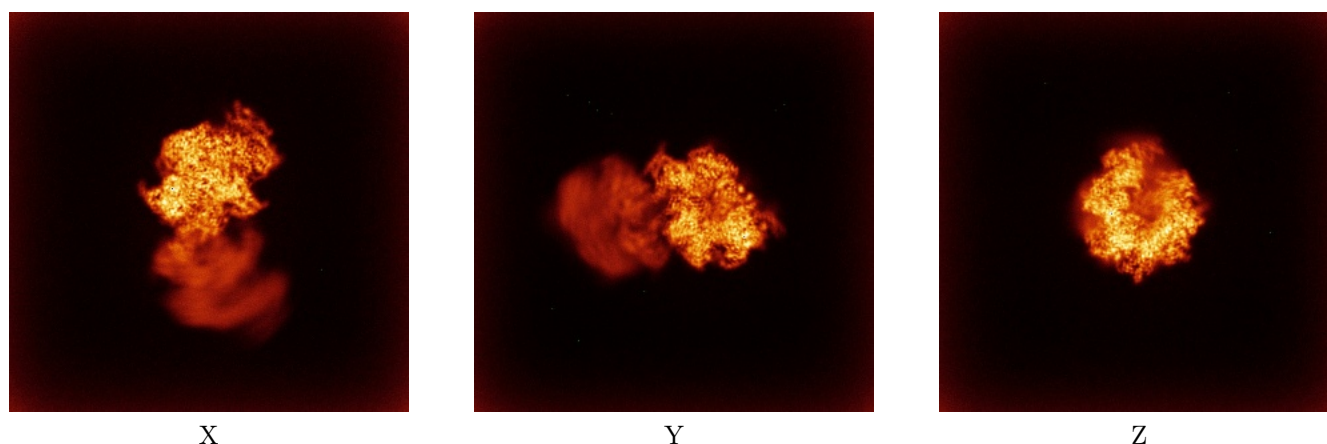


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 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](#)

This section was not generated.

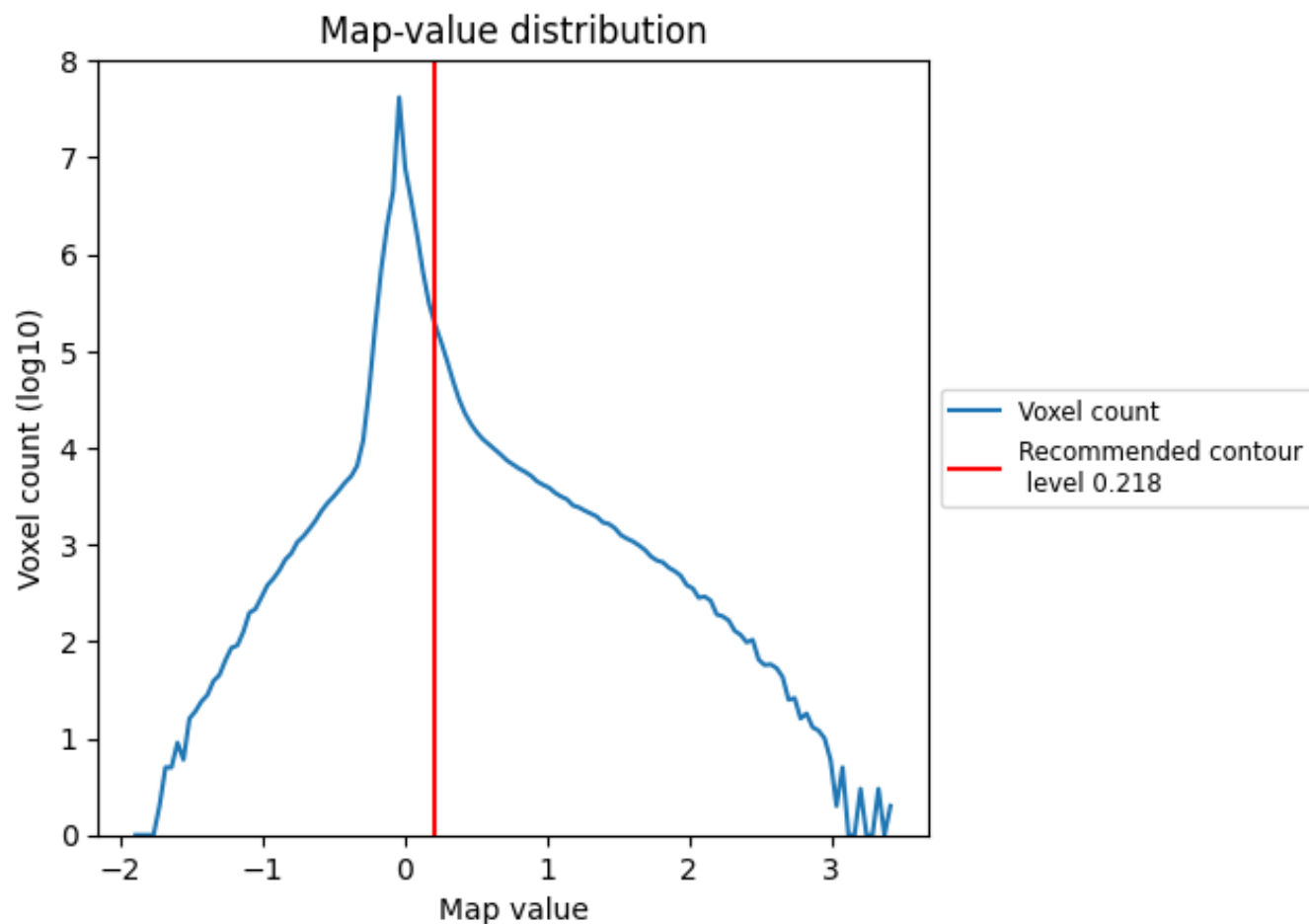
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

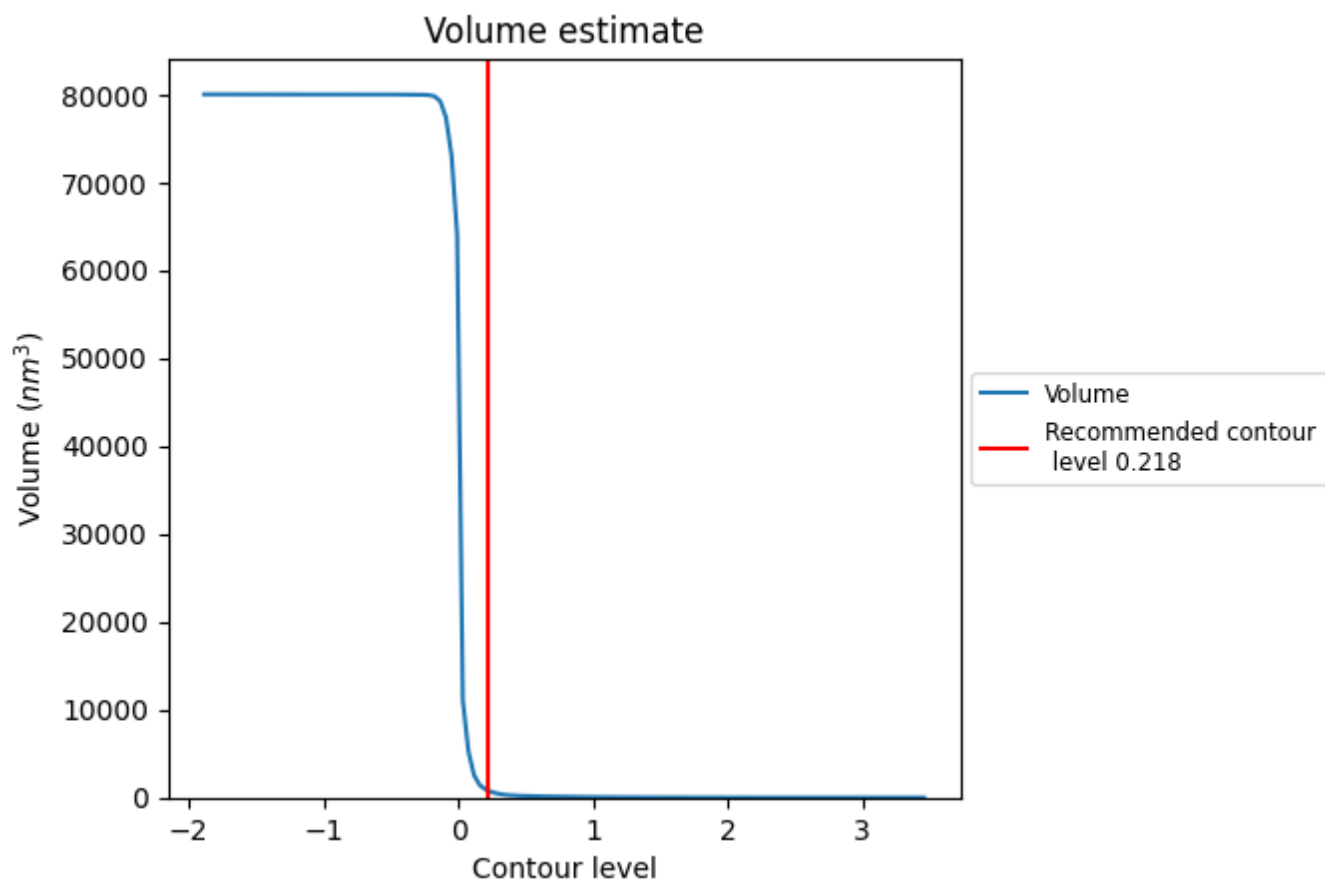
This section contains the results of statistical analysis of the map.

### 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](#)

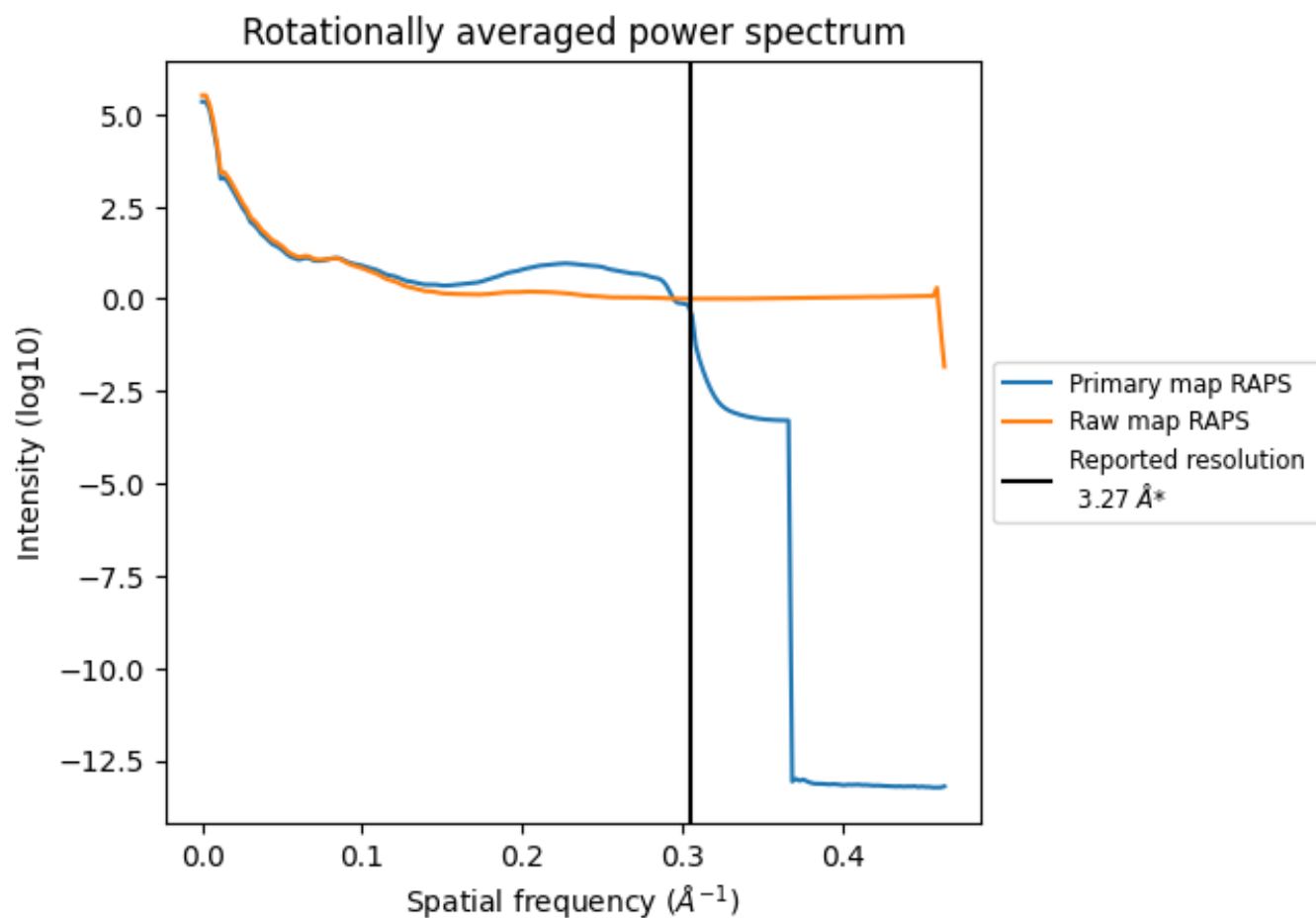


The volume at the recommended contour level is 814 nm<sup>3</sup>; this corresponds to an approximate mass of 735 kDa.

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 ⓘ

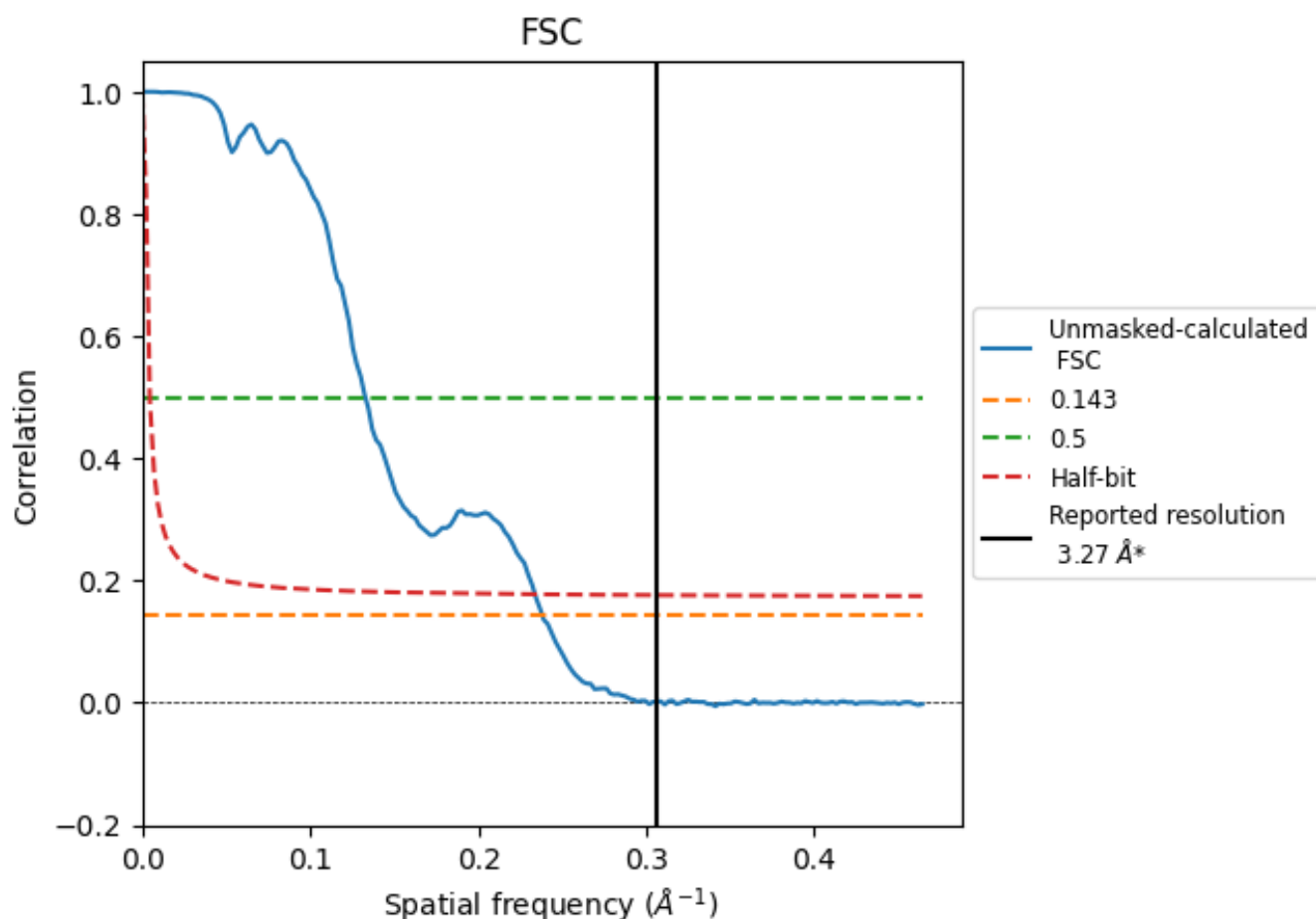


\*Reported resolution corresponds to spatial frequency of 0.306 Å<sup>-1</sup>

## 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 0.306 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

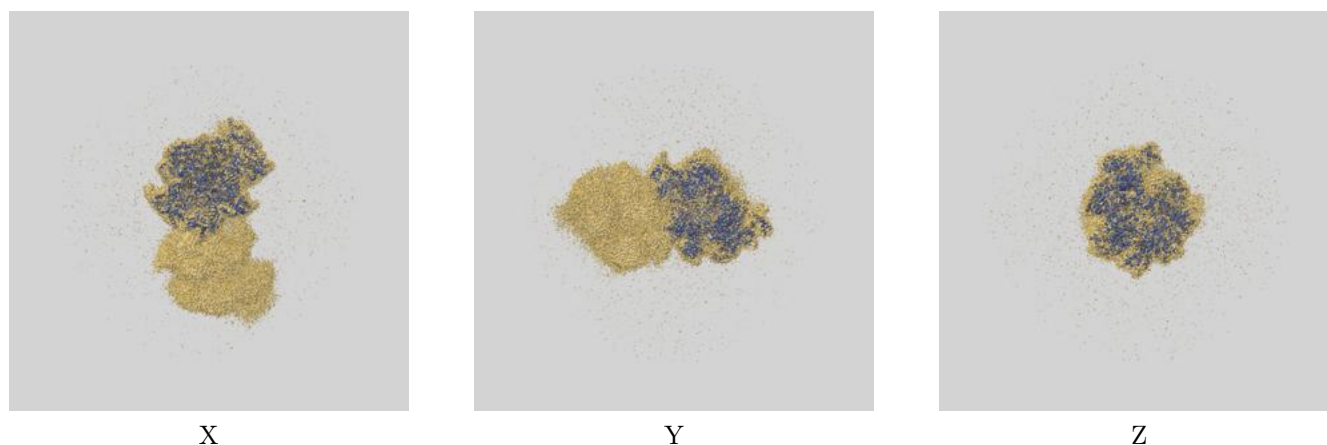
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	7.54	4.28

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.20 differs from the reported value 3.27 by more than 10 %

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

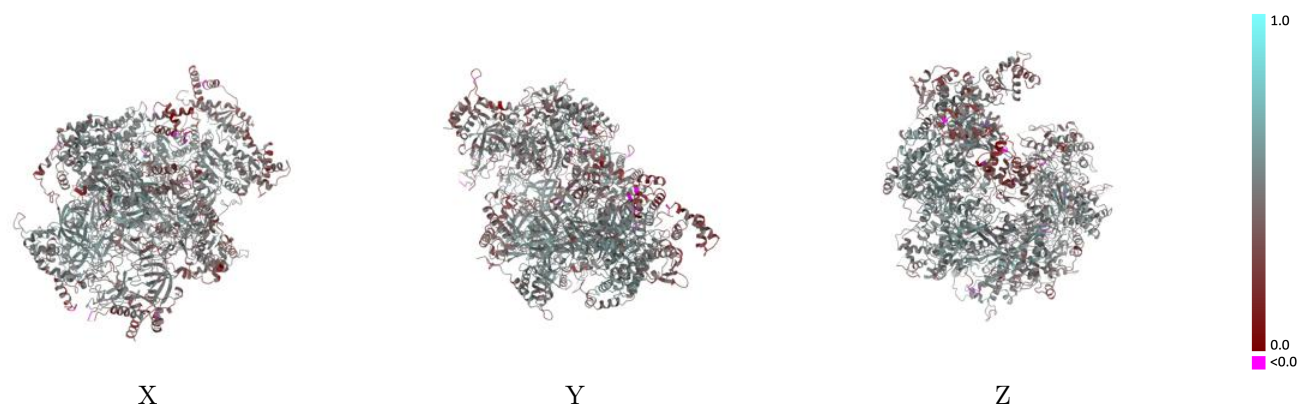
This section contains information regarding the fit between EMDB map EMD-63474 and PDB model 9LXD. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.218 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](#)

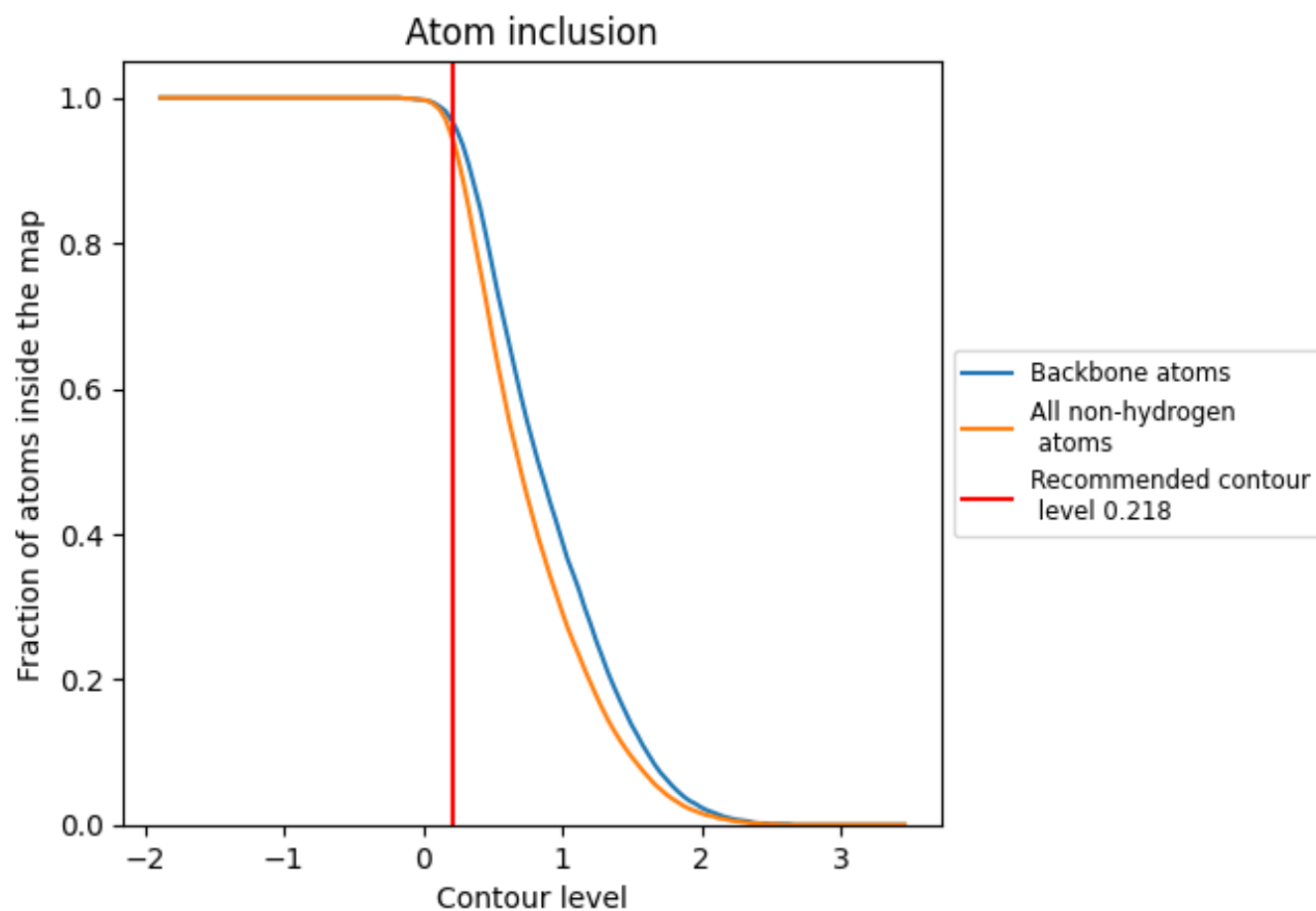


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 96% of all backbone atoms, 94% 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 (0.218) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9390	<div><div></div></div> 0.4620
2	<div><div></div></div> 0.9450	<div><div></div></div> 0.4480
3	<div><div></div></div> 0.9320	<div><div></div></div> 0.4750
4	<div><div></div></div> 0.9270	<div><div></div></div> 0.4770
5	<div><div></div></div> 0.9420	<div><div></div></div> 0.4130
6	<div><div></div></div> 0.9540	<div><div></div></div> 0.4830
7	<div><div></div></div> 0.9450	<div><div></div></div> 0.4790
B	<div><div></div></div> 0.8680	<div><div></div></div> 0.3870

1.0

0.0

<0.0