Full wwPDB EM Validation Report (i)

Feb 26, 2024 – 01:32 AM EST

PDB ID	:	6WGC
EMDB ID	:	EMD-21662
Title	:	Atomic model of semi-attached mutant OCCM-DNA complex (ORC-Cdc6-Cdt1-Mcm2-7 with Mcm6 WHD truncation)
Authors	:	Yuan, Z.; Schneider, S.; Dodd, T.; Riera, A.; Bai, L.; Yan, C.; Magdalou, I.; Ivanov, I.; Stillman, B.; Li, H.; Speck, C.
Deposited on	:	2020-04-05
Resolution	:	4.30 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:

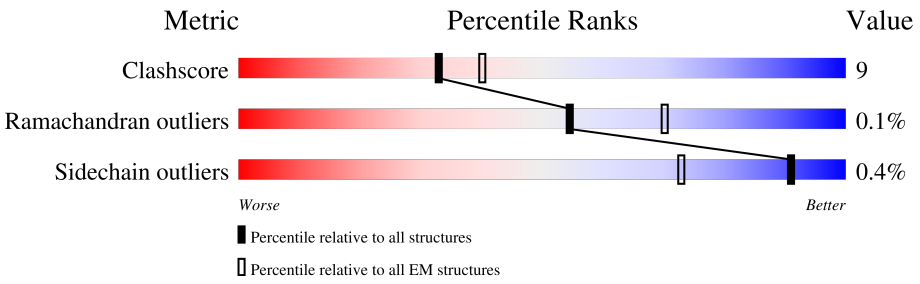
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.30 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	9	513	24% 49% 22% • 27%
2	A	913	• 38% 9% 53%
3	B	620	12% 40% 13% 47%
4	C	616	11% 72% 16% 12%
5	E	479	9% 70% 18% 12%
6	D	529	6% 63% 20% 18%
7	F	435	14% 26% 10% 64%
8	3	971	5% 5% • 93%

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Mol	Chain	Length	Quality of chain
9	7	845	5% 94%
10	G	41	93% 95% 5%
11	H	41	90% 98%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 24605 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 Cell division control protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	9	373	2976	1910	496	553	17	0	0

- Molecule 2 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	425	3386	2163	571	634	18	0	0

- Molecule 3 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	326	2663	1721	442	484	16	0	0

- Molecule 4 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	544	4505	2909	743	838	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	422	3425	2226	545	641	13	0	0

- Molecule 6 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	436	3551	2275	603	660	13	0	0

- Molecule 7 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	157	1315	846	222	235	12	0	0

- Molecule 8 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	3	69	565	358	93	111	3	0	0

- Molecule 9 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	7	52	417	267	70	77	3	0	0

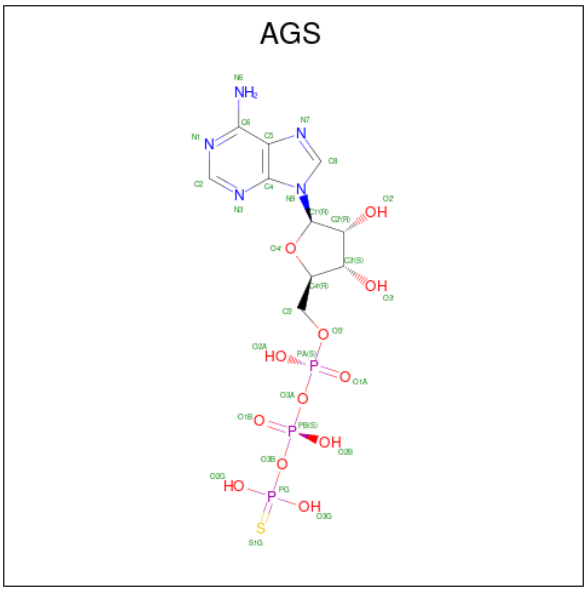
- Molecule 10 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	G	41	831	407	118	266	40	0	0

- Molecule 11 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	H	41	847	404	178	224	41	0	0

- Molecule 12 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).



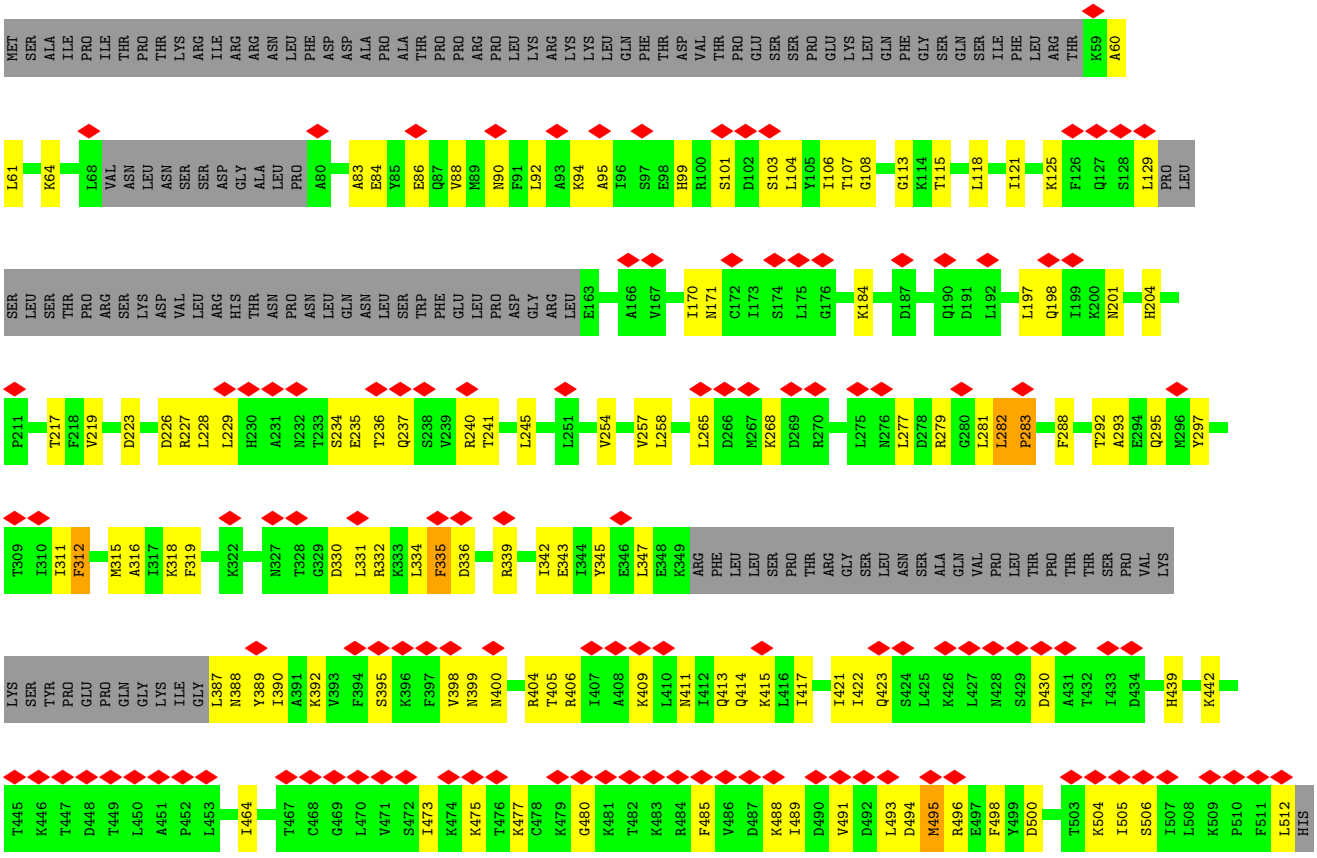
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
12	9	1	31	10	5	12	3	1	0
			Total	C	N	O	P	S	
12	A	1	31	10	5	12	3	1	0
			Total	C	N	O	P	S	
12	E	1	31	10	5	12	3	1	0
			Total	C	N	O	P	S	
12	D	1	31	10	5	12	3	1	0

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.

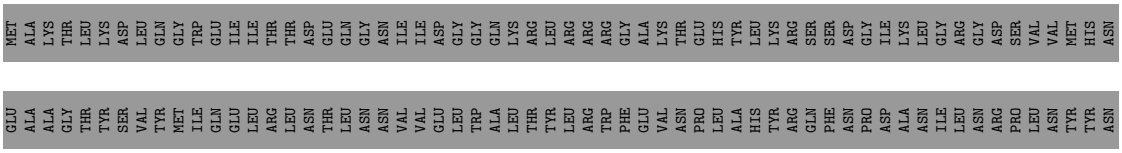
• Molecule 1: Cell division control protein 6

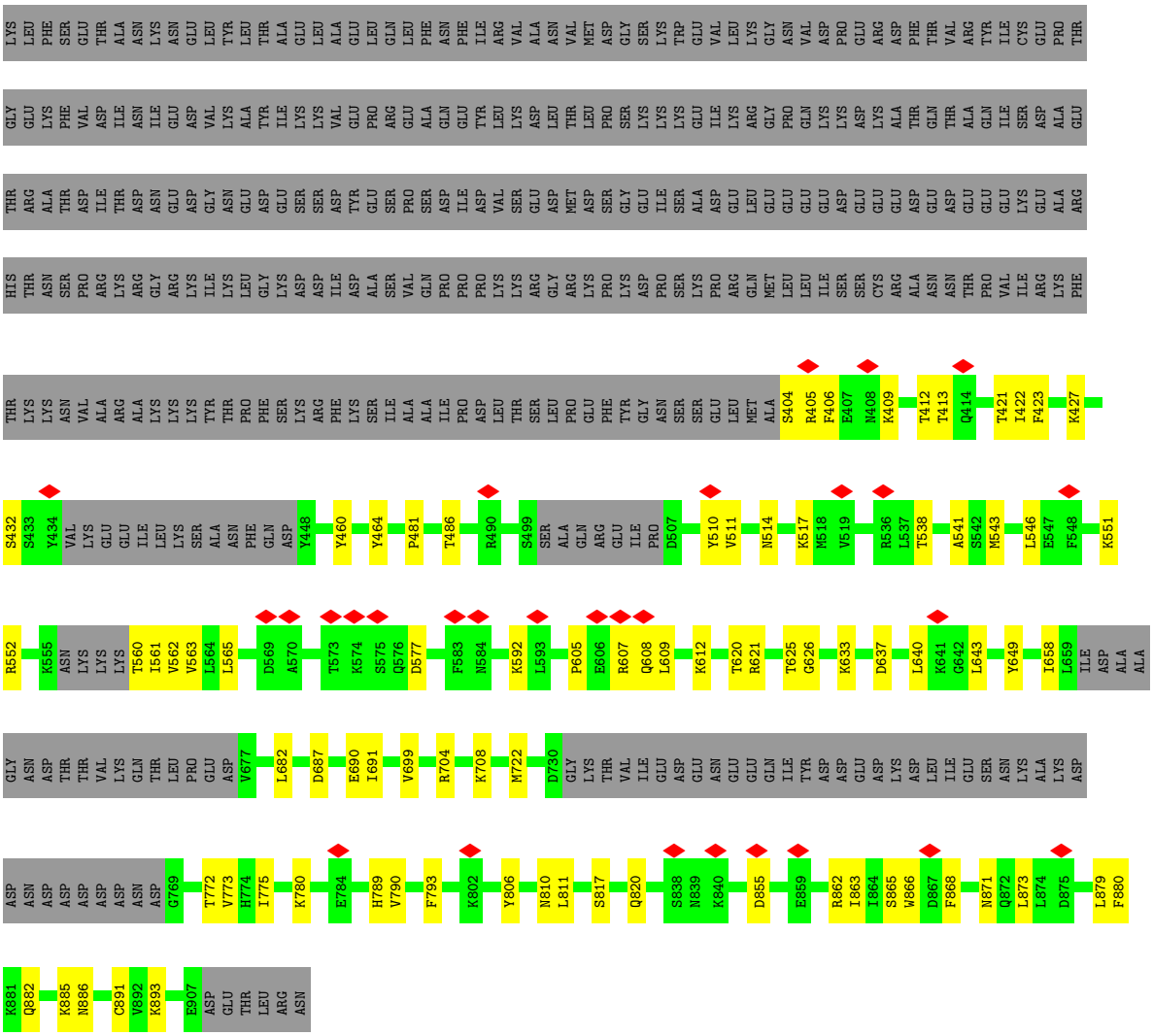
Chain 9:



• Molecule 2: Origin recognition complex subunit 1

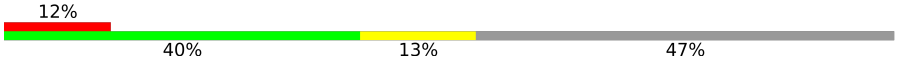
Chain A:

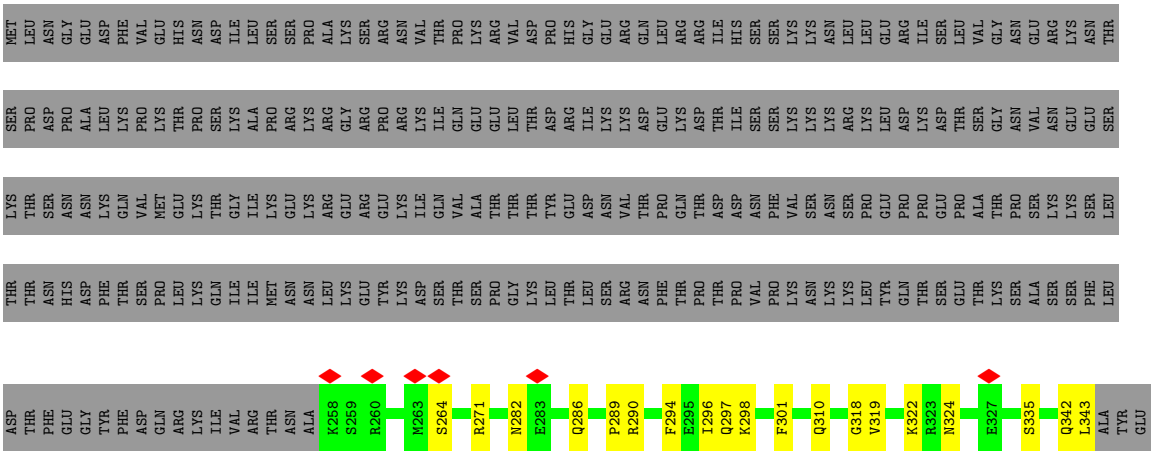


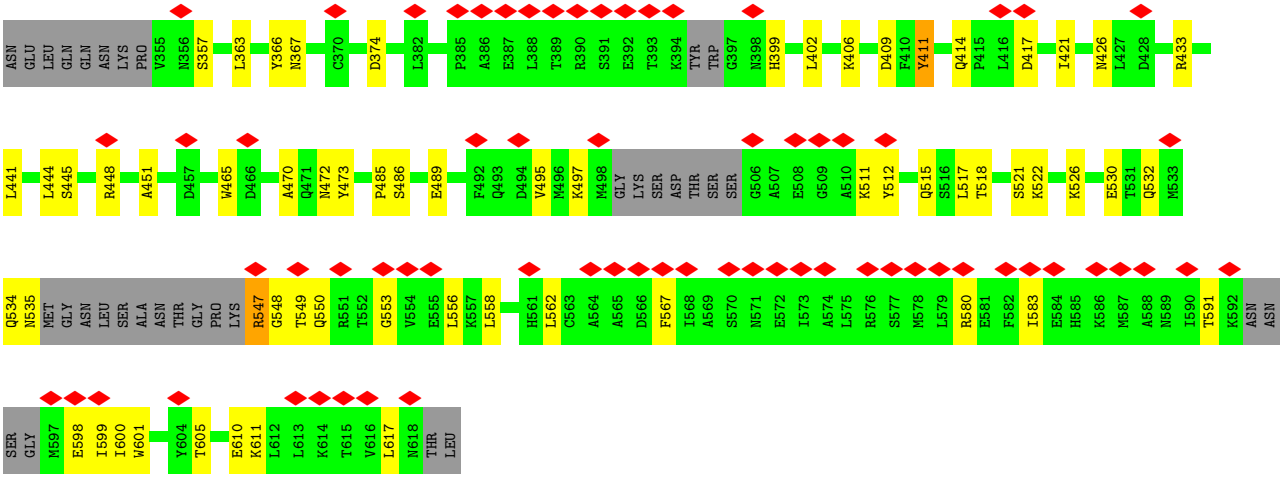


• Molecule 3: Origin recognition complex subunit 2

Chain B:

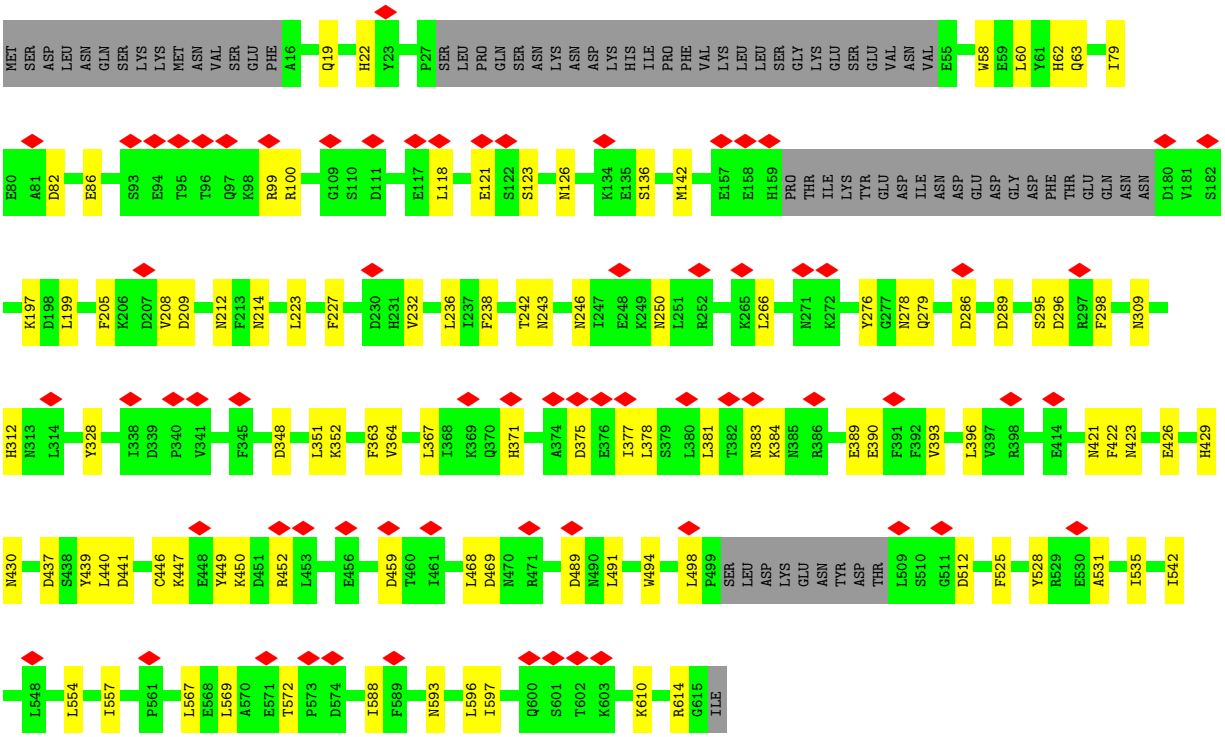






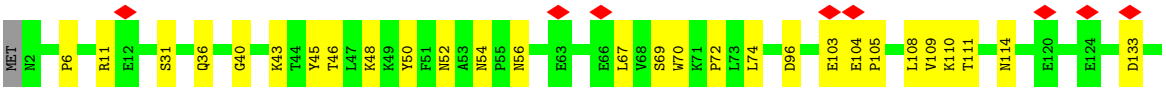
- Molecule 4: Origin recognition complex subunit 3

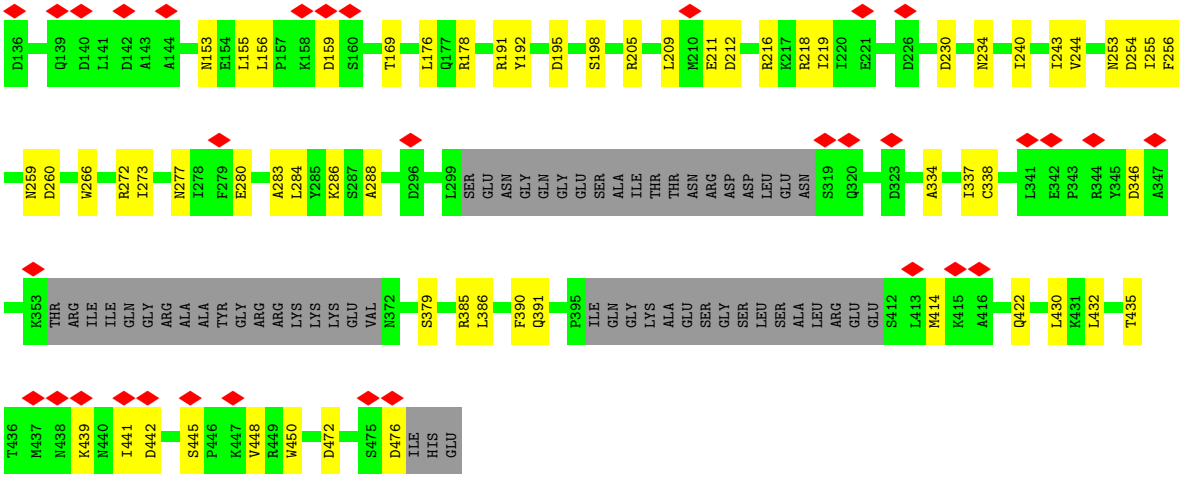
Chain C:



- Molecule 5: Origin recognition complex subunit 5

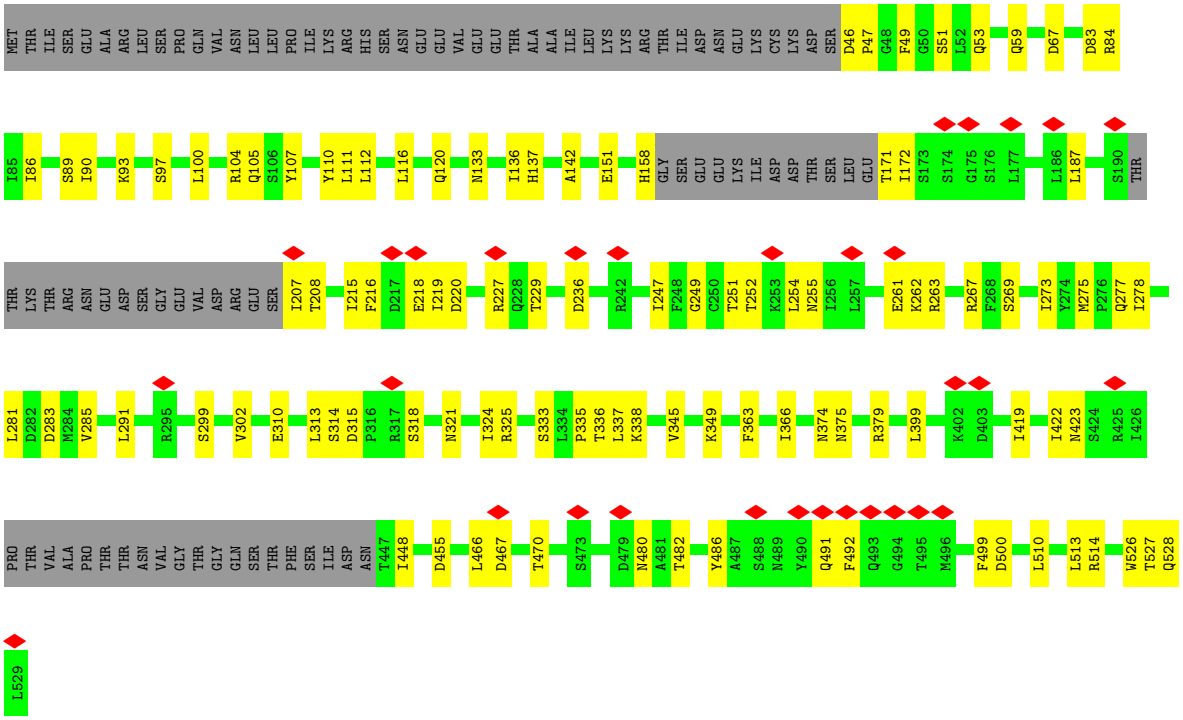
Chain E:





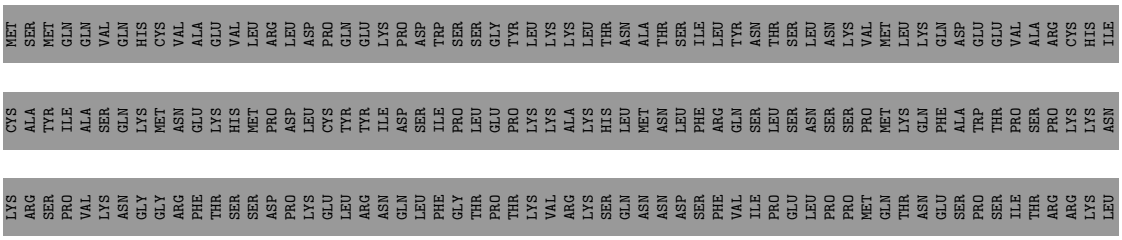
- Molecule 6: Origin recognition complex subunit 4

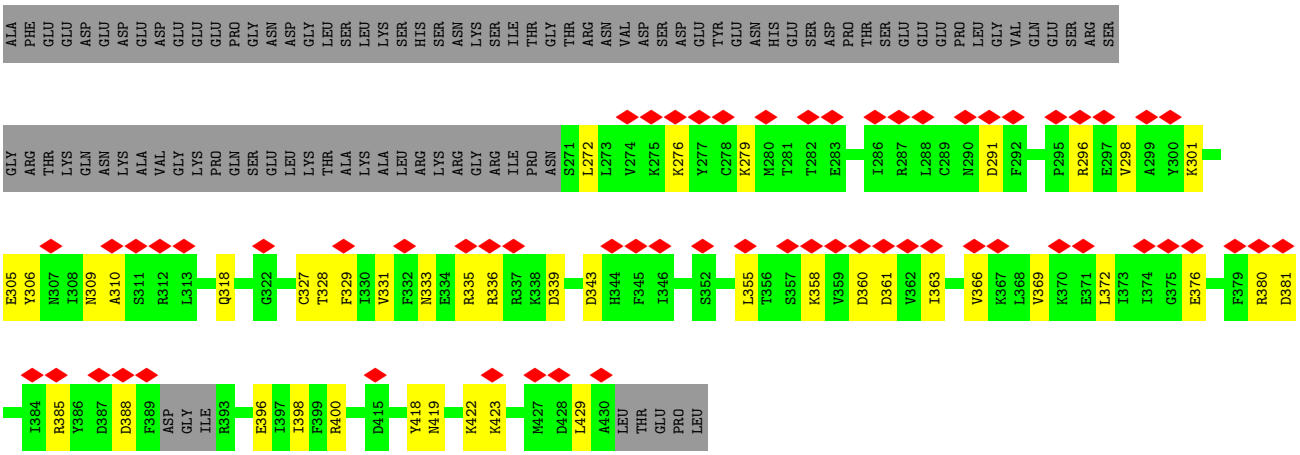
Chain D:



- Molecule 7: Origin recognition complex subunit 6

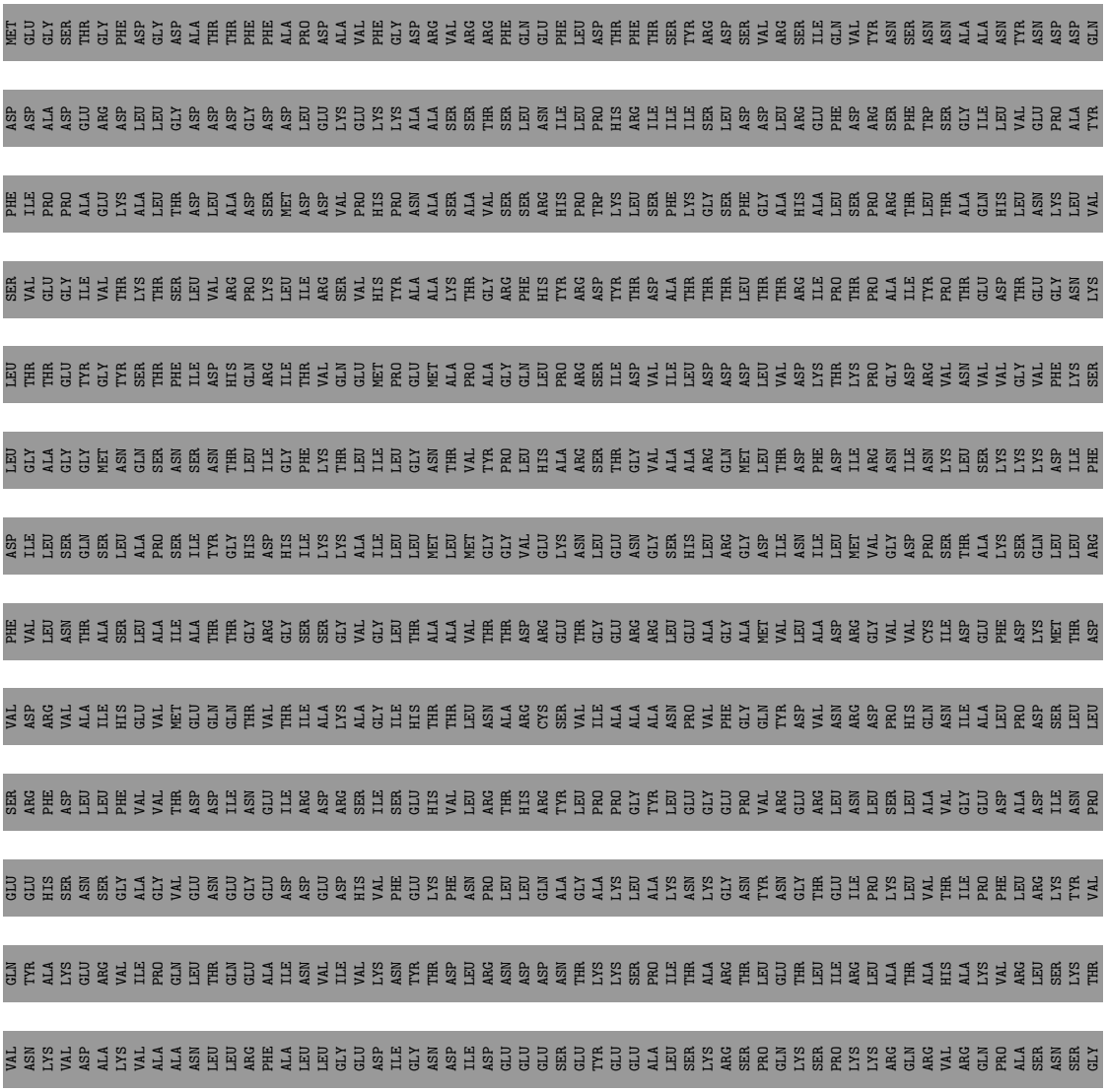
Chain F:

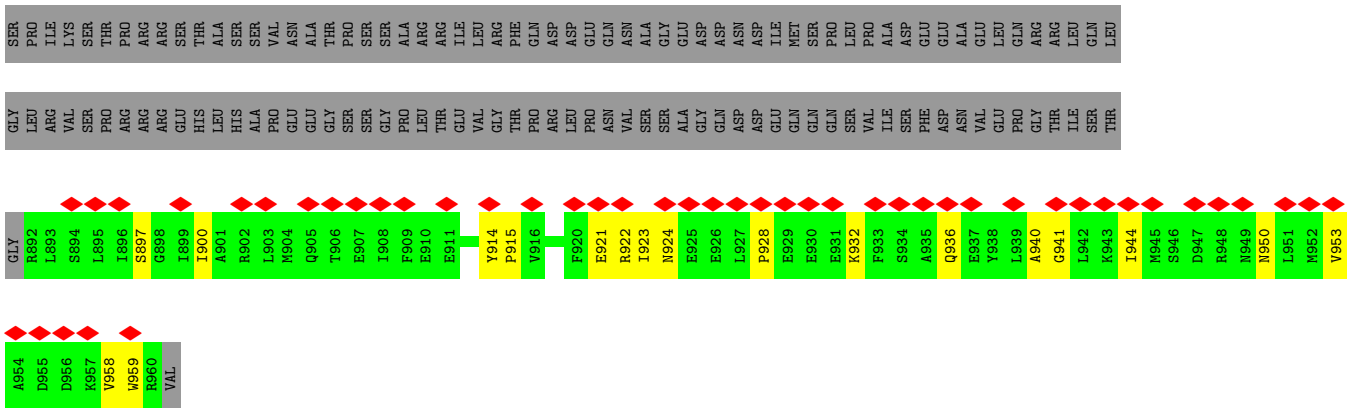




- Molecule 8: DNA replication licensing factor MCM3

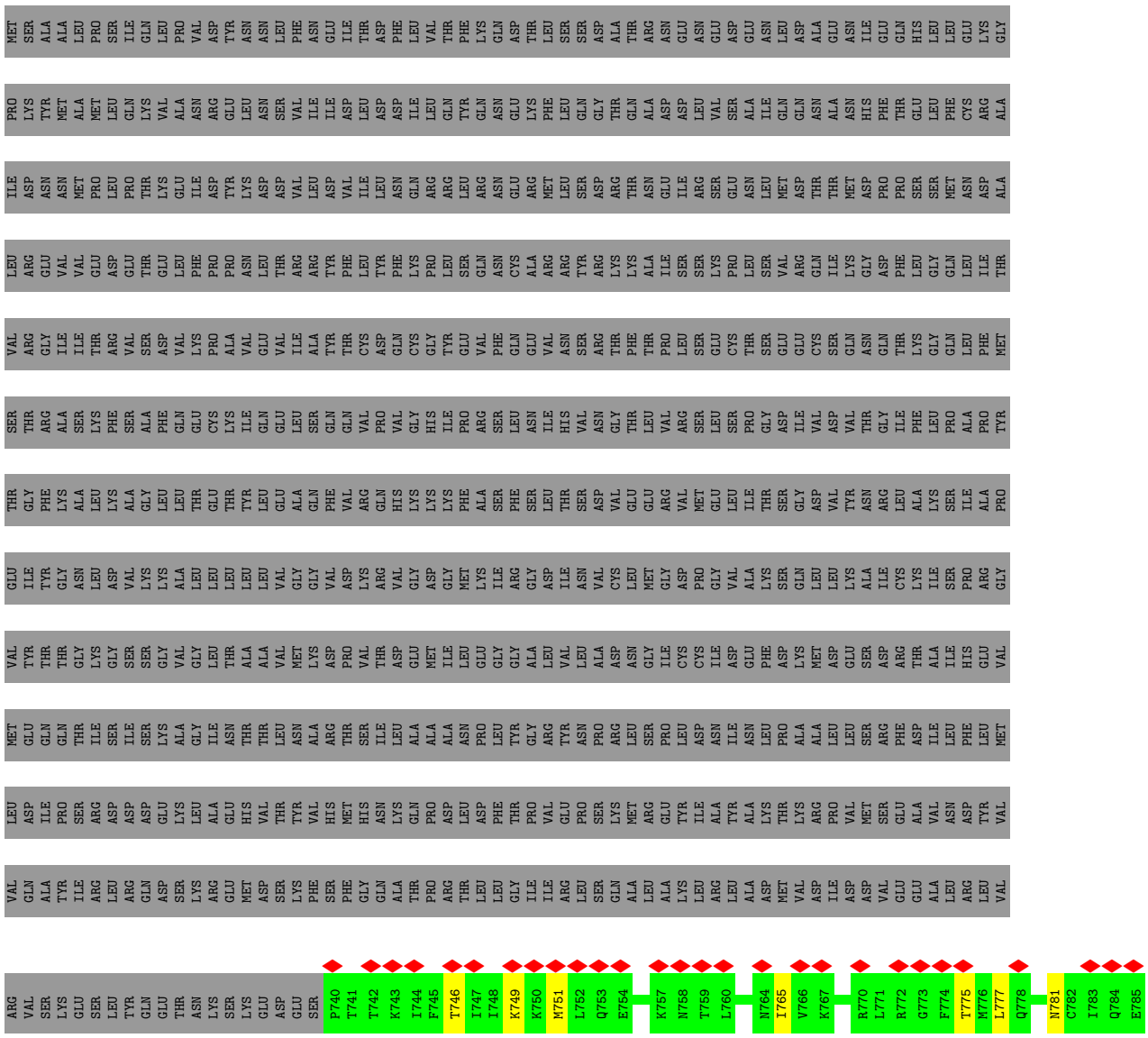
Chain 3: 5% 5% 93%

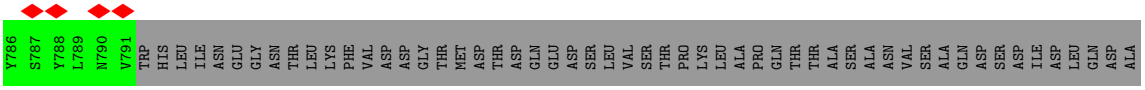




• Molecule 9: DNA replication licensing factor MCM7

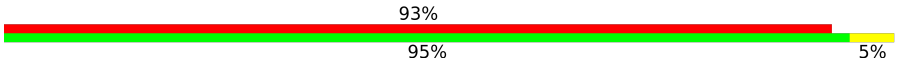
Chain 7: 5% • 94%

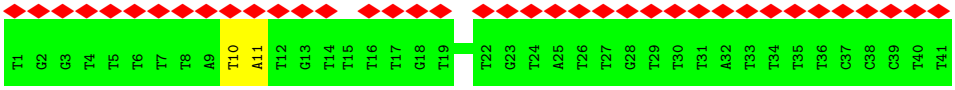




- Molecule 10: DNA (41-MER)

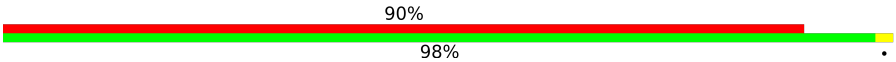
Chain G:

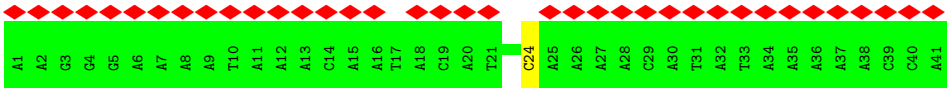




- Molecule 11: DNA (41-MER)

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86074	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	262.0, 262.0, 262.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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: AGS

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	9	0.32	0/3018	0.58	0/4059
2	A	0.34	0/3434	0.54	0/4621
3	B	0.34	0/2717	0.53	0/3662
4	C	0.35	0/4602	0.55	0/6212
5	E	0.38	0/3505	0.55	0/4767
6	D	0.36	0/3612	0.52	0/4879
7	F	0.29	0/1336	0.50	0/1798
8	3	0.29	0/573	0.60	0/770
9	7	0.30	0/421	0.49	0/565
10	G	0.78	0/923	1.16	0/1425
11	H	0.76	0/958	0.94	0/1474
All	All	0.39	0/25099	0.60	0/34232

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	9	2976	0	3093	88	0
2	A	3386	0	3454	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2663	0	2673	53	0
4	C	4505	0	4458	71	0
5	E	3425	0	3402	62	0
6	D	3551	0	3615	80	0
7	F	1315	0	1353	30	0
8	3	565	0	560	13	0
9	7	417	0	443	6	0
10	G	831	0	480	6	0
11	H	847	0	457	7	0
12	9	31	0	12	4	0
12	A	31	0	12	7	0
12	D	31	0	12	4	0
12	E	31	0	12	5	0
All	All	24605	0	24036	446	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 9.

All (446) 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)
2:A:541:ALA:HB2	10:G:10:DT:OP1	1.57	1.03
1:9:311:ILE:HG23	1:9:312:PHE:H	1.30	0.97
2:A:538:THR:HA	10:G:11:DA:OP1	1.61	0.97
2:A:538:THR:CB	10:G:10:DT:H3'	1.97	0.95
1:9:282:LEU:CB	1:9:283:PRO:CD	2.43	0.94
1:9:311:ILE:CG2	1:9:312:PHE:H	1.96	0.78
1:9:282:LEU:CB	1:9:283:PRO:HD3	2.16	0.76
1:9:311:ILE:HG23	1:9:312:PHE:N	2.03	0.74
1:9:282:LEU:CB	1:9:283:PRO:HD2	2.21	0.71
2:A:538:THR:CB	10:G:10:DT:C3'	2.70	0.70
2:A:538:THR:CA	10:G:11:DA:OP1	2.32	0.70
5:E:435:THR:HG22	5:E:450:TRP:HE1	1.58	0.67
1:9:118:LEU:HA	1:9:121:ILE:HD12	1.77	0.66
6:D:324:ILE:HG12	6:D:337:LEU:HD11	1.79	0.65
7:F:333:ASN:HA	7:F:336:ARG:HB2	1.77	0.65
1:9:245:LEU:HB3	1:9:258:LEU:HD11	1.79	0.64
3:B:421:ILE:HG22	3:B:451:ALA:HB3	1.78	0.64
4:C:298:PHE:HB2	4:C:469:ASP:HA	1.79	0.64
1:9:113:GLY:HA2	12:9:2001:AGS:H3'	1.80	0.63
5:E:338:CYS:SG	5:E:385:ARG:NH1	2.71	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:486:TYR:CE2	11:H:24:DC:H6	2.16	0.63
8:3:915:PRO:HA	8:3:958:VAL:HA	1.80	0.63
3:B:294:PHE:HA	3:B:297:GLN:HE21	1.65	0.62
3:B:319:VAL:HG21	4:C:491:LEU:HD21	1.82	0.61
1:9:315:MET:HA	1:9:318:LYS:HD2	1.82	0.61
1:9:171:ASN:HA	1:9:223:ASP:HB2	1.83	0.61
1:9:505:ILE:HG13	1:9:505:ILE:O	1.99	0.60
6:D:278:ILE:HG23	6:D:283:ASP:HB2	1.84	0.60
1:9:331:LEU:O	1:9:335:PHE:N	2.35	0.59
6:D:379:ARG:HH12	6:D:467:ASP:HB2	1.68	0.59
4:C:328:TYR:HB2	4:C:468:LEU:HD21	1.84	0.59
6:D:133:ASN:HB3	6:D:136:ILE:HG22	1.85	0.59
3:B:470:ALA:HA	3:B:473:TYR:HB2	1.85	0.58
1:9:115:THR:OG1	12:9:2001:AGS:S1G	2.62	0.58
2:A:790:VAL:HG12	6:D:254:LEU:HD13	1.85	0.58
1:9:240:ARG:NH2	1:9:241:THR:OG1	2.35	0.58
2:A:722:MET:HB3	6:D:84:ARG:HH22	1.67	0.58
3:B:486:SER:HB2	3:B:489:GLU:HB2	1.85	0.58
12:E:2001:AGS:S1G	12:E:2001:AGS:O2B	2.62	0.58
5:E:50:TYR:O	5:E:54:ASN:ND2	2.35	0.58
6:D:486:TYR:CE2	11:H:24:DC:C6	2.91	0.58
9:7:777:LEU:O	9:7:781:ASN:ND2	2.37	0.58
3:B:318:GLY:O	3:B:322:LYS:NZ	2.37	0.57
6:D:486:TYR:CZ	11:H:24:DC:C6	2.93	0.57
5:E:283:ALA:HA	5:E:286:LYS:HD2	1.86	0.57
6:D:486:TYR:CD1	11:H:24:DC:H5	2.22	0.57
8:3:928:PRO:O	8:3:932:LYS:NZ	2.34	0.57
1:9:104:LEU:H	1:9:281:LEU:HD12	1.70	0.57
2:A:607:ARG:HE	2:A:608:GLN:HE22	1.51	0.57
8:3:923:ILE:HG13	8:3:924:ASN:N	2.18	0.57
5:E:346:ASP:OD2	5:E:385:ARG:NH2	2.38	0.57
1:9:292:THR:OG1	1:9:293:ALA:N	2.38	0.57
2:A:625:THR:OG1	2:A:626:GLY:N	2.38	0.57
2:A:775:ILE:HG12	9:7:749:LYS:HG3	1.87	0.57
8:3:941:GLY:HA2	8:3:944:ILE:HD12	1.86	0.57
2:A:806:TYR:O	2:A:810:ASN:ND2	2.37	0.57
12:A:2001:AGS:O2G	6:D:267:ARG:NH1	2.37	0.56
4:C:378:LEU:O	4:C:383:ASN:ND2	2.38	0.56
6:D:455:ASP:OD1	6:D:455:ASP:N	2.38	0.56
7:F:328:THR:HA	7:F:331:VAL:HG12	1.88	0.56
4:C:309:ASN:ND2	4:C:312:HIS:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:197:LEU:O	1:9:204:HIS:ND1	2.36	0.56
2:A:421:THR:OG1	2:A:422:ILE:N	2.39	0.56
2:A:704:ARG:NH2	12:A:2001:AGS:O3A	2.39	0.56
5:E:31:SER:OG	5:E:153:ASN:ND2	2.39	0.55
2:A:560:THR:HG23	2:A:592:LYS:HB3	1.88	0.55
2:A:704:ARG:HG3	12:A:2001:AGS:H5'2	1.88	0.55
1:9:94:LYS:HB3	1:9:99:HIS:HB3	1.89	0.55
5:E:103:GLU:HG2	5:E:104:GLU:HG2	1.87	0.55
4:C:199:LEU:HB3	4:C:232:VAL:HG12	1.88	0.55
4:C:242:THR:OG1	4:C:243:ASN:N	2.40	0.55
4:C:528:TYR:O	4:C:610:LYS:NZ	2.38	0.55
5:E:435:THR:HG21	5:E:442:ASP:CG	2.26	0.55
6:D:261:GLU:OE2	6:D:263:ARG:NH1	2.38	0.55
1:9:464:ILE:HG12	2:A:699:VAL:HA	1.89	0.55
4:C:375:ASP:N	4:C:375:ASP:OD1	2.40	0.55
6:D:375:ASN:O	6:D:379:ARG:NE	2.40	0.55
5:E:159:ASP:OD1	5:E:159:ASP:N	2.40	0.55
5:E:430:LEU:HB3	5:E:432:LEU:HG	1.89	0.54
2:A:404:SER:OG	2:A:405:ARG:N	2.40	0.54
1:9:60:ALA:O	1:9:64:LYS:N	2.40	0.54
1:9:473:ILE:HG22	1:9:489:ILE:HG22	1.89	0.54
2:A:789:HIS:O	2:A:793:PHE:N	2.32	0.54
1:9:491:VAL:HG22	1:9:493:LEU:H	1.73	0.54
12:A:2001:AGS:O2A	12:A:2001:AGS:O1B	2.25	0.54
2:A:413:THR:HA	6:D:207:ILE:HD12	1.88	0.54
3:B:282:ASN:HB3	3:B:485:PRO:HG3	1.89	0.54
5:E:216:ARG:HA	5:E:219:ILE:HD12	1.88	0.54
6:D:486:TYR:CG	11:H:24:DC:H5	2.25	0.54
1:9:475:LYS:HB3	1:9:485:PHE:HB3	1.90	0.54
5:E:195:ASP:N	5:E:195:ASP:OD1	2.40	0.54
1:9:234:SER:OG	1:9:235:GLU:N	2.40	0.53
5:E:6:PRO:HG3	5:E:50:TYR:HA	1.89	0.53
6:D:313:LEU:O	6:D:321:ASN:ND2	2.41	0.53
7:F:291:ASP:OD1	7:F:291:ASP:N	2.38	0.53
1:9:494:ASP:N	1:9:494:ASP:OD1	2.41	0.53
7:F:376:GLU:O	7:F:380:ARG:NH2	2.41	0.53
1:9:311:ILE:CG2	1:9:312:PHE:N	2.66	0.53
4:C:381:LEU:HD21	7:F:422:LYS:HE3	1.90	0.53
5:E:153:ASN:OD1	5:E:153:ASN:N	2.40	0.53
6:D:53:GLN:NE2	6:D:345:VAL:O	2.42	0.53
9:7:751:MET:HG3	9:7:765:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:442:ASP:HA	5:E:448:VAL:HG21	1.91	0.53
1:9:226:ASP:HA	1:9:229:LEU:HB2	1.91	0.53
5:E:218:ARG:NH2	5:E:273:ILE:O	2.40	0.53
8:3:923:ILE:HG13	8:3:924:ASN:H	1.74	0.53
5:E:56:ASN:OD1	5:E:56:ASN:N	2.41	0.53
1:9:103:SER:HB3	1:9:281:LEU:HA	1.90	0.53
3:B:363:LEU:HD13	4:C:22:HIS:HB3	1.91	0.53
3:B:547:ARG:NH1	3:B:548:GLY:O	2.42	0.53
5:E:230:ASP:O	5:E:234:ASN:ND2	2.41	0.53
7:F:329:PHE:O	7:F:336:ARG:NH2	2.42	0.52
1:9:61:LEU:HA	1:9:64:LYS:HB2	1.92	0.52
5:E:111:THR:HA	5:E:114:ASN:HD22	1.73	0.52
1:9:330:ASP:OD1	1:9:330:ASP:N	2.41	0.52
1:9:345:TYR:OH	1:9:388:ASN:ND2	2.42	0.52
12:9:2001:AGS:S1G	12:9:2001:AGS:O2B	2.67	0.52
6:D:236:ASP:OD2	6:D:267:ARG:NE	2.39	0.52
3:B:342:GLN:NE2	3:B:417:ASP:OD1	2.43	0.52
5:E:192:TYR:O	5:E:253:ASN:ND2	2.43	0.52
3:B:367:ASN:ND2	4:C:19:GLN:O	2.43	0.52
4:C:209:ASP:OD1	4:C:209:ASP:N	2.37	0.52
6:D:251:THR:OG1	6:D:252:THR:N	2.43	0.52
7:F:305:GLU:O	7:F:309:ASN:ND2	2.43	0.52
1:9:226:ASP:OD2	2:A:612:LYS:NZ	2.43	0.51
12:E:2001:AGS:O2B	12:E:2001:AGS:O1A	2.28	0.51
6:D:97:SER:HB2	6:D:247:ILE:HB	1.91	0.51
1:9:495:MET:SD	1:9:495:MET:N	2.82	0.51
2:A:637:ASP:OD1	2:A:637:ASP:N	2.43	0.51
5:E:96:ASP:OD1	5:E:96:ASP:N	2.43	0.51
3:B:433:ARG:HH21	5:E:441:ILE:HD11	1.76	0.51
3:B:556:LEU:CD2	3:B:600:ILE:HG23	2.41	0.51
5:E:205:ARG:NH1	5:E:259:ASN:OD1	2.40	0.51
8:3:897:SER:HA	8:3:900:ILE:HD12	1.91	0.51
1:9:234:SER:OG	1:9:235:GLU:OE1	2.28	0.51
1:9:268:LYS:NZ	3:B:512:TYR:OH	2.40	0.51
2:A:481:PRO:O	6:D:262:LYS:NZ	2.43	0.51
2:A:543:MET:HA	2:A:546:LEU:HB2	1.91	0.51
6:D:486:TYR:CD1	11:H:24:DC:C5	2.98	0.51
1:9:227:ARG:NH2	2:A:577:ASP:OD1	2.41	0.51
2:A:620:THR:OG1	2:A:621:ARG:N	2.43	0.51
6:D:107:TYR:HB3	6:D:110:TYR:HD2	1.76	0.51
6:D:399:LEU:HD22	6:D:510:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:811:LEU:HB3	2:A:820:GLN:HG3	1.93	0.51
4:C:554:LEU:HA	4:C:557:ILE:HG22	1.93	0.51
1:9:331:LEU:HA	1:9:334:LEU:HB2	1.93	0.51
4:C:393:VAL:HA	4:C:396:LEU:HB2	1.93	0.51
6:D:112:LEU:HD13	6:D:215:ILE:HD12	1.93	0.51
7:F:306:TYR:O	7:F:310:ALA:N	2.43	0.51
6:D:171:THR:HG23	6:D:172:ILE:HG13	1.92	0.51
6:D:491:GLN:NE2	6:D:492:PHE:O	2.43	0.51
2:A:873:LEU:HB3	2:A:879:LEU:HD23	1.93	0.51
1:9:423:GLN:NE2	1:9:512:LEU:O	2.44	0.50
2:A:486:THR:OG1	12:A:2001:AGS:O2B	2.30	0.50
5:E:439:LYS:NZ	6:D:491:GLN:OE1	2.41	0.50
1:9:343:GLU:O	1:9:347:LEU:N	2.40	0.50
5:E:133:ASP:HA	5:E:169:THR:HB	1.93	0.50
1:9:88:VAL:O	1:9:92:LEU:N	2.44	0.50
3:B:534:GLN:OE1	3:B:535:ASN:ND2	2.44	0.50
6:D:500:ASP:OD1	6:D:500:ASP:N	2.36	0.50
4:C:512:ASP:OD1	4:C:512:ASP:N	2.44	0.50
3:B:599:ILE:HG22	3:B:601:TRP:HD1	1.77	0.50
6:D:83:ASP:HA	6:D:86:ILE:HG22	1.93	0.50
1:9:399:ASN:O	1:9:404:ARG:NH1	2.45	0.50
4:C:426:GLU:HA	4:C:429:HIS:HB3	1.93	0.50
4:C:447:LYS:HA	4:C:450:LYS:HD3	1.92	0.50
1:9:88:VAL:HG22	1:9:92:LEU:HD23	1.93	0.50
1:9:395:SER:HA	1:9:398:VAL:HG22	1.94	0.49
5:E:272:ARG:HH21	5:E:288:ALA:HA	1.77	0.49
6:D:151:GLU:HB3	6:D:172:ILE:HD12	1.94	0.49
5:E:338:CYS:O	5:E:379:SER:OG	2.29	0.49
1:9:107:THR:OG1	1:9:108:GLY:N	2.45	0.49
1:9:226:ASP:OD1	1:9:226:ASP:N	2.43	0.49
1:9:237:GLN:HA	1:9:240:ARG:HE	1.77	0.49
1:9:332:ARG:O	1:9:336:ASP:N	2.46	0.49
6:D:47:PRO:O	6:D:51:SER:N	2.40	0.49
6:D:486:TYR:CE1	11:H:24:DC:C5	3.00	0.49
6:D:59:GLN:NE2	6:D:291:LEU:O	2.45	0.49
3:B:399:HIS:HB2	3:B:402:LEU:HD22	1.95	0.49
4:C:296:ASP:OD1	4:C:296:ASP:N	2.44	0.49
4:C:449:TYR:HD1	4:C:452:ARG:HD3	1.77	0.49
5:E:69:SER:OG	5:E:70:TRP:N	2.46	0.49
5:E:472:ASP:OD1	5:E:472:ASP:N	2.44	0.49
2:A:708:LYS:HD3	6:D:269:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:500:ASP:OD1	1:9:500:ASP:N	2.45	0.49
2:A:880:PHE:HD2	2:A:893:LYS:HB3	1.78	0.49
4:C:371:HIS:HB2	4:C:377:ILE:HD11	1.94	0.49
4:C:489:ASP:OD2	4:C:614:ARG:NH1	2.45	0.49
6:D:299:SER:HB3	6:D:302:VAL:HG23	1.95	0.49
1:9:506:SER:O	1:9:506:SER:OG	2.31	0.49
2:A:412:THR:HG23	6:D:208:THR:HG23	1.95	0.49
5:E:67:LEU:HD23	5:E:72:PRO:HB2	1.95	0.49
5:E:212:ASP:N	5:E:212:ASP:OD1	2.45	0.49
3:B:286:GLN:H	3:B:290:ARG:HH21	1.61	0.48
3:B:409:ASP:N	3:B:409:ASP:OD1	2.46	0.48
6:D:104:ARG:NH2	6:D:218:GLU:OE2	2.46	0.48
6:D:379:ARG:NH1	6:D:466:LEU:O	2.45	0.48
12:D:2001:AGS:O1B	12:D:2001:AGS:O3G	2.31	0.48
2:A:541:ALA:CB	10:G:10:DT:OP1	2.46	0.48
4:C:423:ASN:O	4:C:439:TYR:OH	2.32	0.48
5:E:109:VAL:HG23	5:E:156:LEU:HD22	1.94	0.48
1:9:92:LEU:HD12	1:9:95:ALA:HB2	1.94	0.48
2:A:865:SER:HB2	2:A:868:PHE:HB3	1.95	0.48
2:A:871:ASN:ND2	5:E:178:ARG:O	2.46	0.48
6:D:315:ASP:O	6:D:318:SER:OG	2.32	0.48
6:D:333:SER:O	6:D:336:THR:OG1	2.31	0.48
1:9:495:MET:HA	1:9:498:PHE:HB2	1.96	0.48
5:E:212:ASP:OD2	5:E:266:TRP:NE1	2.47	0.48
2:A:817:SER:OG	2:A:820:GLN:OE1	2.31	0.48
2:A:882:GLN:NE2	2:A:891:CYS:SG	2.86	0.48
2:A:432:SER:O	12:A:2001:AGS:O2'	2.32	0.48
5:E:74:LEU:HD23	5:E:108:LEU:HB2	1.96	0.48
6:D:275:MET:O	6:D:277:GLN:NE2	2.47	0.48
1:9:316:ALA:HA	1:9:319:PHE:HB3	1.96	0.47
3:B:526:LYS:NZ	3:B:530:GLU:OE2	2.40	0.47
5:E:254:ASP:OD2	5:E:255:ILE:N	2.47	0.47
7:F:336:ARG:NE	7:F:343:ASP:OD1	2.38	0.47
2:A:708:LYS:NZ	6:D:267:ARG:O	2.47	0.47
4:C:441:ASP:OD1	4:C:441:ASP:N	2.46	0.47
5:E:11:ARG:NH2	5:E:192:TYR:OH	2.42	0.47
6:D:116:LEU:O	6:D:120:GLN:N	2.46	0.47
3:B:445:SER:OG	3:B:472:ASN:O	2.31	0.47
6:D:419:ILE:O	6:D:423:ASN:ND2	2.47	0.47
2:A:486:THR:OG1	12:A:2001:AGS:O3G	2.31	0.47
5:E:43:LYS:HA	5:E:46:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:74:LEU:HD21	5:E:105:PRO:HA	1.96	0.47
5:E:109:VAL:HG21	5:E:155:LEU:HB3	1.96	0.47
1:9:170:ILE:HG12	1:9:184:LYS:HG3	1.97	0.47
6:D:220:ASP:OD1	6:D:220:ASP:N	2.47	0.47
2:A:886:ASN:HA	6:D:470:THR:HG21	1.97	0.47
3:B:264:SER:HB2	3:B:605:THR:HG21	1.97	0.47
3:B:296:ILE:HD13	7:F:398:ILE:HD12	1.95	0.47
6:D:281:LEU:HD21	6:D:325:ARG:HH21	1.79	0.47
7:F:333:ASN:HD21	7:F:388:ASP:HB3	1.80	0.47
8:3:921:GLU:O	8:3:922:ARG:NH2	2.38	0.47
1:9:219:VAL:HG13	1:9:257:VAL:HB	1.97	0.47
3:B:289:PRO:HB2	4:C:498:LEU:HD12	1.96	0.47
3:B:580:ARG:HA	3:B:583:ILE:HB	1.97	0.47
5:E:211:GLU:O	5:E:216:ARG:NH2	2.48	0.47
9:7:775:THR:HG23	9:7:777:LEU:H	1.80	0.47
1:9:277:LEU:O	1:9:279:ARG:NH1	2.43	0.47
4:C:351:LEU:HD21	4:C:389:GLU:HB3	1.97	0.47
4:C:390:GLU:HA	4:C:393:VAL:HG22	1.97	0.47
5:E:110:LYS:O	5:E:114:ASN:ND2	2.48	0.47
6:D:67:ASP:OD1	6:D:67:ASP:N	2.48	0.47
2:A:633:LYS:HD3	2:A:690:GLU:HG2	1.97	0.47
12:9:2001:AGS:O1B	12:9:2001:AGS:O2A	2.31	0.46
3:B:335:SER:O	3:B:357:SER:OG	2.34	0.46
8:3:936:GLN:O	8:3:940:ALA:N	2.48	0.46
3:B:518:THR:HG23	3:B:521:SER:H	1.81	0.46
4:C:123:SER:HA	4:C:197:LYS:HD3	1.97	0.46
1:9:198:GLN:HA	1:9:204:HIS:HB3	1.98	0.46
1:9:257:VAL:HG13	1:9:281:LEU:HD11	1.96	0.46
1:9:430:ASP:HA	1:9:488:LYS:HD3	1.97	0.46
1:9:439:HIS:HA	1:9:442:LYS:HG2	1.96	0.46
1:9:504:LYS:HG3	1:9:505:ILE:HG23	1.97	0.46
2:A:514:ASN:HB3	2:A:517:LYS:HB2	1.96	0.46
12:E:2001:AGS:O2G	12:E:2001:AGS:O2A	2.32	0.46
1:9:387:LEU:HD22	1:9:390:ILE:HG13	1.98	0.46
1:9:399:ASN:HB3	1:9:404:ARG:HD3	1.97	0.46
3:B:374:ASP:OD1	3:B:374:ASP:N	2.48	0.46
4:C:569:LEU:O	4:C:572:THR:OG1	2.31	0.46
5:E:277:ASN:HA	5:E:280:GLU:HB2	1.98	0.46
6:D:527:THR:OG1	6:D:528:GLN:N	2.48	0.46
3:B:549:THR:OG1	3:B:550:GLN:N	2.48	0.46
6:D:338:LYS:NZ	12:D:2001:AGS:O3'	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:TYR:HB2	12:E:2001:AGS:H3'	1.98	0.46
6:D:335:PRO:HA	6:D:338:LYS:HB3	1.98	0.45
1:9:217:THR:HA	1:9:254:VAL:HG12	1.97	0.45
1:9:400:ASN:ND2	1:9:404:ARG:O	2.49	0.45
2:A:855:ASP:OD1	2:A:855:ASP:N	2.50	0.45
4:C:60:LEU:HA	4:C:63:GLN:HE21	1.82	0.45
4:C:348:ASP:HA	4:C:351:LEU:HB2	1.98	0.45
7:F:369:VAL:HA	7:F:372:LEU:HD12	1.97	0.45
2:A:422:ILE:HG22	2:A:682:LEU:HD22	1.98	0.45
4:C:136:SER:O	4:C:136:SER:OG	2.32	0.45
1:9:201:ASN:HB3	1:9:204:HIS:CG	2.52	0.45
4:C:459:ASP:OD1	4:C:459:ASP:N	2.49	0.45
6:D:349:LYS:HA	6:D:349:LYS:HD3	1.82	0.45
3:B:310:GLN:O	3:B:448:ARG:NH1	2.43	0.45
3:B:600:ILE:O	3:B:600:ILE:HG13	2.16	0.45
1:9:409:LYS:O	1:9:415:LYS:NZ	2.39	0.45
3:B:558:LEU:O	3:B:562:LEU:N	2.46	0.45
1:9:84:GLU:HB3	1:9:288:PHE:HE1	1.81	0.45
4:C:352:LYS:HE2	4:C:352:LYS:HB3	1.82	0.45
6:D:86:ILE:O	6:D:89:SER:OG	2.29	0.45
6:D:100:LEU:N	6:D:249:GLY:O	2.42	0.45
7:F:363:ILE:HA	7:F:366:VAL:HG12	1.98	0.45
4:C:58:TRP:O	4:C:62:HIS:ND1	2.49	0.45
5:E:260:ASP:OD1	5:E:260:ASP:N	2.42	0.45
5:E:334:ALA:HA	5:E:337:ILE:HD12	1.99	0.45
4:C:596:LEU:HB3	4:C:597:ILE:HD12	1.98	0.44
8:3:953:VAL:HA	8:3:959:TRP:HB3	1.99	0.44
4:C:276:TYR:HA	4:C:279:GLN:HB3	2.00	0.44
4:C:278:ASN:ND2	4:C:422:PHE:O	2.36	0.44
1:9:335:PHE:O	1:9:339:ARG:N	2.49	0.44
3:B:556:LEU:HD21	3:B:600:ILE:HG23	1.99	0.44
6:D:255:ASN:OD1	6:D:255:ASN:N	2.50	0.44
2:A:561:ILE:HG22	2:A:563:VAL:HG23	1.99	0.44
2:A:605:PRO:HA	2:A:609:LEU:HB2	1.98	0.44
2:A:640:LEU:HD22	2:A:643:LEU:HD11	2.00	0.44
3:B:406:LYS:HE3	3:B:406:LYS:HB3	1.86	0.44
3:B:495:VAL:HG13	3:B:497:LYS:H	1.82	0.44
4:C:363:PHE:O	4:C:367:LEU:N	2.51	0.44
4:C:384:LYS:HA	4:C:384:LYS:HD3	1.85	0.44
6:D:105:GLN:N	12:D:2001:AGS:O1B	2.43	0.44
3:B:324:ASN:OD1	3:B:324:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:246:ASN:O	4:C:250:ASN:ND2	2.47	0.44
5:E:476:ASP:N	5:E:476:ASP:OD1	2.47	0.44
6:D:480:ASN:HD21	6:D:482:THR:HG22	1.82	0.44
7:F:381:ASP:O	7:F:385:ARG:N	2.44	0.44
8:3:923:ILE:HB	8:3:932:LYS:HE2	1.99	0.44
9:7:751:MET:HG3	9:7:765:ILE:HD11	1.99	0.44
2:A:460:TYR:O	2:A:464:TYR:N	2.45	0.44
4:C:86:GLU:HG3	4:C:266:LEU:HD21	2.00	0.44
4:C:118:LEU:HD23	4:C:118:LEU:HA	1.88	0.44
5:E:254:ASP:OD2	5:E:256:PHE:N	2.50	0.44
2:A:772:THR:OG1	2:A:773:VAL:N	2.50	0.44
3:B:522:LYS:HG2	3:B:617:LEU:HD23	1.99	0.44
1:9:312:PHE:HD1	1:9:312:PHE:HA	1.66	0.44
2:A:780:LYS:HZ3	2:A:780:LYS:HG2	1.64	0.44
3:B:298:LYS:HE2	3:B:301:PHE:HE2	1.83	0.44
5:E:40:GLY:N	12:E:2001:AGS:O1B	2.42	0.44
5:E:240:ILE:HA	5:E:243:ILE:HG22	1.99	0.44
6:D:90:ILE:O	6:D:93:LYS:NZ	2.43	0.44
7:F:276:LYS:HD2	7:F:318:GLN:HE22	1.83	0.44
9:7:746:THR:HA	9:7:749:LYS:HB2	1.99	0.44
5:E:346:ASP:N	5:E:346:ASP:OD1	2.50	0.43
1:9:106:ILE:HD12	1:9:118:LEU:HD21	1.99	0.43
2:A:649:TYR:N	2:A:658:ILE:O	2.43	0.43
7:F:422:LYS:HB3	7:F:423:LYS:HZ2	1.83	0.43
1:9:236:THR:OG1	1:9:237:GLN:N	2.51	0.43
4:C:593:ASN:OD1	4:C:593:ASN:N	2.50	0.43
7:F:279:LYS:HA	7:F:279:LYS:HD3	1.86	0.43
7:F:361:ASP:OD1	7:F:361:ASP:N	2.50	0.43
5:E:198:SER:HB3	5:E:244:VAL:HG21	2.00	0.43
6:D:514:ARG:HH11	6:D:527:THR:HG1	1.65	0.43
7:F:396:GLU:O	7:F:400:ARG:N	2.47	0.43
4:C:437:ASP:OD1	4:C:437:ASP:N	2.52	0.43
5:E:273:ILE:HA	5:E:284:LEU:HD11	2.01	0.43
8:3:922:ARG:HA	8:3:922:ARG:HD3	1.85	0.43
3:B:271:ARG:NH2	3:B:497:LYS:O	2.49	0.43
4:C:79:ILE:HA	4:C:82:ASP:HB3	2.00	0.43
4:C:367:LEU:HB3	4:C:377:ILE:HD13	2.01	0.43
1:9:107:THR:HG21	1:9:265:LEU:HD11	2.01	0.43
12:D:2001:AGS:O2B	12:D:2001:AGS:O1A	2.34	0.43
5:E:48:LYS:HD2	5:E:52:ASN:HD21	1.84	0.43
4:C:236:LEU:HD23	4:C:238:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:46:ASP:OD2	6:D:49:PHE:N	2.45	0.43
6:D:112:LEU:HD23	6:D:112:LEU:HA	1.83	0.43
3:B:465:TRP:O	5:E:422:GLN:NE2	2.52	0.42
3:B:550:GLN:HA	3:B:601:TRP:CG	2.54	0.42
4:C:364:VAL:HA	4:C:367:LEU:HD12	2.01	0.42
5:E:209:LEU:HD12	5:E:266:TRP:CE2	2.54	0.42
6:D:310:GLU:O	6:D:314:SER:N	2.43	0.42
1:9:342:ILE:HD12	1:9:342:ILE:HA	1.82	0.42
7:F:272:LEU:HG	7:F:355:LEU:HB2	2.00	0.42
7:F:418:TYR:O	7:F:422:LYS:N	2.50	0.42
4:C:557:ILE:HD12	4:C:557:ILE:HA	1.90	0.42
3:B:411:TYR:HA	3:B:414:GLN:HG2	2.01	0.42
3:B:556:LEU:HD23	3:B:598:GLU:HG2	2.02	0.42
4:C:588:ILE:HD12	4:C:588:ILE:HA	1.91	0.42
4:C:214:ASN:N	4:C:214:ASN:OD1	2.53	0.42
2:A:511:VAL:CG2	2:A:563:VAL:HG22	2.50	0.42
5:E:386:LEU:O	5:E:390:PHE:N	2.48	0.42
1:9:228:LEU:HD11	1:9:241:THR:HG21	2.01	0.42
2:A:551:LYS:O	2:A:552:ARG:NH1	2.53	0.42
4:C:426:GLU:O	4:C:430:ASN:ND2	2.34	0.42
1:9:411:ASN:HB3	1:9:414:GLN:HB2	2.01	0.42
2:A:481:PRO:HD2	6:D:262:LYS:HD2	2.00	0.42
6:D:111:LEU:HA	6:D:111:LEU:HD23	1.83	0.42
3:B:343:LEU:HD23	3:B:343:LEU:HA	1.91	0.42
3:B:366:TYR:HB3	3:B:426:ASN:HD22	1.85	0.42
5:E:36:GLN:HG3	5:E:176:LEU:HD22	2.02	0.42
6:D:137:HIS:HB3	6:D:142:ALA:HB2	2.01	0.42
1:9:400:ASN:O	1:9:405:THR:OG1	2.33	0.41
4:C:99:ARG:O	4:C:100:ARG:NE	2.53	0.41
5:E:191:ARG:HH21	5:E:253:ASN:HB2	1.85	0.41
1:9:480:GLY:HA3	2:A:880:PHE:HZ	1.85	0.41
3:B:511:LYS:O	3:B:515:GLN:NE2	2.46	0.41
3:B:591:THR:OG1	3:B:601:TRP:NE1	2.36	0.41
3:B:610:GLU:OE2	3:B:611:LYS:NZ	2.36	0.41
1:9:125:LYS:HG2	1:9:129:LEU:HD13	2.01	0.41
2:A:691:ILE:HD12	2:A:691:ILE:HA	1.93	0.41
4:C:446:CYS:O	4:C:450:LYS:N	2.53	0.41
5:E:391:GLN:NE2	5:E:414:MET:SD	2.93	0.41
7:F:335:ARG:O	7:F:339:ASP:N	2.52	0.41
1:9:421:ILE:HG22	1:9:422:ILE:HD13	2.02	0.41
2:A:885:LYS:HZ1	6:D:470:THR:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:567:PHE:HB3	8:3:950:ASN:HB3	2.01	0.41
4:C:212:ASN:OD1	4:C:212:ASN:N	2.53	0.41
4:C:223:LEU:HD23	4:C:223:LEU:HA	1.86	0.41
4:C:494:TRP:HZ2	7:F:380:ARG:HH11	1.68	0.41
6:D:227:ARG:HB3	6:D:229:THR:HG23	2.02	0.41
6:D:514:ARG:NH1	6:D:527:THR:OG1	2.44	0.41
2:A:406:PHE:HB2	6:D:187:LEU:HD22	2.03	0.41
3:B:517:LEU:HD12	3:B:517:LEU:HA	1.84	0.41
7:F:296:ARG:H	7:F:296:ARG:HG2	1.60	0.41
2:A:863:ILE:HG12	2:A:866:TRP:HB2	2.01	0.41
4:C:100:ARG:NH2	4:C:227:PHE:O	2.47	0.41
4:C:542:ILE:HD13	4:C:542:ILE:HA	1.95	0.41
6:D:422:ILE:HD11	6:D:526:TRP:HE1	1.86	0.41
1:9:86:GLU:O	1:9:90:ASN:ND2	2.54	0.41
3:B:441:LEU:HD13	3:B:444:LEU:HD12	2.02	0.41
4:C:99:ARG:HD3	4:C:99:ARG:HA	1.85	0.41
8:3:914:TYR:O	8:3:959:TRP:N	2.49	0.41
1:9:332:ARG:HA	1:9:335:PHE:HB3	2.02	0.41
1:9:414:GLN:HA	1:9:417:ILE:HG22	2.03	0.41
4:C:121:GLU:HB3	4:C:126:ASN:HD21	1.86	0.41
6:D:285:VAL:HG13	6:D:313:LEU:HD11	2.02	0.41
7:F:298:VAL:HA	7:F:301:LYS:HB2	2.03	0.41
7:F:419:ASN:OD1	7:F:423:LYS:NZ	2.42	0.41
2:A:565:LEU:HD12	2:A:565:LEU:HA	1.84	0.41
2:A:687:ASP:OD1	2:A:687:ASP:N	2.52	0.41
4:C:136:SER:HA	4:C:142:MET:HG3	2.03	0.41
4:C:295:SER:OG	4:C:296:ASP:N	2.53	0.41
4:C:525:PHE:HA	4:C:528:TYR:HB3	2.02	0.41
6:D:100:LEU:HD23	6:D:273:ILE:HG23	2.03	0.41
6:D:448:ILE:HD13	6:D:448:ILE:HA	1.88	0.41
6:D:510:LEU:HD12	6:D:513:LEU:HD12	2.03	0.41
7:F:327:CYS:O	7:F:331:VAL:N	2.52	0.41
7:F:358:LYS:HD2	7:F:358:LYS:HA	1.98	0.41
7:F:360:ASP:OD1	7:F:360:ASP:N	2.54	0.41
7:F:429:LEU:HD12	7:F:429:LEU:HA	1.89	0.41
2:A:510:TYR:HA	2:A:562:VAL:HG13	2.03	0.41
4:C:531:ALA:HB1	4:C:535:ILE:HG21	2.01	0.41
3:B:532:GLN:HG2	3:B:553:GLY:HA2	2.03	0.40
4:C:440:LEU:HD13	4:C:446:CYS:HB3	2.03	0.40
5:E:435:THR:HG22	5:E:450:TRP:NE1	2.30	0.40
4:C:286:ASP:HA	4:C:289:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:567:LEU:HD23	4:C:567:LEU:HA	1.88	0.40
5:E:256:PHE:HD1	5:E:256:PHE:HA	1.78	0.40
6:D:216:PHE:HD2	6:D:219:ILE:HG13	1.86	0.40
6:D:374:ASN:OD1	6:D:374:ASN:N	2.55	0.40
2:A:423:PHE:O	2:A:427:LYS:NZ	2.41	0.40
4:C:205:PHE:HB3	4:C:208:VAL:HG12	2.04	0.40
1:9:389:TYR:HA	1:9:392:LYS:HG2	2.02	0.40
1:9:411:ASN:HD21	1:9:413:GLN:HB3	1.86	0.40
2:A:409:LYS:HB3	6:D:158:HIS:HE1	1.84	0.40
1:9:83:ALA:H	1:9:295:GLN:NE2	2.19	0.40
1:9:94:LYS:HB2	1:9:101:SER:HA	2.02	0.40
1:9:496:ARG:O	1:9:496:ARG:NH1	2.53	0.40
2:A:862:ARG:H	2:A:862:ARG:HG2	1.70	0.40
3:B:489:GLU:OE1	3:B:489:GLU:N	2.52	0.40
4:C:421:ASN:OD1	4:C:421:ASN:N	2.52	0.40
6:D:363:PHE:HA	6:D:366:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	9	363/513 (71%)	318 (88%)	43 (12%)	2 (1%)	25 65
2	A	413/913 (45%)	380 (92%)	33 (8%)	0	100 100
3	B	314/620 (51%)	291 (93%)	23 (7%)	0	100 100
4	C	536/616 (87%)	506 (94%)	30 (6%)	0	100 100
5	E	414/479 (86%)	385 (93%)	28 (7%)	1 (0%)	47 81
6	D	428/529 (81%)	403 (94%)	25 (6%)	0	100 100
7	F	153/435 (35%)	146 (95%)	7 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	3	67/971 (7%)	60 (90%)	7 (10%)	0	100	100
9	7	50/845 (6%)	47 (94%)	3 (6%)	0	100	100
All	All	2738/5921 (46%)	2536 (93%)	199 (7%)	3 (0%)	54	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	445	SER
1	9	282	LEU
1	9	283	PRO

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	9	339/470 (72%)	333 (98%)	6 (2%)	59	77
2	A	373/812 (46%)	373 (100%)	0	100	100
3	B	298/573 (52%)	296 (99%)	2 (1%)	84	90
4	C	505/576 (88%)	505 (100%)	0	100	100
5	E	387/440 (88%)	387 (100%)	0	100	100
6	D	402/488 (82%)	401 (100%)	1 (0%)	93	96
7	F	151/406 (37%)	151 (100%)	0	100	100
8	3	62/835 (7%)	62 (100%)	0	100	100
9	7	49/753 (6%)	49 (100%)	0	100	100
All	All	2566/5353 (48%)	2557 (100%)	9 (0%)	91	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	9	297	TYR
1	9	312	PHE
1	9	335	PHE

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Mol	Chain	Res	Type
1	9	406	ARG
1	9	477	LYS
1	9	495	MET
3	B	411	TYR
3	B	547	ARG
6	D	499	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	9	90	ASN
1	9	295	GLN
1	9	388	ASN
2	A	530	ASN
2	A	882	GLN
2	A	906	ASN
3	B	279	ASN
3	B	282	ASN
3	B	297	GLN
3	B	310	GLN
3	B	364	ASN
3	B	398	ASN
3	B	426	ASN
3	B	458	HIS
3	B	535	ASN
3	B	585	HIS
4	C	63	GLN
4	C	65	HIS
4	C	69	HIS
4	C	78	ASN
4	C	243	ASN
4	C	253	GLN
4	C	486	ASN
5	E	52	ASN
5	E	114	ASN
5	E	193	ASN
5	E	253	ASN
5	E	277	ASN
5	E	320	GLN
5	E	422	GLN
5	E	453	ASN
6	D	80	GLN

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Mol	Chain	Res	Type
6	D	105	GLN
6	D	158	HIS
6	D	277	GLN
6	D	321	ASN
6	D	327	ASN
6	D	409	ASN
6	D	423	ASN
6	D	511	GLN
7	F	318	GLN
7	F	326	ASN
7	F	407	GLN
8	3	924	ASN
8	3	950	ASN
9	7	781	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)

4 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	$\#\|Z\| > 2$
12	AGS	9	2001	-	26,33,33	0.73	1 (3%)	26,52,52	1.30	2 (7%)
12	AGS	E	2001	-	26,33,33	0.68	0	26,52,52	1.33	2 (7%)
12	AGS	A	2001	-	26,33,33	0.72	1 (3%)	26,52,52	1.07	2 (7%)
12	AGS	D	2001	-	26,33,33	0.75	0	26,52,52	1.41	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
12	AGS	9	2001	-	-	7/17/38/38	0/3/3/3
12	AGS	E	2001	-	-	7/17/38/38	0/3/3/3
12	AGS	A	2001	-	-	7/17/38/38	0/3/3/3
12	AGS	D	2001	-	-	2/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	2001	AGS	C8-N7	-2.01	1.31	1.34
12	9	2001	AGS	C8-N7	-2.01	1.31	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	2001	AGS	PA-O3A-PB	-5.97	112.33	132.83
12	9	2001	AGS	PA-O3A-PB	-5.46	114.09	132.83
12	E	2001	AGS	PA-O3A-PB	-5.22	114.92	132.83
12	A	2001	AGS	PA-O3A-PB	-3.83	119.67	132.83
12	D	2001	AGS	C5-C6-N6	2.30	123.84	120.35
12	A	2001	AGS	C5-C6-N6	2.22	123.73	120.35
12	E	2001	AGS	C5-C6-N6	2.22	123.73	120.35
12	9	2001	AGS	C5-C6-N6	2.18	123.67	120.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	9	2001	AGS	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
12	9	2001	AGS	C5'-O5'-PA-O3A
12	A	2001	AGS	C5'-O5'-PA-O1A
12	A	2001	AGS	C5'-O5'-PA-O2A
12	A	2001	AGS	O4'-C4'-C5'-O5'
12	E	2001	AGS	C5'-O5'-PA-O1A
12	E	2001	AGS	C5'-O5'-PA-O2A
12	E	2001	AGS	C5'-O5'-PA-O3A
12	9	2001	AGS	O4'-C4'-C5'-O5'
12	E	2001	AGS	O4'-C4'-C5'-O5'
12	9	2001	AGS	C3'-C4'-C5'-O5'
12	E	2001	AGS	C3'-C4'-C5'-O5'
12	9	2001	AGS	PB-O3A-PA-O1A
12	A	2001	AGS	PG-O3B-PB-O1B
12	9	2001	AGS	C4'-C5'-O5'-PA
12	D	2001	AGS	C4'-C5'-O5'-PA
12	E	2001	AGS	PG-O3B-PB-O2B
12	D	2001	AGS	C3'-C4'-C5'-O5'
12	9	2001	AGS	PB-O3A-PA-O2A
12	A	2001	AGS	PA-O3A-PB-O1B
12	A	2001	AGS	C5'-O5'-PA-O3A
12	E	2001	AGS	PA-O3A-PB-O1B
12	A	2001	AGS	C3'-C4'-C5'-O5'

There are no ring outliers.

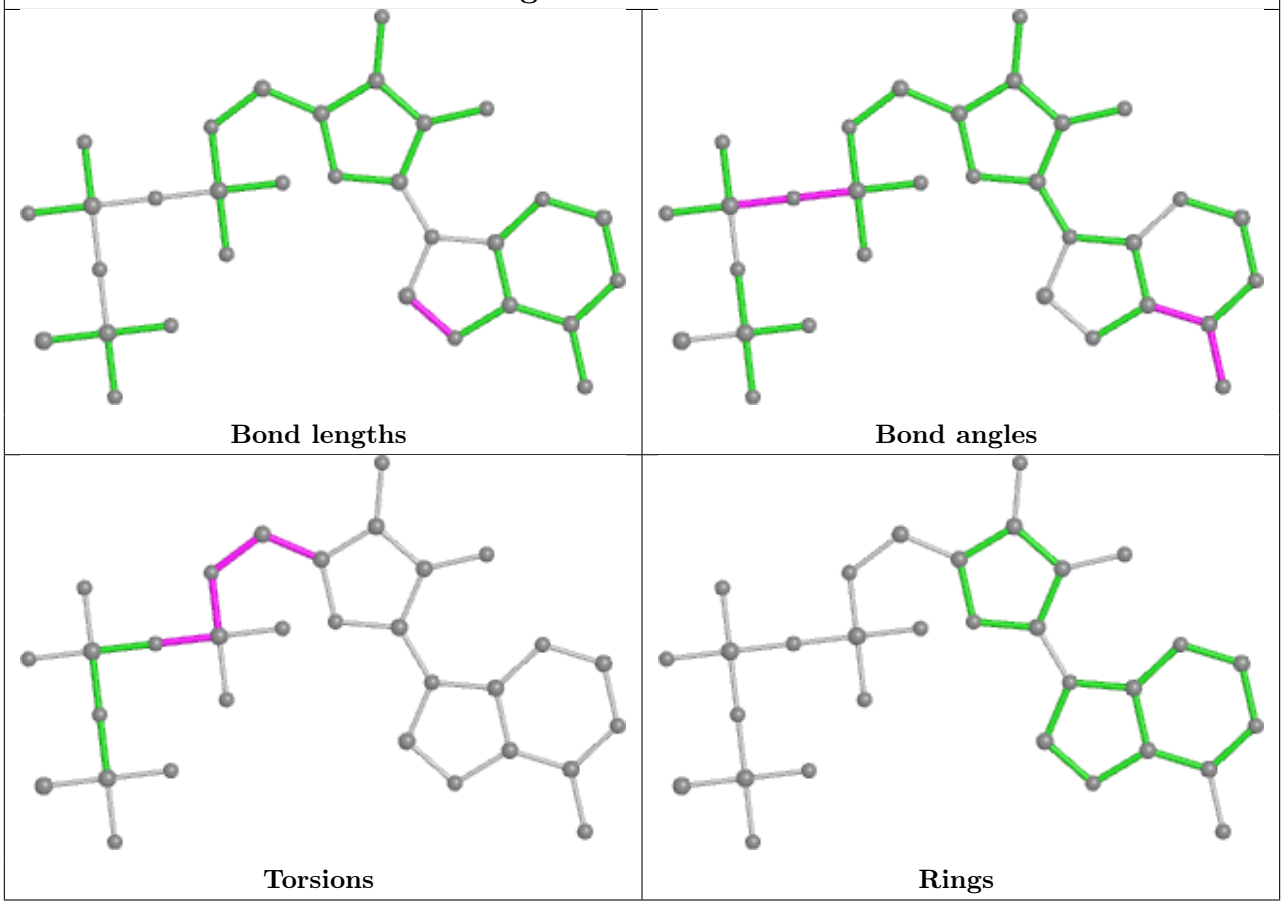
4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	9	2001	AGS	4	0
12	E	2001	AGS	5	0
12	A	2001	AGS	7	0
12	D	2001	AGS	4	0

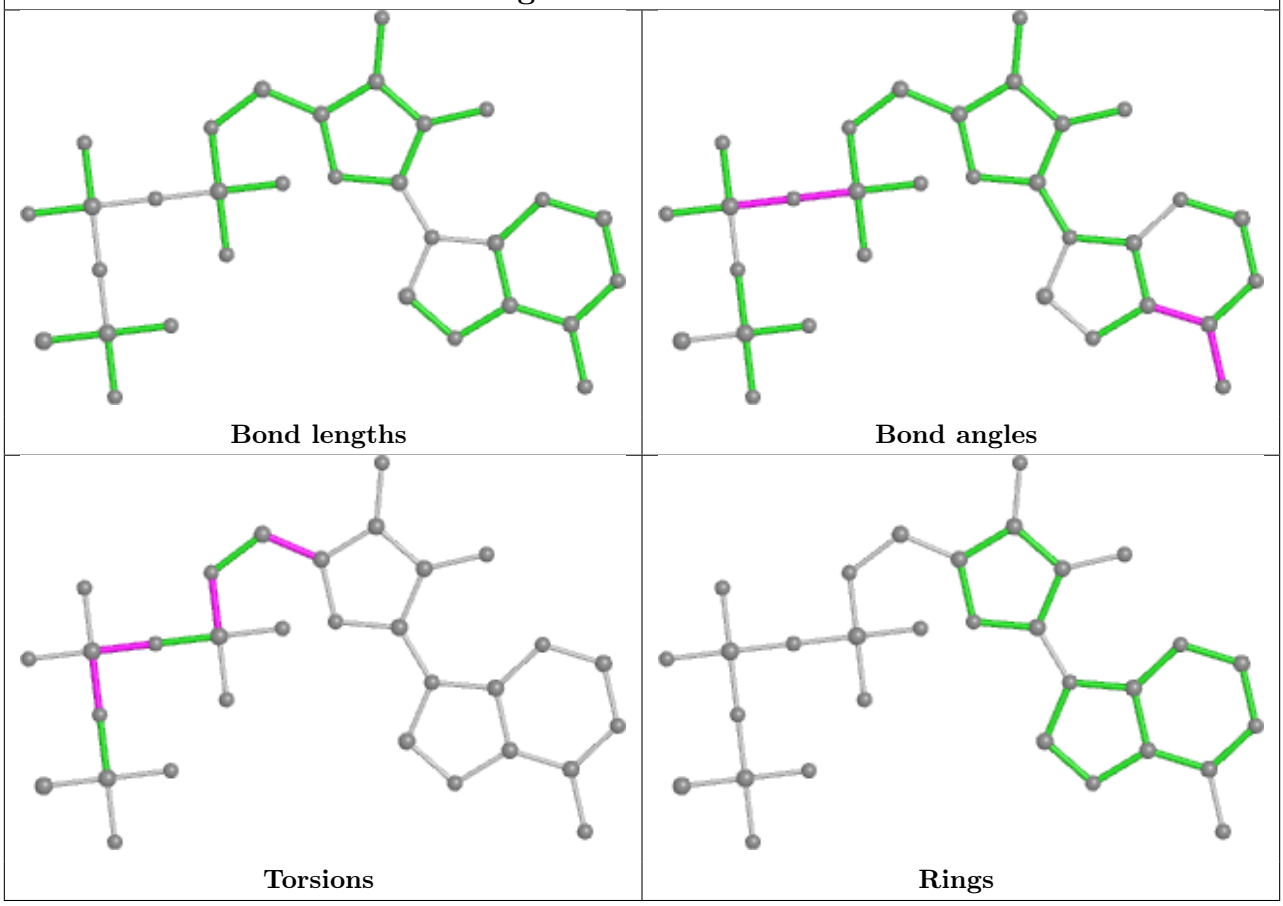
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

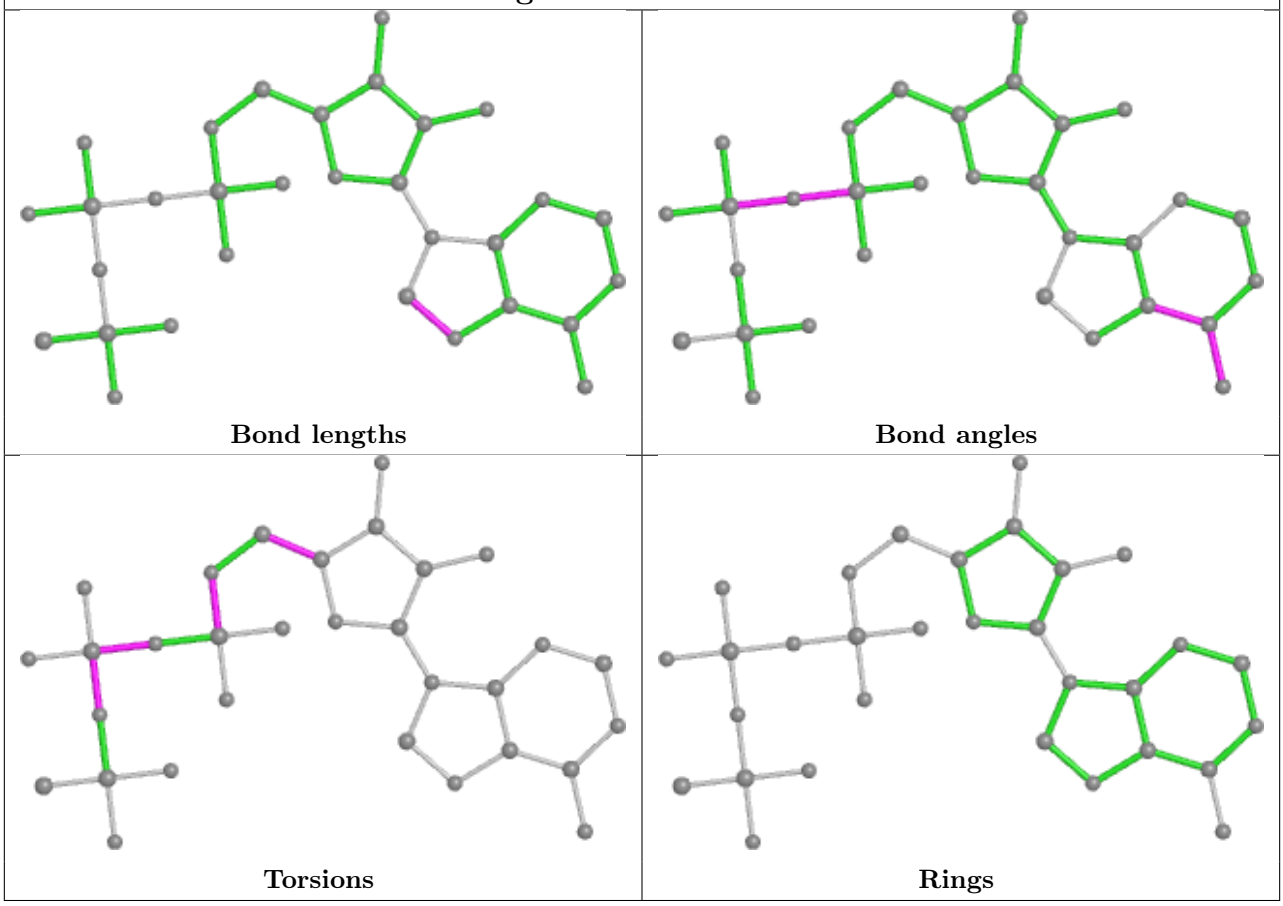
Ligand AGS 9 2001

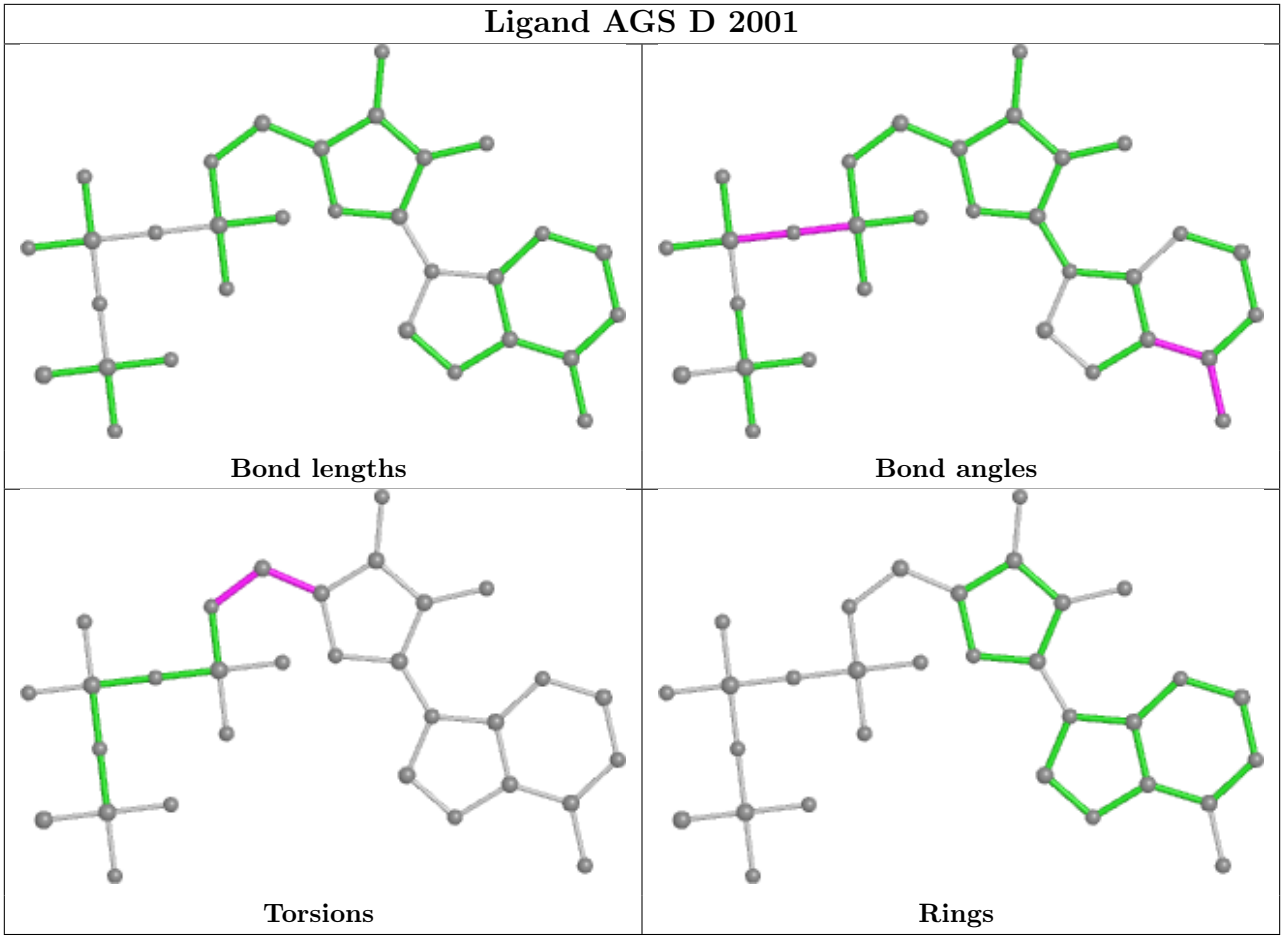


Ligand AGS E 2001



Ligand AGS A 2001





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	9	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	399:ASN	C	400:ASN	N	3.97

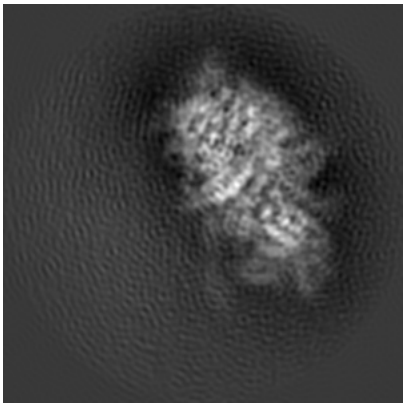
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21662. These allow visual inspection of the internal detail of the map and identification of artifacts.

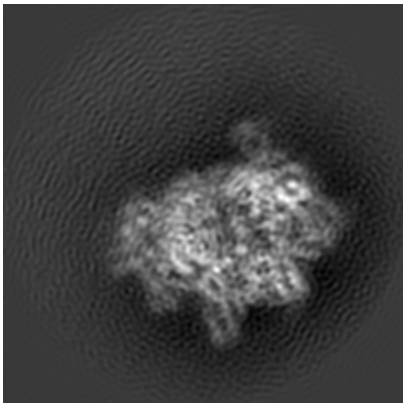
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

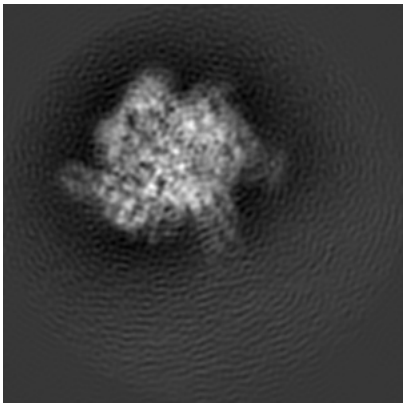
6.1.1 Primary map



X



Y

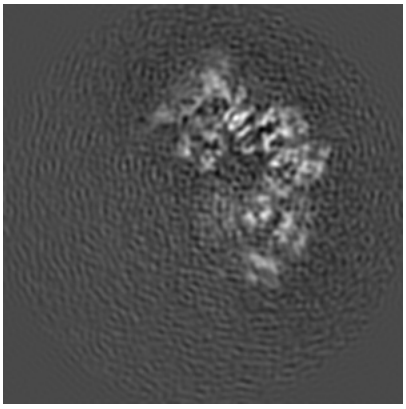


Z

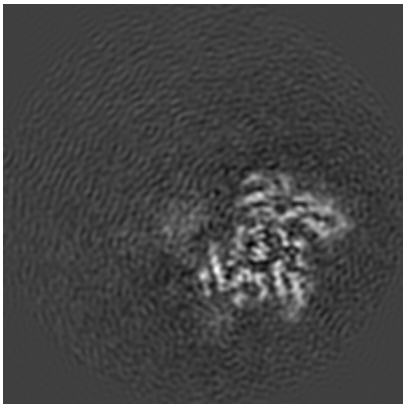
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

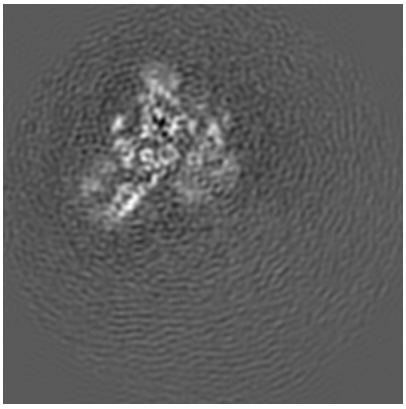
6.2.1 Primary map



X Index: 100



Y Index: 100

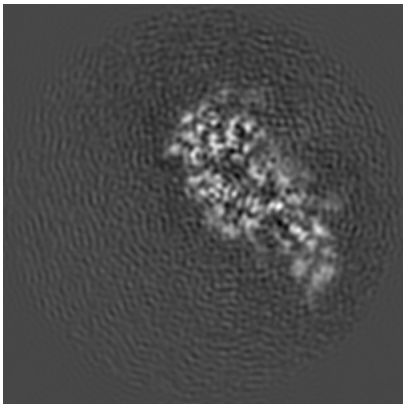


Z Index: 100

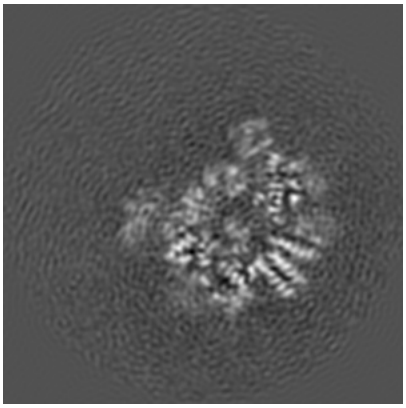
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

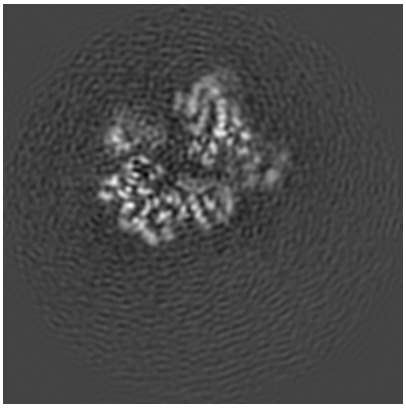
6.3.1 Primary map



X Index: 71



Y Index: 122

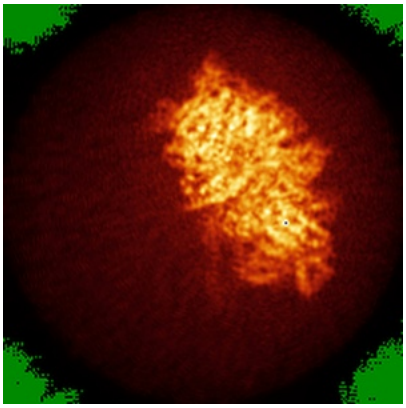


Z Index: 126

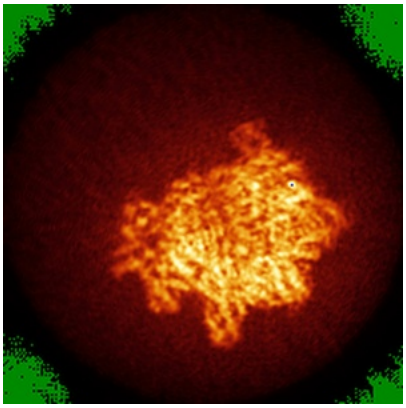
The images above show the largest variance slices of the map in three orthogonal directions.

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

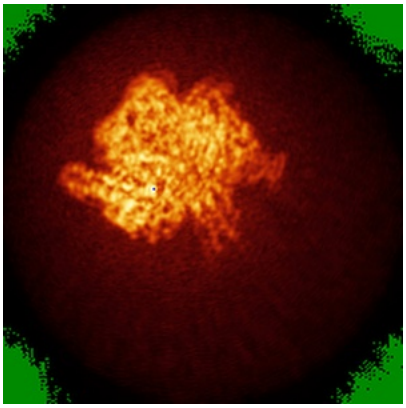
6.4.1 Primary map



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

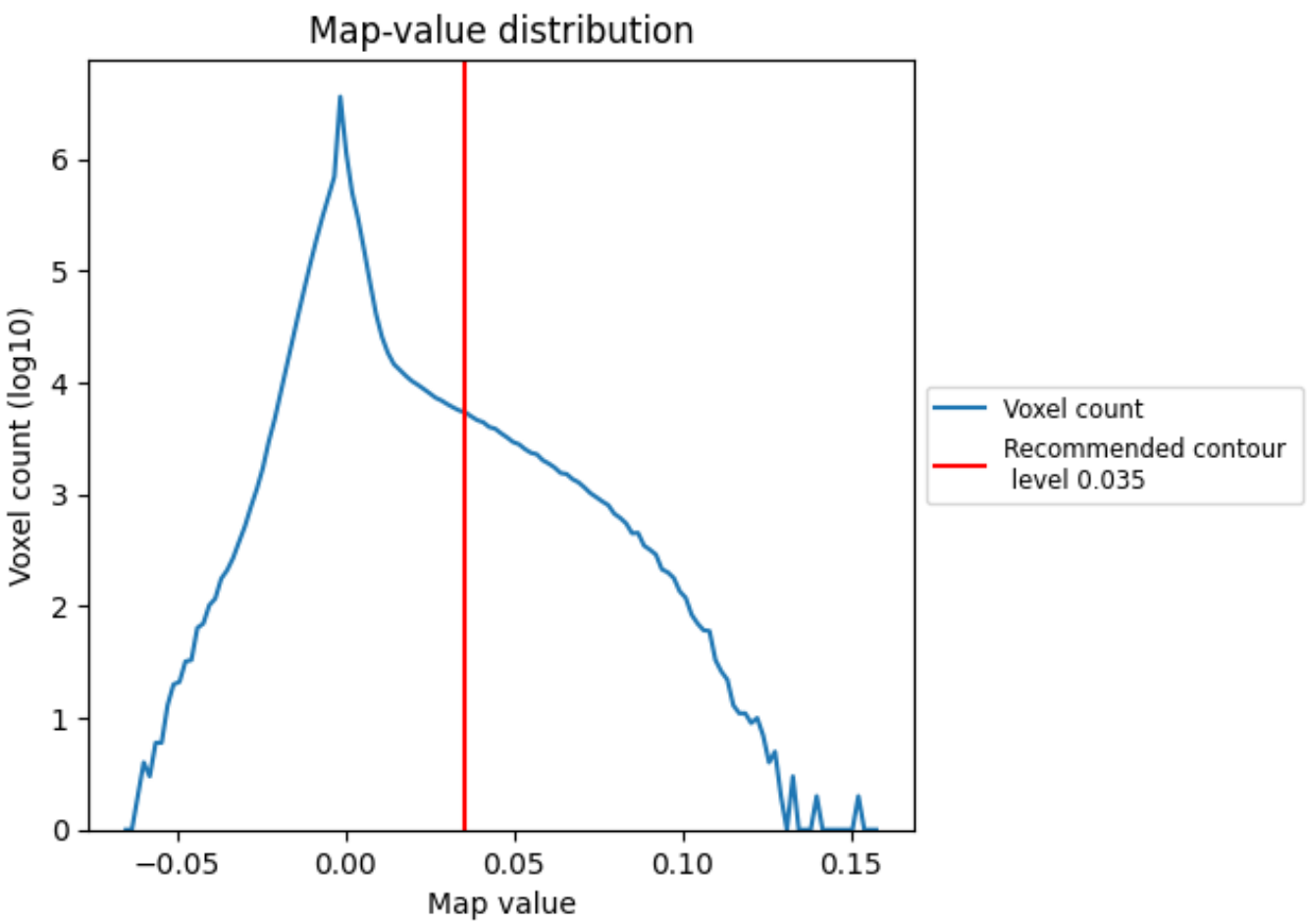
6.6 Mask visualisation (i)

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

7 Map analysis (i)

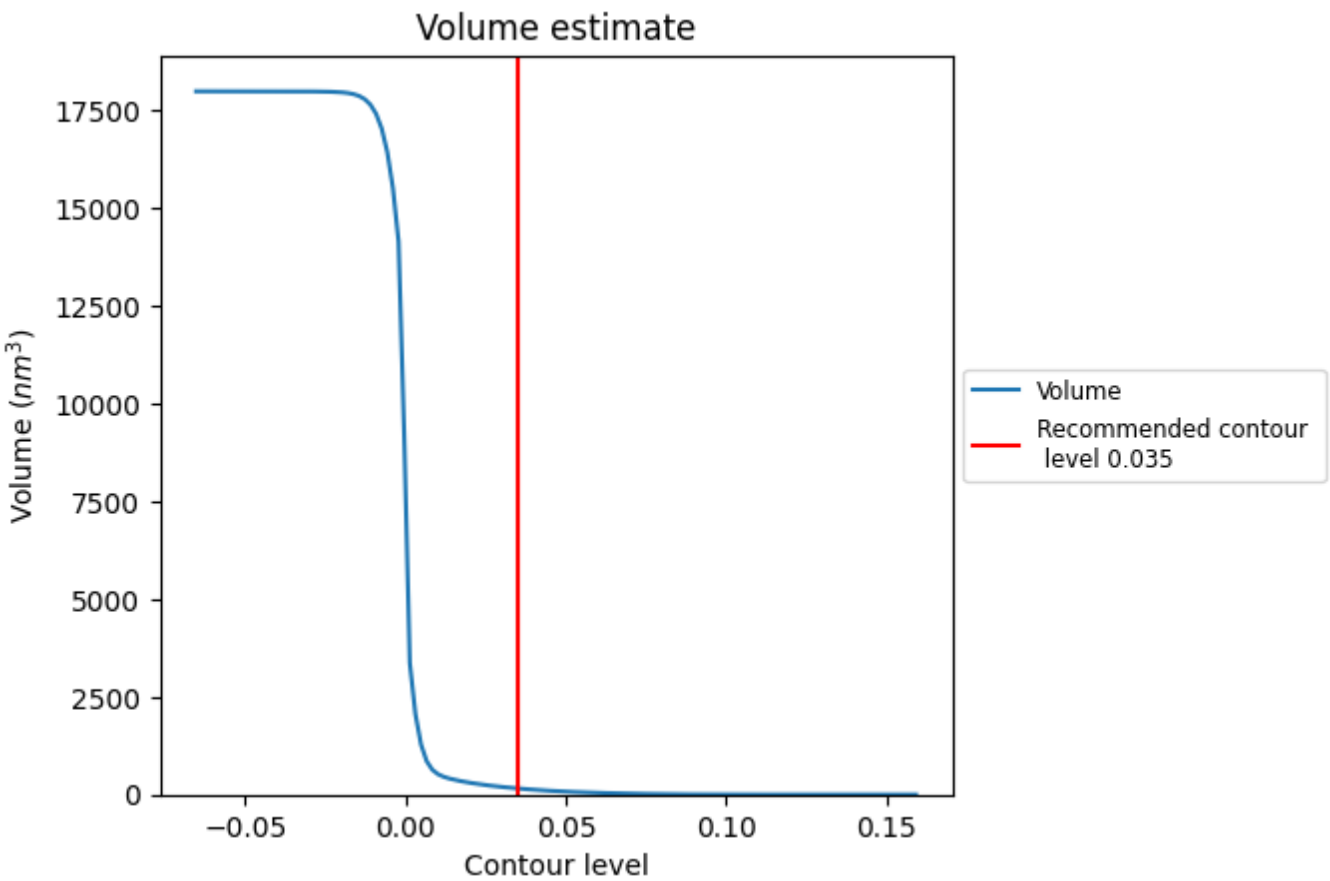
This section contains the results of statistical analysis of the map.

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.

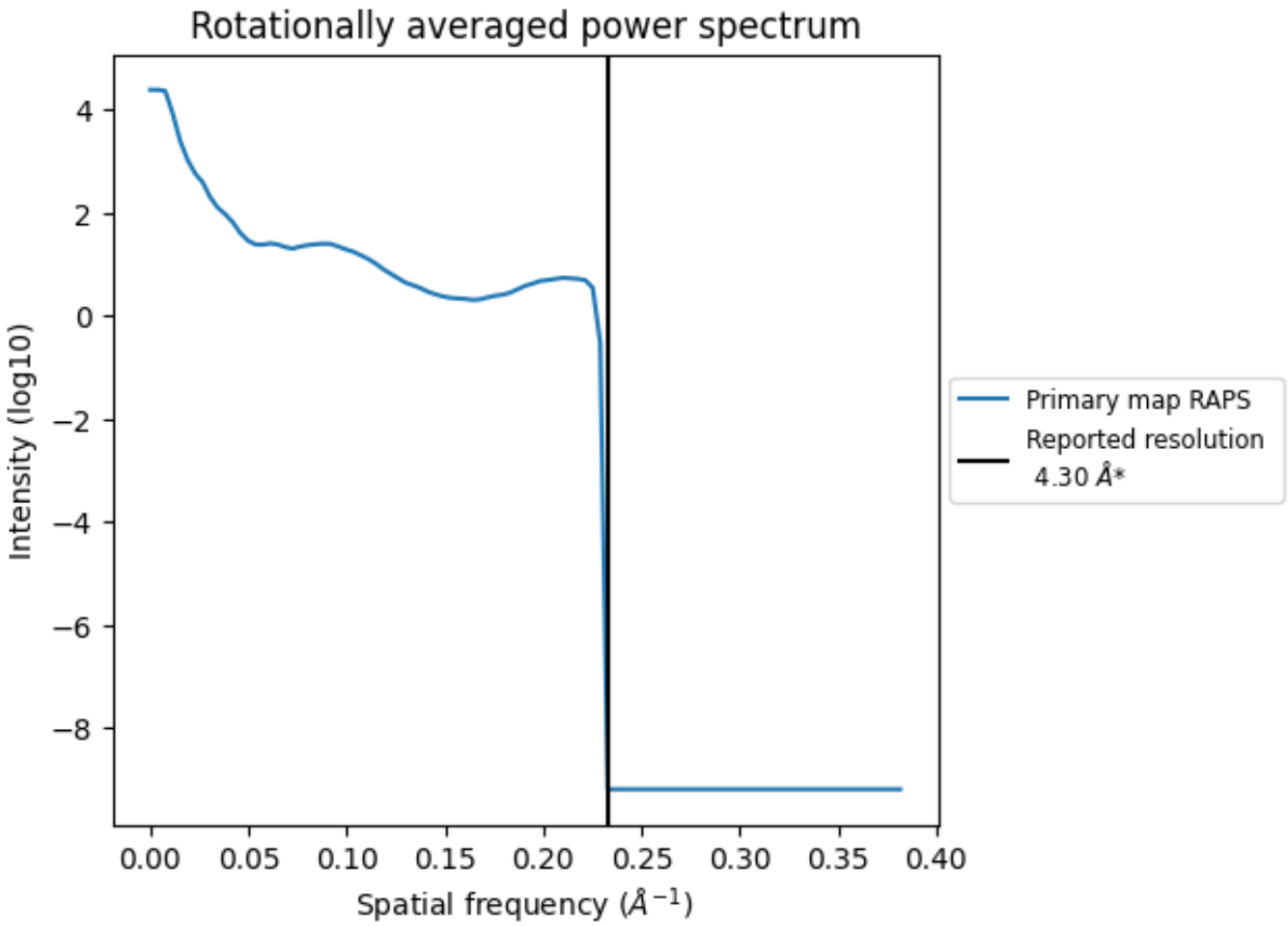
7.2 Volume estimate (i)



The volume at the recommended contour level is 157 nm^3; this corresponds to an approximate mass of 142 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 0.233 Å^{-1}

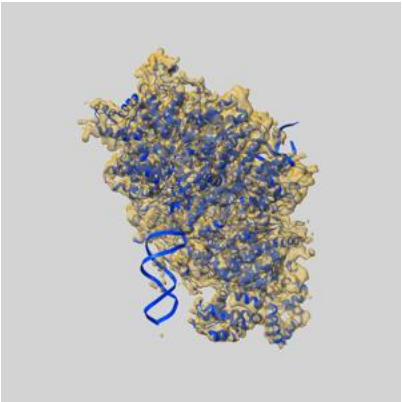
8 Fourier-Shell correlation (i)

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

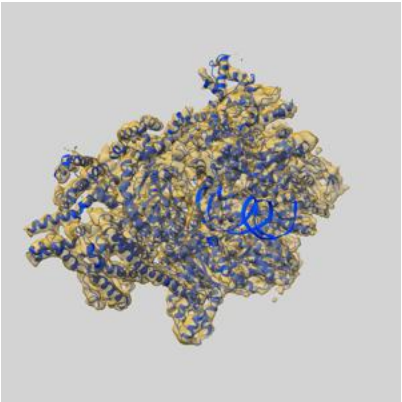
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21662 and PDB model 6WGC. Per-residue inclusion information can be found in section 3 on page 7.

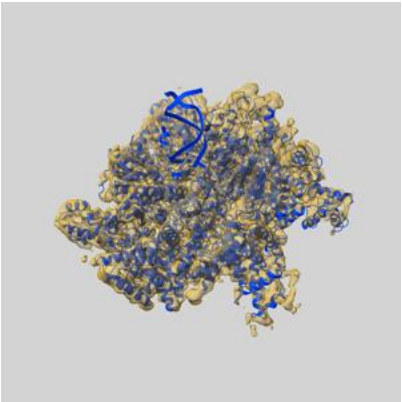
9.1 Map-model overlay (i)



X



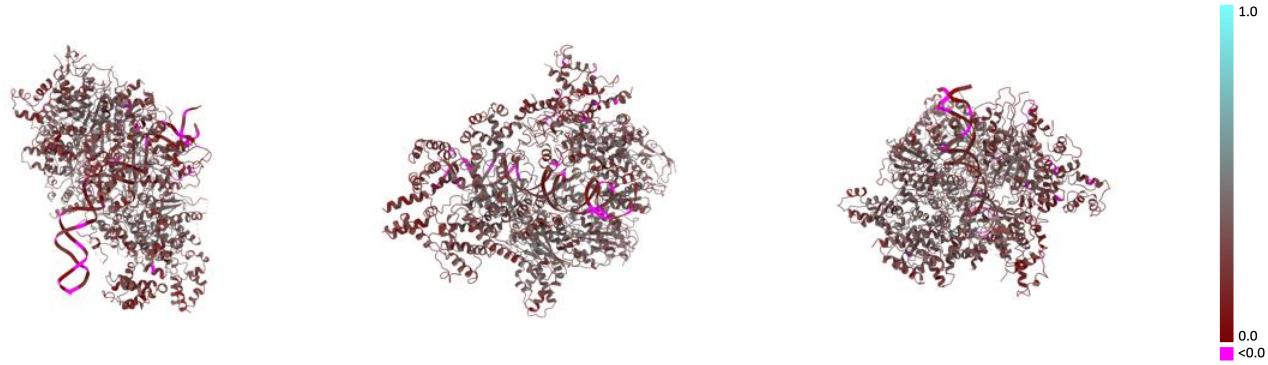
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

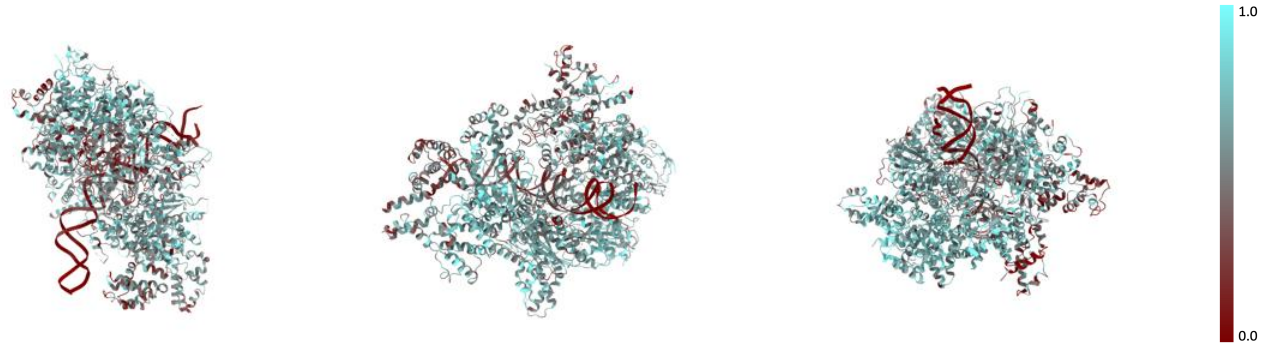
9.2 Q-score mapped to coordinate model (i)



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.

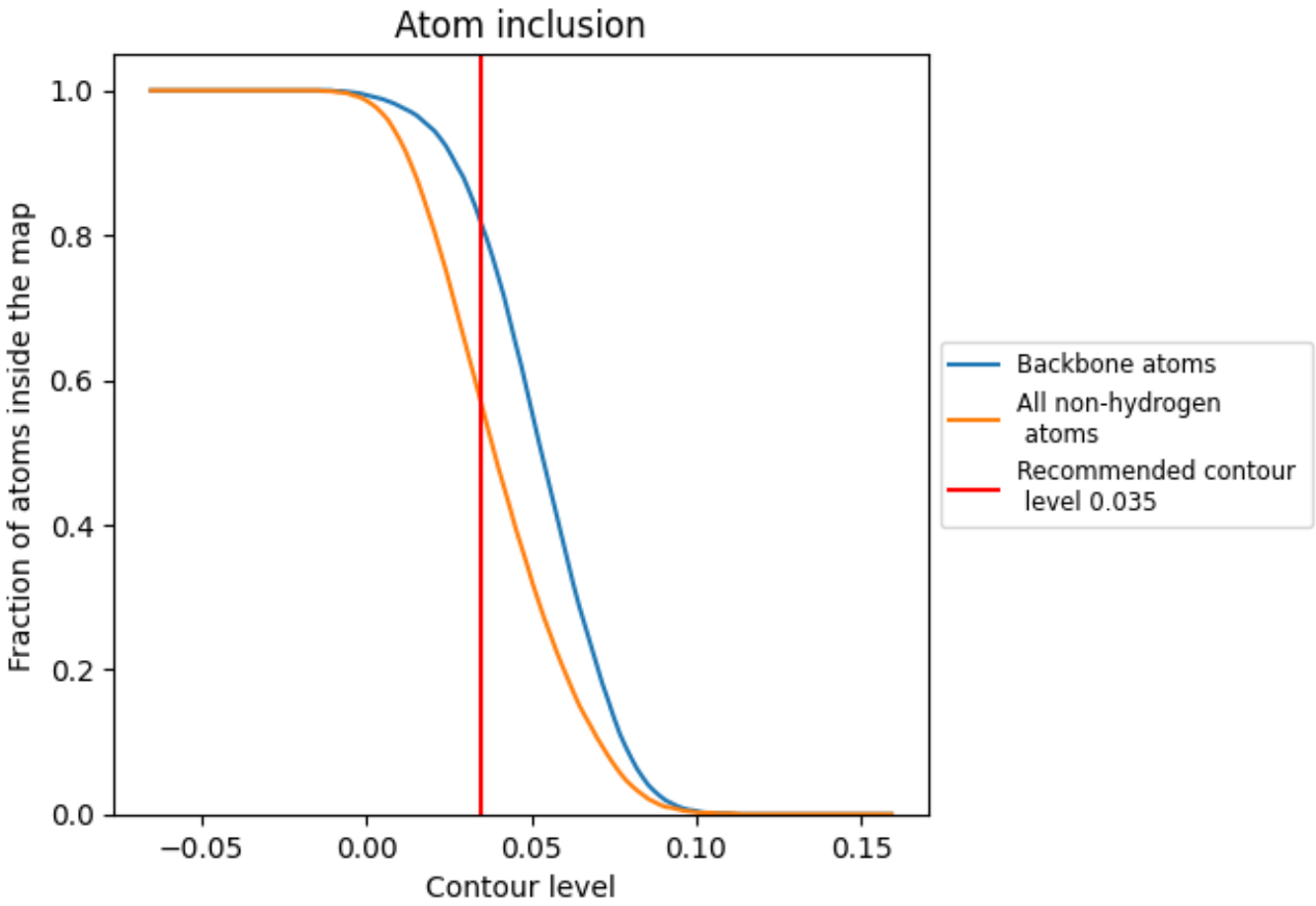
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 56% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5650	0.3010
3	0.3120	0.2500
7	0.3020	0.2250
9	0.5100	0.2600
A	0.6560	0.3400
B	0.5620	0.3080
C	0.6200	0.3150
D	0.6790	0.3550
E	0.6660	0.3490
F	0.4670	0.2500
G	0.1130	0.1290
H	0.1200	0.0950