Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 11:28 PM JST

PDB ID	:	7W8G
EMDB ID	:	EMD-32355
Title	:	Cryo-EM structure of MCM double hexamer
Authors	:	Cheng, J.; Li, N.; Tye, B.; Zhai, Y.; Gao, N.
Deposited on	:	2021-12-07
Resolution	:	2.52 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:

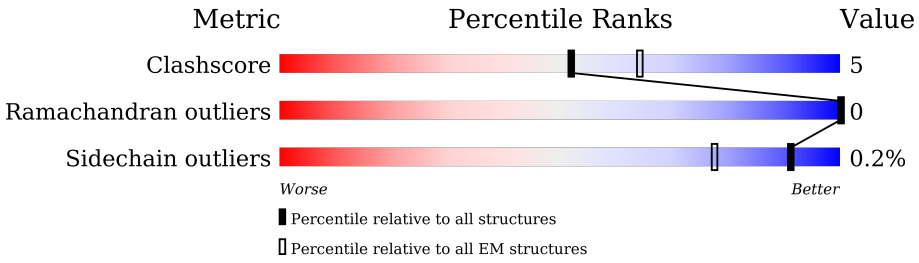
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.52 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	27% 61% 11% 28%
1	B	868	28% 59% 13% 28%
2	3	971	15% 57% 9% 34%
2	C	971	14% 57% 8% 34%
3	4	933	13% 62% 10% 28%
3	D	933	13% 62% 9% 28%
4	5	775	26% 73% 11% 15%
4	E	775	26% 74% 11% 15%

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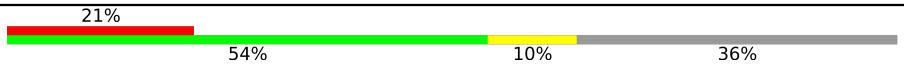
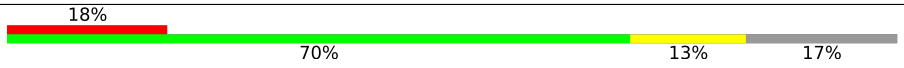
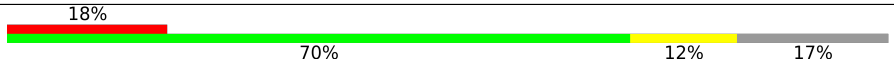
Mol	Chain	Length	Quality of chain
5	6	1017	
5	F	1017	
6	7	845	
6	G	845	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 62460 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	628	Total	C	N	O	S	0	0
			4970	3133	883	935	19		
1	B	628	Total	C	N	O	S	0	0
			4970	3133	883	935	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	637	Total	C	N	O	S	0	0
			4987	3142	889	943	13		
2	C	637	Total	C	N	O	S	0	0
			4987	3142	889	943	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	670	Total	C	N	O	S	0	0
			5323	3339	918	1036	30		
3	D	670	Total	C	N	O	S	0	0
			5323	3339	918	1036	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	658	Total	C	N	O	S	0	0
			5143	3226	882	1010	25		
4	E	658	Total	C	N	O	S	0	0
			5143	3226	882	1010	25		

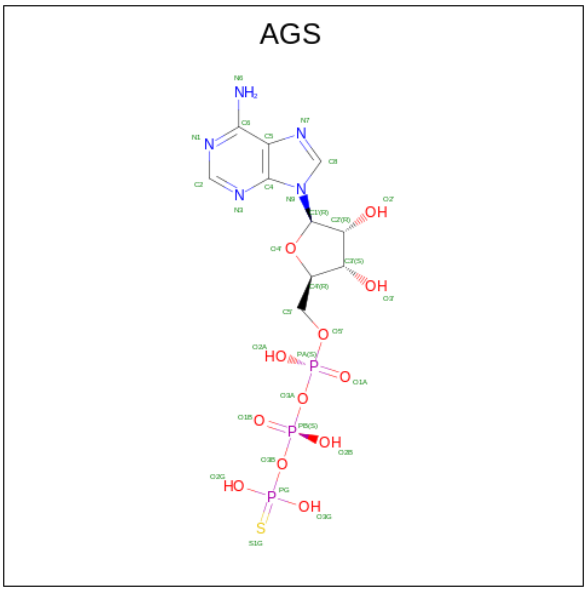
- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	646	Total	C	N	O	S	0	0
			5109	3215	892	977	25		
5	F	646	Total	C	N	O	S	0	0
			5109	3215	892	977	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	699	Total	C	N	O	S	0	0
			5505	3463	952	1059	31		
6	G	699	Total	C	N	O	S	0	0
			5505	3463	952	1059	31		

- Molecule 7 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
7	2	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	4	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	7	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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Mol	Chain	Residues	Atoms						AltConf
7	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	G	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

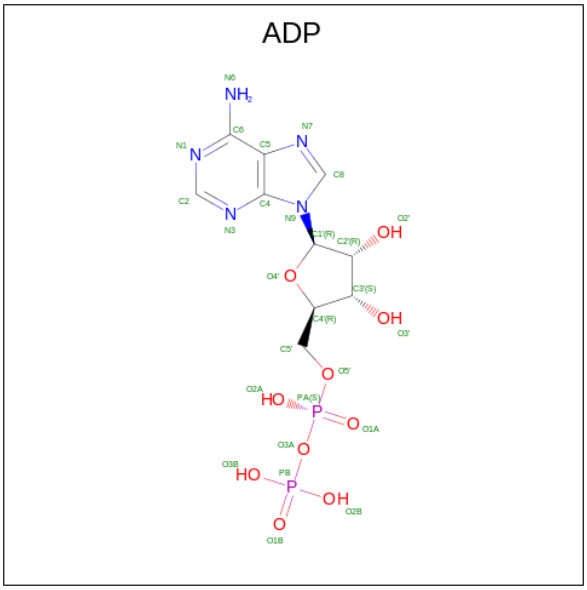
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	2	1	Total	Mg	0
			1	1	
8	3	1	Total	Mg	0
			1	1	
8	4	1	Total	Mg	0
			1	1	
8	5	1	Total	Mg	0
			1	1	
8	6	1	Total	Mg	0
			1	1	
8	7	1	Total	Mg	0
			1	1	
8	B	1	Total	Mg	0
			1	1	
8	C	1	Total	Mg	0
			1	1	
8	D	1	Total	Mg	0
			1	1	
8	E	1	Total	Mg	0
			1	1	
8	F	1	Total	Mg	0
			1	1	
8	G	1	Total	Mg	0
			1	1	

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
9	2	1	Total Zn 1 1	0
9	4	1	Total Zn 1 1	0
9	5	1	Total Zn 1 1	0
9	6	1	Total Zn 1 1	0
9	7	1	Total Zn 1 1	0
9	B	1	Total Zn 1 1	0
9	D	1	Total Zn 1 1	0
9	E	1	Total Zn 1 1	0
9	F	1	Total Zn 1 1	0
9	G	1	Total Zn 1 1	0

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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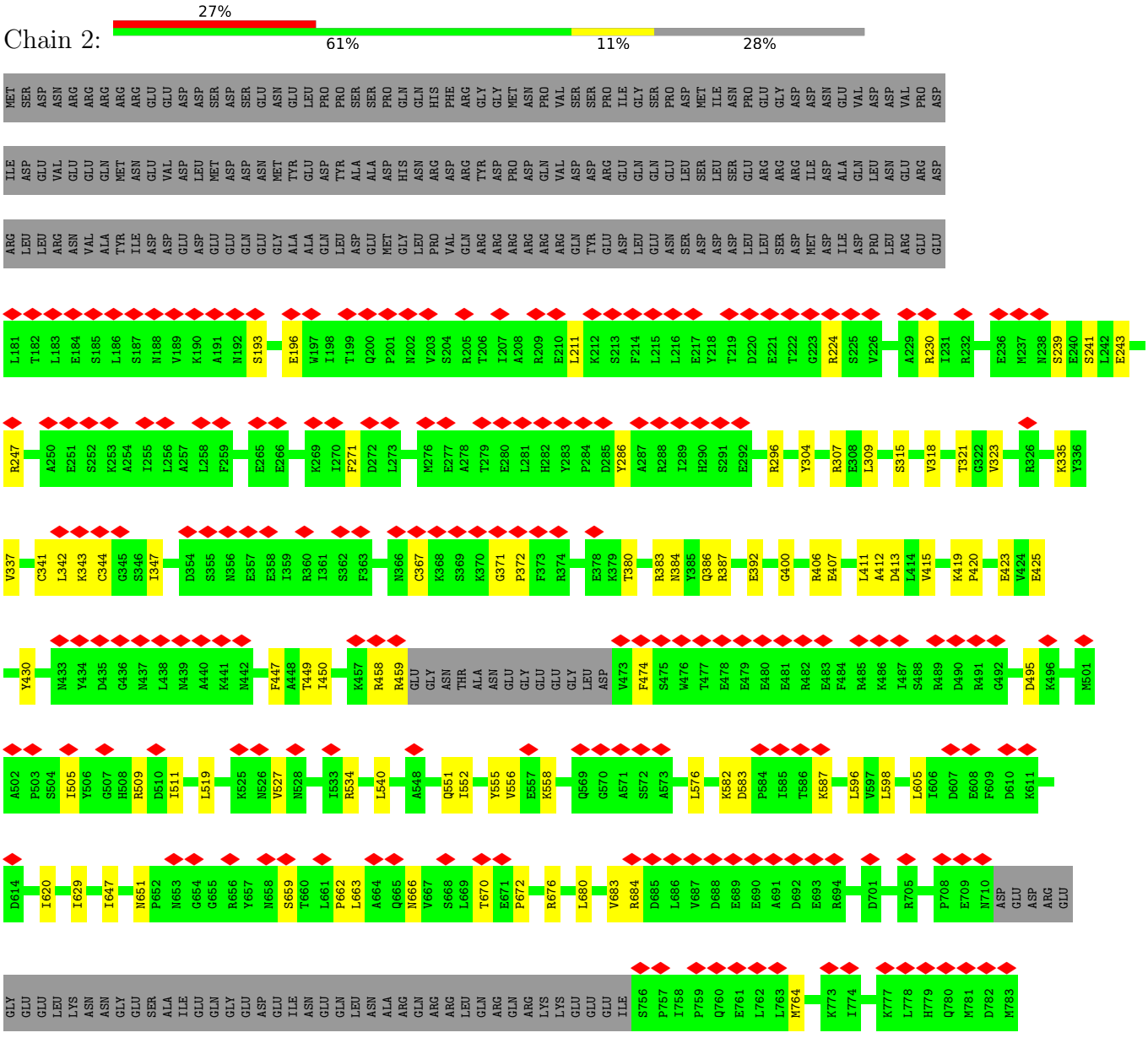
Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

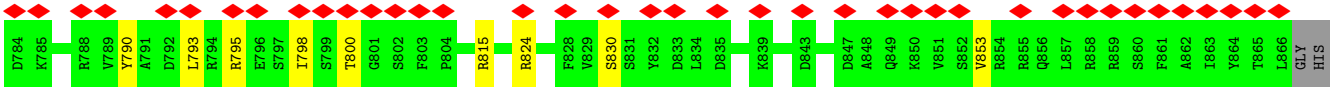
3 Residue-property plots (i)

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

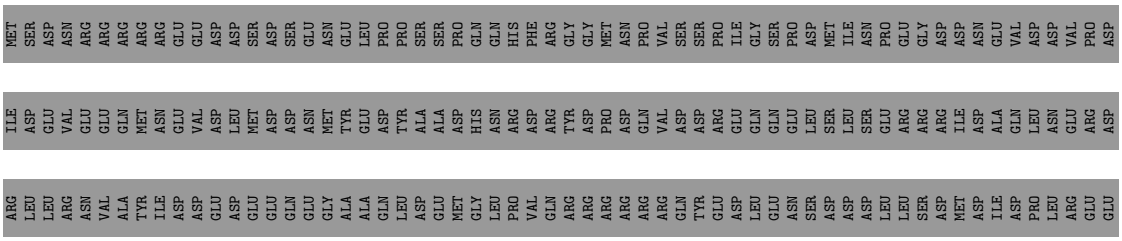
Chain 2:

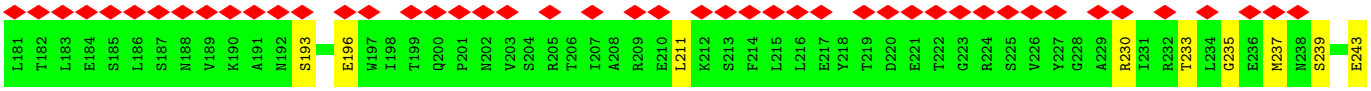


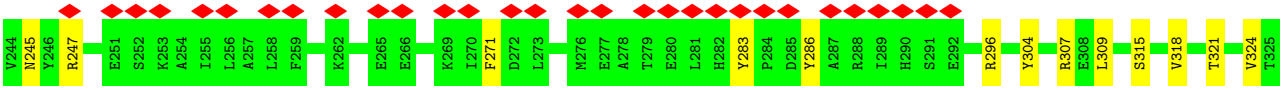


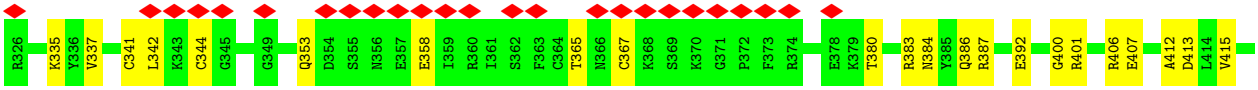
• Molecule 1: DNA replication licensing factor MCM2

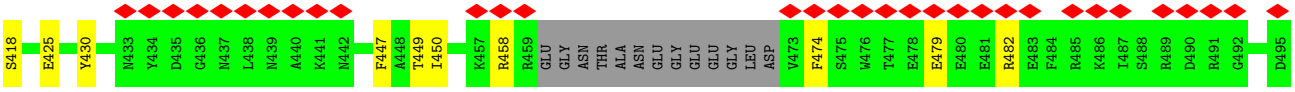
Chain B:

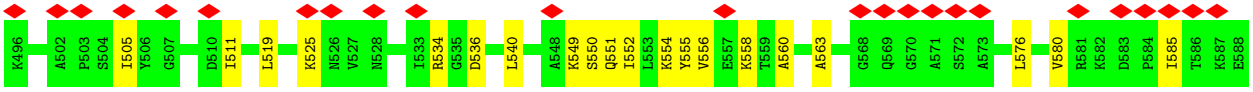


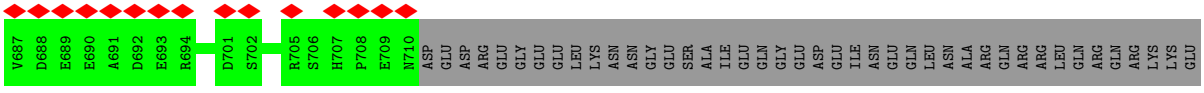


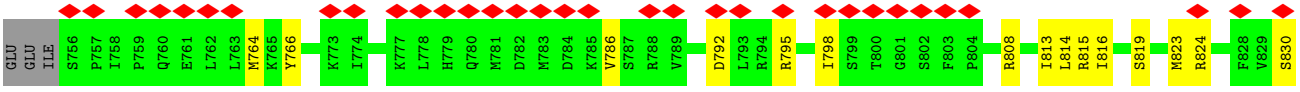


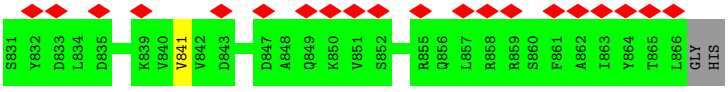






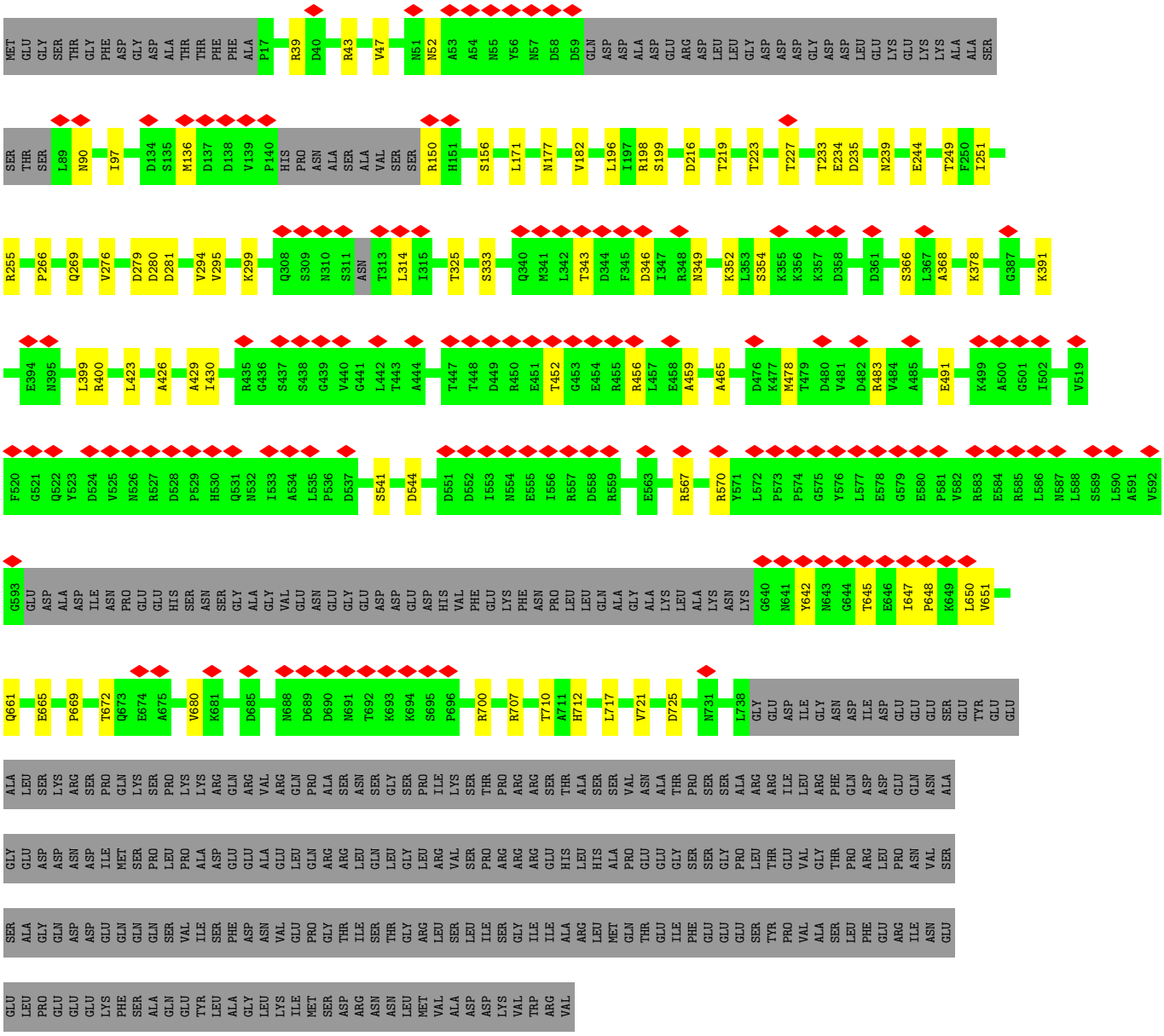






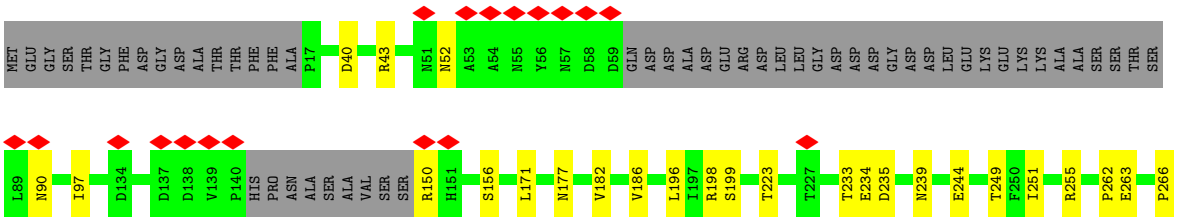
• Molecule 2: DNA replication licensing factor MCM3

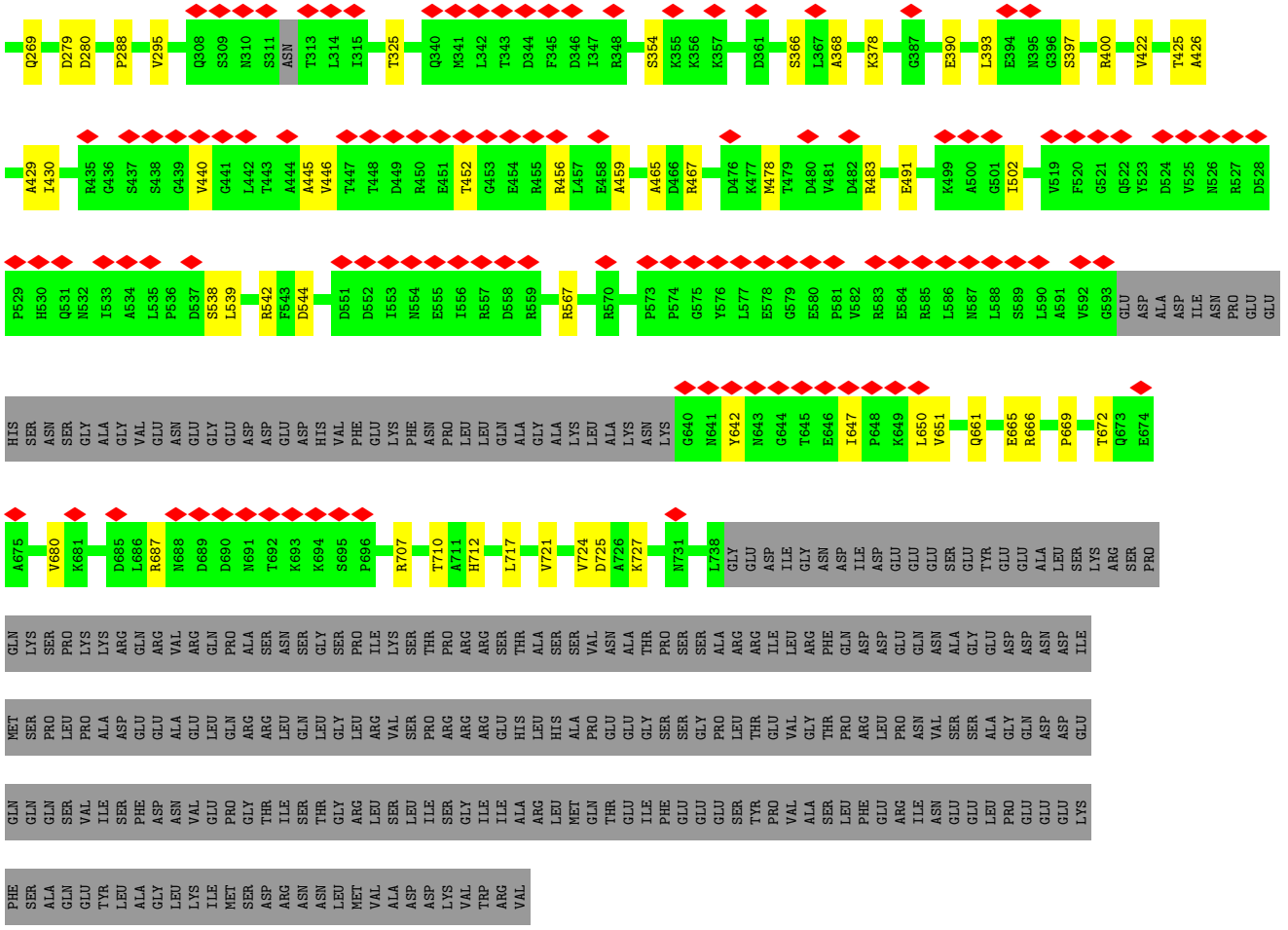
Chain 3:



• Molecule 2: DNA replication licensing factor MCM3

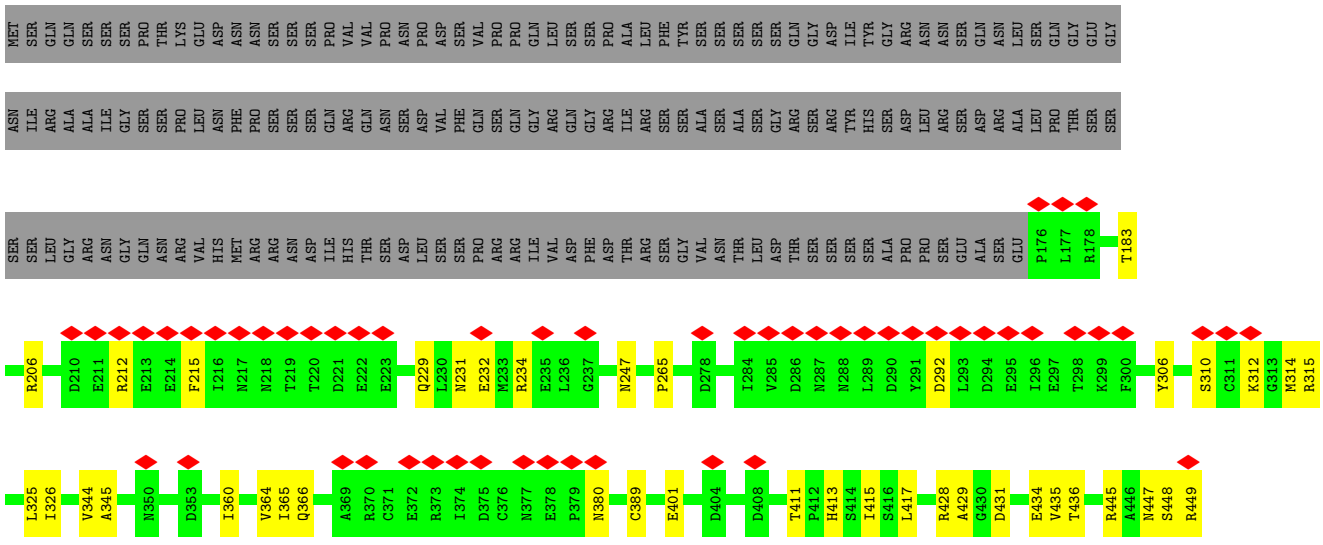
Chain C:

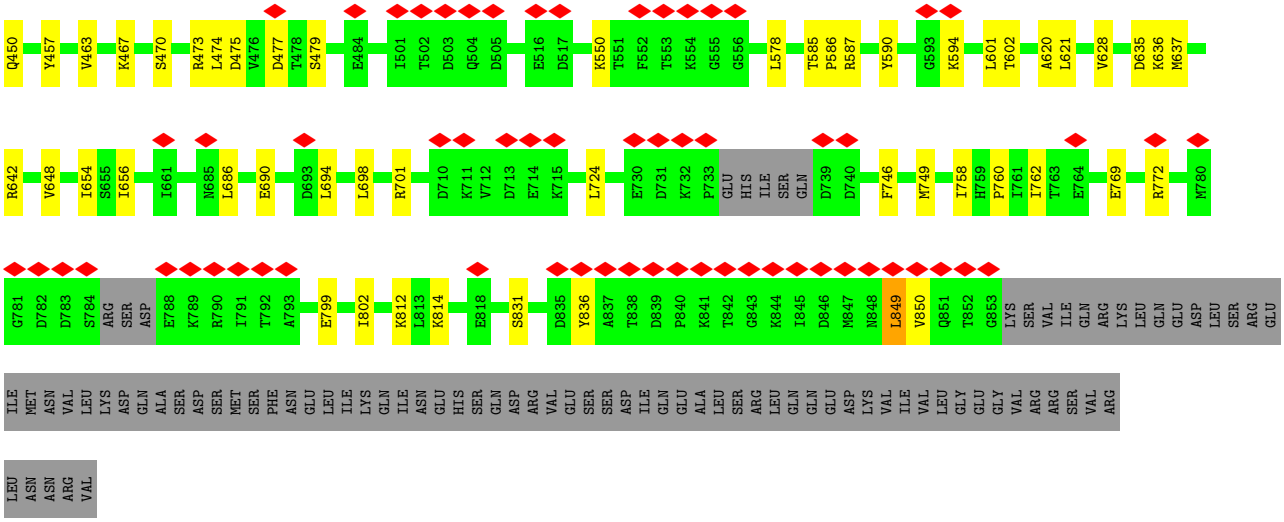




• Molecule 3: DNA replication licensing factor MCM4

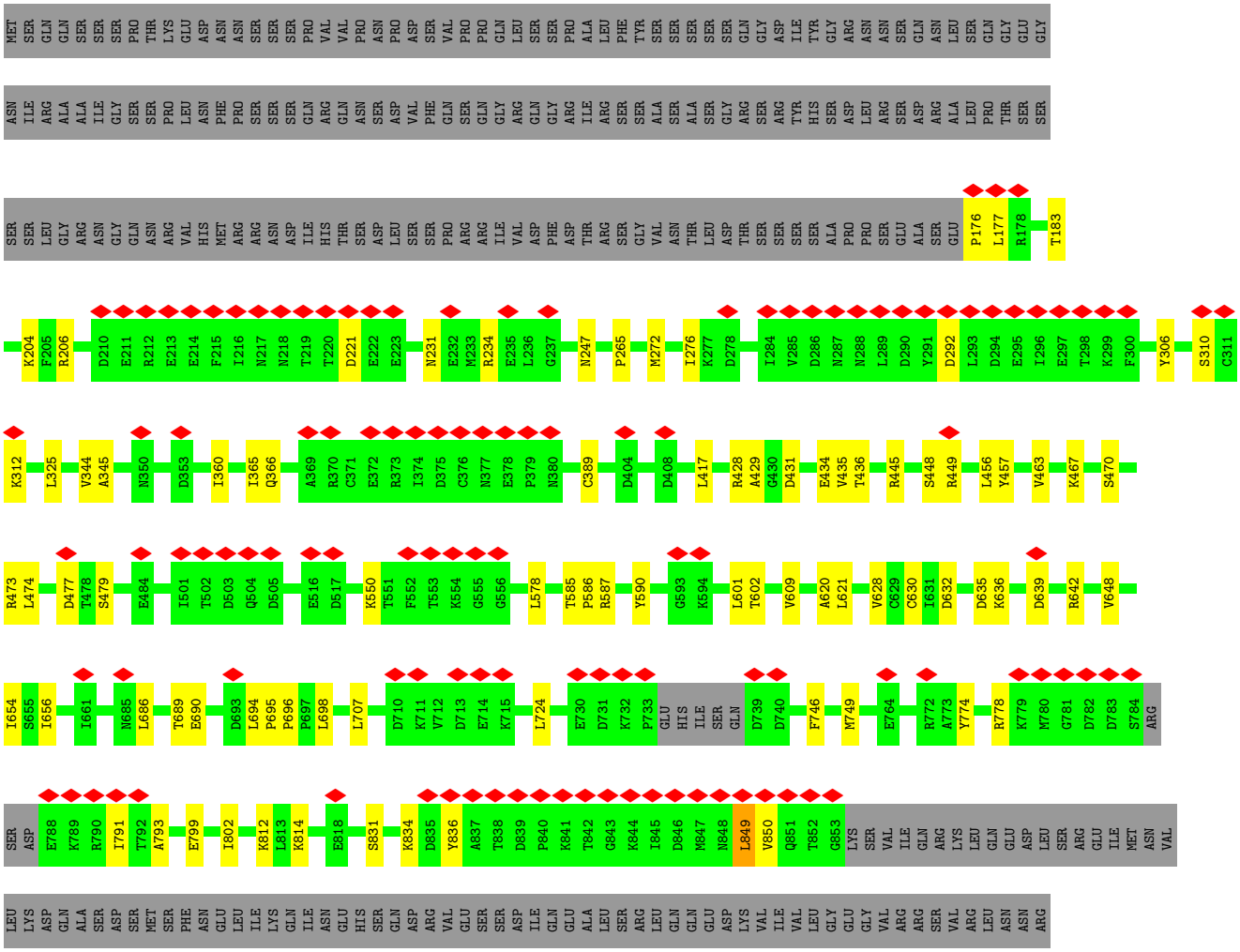
Chain 4:





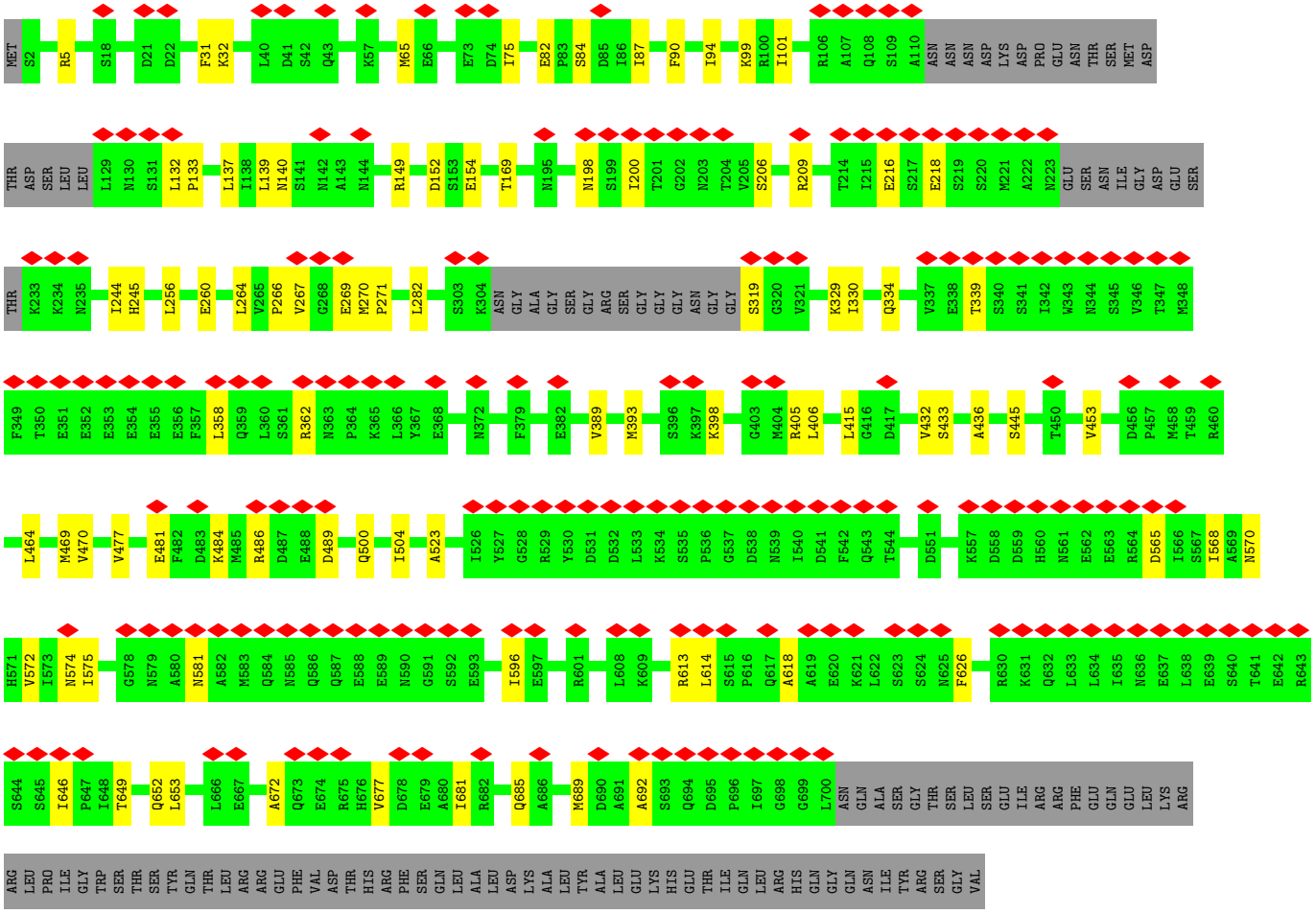
• Molecule 3: DNA replication licensing factor MCM4

Chain D:



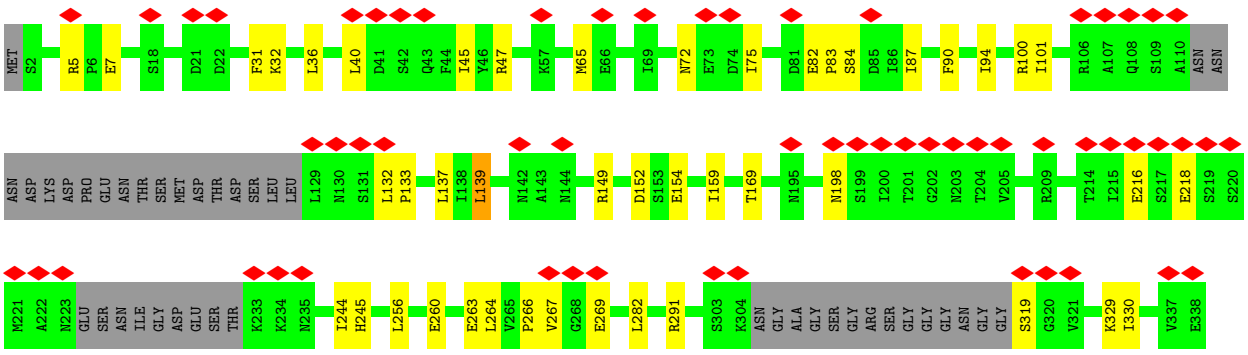
• Molecule 4: Minichromosome maintenance protein 5

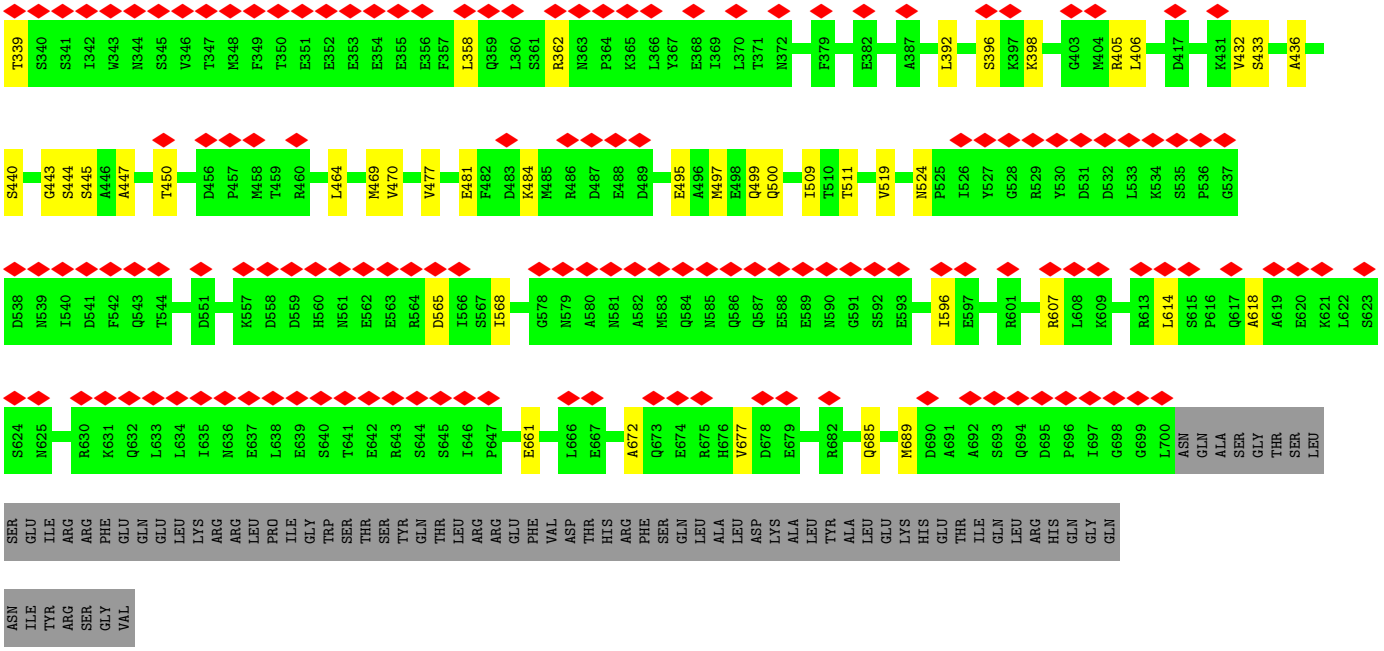
Chain 5:



• Molecule 4: Minichromosome maintenance protein 5

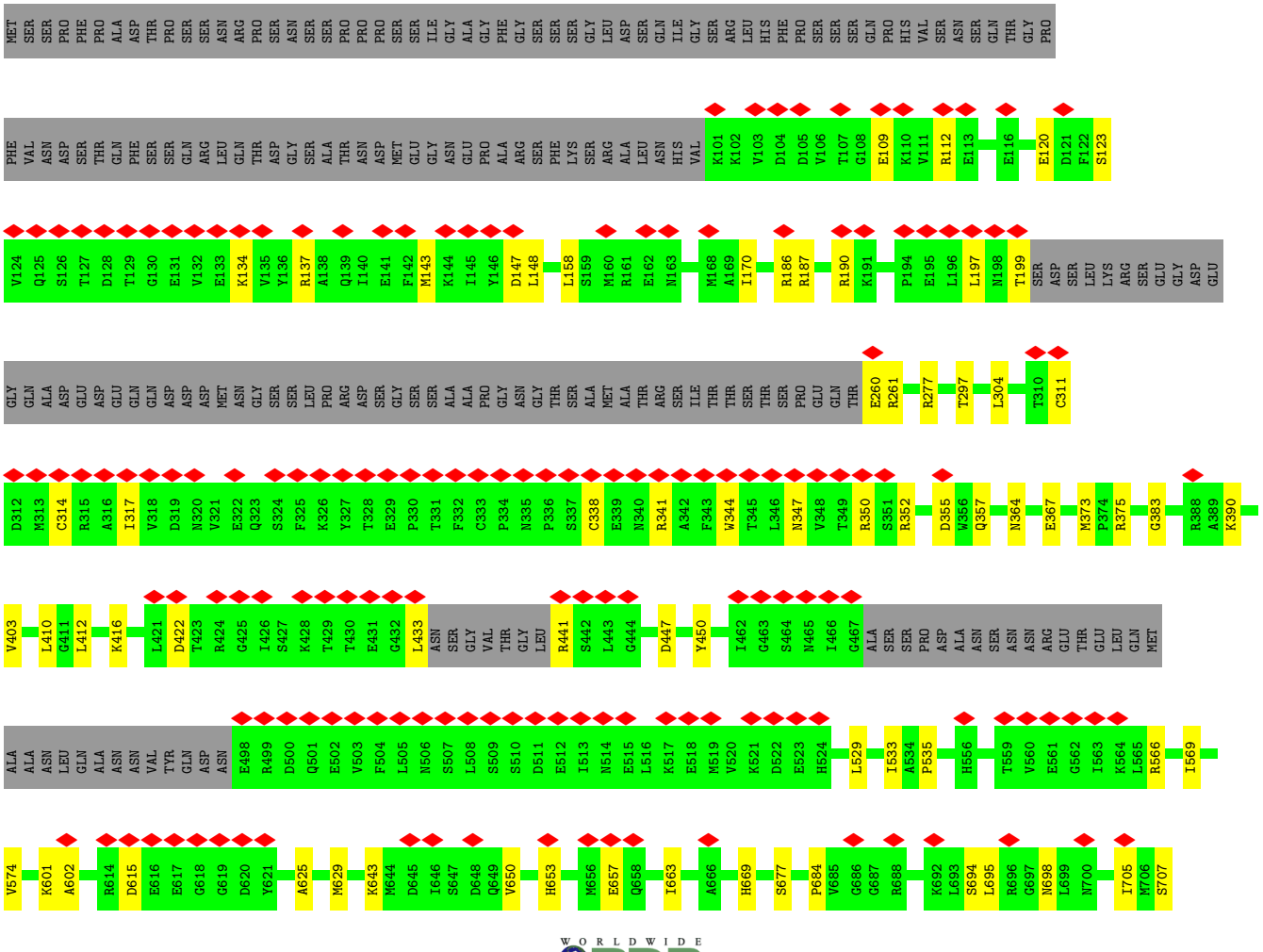
Chain E:

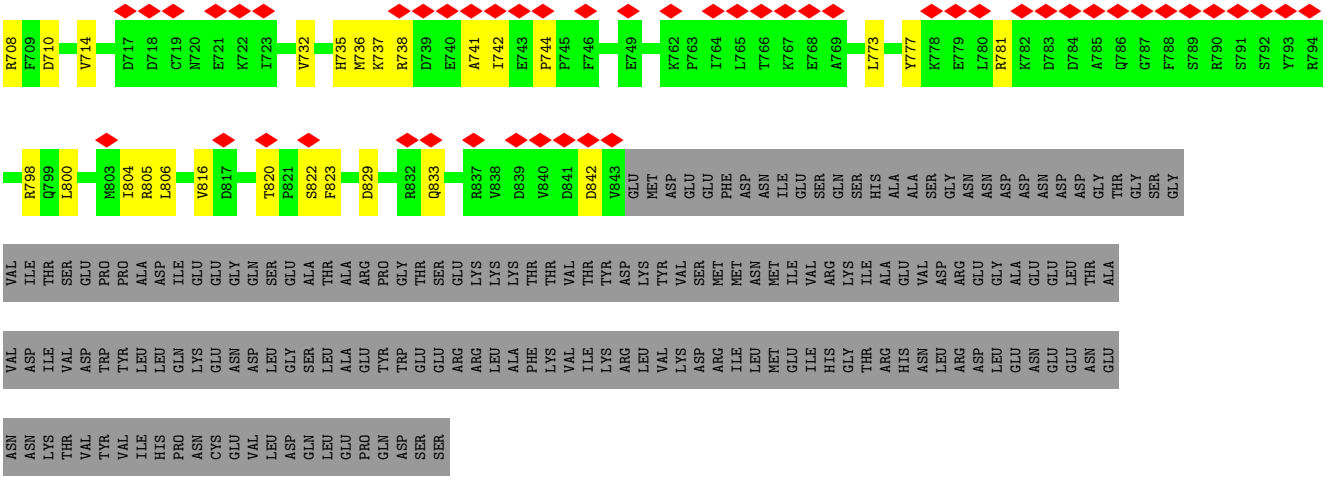




• Molecule 5: DNA replication licensing factor MCM6

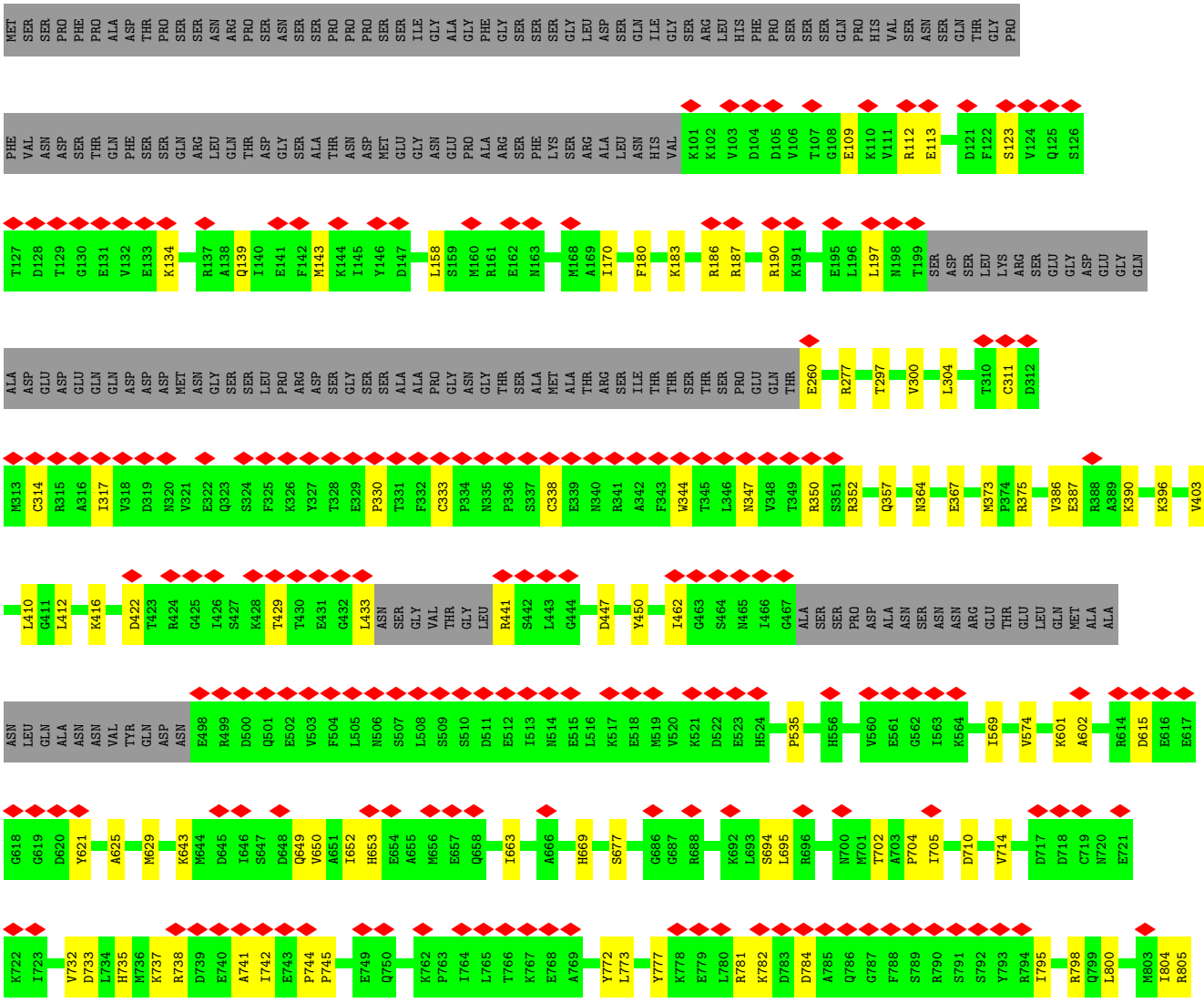
Chain 6:

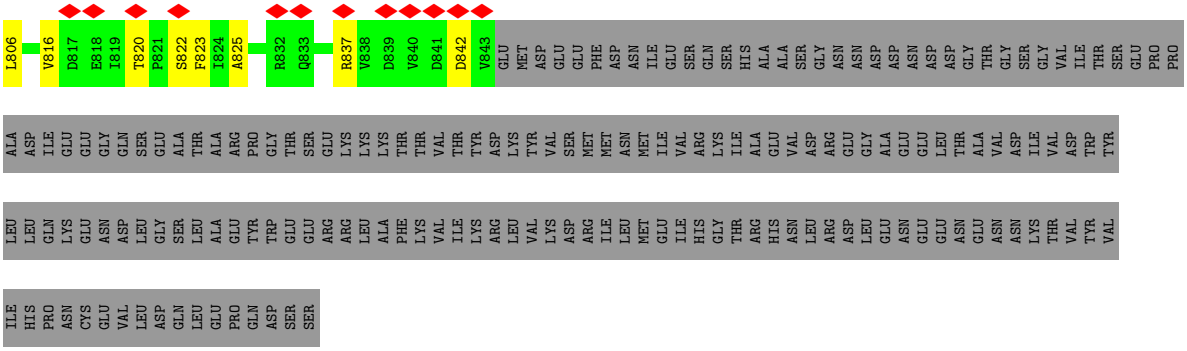




• Molecule 5: DNA replication licensing factor MCM6

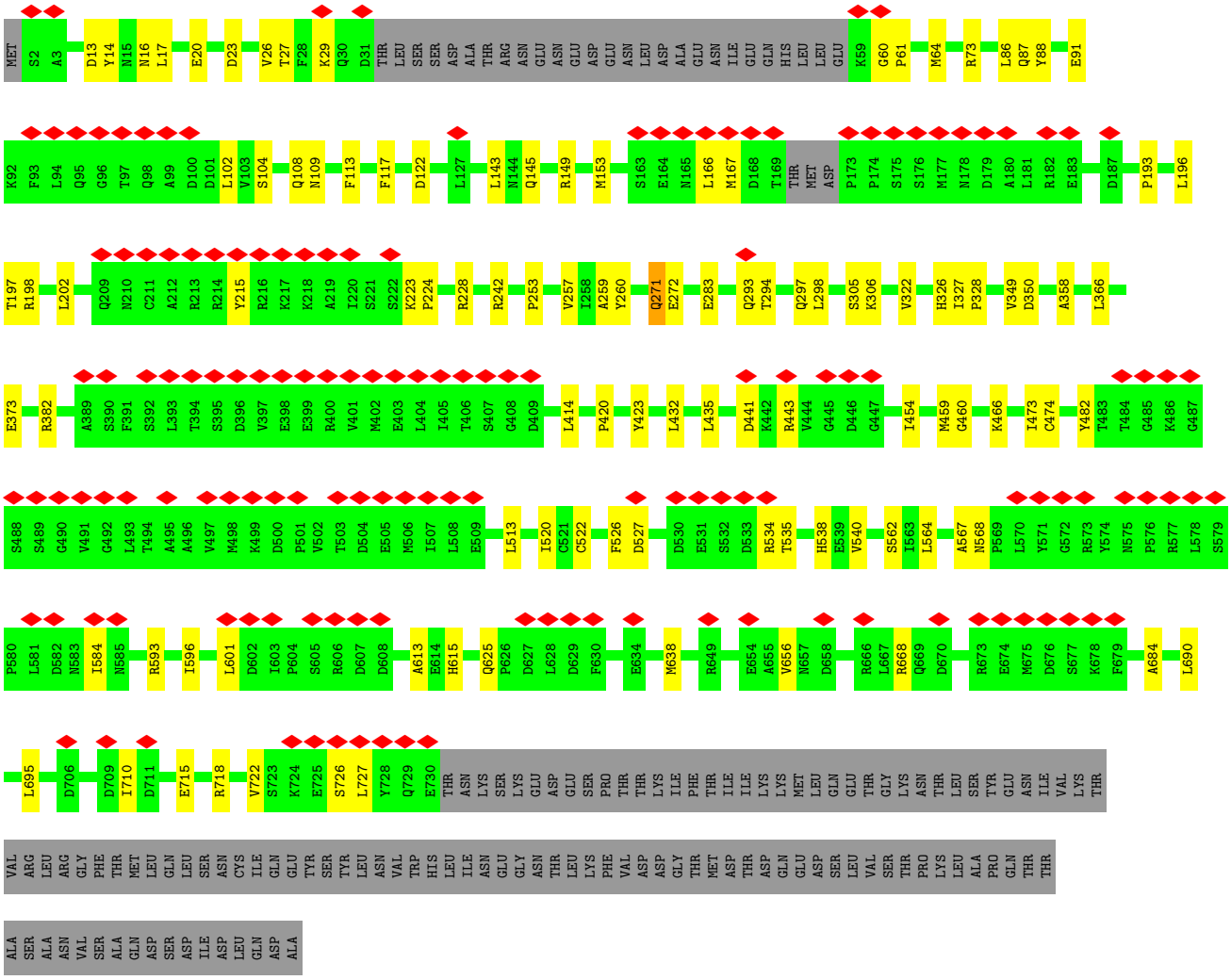
Chain F:





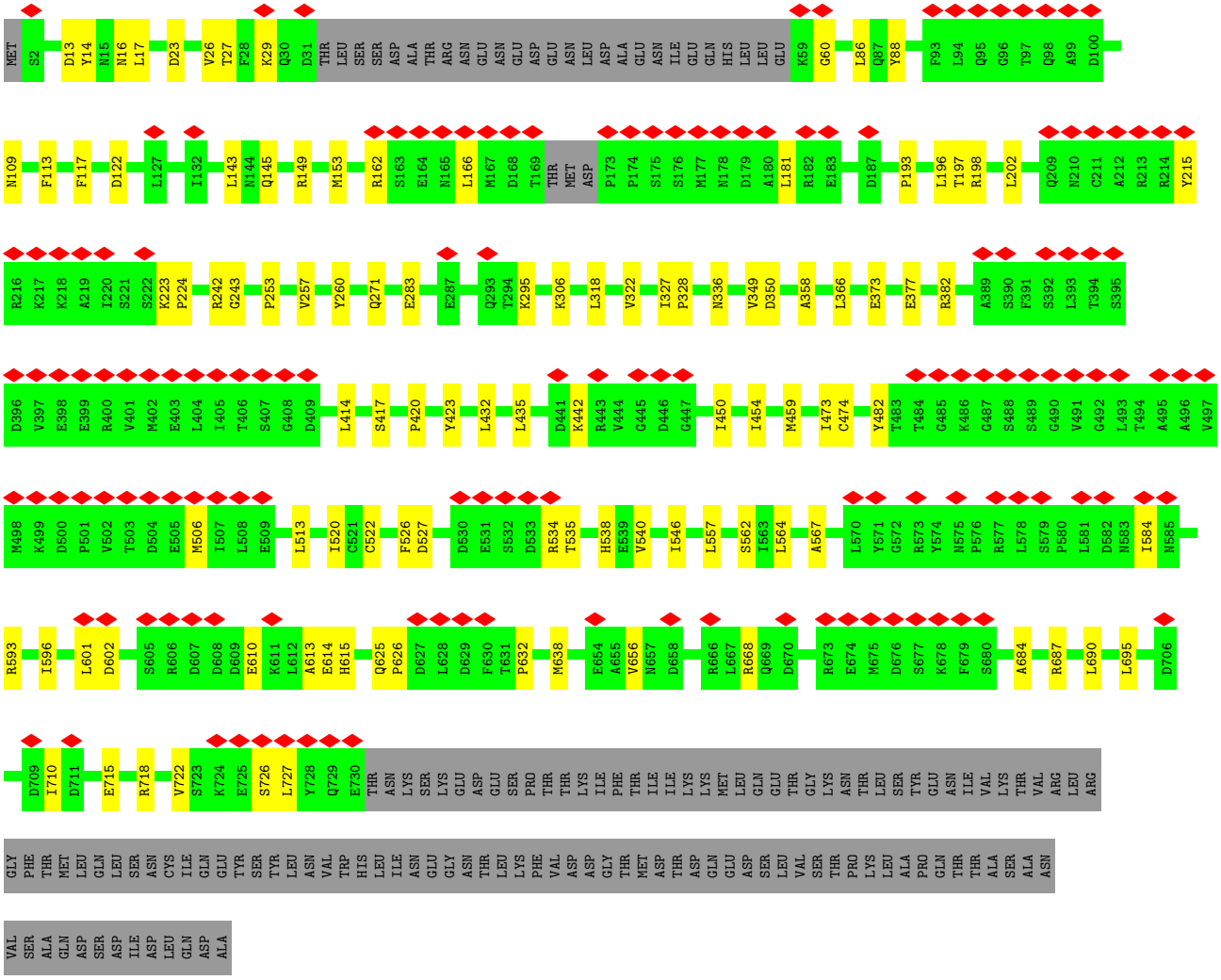
• Molecule 6: DNA replication licensing factor MCM7

Chain 7:



• Molecule 6: DNA replication licensing factor MCM7

Chain G: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N109 F113 F117 D122 L127 I132 L143 N144 Q145 R149 M153 R162 S163 E164 N165 L166 M167 D168 T169 THR MET ASP P173 P174 S175 S176 M177 N178 D179 A180 L181 R182 E183 D187 P193 L196 T197 R198 L202 Q209 N210 C211 A212 R213 R214 Y215
R216 K217 K218 A219 I220 S221 S222 K223 P224 R242 G243 P253 V257 Y260 Q271 E283 E287 Q293 T294 K295 K306 L318 V322 I327 P328 N336 V349 D350 A358 L366 E373 E377 R382 A389 S390 F391 S392 L393 T394 S395
D396 V397 E398 E399 R400 V401 M402 E403 L404 I405 T406 S407 G408 D409 L414 S417 P420 Y423 L432 L435 D441 K442 R443 V444 G445 D446 G447 I450 I454 M459 I473 C474 Y482 T483 T484 G485 K486 G487 S488 S489 G490 V491 G492 L493 T494 A495 A496 V497
M498 K499 D500 P501 V502 T503 D504 E505 M506 I507 L508 E509 L513 I520 C521 C522 F526 D527 D530 E531 S532 D533 R534 T535 H538 E539 V540 I546 L557 S562 I563 L564 A567 L570 Y571 G572 R573 Y574 N575 P576 R577 L578 S579 P580 L581 D582 N583 I584 N585
R593 I596 L601 D602 S605 R606 D607 D608 D609 E610 K611 L612 A613 E614 H615 Q625 P626 D627 L628 D629 F630 T631 P632 M638 E654 A655 V656 N657 D658 R666 L667 R668 Q669 D670 R673 E674 M675 D676 S677 K678 F679 S680 A684 R687 L690 L695 D706
D709 I710 D711 E715 R718 V722 S723 K724 E725 S726 L727 Y728 Q729 E730 THR ASN LYS SER LYS GLU ASP GLU SER PRO THR THR LYS ILE PHE THR ILE ILE LYS LYS MET LEU GLN GLU GLN GLU THR GLY LYS ASN THR LEU SER TYR GLU ASN ILE VAL LYS THR VAL ARG 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, Not provided	
Number of particles used	94859	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.287	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	378.72003, 378.72003, 378.72003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	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, AGS, ZN, MG

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	0.27	0/5057	0.57	1/6834 (0.0%)
1	B	0.27	0/5057	0.55	0/6834
2	3	0.27	0/5073	0.56	0/6880
2	C	0.27	0/5073	0.55	0/6880
3	4	0.27	0/5400	0.54	2/7300 (0.0%)
3	D	0.27	0/5400	0.55	2/7300 (0.0%)
4	5	0.27	0/5217	0.55	1/7054 (0.0%)
4	E	0.27	0/5217	0.55	2/7054 (0.0%)
5	6	0.28	0/5190	0.56	0/7001
5	F	0.28	0/5190	0.57	1/7001 (0.0%)
6	7	0.28	1/5590 (0.0%)	0.53	1/7554 (0.0%)
6	G	0.29	0/5590	0.54	2/7554 (0.0%)
All	All	0.27	1/63054 (0.0%)	0.55	12/85246 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	7	474	CYS	CB-SG	-5.03	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	264	LEU	CA-CB-CG	6.70	130.70	115.30
4	E	264	LEU	CA-CB-CG	6.69	130.69	115.30
5	F	745	PRO	N-CD-CG	-5.98	94.23	103.20
3	D	431	ASP	CB-CG-OD1	5.69	123.42	118.30
3	4	431	ASP	CB-CG-OD1	5.65	123.39	118.30
6	7	474	CYS	CA-CB-SG	5.49	123.88	114.00
4	E	139	LEU	CA-CB-CG	5.16	127.17	115.30
6	G	474	CYS	CA-CB-SG	5.15	123.26	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	583	ASP	CB-CG-OD2	5.12	122.91	118.30
3	4	849	LEU	CA-CB-CG	5.09	127.02	115.30
6	G	632	PRO	CA-N-CD	-5.07	104.40	111.50
3	D	849	LEU	CA-CB-CG	5.05	126.92	115.30

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	2	4970	0	5026	62	0
1	B	4970	0	5026	71	0
2	3	4987	0	5049	52	0
2	C	4987	0	5049	50	0
3	4	5323	0	5373	57	0
3	D	5323	0	5373	53	0
4	5	5143	0	5191	56	0
4	E	5143	0	5191	58	0
5	6	5109	0	5134	62	0
5	F	5109	0	5134	65	0
6	7	5505	0	5563	71	0
6	G	5505	0	5563	66	0
7	2	31	0	12	2	0
7	4	31	0	12	1	0
7	5	31	0	12	1	0
7	6	31	0	12	1	0
7	7	31	0	12	1	0
7	B	31	0	12	1	0
7	D	31	0	12	2	0
7	E	31	0	12	3	0
7	F	31	0	12	0	0
7	G	31	0	12	1	0
8	2	1	0	0	0	0
8	3	1	0	0	0	0
8	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	5	1	0	0	0	0
8	6	1	0	0	0	0
8	7	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
9	2	1	0	0	0	0
9	4	1	0	0	0	0
9	5	1	0	0	0	0
9	6	1	0	0	0	0
9	7	1	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
10	3	27	0	12	0	0
10	C	27	0	12	0	0
All	All	62460	0	62816	652	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (652) 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:B:344:CYS:HB3	1:B:367:CYS:SG	1.99	1.02
1:2:344:CYS:HB3	1:2:367:CYS:SG	1.99	1.01
6:7:482:TYR:HA	6:7:522:CYS:HB2	1.65	0.79
6:G:482:TYR:HA	6:G:522:CYS:HB2	1.66	0.76
5:F:702:THR:HG22	5:F:704:PRO:HD2	1.69	0.75
1:2:670:THR:HG22	1:2:672:PRO:HD2	1.70	0.73
1:B:670:THR:HG22	1:B:672:PRO:HD2	1.70	0.73
1:2:384:ASN:HB2	1:2:412:ALA:HA	1.73	0.70
5:6:657:GLU:HG3	5:6:708:ARG:HE	1.55	0.70
2:3:478:MET:HB2	2:3:483:ARG:HE	1.55	0.70
6:7:166:LEU:HA	4:E:47:ARG:HH11	1.57	0.70
5:6:773:LEU:HD21	5:6:804:ILE:HG12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ASN:HB2	1:B:412:ALA:HA	1.75	0.69
3:4:637:MET:O	3:4:642:ARG:NH1	2.26	0.68
1:2:341:CYS:HB3	1:2:344:CYS:SG	2.34	0.67
5:F:773:LEU:HD21	5:F:804:ILE:HG12	1.76	0.67
2:C:478:MET:HB2	2:C:483:ARG:HE	1.59	0.66
3:D:849:LEU:HD12	3:D:850:VAL:HG23	1.76	0.66
1:B:341:CYS:HB3	1:B:344:CYS:SG	2.35	0.66
2:3:234:GLU:OE2	4:E:5:ARG:NH1	2.29	0.66
3:4:849:LEU:HD12	3:4:850:VAL:HG23	1.77	0.66
1:2:400:GLY:HA3	5:6:390:LYS:HD3	1.78	0.66
4:E:464:LEU:HD21	4:E:470:VAL:HG11	1.77	0.65
6:G:26:VAL:HG23	6:G:27:THR:HG23	1.77	0.65
1:2:307:ARG:NH1	1:2:392:GLU:OE2	2.28	0.65
3:4:434:GLU:HB3	3:4:467:LYS:HB3	1.78	0.65
3:4:417:LEU:HD13	3:4:463:VAL:HG21	1.79	0.65
5:6:364:ASN:HB2	5:6:367:GLU:HG3	1.78	0.64
2:C:40:ASP:OD2	2:C:43:ARG:NH2	2.30	0.64
3:D:434:GLU:HB3	3:D:467:LYS:HB3	1.79	0.64
6:7:166:LEU:HD12	6:7:167:MET:HG3	1.80	0.64
3:D:417:LEU:HD13	3:D:463:VAL:HG21	1.79	0.64
5:F:364:ASN:HB2	5:F:367:GLU:HG3	1.78	0.64
6:G:420:PRO:HB2	6:G:625:GLN:HG2	1.77	0.64
2:C:266:PRO:HB2	2:C:269:GLN:HG3	1.78	0.64
5:F:650:VAL:HA	5:F:653:HIS:CE1	2.33	0.64
6:G:435:LEU:HD21	6:G:564:LEU:HB2	1.80	0.63
6:7:420:PRO:HB2	6:7:625:GLN:HG2	1.81	0.63
6:7:435:LEU:HD21	6:7:564:LEU:HB2	1.81	0.63
1:2:511:ILE:HD11	1:2:683:VAL:HG21	1.81	0.63
2:3:368:ALA:HB3	2:3:378:LYS:HE2	1.80	0.63
7:D:2001:AGS:H5'2	6:G:687:ARG:HE	1.63	0.62
1:B:307:ARG:NH1	1:B:392:GLU:OE2	2.31	0.62
3:D:445:ARG:HD3	5:F:410:LEU:HD11	1.81	0.62
2:C:368:ALA:HB3	2:C:378:LYS:HE2	1.79	0.62
3:4:445:ARG:HD3	5:6:410:LEU:HD11	1.82	0.62
2:C:223:THR:HG21	4:E:244:ILE:HA	1.81	0.62
3:D:621:LEU:HD13	3:D:648:VAL:HG21	1.81	0.62
6:G:162:ARG:HE	6:G:181:LEU:HD21	1.65	0.62
5:F:737:LYS:HB2	5:F:741:ALA:HB2	1.82	0.62
5:F:109:GLU:OE1	5:F:112:ARG:NH1	2.33	0.62
3:D:445:ARG:NH1	5:F:447:ASP:OD2	2.33	0.62
2:3:567:ARG:O	2:3:642:TYR:OH	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:398:LYS:NZ	4:E:661:GLU:OE1	2.33	0.62
2:3:266:PRO:HB2	2:3:269:GLN:HG3	1.82	0.61
5:F:403:VAL:HG22	5:F:450:TYR:HB3	1.80	0.61
6:7:26:VAL:HG23	6:7:27:THR:HG23	1.82	0.61
2:C:567:ARG:O	2:C:642:TYR:OH	2.18	0.61
4:E:198:ASN:HA	4:E:329:LYS:HD3	1.82	0.61
5:6:710:ASP:OD2	5:6:805:ARG:NH1	2.33	0.61
1:B:576:LEU:HD13	1:B:620:ILE:HD11	1.83	0.61
4:E:72:ASN:HB3	4:E:75:ILE:HG12	1.83	0.61
2:3:223:THR:HG21	4:5:244:ILE:HA	1.83	0.61
3:4:656:ILE:HD13	5:6:602:ALA:HB1	1.83	0.61
6:7:166:LEU:HD13	4:E:101:ILE:HG12	1.82	0.61
1:B:406:ARG:NH1	1:B:449:THR:OG1	2.34	0.61
5:6:109:GLU:OE1	5:6:112:ARG:NH1	2.34	0.60
5:6:314:CYS:SG	5:6:338:CYS:HB3	2.41	0.60
3:4:314:MET:HG2	3:4:415:ILE:HG21	1.83	0.60
3:4:621:LEU:HD13	3:4:648:VAL:HG21	1.82	0.60
1:2:406:ARG:NH1	1:2:449:THR:OG1	2.34	0.60
6:7:350:ASP:OD2	6:7:382:ARG:NH2	2.35	0.60
2:3:712:HIS:ND1	2:3:725:ASP:OD1	2.33	0.60
1:B:400:GLY:HA3	5:F:390:LYS:HD3	1.83	0.60
2:C:712:HIS:ND1	2:C:725:ASP:OD1	2.34	0.60
2:3:647:ILE:HG22	2:3:651:VAL:HG12	1.82	0.60
5:6:403:VAL:HG22	5:6:450:TYR:HB3	1.81	0.60
6:G:414:LEU:HD22	6:G:638:MET:HG3	1.83	0.60
5:6:829:ASP:O	5:6:833:GLN:NE2	2.34	0.60
4:5:433:SER:HB3	4:5:436:ALA:HB2	1.82	0.60
2:3:295:VAL:HB	2:3:325:THR:HB	1.84	0.60
5:F:710:ASP:OD2	5:F:805:ARG:NH1	2.35	0.60
4:5:101:ILE:HG12	6:G:166:LEU:HD13	1.84	0.59
4:E:433:SER:HB3	4:E:436:ALA:HB2	1.82	0.59
4:E:152:ASP:HB3	4:E:154:GLU:HG2	1.83	0.59
1:2:321:THR:HG22	1:2:425:GLU:HG2	1.84	0.59
1:2:519:LEU:HD21	1:2:556:VAL:HG13	1.85	0.59
4:5:464:LEU:HD21	4:5:470:VAL:HG11	1.85	0.59
1:B:519:LEU:HD21	1:B:556:VAL:HG13	1.85	0.59
4:5:152:ASP:HB3	4:5:154:GLU:HG2	1.83	0.59
5:6:143:MET:HG2	5:6:148:LEU:HB2	1.84	0.59
5:F:311:CYS:HB3	5:F:314:CYS:HB2	1.82	0.59
5:F:314:CYS:SG	5:F:338:CYS:HB3	2.42	0.59
6:G:350:ASP:OD2	6:G:382:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:390:GLU:OE1	2:C:467:ARG:NH1	2.35	0.58
3:4:310:SER:HB2	3:4:312:LYS:HE3	1.85	0.58
5:6:650:VAL:HA	5:6:653:HIS:CE1	2.38	0.58
6:G:432:LEU:HD22	6:G:473:ILE:HG13	1.85	0.58
5:6:601:LYS:HG2	5:6:643:LYS:HB3	1.85	0.58
5:6:737:LYS:HB2	5:6:741:ALA:HB2	1.85	0.58
1:B:321:THR:HG22	1:B:425:GLU:HG2	1.85	0.58
2:3:244:GLU:OE1	6:7:109:ASN:ND2	2.36	0.58
5:F:742:ILE:HG22	5:F:744:PRO:HD3	1.84	0.58
6:G:14:TYR:OH	6:G:109:ASN:ND2	2.36	0.58
7:B:2001:AGS:O2G	5:F:798:ARG:NH2	2.34	0.58
5:6:311:CYS:HB3	5:6:314:CYS:HB2	1.85	0.58
6:7:14:TYR:OH	6:7:109:ASN:ND2	2.36	0.58
6:7:414:LEU:HD22	6:7:638:MET:HG3	1.85	0.58
2:C:483:ARG:HD2	2:C:539:LEU:HD11	1.85	0.57
4:E:392:LEU:O	4:E:607:ARG:NH2	2.36	0.57
3:4:345:ALA:HB2	3:4:365:ILE:HD13	1.87	0.57
1:B:616:ASP:O	1:B:620:ILE:HD12	2.05	0.57
2:C:647:ILE:HG22	2:C:651:VAL:HG12	1.86	0.57
7:E:2001:AGS:S1G	7:E:2001:AGS:O2B	2.62	0.57
1:2:659:SER:OG	1:2:684:ARG:NH1	2.37	0.57
2:3:177:ASN:ND2	4:5:245:HIS:O	2.37	0.57
6:7:432:LEU:HD22	6:7:473:ILE:HG13	1.85	0.57
2:3:541:SER:HB2	2:3:700:ARG:HD2	1.86	0.57
3:D:601:LEU:HD23	3:D:620:ALA:HB3	1.87	0.57
2:C:244:GLU:OE1	6:G:109:ASN:ND2	2.36	0.57
3:4:429:ALA:O	3:4:587:ARG:NH2	2.38	0.57
5:6:147:ASP:OD1	5:6:261:ARG:NH1	2.38	0.57
6:7:466:LYS:NZ	7:7:2001:AGS:S1G	2.71	0.57
6:7:596:ILE:HD11	6:7:695:LEU:HD21	1.87	0.56
2:C:177:ASN:ND2	4:E:245:HIS:O	2.38	0.56
5:F:663:ILE:O	5:F:669:HIS:HA	2.04	0.56
4:5:206:SER:OG	4:5:209:ARG:NH2	2.38	0.56
1:2:598:LEU:HD21	4:5:267:VAL:HA	1.86	0.56
3:D:345:ALA:HB2	3:D:365:ILE:HD13	1.87	0.56
5:F:777:TYR:OH	5:F:781:ARG:NH1	2.38	0.56
5:F:820:THR:HG22	5:F:822:SER:H	1.71	0.56
6:G:593:ARG:NH1	6:G:687:ARG:HH12	2.03	0.56
3:D:310:SER:HB2	3:D:312:LYS:HE3	1.86	0.56
1:2:419:LYS:HD2	1:2:420:PRO:HD2	1.87	0.56
3:4:445:ARG:NH1	5:6:447:ASP:OD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:295:VAL:HB	2:C:325:THR:HB	1.87	0.56
1:2:596:LEU:HD11	1:2:620:ILE:HG13	1.88	0.56
1:B:505:ILE:HD11	1:B:551:GLN:HB2	1.86	0.56
1:B:511:ILE:HD11	1:B:683:VAL:HG21	1.88	0.56
3:D:639:ASP:OD1	3:D:642:ARG:NH2	2.36	0.56
6:7:260:TYR:HE2	6:7:271:GLN:HG2	1.70	0.56
1:B:612:MET:O	1:B:617:ARG:NH1	2.38	0.56
1:B:598:LEU:HD21	4:E:267:VAL:HA	1.88	0.55
6:G:149:ARG:O	6:G:153:MET:HG3	2.07	0.55
2:3:196:LEU:HD21	2:3:199:SER:HB3	1.89	0.55
4:E:432:VAL:HG23	4:E:596:ILE:HG13	1.88	0.55
1:2:342:LEU:HB3	5:F:433:LEU:HD13	1.88	0.55
3:4:601:LEU:HD23	3:4:620:ALA:HB3	1.89	0.55
4:5:398:LYS:HB2	4:5:406:LEU:HB2	1.88	0.55
7:2:2001:AGS:O2G	5:6:798:ARG:NH2	2.36	0.55
5:6:433:LEU:HD13	1:B:342:LEU:HB3	1.88	0.55
6:7:441:ASP:OD2	6:7:443:ARG:NH1	2.39	0.55
3:D:656:ILE:HD13	5:F:602:ALA:HB1	1.88	0.55
1:2:527:VAL:HG23	4:5:581:ASN:HB2	1.88	0.55
3:4:470:SER:HB3	3:4:473:ARG:HG2	1.88	0.55
3:D:470:SER:HB3	3:D:473:ARG:HG2	1.89	0.55
1:2:337:VAL:HA	1:2:380:THR:HG23	1.89	0.54
2:C:196:LEU:HD21	2:C:199:SER:HB3	1.88	0.54
1:B:230:ARG:NH1	1:B:243:GLU:O	2.40	0.54
6:7:272:GLU:HB2	4:E:7:GLU:H	1.72	0.54
2:C:680:VAL:HG22	6:G:613:ALA:HB1	1.90	0.54
3:D:477:ASP:OD2	3:D:479:SER:OG	2.25	0.54
6:G:596:ILE:HD11	6:G:695:LEU:HD21	1.90	0.54
6:G:260:TYR:HE2	6:G:271:GLN:HG2	1.72	0.54
3:4:799:GLU:OE1	5:6:735:HIS:NE2	2.41	0.54
4:5:5:ARG:HG2	4:5:218:GLU:HB3	1.90	0.54
2:C:459:ALA:HB2	6:G:327:ILE:HD11	1.90	0.54
1:B:337:VAL:HA	1:B:380:THR:HG23	1.90	0.54
6:G:336:ASN:ND2	6:G:377:GLU:OE2	2.41	0.54
3:4:769:GLU:OE2	3:4:772:ARG:NH2	2.41	0.54
4:5:481:GLU:OE1	4:5:484:LYS:NZ	2.41	0.54
2:C:542:ARG:NH1	7:G:2001:AGS:O3G	2.40	0.54
4:E:36:LEU:O	4:E:47:ARG:NH2	2.41	0.54
3:D:429:ALA:O	3:D:587:ARG:NH2	2.38	0.54
6:G:513:LEU:HD13	6:G:540:VAL:HG21	1.89	0.54
6:G:526:PHE:HB3	6:G:567:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:491:GLU:OE1	2:3:700:ARG:NH1	2.41	0.53
3:D:707:LEU:O	3:D:834:LYS:NZ	2.37	0.53
1:2:534:ARG:O	1:2:815:ARG:NH1	2.39	0.53
3:D:774:TYR:OH	3:D:778:ARG:NH1	2.40	0.53
5:6:569:ILE:O	5:6:677:SER:OG	2.26	0.53
5:F:277:ARG:NH2	5:F:373:MET:O	2.41	0.53
3:4:206:ARG:NH1	3:4:247:ASN:OD1	2.40	0.53
4:5:216:GLU:HB3	4:5:218:GLU:HG2	1.90	0.53
5:6:820:THR:HG22	5:6:822:SER:H	1.74	0.53
1:B:795:ARG:HA	1:B:798:ILE:HD12	1.89	0.53
3:D:231:ASN:OD1	3:D:234:ARG:NH2	2.41	0.53
5:F:569:ILE:O	5:F:677:SER:OG	2.27	0.53
1:B:813:ILE:HG12	1:B:841:VAL:HG11	1.90	0.53
3:4:724:LEU:HD12	6:7:690:LEU:HD21	1.90	0.53
4:5:358:LEU:HB3	4:5:362:ARG:HH12	1.74	0.53
1:B:659:SER:OG	1:B:684:ARG:NH1	2.42	0.53
1:2:384:ASN:ND2	4:5:152:ASP:OD2	2.42	0.53
5:6:260:GLU:O	5:6:352:ARG:NH2	2.41	0.52
4:E:524:ASN:ND2	7:E:2001:AGS:O2G	2.41	0.52
4:5:432:VAL:HG23	4:5:596:ILE:HG13	1.90	0.52
1:2:505:ILE:HD11	1:2:551:GLN:HB2	1.92	0.52
3:4:694:LEU:HD22	3:4:698:LEU:HD23	1.91	0.52
4:E:358:LEU:HB3	4:E:362:ARG:HH12	1.74	0.52
4:E:495:GLU:O	4:E:499:GLN:HB2	2.10	0.52
3:4:636:LYS:HD3	6:7:535:THR:HG22	1.91	0.52
4:5:198:ASN:HA	4:5:329:LYS:HD3	1.90	0.52
1:B:824:ARG:NH1	1:B:830:SER:OG	2.43	0.52
3:D:204:LYS:HB3	3:D:221:ASP:HB3	1.92	0.52
3:D:306:TYR:HA	3:D:436:THR:HG21	1.91	0.52
6:G:715:GLU:HA	6:G:718:ARG:HG2	1.91	0.52
4:5:486:ARG:NH2	4:5:489:ASP:OD1	2.43	0.52
2:3:366:SER:HB3	2:3:650:LEU:HB2	1.92	0.52
5:6:277:ARG:HG2	5:6:375:ARG:HD2	1.92	0.52
3:4:231:ASN:OD1	3:4:234:ARG:NH2	2.43	0.52
5:6:277:ARG:NH2	5:6:373:MET:O	2.42	0.52
1:2:335:LYS:HE3	1:2:383:ARG:HB3	1.91	0.51
5:6:186:ARG:HE	5:6:197:LEU:HD22	1.74	0.51
3:4:183:THR:O	6:7:145:GLN:NE2	2.43	0.51
6:G:117:PHE:HB3	6:G:202:LEU:HD11	1.91	0.51
6:7:513:LEU:HD13	6:7:540:VAL:HG21	1.91	0.51
3:D:636:LYS:HD3	6:G:535:THR:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:401:GLU:OE1	3:4:413:HIS:NE2	2.40	0.51
6:7:122:ASP:OD1	6:7:198:ARG:NE	2.42	0.51
2:C:672:THR:OG1	2:C:721:VAL:O	2.28	0.51
3:D:183:THR:O	6:G:145:GLN:NE2	2.43	0.51
5:F:123:SER:HB3	5:F:134:LYS:HG2	1.91	0.51
6:7:149:ARG:O	6:7:153:MET:HG3	2.11	0.51
3:D:445:ARG:NH2	3:D:448:SER:O	2.43	0.51
4:E:398:LYS:HB2	4:E:406:LEU:HB2	1.92	0.51
6:G:23:ASP:OD2	6:G:88:TYR:OH	2.26	0.51
3:4:477:ASP:OD2	3:4:479:SER:OG	2.27	0.51
6:7:117:PHE:HB3	6:7:202:LEU:HD11	1.91	0.51
6:G:534:ARG:O	6:G:538:HIS:HB2	2.09	0.51
3:4:445:ARG:NH2	3:4:448:SER:O	2.43	0.51
1:B:383:ARG:HB2	1:B:412:ALA:HB2	1.93	0.51
3:4:364:VAL:HG11	6:7:297:GLN:HE22	1.75	0.51
5:6:742:ILE:HG22	5:6:744:PRO:HD3	1.92	0.51
2:C:422:VAL:HA	2:C:425:THR:HG22	1.93	0.51
1:2:824:ARG:NH1	1:2:830:SER:OG	2.42	0.51
4:5:614:LEU:HA	4:5:672:ALA:HB3	1.93	0.51
6:7:228:ARG:HH21	6:7:326:HIS:HB3	1.76	0.50
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.93	0.50
4:E:396:SER:OG	4:E:661:GLU:OE1	2.29	0.50
4:E:169:THR:HG22	4:E:256:LEU:HD22	1.92	0.50
4:E:216:GLU:HB3	4:E:218:GLU:HG2	1.93	0.50
2:3:255:ARG:NH2	6:7:366:LEU:O	2.45	0.50
2:3:661:GLN:O	2:3:665:GLU:HG2	2.11	0.50
1:B:309:LEU:HD21	1:B:318:VAL:HG21	1.93	0.50
1:B:384:ASN:ND2	4:E:152:ASP:OD2	2.43	0.50
1:B:792:ASP:OD1	1:B:795:ARG:NH1	2.43	0.50
3:D:206:ARG:NH1	3:D:247:ASN:OD1	2.40	0.50
6:G:596:ILE:HD11	6:G:695:LEU:HD11	1.94	0.50
3:4:306:TYR:HA	3:4:436:THR:HG21	1.92	0.50
1:2:605:LEU:HD23	1:2:647:ILE:HB	1.94	0.50
2:3:459:ALA:HB2	6:7:327:ILE:HD11	1.92	0.50
6:G:122:ASP:OD1	6:G:198:ARG:NE	2.42	0.50
1:2:239:SER:O	1:2:286:TYR:OH	2.29	0.50
2:3:39:ARG:HH12	2:3:136:MET:HB2	1.77	0.50
2:3:391:LYS:HB2	2:3:399:LEU:HB2	1.94	0.50
5:6:777:TYR:OH	5:6:781:ARG:NH1	2.41	0.50
2:C:661:GLN:O	2:C:665:GLU:HG2	2.12	0.50
5:F:277:ARG:HG2	5:F:375:ARG:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:235:ASP:OD1	2:3:239:ASN:N	2.45	0.50
4:5:169:THR:HG22	4:5:256:LEU:HD22	1.94	0.50
6:7:13:ASP:OD2	6:7:16:ASN:ND2	2.45	0.50
5:F:297:THR:OG1	5:F:357:GLN:NE2	2.44	0.49
1:2:309:LEU:HD21	1:2:318:VAL:HG21	1.94	0.49
2:3:52:ASN:ND2	2:3:90:ASN:O	2.44	0.49
4:5:570:ASN:O	4:5:574:ASN:ND2	2.45	0.49
1:B:534:ARG:O	1:B:815:ARG:NH1	2.41	0.49
3:D:292:ASP:OD1	3:D:292:ASP:N	2.43	0.49
3:4:594:LYS:HD2	6:7:535:THR:HG21	1.93	0.49
3:D:474:LEU:HB2	3:D:586:PRO:HD3	1.94	0.49
2:3:570:ARG:O	4:5:613:ARG:NH2	2.46	0.49
7:5:2001:AGS:S1G	7:5:2001:AGS:O2B	2.70	0.49
2:C:52:ASN:ND2	2:C:90:ASN:O	2.45	0.49
2:C:366:SER:HB3	2:C:650:LEU:HB2	1.95	0.49
3:D:799:GLU:OE2	5:F:735:HIS:NE2	2.46	0.49
6:G:459:MET:HA	6:G:567:ALA:O	2.13	0.49
1:2:495:ASP:OD1	1:2:509:ARG:NH2	2.45	0.49
2:3:672:THR:OG1	2:3:721:VAL:O	2.29	0.49
3:4:360:ILE:HG13	3:4:365:ILE:HG13	1.95	0.49
3:D:585:THR:HG21	3:D:628:VAL:HB	1.95	0.49
4:E:481:GLU:OE1	4:E:484:LYS:NZ	2.42	0.49
1:B:239:SER:O	1:B:286:TYR:OH	2.29	0.49
3:4:585:THR:HG21	3:4:628:VAL:HB	1.94	0.49
3:4:701:ARG:NH2	7:6:2001:AGS:S1G	2.86	0.49
6:G:454:ILE:O	6:G:562:SER:OG	2.27	0.49
1:2:662:PRO:O	1:2:666:ASN:ND2	2.46	0.48
5:F:615:ASP:OD1	5:F:615:ASP:N	2.45	0.48
6:G:13:ASP:OD2	6:G:16:ASN:ND2	2.46	0.48
6:7:193:PRO:HD2	6:7:196:LEU:HD12	1.95	0.48
2:C:400:ARG:HB2	2:C:707:ARG:HH21	1.79	0.48
2:C:426:ALA:HB3	2:C:429:ALA:HB2	1.95	0.48
5:6:535:PRO:HB2	5:6:742:ILE:HG23	1.95	0.48
1:B:479:GLU:OE2	1:B:482:ARG:NH2	2.38	0.48
2:C:255:ARG:NH2	6:G:366:LEU:O	2.47	0.48
2:C:440:VAL:HB	2:C:445:ALA:HB2	1.95	0.48
3:D:812:LYS:HD3	3:D:814:LYS:HE2	1.94	0.48
2:3:669:PRO:HG2	2:3:710:THR:HG23	1.95	0.48
5:6:199:THR:OG1	5:6:261:ARG:NH2	2.46	0.48
3:D:360:ILE:HG13	3:D:365:ILE:HG13	1.95	0.48
5:F:733:ASP:OD2	5:F:737:LYS:NZ	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:474:LEU:HB2	3:4:586:PRO:HD3	1.94	0.48
5:6:441:ARG:HH22	6:7:283:GLU:HG3	1.79	0.48
1:B:296:ARG:HH21	1:B:413:ASP:HB3	1.78	0.48
1:2:555:TYR:HA	1:2:558:LYS:HE2	1.96	0.48
3:4:212:ARG:HB3	3:4:215:PHE:HD1	1.78	0.48
2:3:430:ILE:HD12	2:3:465:ALA:HB2	1.95	0.48
1:2:795:ARG:HA	1:2:798:ILE:HD12	1.95	0.48
1:B:335:LYS:HE3	1:B:383:ARG:HB3	1.95	0.48
3:D:457:TYR:HB2	6:G:253:PRO:HG2	1.96	0.48
5:F:601:LYS:HG2	5:F:643:LYS:HB3	1.95	0.48
1:2:386:GLN:HB2	1:2:415:VAL:HG12	1.96	0.48
4:5:685:GLN:HA	4:5:689:MET:HB2	1.95	0.48
2:C:669:PRO:HG2	2:C:710:THR:HG23	1.95	0.48
4:5:99:LYS:HG3	4:5:132:LEU:HD23	1.96	0.48
6:7:715:GLU:HA	6:7:718:ARG:HG2	1.96	0.48
4:E:282:LEU:HD13	4:E:330:ILE:HG22	1.96	0.48
1:2:296:ARG:HH21	1:2:413:ASP:HB3	1.79	0.47
4:5:469:MET:HA	4:5:477:VAL:HG21	1.96	0.47
5:6:123:SER:HB3	5:6:134:LYS:HG2	1.95	0.47
3:4:602:THR:HG22	3:4:654:ILE:HD13	1.96	0.47
1:B:605:LEU:HD23	1:B:647:ILE:HB	1.95	0.47
5:F:653:HIS:HB3	5:F:705:ILE:HD13	1.96	0.47
6:7:656:VAL:HG12	6:7:710:ILE:HD13	1.96	0.47
6:G:656:VAL:HG12	6:G:710:ILE:HD13	1.96	0.47
1:B:315:SER:N	1:B:430:TYR:O	2.46	0.47
2:C:198:ARG:HB3	2:C:249:THR:HG22	1.96	0.47
3:D:435:VAL:HG13	3:D:463:VAL:HG13	1.96	0.47
4:E:497:MET:HG2	4:E:519:VAL:HG21	1.97	0.47
2:3:171:LEU:HD11	2:3:182:VAL:HG21	1.96	0.47
7:4:2001:AGS:O3G	6:7:593:ARG:NH2	2.36	0.47
4:5:646:ILE:HG21	4:5:692:ALA:HA	1.96	0.47
2:C:171:LEU:HD11	2:C:182:VAL:HG21	1.95	0.47
5:6:615:ASP:OD1	5:6:615:ASP:N	2.45	0.47
6:7:242:ARG:HB3	6:7:350:ASP:OD1	2.15	0.47
6:7:322:VAL:HG21	6:7:328:PRO:HG3	1.96	0.47
1:B:596:LEU:HD11	1:B:620:ILE:HG13	1.97	0.47
3:D:746:PHE:HA	3:D:749:MET:HG2	1.97	0.47
6:G:193:PRO:HD2	6:G:196:LEU:HD12	1.97	0.47
1:2:419:LYS:NZ	1:2:420:PRO:O	2.38	0.47
4:E:32:LYS:HD3	4:E:100:ARG:HH12	1.79	0.47
2:3:198:ARG:HB3	2:3:249:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:263:GLU:OE2	4:E:511:THR:OG1	2.29	0.47
6:G:257:VAL:HG12	6:G:306:LYS:HB3	1.97	0.47
1:B:629:ILE:HG23	4:E:445:SER:HB3	1.97	0.47
2:C:235:ASP:OD2	2:C:239:ASN:N	2.48	0.47
2:3:251:ILE:HG23	2:3:280:ASP:HB2	1.96	0.46
3:4:292:ASP:OD1	3:4:292:ASP:N	2.43	0.46
1:B:576:LEU:HD23	1:B:595:ALA:HB3	1.96	0.46
5:F:139:GLN:O	5:F:143:MET:HG3	2.15	0.46
5:F:186:ARG:HE	5:F:197:LEU:HD22	1.80	0.46
6:G:29:LYS:HE3	6:G:60:GLY:HA2	1.97	0.46
4:E:65:MET:HE1	4:E:159:ILE:HG21	1.96	0.46
4:E:82:GLU:OE2	4:E:84:SER:OG	2.33	0.46
4:E:614:LEU:HA	4:E:672:ALA:HB3	1.98	0.46
6:G:223:LYS:HD2	6:G:224:PRO:HD2	1.97	0.46
3:4:457:TYR:HB2	6:7:253:PRO:HG2	1.97	0.46
3:4:578:LEU:HB3	3:4:590:TYR:HE2	1.79	0.46
5:F:330:PRO:O	5:F:344:TRP:NE1	2.48	0.46
5:F:535:PRO:HB2	5:F:742:ILE:HG23	1.97	0.46
5:6:187:ARG:HG2	5:6:190:ARG:HH22	1.80	0.46
6:7:293:GLN:HG2	6:7:294:THR:HG23	1.97	0.46
2:C:251:ILE:HG23	2:C:280:ASP:HB2	1.97	0.46
4:E:40:LEU:HB2	4:E:45:ILE:HD13	1.97	0.46
3:4:812:LYS:HD3	3:4:814:LYS:HE2	1.98	0.46
1:2:576:LEU:HD13	1:2:620:ILE:HD11	1.97	0.46
2:3:279:ASP:OD1	2:3:279:ASP:N	2.48	0.46
3:4:746:PHE:HA	3:4:749:MET:HG2	1.97	0.46
1:B:580:VAL:HG12	1:B:589:TRP:HE3	1.79	0.46
1:B:609:PHE:HB3	1:B:650:ALA:HB2	1.98	0.46
5:F:187:ARG:HG2	5:F:190:ARG:HH22	1.81	0.46
1:2:406:ARG:NH1	1:2:430:TYR:OH	2.47	0.46
5:F:396:LYS:HB2	5:F:462:ILE:HD11	1.98	0.46
3:D:344:VAL:O	3:D:389:CYS:HB2	2.16	0.46
3:4:366:GLN:HB3	5:6:422:ASP:HB2	1.98	0.46
5:6:341:ARG:O	5:6:344:TRP:NE1	2.49	0.46
3:D:272:MET:O	3:D:276:ILE:HG12	2.15	0.46
4:E:469:MET:HA	4:E:477:VAL:HG21	1.98	0.46
5:F:837:ARG:HA	5:F:837:ARG:HD2	1.80	0.46
1:2:629:ILE:HG23	4:5:445:SER:HB3	1.97	0.45
6:7:223:LYS:HD2	6:7:224:PRO:HD2	1.97	0.45
2:C:354:SER:HB3	2:C:717:LEU:HD12	1.98	0.45
5:F:441:ARG:HH22	6:G:283:GLU:HG2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:423:GLU:OE1	1:2:459:ARG:NH1	2.50	0.45
3:4:435:VAL:HG13	3:4:463:VAL:HG13	1.97	0.45
3:4:686:LEU:HD12	3:4:690:GLU:HG2	1.98	0.45
2:C:97:ILE:HD13	2:C:156:SER:HB2	1.99	0.45
2:C:279:ASP:N	2:C:279:ASP:OD1	2.48	0.45
3:D:694:LEU:HD22	3:D:698:LEU:HD23	1.98	0.45
6:7:596:ILE:HD11	6:7:695:LEU:HD11	1.97	0.45
6:G:143:LEU:HG	6:G:197:THR:HA	1.99	0.45
2:3:400:ARG:NH2	2:3:544:ASP:OD1	2.44	0.45
2:3:400:ARG:HB2	2:3:707:ARG:HH21	1.82	0.45
2:3:680:VAL:HG22	6:7:613:ALA:HB1	1.98	0.45
4:5:90:PHE:CE2	4:5:137:LEU:HD13	2.51	0.45
1:B:324:VAL:HG21	1:B:418:SER:HB2	1.99	0.45
3:D:265:PRO:HB3	3:D:325:LEU:HG	1.99	0.45
1:2:230:ARG:NH1	1:2:243:GLU:O	2.50	0.45
4:5:87:ILE:HG12	4:5:137:LEU:HD23	1.98	0.45
4:E:90:PHE:CE2	4:E:137:LEU:HD13	2.52	0.45
5:F:842:ASP:OD1	5:F:842:ASP:N	2.50	0.45
6:G:283:GLU:OE2	6:G:295:LYS:HB2	2.16	0.45
1:2:224:ARG:HE	1:2:224:ARG:HB3	1.67	0.45
6:7:143:LEU:HG	6:7:197:THR:HA	1.98	0.45
6:7:257:VAL:HG12	6:7:306:LYS:HB3	1.99	0.45
6:7:460:GLY:O	6:7:568:ASN:ND2	2.48	0.45
1:B:550:SER:O	1:B:554:LYS:HG2	2.17	0.45
5:F:569:ILE:HD13	5:F:806:LEU:HD23	1.99	0.45
5:F:782:LYS:HB3	5:F:782:LYS:HE3	1.83	0.45
4:5:5:ARG:NE	2:C:234:GLU:OE2	2.49	0.45
3:D:686:LEU:HD12	3:D:690:GLU:HG2	1.98	0.45
4:5:626:PHE:CG	4:5:653:LEU:HD12	2.51	0.45
5:6:663:ILE:O	5:6:669:HIS:HA	2.17	0.45
6:7:454:ILE:O	6:7:562:SER:OG	2.26	0.45
5:F:260:GLU:O	5:F:352:ARG:NH2	2.48	0.45
6:G:610:GLU:O	6:G:614:GLU:HG3	2.17	0.45
5:6:574:VAL:O	5:6:714:VAL:HA	2.17	0.45
2:3:216:ASP:O	2:3:219:THR:OG1	2.33	0.44
2:3:354:SER:HB3	2:3:717:LEU:HD12	1.99	0.44
5:6:297:THR:OG1	5:6:357:GLN:NE2	2.50	0.44
6:7:534:ARG:O	6:7:538:HIS:HB2	2.17	0.44
1:B:447:PHE:HE1	5:F:304:LEU:HB2	1.83	0.44
3:D:366:GLN:HB3	5:F:422:ASP:HB2	2.00	0.44
1:2:511:ILE:HG21	1:2:552:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:140:ASN:OD1	4:5:334:GLN:NE2	2.50	0.44
4:5:453:VAL:HG21	4:5:504:ILE:HG21	1.99	0.44
1:B:407:GLU:HB2	1:B:450:ILE:HG22	1.98	0.44
1:B:560:ALA:HB3	1:B:563:ALA:HB2	2.00	0.44
2:3:97:ILE:HD13	2:3:156:SER:HB2	1.98	0.44
5:6:569:ILE:HD13	5:6:806:LEU:HD23	1.99	0.44
5:6:707:SER:OG	5:6:708:ARG:NH1	2.49	0.44
6:7:23:ASP:OD2	6:7:88:TYR:OH	2.23	0.44
1:B:474:PHE:CE1	1:B:764:MET:HB3	2.52	0.44
2:C:430:ILE:HD12	2:C:465:ALA:HB2	1.98	0.44
4:E:263:GLU:OE2	4:E:291:ARG:NH2	2.40	0.44
1:2:582:LYS:HE3	1:2:587:LYS:HD3	1.98	0.44
2:3:227:THR:O	2:3:227:THR:OG1	2.35	0.44
1:B:211:LEU:HD13	1:B:271:PHE:HB2	1.99	0.44
6:G:546:ILE:HD12	6:G:557:LEU:HD11	2.00	0.44
3:4:344:VAL:O	3:4:389:CYS:HB2	2.17	0.44
6:7:20:GLU:HG2	6:7:102:LEU:HD22	1.99	0.44
2:3:314:LEU:HD11	4:5:200:ILE:HA	2.00	0.44
4:5:149:ARG:NH2	4:5:260:GLU:OE2	2.43	0.44
6:7:104:SER:O	6:7:108:GLN:HG2	2.17	0.44
1:B:245:ASN:HD21	1:B:247:ARG:HH21	1.66	0.44
1:2:193:SER:HB3	1:2:196:GLU:OE1	2.18	0.44
2:3:52:ASN:HD22	2:3:90:ASN:H	1.66	0.44
1:B:406:ARG:NH1	1:B:430:TYR:OH	2.51	0.44
1:B:525:LYS:HB3	1:B:525:LYS:HE3	1.86	0.44
6:G:358:ALA:HB3	6:G:373:GLU:HB2	2.00	0.44
1:2:474:PHE:CE1	1:2:764:MET:HB3	2.52	0.44
1:2:676:ARG:HA	1:2:676:ARG:HD2	1.87	0.44
4:5:82:GLU:OE2	4:5:84:SER:OG	2.35	0.44
4:5:415:LEU:HD23	4:5:523:ALA:HB3	1.99	0.44
4:5:677:VAL:O	4:5:681:ILE:HG12	2.17	0.44
1:B:816:ILE:O	1:B:819:SER:OG	2.33	0.44
4:E:31:PHE:CE1	4:E:75:ILE:HD12	2.53	0.44
5:6:355:ASP:HB2	5:6:383:GLY:H	1.83	0.43
5:6:653:HIS:HB3	5:6:705:ILE:HD13	1.99	0.43
1:B:555:TYR:HA	1:B:558:LYS:HE2	2.00	0.43
3:D:778:ARG:HD2	3:D:793:ALA:HB3	1.99	0.43
5:F:158:LEU:HD21	5:F:170:ILE:HD12	1.99	0.43
5:F:694:SER:OG	5:F:695:LEU:N	2.51	0.43
5:6:777:TYR:HB2	5:6:800:LEU:HD13	2.00	0.43
2:3:43:ARG:O	2:3:47:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:601:LEU:H	6:7:727:LEU:HD21	1.82	0.43
4:E:266:PRO:HG2	4:E:269:GLU:HB2	2.00	0.43
1:B:193:SER:HB3	1:B:196:GLU:OE1	2.19	0.43
4:E:618:ALA:HB1	4:E:677:VAL:HG21	2.00	0.43
5:F:625:ALA:HB1	5:F:629:MET:HB2	2.00	0.43
6:G:520:ILE:HA	6:G:562:SER:O	2.19	0.43
1:2:663:LEU:HD12	1:2:663:LEU:HA	1.83	0.43
2:3:400:ARG:HD2	2:3:491:GLU:HA	1.99	0.43
6:7:17:LEU:HD13	6:7:113:PHE:HZ	1.84	0.43
6:7:459:MET:HA	6:7:567:ALA:O	2.18	0.43
6:7:527:ASP:OD1	6:7:527:ASP:N	2.52	0.43
6:7:722:VAL:HA	6:7:726:SER:HB3	2.01	0.43
1:B:304:TYR:HD2	1:B:318:VAL:HG23	1.84	0.43
1:2:527:VAL:HG11	4:5:575:ILE:HG23	2.00	0.43
6:7:668:ARG:NH1	6:7:684:ALA:O	2.43	0.43
1:B:386:GLN:HB2	1:B:415:VAL:HG12	2.00	0.43
5:6:566:ARG:O	5:6:805:ARG:NE	2.52	0.43
2:C:400:ARG:HD2	2:C:491:GLU:HA	2.00	0.43
4:E:132:LEU:HD12	4:E:133:PRO:HD2	2.01	0.43
5:F:772:TYR:HE1	5:F:825:ALA:HB2	1.83	0.43
1:2:651:ASN:ND2	7:2:2001:AGS:S1G	2.82	0.43
5:6:694:SER:OG	5:6:695:LEU:N	2.52	0.43
6:G:322:VAL:HG21	6:G:328:PRO:HG3	2.01	0.43
6:G:668:ARG:NH1	6:G:684:ALA:O	2.44	0.43
1:2:447:PHE:HE1	5:6:304:LEU:HB2	1.83	0.43
4:E:685:GLN:HA	4:E:689:MET:HB2	2.00	0.43
1:2:241:SER:OG	1:2:413:ASP:OD2	2.31	0.43
1:2:323:VAL:HG22	1:2:423:GLU:HB2	2.01	0.43
1:2:387:ARG:NH1	4:5:319:SER:OG	2.50	0.43
1:2:790:TYR:HA	1:2:793:LEU:HD12	2.01	0.43
3:4:635:ASP:OD1	3:4:635:ASP:N	2.50	0.43
4:5:132:LEU:HD12	4:5:133:PRO:HD2	2.01	0.43
4:5:282:LEU:HD13	4:5:330:ILE:HG22	2.00	0.43
5:6:625:ALA:HB1	5:6:629:MET:HB2	2.01	0.43
1:B:401:ARG:NH2	5:F:387:GLU:O	2.52	0.43
6:7:358:ALA:HB3	6:7:373:GLU:HB2	2.01	0.42
3:D:176:PRO:HB2	3:D:177:LEU:H	1.63	0.42
5:F:777:TYR:HB2	5:F:800:LEU:HD13	2.00	0.42
6:G:615:HIS:CD2	6:G:626:PRO:HG2	2.54	0.42
1:2:315:SER:N	1:2:430:TYR:O	2.45	0.42
1:2:407:GLU:HB2	1:2:450:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:800:THR:HG21	1:2:853:VAL:HG13	2.01	0.42
3:4:831:SER:HA	3:4:836:TYR:HE1	1.85	0.42
6:7:224:PRO:HB2	6:7:242:ARG:HG2	2.01	0.42
6:7:242:ARG:HA	6:7:349:VAL:O	2.19	0.42
6:7:520:ILE:HA	6:7:562:SER:O	2.19	0.42
1:B:766:TYR:OH	1:B:823:MET:O	2.32	0.42
2:C:446:VAL:HG21	2:C:502:ILE:HG21	2.01	0.42
2:C:687:ARG:NH1	6:G:602:ASP:OD1	2.44	0.42
4:E:87:ILE:HG12	4:E:137:LEU:HD23	2.01	0.42
5:F:109:GLU:O	5:F:113:GLU:HG3	2.18	0.42
6:G:527:ASP:OD1	6:G:527:ASP:N	2.52	0.42
2:3:299:LYS:HD2	2:3:299:LYS:HA	1.81	0.42
5:F:317:ILE:HD12	5:F:350:ARG:NH2	2.35	0.42
4:5:266:PRO:HG2	4:5:269:GLU:HB2	2.00	0.42
6:7:29:LYS:HE3	6:7:60:GLY:HA2	2.01	0.42
1:B:235:GLY:HA3	1:B:283:TYR:CE1	2.54	0.42
1:B:536:ASP:HB2	1:B:645:SER:HB2	2.00	0.42
3:D:635:ASP:OD1	3:D:635:ASP:N	2.51	0.42
3:D:724:LEU:HD22	6:G:690:LEU:HD21	2.02	0.42
1:2:304:TYR:HD2	1:2:318:VAL:HG23	1.85	0.42
6:7:259:ALA:H	6:7:305:SER:HB3	1.85	0.42
3:D:550:LYS:HG2	5:F:738:ARG:HH21	1.84	0.42
3:D:578:LEU:HD23	3:D:630:CYS:HB3	2.00	0.42
5:F:347:ASN:HD21	5:F:350:ARG:HD3	1.85	0.42
6:G:601:LEU:H	6:G:727:LEU:HD21	1.85	0.42
6:G:722:VAL:HA	6:G:726:SER:HB3	2.02	0.42
1:B:610:ASP:OD1	1:B:610:ASP:N	2.53	0.42
3:D:609:VAL:HG11	6:G:506:MET:H	1.84	0.42
6:G:17:LEU:HD13	6:G:113:PHE:HZ	1.85	0.42
3:4:326:ILE:O	3:4:436:THR:HA	2.20	0.42
4:5:90:PHE:CE2	4:5:94:ILE:HD11	2.54	0.42
1:B:540:LEU:HB3	1:B:680:LEU:HD23	2.02	0.42
3:D:802:ILE:HD11	5:F:732:VAL:HG22	2.02	0.42
4:E:32:LYS:HE3	4:E:32:LYS:HB2	1.84	0.42
4:5:5:ARG:HG3	2:C:233:THR:HB	2.02	0.42
5:6:120:GLU:HB3	5:6:137:ARG:HH21	1.84	0.42
6:G:423:TYR:HB2	6:G:615:HIS:CG	2.55	0.42
1:2:347:ILE:HD11	5:F:429:THR:HG23	2.02	0.42
2:3:233:THR:HB	4:E:5:ARG:HG3	2.01	0.42
3:4:265:PRO:HB3	3:4:325:LEU:HG	2.01	0.42
3:D:590:TYR:OH	3:D:632:ASP:OD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:90:PHE:CE2	4:E:94:ILE:HD11	2.55	0.42
4:E:565:ASP:HA	4:E:568:ILE:HG22	2.02	0.42
3:4:229:GLN:HA	3:4:232:GLU:HG2	2.02	0.41
3:4:550:LYS:HG2	5:6:738:ARG:HH21	1.84	0.41
3:4:762:ILE:HB	5:6:736:MET:HG2	2.02	0.41
5:6:158:LEU:HD21	5:6:170:ILE:HD12	2.02	0.41
5:6:317:ILE:HD12	5:6:350:ARG:NH2	2.34	0.41
5:6:842:ASP:N	5:6:842:ASP:OD1	2.50	0.41
1:B:808:ARG:NH2	7:E:2001:AGS:S1G	2.81	0.41
6:G:459:MET:SD	6:G:584:ILE:HG12	2.60	0.41
4:5:31:PHE:CE1	4:5:75:ILE:HD12	2.55	0.41
4:5:31:PHE:CG	4:5:90:PHE:HD1	2.38	0.41
4:5:405:ARG:HH12	4:5:500:GLN:HG3	1.85	0.41
1:B:353:GLN:HE22	1:B:358:GLU:HA	1.85	0.41
1:B:600:ASP:OD2	1:B:643:ARG:NH2	2.40	0.41
2:C:724:VAL:HA	2:C:727:LYS:HG2	2.00	0.41
3:D:602:THR:HG22	3:D:654:ILE:HD13	2.01	0.41
3:D:831:SER:HA	3:D:836:TYR:HE1	1.85	0.41
4:E:83:PRO:HG3	4:E:159:ILE:HG13	2.02	0.41
4:E:149:ARG:NH2	4:E:260:GLU:OE2	2.43	0.41
5:F:574:VAL:O	5:F:714:VAL:HA	2.20	0.41
6:G:417:SER:HA	6:G:420:PRO:HG3	2.02	0.41
3:4:802:ILE:HD11	5:6:732:VAL:HG22	2.00	0.41
2:C:150:ARG:HD3	2:C:150:ARG:HA	1.91	0.41
4:E:31:PHE:CG	4:E:90:PHE:HD1	2.39	0.41
6:G:242:ARG:HA	6:G:349:VAL:O	2.20	0.41
3:4:315:ARG:NH2	3:4:411:THR:O	2.35	0.41
4:5:65:MET:HG2	4:5:139:LEU:HD12	2.01	0.41
2:C:186:VAL:HG12	2:C:288:PRO:HA	2.02	0.41
3:D:689:THR:HG22	3:D:791:ILE:HG12	2.02	0.41
1:2:211:LEU:HD13	1:2:271:PHE:HB2	2.01	0.41
1:B:387:ARG:NH1	4:E:319:SER:OG	2.48	0.41
1:B:558:LYS:HE3	1:B:558:LYS:HB2	1.81	0.41
2:C:666:ARG:HA	2:C:666:ARG:HD3	1.87	0.41
3:D:456:LEU:HD12	3:D:456:LEU:HA	1.95	0.41
7:D:2001:AGS:O3A	6:G:687:ARG:NH2	2.53	0.41
4:E:450:THR:HA	4:E:469:MET:HB2	2.02	0.41
5:F:333:CYS:HB2	5:F:344:TRP:CZ2	2.56	0.41
6:G:442:LYS:HB3	6:G:450:ILE:HB	2.03	0.41
2:3:276:VAL:HG11	2:3:294:VAL:HG11	2.02	0.41
1:B:563:ALA:HA	1:B:603:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:ILE:HD11	5:F:621:TYR:HE2	1.84	0.41
3:D:707:LEU:HD23	3:D:707:LEU:HA	1.95	0.41
4:E:685:GLN:OE1	4:E:689:MET:HG3	2.21	0.41
6:G:86:LEU:HG	6:G:215:TYR:HD2	1.86	0.41
1:2:540:LEU:HB3	1:2:680:LEU:HD23	2.03	0.41
3:4:447:ASN:HB2	3:4:450:GLN:HB2	2.03	0.41
3:4:475:ASP:OD1	3:4:475:ASP:N	2.51	0.41
4:5:565:ASP:HA	4:5:568:ILE:HG22	2.03	0.41
6:7:459:MET:SD	6:7:584:ILE:HG12	2.61	0.41
5:6:347:ASN:HD21	5:6:350:ARG:HD3	1.85	0.41
2:C:452:THR:HG21	2:C:456:ARG:HH22	1.85	0.41
3:D:695:PRO:HA	3:D:696:PRO:HD3	1.98	0.41
5:F:784:ASP:OD2	5:F:795:ILE:HG12	2.20	0.41
1:2:558:LYS:HE3	1:2:558:LYS:HB2	1.81	0.41
3:4:380:ASN:ND2	1:B:365:THR:O	2.54	0.41
4:5:32:LYS:HB2	4:5:32:LYS:HE3	1.83	0.41
4:5:572:VAL:HA	4:5:575:ILE:HD12	2.02	0.41
5:6:684:PRO:HB3	5:6:698:ASN:HB3	2.03	0.41
6:7:61:PRO:HB2	6:7:64:MET:HB2	2.02	0.41
6:7:260:TYR:HB3	6:7:298:LEU:HB3	2.02	0.41
6:7:432:LEU:HB3	6:7:473:ILE:HD11	2.03	0.41
2:C:393:LEU:HD12	2:C:397:SER:HB3	2.03	0.41
2:C:538:SER:O	2:C:542:ARG:HG2	2.21	0.41
4:E:137:LEU:HG	4:E:139:LEU:HD22	2.03	0.41
5:F:180:PHE:HA	5:F:183:LYS:HE2	2.03	0.41
5:F:412:LEU:O	5:F:416:LYS:NZ	2.48	0.41
4:5:389:VAL:O	4:5:393:MET:HG2	2.21	0.41
4:5:618:ALA:HB1	4:5:677:VAL:HG21	2.02	0.41
4:5:649:THR:H	4:5:652:GLN:HG2	1.86	0.41
1:B:233:THR:O	1:B:237:MET:HG2	2.21	0.41
5:F:649:GLN:HA	5:F:652:ILE:HG12	2.02	0.41
1:2:342:LEU:HD12	1:2:372:PRO:HB2	2.03	0.40
2:3:645:THR:H	2:3:648:PRO:HG3	1.86	0.40
1:B:549:LYS:HB2	1:B:549:LYS:HE2	1.92	0.40
2:C:262:PRO:HG3	4:E:509:ILE:HD11	2.02	0.40
5:F:300:VAL:HG13	5:F:386:VAL:HG11	2.03	0.40
6:G:243:GLY:HA2	6:G:318:LEU:HG	2.03	0.40
2:3:349:ASN:HA	2:3:352:LYS:HG2	2.04	0.40
5:6:816:VAL:HG21	5:6:823:PHE:HE2	1.86	0.40
4:E:405:ARG:HH12	4:E:500:GLN:HG3	1.86	0.40
4:E:440:SER:OG	4:E:443:GLY:O	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:383:ARG:HD2	1:2:411:LEU:HD12	2.04	0.40
2:3:150:ARG:HD3	2:3:150:ARG:HA	1.91	0.40
2:3:343:THR:OG1	2:3:346:ASP:OD2	2.30	0.40
3:4:315:ARG:NH2	3:4:413:HIS:HD2	2.19	0.40
4:5:270:MET:SD	4:5:271:PRO:HD2	2.62	0.40
5:6:412:LEU:O	5:6:416:LYS:NZ	2.49	0.40
5:6:742:ILE:HD13	5:6:742:ILE:HA	1.88	0.40
1:B:511:ILE:HG21	1:B:552:ILE:HD13	2.03	0.40
2:C:400:ARG:NH2	2:C:544:ASP:OD1	2.44	0.40
2:3:333:SER:HB2	2:3:423:LEU:HD11	2.04	0.40
2:3:426:ALA:HB3	2:3:429:ALA:HB2	2.03	0.40
1:B:786:VAL:HG11	1:B:814:LEU:HD11	2.04	0.40
5:F:816:VAL:HG21	5:F:823:PHE:HE2	1.86	0.40
6:G:432:LEU:HB3	6:G:473:ILE:HD11	2.02	0.40
1:2:343:LYS:HE3	1:2:371:GLY:HA3	2.04	0.40
2:3:281:ASP:OD1	2:3:281:ASP:N	2.50	0.40
2:3:452:THR:HG21	2:3:456:ARG:HH22	1.85	0.40
3:4:758:ILE:HG22	3:4:760:PRO:HD3	2.02	0.40
5:6:529:LEU:O	5:6:533:ILE:HG12	2.21	0.40
6:7:86:LEU:HG	6:7:215:TYR:HD2	1.87	0.40
6:7:87:GLN:NE2	6:7:91:GLU:OE2	2.48	0.40
6:7:271:GLN:HE21	6:7:271:GLN:HB2	1.64	0.40
6:7:423:TYR:HB2	6:7:615:HIS:CG	2.57	0.40
4:E:444:SER:HB2	4:E:447:ALA:HB3	2.04	0.40
6:G:224:PRO:HB2	6:G:242:ARG:HG2	2.03	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	622/868 (72%)	609 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	622/868 (72%)	607 (98%)	15 (2%)	0	100	100
2	3	627/971 (65%)	607 (97%)	20 (3%)	0	100	100
2	C	627/971 (65%)	603 (96%)	24 (4%)	0	100	100
3	4	664/933 (71%)	650 (98%)	14 (2%)	0	100	100
3	D	664/933 (71%)	649 (98%)	15 (2%)	0	100	100
4	5	650/775 (84%)	637 (98%)	13 (2%)	0	100	100
4	E	650/775 (84%)	637 (98%)	13 (2%)	0	100	100
5	6	638/1017 (63%)	621 (97%)	17 (3%)	0	100	100
5	F	638/1017 (63%)	621 (97%)	17 (3%)	0	100	100
6	7	693/845 (82%)	685 (99%)	8 (1%)	0	100	100
6	G	693/845 (82%)	683 (99%)	10 (1%)	0	100	100
All	All	7788/10818 (72%)	7609 (98%)	179 (2%)	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	552/770 (72%)	550 (100%)	2 (0%)	89	96
1	B	552/770 (72%)	551 (100%)	1 (0%)	92	97
2	3	550/835 (66%)	550 (100%)	0	100	100
2	C	550/835 (66%)	550 (100%)	0	100	100
3	4	606/848 (72%)	604 (100%)	2 (0%)	91	96
3	D	606/848 (72%)	604 (100%)	2 (0%)	91	96
4	5	588/688 (86%)	587 (100%)	1 (0%)	92	97
4	E	588/688 (86%)	587 (100%)	1 (0%)	92	97
5	6	565/886 (64%)	565 (100%)	0	100	100
5	F	565/886 (64%)	565 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	7	618/753 (82%)	616 (100%)	2 (0%)	91 96
6	G	618/753 (82%)	618 (100%)	0	100 100
All	All	6958/9560 (73%)	6947 (100%)	11 (0%)	91 97

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	247	ARG
1	2	458	ARG
3	4	428	ARG
3	4	449	ARG
4	5	339	THR
6	7	73	ARG
6	7	271	GLN
1	B	458	ARG
3	D	428	ARG
3	D	449	ARG
4	E	339	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	3	330	HIS
4	5	574	ASN
4	5	579	ASN
5	6	653	HIS
5	6	833	GLN
6	7	109	ASN
6	7	271	GLN
6	7	615	HIS
6	G	109	ASN
6	G	615	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 22 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
7	AGS	2	2001	8	26,33,33	0.70	0	26,52,52	1.03	2 (7%)
7	AGS	7	2001	8	26,33,33	0.72	1 (3%)	26,52,52	1.01	2 (7%)
7	AGS	E	2001	8	26,33,33	0.72	1 (3%)	26,52,52	1.11	2 (7%)
7	AGS	5	2001	8	26,33,33	0.72	1 (3%)	26,52,52	1.11	2 (7%)
7	AGS	B	2001	8	26,33,33	0.69	0	26,52,52	1.04	2 (7%)
7	AGS	D	2001	8	26,33,33	0.70	1 (3%)	26,52,52	1.08	2 (7%)
7	AGS	F	2001	8	26,33,33	0.69	0	26,52,52	1.00	2 (7%)
10	ADP	3	2001	8	24,29,29	0.96	1 (4%)	29,45,45	1.44	4 (13%)
7	AGS	4	2001	8	26,33,33	0.70	1 (3%)	26,52,52	1.14	2 (7%)
7	AGS	G	2001	8	26,33,33	0.72	1 (3%)	26,52,52	0.99	2 (7%)
10	ADP	C	2001	8	24,29,29	0.95	1 (4%)	29,45,45	1.44	4 (13%)
7	AGS	6	2001	8	26,33,33	0.70	1 (3%)	26,52,52	1.00	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AGS	2	2001	8	-	4/17/38/38	0/3/3/3
7	AGS	7	2001	8	-	5/17/38/38	0/3/3/3
7	AGS	E	2001	8	-	4/17/38/38	0/3/3/3
7	AGS	5	2001	8	-	3/17/38/38	0/3/3/3
7	AGS	B	2001	8	-	4/17/38/38	0/3/3/3
7	AGS	D	2001	8	-	6/17/38/38	0/3/3/3
7	AGS	F	2001	8	-	6/17/38/38	0/3/3/3
10	ADP	3	2001	8	-	6/12/32/32	0/3/3/3
7	AGS	4	2001	8	-	6/17/38/38	0/3/3/3
7	AGS	G	2001	8	-	5/17/38/38	0/3/3/3
10	ADP	C	2001	8	-	6/12/32/32	0/3/3/3
7	AGS	6	2001	8	-	6/17/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	2001	ADP	C5-C4	2.49	1.47	1.40
10	C	2001	ADP	C5-C4	2.45	1.47	1.40
7	G	2001	AGS	PG-S1G	2.12	1.95	1.90
7	E	2001	AGS	PG-S1G	2.12	1.95	1.90
7	7	2001	AGS	PG-S1G	2.10	1.95	1.90
7	4	2001	AGS	PG-S1G	2.09	1.95	1.90
7	5	2001	AGS	PG-S1G	2.08	1.95	1.90
7	D	2001	AGS	PG-S1G	2.07	1.95	1.90
7	6	2001	AGS	PG-S1G	2.05	1.95	1.90

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	2001	AGS	PA-O3A-PB	-4.21	118.39	132.83
7	5	2001	AGS	PA-O3A-PB	-4.15	118.57	132.83
7	4	2001	AGS	PA-O3A-PB	-4.03	119.00	132.83
7	D	2001	AGS	PA-O3A-PB	-3.82	119.73	132.83
7	B	2001	AGS	PA-O3A-PB	-3.64	120.34	132.83
7	2	2001	AGS	PA-O3A-PB	-3.57	120.57	132.83
7	7	2001	AGS	PA-O3A-PB	-3.55	120.63	132.83
7	G	2001	AGS	PA-O3A-PB	-3.52	120.76	132.83
7	6	2001	AGS	PA-O3A-PB	-3.42	121.10	132.83
7	F	2001	AGS	PA-O3A-PB	-3.38	121.23	132.83
10	C	2001	ADP	N3-C2-N1	-3.28	123.56	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	2001	ADP	N3-C2-N1	-3.23	123.64	128.68
10	C	2001	ADP	C3'-C2'-C1'	3.21	105.81	100.98
10	3	2001	ADP	C3'-C2'-C1'	3.17	105.75	100.98
10	3	2001	ADP	PA-O3A-PB	-3.09	122.24	132.83
10	C	2001	ADP	PA-O3A-PB	-3.02	122.46	132.83
10	3	2001	ADP	C4-C5-N7	-2.79	106.49	109.40
10	C	2001	ADP	C4-C5-N7	-2.73	106.56	109.40
7	4	2001	AGS	C5-C6-N6	2.37	123.96	120.35
7	G	2001	AGS	C5-C6-N6	2.34	123.91	120.35
7	D	2001	AGS	C5-C6-N6	2.32	123.89	120.35
7	2	2001	AGS	C5-C6-N6	2.32	123.88	120.35
7	F	2001	AGS	C5-C6-N6	2.32	123.88	120.35
7	5	2001	AGS	C5-C6-N6	2.31	123.87	120.35
7	6	2001	AGS	C5-C6-N6	2.30	123.84	120.35
7	E	2001	AGS	C5-C6-N6	2.28	123.82	120.35
7	7	2001	AGS	C5-C6-N6	2.25	123.77	120.35
7	B	2001	AGS	C5-C6-N6	2.23	123.74	120.35

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	2	2001	AGS	PB-O3B-PG-O2G
7	2	2001	AGS	PB-O3B-PG-O3G
7	4	2001	AGS	C5'-O5'-PA-O2A
7	6	2001	AGS	C5'-O5'-PA-O1A
7	6	2001	AGS	C5'-O5'-PA-O2A
7	6	2001	AGS	C5'-O5'-PA-O3A
7	7	2001	AGS	C5'-O5'-PA-O1A
7	7	2001	AGS	C5'-O5'-PA-O2A
7	7	2001	AGS	C5'-O5'-PA-O3A
7	7	2001	AGS	O4'-C4'-C5'-O5'
7	B	2001	AGS	PB-O3B-PG-O2G
7	B	2001	AGS	PB-O3B-PG-O3G
7	D	2001	AGS	C5'-O5'-PA-O2A
7	D	2001	AGS	O4'-C4'-C5'-O5'
7	E	2001	AGS	O4'-C4'-C5'-O5'
7	F	2001	AGS	PB-O3B-PG-O2G
7	F	2001	AGS	C5'-O5'-PA-O3A
7	F	2001	AGS	O4'-C4'-C5'-O5'
7	G	2001	AGS	C5'-O5'-PA-O1A
7	G	2001	AGS	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
7	G	2001	AGS	C5'-O5'-PA-O3A
10	3	2001	ADP	O4'-C4'-C5'-O5'
10	C	2001	ADP	C5'-O5'-PA-O2A
10	C	2001	ADP	O4'-C4'-C5'-O5'
7	4	2001	AGS	O4'-C4'-C5'-O5'
7	6	2001	AGS	O4'-C4'-C5'-O5'
7	E	2001	AGS	C3'-C4'-C5'-O5'
7	G	2001	AGS	O4'-C4'-C5'-O5'
10	3	2001	ADP	C3'-C4'-C5'-O5'
10	C	2001	ADP	C3'-C4'-C5'-O5'
7	5	2001	AGS	O4'-C4'-C5'-O5'
7	5	2001	AGS	C3'-C4'-C5'-O5'
7	4	2001	AGS	C3'-C4'-C5'-O5'
7	7	2001	AGS	PA-O3A-PB-O1B
7	G	2001	AGS	PA-O3A-PB-O1B
7	6	2001	AGS	C3'-C4'-C5'-O5'
7	B	2001	AGS	O4'-C4'-C5'-O5'
7	4	2001	AGS	C5'-O5'-PA-O3A
7	D	2001	AGS	C5'-O5'-PA-O3A
10	3	2001	ADP	C5'-O5'-PA-O3A
7	4	2001	AGS	C5'-O5'-PA-O1A
7	D	2001	AGS	C5'-O5'-PA-O1A
7	F	2001	AGS	C5'-O5'-PA-O1A
7	F	2001	AGS	C5'-O5'-PA-O2A
10	3	2001	ADP	C5'-O5'-PA-O2A
7	D	2001	AGS	C3'-C4'-C5'-O5'
7	2	2001	AGS	O4'-C4'-C5'-O5'
7	B	2001	AGS	PB-O3A-PA-O2A
10	3	2001	ADP	C4'-C5'-O5'-PA
10	C	2001	ADP	C4'-C5'-O5'-PA
7	F	2001	AGS	C3'-C4'-C5'-O5'
7	5	2001	AGS	PG-O3B-PB-O2B
7	E	2001	AGS	PG-O3B-PB-O2B
7	6	2001	AGS	PB-O3B-PG-O2G
7	4	2001	AGS	C4'-C5'-O5'-PA
10	C	2001	ADP	C5'-O5'-PA-O3A
7	2	2001	AGS	PB-O3A-PA-O2A
7	E	2001	AGS	C5'-O5'-PA-O1A
10	3	2001	ADP	C5'-O5'-PA-O1A
10	C	2001	ADP	C5'-O5'-PA-O1A
7	D	2001	AGS	C4'-C5'-O5'-PA

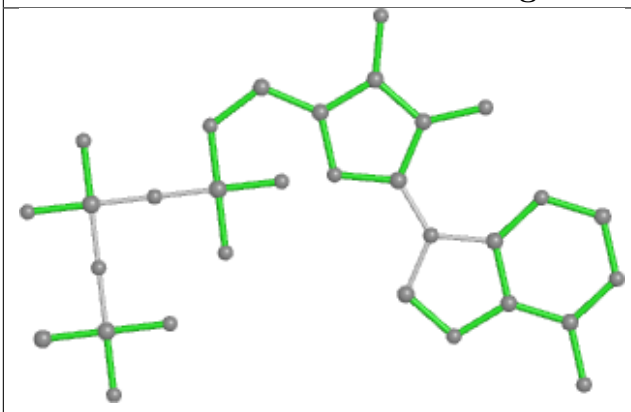
There are no ring outliers.

9 monomers are involved in 13 short contacts:

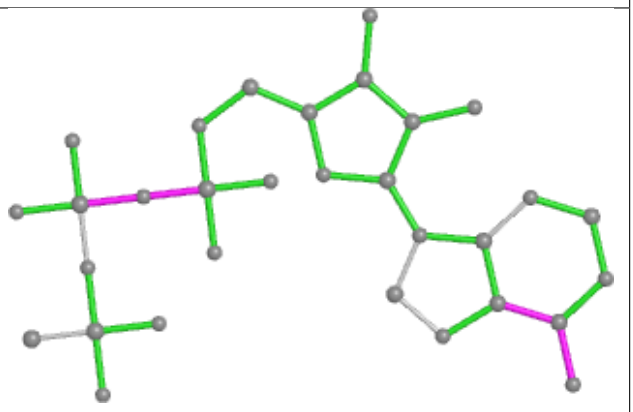
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	2	2001	AGS	2	0
7	7	2001	AGS	1	0
7	E	2001	AGS	3	0
7	5	2001	AGS	1	0
7	B	2001	AGS	1	0
7	D	2001	AGS	2	0
7	4	2001	AGS	1	0
7	G	2001	AGS	1	0
7	6	2001	AGS	1	0

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.

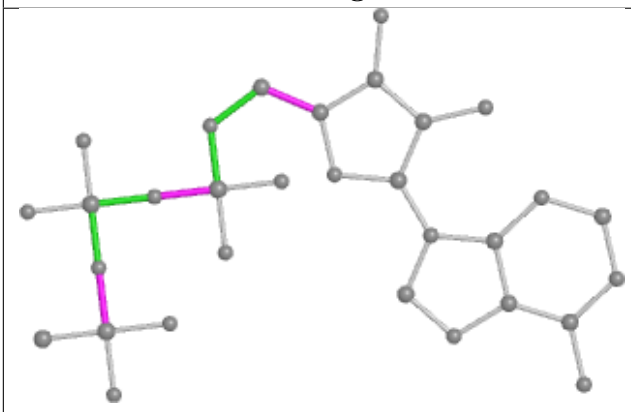
Ligand AGS 2 2001



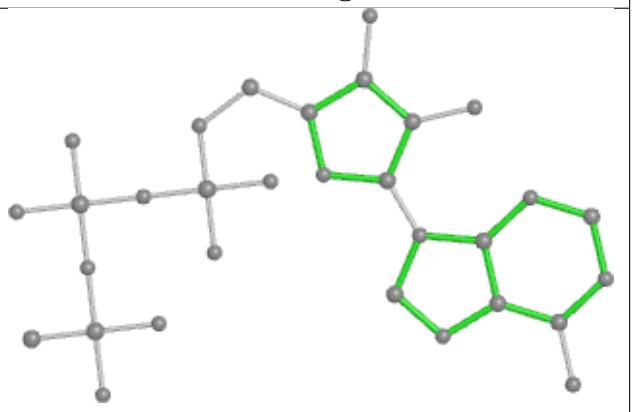
Bond lengths



Bond angles

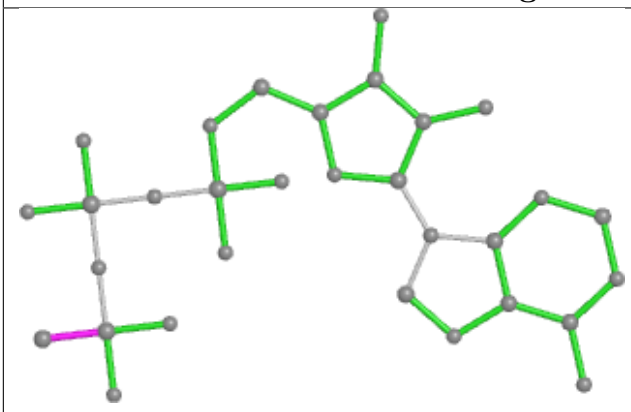


Torsions



Rings

Ligand AGS 7 2001



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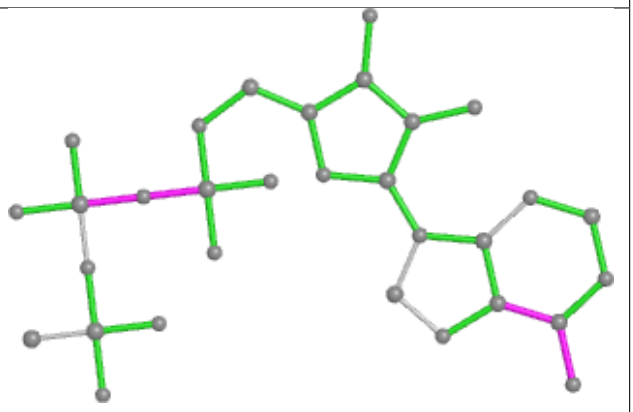

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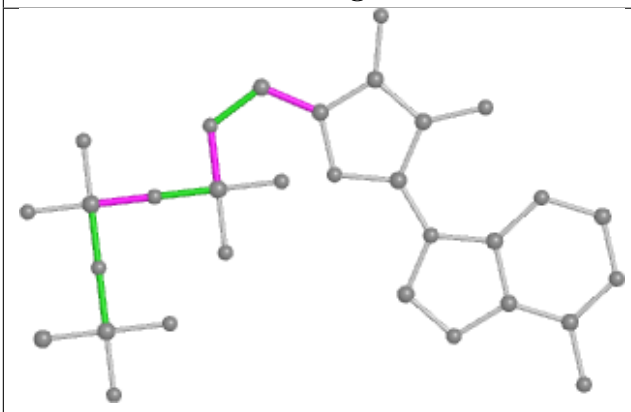

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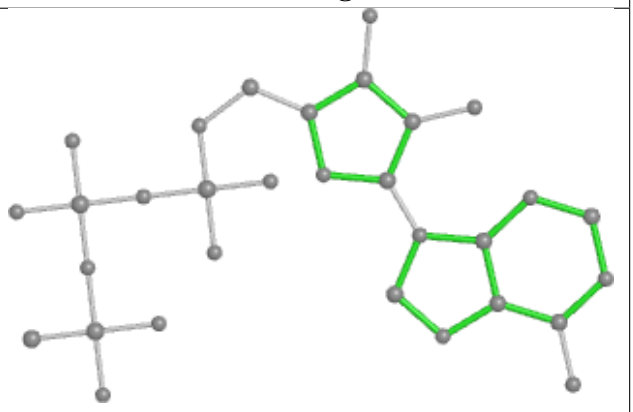

Rings

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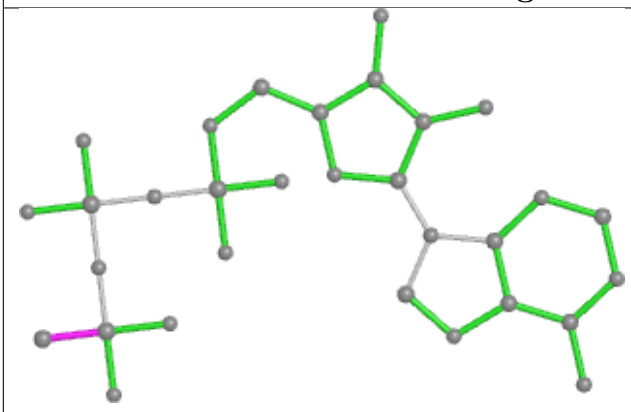

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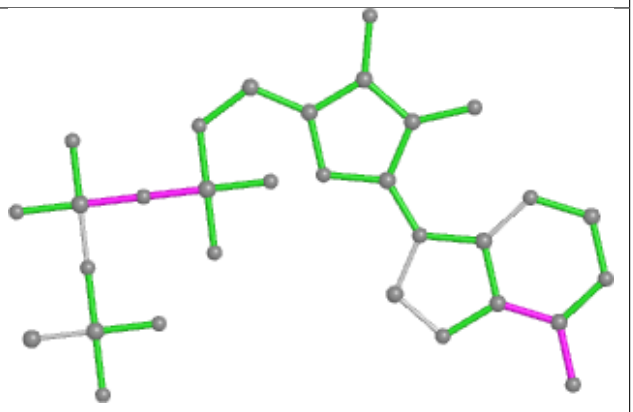
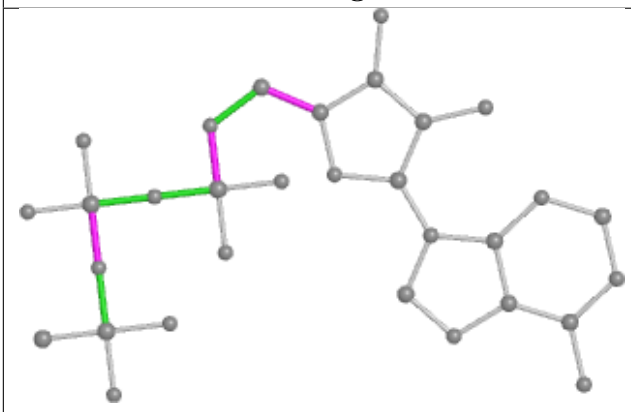


Bond angles



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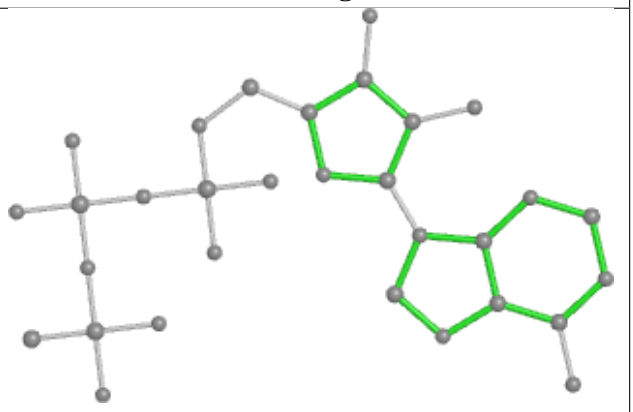
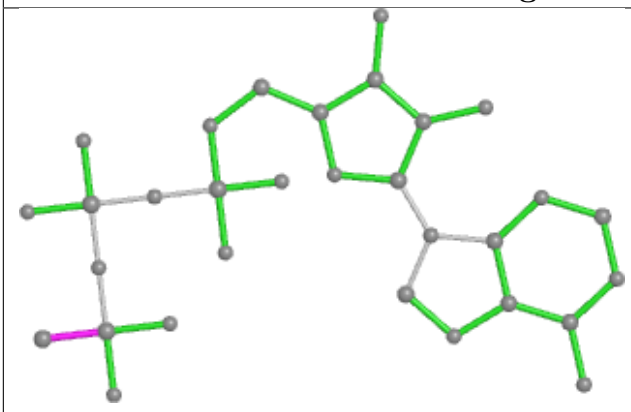


Rings

Ligand AGS 5 2001



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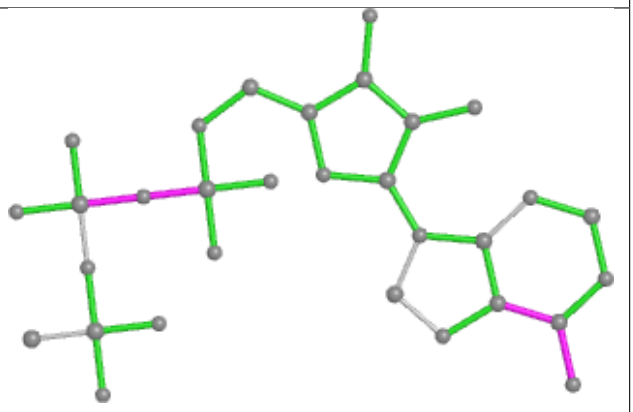
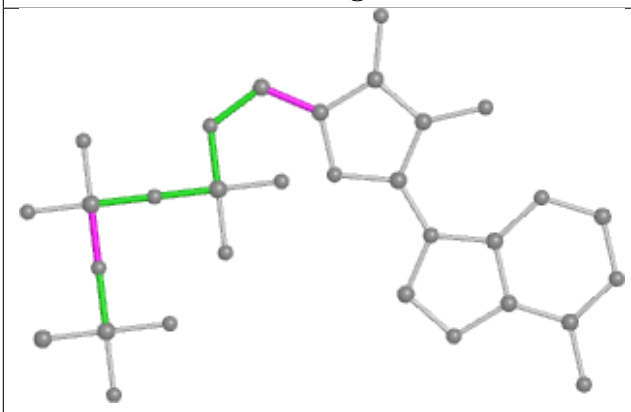


Bond angles



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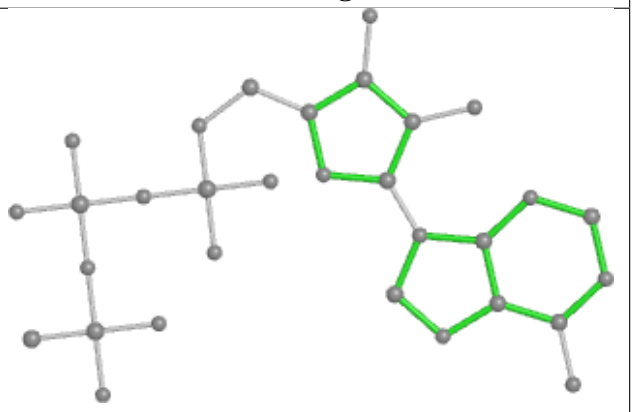

Rings

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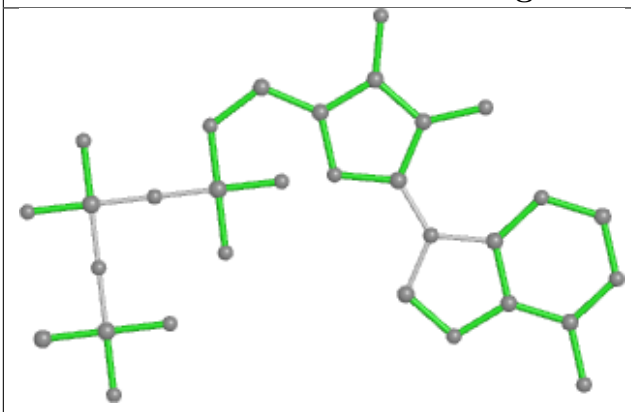
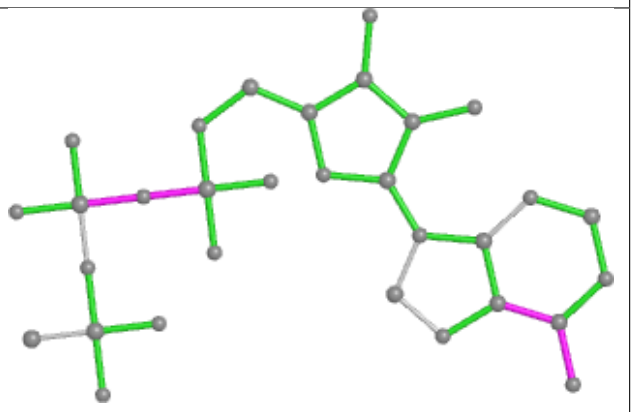
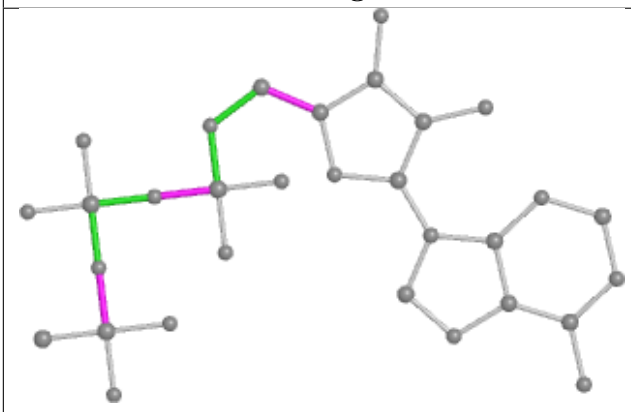


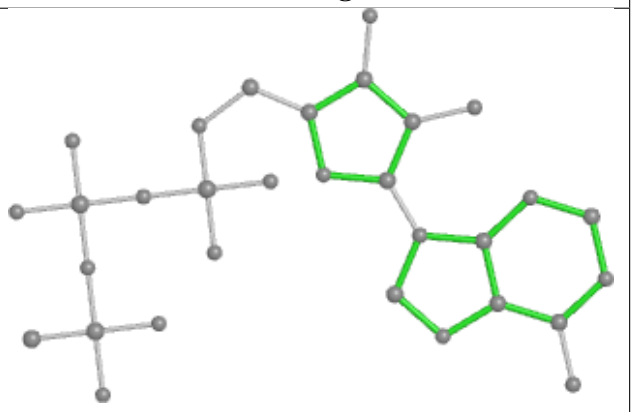
Bond lengths



Bond angles

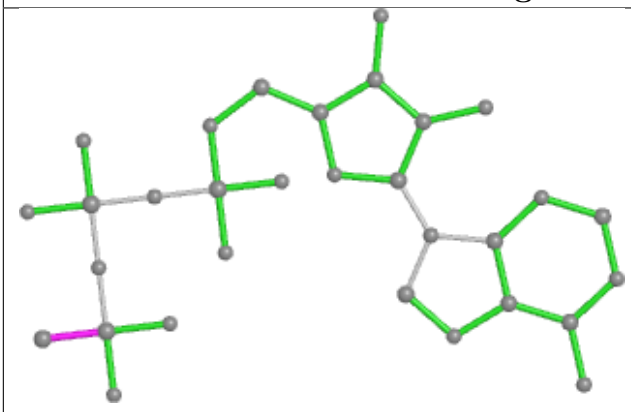


Torsions

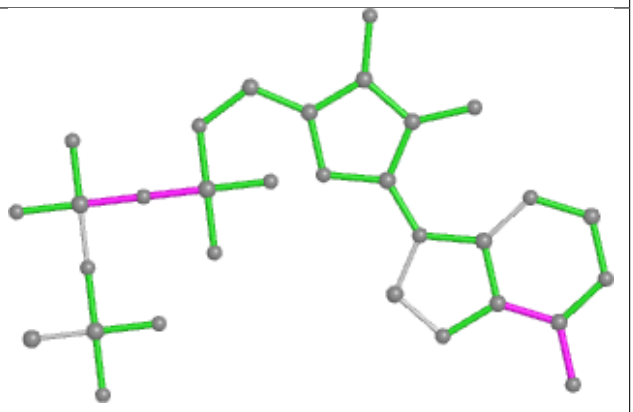


Rings

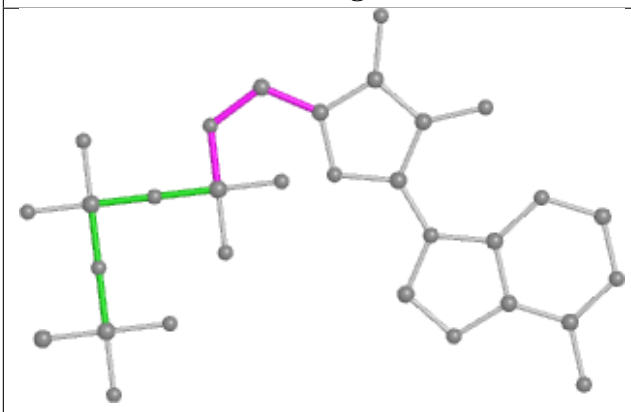
Ligand AGS D 2001



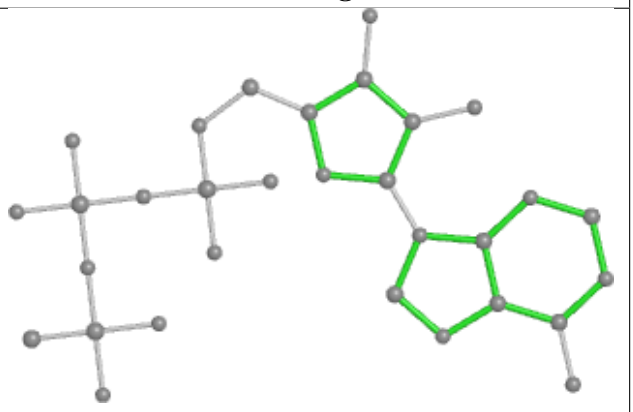
Bond lengths



Bond angles

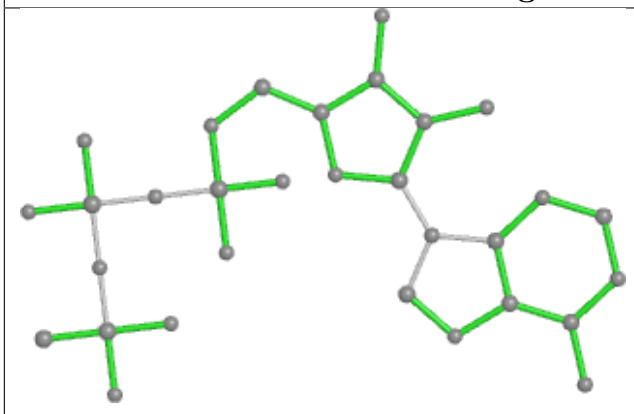


Torsions

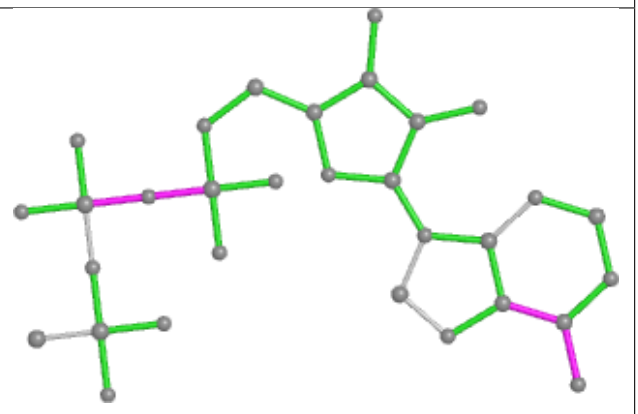


Rings

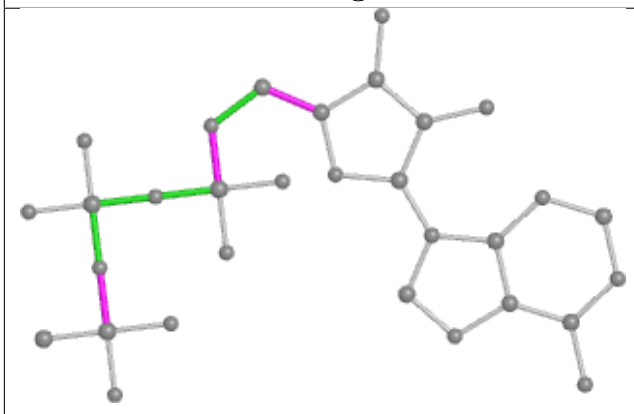
Ligand AGS F 2001



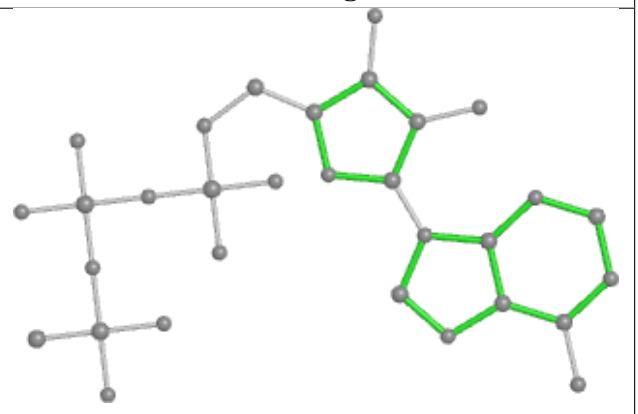
Bond lengths



Bond angles

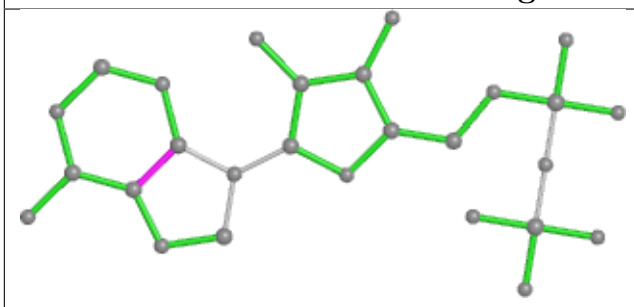


Torsions

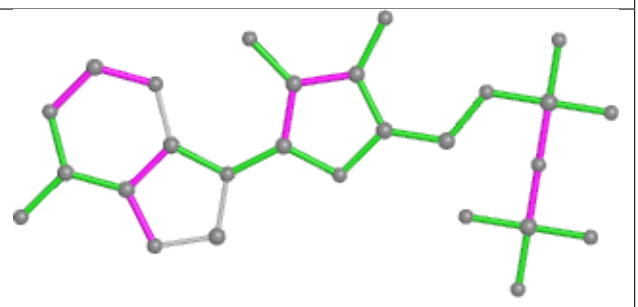


Rings

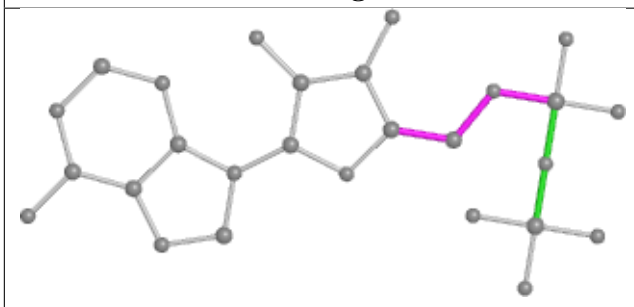
Ligand ADP 3 2001



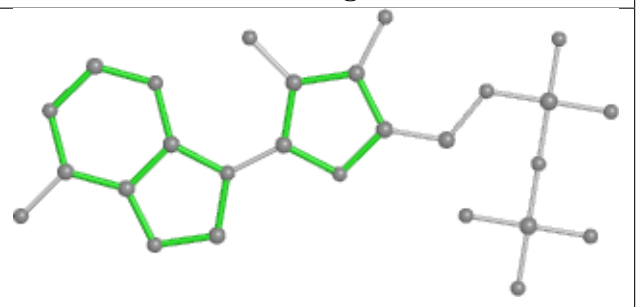
Bond lengths



Bond angles

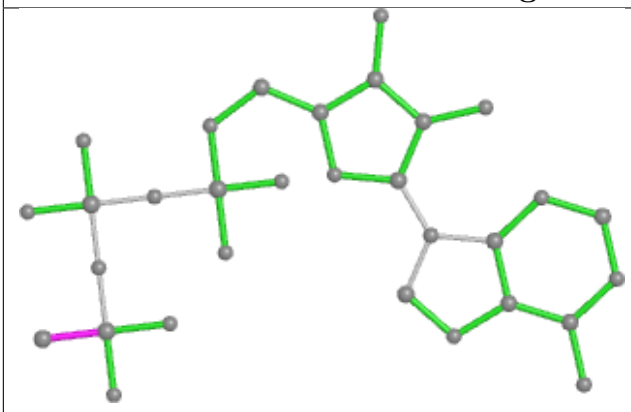


Torsions

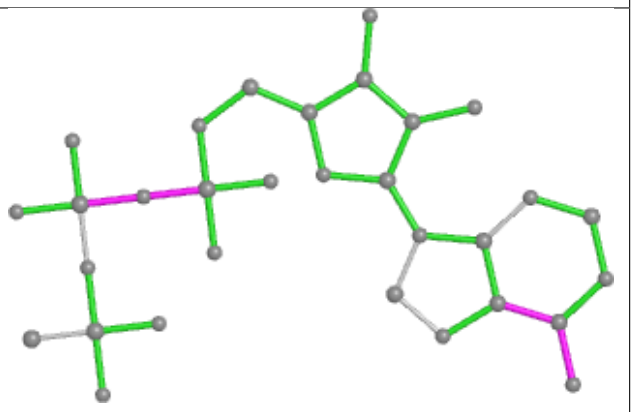


Rings

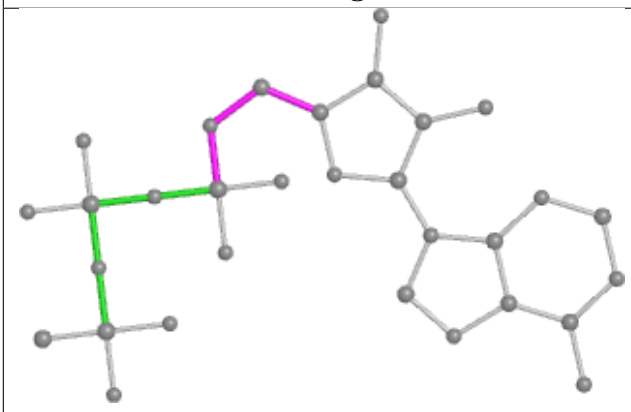
Ligand AGS 4 2001



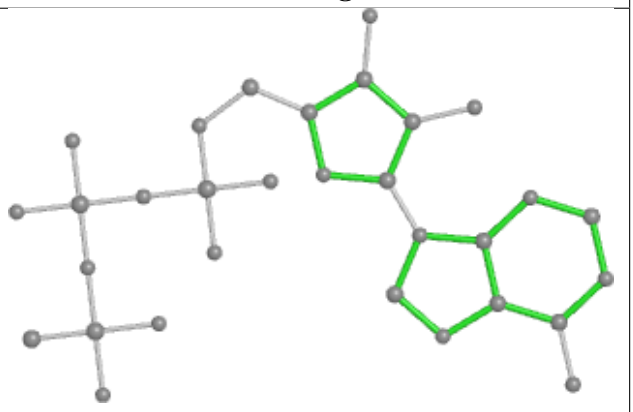
Bond lengths



Bond angles

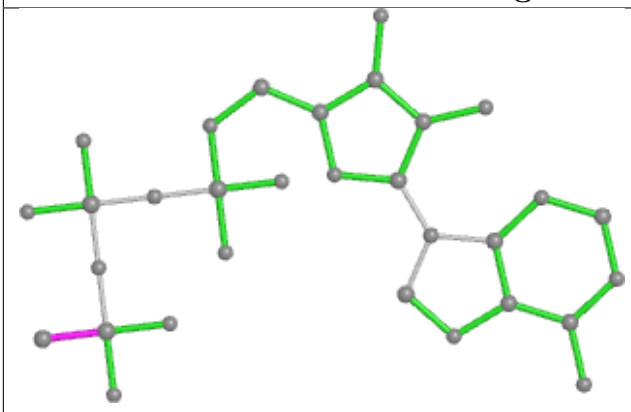


Torsions

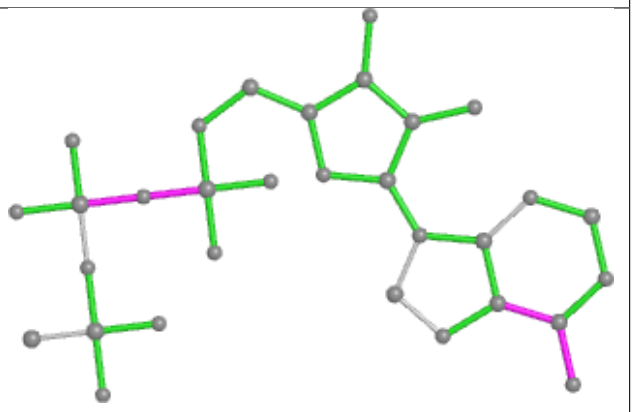


Rings

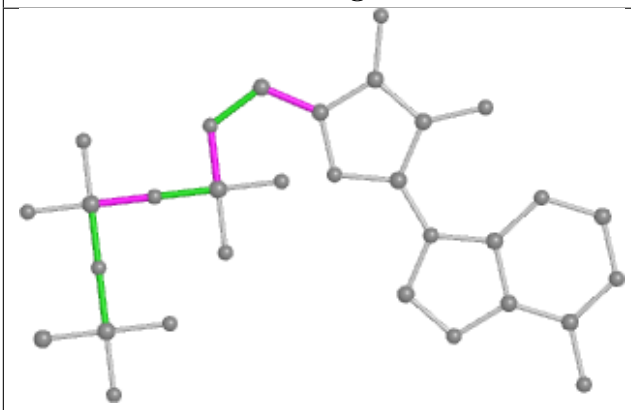
Ligand AGS G 2001



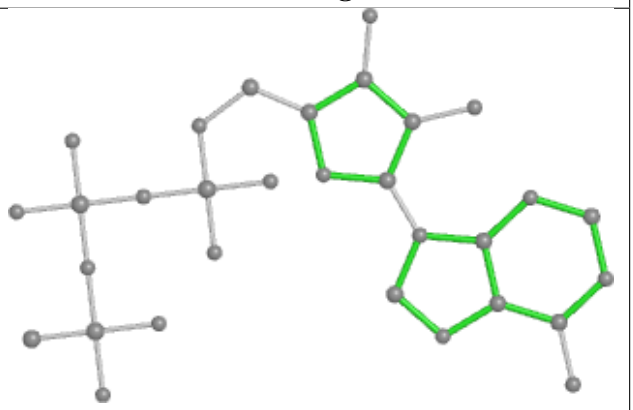
Bond lengths



Bond angles

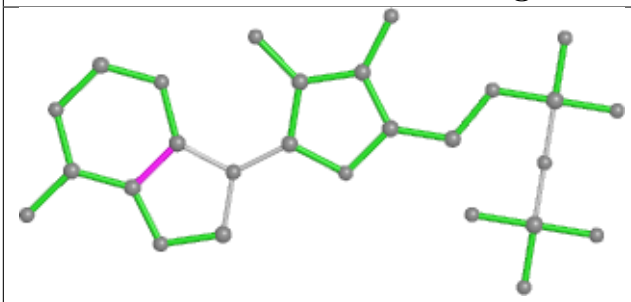


Torsions

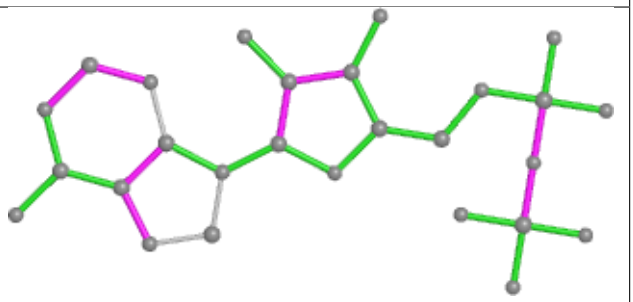


Rings

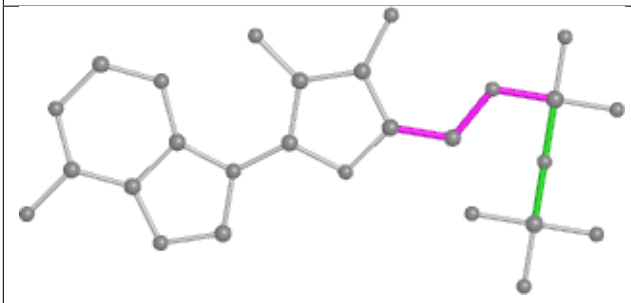
Ligand ADP C 2001



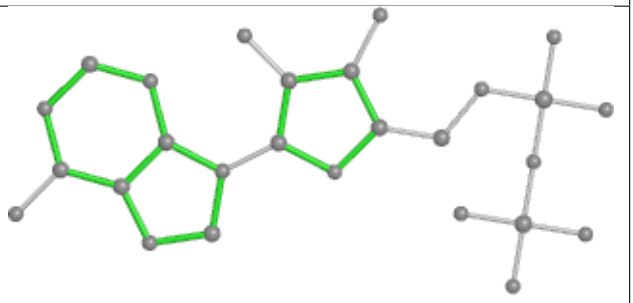
Bond lengths



Bond angles

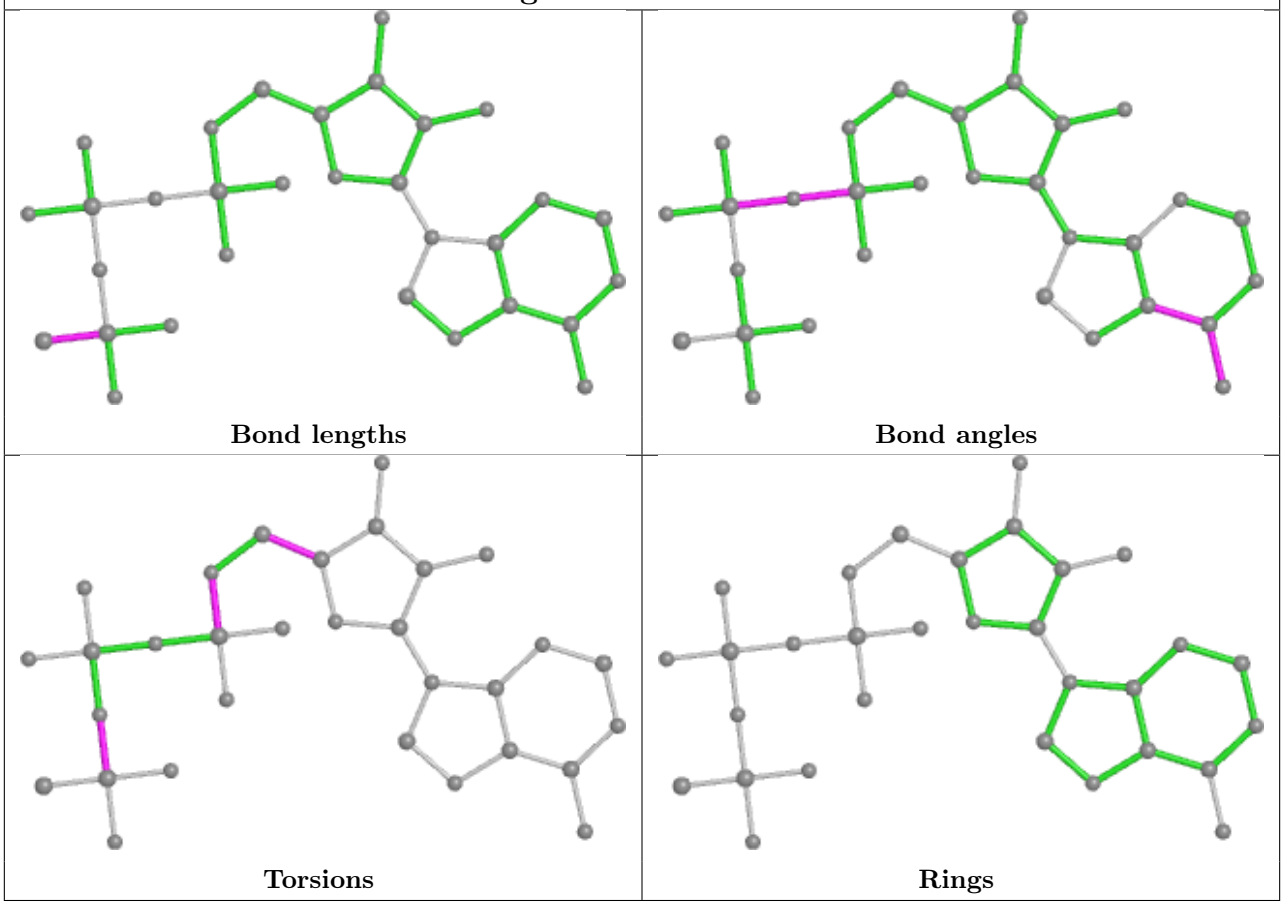


Torsions



Rings

Ligand AGS 6 2001



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.

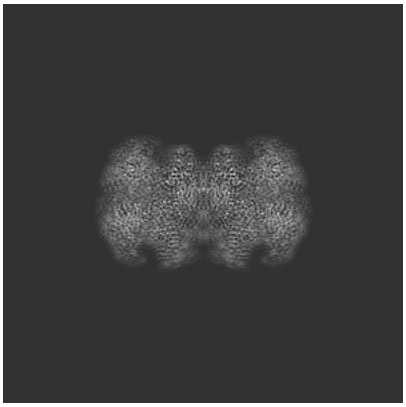
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32355. These allow visual inspection of the internal detail of the map and identification of artifacts.

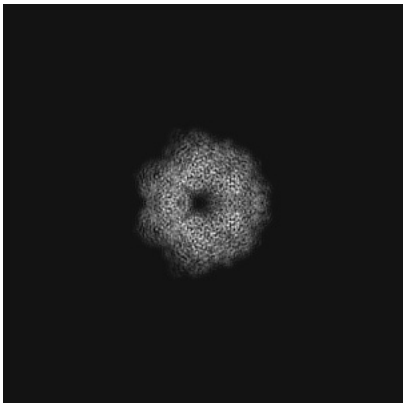
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

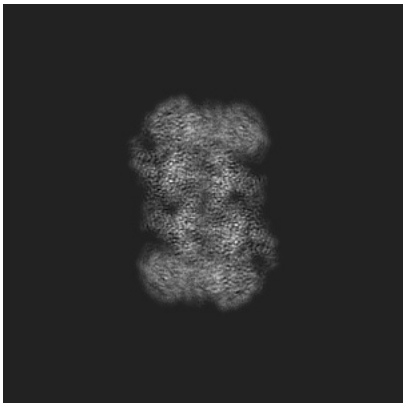
6.1.1 Primary map



X



Y



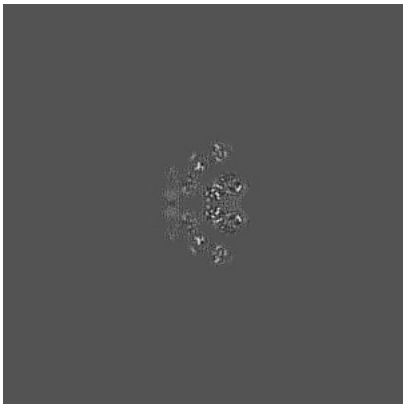
Z

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

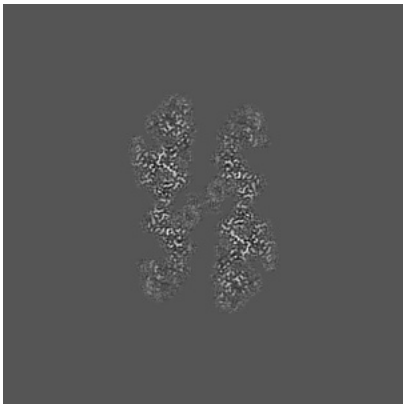
6.2 Central slices

6.2.1 Primary map

X Index: 180



Y Index: 180

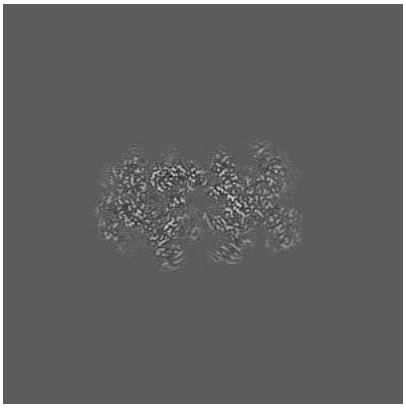


Z Index: 180

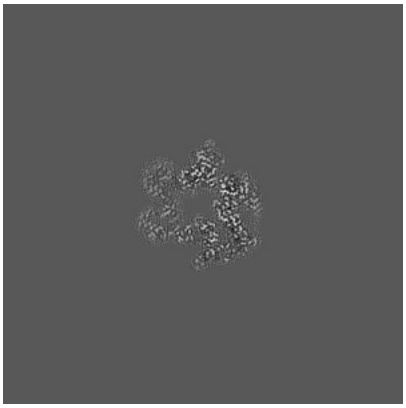
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

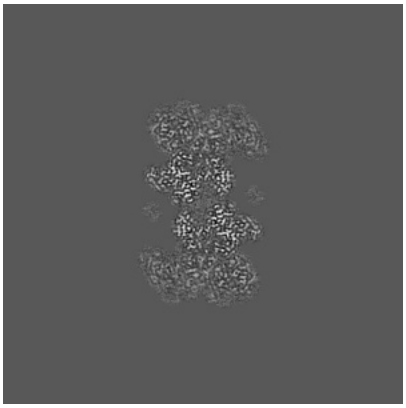
6.3.1 Primary map



X Index: 201



Y Index: 203

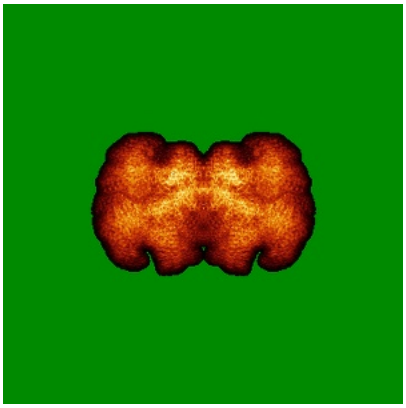


Z Index: 206

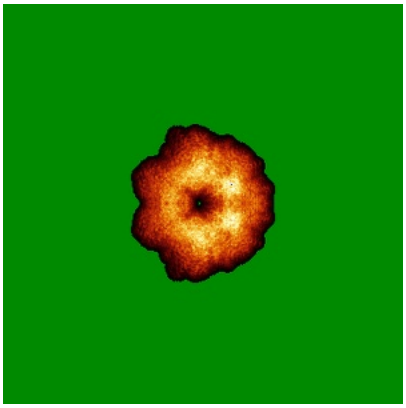
The images above show the largest variance slices of the map in three orthogonal directions.

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

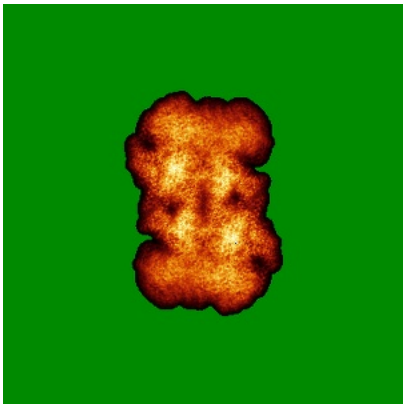
6.4.1 Primary map



X



Y

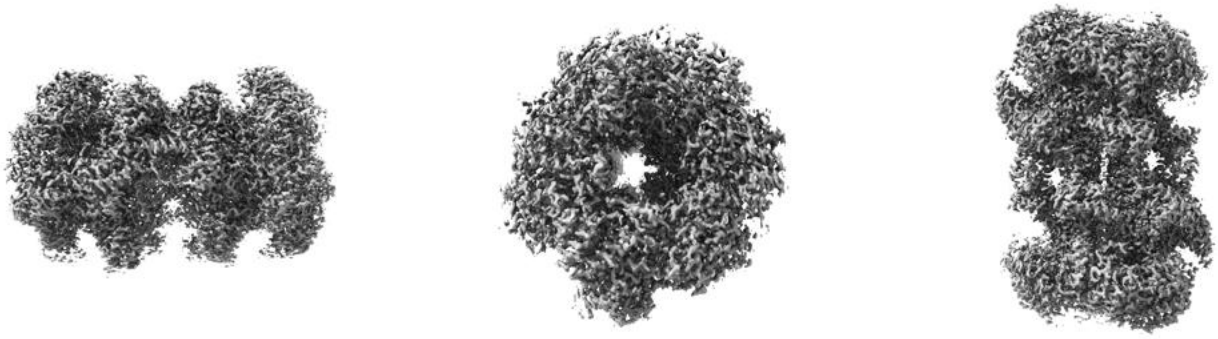


Z

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 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

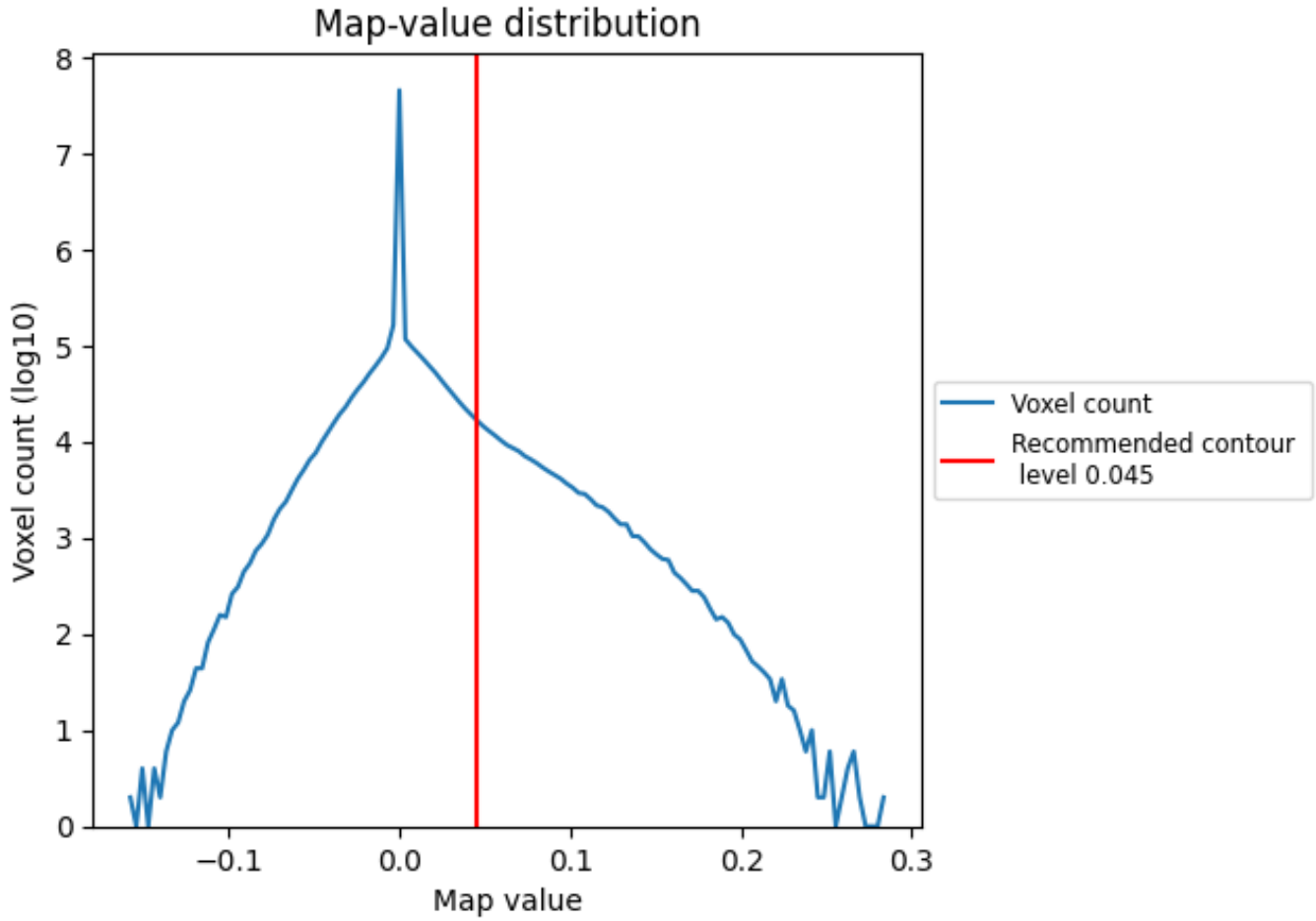
6.6 Mask visualisation (i)

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

7 Map analysis

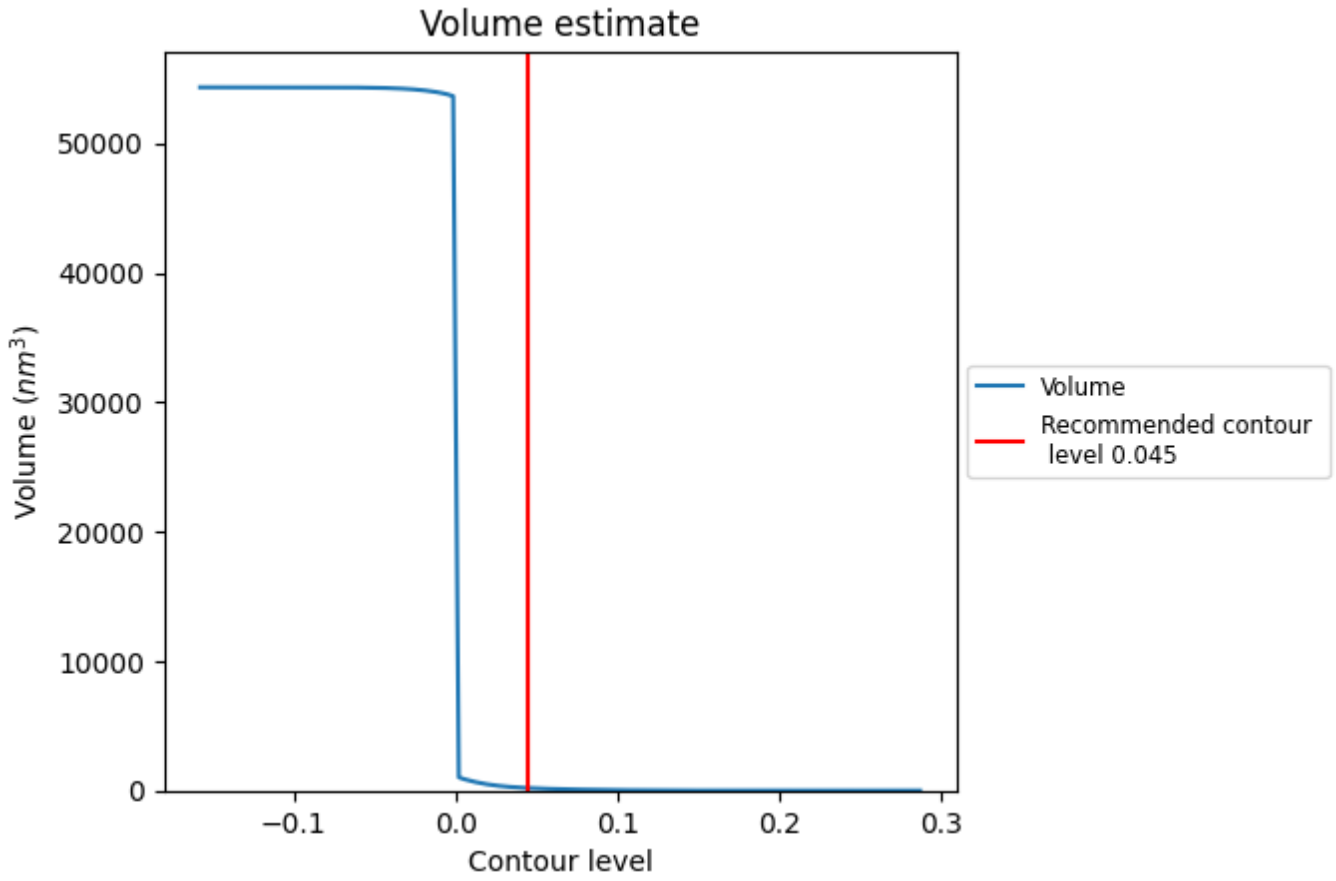
This section contains the results of statistical analysis of the map.

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.

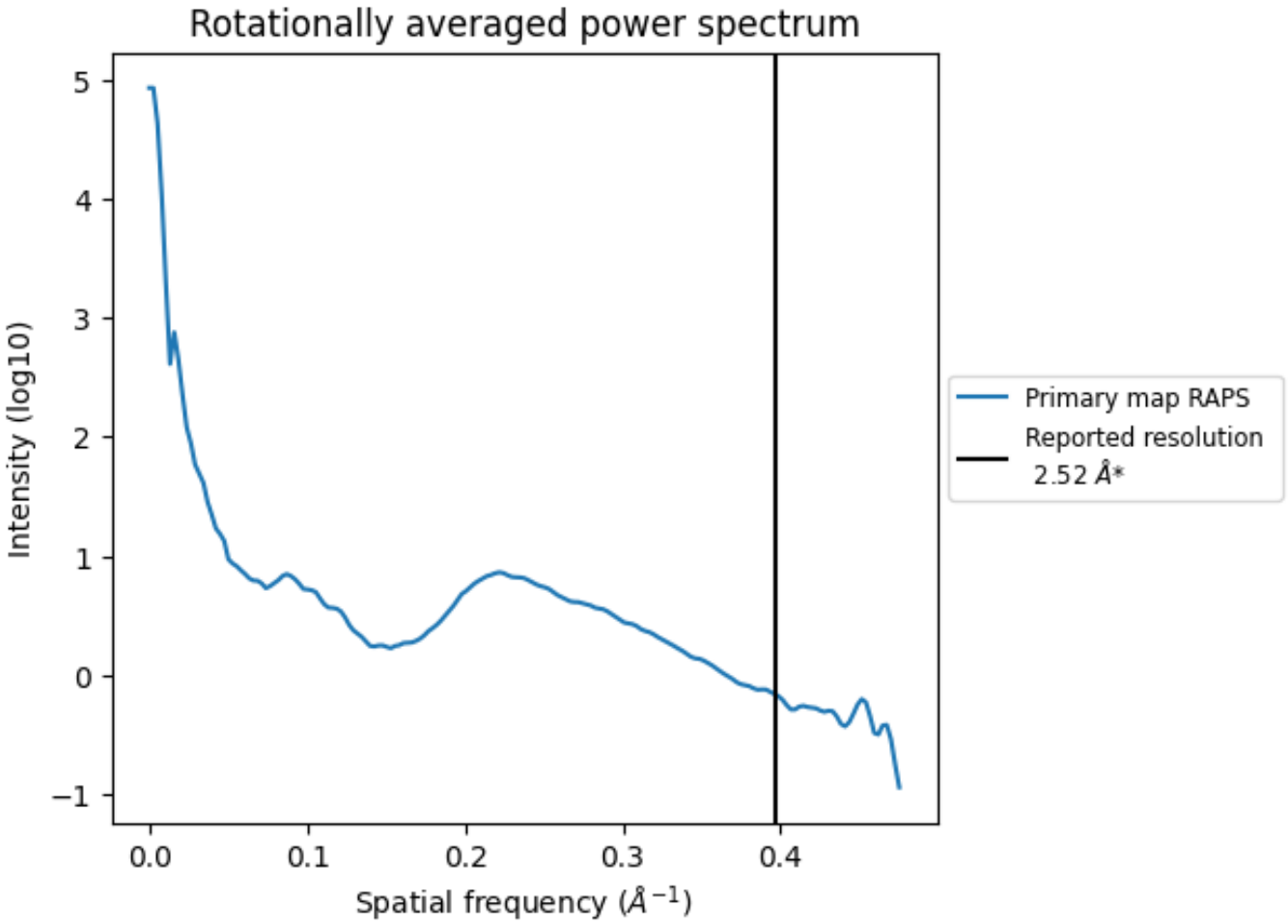
7.2 Volume estimate



The volume at the recommended contour level is 194 nm^3; this corresponds to an approximate mass of 176 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 0.397 $Å^{-1}$

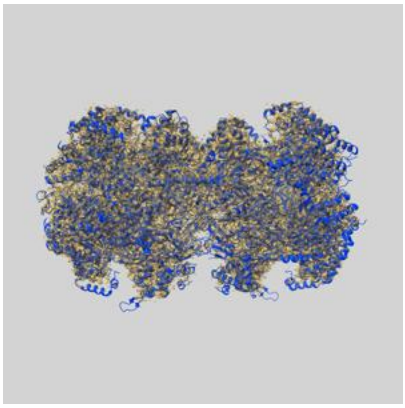
8 Fourier-Shell correlation (i)

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

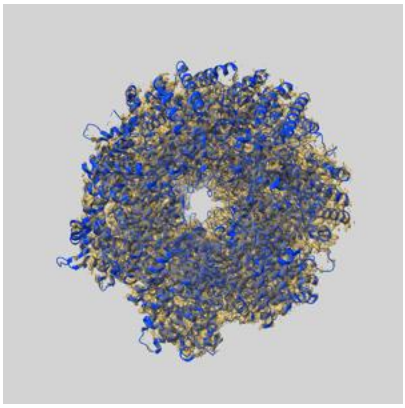
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32355 and PDB model 7W8G. Per-residue inclusion information can be found in section 3 on page 9.

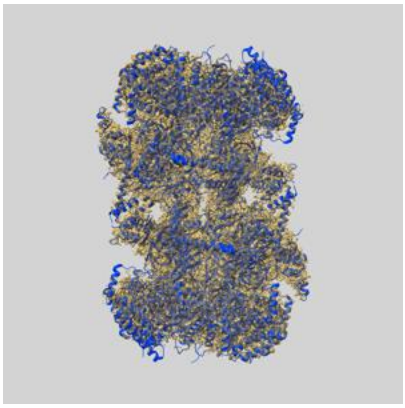
9.1 Map-model overlay



X



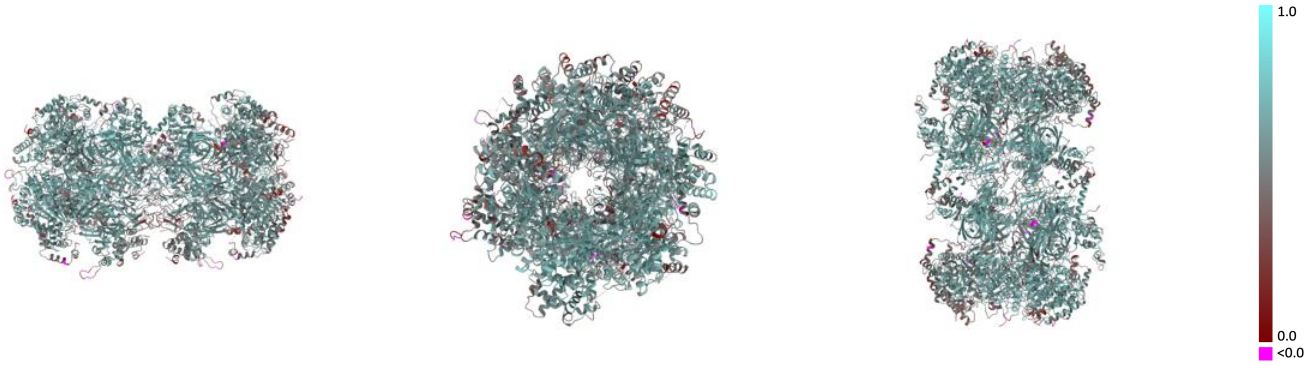
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

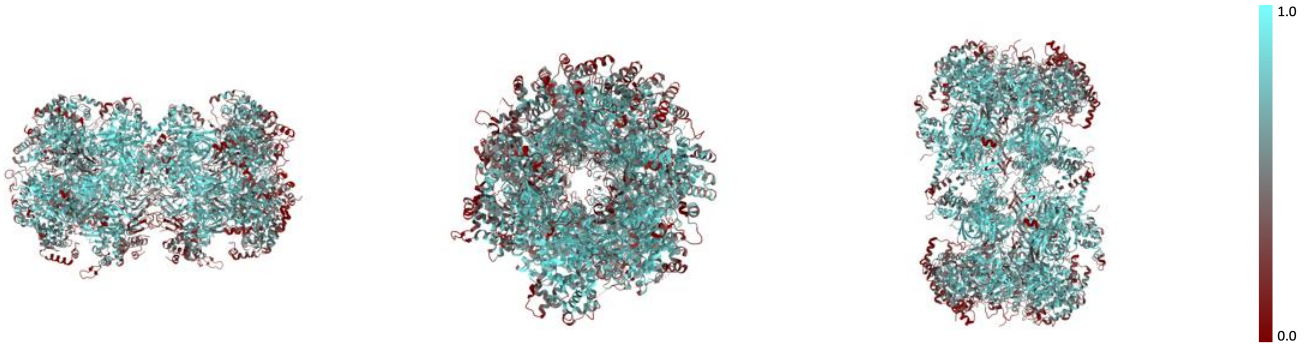
9.2 Q-score mapped to coordinate model



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.

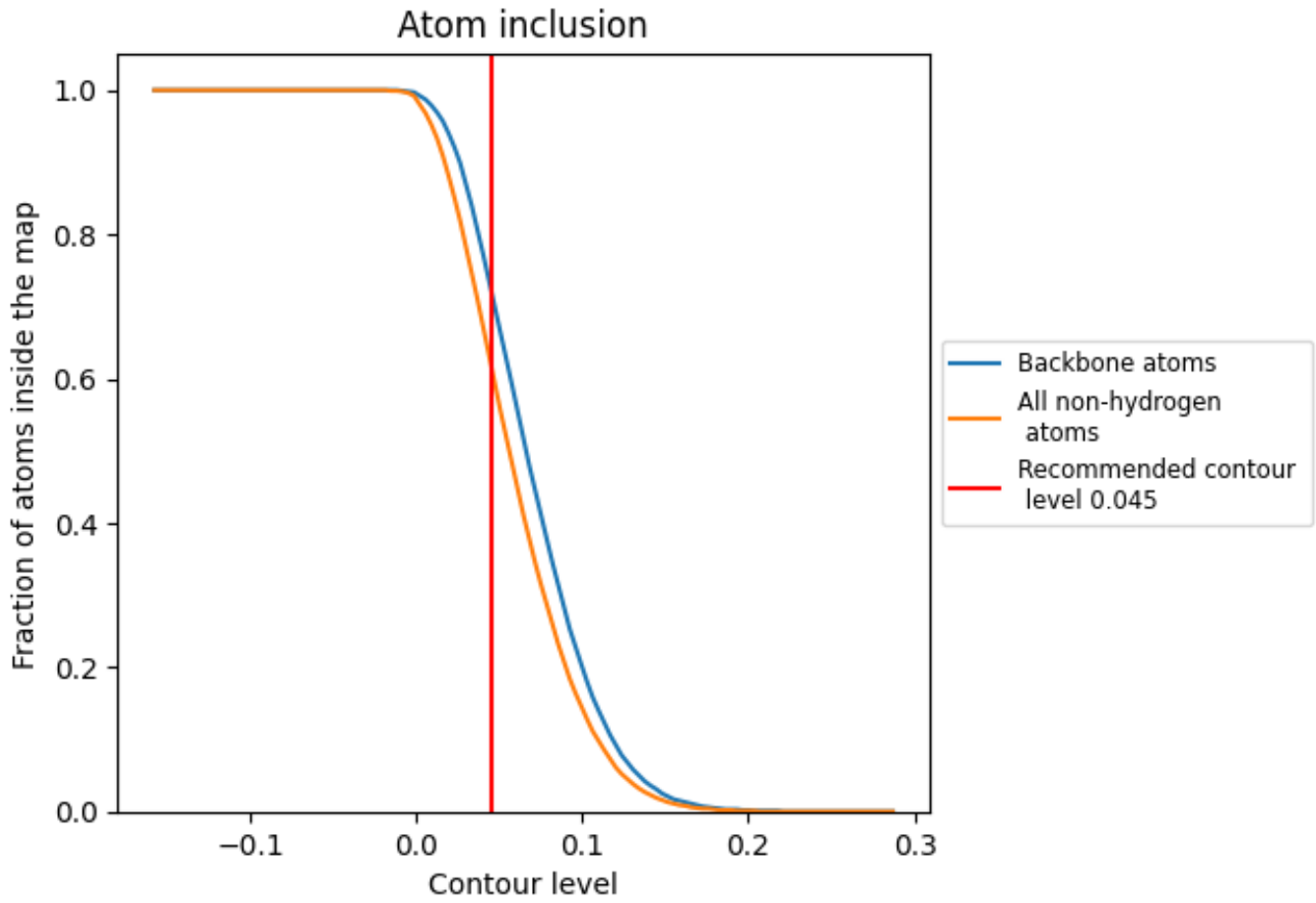
9.3 Atom inclusion mapped to coordinate model



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6190	0.5740
2	0.5180	0.5420
3	0.6680	0.5940
4	0.6920	0.6030
5	0.5940	0.5640
6	0.5530	0.5360
7	0.6820	0.6010
B	0.5160	0.5430
C	0.6650	0.5950
D	0.6910	0.6030
E	0.5920	0.5610
F	0.5540	0.5360
G	0.6820	0.6040