Full wwPDB EM Validation Report (i)

Mar 4, 2024 – 04:50 PM EST

PDB ID	:	6D00
EMDB ID	:	EMD-7782
Title	:	Calcarisporiella thermophila Hsp104
Authors	:	Zhang, K.; Pintilie, G.
Deposited on	:	2018-04-09
Resolution	:	4.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

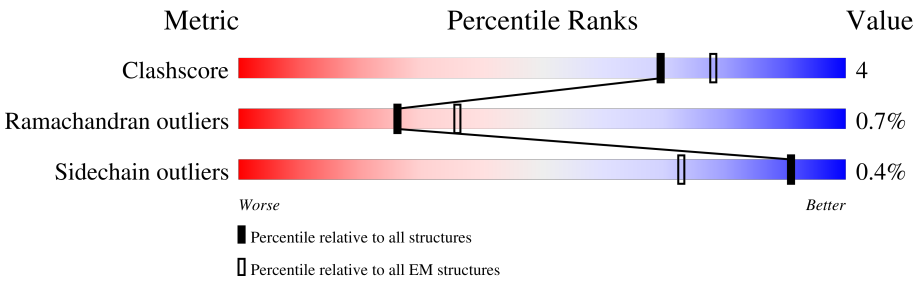
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	1	883	45% / 81% / 10% / 9%
1	2	883	50% / 80% / 11% / 9%
1	3	883	40% / 80% / 11% / 9%
1	4	883	38% / 81% / 10% / 9%
1	5	883	45% / 80% / 11% / 9%
1	6	883	38% / 81% / 10% / 9%

2 Entry composition (i)

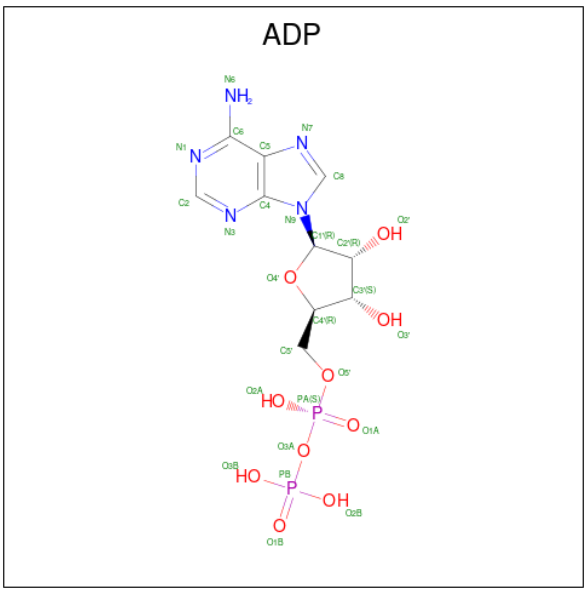
There are 2 unique types of molecules in this entry. The entry contains 38328 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Calcarisporiella thermophila Hsp104.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	804	6334	3965	1150	1194	25	0	0
1	2	804	6334	3965	1150	1194	25	0	0
1	3	804	6334	3965	1150	1194	25	0	0
1	4	804	6334	3965	1150	1194	25	0	0
1	5	804	6334	3965	1150	1194	25	0	0
1	6	804	6334	3965	1150	1194	25	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



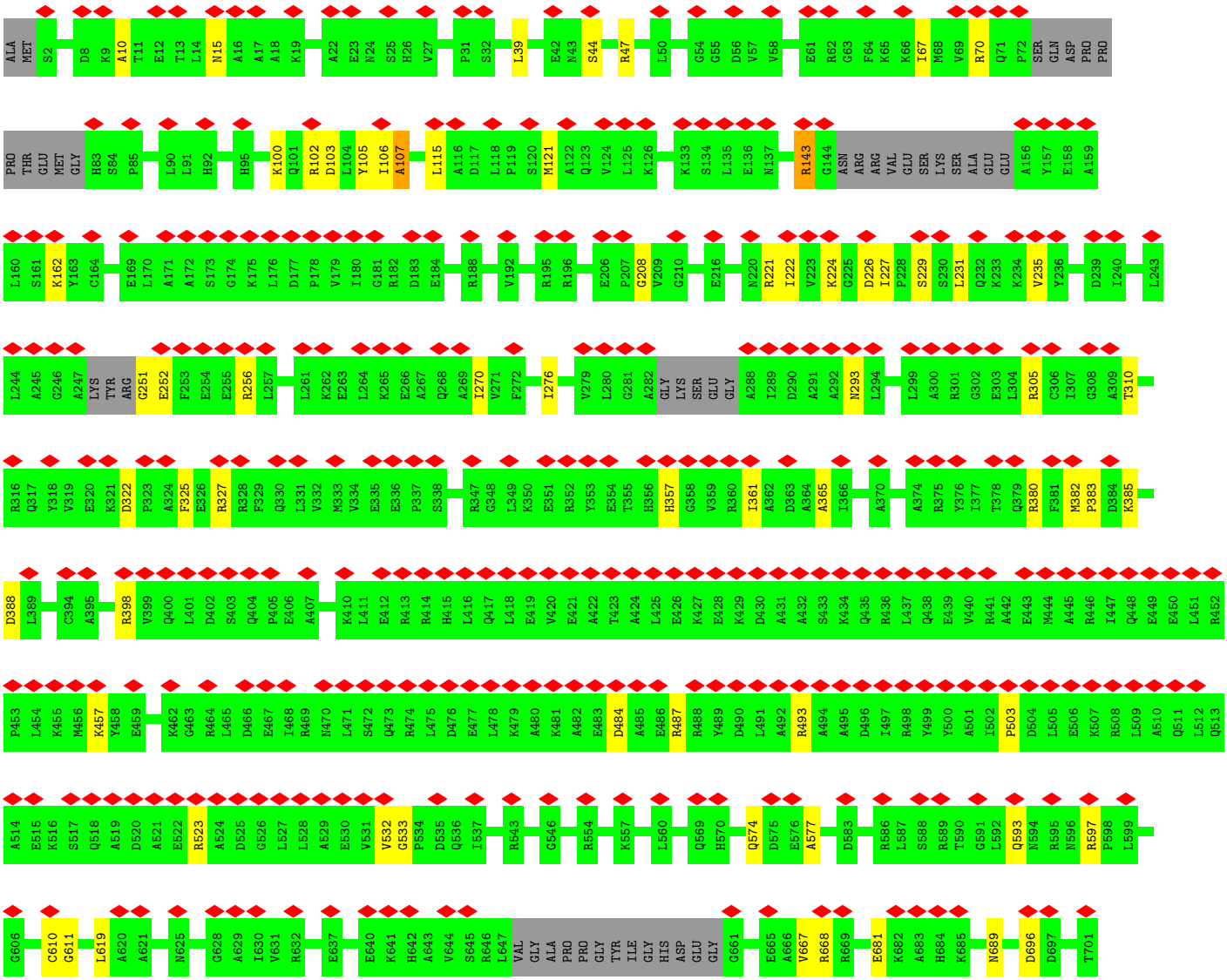
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	1	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	1	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	2	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	2	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	3	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	3	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	4	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	4	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	5	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	5	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	6	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	6	1	27	10	5	10	2	0

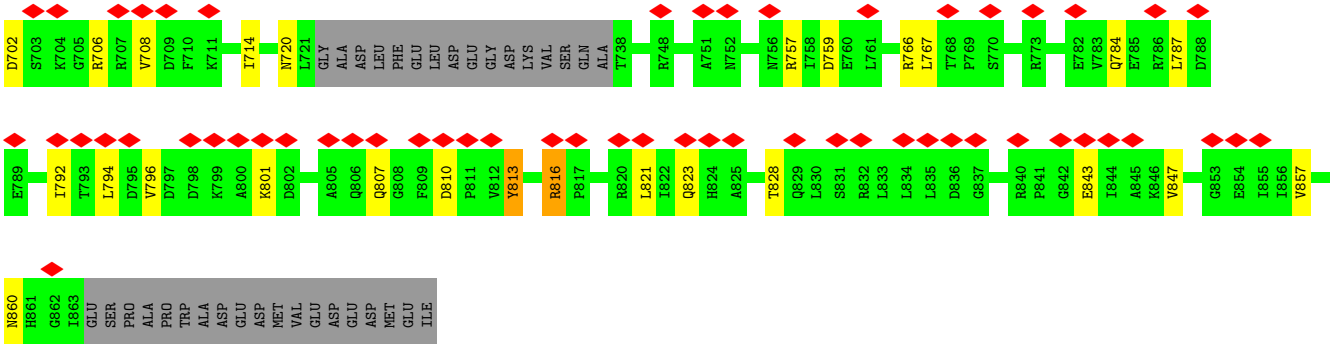
3 Residue-property plots (i)

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: Calcarisporiella thermophila Hsp104

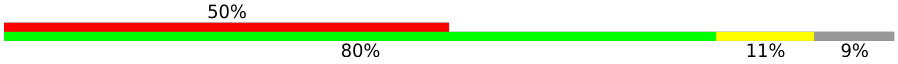
Chain 1:

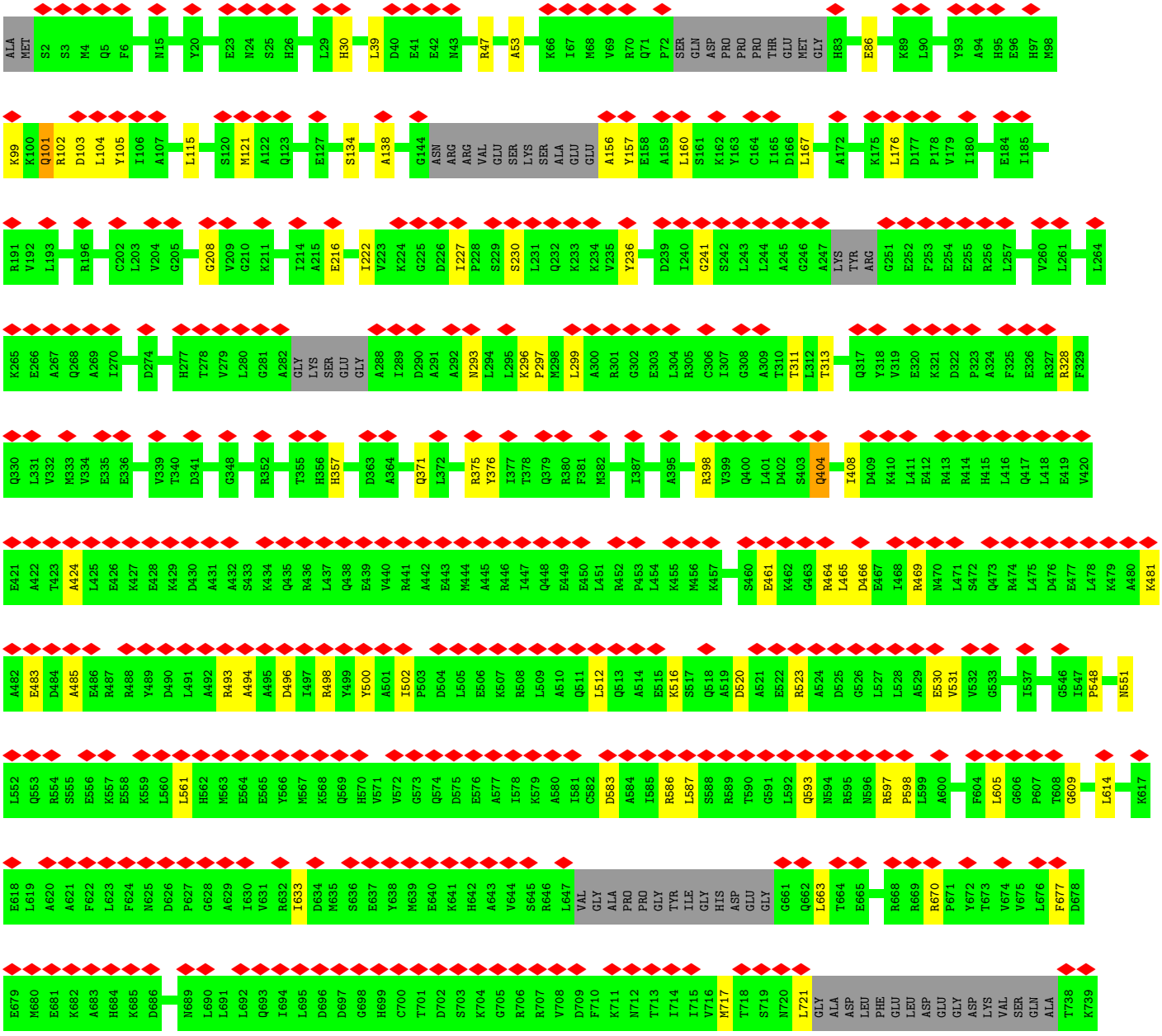


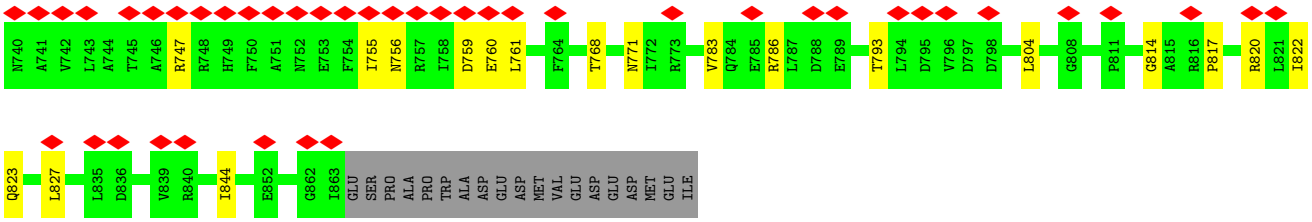


- Molecule 1: Calcarisporiella thermophila Hsp104

Chain 2:

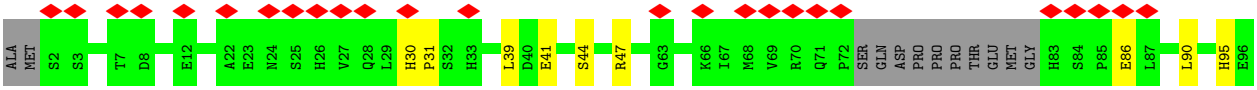


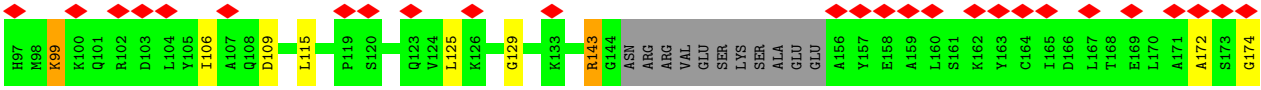


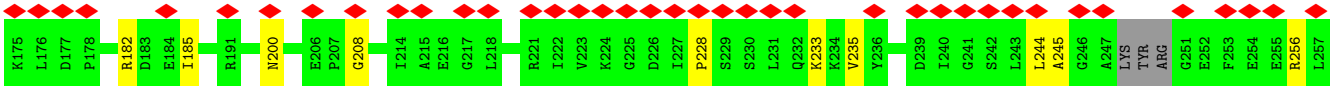


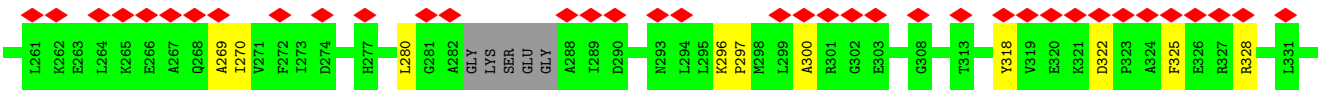
• Molecule 1: Calcarisporiella thermophila Hsp104

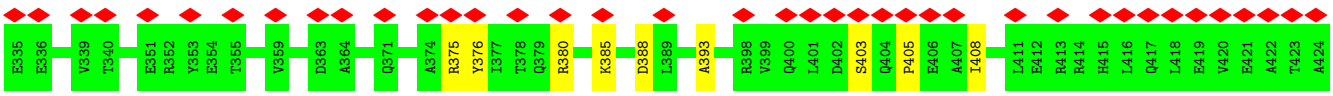
Chain 3:

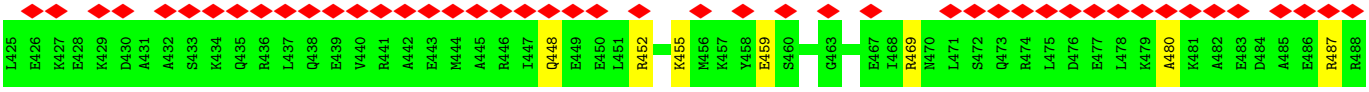


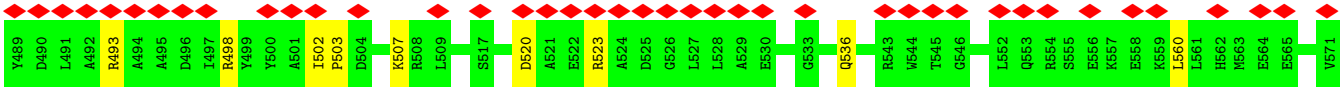


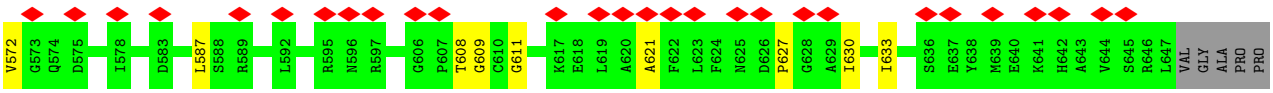


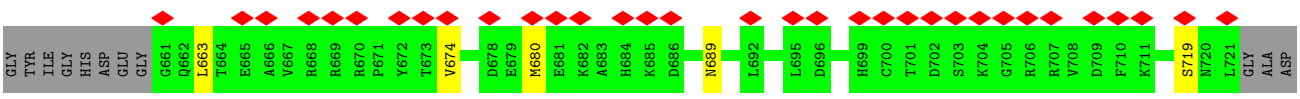


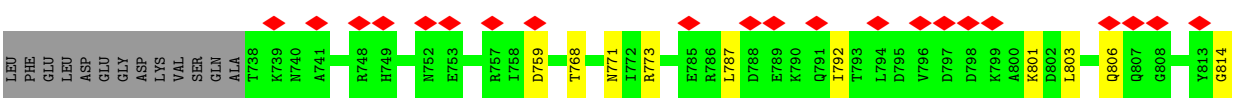


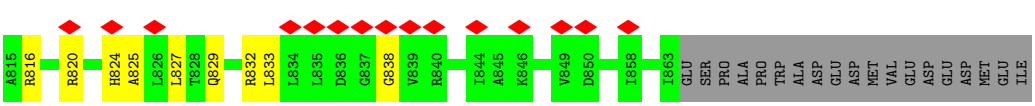






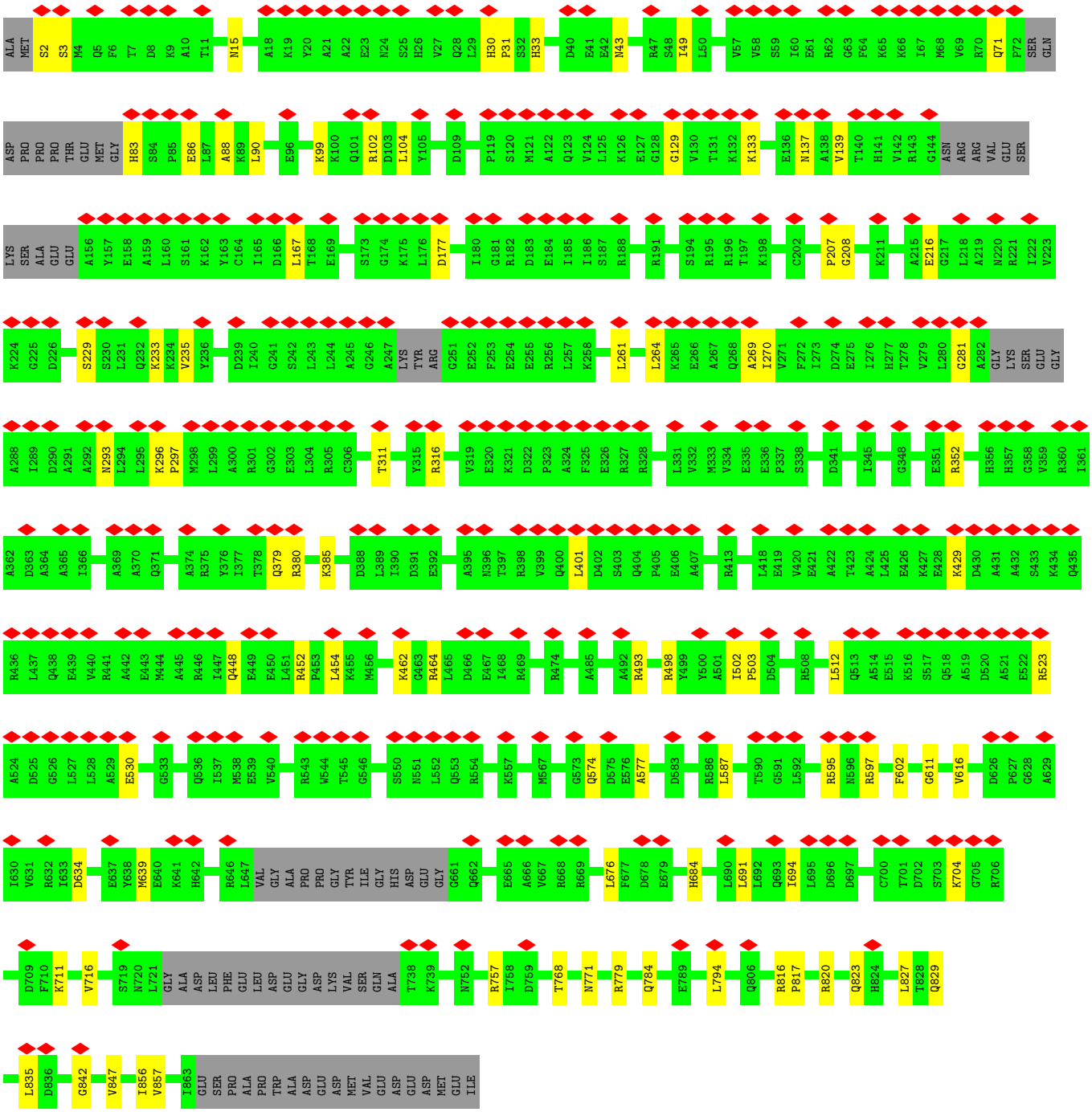






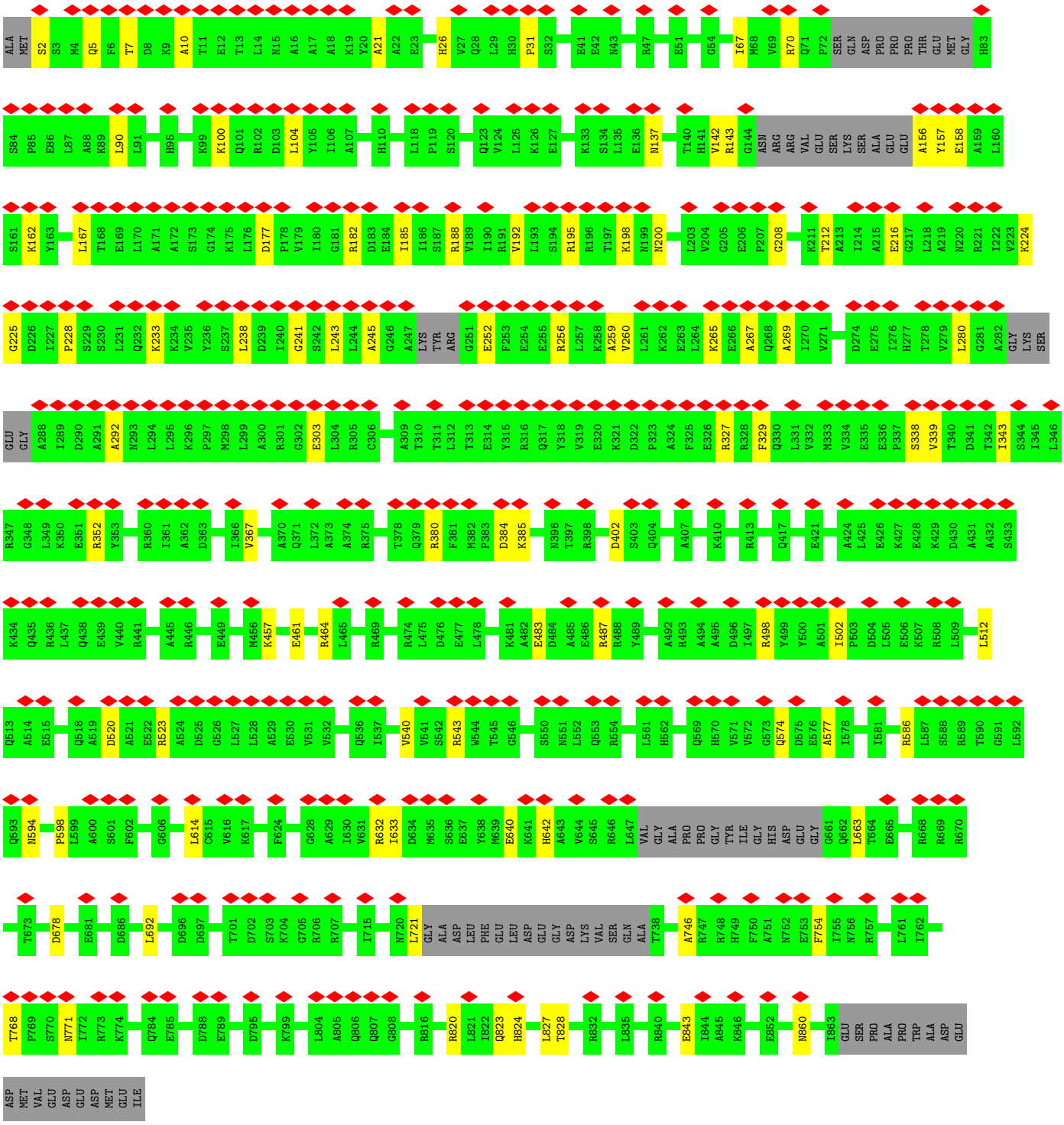
- Molecule 1: Calcarisporiella thermophila Hsp104

Chain 4:



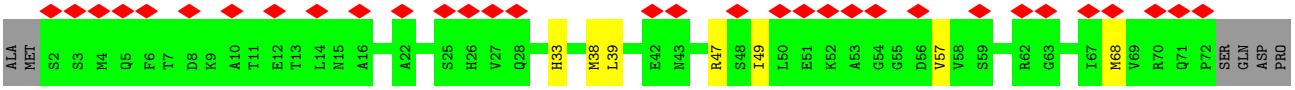
- Molecule 1: Calcarisporiella thermophila Hsp104

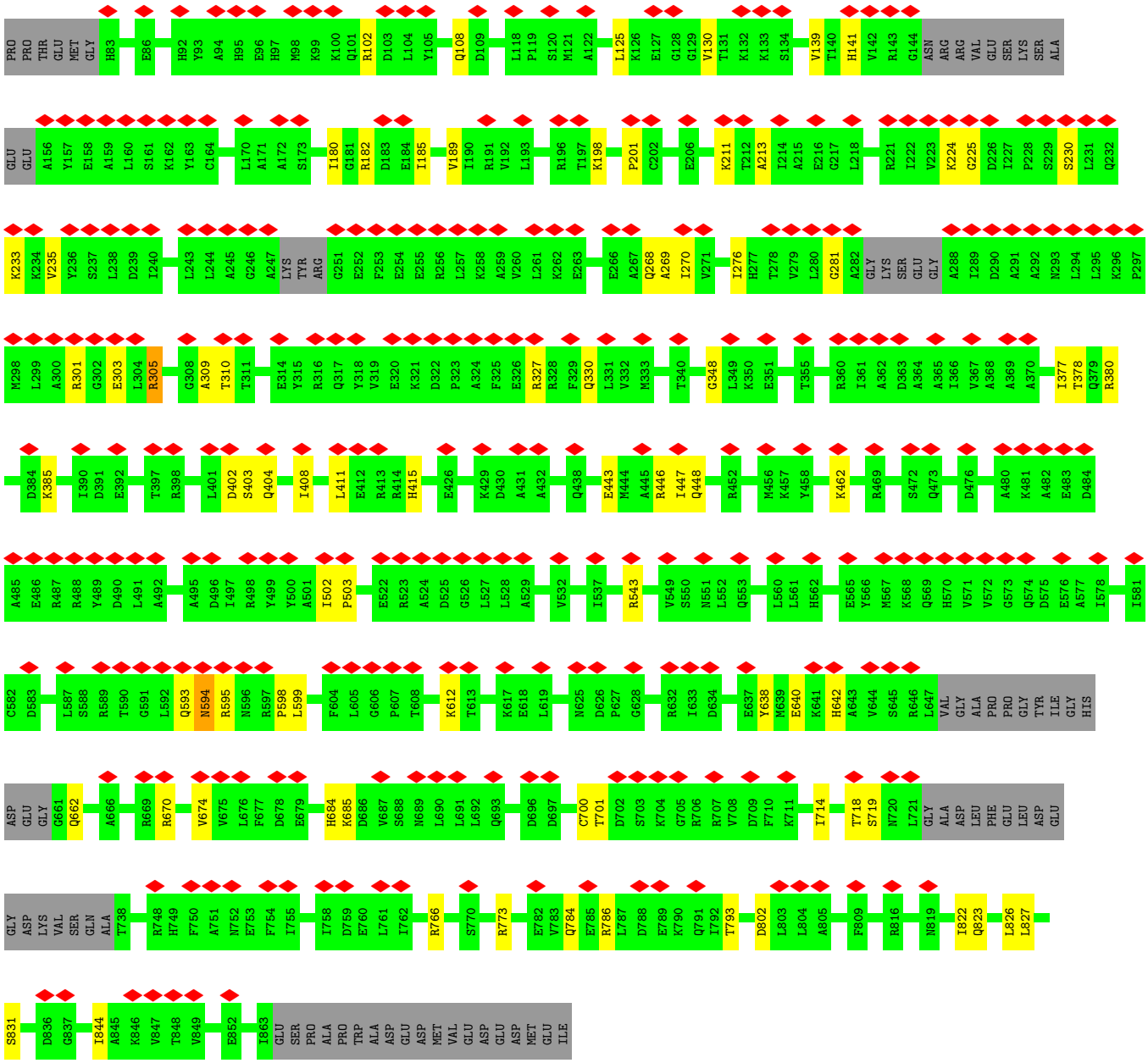
Chain 5:



- Molecule 1: Calcarisporiella thermophila Hsp104

Chain 6:




PRO PRO THR GLU MET GLY H83 E86 H92 Y93 A94 H95 E96 H97 M98 K99 K100 Q101 R102 D103 L104 Y105 Q108 D109 L118 P119 S120 M121 A122 L125 K126 E127 G128 G129 V130 T131 K132 K133 S134 V139 T140 H141 V142 R143 G144 ASN ARG ARG VAL GLU SER LYS SER ALA
GLU GLU A156 Y157 E158 A159 L160 S161 K162 Y163 C164 L170 A171 A172 S173 I180 G181 R182 D183 E184 I185 V189 I190 R191 V192 L193 R196 T197 K198 P201 C202 E206 K211 T212 A213 I214 A215 E216 G217 L218 R221 I222 V223 K224 G225 D226 I227 P228 S229 S230 L231 Q232
K233 K234 V235 Y236 S237 L238 D239 I240 L243 L244 A245 G246 A247 LYS TYR ARG G251 E252 F253 E254 E255 R256 L257 K258 A259 V260 L261 K262 E263 E266 A267 Q268 A269 I270 V271 I276 H277 T278 V279 L280 G281 A282 GLY LYS SER GLU GLY A288 I289 D290 A291 A292 N293 L294 L295 K296 P297
M298 L299 A300 R301 G302 E303 L304 R305 G308 A309 T310 T311 E314 Y315 R316 Q317 Y318 V319 E320 K321 D322 P323 A324 F325 E326 R327 R328 F329 Q330 L331 V332 M333 T340 G348 L349 K350 E351 T355 R360 I361 A362 D363 A364 A365 I366 V367 A368 A369 A370 I377 T378 Q379 R380
D384 K385 I390 D391 E392 T397 R398 L401 D402 S403 Q404 I408 L411 E412 R413 R414 H415 E426 K429 D430 A431 A432 Q438 E443 M444 A445 R446 I447 Q448 R452 M456 K457 Y458 K462 R469 S472 Q473 D476 A480 K481 A482 E483 D484
A485 E486 R487 R488 Y489 D490 L491 A492 A495 D496 I497 R498 Y499 Y500 A501 I502 P503 E522 R523 A524 D525 G526 L527 L528 A529 V532 I537 R543 V549 S550 N551 L552 Q553 L560 L561 H562 E565 Y566 H567 K568 Q569 H570 V571 V572 G573 Q574 D575 E576 A577 I578 I581
C582 D583 L587 S588 R589 T590 G591 L592 Q593 N594 R595 N596 R597 P598 L599 F604 L605 G606 P607 T608 K612 T613 K617 E618 L619 M625 D626 P627 G628 R632 I633 D634 E637 Y638 M639 E640 K641 H642 A643 V644 S645 R646 L647 VAL GLY ALA PRO PRO GLY TYR ILE GLY HIS
ASP GLU GLY G661 Q662 A666 R669 R670 V674 V675 L676 F677 D678 E679 H684 K685 D686 V687 S688 N689 L690 L691 L692 Q693 D696 D697 C700 T701 D702 S703 K704 G705 R706 R707 V708 D709 F710 K711 I714 T718 S719 N720 L721 GLY ALA ASP LEU PHE GLU LEU ASP GLU
GLY ASP LYS VAL SER GLN ALA T738 R748 H749 F750 A751 N752 E753 F754 I755 I758 D759 E760 L761 I762 R766 S770 R773 E782 V783 Q784 E785 R786 L787 D788 E789 K790 Q791 I792 T793 D802 L803 L804 A805 F809 R816 N819 I822 Q823 L826 L827
S831 D836 G837 I844 A845 K846 V847 T848 V849 E852 I863 GLU SER PRO ALA PRO TRP ALA ASP GLU ASP MET VAL GLU ASP GLU ASP MET GLU ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224915	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Gctf	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	31.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1	0.22	0/6411	0.38	0/8631
1	2	0.23	0/6411	0.37	0/8631
1	3	0.22	0/6411	0.37	0/8631
1	4	0.22	0/6411	0.37	0/8631
1	5	0.22	0/6411	0.37	0/8631
1	6	0.22	0/6411	0.37	0/8631
All	All	0.22	0/38466	0.37	0/51786

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	6334	0	6497	53	0
1	2	6334	0	6497	58	0
1	3	6334	0	6497	56	0
1	4	6334	0	6497	49	0
1	5	6334	0	6497	56	0
1	6	6334	0	6497	50	0
2	1	54	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	54	0	24	3	0
2	3	54	0	24	3	0
2	4	54	0	24	1	0
2	5	54	0	24	2	0
2	6	54	0	24	2	0
All	All	38328	0	39126	287	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 4.

All (287) 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)
1:2:156:ALA:N	1:2:236:TYR:HH	1.72	0.88
1:3:106:ILE:HG13	1:4:102:ARG:HH21	1.58	0.69
1:1:816:ARG:HH21	1:6:303:GLU:HG2	1.61	0.65
1:4:784:GLN:HE22	1:4:794:LEU:H	1.42	0.65
1:6:404:GLN:HE21	1:6:408:ILE:HG22	1.62	0.64
1:2:157:TYR:H	1:2:160:LEU:HB2	1.63	0.62
1:5:594:ASN:HD22	1:6:786:ARG:HH21	1.44	0.62
1:1:102:ARG:HH11	1:2:103:ASP:HA	1.65	0.61
1:1:457:LYS:HG3	1:1:523:ARG:HH21	1.65	0.61
1:3:31:PRO:HB3	1:3:90:LEU:HD22	1.83	0.61
1:4:779:ARG:NH1	2:4:902:ADP:N3	2.49	0.60
1:3:300:ALA:HA	1:3:328:ARG:HE	1.67	0.60
1:2:481:LYS:HB3	1:2:493:ARG:HH12	1.66	0.60
1:1:821:LEU:HD13	1:6:230:SER:HB3	1.84	0.60
1:2:357:HIS:O	1:2:398:ARG:NH2	2.34	0.60
1:1:784:GLN:HE22	1:1:794:LEU:H	1.51	0.58
1:6:443:GLU:OE1	1:6:446:ARG:NH2	2.36	0.58
1:1:668:ARG:HD2	1:1:708:VAL:HG22	1.85	0.58
1:1:357:HIS:O	1:1:398:ARG:NH2	2.36	0.58
1:4:602:PHE:HB2	1:4:716:VAL:HG12	1.84	0.58
1:2:39:LEU:HD22	1:2:47:ARG:HH21	1.69	0.58
1:5:633:ILE:HG13	1:5:663:LEU:HD12	1.84	0.58
1:3:95:HIS:HB3	1:4:99:LYS:HB3	1.86	0.57
1:6:674:VAL:HG22	1:6:714:ILE:HD11	1.86	0.57
1:2:53:ALA:HB1	1:2:134:SER:HB3	1.87	0.57
1:6:38:MET:SD	1:6:108:GLN:NE2	2.75	0.57
1:3:448:GLN:HE22	1:3:452:ARG:HE	1.52	0.57
1:5:7:THR:OG1	1:5:162:LYS:NZ	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:41:GLU:HB2	1:3:44:SER:HB2	1.86	0.57
1:4:380:ARG:HB2	1:4:385:LYS:HB3	1.86	0.56
1:2:593:GLN:HE22	1:2:597:ARG:HH21	1.53	0.56
1:5:192:VAL:HG13	1:5:195:ARG:HH21	1.69	0.56
1:6:213:ALA:HB2	2:6:901:ADP:H2'	1.86	0.56
1:5:245:ALA:O	1:5:256:ARG:NH2	2.39	0.56
1:6:700:CYS:SG	1:6:701:THR:N	2.78	0.56
1:2:404:GLN:HE21	1:2:408:ILE:HG22	1.70	0.56
1:3:816:ARG:NH2	2:3:902:ADP:O2B	2.39	0.56
1:4:464:ARG:HG3	1:4:512:LEU:HD22	1.87	0.56
1:3:109:ASP:OD2	1:3:143:ARG:NH1	2.39	0.55
1:4:823:GLN:HA	1:4:827:LEU:HB2	1.88	0.55
1:5:632:ARG:NH1	1:5:678:ASP:OD2	2.40	0.55
1:5:233:LYS:HB3	1:5:269:ALA:HA	1.89	0.55
1:1:696:ASP:OD2	1:1:757:ARG:NH1	2.40	0.54
1:1:39:LEU:O	1:1:47:ARG:NH2	2.41	0.54
1:5:185:ILE:HG12	1:5:188:ARG:HH21	1.72	0.54
1:2:759:ASP:O	1:3:820:ARG:NH2	2.40	0.54
1:2:167:LEU:HD21	1:2:216:GLU:HA	1.90	0.54
1:3:787:LEU:HB3	1:3:792:ILE:HB	1.90	0.54
1:3:609:GLY:HA3	1:3:814:GLY:HA3	1.90	0.54
1:6:39:LEU:O	1:6:47:ARG:NH2	2.41	0.54
1:6:49:ILE:HD13	1:6:139:VAL:HG12	1.90	0.54
1:1:327:ARG:NH2	2:2:901:ADP:O3A	2.41	0.54
1:2:376:TYR:O	1:2:670:ARG:NH1	2.41	0.54
1:5:21:ALA:HB1	1:5:26:HIS:HB2	1.89	0.53
1:1:235:VAL:HG22	1:1:270:ILE:HD11	1.91	0.53
1:5:457:LYS:NZ	1:5:461:GLU:OE2	2.41	0.53
1:3:39:LEU:HD11	1:3:47:ARG:HE	1.73	0.53
1:5:380:ARG:HH21	1:5:384:ASP:HB3	1.74	0.53
1:4:31:PRO:HB3	1:4:90:LEU:HD22	1.90	0.53
1:2:747:ARG:HH21	1:2:761:LEU:HD22	1.74	0.53
1:6:211:LYS:HD2	1:6:309:ALA:HB1	1.91	0.52
1:5:228:PRO:HG3	1:6:403:SER:HB2	1.90	0.52
1:5:252:GLU:OE2	1:5:256:ARG:NH1	2.43	0.52
1:1:484:ASP:OD1	1:1:487:ARG:NH2	2.38	0.52
1:6:402:ASP:OD1	1:6:462:LYS:NZ	2.42	0.52
1:3:825:ALA:O	1:3:829:GLN:NE2	2.43	0.52
1:3:393:ALA:HB1	1:3:536:GLN:HG3	1.92	0.52
1:3:455:LYS:NZ	1:3:459:GLU:OE2	2.43	0.52
1:3:680:MET:HB3	1:3:719:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:691:LEU:HD13	1:4:694:ILE:HD12	1.92	0.52
1:5:200:ASN:HB2	1:5:329:PHE:HA	1.91	0.52
1:1:224:LYS:HA	1:1:487:ARG:HA	1.92	0.51
1:2:465:LEU:HD12	1:2:516:LYS:HE3	1.92	0.51
1:4:847:VAL:HG22	1:4:857:VAL:HG22	1.93	0.51
1:5:167:LEU:HD21	1:5:216:GLU:HA	1.90	0.51
1:6:233:LYS:HB3	1:6:269:ALA:HA	1.92	0.51
1:1:221:ARG:HB3	1:1:226:ASP:HB2	1.92	0.51
1:1:847:VAL:HG22	1:1:857:VAL:HG22	1.92	0.51
1:5:67:ILE:HG12	1:5:70:ARG:HH11	1.75	0.51
1:5:100:LYS:HD3	1:6:102:ARG:HB3	1.91	0.51
1:1:143:ARG:HD2	1:2:99:LYS:HE3	1.93	0.51
1:3:245:ALA:O	1:3:256:ARG:NH2	2.43	0.51
1:4:177:ASP:OD1	1:4:352:ARG:NE	2.43	0.51
1:6:793:THR:HB	1:6:844:ILE:HG12	1.93	0.51
1:6:773:ARG:NH2	1:6:802:ASP:OD1	2.44	0.51
1:4:49:ILE:HD13	1:4:139:VAL:HG12	1.91	0.51
1:1:231:LEU:HD22	1:2:469:ARG:HH22	1.75	0.51
1:2:614:LEU:HD22	2:2:902:ADP:H2'	1.93	0.51
1:6:198:LYS:HB3	1:6:330:GLN:HB2	1.93	0.50
1:6:380:ARG:HB2	1:6:385:LYS:HB3	1.93	0.50
1:1:807:GLN:NE2	1:6:230:SER:OG	2.44	0.50
1:5:327:ARG:NH2	2:6:901:ADP:O2B	2.44	0.50
1:1:810:ASP:HB3	1:1:813:TYR:HB3	1.93	0.50
1:3:322:ASP:HB2	1:3:325:PHE:HD2	1.76	0.50
1:3:633:ILE:HG13	1:3:663:LEU:HD12	1.92	0.50
1:5:843:GLU:OE2	1:5:860:ASN:ND2	2.45	0.50
1:1:115:LEU:HD12	1:1:121:MET:HG3	1.92	0.50
1:2:520:ASP:OD1	1:2:523:ARG:NH2	2.45	0.50
1:5:614:LEU:HD22	2:5:902:ADP:H2'	1.94	0.50
1:6:182:ARG:HD2	1:6:185:ILE:HD12	1.92	0.50
1:6:640:GLU:HG3	1:6:642:HIS:H	1.74	0.50
1:5:520:ASP:OD1	1:5:523:ARG:NH2	2.45	0.49
1:3:99:LYS:HD3	1:4:104:LEU:HA	1.94	0.49
1:3:689:ASN:ND2	1:4:634:ASP:OD2	2.45	0.49
1:3:773:ARG:HH21	1:3:801:LYS:HE3	1.77	0.49
1:6:189:VAL:HG13	1:6:201:PRO:HG3	1.94	0.49
1:6:784:GLN:HE22	1:6:793:THR:HA	1.76	0.49
1:2:823:GLN:HA	1:2:827:LEU:HB2	1.94	0.49
1:6:612:LYS:HD2	1:6:718:THR:HG23	1.94	0.49
1:4:316:ARG:NH2	1:4:704:LYS:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:182:ARG:HD2	1:5:185:ILE:HD12	1.94	0.49
1:6:593:GLN:NE2	1:6:598:PRO:O	2.46	0.49
1:1:787:LEU:HB3	1:1:792:ILE:HB	1.93	0.49
1:2:530:GLU:HG2	1:2:531:VAL:HG23	1.93	0.49
1:3:520:ASP:OD1	1:3:523:ARG:NH2	2.45	0.49
1:3:200:ASN:HD22	1:3:328:ARG:HB3	1.78	0.49
1:3:507:LYS:NZ	1:4:429:LYS:O	2.44	0.49
1:4:233:LYS:HB3	1:4:269:ALA:HA	1.94	0.49
1:3:768:THR:OG1	1:3:771:ASN:OD1	2.31	0.49
1:1:293:ASN:ND2	1:2:241:GLY:O	2.45	0.49
1:2:498:ARG:HD3	1:2:502:ILE:HD12	1.95	0.49
1:5:265:LYS:HD3	1:5:303:GLU:HB3	1.94	0.49
1:5:195:ARG:NH2	1:5:198:LYS:O	2.46	0.48
1:1:102:ARG:HE	1:1:143:ARG:HH21	1.61	0.48
1:1:105:TYR:HH	1:1:251:GLY:N	2.12	0.48
1:1:222:ILE:HG12	1:1:227:ILE:HD13	1.96	0.48
1:4:379:GLN:HG3	1:4:380:ARG:HG2	1.95	0.48
1:4:498:ARG:HD3	1:4:502:ILE:HD12	1.95	0.48
1:1:67:ILE:HG12	1:1:70:ARG:HH11	1.77	0.48
1:2:583:ASP:OD1	1:2:586:ARG:NH2	2.45	0.48
1:5:2:SER:HA	1:6:141:HIS:HB2	1.96	0.48
1:2:817:PRO:HA	1:2:820:ARG:HE	1.77	0.48
1:4:261:LEU:HD13	1:4:264:LEU:HD12	1.94	0.48
1:5:586:ARG:NH1	1:6:831:SER:OG	2.46	0.48
1:3:115:LEU:HB3	1:3:125:LEU:HD11	1.95	0.48
1:1:322:ASP:HB3	1:1:325:PHE:HD2	1.78	0.48
1:2:633:ILE:HG13	1:2:663:LEU:HD12	1.94	0.48
1:4:639:MET:HA	1:4:684:HIS:HB2	1.96	0.48
1:3:233:LYS:HB3	1:3:269:ALA:HA	1.96	0.48
1:3:405:PRO:HD2	1:3:408:ILE:HD12	1.95	0.48
1:2:548:PRO:HD2	1:2:551:ASN:HD22	1.78	0.48
1:2:804:LEU:HD13	1:2:822:ILE:HG12	1.95	0.48
1:5:143:ARG:HG3	1:5:157:TYR:HA	1.96	0.48
1:1:667:VAL:HG23	1:1:708:VAL:HG11	1.96	0.47
1:1:702:ASP:HB3	1:1:706:ARG:H	1.79	0.47
1:1:796:VAL:O	1:1:801:LYS:NZ	2.47	0.47
1:3:182:ARG:HD2	1:3:185:ILE:HD12	1.95	0.47
1:4:448:GLN:HB3	1:4:452:ARG:HE	1.79	0.47
1:2:768:THR:OG1	1:2:771:ASN:OD1	2.31	0.47
1:4:587:LEU:HD11	1:5:827:LEU:HB3	1.95	0.47
1:2:747:ARG:HA	1:2:755:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:759:ASP:O	1:4:820:ARG:NH2	2.47	0.47
1:4:207:PRO:HD3	1:4:311:THR:HG23	1.96	0.47
1:6:411:LEU:HD22	1:6:447:ILE:HG23	1.96	0.47
1:2:293:ASN:HD21	1:3:244:LEU:HD23	1.78	0.47
1:1:843:GLU:OE1	1:1:860:ASN:ND2	2.48	0.47
1:4:2:SER:OG	1:4:3:SER:N	2.45	0.47
1:4:293:ASN:ND2	1:5:241:GLY:O	2.48	0.47
1:5:498:ARG:HA	1:5:502:ILE:HD12	1.96	0.47
1:6:33:HIS:NE2	1:6:68:MET:SD	2.76	0.47
1:3:380:ARG:NH1	1:3:388:ASP:OD2	2.38	0.46
1:2:230:SER:HA	1:3:469:ARG:HH12	1.81	0.46
1:2:609:GLY:N	2:2:902:ADP:O1B	2.43	0.46
1:4:71:GLN:NE2	1:4:86:GLU:OE1	2.48	0.46
1:1:574:GLN:HB3	1:1:577:ALA:HB3	1.96	0.46
1:2:30:HIS:NE2	1:2:86:GLU:OE1	2.47	0.46
1:2:677:PHE:HB2	1:2:717:MET:HG2	1.97	0.46
1:5:104:LEU:HD23	1:5:259:ALA:HB2	1.96	0.46
1:2:464:ARG:HG3	1:2:512:LEU:HD22	1.97	0.46
1:3:498:ARG:HD3	1:3:502:ILE:HD12	1.98	0.46
1:3:608:THR:OG1	2:3:902:ADP:O2B	2.30	0.46
1:4:574:GLN:HB3	1:4:577:ALA:HB3	1.97	0.46
1:6:235:VAL:HG22	1:6:270:ILE:HD11	1.98	0.46
1:1:252:GLU:OE2	1:1:256:ARG:NE	2.49	0.46
1:6:378:THR:HG21	1:6:670:ARG:HG3	1.98	0.46
1:6:594:ASN:HD22	1:6:595:ARG:H	1.63	0.46
1:1:720:ASN:HB3	1:6:301:ARG:HD3	1.96	0.45
1:2:299:LEU:HB2	1:2:328:ARG:HH11	1.82	0.45
1:3:380:ARG:HB2	1:3:385:LYS:HB3	1.97	0.45
1:4:167:LEU:HD21	1:4:216:GLU:HA	1.97	0.45
1:1:610:CYS:HA	1:1:767:LEU:HD21	1.96	0.45
1:2:587:LEU:HD11	1:3:827:LEU:HB3	1.98	0.45
1:5:31:PRO:HB3	1:5:90:LEU:HD22	1.98	0.45
1:5:158:GLU:HG3	1:5:162:LYS:HE2	1.98	0.45
1:5:343:ILE:HD13	1:5:367:VAL:HG22	1.98	0.45
1:1:10:ALA:HB2	1:1:107:ALA:HA	1.98	0.45
1:5:820:ARG:HH11	1:5:824:HIS:HE1	1.65	0.45
1:6:125:LEU:HB3	1:6:130:VAL:HB	1.98	0.45
1:2:760:GLU:OE2	1:3:824:HIS:NE2	2.50	0.45
1:5:177:ASP:OD1	1:5:352:ARG:NE	2.49	0.45
1:2:485:ALA:HB3	1:2:494:ALA:HB2	1.99	0.45
1:6:612:LYS:NZ	1:6:719:SER:O	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:44:SER:O	1:1:162:LYS:NZ	2.44	0.45
1:5:768:THR:OG1	1:5:771:ASN:OD1	2.34	0.45
1:6:47:ARG:HG3	1:6:57:VAL:HG11	1.98	0.45
1:1:597:ARG:NH1	1:1:759:ASP:OD1	2.45	0.45
1:2:561:LEU:HA	1:3:832:ARG:HH12	1.82	0.45
1:2:783:VAL:HG22	1:2:786:ARG:HH21	1.82	0.45
1:6:823:GLN:HA	1:6:827:LEU:HB2	1.99	0.45
1:5:380:ARG:HB2	1:5:385:LYS:HB3	1.99	0.45
1:5:157:TYR:HE2	1:5:267:ALA:HB2	1.82	0.44
1:5:692:LEU:HD13	1:5:754:PHE:HD1	1.82	0.44
1:6:684:HIS:CD2	1:6:685:LYS:H	2.36	0.44
1:4:829:GLN:HE22	1:4:856:ILE:HG13	1.82	0.44
1:3:296:LYS:HB3	1:3:297:PRO:HD3	1.99	0.44
1:5:721:LEU:HD23	1:5:746:ALA:HA	2.00	0.44
1:1:100:LYS:HB2	1:2:101:GLN:HB2	2.00	0.44
1:3:587:LEU:HD11	1:4:827:LEU:HB3	1.99	0.44
1:5:5:GLN:NE2	1:5:104:LEU:O	2.51	0.44
1:1:270:ILE:HG22	1:1:305:ARG:HB3	2.00	0.44
1:2:311:THR:HG22	1:2:313:THR:H	1.83	0.44
1:4:83:HIS:HE1	1:4:88:ALA:HB2	1.83	0.44
1:4:133:LYS:NZ	1:4:137:ASN:OD1	2.49	0.44
1:6:377:ILE:HG21	1:6:380:ARG:HH21	1.82	0.44
1:5:280:LEU:HD13	1:5:292:ALA:HA	1.99	0.44
1:2:609:GLY:HA3	1:2:814:GLY:HA3	1.99	0.44
1:6:305:ARG:H	1:6:305:ARG:HD2	1.83	0.44
1:3:630:ILE:HG12	1:3:674:VAL:HB	2.00	0.44
1:2:793:THR:HB	1:2:844:ILE:HG12	2.00	0.43
1:3:621:ALA:HB2	1:3:627:PRO:HG3	2.00	0.43
1:5:823:GLN:O	1:5:828:THR:OG1	2.36	0.43
1:3:803:LEU:HD12	1:3:806:GLN:HE21	1.83	0.43
1:4:296:LYS:HB3	1:4:297:PRO:HD3	1.98	0.43
1:6:822:ILE:HG23	1:6:826:LEU:HD23	2.00	0.43
1:3:560:LEU:HB3	1:4:835:LEU:HD21	1.99	0.43
1:2:222:ILE:HG12	1:2:227:ILE:HD13	2.01	0.43
1:2:461:GLU:HB3	1:2:516:LYS:HE2	2.00	0.43
1:3:280:LEU:HD22	1:3:318:TYR:HB3	2.01	0.43
1:4:768:THR:OG1	1:4:771:ASN:ND2	2.52	0.43
1:5:7:THR:HG23	1:5:10:ALA:H	1.84	0.43
1:4:597:ARG:HH22	1:4:757:ARG:HE	1.67	0.43
1:5:238:LEU:HD13	1:5:260:VAL:HG11	2.01	0.43
1:5:483:GLU:HB3	1:5:487:ARG:HH12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:483:GLU:HG3	1:2:498:ARG:HH21	1.84	0.43
1:5:464:ARG:HG2	1:5:512:LEU:HD22	2.01	0.43
1:6:270:ILE:HG22	1:6:305:ARG:HD3	2.01	0.43
1:4:229:SER:H	1:5:402:ASP:HB3	1.84	0.43
1:5:142:VAL:O	1:5:156:ALA:N	2.52	0.43
1:2:176:LEU:HD21	1:2:216:GLU:HB3	2.00	0.42
1:3:228:PRO:HG3	1:4:462:LYS:HD2	2.01	0.42
1:4:502:ILE:HB	1:4:503:PRO:HD3	2.01	0.42
1:5:574:GLN:HB3	1:5:577:ALA:HB3	2.00	0.42
1:3:572:VAL:O	2:3:902:ADP:N6	2.52	0.42
1:3:375:ARG:HH11	1:3:376:TYR:HE2	1.66	0.42
1:1:382:MET:HA	1:1:383:PRO:HA	1.87	0.42
1:3:172:ALA:O	1:3:487:ARG:NH2	2.53	0.42
1:1:593:GLN:HE21	1:1:597:ARG:HD3	1.85	0.42
1:4:401:LEU:HD12	1:4:530:GLU:HG2	2.02	0.42
1:6:233:LYS:HE3	1:6:268:GLN:HG2	2.01	0.42
1:2:53:ALA:HB2	1:2:138:ALA:HB2	2.02	0.42
1:5:338:SER:OG	1:5:339:VAL:N	2.53	0.41
1:4:816:ARG:HB3	1:4:817:PRO:HD3	2.02	0.41
1:1:106:ILE:HD12	1:2:102:ARG:HH21	1.85	0.41
1:6:276:ILE:HG22	1:6:310:THR:HB	2.02	0.41
1:6:638:TYR:OH	1:6:662:GLN:OE1	2.38	0.41
1:3:174:GLY:HA3	1:3:480:ALA:HB1	2.02	0.41
1:4:454:LEU:HD22	1:4:523:ARG:HH12	1.85	0.41
1:5:212:THR:HB	2:5:901:ADP:H3'	2.02	0.41
1:1:361:ILE:HA	1:1:532:VAL:HB	2.02	0.41
1:1:380:ARG:HH22	1:1:388:ASP:HB3	1.86	0.41
1:1:823:GLN:O	1:1:828:THR:OG1	2.35	0.41
1:4:30:HIS:HB2	1:4:33:HIS:HD1	1.85	0.41
1:1:105:TYR:OH	1:1:251:GLY:N	2.54	0.41
1:2:605:LEU:HD22	1:2:721:LEU:HB2	2.01	0.41
1:6:502:ILE:HB	1:6:503:PRO:HD3	2.02	0.41
1:2:496:ASP:HA	1:2:500:TYR:HD2	1.85	0.41
1:3:502:ILE:HB	1:3:503:PRO:HD3	2.02	0.41
1:3:833:LEU:HD22	1:3:838:GLY:HA3	2.03	0.41
1:4:595:ARG:O	1:4:711:LYS:NZ	2.41	0.41
1:4:616:VAL:HG21	1:4:676:LEU:HD13	2.02	0.41
1:6:180:ILE:HD13	1:6:348:GLY:HA3	2.02	0.41
1:1:380:ARG:HB2	1:1:385:LYS:HB3	2.03	0.40
1:2:296:LYS:HB3	1:2:297:PRO:HD3	2.03	0.40
1:4:235:VAL:HG22	1:4:270:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:365:ALA:HB2	1:1:533:GLY:HA2	2.02	0.40
1:1:503:PRO:HB3	1:2:424:ALA:HB2	2.03	0.40
1:3:30:HIS:NE2	1:3:86:GLU:OE1	2.55	0.40
1:5:243:LEU:HD22	1:5:256:ARG:HB3	2.02	0.40
1:6:415:HIS:CD2	1:6:448:GLN:HE21	2.39	0.40
1:1:229:SER:OG	1:2:466:ASP:OD2	2.38	0.40
1:1:619:LEU:HD21	1:1:714:ILE:HD13	2.03	0.40
1:2:371:GLN:O	1:2:375:ARG:NE	2.50	0.40
1:3:235:VAL:HG22	1:3:270:ILE:HD11	2.03	0.40
1:5:640:GLU:HG2	1:5:642:HIS:H	1.86	0.40
1:1:276:ILE:HG22	1:1:310:THR:HB	2.02	0.40
1:2:115:LEU:HD12	1:2:121:MET:HG3	2.03	0.40
1:5:540:VAL:HG22	1:5:543:ARG:HH11	1.84	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	1	790/883 (90%)	716 (91%)	66 (8%)	8 (1%)	15	53
1	2	790/883 (90%)	740 (94%)	44 (6%)	6 (1%)	19	58
1	3	790/883 (90%)	732 (93%)	53 (7%)	5 (1%)	25	63
1	4	790/883 (90%)	747 (95%)	38 (5%)	5 (1%)	25	63
1	5	790/883 (90%)	736 (93%)	50 (6%)	4 (0%)	29	67
1	6	790/883 (90%)	729 (92%)	57 (7%)	4 (0%)	29	67
All	All	4740/5298 (90%)	4400 (93%)	308 (6%)	32 (1%)	26	61

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	103	ASP
1	2	101	GLN
1	2	105	TYR
1	6	224	LYS
1	1	611	GLY
1	2	104	LEU
1	2	404	GLN
1	4	611	GLY
1	5	225	GLY
1	6	225	GLY
1	6	599	LEU
1	1	107	ALA
1	1	143	ARG
1	1	813	TYR
1	2	598	PRO
1	3	403	SER
1	4	129	GLY
1	5	208	GLY
1	1	681	GLU
1	1	816	ARG
1	3	208	GLY
1	5	598	PRO
1	3	143	ARG
1	5	224	LYS
1	1	208	GLY
1	3	611	GLY
1	4	281	GLY
1	6	281	GLY
1	3	129	GLY
1	4	842	GLY
1	4	208	GLY
1	2	208	GLY

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	1	679/742 (92%)	675 (99%)	4 (1%)	86	92
1	2	679/742 (92%)	678 (100%)	1 (0%)	93	97
1	3	679/742 (92%)	677 (100%)	2 (0%)	92	95
1	4	679/742 (92%)	676 (100%)	3 (0%)	91	94
1	5	679/742 (92%)	678 (100%)	1 (0%)	93	97
1	6	679/742 (92%)	674 (99%)	5 (1%)	84	90
All	All	4074/4452 (92%)	4058 (100%)	16 (0%)	91	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	15	ASN
1	1	493	ARG
1	1	689	ASN
1	1	766	ARG
1	2	756	ASN
1	3	99	LYS
1	3	493	ARG
1	4	15	ASN
1	4	43	ASN
1	4	493	ARG
1	5	137	ASN
1	6	305	ARG
1	6	327	ARG
1	6	543	ARG
1	6	594	ASN
1	6	766	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	15	ASN
1	1	71	GLN
1	1	101	GLN
1	1	415	HIS
1	1	551	ASN
1	1	593	GLN
1	1	689	ASN
1	1	784	GLN
1	1	807	GLN

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Mol	Chain	Res	Type
1	1	824	HIS
1	2	293	ASN
1	2	551	ASN
1	2	593	GLN
1	2	625	ASN
1	2	756	ASN
1	2	806	GLN
1	3	108	GLN
1	3	200	ASN
1	3	806	GLN
1	3	829	GLN
1	4	15	ASN
1	4	43	ASN
1	4	83	HIS
1	4	293	ASN
1	4	756	ASN
1	4	771	ASN
1	4	784	GLN
1	5	137	ASN
1	5	293	ASN
1	5	536	GLN
1	5	594	ASN
1	6	26	HIS
1	6	200	ASN
1	6	415	HIS
1	6	536	GLN
1	6	594	ASN
1	6	684	HIS
1	6	720	ASN
1	6	771	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)

12 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	$\#\|Z\| > 2$
2	ADP	3	901	-	24,29,29	0.97	1 (4%)	29,45,45	1.40	4 (13%)
2	ADP	2	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.40	4 (13%)
2	ADP	3	902	-	24,29,29	0.96	1 (4%)	29,45,45	1.46	4 (13%)
2	ADP	5	902	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	1	901	-	24,29,29	0.95	1 (4%)	29,45,45	1.39	4 (13%)
2	ADP	1	902	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	4	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)
2	ADP	6	901	-	24,29,29	0.95	1 (4%)	29,45,45	1.39	4 (13%)
2	ADP	6	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	2	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
2	ADP	4	902	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	5	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.42	4 (13%)

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
2	ADP	3	901	-	-	5/12/32/32	0/3/3/3
2	ADP	2	901	-	-	5/12/32/32	0/3/3/3
2	ADP	3	902	-	-	1/12/32/32	0/3/3/3
2	ADP	5	902	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	1	901	-	-	5/12/32/32	0/3/3/3
2	ADP	1	902	-	-	2/12/32/32	0/3/3/3
2	ADP	4	901	-	-	3/12/32/32	0/3/3/3
2	ADP	6	901	-	-	4/12/32/32	0/3/3/3
2	ADP	6	902	-	-	2/12/32/32	0/3/3/3
2	ADP	2	902	-	-	1/12/32/32	0/3/3/3
2	ADP	4	902	-	-	0/12/32/32	0/3/3/3
2	ADP	5	901	-	-	2/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	901	ADP	C5-C4	2.53	1.47	1.40
2	2	901	ADP	C5-C4	2.50	1.47	1.40
2	2	902	ADP	C5-C4	2.50	1.47	1.40
2	1	902	ADP	C5-C4	2.50	1.47	1.40
2	4	901	ADP	C5-C4	2.49	1.47	1.40
2	1	901	ADP	C5-C4	2.49	1.47	1.40
2	5	902	ADP	C5-C4	2.49	1.47	1.40
2	6	902	ADP	C5-C4	2.49	1.47	1.40
2	3	902	ADP	C5-C4	2.48	1.47	1.40
2	5	901	ADP	C5-C4	2.48	1.47	1.40
2	4	902	ADP	C5-C4	2.48	1.47	1.40
2	6	901	ADP	C5-C4	2.47	1.47	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	902	ADP	PA-O3A-PB	-3.56	120.62	132.83
2	3	902	ADP	PA-O3A-PB	-3.51	120.77	132.83
2	5	902	ADP	PA-O3A-PB	-3.49	120.86	132.83
2	1	902	ADP	PA-O3A-PB	-3.48	120.88	132.83
2	4	902	ADP	PA-O3A-PB	-3.46	120.95	132.83
2	6	902	ADP	PA-O3A-PB	-3.46	120.95	132.83
2	2	901	ADP	C3'-C2'-C1'	3.33	105.99	100.98
2	3	901	ADP	C3'-C2'-C1'	3.32	105.98	100.98
2	2	902	ADP	C3'-C2'-C1'	3.32	105.98	100.98
2	6	901	ADP	C3'-C2'-C1'	3.31	105.97	100.98
2	3	902	ADP	C3'-C2'-C1'	3.30	105.94	100.98
2	6	902	ADP	C3'-C2'-C1'	3.30	105.94	100.98
2	5	902	ADP	C3'-C2'-C1'	3.29	105.93	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	4	902	ADP	C3'-C2'-C1'	3.28	105.92	100.98
2	4	901	ADP	C3'-C2'-C1'	3.28	105.91	100.98
2	4	901	ADP	PA-O3A-PB	-3.27	121.61	132.83
2	5	901	ADP	C3'-C2'-C1'	3.24	105.86	100.98
2	5	901	ADP	PA-O3A-PB	-3.23	121.76	132.83
2	1	902	ADP	C3'-C2'-C1'	3.23	105.83	100.98
2	1	901	ADP	N3-C2-N1	-3.19	123.69	128.68
2	2	901	ADP	N3-C2-N1	-3.19	123.70	128.68
2	4	901	ADP	N3-C2-N1	-3.18	123.70	128.68
2	1	901	ADP	C3'-C2'-C1'	3.18	105.77	100.98
2	6	901	ADP	N3-C2-N1	-3.18	123.71	128.68
2	5	902	ADP	N3-C2-N1	-3.18	123.71	128.68
2	4	902	ADP	N3-C2-N1	-3.17	123.72	128.68
2	3	902	ADP	N3-C2-N1	-3.17	123.72	128.68
2	2	902	ADP	N3-C2-N1	-3.17	123.73	128.68
2	3	901	ADP	N3-C2-N1	-3.17	123.73	128.68
2	5	901	ADP	N3-C2-N1	-3.17	123.73	128.68
2	1	902	ADP	N3-C2-N1	-3.16	123.73	128.68
2	6	902	ADP	N3-C2-N1	-3.14	123.77	128.68
2	3	901	ADP	PA-O3A-PB	-2.91	122.84	132.83
2	1	901	ADP	PA-O3A-PB	-2.90	122.89	132.83
2	2	901	ADP	PA-O3A-PB	-2.80	123.23	132.83
2	6	901	ADP	PA-O3A-PB	-2.76	123.35	132.83
2	3	902	ADP	C4-C5-N7	-2.72	106.56	109.40
2	1	901	ADP	C4-C5-N7	-2.72	106.56	109.40
2	3	901	ADP	C4-C5-N7	-2.71	106.58	109.40
2	4	902	ADP	C4-C5-N7	-2.69	106.59	109.40
2	6	901	ADP	C4-C5-N7	-2.69	106.59	109.40
2	5	901	ADP	C4-C5-N7	-2.69	106.60	109.40
2	5	902	ADP	C4-C5-N7	-2.69	106.60	109.40
2	2	901	ADP	C4-C5-N7	-2.68	106.61	109.40
2	6	902	ADP	C4-C5-N7	-2.67	106.61	109.40
2	1	902	ADP	C4-C5-N7	-2.67	106.61	109.40
2	4	901	ADP	C4-C5-N7	-2.65	106.64	109.40
2	2	902	ADP	C4-C5-N7	-2.62	106.67	109.40

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	901	ADP	PB-O3A-PA-O5'
2	1	901	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	2	901	ADP	C5'-O5'-PA-O1A
2	3	901	ADP	PB-O3A-PA-O5'
2	3	901	ADP	C5'-O5'-PA-O1A
2	3	902	ADP	C5'-O5'-PA-O1A
2	6	902	ADP	C5'-O5'-PA-O1A
2	2	901	ADP	PB-O3A-PA-O5'
2	6	901	ADP	PB-O3A-PA-O5'
2	1	901	ADP	C5'-O5'-PA-O3A
2	2	901	ADP	C5'-O5'-PA-O3A
2	3	901	ADP	C5'-O5'-PA-O3A
2	6	901	ADP	C5'-O5'-PA-O3A
2	6	901	ADP	C5'-O5'-PA-O1A
2	1	901	ADP	O4'-C4'-C5'-O5'
2	5	901	ADP	PB-O3A-PA-O2A
2	2	901	ADP	O4'-C4'-C5'-O5'
2	6	902	ADP	C5'-O5'-PA-O3A
2	1	902	ADP	O4'-C4'-C5'-O5'
2	6	901	ADP	O4'-C4'-C5'-O5'
2	4	901	ADP	PB-O3A-PA-O1A
2	4	901	ADP	PB-O3A-PA-O2A
2	5	901	ADP	PB-O3A-PA-O1A
2	1	901	ADP	C5'-O5'-PA-O2A
2	1	902	ADP	C5'-O5'-PA-O1A
2	2	901	ADP	C5'-O5'-PA-O2A
2	2	902	ADP	C5'-O5'-PA-O1A
2	3	901	ADP	C5'-O5'-PA-O2A
2	4	901	ADP	C5'-O5'-PA-O1A
2	5	902	ADP	C5'-O5'-PA-O1A
2	3	901	ADP	O4'-C4'-C5'-O5'

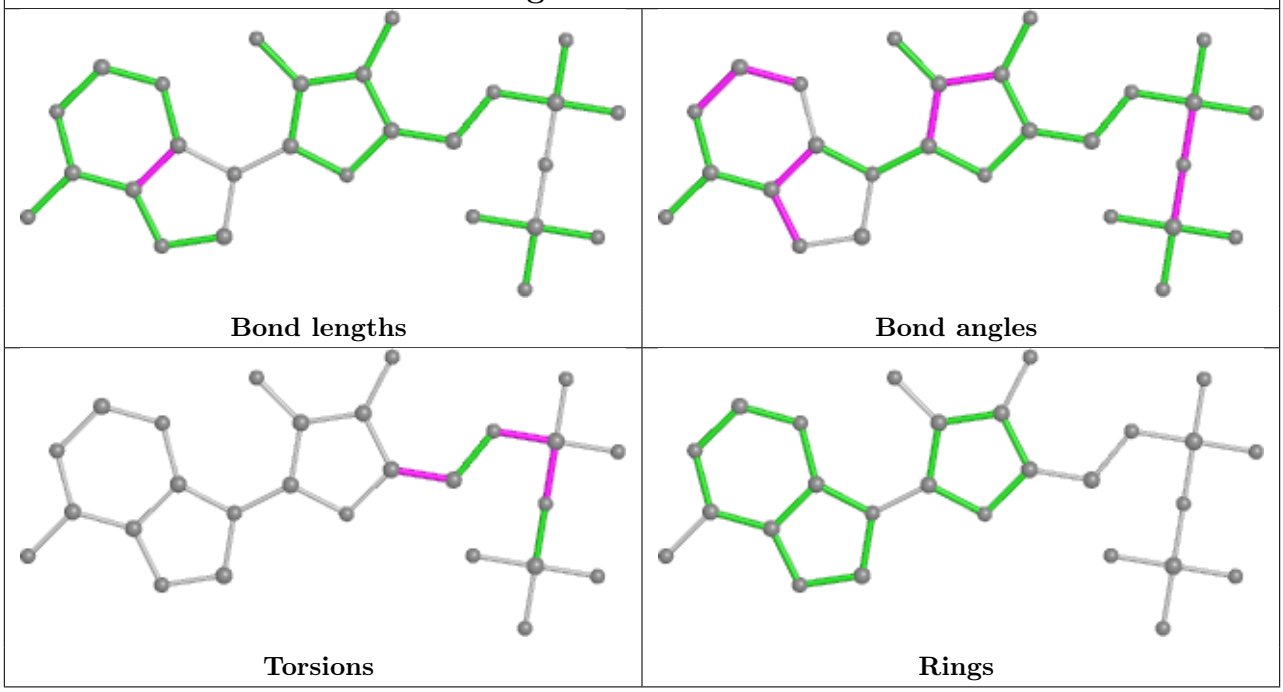
There are no ring outliers.

7 monomers are involved in 11 short contacts:

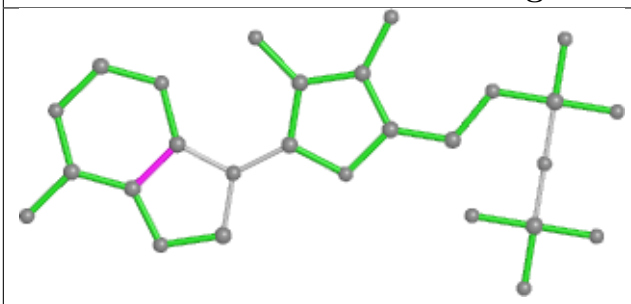
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	901	ADP	1	0
2	3	902	ADP	3	0
2	5	902	ADP	1	0
2	6	901	ADP	2	0
2	2	902	ADP	2	0
2	4	902	ADP	1	0
2	5	901	ADP	1	0

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

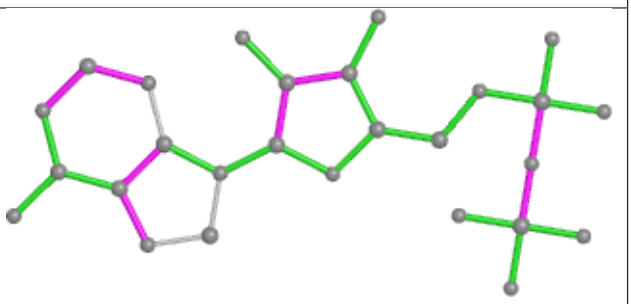
Ligand ADP 3 901



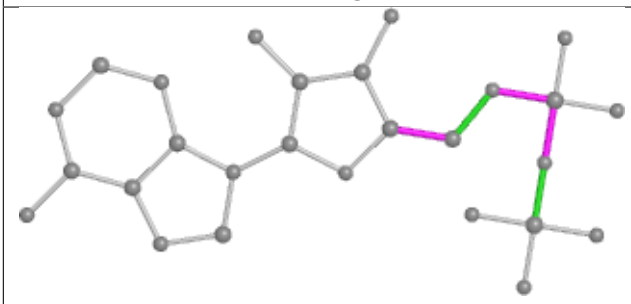
Ligand ADP 2 901



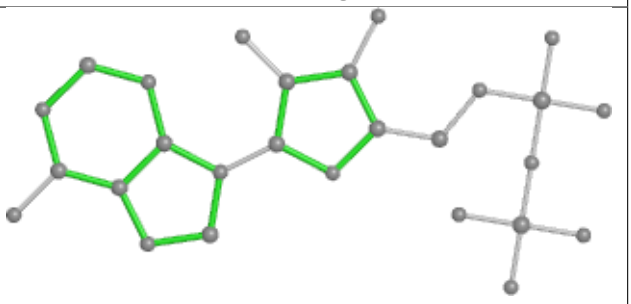
Bond lengths



Bond angles

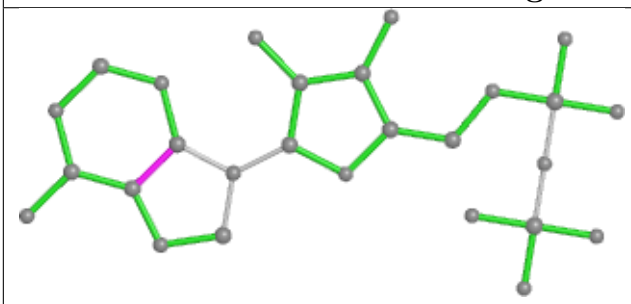


Torsions

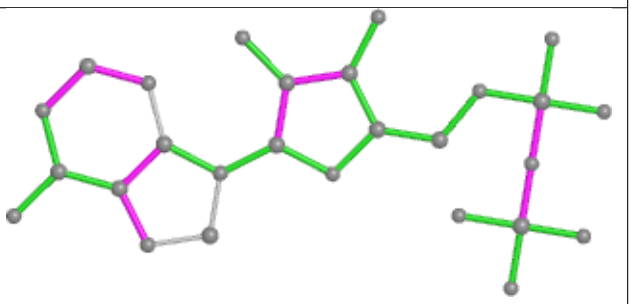


Rings

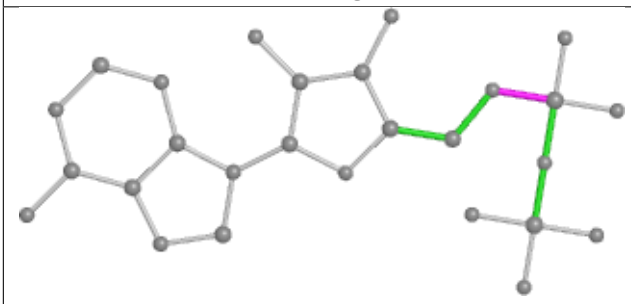
Ligand ADP 3 902



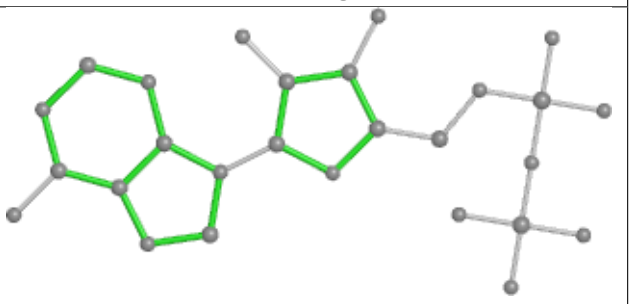
Bond lengths



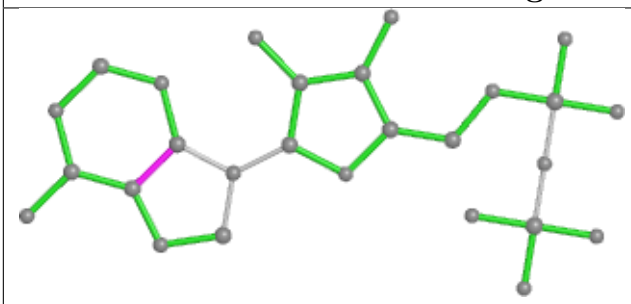
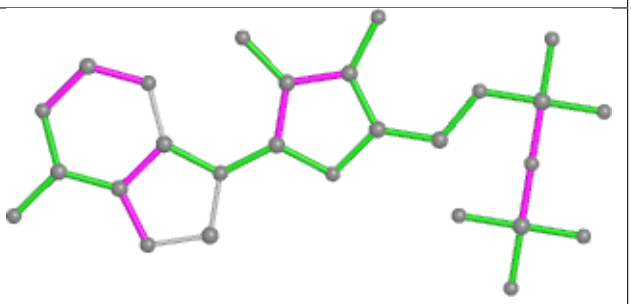
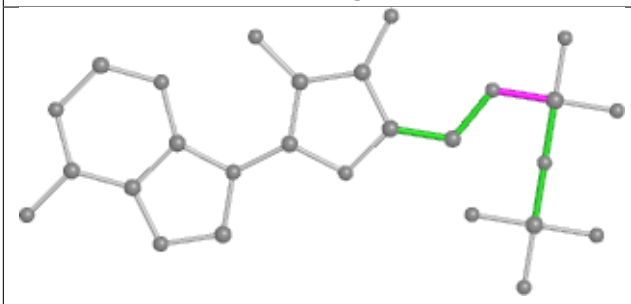
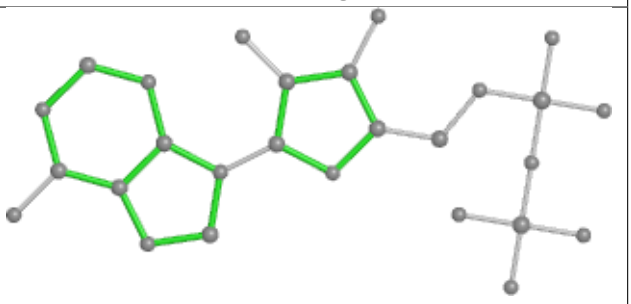
Bond angles

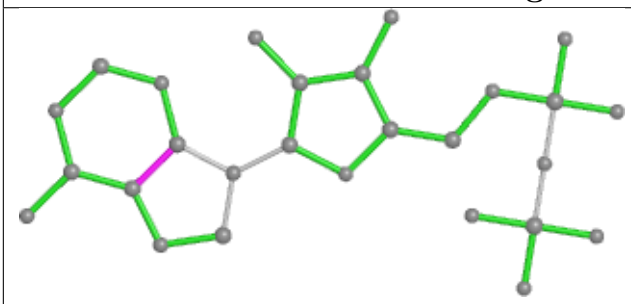
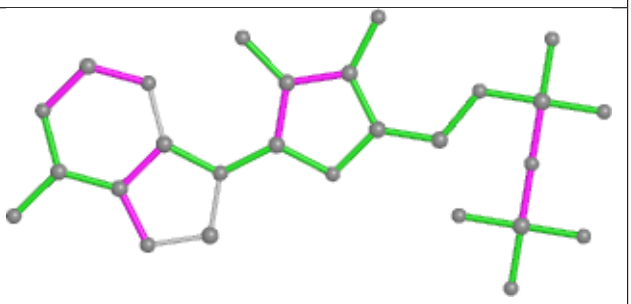
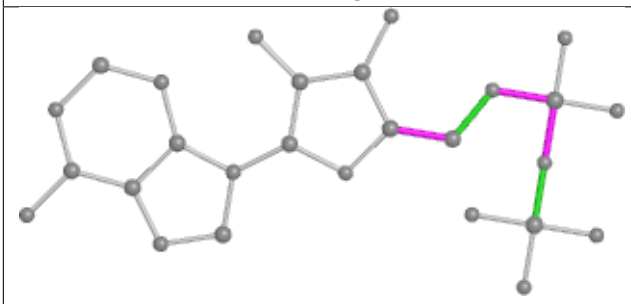
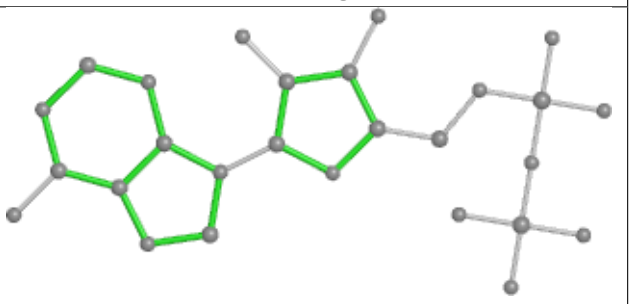


Torsions

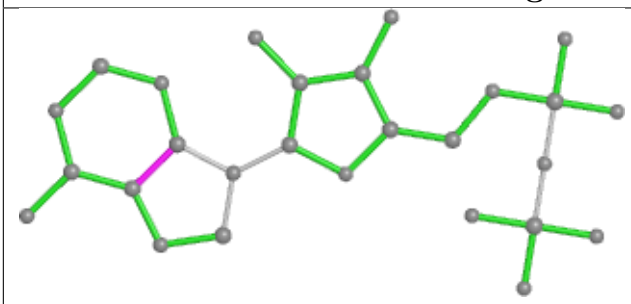


Rings

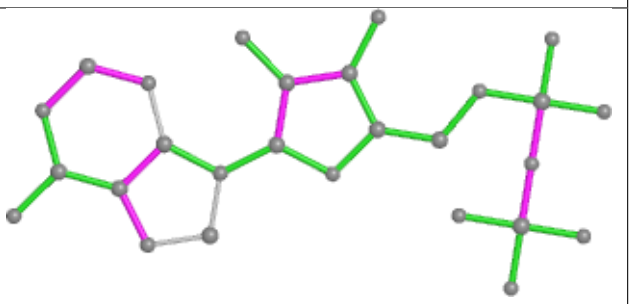
Ligand ADP 5 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP 1 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

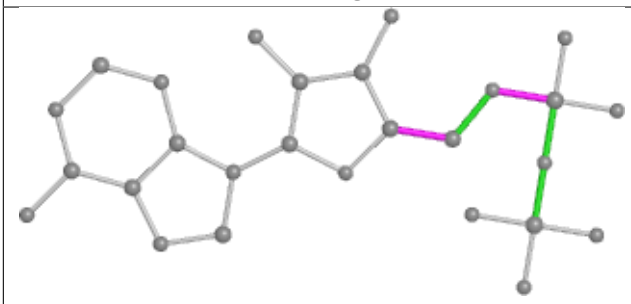
Ligand ADP 1 902



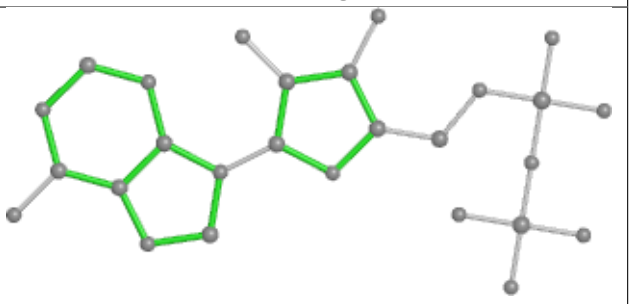
Bond lengths



Bond angles

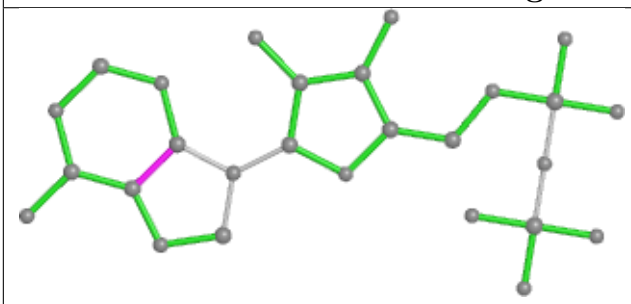


Torsions

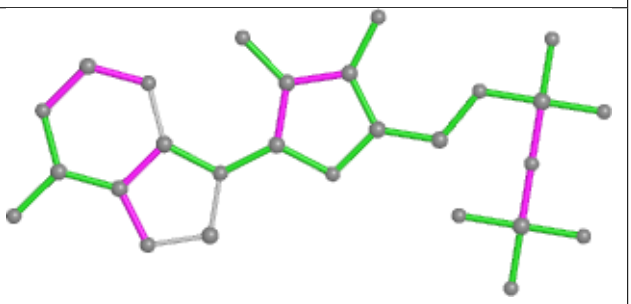


Rings

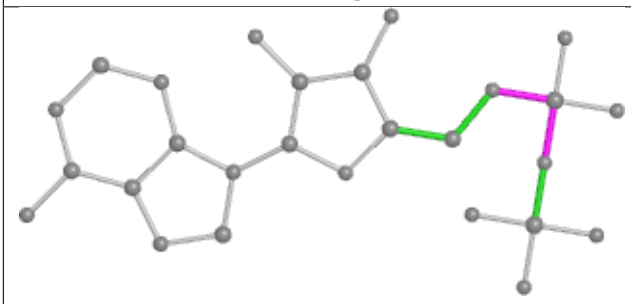
Ligand ADP 4 901



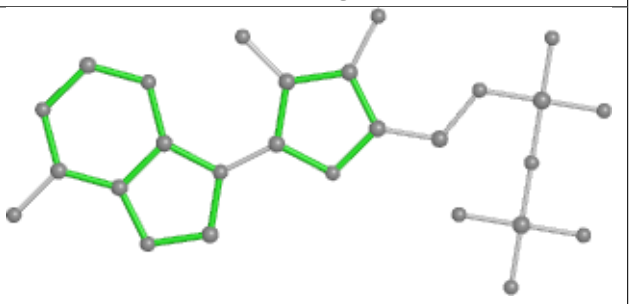
Bond lengths



Bond angles

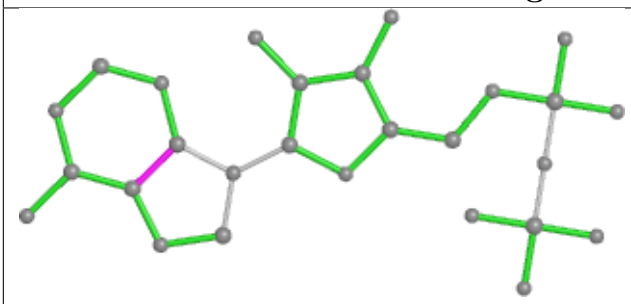


Torsions

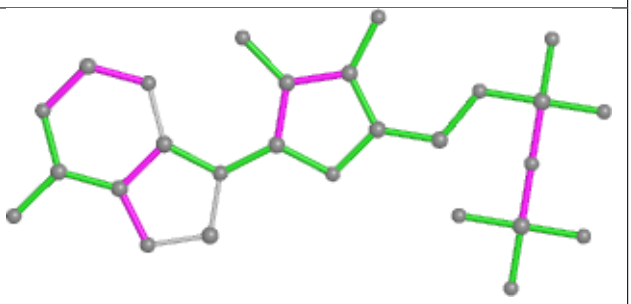


Rings

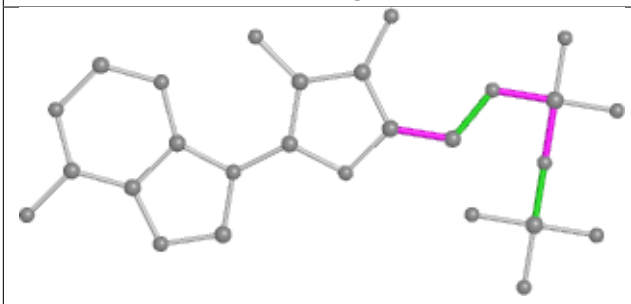
Ligand ADP 6 901



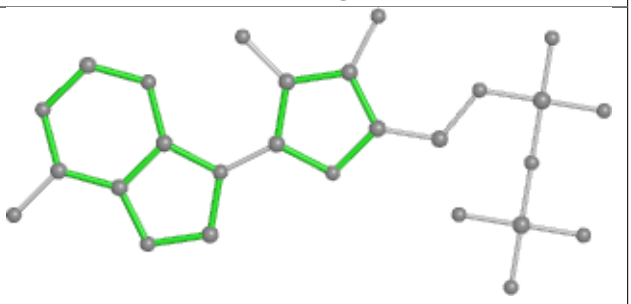
Bond lengths



Bond angles

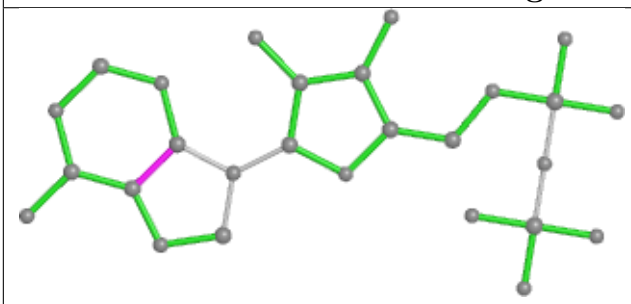


Torsions

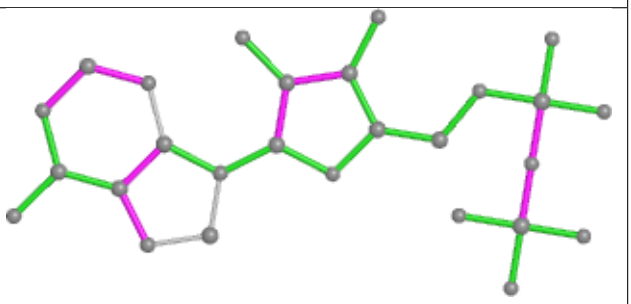


Rings

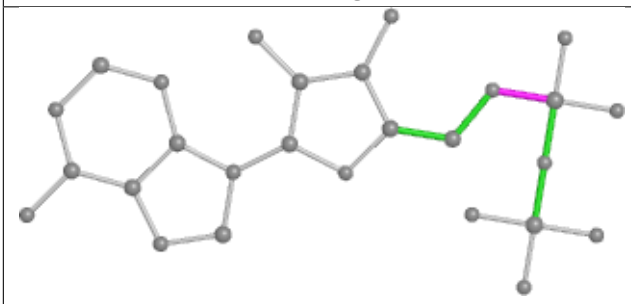
Ligand ADP 6 902



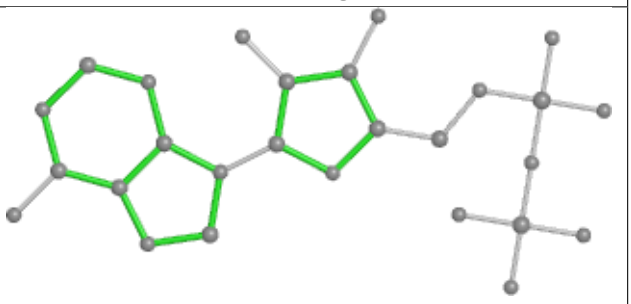
Bond lengths



Bond angles

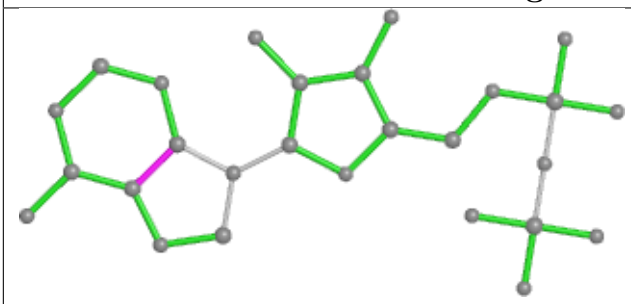


Torsions

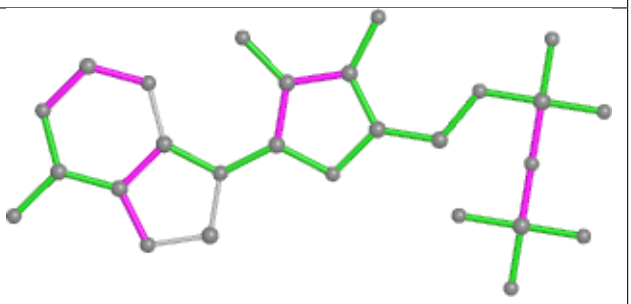


Rings

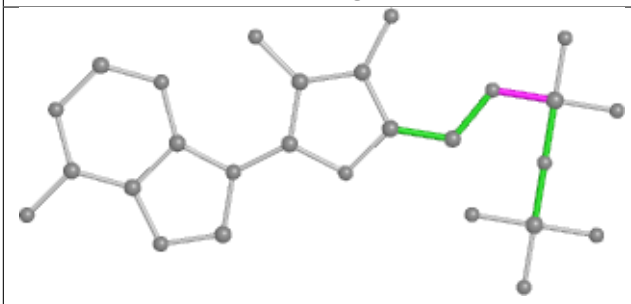
Ligand ADP 2 902



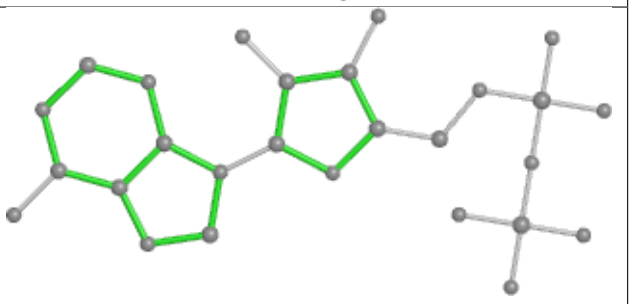
Bond lengths



Bond angles

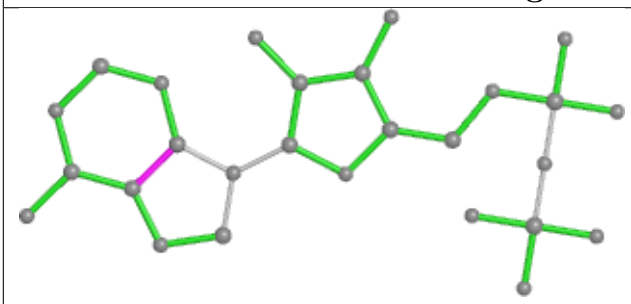


Torsions

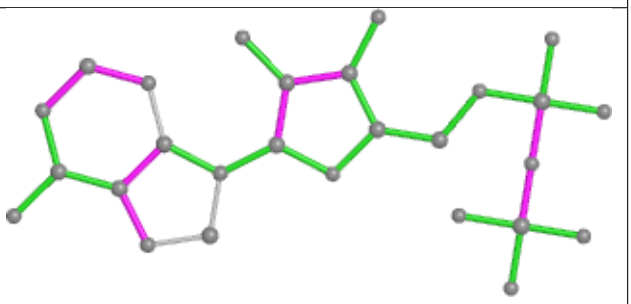


Rings

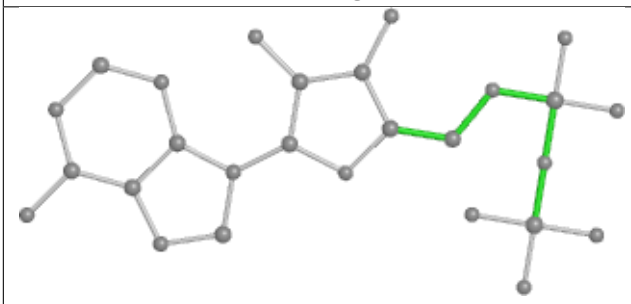
Ligand ADP 4 902



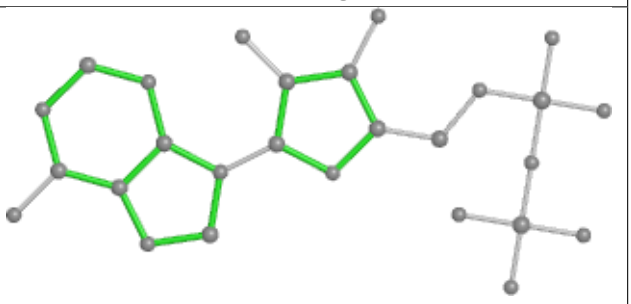
Bond lengths



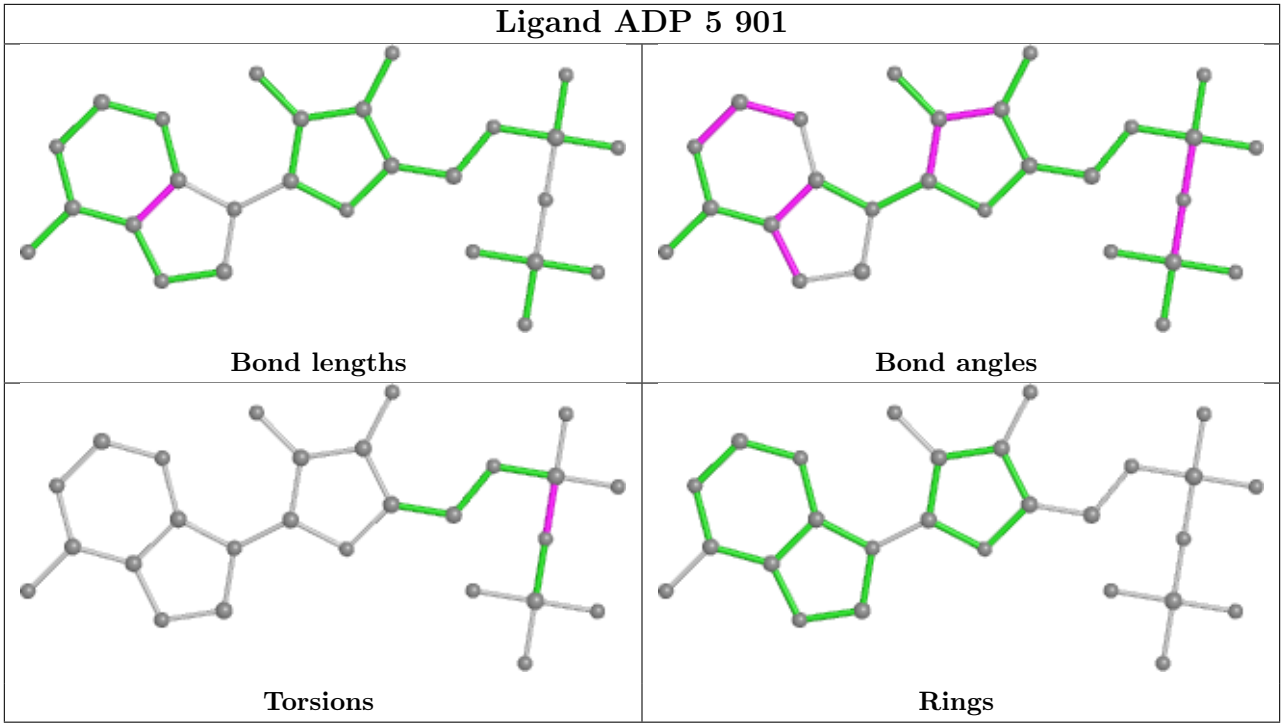
Bond angles



Torsions



Rings



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.

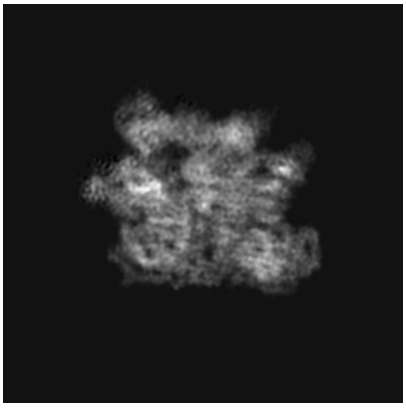
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7782. These allow visual inspection of the internal detail of the map and identification of artifacts.

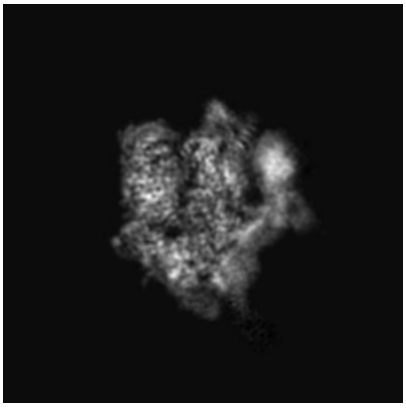
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

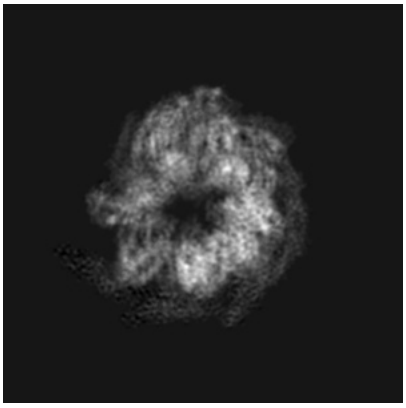
6.1.1 Primary map



X



Y

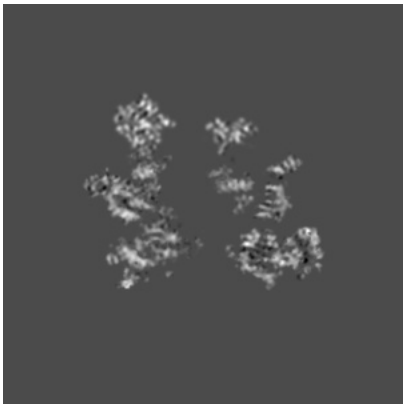


Z

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

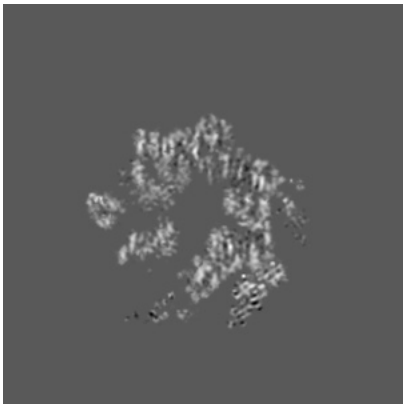
6.2 Central slices (i)

6.2.1 Primary map



X Index: 128

Y Index: 128

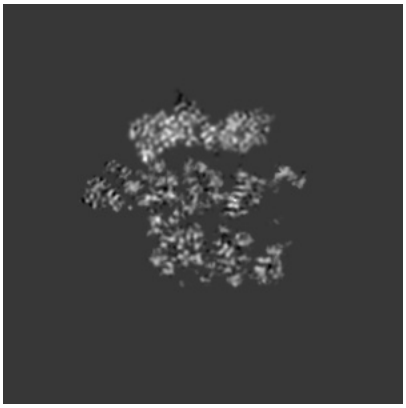


Z Index: 128

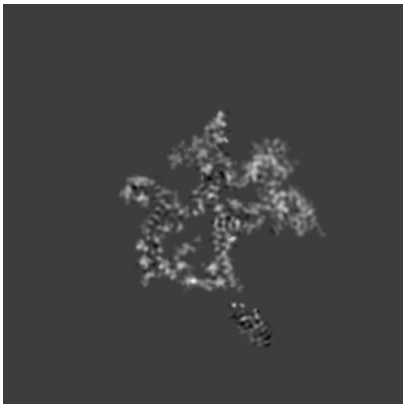
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

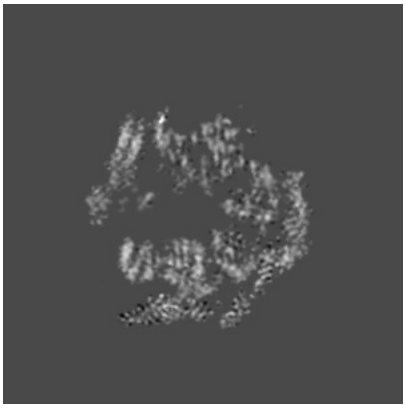
6.3.1 Primary map



X Index: 151



Y Index: 92

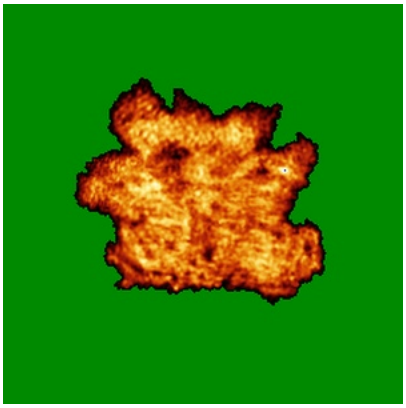


Z Index: 137

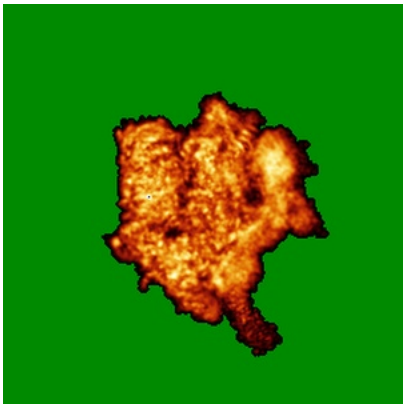
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

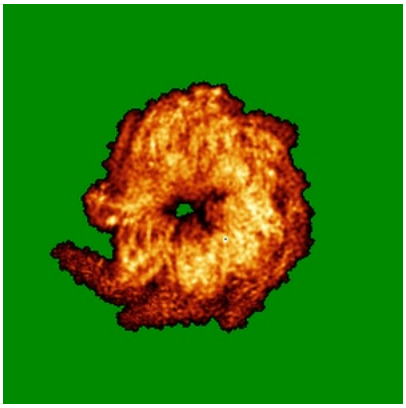
6.4.1 Primary map



X



Y

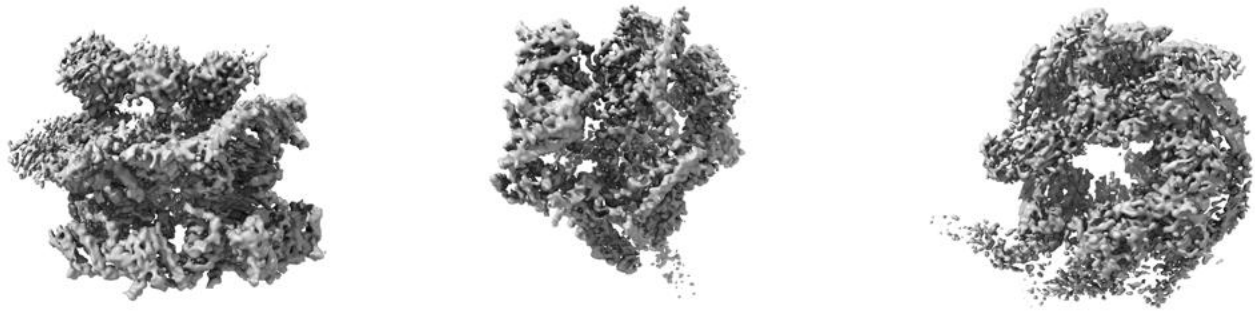


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

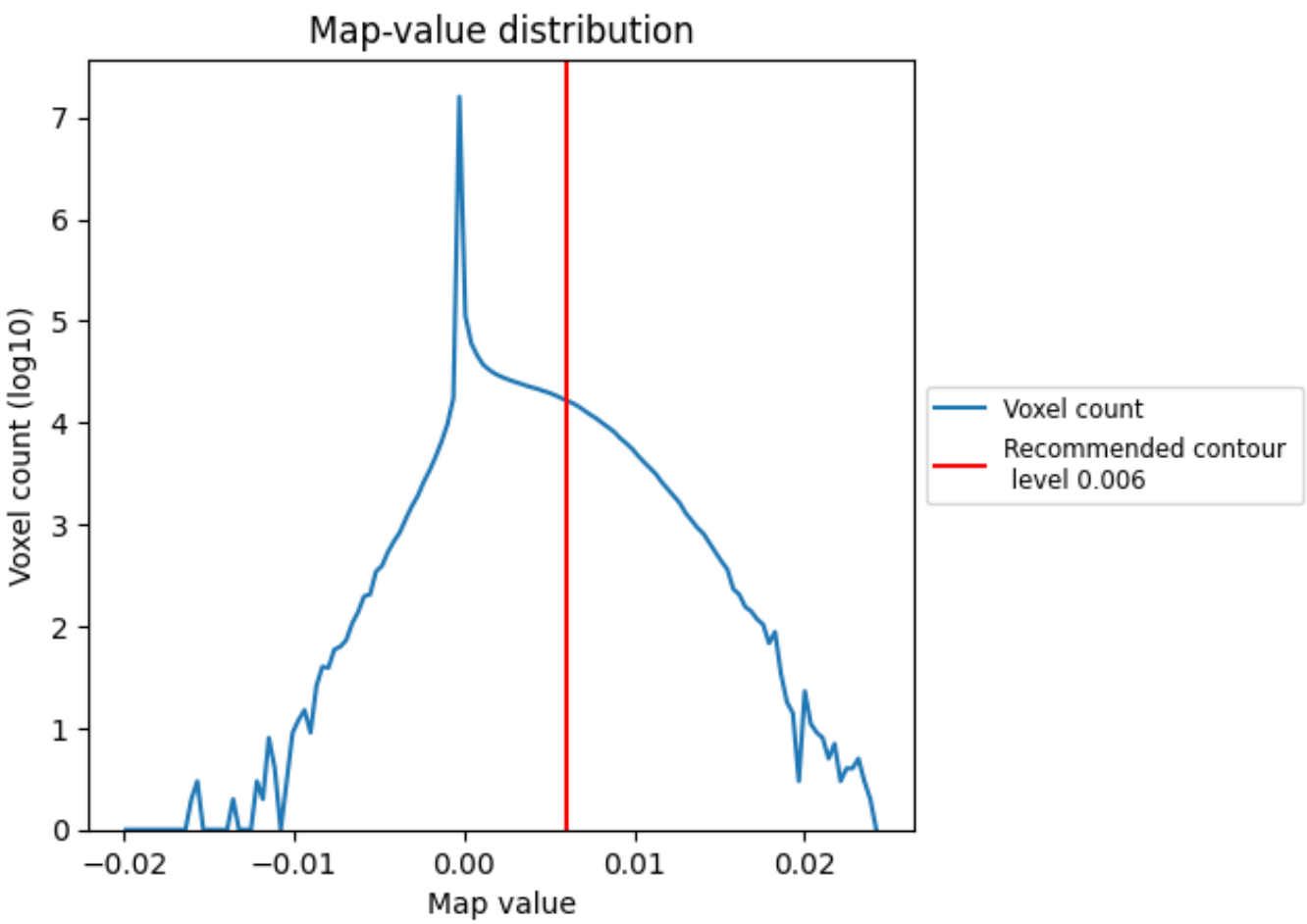
6.6 Mask visualisation (i)

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

7 Map analysis (i)

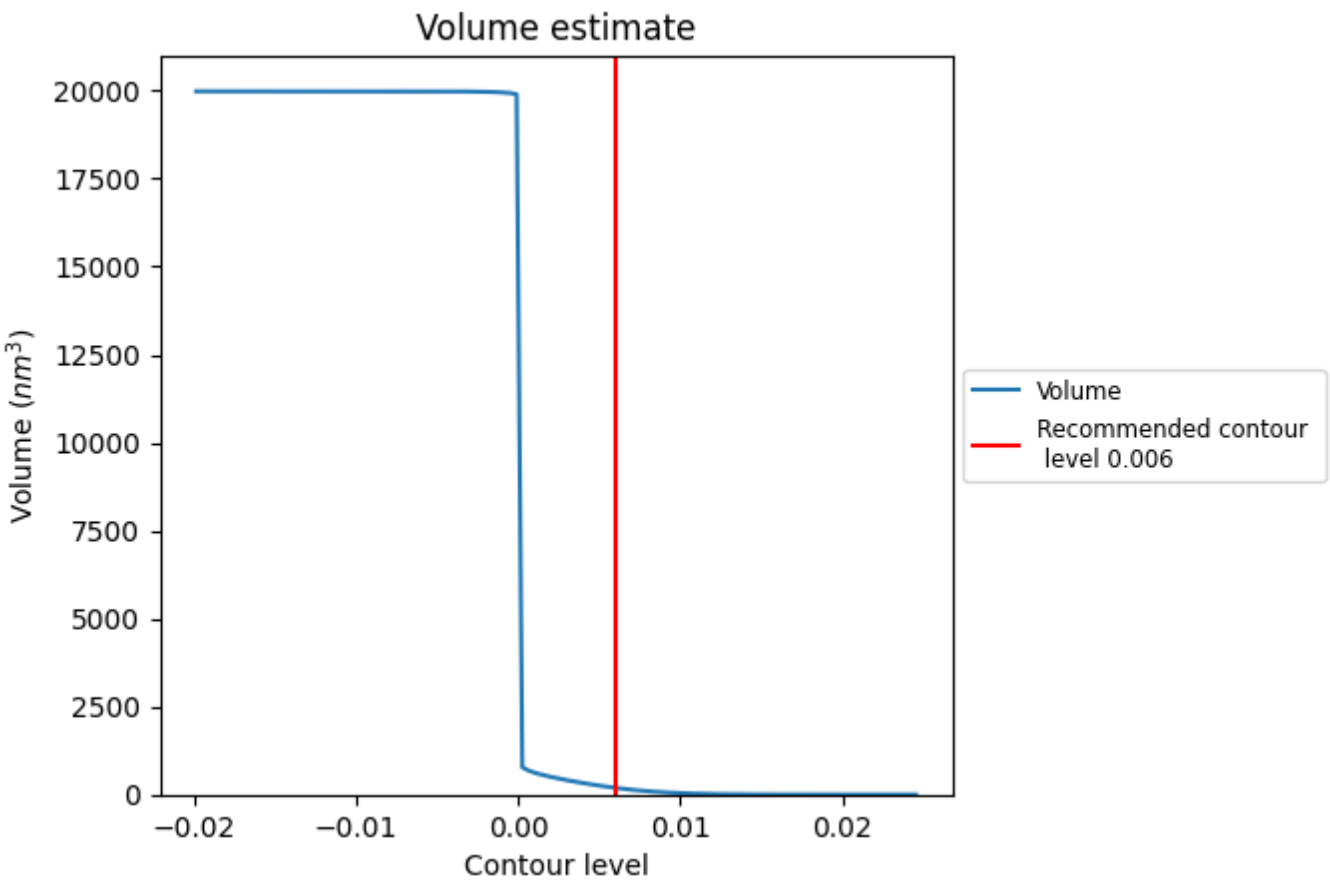
This section contains the results of statistical analysis of the map.

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.

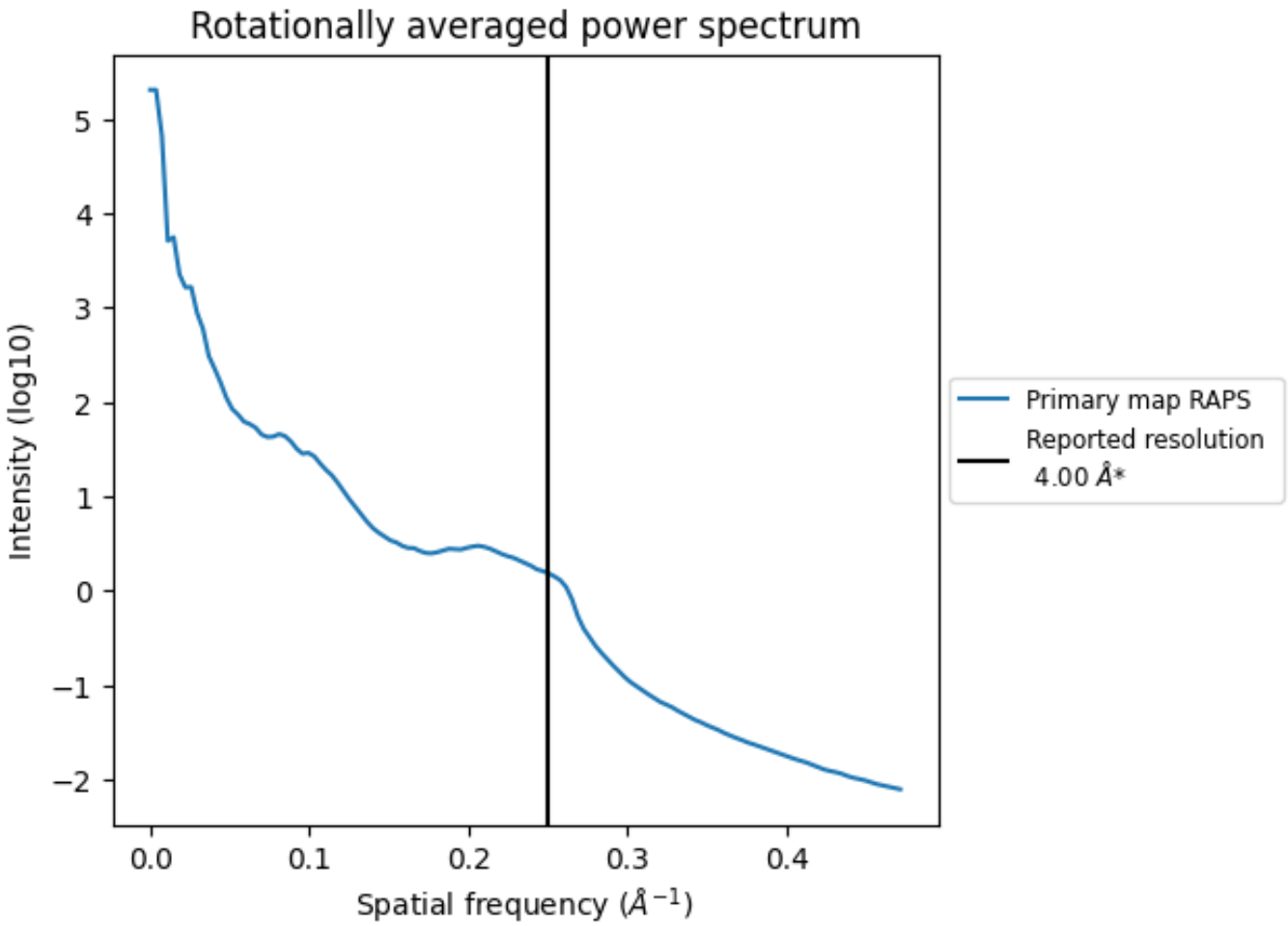
7.2 Volume estimate (i)



The volume at the recommended contour level is 191 nm^3; this corresponds to an approximate mass of 172 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 0.250 Å^{-1}

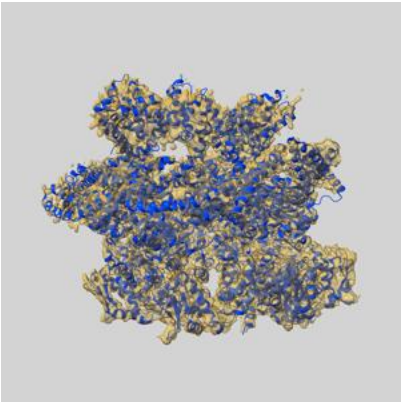
8 Fourier-Shell correlation (i)

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

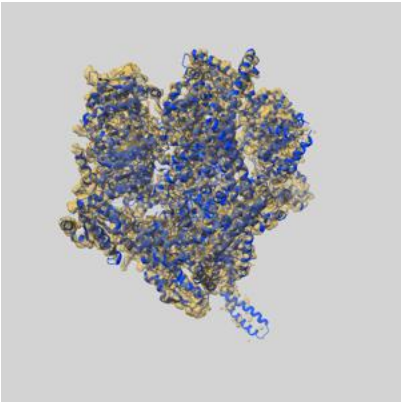
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7782 and PDB model 6D00. Per-residue inclusion information can be found in section 3 on page 5.

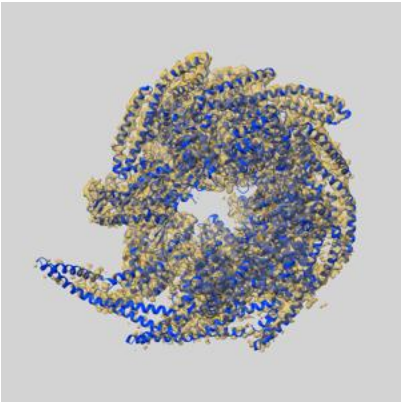
9.1 Map-model overlay (i)



X



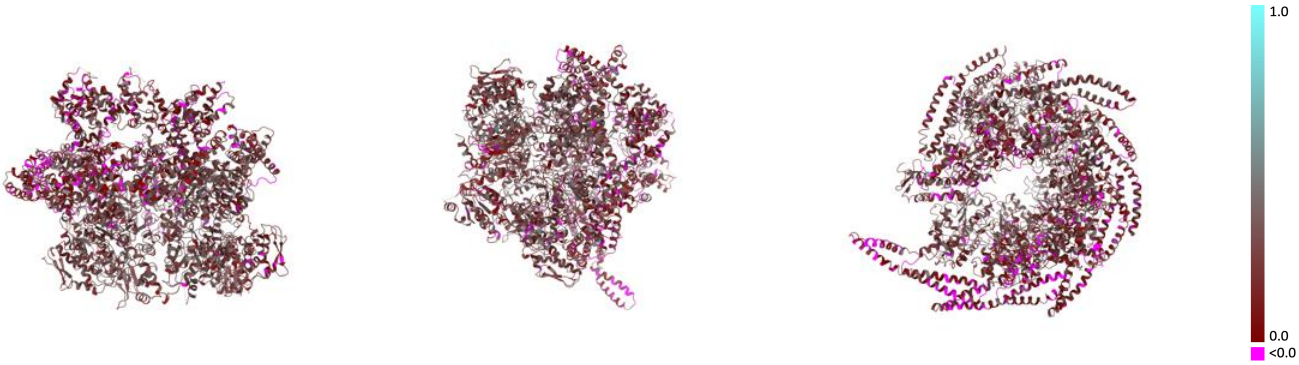
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

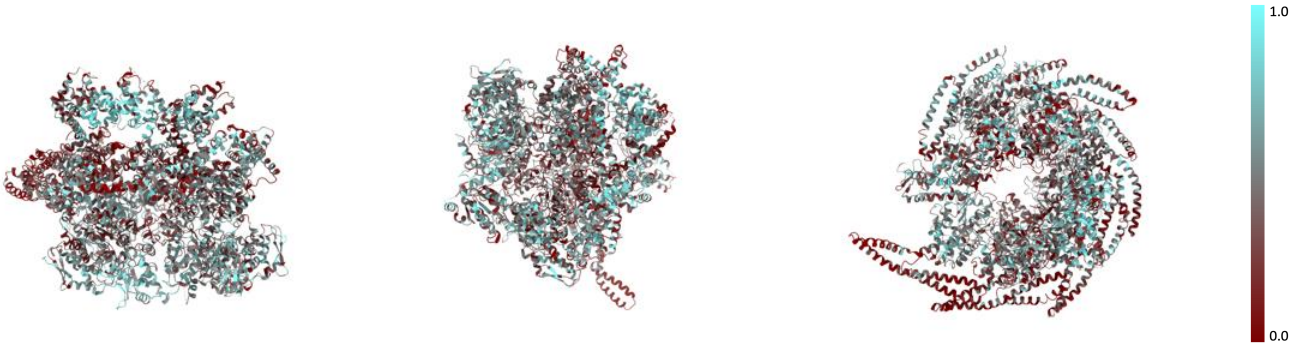
9.2 Q-score mapped to coordinate model (i)



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.

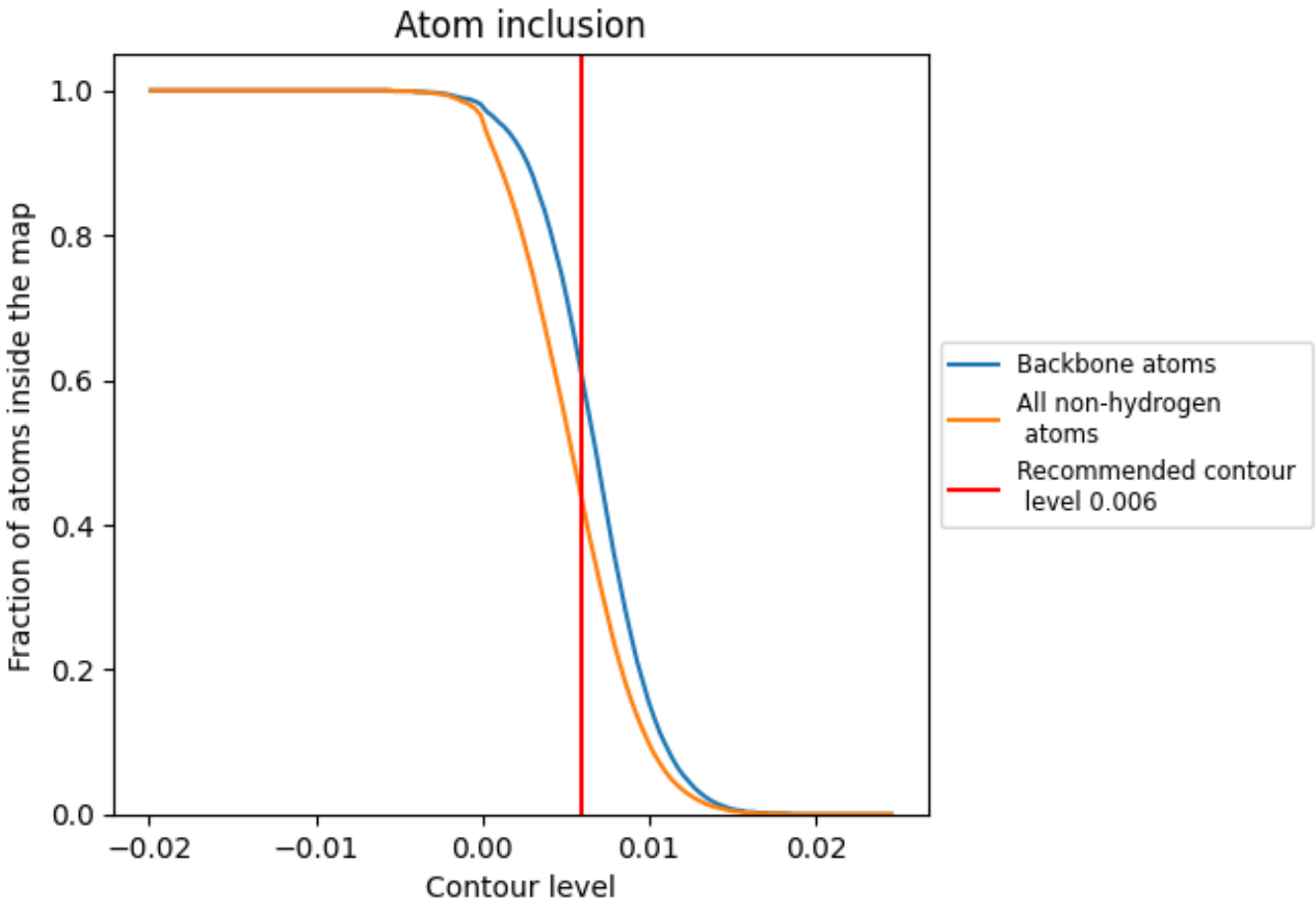
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 43% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4300	0.2320
1	0.4090	0.2030
2	0.3790	0.2150
3	0.4500	0.2470
4	0.4590	0.2660
5	0.4200	0.2410
6	0.4650	0.2240