Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 10:03 pm GMT

PDB ID	:	6EYC
EMDB ID	:	EMD-6338
Title	:	Re-refinement of the MCM2-7 double hexamer using ISOLDE
Authors	:	Croll, T.I.
Deposited on	:	2017-11-11
Resolution	:	3.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

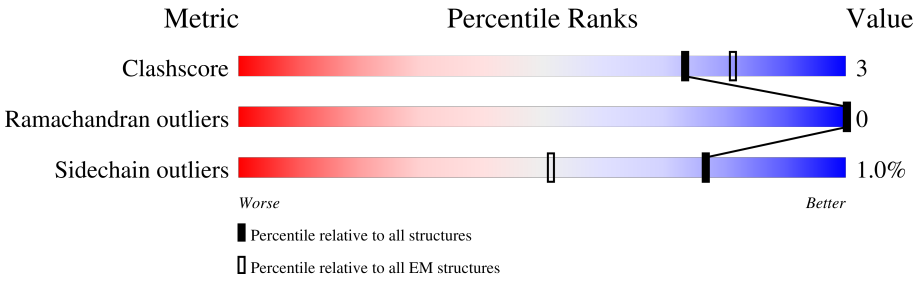
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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 >=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 <=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	868	20% 61% 8% 31%
2	3	971	13% 54% 8% 38%
3	4	933	13% 63% 6% 31%
4	5	775	20% 75% 7% 18%
5	6	1017	18% 57% · 39%
6	7	845	13% 73% 8% 18%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 60365 atoms, of which 30301 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
			Total	C	H	N	O	S		
1	2	603	9619	3007	4849	850	894	19	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	3	605	9561	2990	4816	846	896	13	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	4	641	10296	3210	5186	883	989	28	0	0

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	5	633	9990	3116	5024	855	971	24	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	6	616	9794	3072	4920	853	924	25	0	0

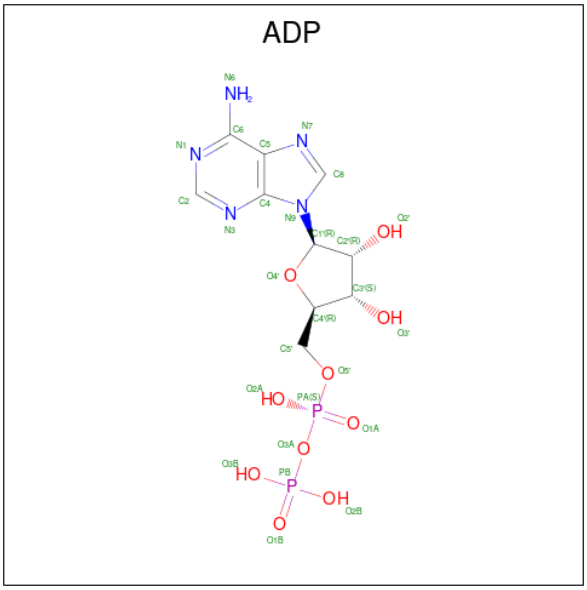
- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	7	689	10938	3419	5506	940	1042	31	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
7	2	1	Total Zn 1 1	0
7	4	1	Total Zn 1 1	0
7	5	1	Total Zn 1 1	0
7	6	1	Total Zn 1 1	0
7	7	1	Total Zn 1 1	0

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



Mol	Chain	Residues	Atoms	AltConf
8	2	1	Total C N O P 27 10 5 10 2	0
8	3	1	Total C N O P 54 20 10 20 4	0
8	3	1	Total C N O P 54 20 10 20 4	0
8	4	1	Total C N O P 27 10 5 10 2	0
8	5	1	Total C N O P 27 10 5 10 2	0

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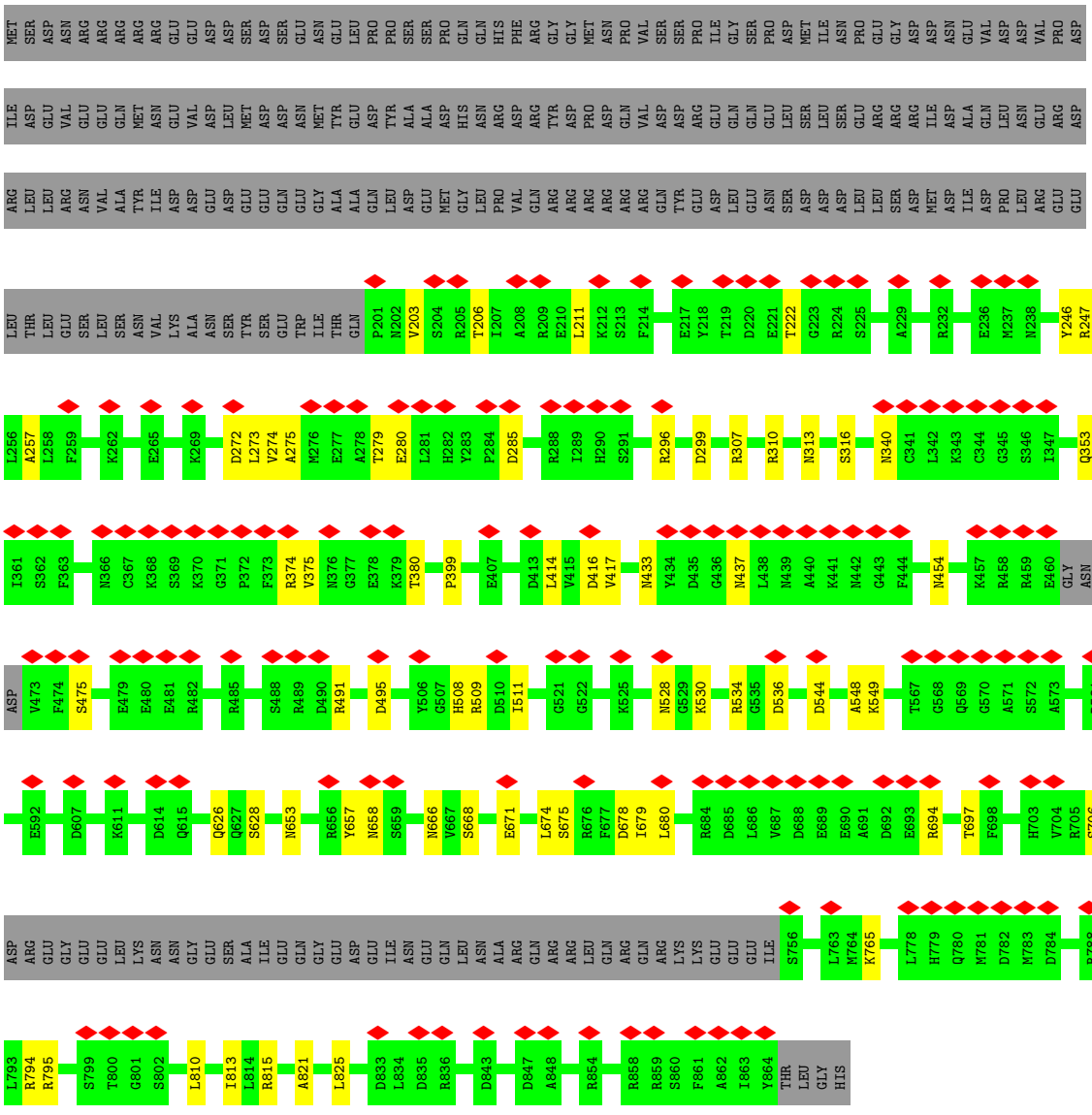
Mol	Chain	Residues	Atoms					AltConf
8	6	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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.

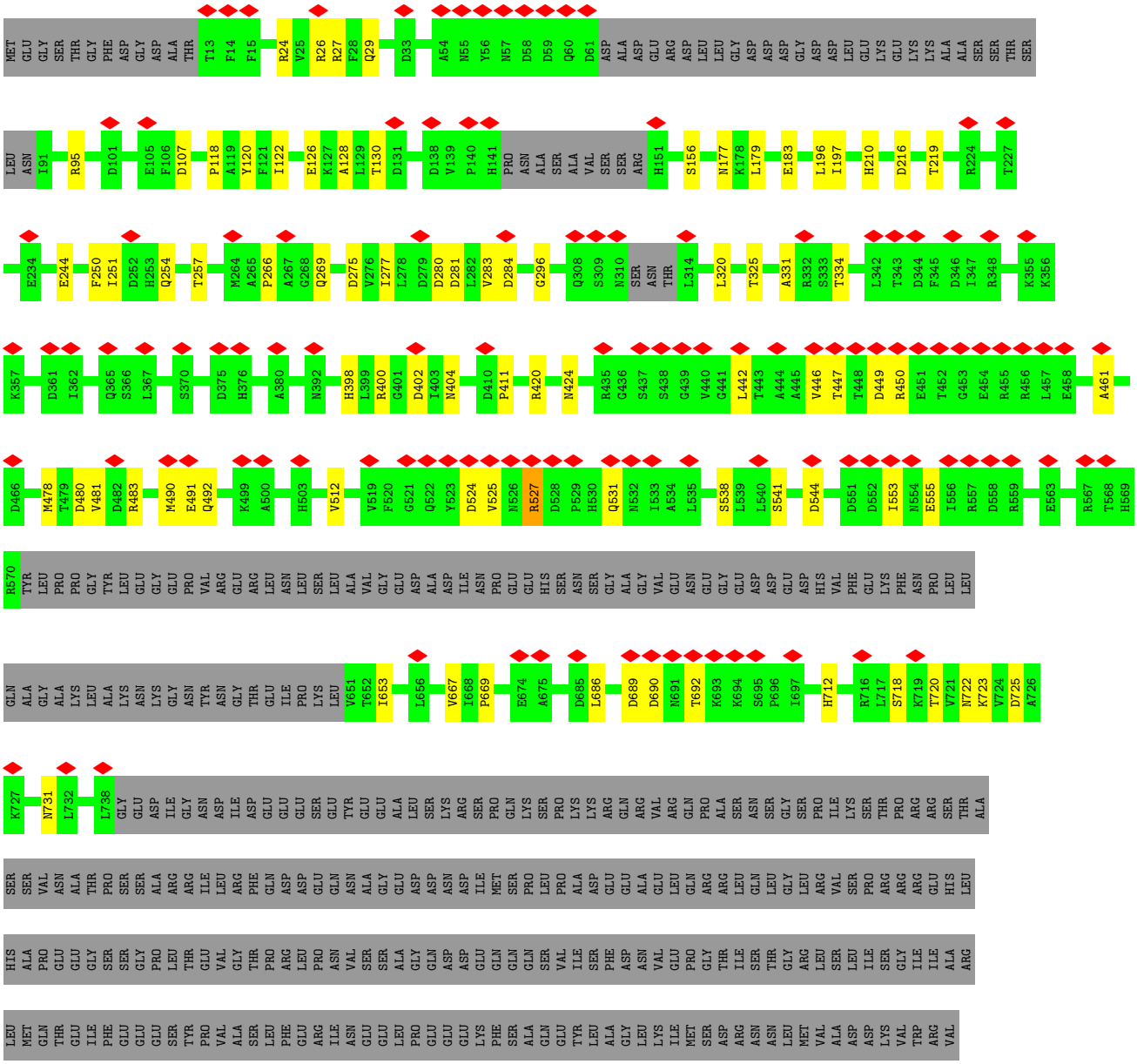
• Molecule 1: DNA replication licensing factor MCM2

Chain 2:



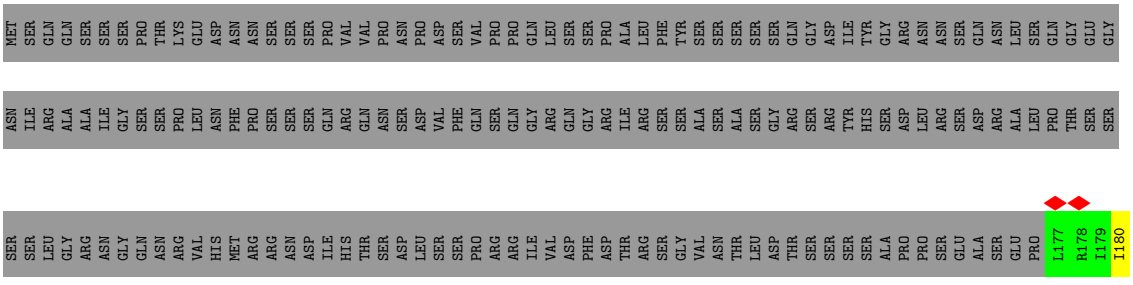
• Molecule 2: DNA replication licensing factor MCM3

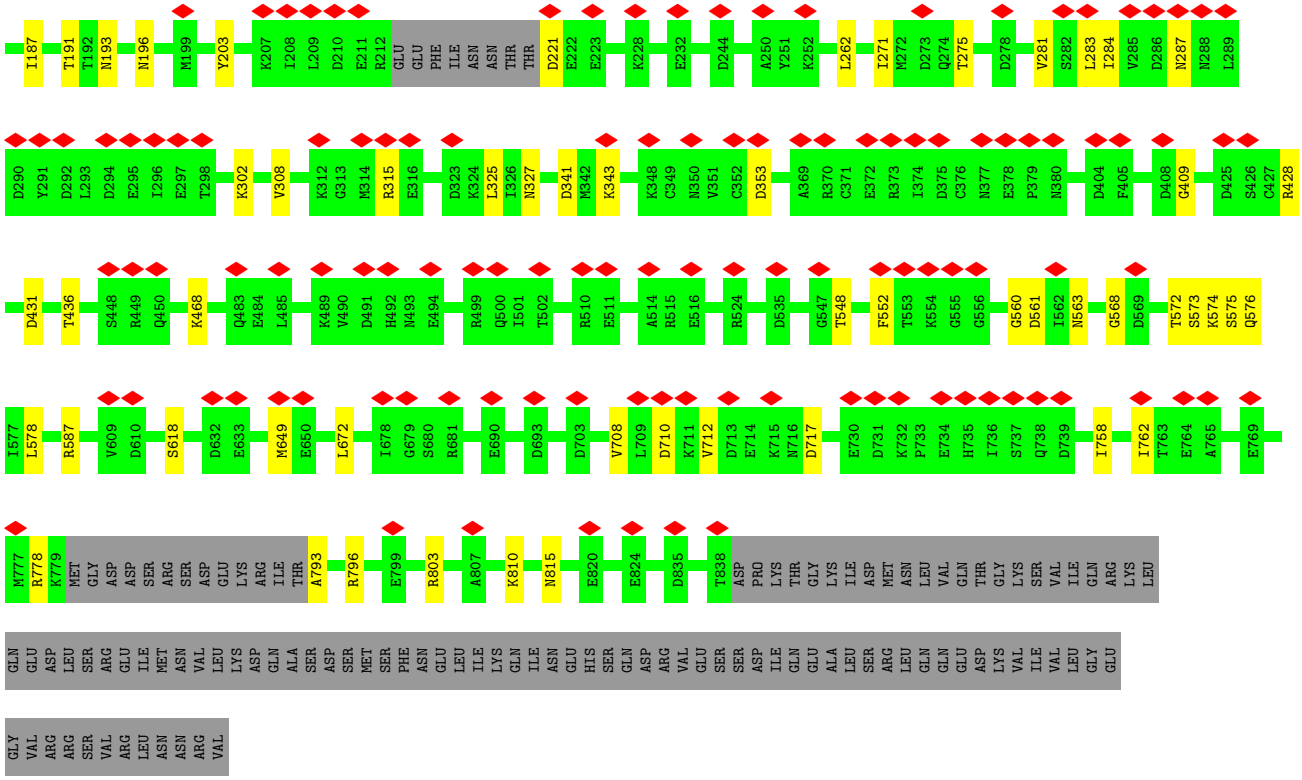
Chain 3:



• Molecule 3: DNA replication licensing factor MCM4

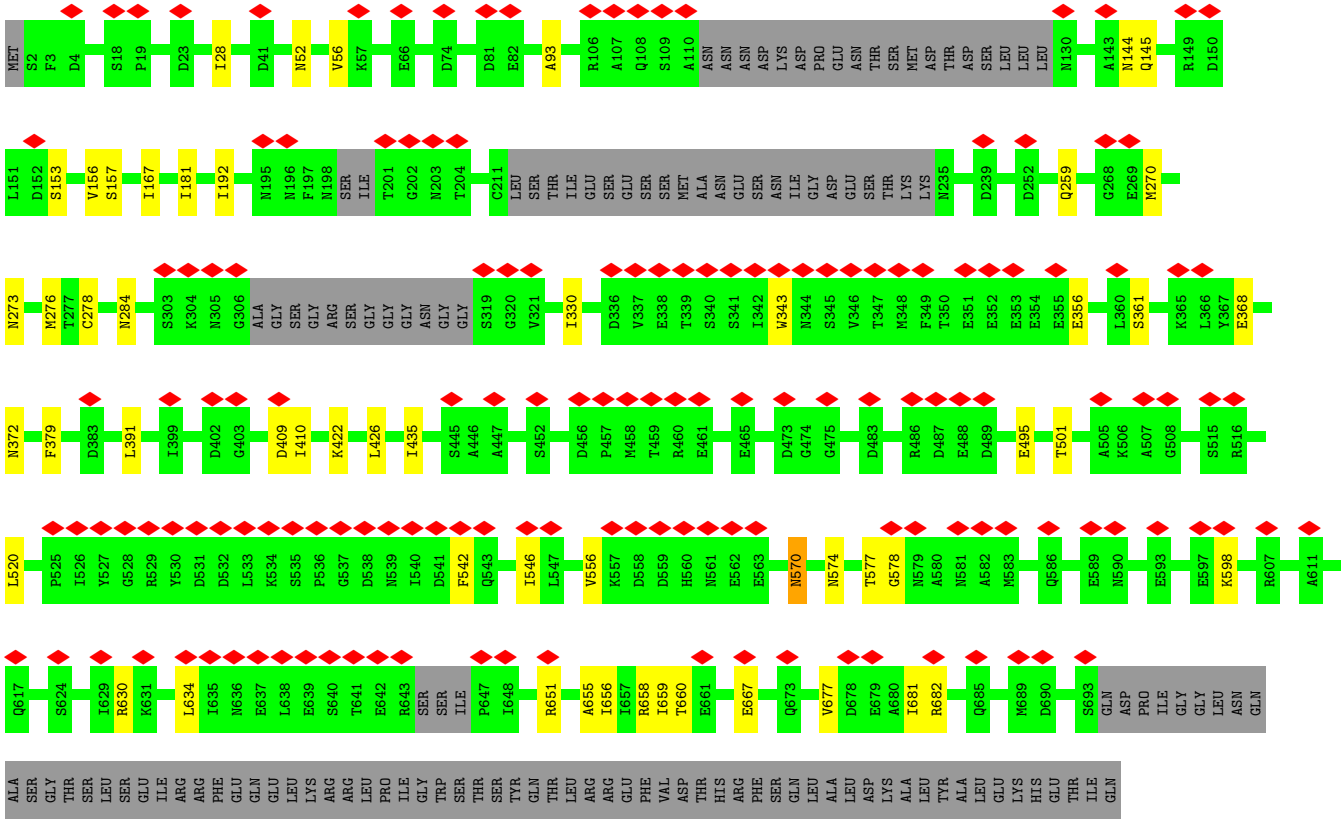
Chain 4:





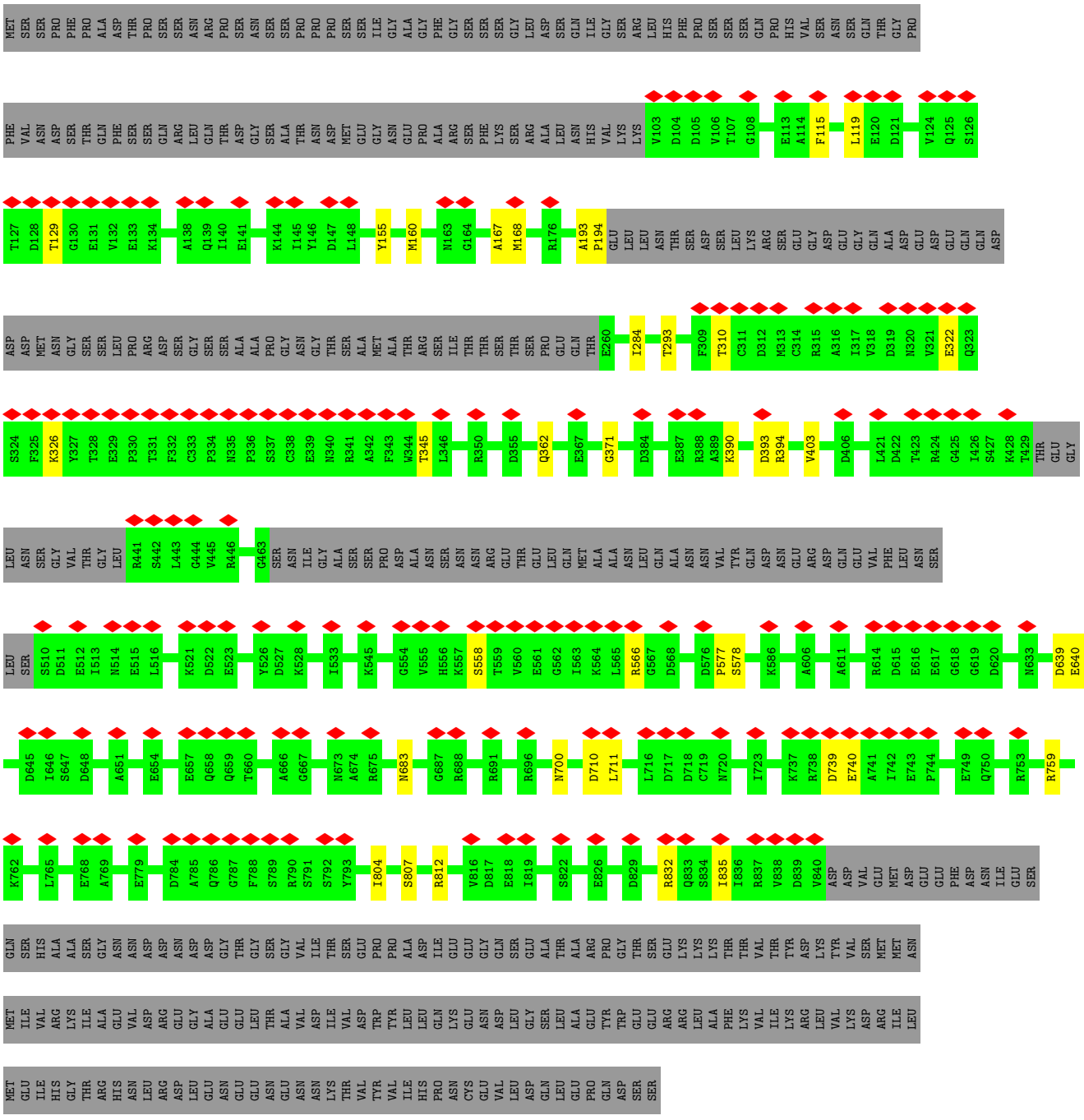
• Molecule 4: Minichromosome maintenance protein 5

Chain 5:



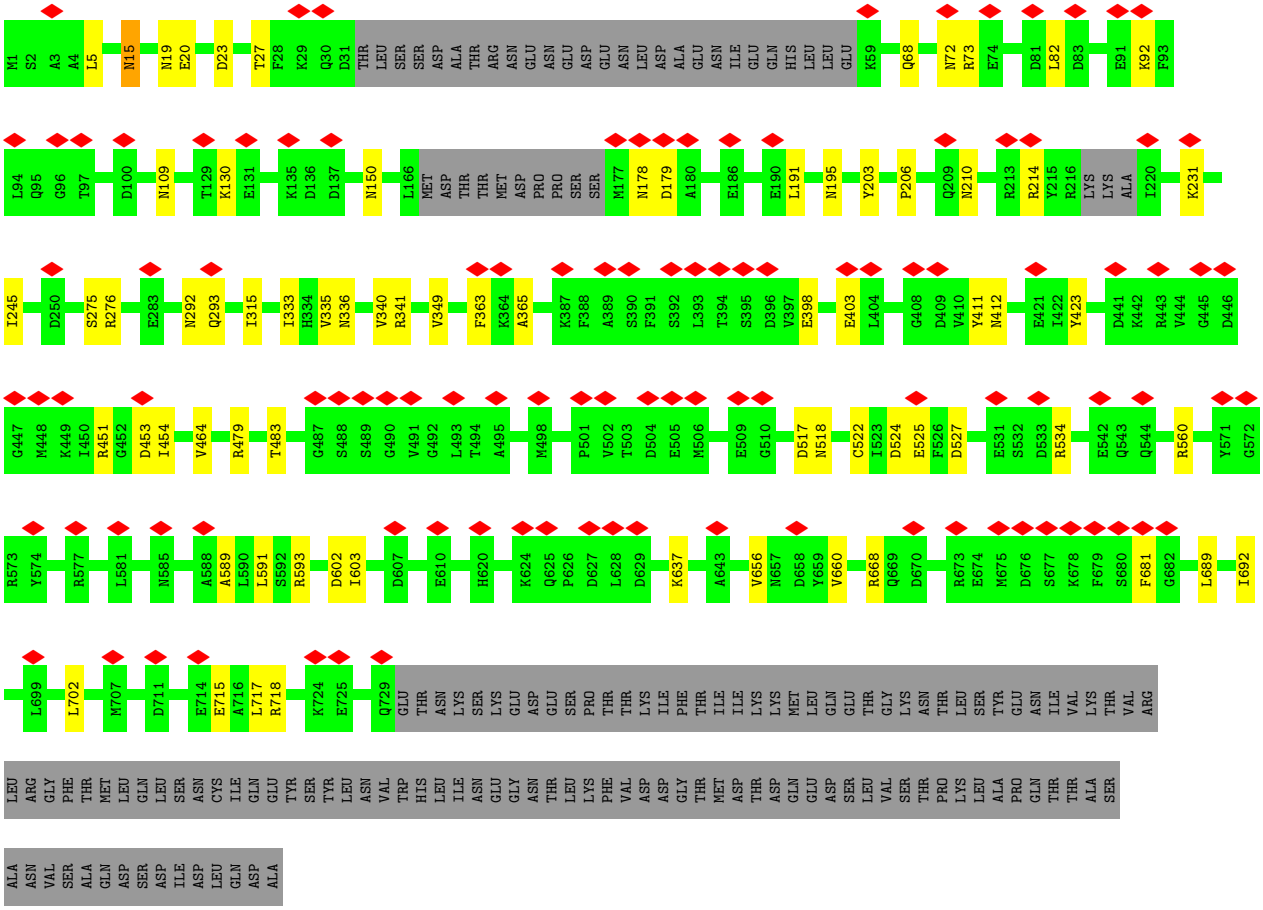
• Molecule 5: DNA replication licensing factor MCM6

Chain 6:



• Molecule 6: DNA replication licensing factor MCM7

Chain 7:


M1 S2 A3 A4 L5 N15 N19 E20 D23 T27 F28 K29 Q30 D31 THR LEU SER SER ASP ALA THR ARG ASN GLU ASN GLU ASP GLU ASN LEU ASP ALA GLU ASN ILE GLU GLN HIS LEU LEU GLU K59 Q68 N72 R73 E74 D81 L82 D83 E91 K92 F93
L94 Q95 G96 T97 D100 N109 T129 K130 E131 K135 D136 D137 N150 L166 MET ASP THR THR MET ASP PRO PRO SER SER M177 N178 D179 A180 E186 E190 L191 N195 Y203 P206 Q209 N210 R213 R214 Y215 R216 LYS LYS ALA I220 K231
I245 D250 S275 R276 E283 N292 Q293 I315 I333 H334 V335 N336 V340 R341 V349 F363 K364 A365 K387 F388 A389 S390 F391 S392 L393 T394 S395 D396 V397 E398 E403 L404 G408 D409 V410 Y411 N412 E421 I422 Y423 D441 K442 R443 V444 G445 D446
G447 M448 K449 I450 R451 G452 D453 I454 V464 R479 T483 G487 S488 S489 G490 V491 G492 L493 T494 A495 M498 P501 V502 T503 D504 E505 M506 E509 G510 D517 N518 C522 I523 D524 E525 F526 D527 E531 S532 D533 R534 E542 Q543 Q544 R560 Y571 G572
R573 Y574 R577 L581 N585 A588 A589 L590 L591 S592 R593 D602 I603 D607 E610 H620 K624 Q625 P626 D627 L628 D629 K637 A643 V656 N657 D658 Y659 V660 R668 Q669 D670 R673 E674 M675 D676 S677 K678 F679 S680 F681 G682 L689 I692
L699 L702 M707 D711 E714 E715 A716 L717 R718 K724 E725 Q729 GLU THR ASN LYS SER LYS GLU ASP GLU SER PRO THR THR LYS ILE PHE THR ILE ILE LYS LYS MET LEU GLN GLU ASP SER LEU VAL SER THR PRO LYS LEU ALA PRO GLN THR THR ALA SER
LEU ARG GLY PHE THR MET LEU GLN LEU SER ASN CYS ILE GLN GLU TYR SER TYR LEU ASN VAL TRP HIS LEU ILE ASN GLU GLY ASN THR LEU LYS PHE VAL ASP ASP GLY THR MET ASP THR ASP GLN GLU ASP SER LEU VAL SER THR PRO LYS LEU ALA PRO GLN THR THR ALA SER
ALA ASN VAL SER ALA GLN ASP SER ASP ILE ASP LEU GLN ASP ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	85365	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	22	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	32.028	Depositor
Minimum map value	-16.136	Depositor
Average map value	-0.058	Depositor
Map value standard deviation	0.697	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	396.00003, 396.00003, 396.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.34	0/4852	0.67	1/6551 (0.0%)
2	3	0.37	0/4827	0.67	0/6545
3	4	0.35	0/5185	0.69	3/7009 (0.0%)
4	5	0.34	0/5037	0.65	0/6809
5	6	0.34	0/4954	0.67	0/6683
6	7	0.36	0/5514	0.65	0/7450
All	All	0.35	0/30369	0.67	4/41047 (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
3	4	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	416	ASP	CB-CG-OD1	6.67	124.30	118.30
3	4	468	LYS	CB-CA-C	6.55	123.49	110.40
3	4	353	ASP	CB-CG-OD1	5.96	123.66	118.30
3	4	573	SER	CB-CA-C	5.55	120.65	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	552	PHE	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	2	4770	4849	4834	35	0
2	3	4745	4816	4793	50	0
3	4	5110	5186	5171	33	0
4	5	4966	5024	5011	34	0
5	6	4874	4920	4909	21	0
6	7	5432	5506	5496	44	0
7	2	1	0	0	0	0
7	4	1	0	0	0	0
7	5	1	0	0	0	0
7	6	1	0	0	0	0
7	7	1	0	0	0	0
8	2	27	0	12	1	0
8	3	54	0	24	4	0
8	4	27	0	12	4	0
8	5	27	0	12	1	0
8	6	27	0	12	2	0
All	All	30064	30301	30286	201	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 3.

All (201) 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)
1:2:353:GLN:NE2	1:2:357:GLU:O	2.15	0.79
1:2:588:GLU:OE2	4:5:273:ASN:ND2	2.16	0.78
4:5:409:ASP:O	4:5:658:ARG:NH1	2.18	0.77
2:3:404:ASN:ND2	2:3:490:MET:SD	2.57	0.77
2:3:284:ASP:OD2	6:7:231:LYS:NZ	2.18	0.76
3:4:315:ARG:O	6:7:341:ARG:NH2	2.21	0.74
3:4:758:ILE:O	3:4:810:LYS:NZ	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4:1002:ADP:O3B	6:7:593:ARG:NH2	2.21	0.73
2:3:244:GLU:OE1	6:7:109:ASN:ND2	2.21	0.73
1:2:536:ASP:O	1:2:815:ARG:NH2	2.21	0.73
1:2:657:TYR:O	1:2:666:ASN:ND2	2.22	0.72
1:2:247:ARG:NH1	1:2:299:ASP:O	2.23	0.72
1:2:313:ASN:O	1:2:316:SER:OG	2.08	0.72
2:3:420:ARG:NH1	4:5:495:GLU:OE2	2.21	0.72
6:7:527:ASP:OD1	6:7:534:ARG:NH2	2.23	0.71
1:2:626:GLN:NE2	1:2:628:SER:O	2.23	0.71
3:4:409:GLY:N	6:7:517:ASP:OD2	2.24	0.70
5:6:759:ARG:O	5:6:812:ARG:NH1	2.24	0.70
3:4:283:LEU:O	3:4:287:ASN:ND2	2.25	0.70
4:5:356:GLU:OE2	4:5:598:LYS:NZ	2.23	0.70
6:7:403:GLU:OE2	6:7:637:LYS:NZ	2.22	0.69
3:4:778:ARG:NH1	3:4:793:ALA:O	2.26	0.69
2:3:266:PRO:O	2:3:269:GLN:NE2	2.26	0.68
2:3:411:PRO:O	4:5:651:ARG:NH1	2.26	0.68
2:3:718:SER:OG	2:3:720:THR:O	2.06	0.68
4:5:368:GLU:O	4:5:372:ASN:ND2	2.26	0.68
6:7:203:TYR:OH	6:7:336:ASN:O	2.08	0.67
2:3:478:MET:O	2:3:483:ARG:NH2	2.27	0.67
6:7:479:ARG:NH1	6:7:517:ASP:OD1	2.29	0.66
1:2:706:SER:O	5:6:558:SER:OG	2.06	0.65
1:2:694:ARG:O	1:2:697:THR:OG1	2.10	0.64
2:3:404:ASN:OD1	2:3:512:VAL:N	2.30	0.63
8:3:2001:ADP:O1A	4:5:651:ARG:NH1	2.30	0.63
2:3:420:ARG:O	2:3:424:ASN:ND2	2.32	0.63
3:4:191:THR:HG23	3:4:275:THR:HG22	1.80	0.62
3:4:572:THR:N	8:4:1002:ADP:O2A	2.33	0.62
1:2:307:ARG:O	1:2:310:ARG:NH1	2.32	0.61
3:4:561:ASP:OD1	3:4:803:ARG:NH1	2.32	0.61
2:3:712:HIS:ND1	2:3:725:ASP:OD1	2.33	0.61
6:7:483:THR:OG1	6:7:522:CYS:O	2.14	0.60
2:3:197:ILE:CD1	2:3:251:ILE:HD12	2.32	0.59
8:3:2001:ADP:O3B	4:5:651:ARG:NH1	2.33	0.59
4:5:167:ILE:HD11	4:5:259:GLN:CG	2.32	0.59
3:4:327:ASN:HB3	3:4:436:THR:HG22	1.83	0.59
2:3:420:ARG:NH2	4:5:501:THR:OG1	2.35	0.59
3:4:618:SER:OG	5:6:371:GLY:O	2.10	0.59
2:3:24:ARG:NH1	2:3:120:TYR:O	2.36	0.58
3:4:563:ASN:ND2	3:4:649:MET:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:431:ASP:OD1	3:4:587:ARG:NH2	2.36	0.58
1:2:495:ASP:OD1	1:2:509:ARG:NH1	2.35	0.58
2:3:27:ARG:NE	2:3:107:ASP:OD2	2.37	0.57
4:5:361:SER:OG	4:5:667:GLU:O	2.22	0.56
1:2:534:ARG:O	1:2:815:ARG:NE	2.33	0.56
5:6:804:ILE:O	5:6:807:SER:OG	2.10	0.55
2:3:449:ASP:OD1	2:3:450:ARG:N	2.39	0.55
6:7:715:GLU:OE2	6:7:718:ARG:NH1	2.40	0.55
3:4:575:SER:OG	8:4:1002:ADP:O1A	2.15	0.54
8:6:1102:ADP:H2'	8:6:1102:ADP:N3	2.22	0.54
6:7:451:ARG:NH2	6:7:453:ASP:O	2.40	0.54
2:3:254:GLN:OE1	2:3:283:VAL:HG13	2.08	0.54
1:2:246:TYR:CE1	1:2:257:ALA:HB1	2.43	0.54
3:4:308:VAL:HG21	3:4:325:LEU:CD1	2.38	0.54
2:3:689:ASP:O	2:3:692:THR:OG1	2.15	0.53
2:3:527:ARG:NH2	2:3:531:GLN:OE1	2.40	0.53
3:4:712:VAL:HG12	6:7:668:ARG:NH2	2.23	0.53
6:7:68:GLN:O	6:7:72:ASN:N	2.41	0.53
1:2:548:ALA:HA	8:2:902:ADP:H5'1	1.91	0.53
2:3:555:GLU:N	2:3:555:GLU:OE1	2.42	0.53
3:4:308:VAL:HG11	3:4:325:LEU:HD12	1.89	0.53
4:5:278:CYS:HB3	4:5:330:ILE:HD12	1.91	0.53
6:7:245:ILE:HD11	6:7:349:VAL:HG21	1.90	0.53
2:3:553:ILE:HB	4:5:630:ARG:HE	1.74	0.53
1:2:211:LEU:HD12	1:2:274:VAL:HG11	1.90	0.52
4:5:677:VAL:O	4:5:681:ILE:HD12	2.08	0.52
5:6:193:ALA:HB1	5:6:194:PRO:HD2	1.90	0.52
1:2:544:ASP:O	1:2:549:LYS:NZ	2.43	0.52
5:6:393:ASP:OD1	5:6:394:ARG:N	2.43	0.52
6:7:398:GLU:OE1	6:7:398:GLU:N	2.43	0.52
1:2:414:LEU:O	1:2:417:VAL:HG22	2.10	0.51
1:2:203:VAL:O	1:2:206:THR:OG1	2.21	0.51
6:7:20:GLU:OE1	6:7:92:LYS:NZ	2.44	0.51
2:3:27:ARG:NH2	2:3:107:ASP:OD1	2.42	0.50
2:3:179:LEU:HD12	2:3:296:GLY:O	2.11	0.50
5:6:284:ILE:HD12	5:6:403:VAL:CG1	2.42	0.50
5:6:293:THR:O	5:6:362:GLN:N	2.42	0.50
8:3:2002:ADP:HN62	6:7:423:TYR:HB3	1.76	0.50
2:3:183:GLU:N	2:3:183:GLU:OE1	2.45	0.49
5:6:322:GLU:OE1	5:6:322:GLU:N	2.43	0.49
1:2:296:ARG:NE	1:2:454:ASN:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:491:GLU:OE1	8:3:2002:ADP:H4'	2.12	0.49
2:3:400:ARG:NH1	2:3:544:ASP:OD2	2.45	0.49
2:3:667:VAL:HG12	2:3:669:PRO:HD3	1.95	0.48
1:2:810:LEU:HA	1:2:813:ILE:HD12	1.93	0.48
3:4:308:VAL:HG11	3:4:325:LEU:CD1	2.44	0.48
6:7:178:ASN:OD1	6:7:179:ASP:N	2.46	0.48
1:2:671:GLU:O	1:2:675:SER:N	2.46	0.48
1:2:674:LEU:HD11	1:2:680:LEU:HD21	1.95	0.48
2:3:257:THR:HG22	2:3:275:ASP:OD1	2.13	0.48
4:5:144:ASN:OD1	4:5:145:GLN:N	2.47	0.48
4:5:655:ALA:O	4:5:659:ILE:HD12	2.13	0.48
3:4:708:VAL:O	3:4:708:VAL:HG12	2.14	0.47
2:3:400:ARG:NH1	2:3:402:ASP:O	2.42	0.47
5:6:739:ASP:OD1	5:6:740:GLU:N	2.46	0.47
4:5:343:TRP:HA	4:5:435:ILE:HD12	1.96	0.47
1:2:275:ALA:O	1:2:279:THR:OG1	2.20	0.47
1:2:399:PRO:O	5:6:390:LYS:NZ	2.31	0.47
1:2:653:ASN:OD1	1:2:668:SER:N	2.47	0.47
2:3:156:SER:OG	2:3:325:THR:OG1	2.15	0.47
2:3:251:ILE:HG23	2:3:280:ASP:HB2	1.97	0.47
6:7:315:ILE:HD12	6:7:333:ILE:HD11	1.96	0.47
2:3:216:ASP:OD1	2:3:219:THR:HG23	2.14	0.47
3:4:568:GLY:O	3:4:574:LYS:NZ	2.48	0.47
1:2:508:HIS:CE1	1:2:511:ILE:HD12	2.50	0.47
1:2:222:THR:O	1:2:222:THR:HG22	2.15	0.47
2:3:653:ILE:HD12	2:3:653:ILE:H	1.80	0.46
3:4:327:ASN:CB	3:4:436:THR:HG22	2.45	0.46
6:7:275:SER:OG	6:7:276:ARG:N	2.49	0.46
6:7:292:ASN:OD1	6:7:293:GLN:N	2.48	0.46
2:3:95:ARG:NH2	2:3:281:ASP:OD2	2.45	0.46
4:5:542:PHE:CZ	4:5:546:ILE:HD11	2.50	0.46
6:7:518:ASN:N	6:7:560:ARG:O	2.46	0.46
6:7:453:ASP:OD1	6:7:454:ILE:N	2.47	0.46
2:3:331:ALA:O	2:3:334:THR:OG1	2.25	0.45
3:4:548:THR:O	3:4:560:GLY:N	2.50	0.45
3:4:203:TYR:HH	3:4:221:ASP:N	2.14	0.45
4:5:167:ILE:HD11	4:5:259:GLN:HG2	1.97	0.45
3:4:710:ASP:OD2	6:7:668:ARG:NH2	2.48	0.45
2:3:29:GLN:HE21	2:3:128:ALA:HB1	1.82	0.45
4:5:28:ILE:HG23	4:5:93:ALA:HB2	1.98	0.45
5:6:129:THR:HG22	5:6:129:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:640:GLU:OE1	5:6:683:ASN:ND2	2.49	0.45
2:3:553:ILE:HG13	4:5:634:LEU:HD13	1.97	0.45
3:4:796:ARG:NH2	8:6:1102:ADP:H4'	2.31	0.45
2:3:442:LEU:O	2:3:461:ALA:N	2.50	0.45
4:5:570:ASN:O	4:5:574:ASN:ND2	2.49	0.45
6:7:656:VAL:O	6:7:660:VAL:HG23	2.17	0.44
6:7:150:ASN:OD1	6:7:191:LEU:HD22	2.18	0.44
6:7:73:ARG:NH2	6:7:130:LYS:O	2.49	0.44
6:7:589:ALA:O	6:7:593:ARG:NH1	2.48	0.44
4:5:56:VAL:O	4:5:56:VAL:HG12	2.17	0.44
4:5:426:LEU:CD2	4:5:520:LEU:HD22	2.48	0.44
1:2:340:ASN:N	1:2:374:ARG:O	2.48	0.44
5:6:710:ASP:O	5:6:711:LEU:HD22	2.18	0.44
4:5:556:VAL:HG13	4:5:556:VAL:O	2.17	0.44
1:2:678:ASP:OD1	1:2:679:ILE:N	2.50	0.44
6:7:660:VAL:HG12	6:7:689:LEU:HD11	1.99	0.44
3:4:762:ILE:HG23	3:4:762:ILE:O	2.18	0.43
4:5:577:THR:HG22	4:5:578:GLY:H	1.83	0.43
6:7:524:ASP:OD1	6:7:525:GLU:N	2.49	0.43
6:7:27:THR:HG22	6:7:27:THR:O	2.18	0.43
6:7:335:VAL:HG11	6:7:340:VAL:HA	2.00	0.43
2:3:398:HIS:NE2	2:3:492:GLN:O	2.46	0.43
6:7:602:ASP:OD1	6:7:603:ILE:N	2.52	0.43
3:4:262:LEU:HD22	3:4:325:LEU:HB3	1.99	0.43
2:3:196:LEU:HD23	2:3:250:PHE:CE1	2.54	0.43
2:3:686:LEU:O	2:3:690:ASP:N	2.49	0.43
3:4:180:ILE:HD11	3:4:187:ILE:HD11	2.00	0.43
4:5:153:SER:O	4:5:156:VAL:HG23	2.19	0.43
2:3:277:ILE:HD12	2:3:320:LEU:HD13	2.01	0.43
3:4:717:ASP:OD2	6:7:668:ARG:NE	2.47	0.42
5:6:577:PRO:O	5:6:578:SER:OG	2.32	0.42
1:2:821:ALA:O	1:2:825:LEU:N	2.52	0.42
3:4:187:ILE:HD13	3:4:271:ILE:HD11	2.01	0.42
5:6:155:TYR:OH	5:6:167:ALA:HB1	2.19	0.42
1:2:475:SER:O	1:2:765:LYS:NZ	2.47	0.42
2:3:538:SER:O	2:3:541:SER:OG	2.19	0.42
6:7:692:ILE:HD13	6:7:717:LEU:HD21	2.02	0.42
1:2:246:TYR:CZ	1:2:257:ALA:HB1	2.54	0.42
5:6:310:THR:N	5:6:345:THR:O	2.46	0.42
4:5:379:PHE:H	8:5:802:ADP:HN62	1.67	0.42
1:2:280:GLU:OE2	1:2:285:ASP:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:276:MET:HG2	4:5:330:ILE:HD11	2.01	0.42
5:6:832:ARG:O	5:6:835:ILE:HG22	2.20	0.41
3:4:341:ASP:OD2	3:4:343:LYS:NZ	2.53	0.41
2:3:480:ASP:OD1	2:3:481:VAL:N	2.52	0.41
2:3:524:ASP:OD1	2:3:525:VAL:N	2.52	0.41
2:3:722:ASN:OD1	2:3:723:LYS:N	2.50	0.41
6:7:23:ASP:O	6:7:27:THR:N	2.53	0.41
6:7:82:LEU:HD12	6:7:206:PRO:HA	2.03	0.41
2:3:126:GLU:O	2:3:130:THR:HG23	2.19	0.41
3:4:578:LEU:HD23	3:4:672:LEU:HD22	2.01	0.41
4:5:156:VAL:O	4:5:157:SER:OG	2.32	0.41
5:6:115:PHE:CE2	5:6:119:LEU:HD11	2.55	0.41
6:7:15:ASN:O	6:7:15:ASN:ND2	2.53	0.41
4:5:391:LEU:HA	4:5:410:ILE:HD11	2.03	0.41
2:3:446:VAL:HG22	2:3:447:THR:H	1.84	0.41
1:2:272:ASP:OD1	1:2:273:LEU:N	2.54	0.41
4:5:656:ILE:O	4:5:660:THR:HG23	2.21	0.41
5:6:710:ASP:C	5:6:711:LEU:HD22	2.41	0.41
5:6:639:ASP:OD1	5:6:640:GLU:N	2.54	0.41
6:7:411:TYR:HD1	6:7:702:LEU:HD13	1.85	0.41
2:3:118:PRO:HB2	2:3:122:ILE:HD12	2.03	0.40
2:3:210:HIS:ND1	6:7:5:LEU:O	2.49	0.40
3:4:281:VAL:HA	3:4:284:ILE:HD13	2.03	0.40
4:5:426:LEU:HD21	4:5:520:LEU:HD22	2.03	0.40
6:7:363:PHE:O	6:7:365:ALA:N	2.52	0.40
6:7:591:LEU:HD13	6:7:681:PHE:HZ	1.85	0.40
1:2:375:VAL:HG13	1:2:380:THR:HG21	2.03	0.40
6:7:464:VAL:O	6:7:464:VAL:HG13	2.20	0.40
3:4:576:GLN:HG3	8:4:1002:ADP:H3'	2.03	0.40
4:5:181:ILE:CD1	4:5:192:ILE:HD12	2.52	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	597/868 (69%)	552 (92%)	45 (8%)	0	100	100
2	3	595/971 (61%)	559 (94%)	36 (6%)	0	100	100
3	4	635/933 (68%)	591 (93%)	44 (7%)	0	100	100
4	5	621/775 (80%)	576 (93%)	45 (7%)	0	100	100
5	6	608/1017 (60%)	571 (94%)	37 (6%)	0	100	100
6	7	681/845 (81%)	645 (95%)	36 (5%)	0	100	100
All	All	3737/5409 (69%)	3494 (94%)	243 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	528/770 (69%)	520 (98%)	8 (2%)	65	81
2	3	523/835 (63%)	519 (99%)	4 (1%)	81	89
3	4	582/848 (69%)	577 (99%)	5 (1%)	78	88
4	5	566/688 (82%)	560 (99%)	6 (1%)	73	85
5	6	537/886 (61%)	532 (99%)	5 (1%)	78	88
6	7	609/753 (81%)	603 (99%)	6 (1%)	76	86
All	All	3345/4780 (70%)	3311 (99%)	34 (1%)	77	86

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

Mol	Chain	Res	Type
1	2	433	ASN
1	2	437	ASN
1	2	491	ARG
1	2	528	ASN

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Mol	Chain	Res	Type
1	2	530	LYS
1	2	658	ASN
1	2	794	ARG
1	2	795	ARG
2	3	26	ARG
2	3	177	ASN
2	3	527	ARG
2	3	731	ASN
3	4	193	ASN
3	4	196	ASN
3	4	302	LYS
3	4	428	ARG
3	4	815	ASN
4	5	52	ASN
4	5	270	MET
4	5	284	ASN
4	5	422	LYS
4	5	570	ASN
4	5	682	ARG
5	6	160	MET
5	6	168	MET
5	6	326	LYS
5	6	566	ARG
5	6	700	ASN
6	7	15	ASN
6	7	19	ASN
6	7	195	ASN
6	7	210	ASN
6	7	214	ARG
6	7	412	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	437	ASN
1	2	508	HIS
1	2	528	ASN
1	2	658	ASN
2	3	29	GLN
2	3	269	GLN
2	3	374	HIS
2	3	569	HIS

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Mol	Chain	Res	Type
2	3	673	GLN
2	3	691	ASN
2	3	731	ASN
4	5	198	ASN
4	5	372	ASN
4	5	574	ASN
4	5	585	ASN
5	6	139	GLN
5	6	700	ASN
6	7	90	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	ADP	2	902	-	24,29,29	0.92	1 (4%)	29,45,45	1.54	4 (13%)
8	ADP	3	2001	-	24,29,29	0.98	1 (4%)	29,45,45	1.40	4 (13%)
8	ADP	3	2002	-	24,29,29	0.98	1 (4%)	29,45,45	1.64	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	ADP	5	802	-	24,29,29	0.94	1 (4%)	29,45,45	1.54	4 (13%)
8	ADP	6	1102	-	24,29,29	0.98	1 (4%)	29,45,45	1.48	4 (13%)
8	ADP	4	1002	-	24,29,29	0.95	1 (4%)	29,45,45	1.79	5 (17%)

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
8	ADP	2	902	-	-	4/12/32/32	0/3/3/3
8	ADP	3	2001	-	-	3/12/32/32	0/3/3/3
8	ADP	3	2002	-	-	4/12/32/32	0/3/3/3
8	ADP	5	802	-	-	2/12/32/32	0/3/3/3
8	ADP	6	1102	-	-	3/12/32/32	0/3/3/3
8	ADP	4	1002	-	-	2/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	6	1102	ADP	C5-C4	2.58	1.47	1.40
8	3	2002	ADP	C5-C4	2.46	1.47	1.40
8	2	902	ADP	C5-C4	2.45	1.47	1.40
8	3	2001	ADP	C5-C4	2.41	1.47	1.40
8	4	1002	ADP	C5-C4	2.39	1.47	1.40
8	5	802	ADP	C5-C4	2.33	1.47	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	4	1002	ADP	PA-O3A-PB	-6.37	110.98	132.83
8	3	2002	ADP	PA-O3A-PB	-5.11	115.29	132.83
8	5	802	ADP	PA-O3A-PB	-4.29	118.11	132.83
8	2	902	ADP	C3'-C2'-C1'	3.80	106.70	100.98
8	6	1102	ADP	C3'-C2'-C1'	3.55	106.33	100.98
8	6	1102	ADP	PA-O3A-PB	-3.50	120.80	132.83
8	3	2002	ADP	C3'-C2'-C1'	3.47	106.20	100.98
8	2	902	ADP	PA-O3A-PB	-3.44	121.02	132.83
8	5	802	ADP	C3'-C2'-C1'	3.27	105.91	100.98
8	6	1102	ADP	N3-C2-N1	-3.27	123.57	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	5	802	ADP	N3-C2-N1	-3.19	123.70	128.68
8	2	902	ADP	N3-C2-N1	-3.18	123.71	128.68
8	3	2001	ADP	PA-O3A-PB	-3.14	122.05	132.83
8	3	2001	ADP	N3-C2-N1	-3.11	123.82	128.68
8	4	1002	ADP	N3-C2-N1	-3.06	123.89	128.68
8	3	2001	ADP	C4-C5-N7	-2.95	106.33	109.40
8	3	2001	ADP	C3'-C2'-C1'	2.87	105.30	100.98
8	3	2002	ADP	N3-C2-N1	-2.79	124.32	128.68
8	4	1002	ADP	C4-C5-N7	-2.78	106.50	109.40
8	2	902	ADP	C4-C5-N7	-2.77	106.52	109.40
8	5	802	ADP	C4-C5-N7	-2.49	106.81	109.40
8	6	1102	ADP	C4-C5-N7	-2.39	106.91	109.40
8	3	2002	ADP	C4-C5-N7	-2.39	106.91	109.40
8	4	1002	ADP	C3'-C2'-C1'	2.23	104.33	100.98
8	4	1002	ADP	O5'-C5'-C4'	2.02	115.94	108.99

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	2	902	ADP	C5'-O5'-PA-O3A
8	3	2001	ADP	C5'-O5'-PA-O1A
8	3	2001	ADP	C5'-O5'-PA-O3A
8	3	2002	ADP	C3'-C4'-C5'-O5'
8	4	1002	ADP	C3'-C4'-C5'-O5'
8	5	802	ADP	C5'-O5'-PA-O2A
8	5	802	ADP	C5'-O5'-PA-O3A
8	2	902	ADP	O4'-C4'-C5'-O5'
8	2	902	ADP	C3'-C4'-C5'-O5'
8	3	2002	ADP	O4'-C4'-C5'-O5'
8	4	1002	ADP	O4'-C4'-C5'-O5'
8	6	1102	ADP	C3'-C4'-C5'-O5'
8	3	2002	ADP	PA-O3A-PB-O1B
8	6	1102	ADP	O4'-C4'-C5'-O5'
8	3	2001	ADP	C4'-C5'-O5'-PA
8	3	2002	ADP	PA-O3A-PB-O2B
8	2	902	ADP	C5'-O5'-PA-O2A
8	6	1102	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	2	902	ADP	1	0
8	3	2001	ADP	2	0
8	3	2002	ADP	2	0
8	5	802	ADP	1	0
8	6	1102	ADP	2	0
8	4	1002	ADP	4	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 then 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.

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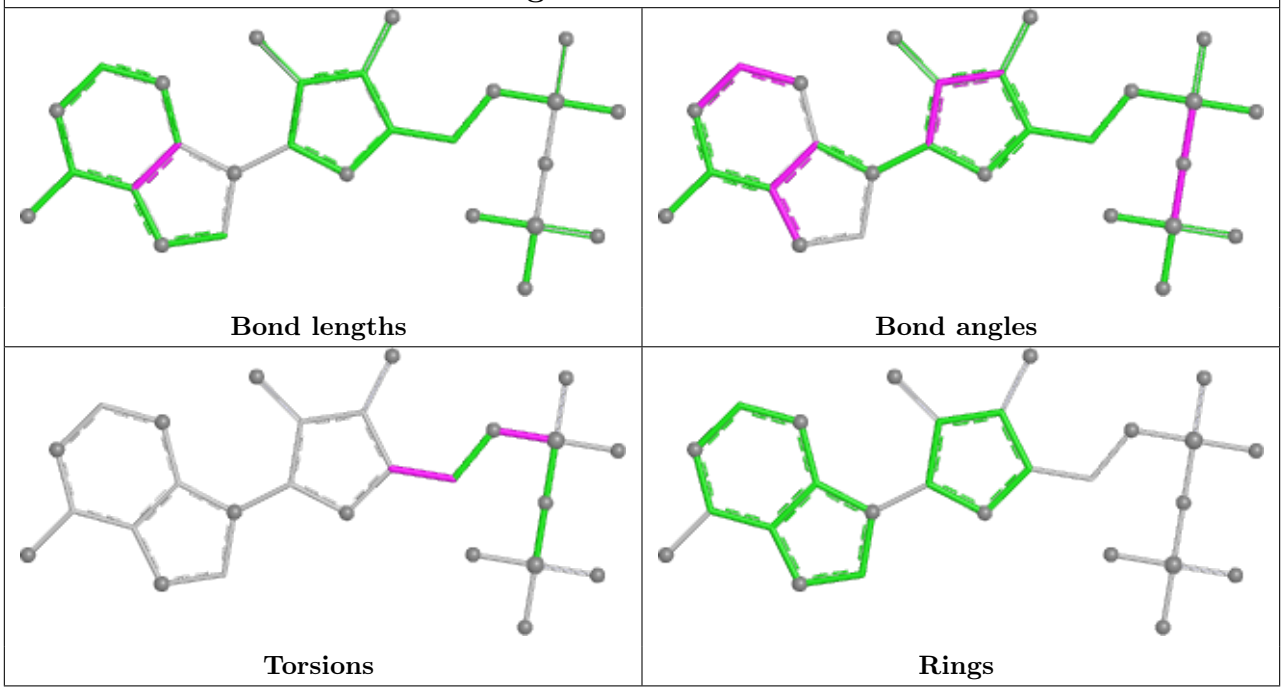
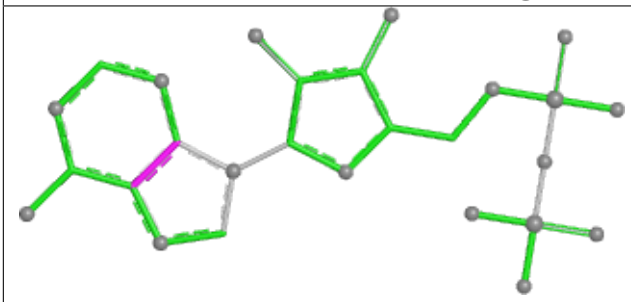
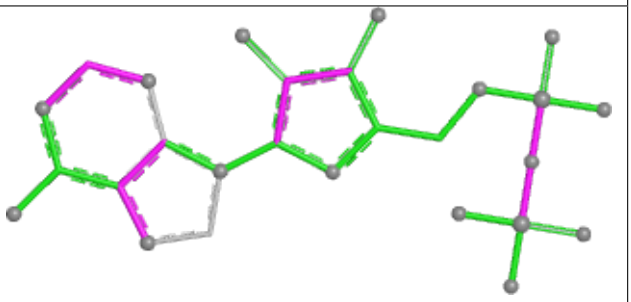
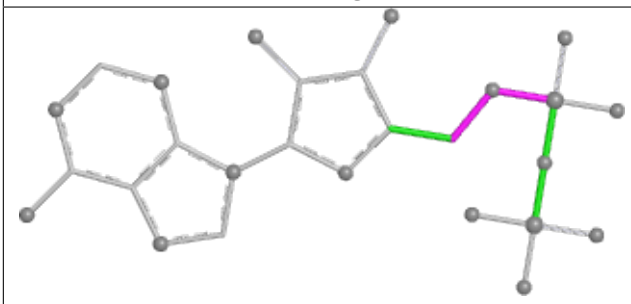
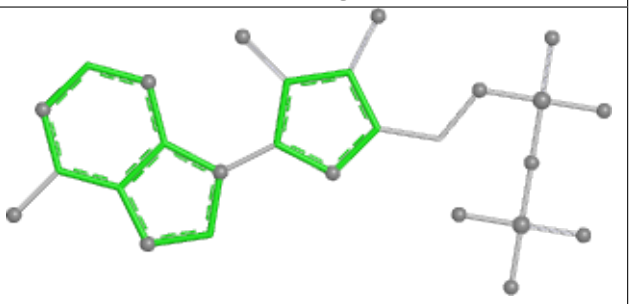
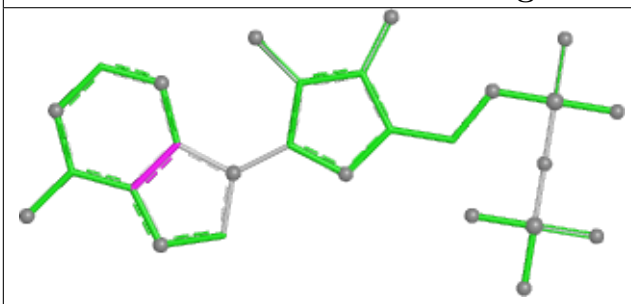
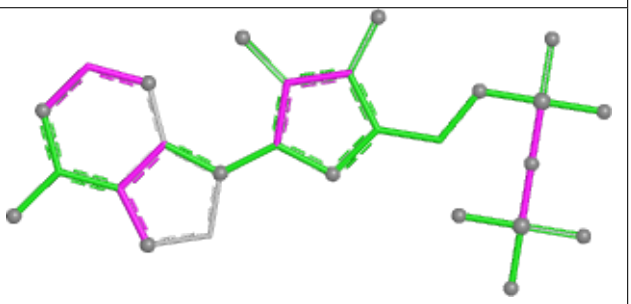
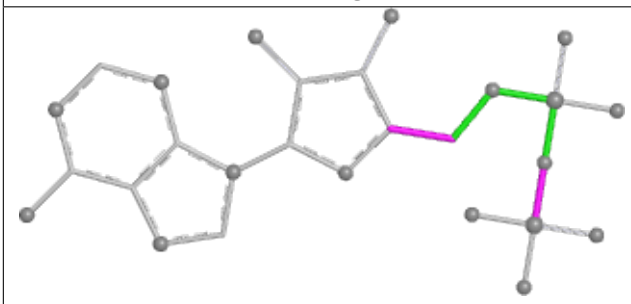
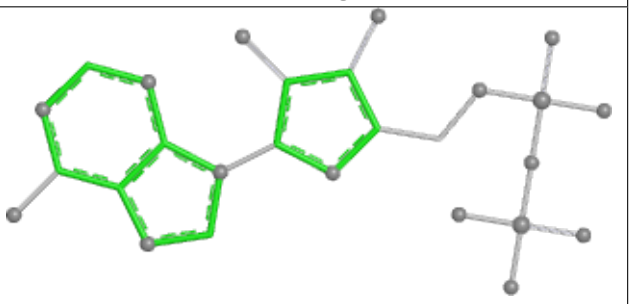
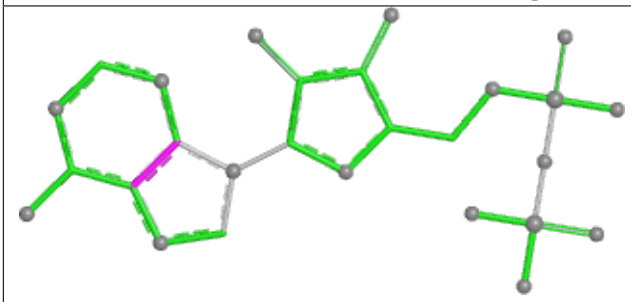
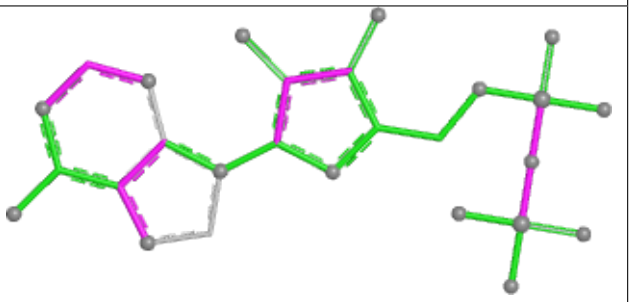
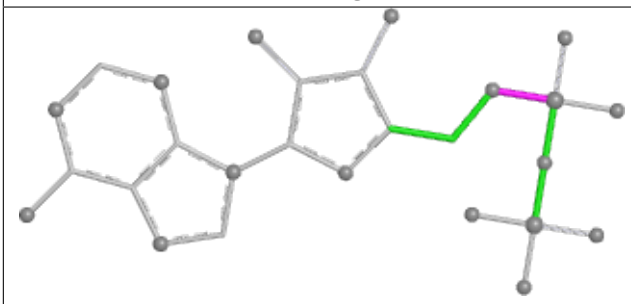
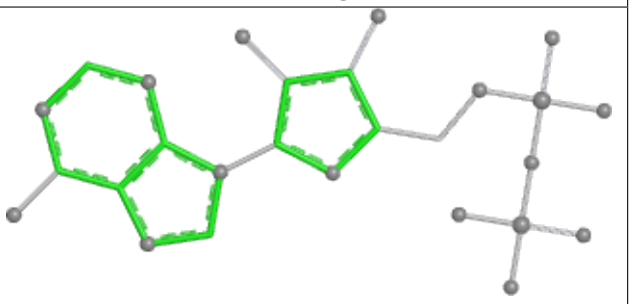
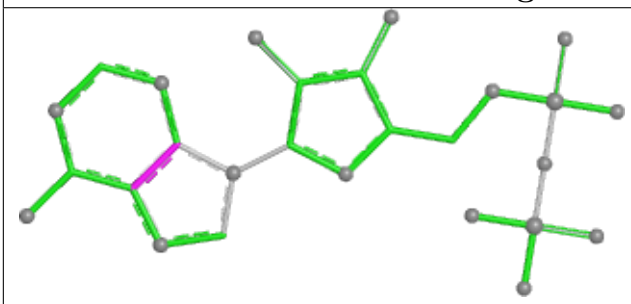
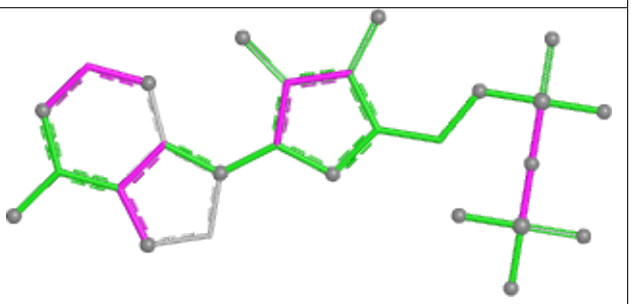
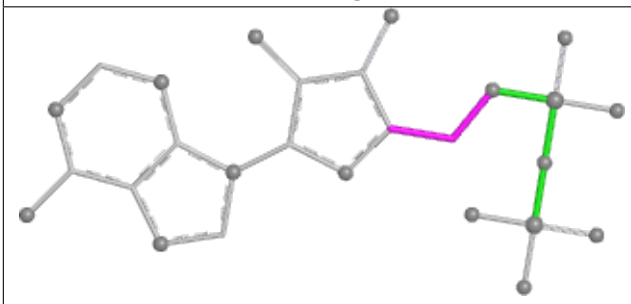
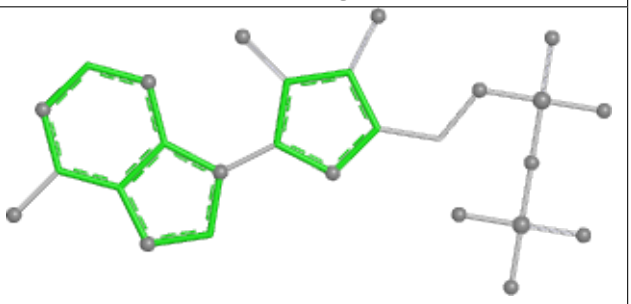
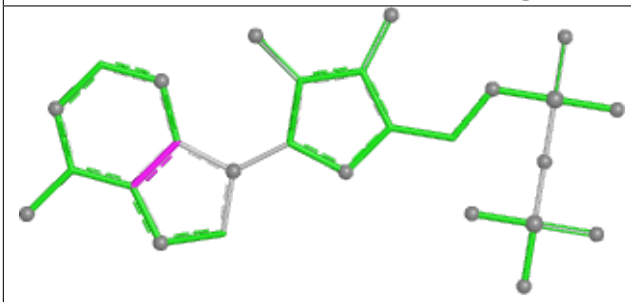
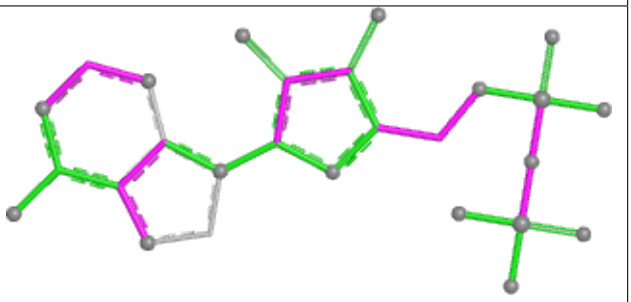
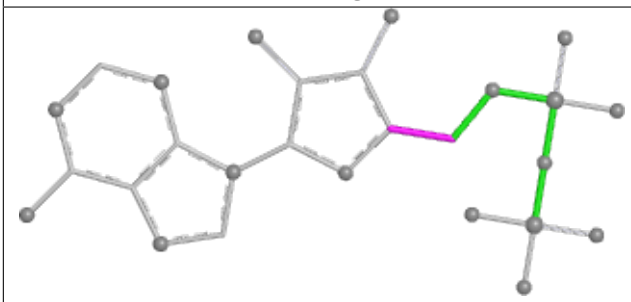
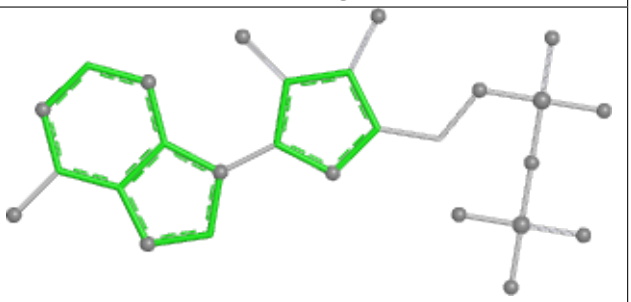


Ligand ADP 3 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP 3 2002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP 5 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP 6 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP 4 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

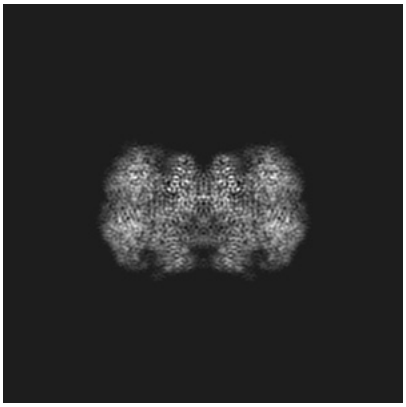
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6338. These allow visual inspection of the internal detail of the map and identification of artifacts.

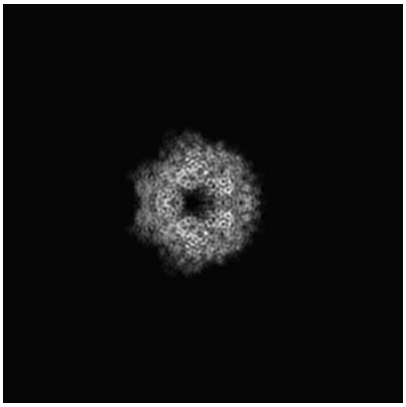
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

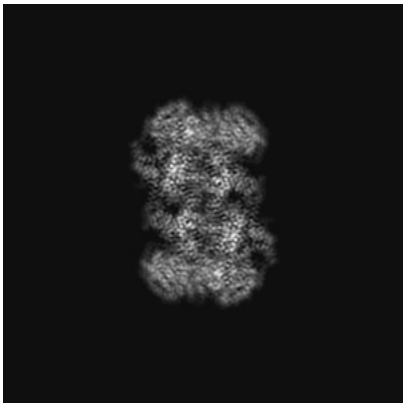
6.1.1 Primary map



X



Y



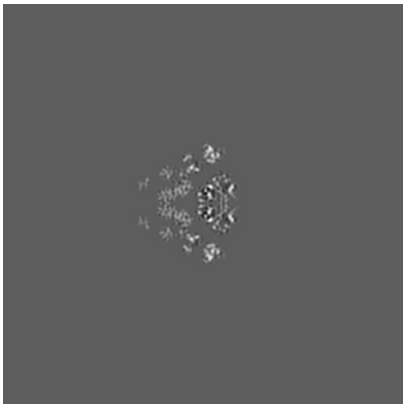
Z

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

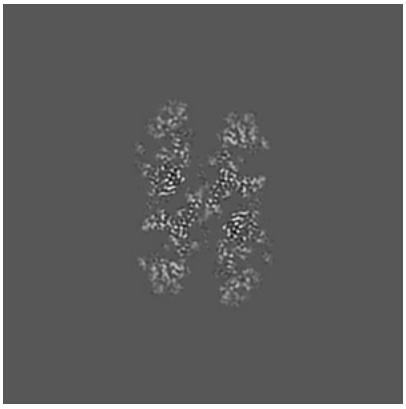
6.2 Central slices

6.2.1 Primary map

X Index: 150



Y Index: 150

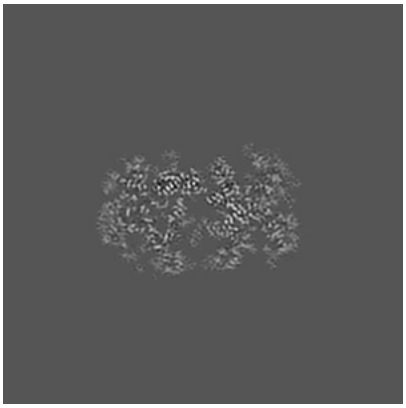


Z Index: 150

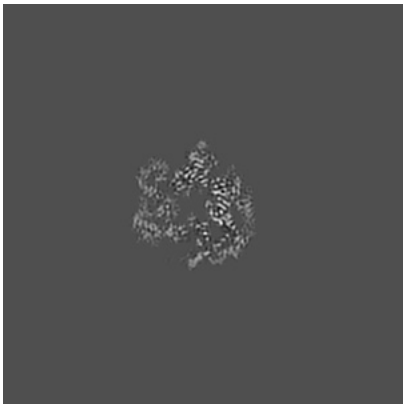
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

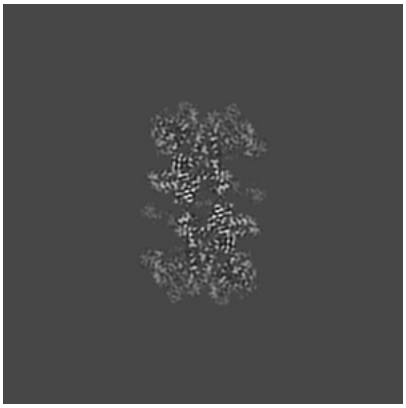
6.3.1 Primary map



X Index: 166



Y Index: 169

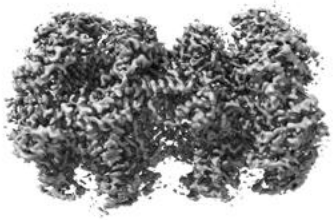


Z Index: 166

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

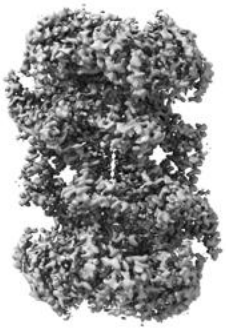
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

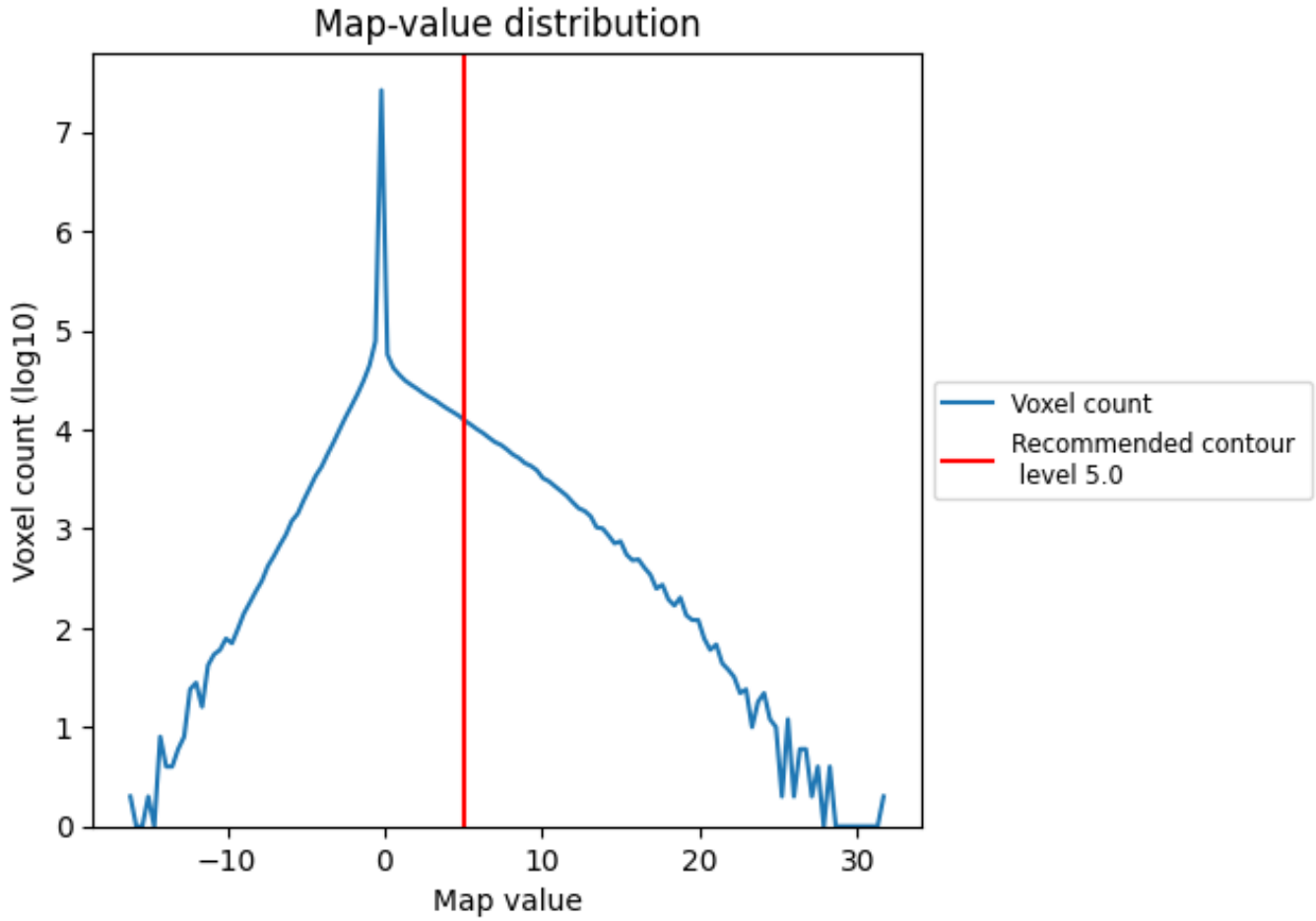
6.5 Mask visualisation (i)

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

7 Map analysis

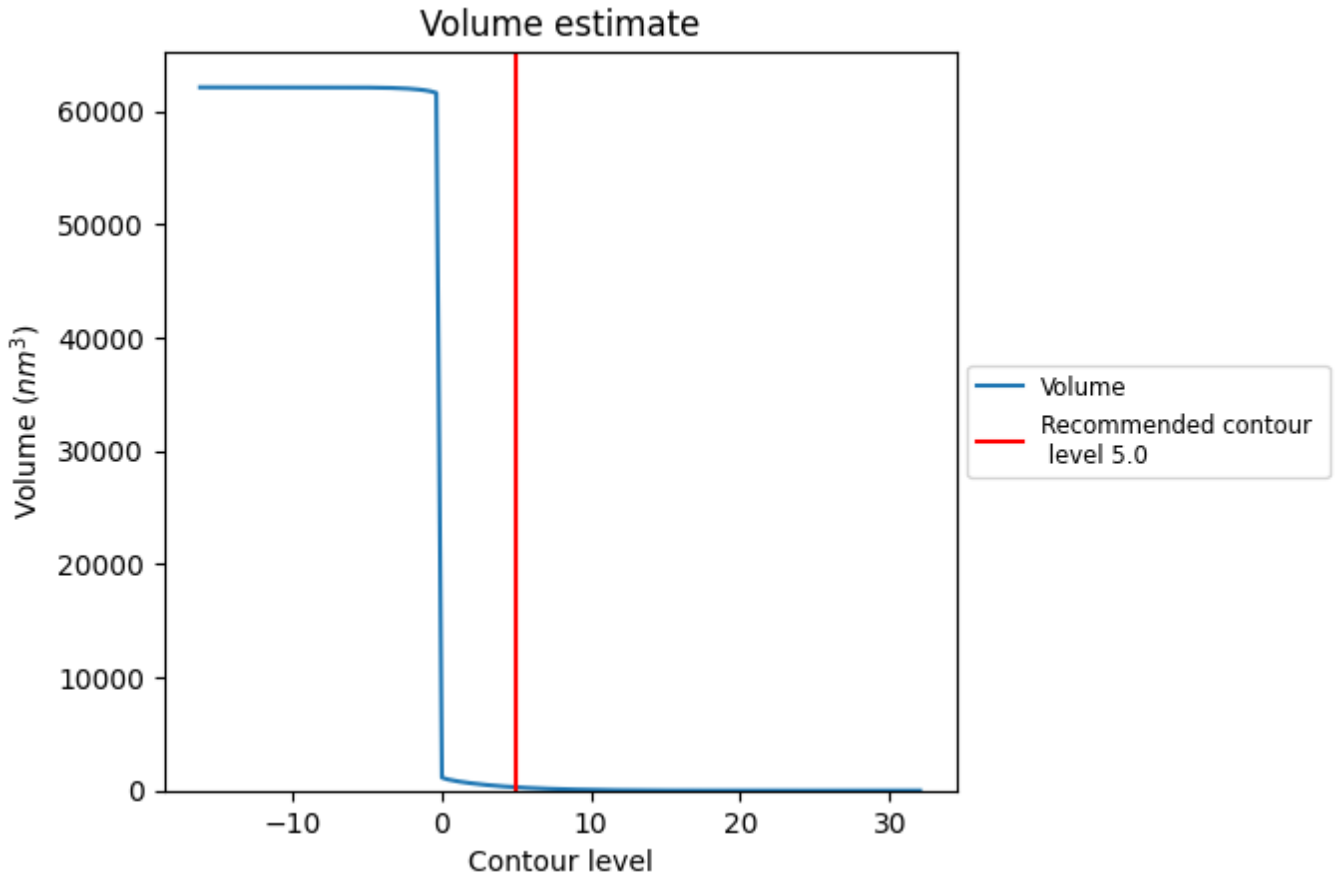
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

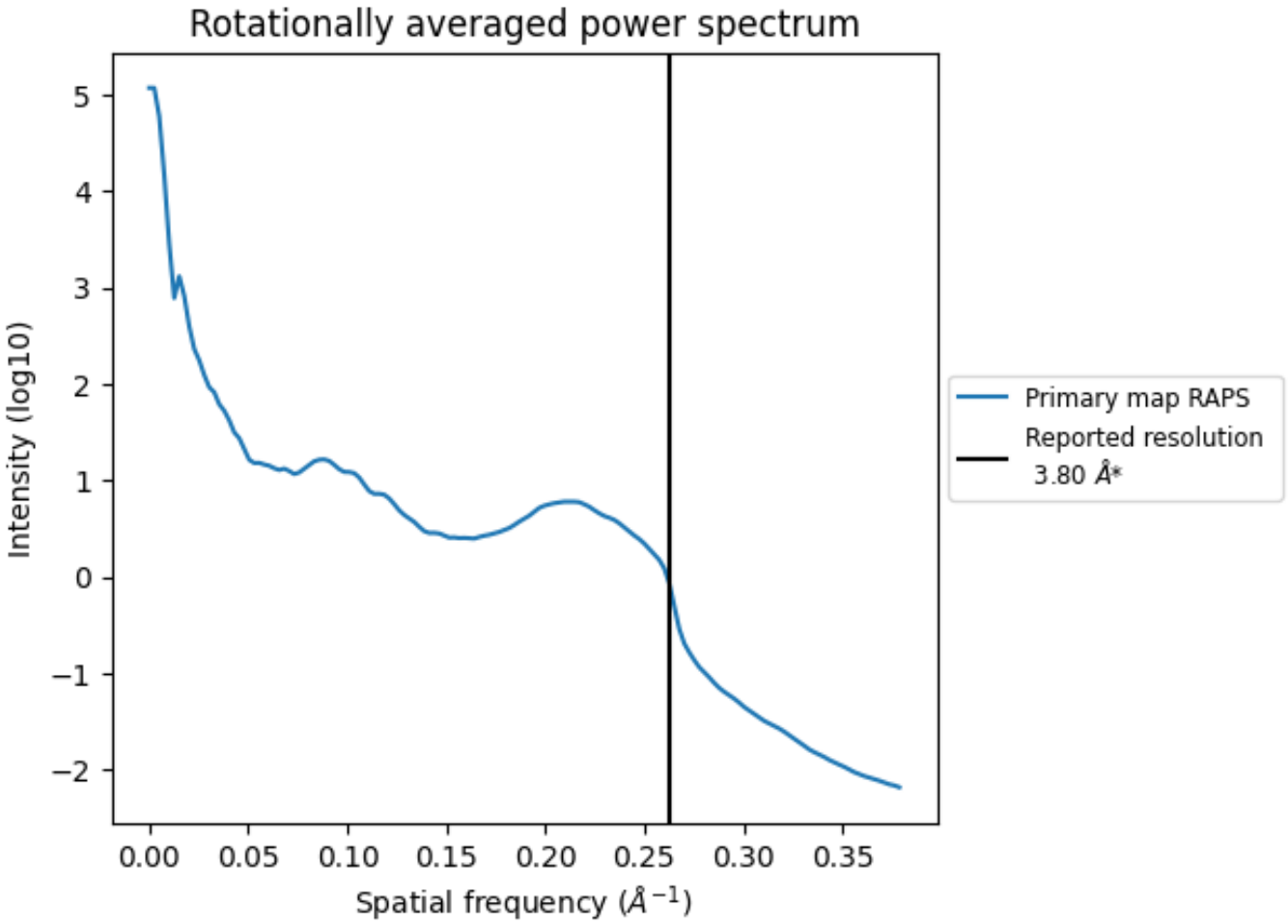
7.2 Volume estimate



The volume at the recommended contour level is 292 nm^3; this corresponds to an approximate mass of 264 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

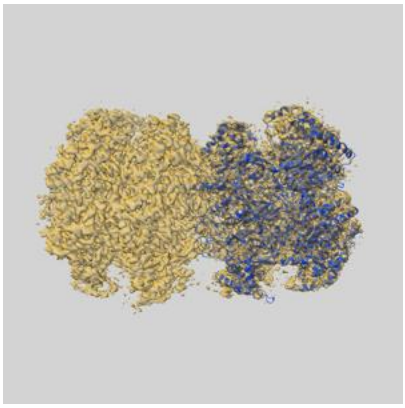
8 Fourier-Shell correlation (i)

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

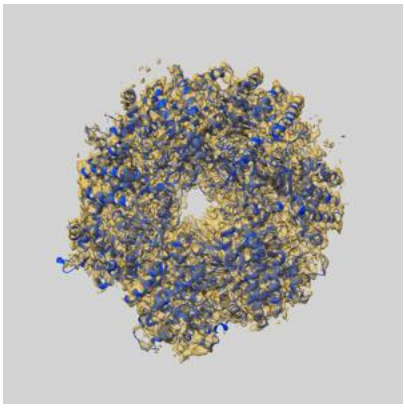
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6338 and PDB model 6EYC. Per-residue inclusion information can be found in section 3 on page 6.

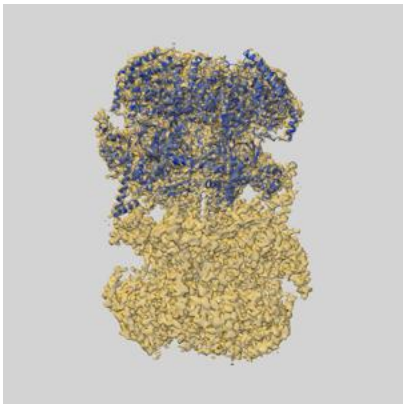
9.1 Map-model overlay



X



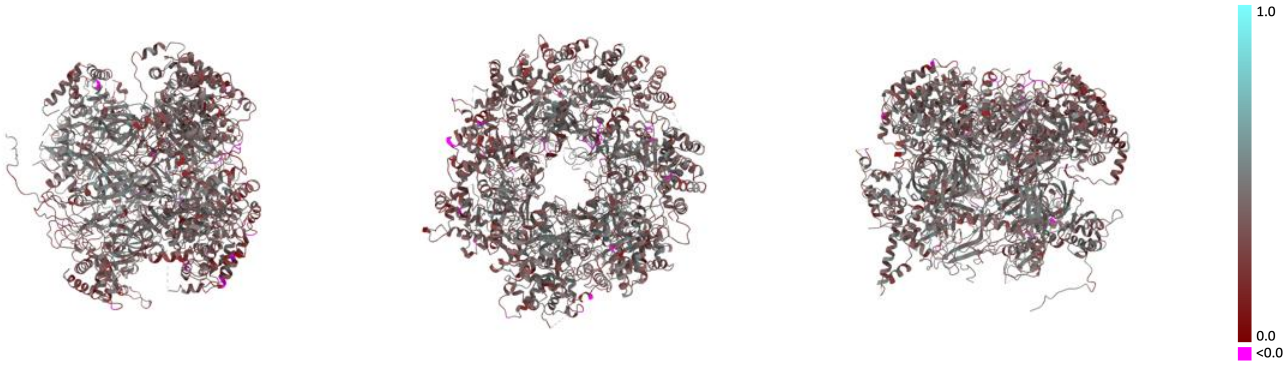
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 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.

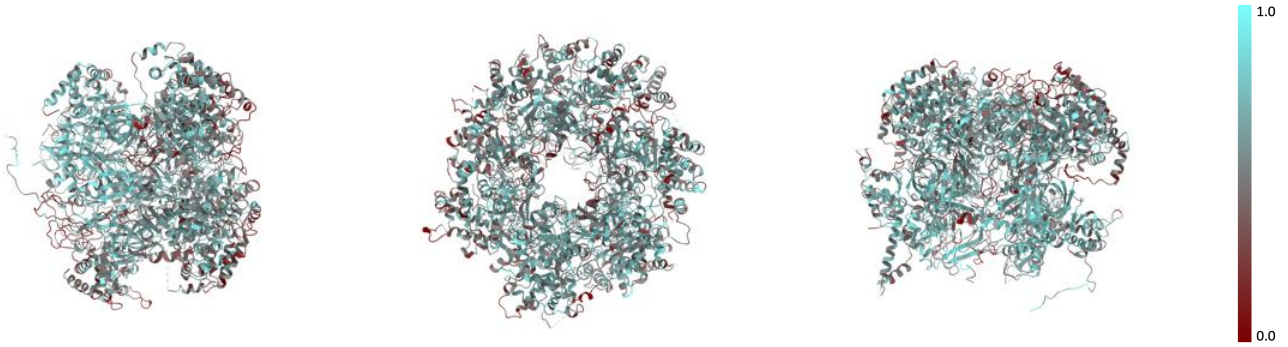
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

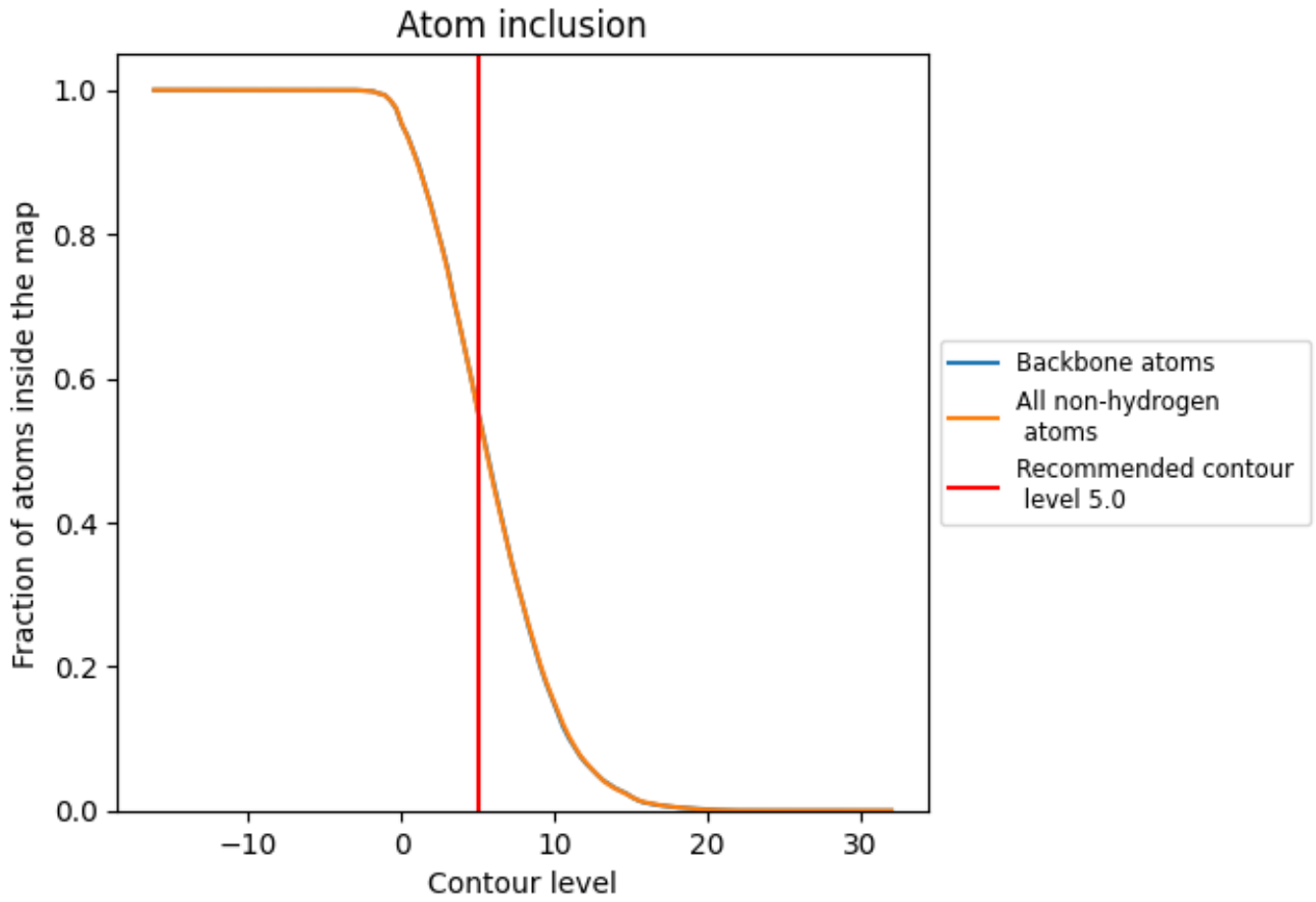
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (5.0).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5547	0.3770
2	0.5214	0.3540
3	0.5861	0.3890
4	0.5850	0.3920
5	0.5552	0.3790
6	0.4909	0.3470
7	0.6109	0.4000