



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 08:26 AM EST

PDB ID : 7MCA
EMDB ID : EMD-23755
Title : Structure of the *S. cerevisiae* origin recognition complex bound to the replication initiator Cdc6 and the ARS1 origin DNA.
Authors : Feng, X.; Li, H.
Deposited on : 2021-04-01
Resolution : 3.60 Å (reported)
Based on initial model : 5V8F

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

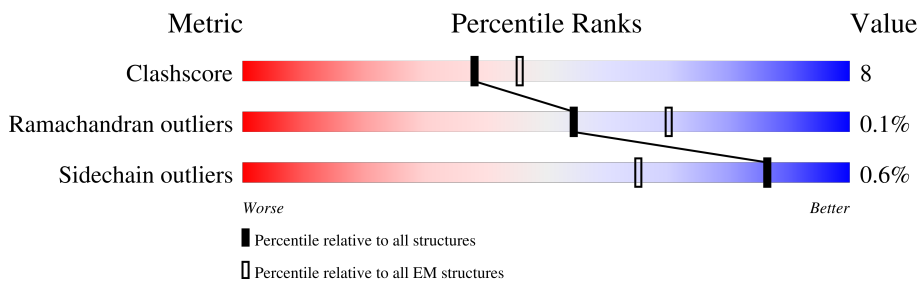
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	914	
2	B	620	
3	C	616	
4	D	529	
5	E	479	
6	F	435	
7	G	85	
8	H	85	

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Mol	Chain	Length	Quality of chain
9	I	513	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	AGS	D	2001	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 24692 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 Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	493	3946	2518	675	734	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	253	2096	1358	347	382	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	584	4830	3112	797	905	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	438	3572	2288	606	665	13	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	452	3702	2403	601	684	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	164	1369	879	233	245	12	0	0

- Molecule 7 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	G	50	1018	493	161	314	50	0	0

- Molecule 8 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	H	50	1032	493	203	286	50	0	0

- Molecule 9 is a protein called Cell division control protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	376	2999	1925	502	555	17	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

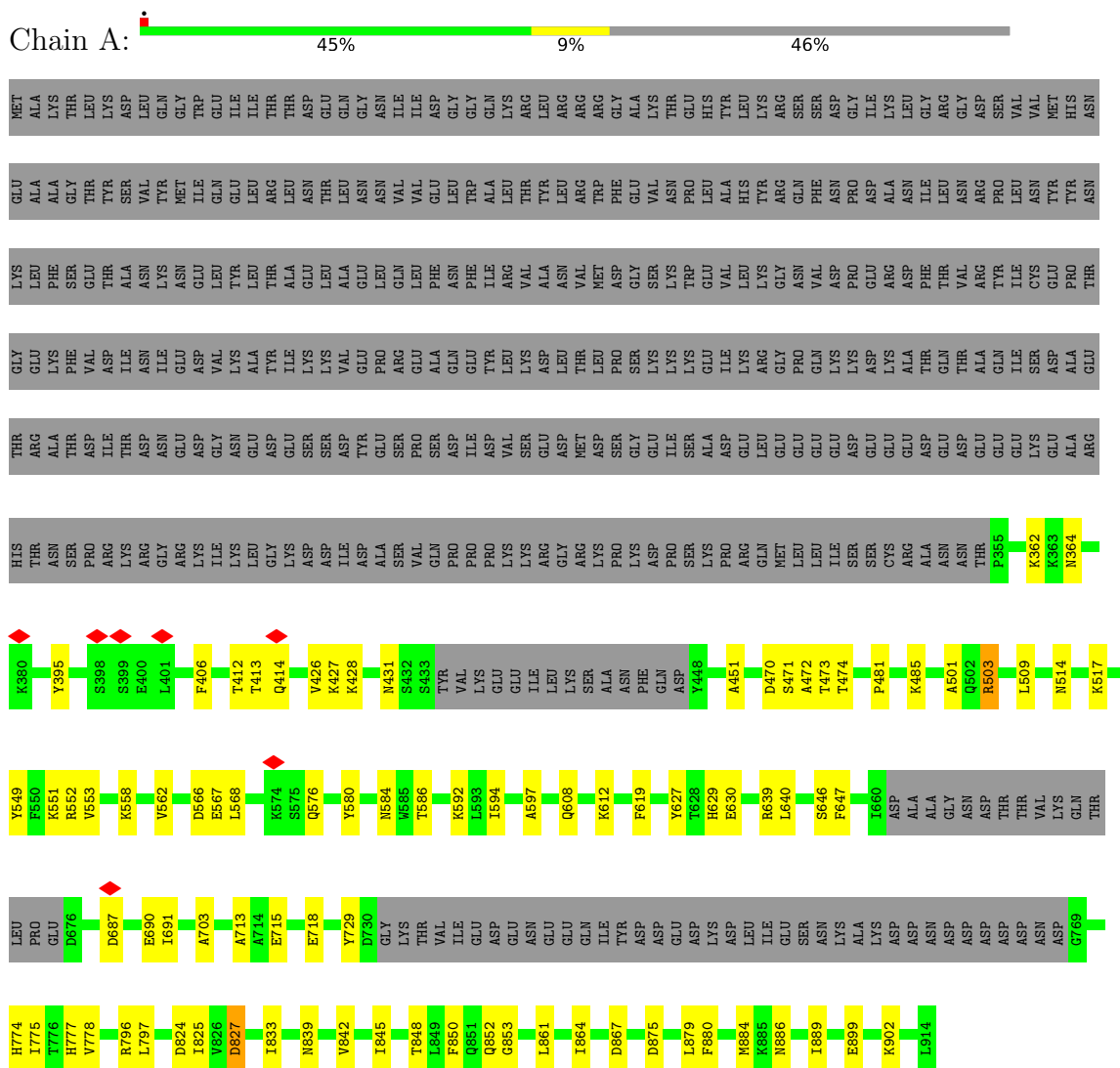
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total 1	Mg 1	0
10	D	1	Total 1	Mg 1	0
10	E	1	Total 1	Mg 1	0
10	I	1	Total 1	Mg 1	0

- Molecule 11 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Origin recognition complex subunit 1



- Molecule 2: Origin recognition complex subunit 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	76	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.011	Depositor
Map size (\AA)	231.84, 231.84, 231.84	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.828, 0.828, 0.828	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, 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	A	0.35	0/4007	0.59	2/5389 (0.0%)
2	B	0.40	0/2149	0.57	1/2905 (0.0%)
3	C	0.35	0/4935	0.56	1/6663 (0.0%)
4	D	0.38	0/3634	0.52	0/4909
5	E	0.39	0/3787	0.56	1/5140 (0.0%)
6	F	0.30	0/1392	0.53	0/1876
7	G	0.79	0/1135	1.04	0/1750
8	H	0.81	0/1163	0.90	0/1792
9	I	0.34	0/3041	0.62	2/4089 (0.0%)
All	All	0.42	0/25243	0.62	7/34513 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	209	LEU	CA-CB-CG	7.22	131.90	115.30
3	C	521	LEU	CA-CB-CG	6.98	131.35	115.30
1	A	875	ASP	CB-CG-OD1	6.47	124.13	118.30
5	E	171	LEU	CA-CB-CG	5.34	127.58	115.30
9	I	282	LEU	CA-CB-CG	5.30	127.49	115.30
2	B	463	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	827	ASP	CB-CG-OD1	5.14	122.93	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	126	PHE	Peptide
9	I	235	GLU	Peptide
9	I	282	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3946	0	4062	60	0
2	B	2096	0	2069	21	0
3	C	4830	0	4782	54	0
4	D	3572	0	3630	44	0
5	E	3702	0	3731	38	0
6	F	1369	0	1409	17	0
7	G	1018	0	574	27	0
8	H	1032	0	560	38	0
9	I	2999	0	3124	139	0
10	A	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	I	1	0	0	0	0
11	D	62	0	24	14	0
11	E	31	0	12	1	0
11	I	31	0	12	1	0
All	All	24692	0	23989	388	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 8.

All (388) 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)
9:I:406:ARG:NH1	9:I:504:LYS:HD2	1.36	1.37
9:I:406:ARG:HH11	9:I:504:LYS:CD	1.40	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:409:LYS:CG	9:I:414:GLN:O	1.79	1.29
1:A:485:LYS:NZ	11:D:2001:AGS:O2B	1.65	1.28
7:G:8:DT:O4	8:H:78:DA:N1	1.65	1.28
9:I:409:LYS:O	9:I:411:ASN:N	1.66	1.27
9:I:401:ASN:ND2	9:I:497:GLU:HB2	1.52	1.24
1:A:485:LYS:NZ	11:D:2001:AGS:PB	2.18	1.16
9:I:393:VAL:CG2	9:I:397:PHE:HE2	1.62	1.12
9:I:165:VAL:HG13	9:I:217:THR:HG21	1.29	1.11
9:I:409:LYS:HG3	9:I:414:GLN:O	1.39	1.10
9:I:402:SER:HB3	9:I:501:GLU:CG	1.84	1.08
9:I:393:VAL:HG22	9:I:397:PHE:CE2	1.90	1.06
9:I:393:VAL:HG22	9:I:397:PHE:HE2	1.16	1.04
9:I:400:ASN:HB2	9:I:404:ARG:CG	1.87	1.04
9:I:388:ASN:O	9:I:392:LYS:HB3	1.58	1.03
8:H:76:DG:H2''	8:H:77:DT:OP2	1.59	1.00
9:I:402:SER:HB3	9:I:501:GLU:CB	1.91	1.00
9:I:165:VAL:HA	9:I:217:THR:HB	1.44	0.98
9:I:393:VAL:O	9:I:397:PHE:HD2	1.48	0.97
9:I:409:LYS:HG3	9:I:414:GLN:C	1.84	0.96
9:I:406:ARG:HD3	9:I:504:LYS:CE	1.94	0.96
9:I:165:VAL:HG13	9:I:217:THR:CG2	1.95	0.95
9:I:393:VAL:CG2	9:I:397:PHE:CE2	2.51	0.93
9:I:402:SER:CB	9:I:501:GLU:HB2	1.99	0.92
8:H:78:DA:N3	8:H:79:DA:C8	2.37	0.92
9:I:409:LYS:CD	9:I:414:GLN:O	2.18	0.91
1:A:485:LYS:HZ2	11:D:2001:AGS:PB	1.95	0.89
9:I:402:SER:OG	9:I:501:GLU:HB2	1.71	0.89
9:I:400:ASN:HB2	9:I:404:ARG:HG3	1.55	0.88
9:I:210:GLU:OE1	9:I:210:GLU:N	2.09	0.85
9:I:421:ILE:CG2	9:I:489:ILE:HG21	2.07	0.84
9:I:388:ASN:O	9:I:392:LYS:CB	2.25	0.84
7:G:7:DT:H2''	7:G:8:DT:H5''	1.61	0.82
9:I:404:ARG:HA	9:I:407:ILE:HB	1.61	0.82
9:I:400:ASN:CB	9:I:404:ARG:CG	2.57	0.81
1:A:619:PHE:CE2	9:I:393:VAL:HG11	2.15	0.81
9:I:403:THR:O	9:I:407:ILE:HG12	1.80	0.81
8:H:78:DA:C4	8:H:79:DA:N7	2.50	0.80
6:F:366:VAL:O	6:F:370:LYS:HB2	1.82	0.80
9:I:400:ASN:CB	9:I:404:ARG:HG3	2.11	0.80
9:I:402:SER:HB3	9:I:501:GLU:HB2	1.60	0.80
9:I:401:ASN:ND2	9:I:497:GLU:CB	2.40	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:215:LYS:N	9:I:215:LYS:HE3	1.96	0.79
9:I:212:TYR:CZ	9:I:213:HIS:HD2	2.00	0.79
9:I:389:TYR:O	9:I:393:VAL:N	2.16	0.79
7:G:9:DA:N6	8:H:76:DG:O6	2.15	0.78
9:I:215:LYS:HE3	9:I:215:LYS:CA	2.15	0.77
9:I:402:SER:CB	9:I:501:GLU:CG	2.62	0.77
9:I:409:LYS:HD2	9:I:414:GLN:O	1.85	0.76
9:I:401:ASN:HD21	9:I:497:GLU:HB2	1.49	0.76
7:G:6:DT:H71	8:H:79:DA:N6	2.00	0.76
8:H:76:DG:C2'	8:H:77:DT:H72	2.16	0.76
8:H:76:DG:H2''	8:H:77:DT:H72	1.67	0.76
6:F:378:TRP:O	6:F:382:LEU:HB2	1.85	0.76
9:I:421:ILE:HG23	9:I:489:ILE:HG21	1.65	0.75
9:I:399:ASN:C	9:I:400:ASN:HD22	1.89	0.75
9:I:400:ASN:CG	9:I:404:ARG:HG3	2.07	0.75
9:I:212:TYR:CE2	9:I:213:HIS:HD2	2.04	0.75
9:I:396:LYS:HE3	9:I:396:LYS:HA	1.69	0.74
9:I:409:LYS:HG2	9:I:414:GLN:O	1.85	0.74
9:I:406:ARG:HH11	9:I:504:LYS:HD2	0.61	0.74
9:I:421:ILE:HD13	9:I:421:ILE:N	2.02	0.74
9:I:406:ARG:HD3	9:I:504:LYS:HE2	1.70	0.74
7:G:6:DT:N3	8:H:81:DA:C2	2.56	0.73
8:H:78:DA:C4	8:H:79:DA:C8	2.77	0.73
9:I:388:ASN:O	9:I:392:LYS:N	2.23	0.72
9:I:402:SER:HB3	9:I:501:GLU:HG2	1.70	0.71
9:I:406:ARG:HB3	9:I:501:GLU:OE2	1.91	0.70
11:D:2001:AGS:N3	11:D:2001:AGS:H2'	2.05	0.70
1:A:824:ASP:O	1:A:827:ASP:OD1	2.10	0.70
5:E:68:VAL:HG13	5:E:139:GLN:HB2	1.73	0.69
9:I:406:ARG:NH1	9:I:504:LYS:CD	2.20	0.68
9:I:400:ASN:CG	9:I:404:ARG:CG	2.61	0.68
9:I:402:SER:HA	9:I:501:GLU:HG3	1.75	0.67
9:I:402:SER:CA	9:I:501:GLU:HG3	2.24	0.67
4:D:83:ASP:O	4:D:87:LYS:HB2	1.95	0.66
7:G:6:DT:H71	8:H:79:DA:H61	1.59	0.66
9:I:399:ASN:O	9:I:400:ASN:ND2	2.21	0.66
9:I:406:ARG:HD3	9:I:504:LYS:CD	2.26	0.66
3:C:332:ASN:ND2	3:C:465:LEU:O	2.29	0.66
4:D:232:TYR:O	4:D:236:ASP:HB2	1.96	0.66
9:I:421:ILE:CG2	9:I:489:ILE:CG2	2.73	0.66
9:I:400:ASN:HB2	9:I:404:ARG:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LYS:HZ1	11:D:2001:AGS:PB	2.19	0.65
7:G:6:DT:C7	8:H:79:DA:H61	2.09	0.65
9:I:215:LYS:HE3	9:I:215:LYS:HA	1.79	0.65
9:I:409:LYS:HD2	9:I:414:GLN:HB3	1.79	0.65
5:E:82:GLN:HE22	5:E:97:TYR:H	1.43	0.64
9:I:400:ASN:CB	9:I:404:ARG:HG2	2.27	0.64
2:B:275:SER:O	2:B:279:ASN:ND2	2.30	0.64
2:B:294:PHE:O	2:B:298:LYS:HB2	1.98	0.64
9:I:502:MET:HG2	9:I:508:LEU:HB3	1.80	0.63
9:I:421:ILE:HG21	9:I:489:ILE:CG2	2.28	0.63
9:I:421:ILE:HG21	9:I:489:ILE:HG21	1.79	0.63
4:D:422:ILE:HG21	4:D:448:ILE:HD12	1.80	0.63
7:G:9:DA:C5	7:G:10:DC:N4	2.67	0.62
1:A:395:TYR:HH	1:A:549:TYR:HH	1.46	0.62
9:I:402:SER:CB	9:I:501:GLU:HG3	2.29	0.62
1:A:414:GLN:HB3	4:D:207:ILE:HD12	1.81	0.62
2:B:243:PHE:HB3	5:E:391:GLN:HE21	1.65	0.62
3:C:145:ARG:NH2	7:G:23:DT:OP1	2.32	0.61
9:I:212:TYR:CE2	9:I:213:HIS:CD2	2.86	0.61
9:I:406:ARG:HD3	9:I:504:LYS:HD2	1.82	0.61
9:I:406:ARG:CZ	9:I:504:LYS:HD2	2.26	0.61
3:C:384:LYS:HE3	3:C:386:ARG:HB2	1.81	0.61
9:I:406:ARG:O	9:I:410:LEU:N	2.31	0.61
7:G:9:DA:C2	8:H:78:DA:C2	2.89	0.60
9:I:393:VAL:O	9:I:397:PHE:CD2	2.41	0.60
9:I:400:ASN:HB2	9:I:404:ARG:CB	2.31	0.60
2:B:315:LEU:HD11	2:B:456:THR:HG23	1.84	0.60
9:I:304:MET:HG3	9:I:306:SER:H	1.64	0.60
9:I:212:TYR:CZ	9:I:213:HIS:CD2	2.87	0.60
4:D:286:ASP:OD1	4:D:289:ARG:NH1	2.35	0.59
9:I:406:ARG:CD	9:I:504:LYS:HE2	2.31	0.59
1:A:501:ALA:O	1:A:503:ARG:NH1	2.36	0.59
1:A:729:TYR:OH	4:D:84:ARG:NH2	2.36	0.59
9:I:406:ARG:HD3	9:I:504:LYS:HE3	1.82	0.59
5:E:142:ASP:OD1	5:E:142:ASP:N	2.34	0.59
8:H:76:DG:C2'	8:H:77:DT:OP2	2.41	0.58
9:I:237:GLN:O	9:I:241:THR:OG1	2.21	0.58
3:C:185:LEU:HB2	5:E:66:GLU:HB2	1.84	0.58
7:G:51:DG:N2	8:H:36:DC:O2	2.37	0.58
9:I:409:LYS:C	9:I:411:ASN:N	2.50	0.58
7:G:9:DA:C6	8:H:76:DG:O6	2.56	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:2001:AGS:O2B	11:D:2001:AGS:O2G	2.22	0.57
9:I:84:GLU:HB3	9:I:87:GLN:HB3	1.87	0.57
9:I:210:GLU:OE2	9:I:250:LYS:NZ	2.38	0.57
9:I:402:SER:CB	9:I:501:GLU:CB	2.62	0.57
1:A:485:LYS:NZ	11:D:2001:AGS:O1B	2.24	0.56
2:B:282:ASN:O	2:B:290:ARG:NH2	2.39	0.56
3:C:545:ARG:NH2	3:C:546:GLU:OE2	2.39	0.56
4:D:447:THR:OG1	4:D:448:ILE:N	2.39	0.56
9:I:394:PHE:O	9:I:398:VAL:HG23	2.06	0.56
1:A:612:LYS:NZ	9:I:263:ASN:OD1	2.38	0.56
2:B:261:HIS:HB2	3:C:536:ASN:HD21	1.72	0.55
3:C:17:ASP:OD1	3:C:20:ARG:NH2	2.40	0.55
9:I:400:ASN:OD1	9:I:404:ARG:HG2	2.06	0.55
6:F:334:GLU:O	6:F:338:LYS:NZ	2.39	0.55
3:C:217:ASP:HB2	3:C:255:THR:HG21	1.88	0.55
9:I:396:LYS:HE3	9:I:396:LYS:CA	2.36	0.55
9:I:406:ARG:CD	9:I:504:LYS:HD2	2.35	0.55
8:H:76:DG:C5	8:H:77:DT:C4	2.95	0.55
1:A:880:PHE:HE1	9:I:484:ARG:HD2	1.71	0.55
7:G:8:DT:C4	8:H:78:DA:N1	2.66	0.55
3:C:267:ASP:HB3	3:C:272:LYS:HE2	1.88	0.55
5:E:280:GLU:OE2	5:E:283:ALA:N	2.40	0.55
4:D:318:SER:OG	4:D:319:ASN:N	2.40	0.54
5:E:38:TYR:O	5:E:43:LYS:NZ	2.40	0.54
9:I:401:ASN:HD22	9:I:497:GLU:CD	2.09	0.54
4:D:95:SER:HA	4:D:245:VAL:O	2.08	0.54
5:E:11:ARG:NH1	5:E:190:PRO:O	2.37	0.54
4:D:498:PRO:HD3	5:E:453:ASN:HB2	1.90	0.54
9:I:392:LYS:O	9:I:396:LYS:HB2	2.07	0.54
2:B:395:TYR:O	3:C:145:ARG:NH1	2.40	0.54
4:D:104:ARG:NH1	11:D:2002:AGS:O3G	2.41	0.54
5:E:325:SER:OG	5:E:326:ILE:N	2.41	0.54
2:B:421:ILE:HG22	2:B:451:ALA:HB3	1.90	0.54
8:H:76:DG:H2''	8:H:77:DT:C7	2.35	0.54
3:C:431:LEU:HB2	3:C:436:LEU:HD13	1.89	0.53
9:I:390:ILE:HA	9:I:393:VAL:HG12	1.89	0.53
1:A:431:ASN:O	1:A:639:ARG:NH2	2.41	0.53
5:E:322:TYR:HB2	5:E:462:ILE:HD11	1.90	0.53
4:D:53:GLN:NE2	4:D:345:VAL:O	2.37	0.53
1:A:839:ASN:HB3	1:A:842:VAL:HG12	1.91	0.53
1:A:886:ASN:HB3	1:A:889:ILE:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:302:ILE:HG23	6:F:323:LEU:HD13	1.90	0.53
9:I:400:ASN:OD1	9:I:404:ARG:CG	2.56	0.53
3:C:357:CYS:HG	3:C:359:THR:HG1	1.55	0.53
3:C:529:ARG:HH12	6:F:371:GLU:HB2	1.74	0.53
1:A:514:ASN:HB3	1:A:517:LYS:HB2	1.91	0.53
3:C:74:HIS:O	3:C:78:ASN:HB2	2.09	0.53
2:B:308:LEU:HD22	2:B:451:ALA:HB1	1.91	0.53
4:D:500:ASP:OD1	4:D:500:ASP:N	2.34	0.53
5:E:14:GLN:O	5:E:18:LEU:HB2	2.08	0.53
3:C:409:VAL:HG13	3:C:453:LEU:HD22	1.91	0.52
7:G:12:DG:N2	8:H:75:DT:O2	2.41	0.52
1:A:470:ASP:HB3	1:A:592:LYS:HD3	1.92	0.52
2:B:317:TYR:HE1	2:B:477:PHE:HB3	1.73	0.52
4:D:387:GLU:HB3	4:D:463:LEU:HD11	1.92	0.52
1:A:364:ASN:OD1	5:E:101:GLN:NE2	2.43	0.52
9:I:390:ILE:O	9:I:394:PHE:HB2	2.10	0.52
3:C:112:SER:HB2	3:C:206:LYS:HD2	1.90	0.52
4:D:59:GLN:HG2	4:D:64:LEU:HD11	1.90	0.52
1:A:406:PHE:HB3	4:D:187:LEU:HD13	1.92	0.52
3:C:542:ILE:HD12	3:C:545:ARG:HH21	1.75	0.52
9:I:434:ASP:O	9:I:438:ASP:N	2.42	0.52
1:A:867:ASP:OD1	1:A:867:ASP:N	2.43	0.51
9:I:401:ASN:HD22	9:I:497:GLU:HB2	1.60	0.51
9:I:432:THR:HG22	9:I:434:ASP:H	1.75	0.51
6:F:399:PHE:O	6:F:404:SER:OG	2.25	0.51
5:E:360:ARG:NH1	5:E:363:TYR:OH	2.44	0.51
4:D:400:ARG:NH1	4:D:414:GLU:OE1	2.34	0.51
5:E:60:VAL:HB	5:E:130:LEU:HA	1.93	0.51
3:C:495:GLU:HG2	6:F:384:ILE:HD11	1.92	0.51
11:E:2001:AGS:O2A	11:E:2001:AGS:O2B	2.28	0.51
9:I:395:SER:O	9:I:399:ASN:N	2.38	0.50
1:A:691:ILE:HG21	1:A:775:ILE:HG23	1.93	0.50
9:I:215:LYS:N	9:I:215:LYS:CE	2.73	0.50
1:A:551:LYS:HG2	1:A:552:ARG:HG2	1.94	0.50
1:A:576:GLN:NE2	1:A:608:GLN:O	2.44	0.50
7:G:6:DT:N3	8:H:80:DA:C2	2.80	0.50
9:I:396:LYS:HE3	9:I:396:LYS:O	2.12	0.50
1:A:562:VAL:HG12	1:A:594:ILE:HB	1.93	0.50
1:A:718:GLU:OE1	4:D:84:ARG:NH1	2.45	0.50
3:C:140:ARG:HB3	5:E:68:VAL:HG11	1.92	0.49
9:I:82:THR:OG1	9:I:296:MET:SD	2.69	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LYS:HB2	8:H:69:DA:H5''	1.93	0.49
8:H:76:DG:C4	8:H:77:DT:C4	3.00	0.49
3:C:385:ASN:O	3:C:389:GLU:HB2	2.12	0.49
4:D:90:ILE:HG23	4:D:127:PHE:HB3	1.94	0.49
1:A:412:THR:HG23	1:A:413:THR:HG22	1.92	0.49
3:C:593:ASN:OD1	3:C:593:ASN:N	2.46	0.49
4:D:97:SER:O	4:D:269:SER:OG	2.30	0.49
4:D:335:PRO:O	4:D:339:ASN:ND2	2.46	0.49
6:F:274:VAL:HG13	6:F:275:LYS:HD2	1.95	0.49
1:A:833:ILE:HG21	1:A:850:PHE:HE2	1.78	0.49
4:D:174:SER:O	4:D:183:LYS:NZ	2.42	0.49
9:I:240:ARG:HH12	9:I:244:GLU:HG3	1.76	0.49
1:A:567:GLU:OE2	11:D:2001:AGS:O2G	2.30	0.49
9:I:103:SER:HB2	9:I:281:LEU:HA	1.94	0.49
1:A:553:VAL:HB	1:A:558:LYS:HD3	1.94	0.48
1:A:797:LEU:O	4:D:332:ARG:NH2	2.46	0.48
8:H:78:DA:C2	8:H:79:DA:C4	3.01	0.48
9:I:314:PRO:HA	9:I:317:ILE:HB	1.94	0.48
9:I:400:ASN:CG	9:I:404:ARG:HG2	2.33	0.48
1:A:703:ALA:HB3	11:D:2001:AGS:C8	2.43	0.48
2:B:435:ASN:OD1	2:B:469:LYS:NZ	2.43	0.48
5:E:77:ILE:HG23	5:E:130:LEU:HD11	1.95	0.48
8:H:76:DG:C5	8:H:77:DT:O4	2.66	0.48
4:D:219:ILE:HG22	4:D:251:THR:HB	1.95	0.48
5:E:251:THR:OG1	5:E:252:GLY:N	2.46	0.48
3:C:554:LEU:O	3:C:558:ARG:NH1	2.46	0.48
5:E:438:ASN:HB3	5:E:441:ILE:HD13	1.95	0.48
6:F:416:ASP:OD1	6:F:416:ASP:N	2.44	0.48
9:I:313:GLN:OE1	9:I:383:GLY:N	2.46	0.48
7:G:9:DA:C4	7:G:10:DC:N4	2.82	0.48
1:A:481:PRO:HB3	11:D:2001:AGS:O3G	2.13	0.48
1:A:899:GLU:HG2	9:I:441:ILE:HG13	1.95	0.48
9:I:193:ASN:HD21	9:I:197:LEU:HB3	1.78	0.48
1:A:646:SER:OG	1:A:647:PHE:N	2.46	0.47
7:G:5:DT:H2''	7:G:6:DT:H5''	1.97	0.47
1:A:713:ALA:HB2	1:A:778:VAL:HG23	1.96	0.47
4:D:96:HIS:O	4:D:246:CYS:HA	2.15	0.47
9:I:388:ASN:HA	9:I:391:ALA:HB3	1.96	0.47
3:C:216:LEU:HD21	3:C:238:PHE:HE2	1.80	0.47
6:F:366:VAL:HA	6:F:369:VAL:HG12	1.96	0.47
3:C:598:LYS:HD2	5:E:446:PRO:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:150:LEU:HD13	4:D:187:LEU:HD23	1.97	0.47
5:E:230:ASP:HA	5:E:233:GLN:HG2	1.97	0.47
1:A:471:SER:OG	1:A:472:ALA:N	2.47	0.47
1:A:842:VAL:HA	1:A:845:ILE:HG22	1.96	0.47
2:B:267:PRO:HG2	3:C:577:ASP:HB3	1.95	0.47
2:B:277:VAL:HG11	3:C:579:VAL:HG23	1.97	0.47
2:B:321:SER:H	2:B:484:GLU:HB2	1.79	0.47
11:D:2002:AGS:H8	11:D:2002:AGS:PA	2.55	0.47
1:A:902:LYS:HB2	1:A:902:LYS:HE3	1.72	0.47
7:G:6:DT:N3	8:H:80:DA:H2	2.13	0.47
3:C:484:LYS:HE2	3:C:612:VAL:HG13	1.96	0.47
9:I:409:LYS:C	9:I:410:LEU:HG	2.35	0.47
11:I:601:AGS:O2A	11:I:601:AGS:O2B	2.33	0.47
4:D:105:GLN:HB3	4:D:335:PRO:HG2	1.97	0.46
5:E:356:ILE:HD11	6:F:368:LEU:HD13	1.98	0.46
1:A:427:LYS:NZ	1:A:715:GLU:OE1	2.39	0.46
3:C:34:LYS:HA	3:C:34:LYS:HD2	1.75	0.46
7:G:6:DT:H71	8:H:79:DA:C6	2.50	0.46
1:A:884:MET:HA	4:D:475:VAL:HA	1.96	0.46
2:B:331:ILE:HD11	2:B:362:ILE:HD11	1.97	0.46
7:G:8:DT:O4	8:H:78:DA:C2	2.55	0.46
5:E:153:ASN:ND2	5:E:164:ILE:O	2.49	0.46
7:G:9:DA:H2	8:H:78:DA:C2	2.31	0.46
5:E:435:THR:OG1	5:E:436:THR:N	2.49	0.46
9:I:325:ALA:HA	9:I:329:GLY:HA2	1.97	0.46
3:C:253:GLN:HE21	4:D:457:LYS:HD3	1.81	0.46
3:C:331:GLN:NE2	6:F:405:MET:O	2.49	0.46
6:F:400:ARG:NH2	6:F:408:THR:O	2.49	0.46
3:C:137:PRO:O	4:D:491:GLN:NE2	2.48	0.46
4:D:346:ALA:HB3	5:E:20:SER:HB2	1.98	0.46
9:I:198:GLN:NE2	9:I:204:HIS:O	2.47	0.46
9:I:393:VAL:HG23	9:I:397:PHE:CE2	2.43	0.46
9:I:409:LYS:HA	9:I:409:LYS:HD3	1.68	0.46
9:I:389:TYR:HA	9:I:392:LYS:HB3	1.97	0.45
1:A:568:LEU:HD22	1:A:597:ALA:HB1	1.99	0.45
3:C:315:GLN:HE22	3:C:319:LYS:HD2	1.81	0.45
9:I:496:ARG:HA	9:I:496:ARG:HD3	1.76	0.45
9:I:406:ARG:CB	9:I:501:GLU:OE2	2.63	0.45
4:D:423:ASN:OD1	4:D:447:THR:OG1	2.30	0.45
1:A:472:ALA:O	1:A:586:THR:OG1	2.34	0.45
3:C:572:THR:HG22	3:C:574:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:106:SER:O	4:D:106:SER:OG	2.28	0.45
7:G:6:DT:C4	8:H:81:DA:N1	2.84	0.45
9:I:393:VAL:HG22	9:I:397:PHE:CD2	2.44	0.45
5:E:134:GLY:H	5:E:169:THR:HB	1.82	0.45
9:I:214:LYS:C	9:I:215:LYS:HE3	2.37	0.45
9:I:409:LYS:HB3	9:I:415:LYS:HG3	1.99	0.45
3:C:488:GLU:HB3	3:C:614:ARG:HG3	1.98	0.45
8:H:80:DA:OP2	8:H:80:DA:C8	2.70	0.45
5:E:31:SER:O	5:E:32:ASN:ND2	2.51	0.44
9:I:417:ILE:HG22	9:I:440:TYR:HE2	1.81	0.44
3:C:60:LEU:HD21	3:C:338:ILE:HG12	1.98	0.44
3:C:292:LEU:HD13	3:C:468:LEU:HD21	1.99	0.44
11:D:2002:AGS:O2G	11:D:2002:AGS:O2B	2.35	0.44
3:C:386:ARG:NH2	3:C:389:GLU:OE2	2.51	0.44
9:I:299:ILE:HA	9:I:302:GLN:HG2	1.99	0.44
3:C:273:GLY:O	3:C:275:LYS:N	2.51	0.44
5:E:47:LEU:HB3	5:E:61:TRP:HH2	1.82	0.44
5:E:383:ILE:HD11	5:E:424:LEU:HD21	1.99	0.44
6:F:276:LYS:HB3	6:F:276:LYS:HE2	1.87	0.44
9:I:406:ARG:CD	9:I:504:LYS:CD	2.95	0.44
3:C:189:GLU:HG2	3:C:229:TYR:CZ	2.53	0.44
6:F:334:GLU:HA	6:F:337:ARG:HD2	1.99	0.44
3:C:240:ILE:HG22	3:C:242:THR:H	1.82	0.44
3:C:523:GLN:HE22	3:C:526:LYS:HE3	1.83	0.44
7:G:6:DT:H3	8:H:80:DA:H2	1.66	0.44
7:G:8:DT:H3	8:H:78:DA:H2	1.65	0.44
3:C:411:ARG:HA	3:C:414:GLU:HG3	2.00	0.43
4:D:302:VAL:HG22	4:D:306:ASN:HD21	1.83	0.43
7:G:9:DA:C2	8:H:78:DA:H2	2.35	0.43
7:G:8:DT:N3	8:H:79:DA:N3	2.66	0.43
9:I:406:ARG:CD	9:I:504:LYS:CE	2.79	0.43
3:C:365:GLU:HA	3:C:368:ILE:HD12	2.00	0.43
5:E:164:ILE:HD13	5:E:164:ILE:HA	1.88	0.43
6:F:327:CYS:HA	6:F:330:ILE:HG12	1.99	0.43
1:A:687:ASP:HA	1:A:690:GLU:HG2	2.01	0.43
4:D:340:SER:HB3	4:D:364:LEU:HD22	2.00	0.43
9:I:270:ARG:NH2	9:I:271:PHE:O	2.41	0.43
1:A:426:VAL:HG13	1:A:640:LEU:HD21	2.01	0.43
1:A:629:HIS:NE2	1:A:630:GLU:OE2	2.52	0.43
3:C:469:ASP:OD1	3:C:470:ASN:N	2.52	0.43
9:I:409:LYS:CD	9:I:414:GLN:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:GLN:HG2	1:A:864:ILE:HG13	2.01	0.43
2:B:237:SER:OG	2:B:248:ASP:OD2	2.36	0.43
1:A:861:LEU:HD12	4:D:376:LEU:HD23	2.01	0.43
3:C:217:ASP:HB3	3:C:251:LEU:HD22	2.00	0.43
1:A:774:HIS:CE1	1:A:777:HIS:HB2	2.54	0.42
11:D:2002:AGS:O2B	11:D:2002:AGS:O1A	2.37	0.42
3:C:518:ALA:HB3	3:C:523:GLN:HB2	2.01	0.42
4:D:522:MET:SD	4:D:522:MET:N	2.82	0.42
1:A:451:ALA:HB1	1:A:627:TYR:HE1	1.84	0.42
4:D:85:ILE:HD13	4:D:98:VAL:HG11	2.01	0.42
5:E:79:ARG:HG3	5:E:99:PRO:HG3	2.02	0.42
9:I:315:MET:SD	9:I:315:MET:N	2.92	0.42
3:C:447:LYS:HD3	3:C:447:LYS:HA	1.87	0.42
9:I:213:HIS:O	9:I:216:THR:OG1	2.36	0.42
9:I:251:LEU:HD23	9:I:251:LEU:HA	1.92	0.42
2:B:297:GLN:HG3	2:B:325:PHE:HE2	1.83	0.42
1:A:848:THR:HA	1:A:853:GLY:H	1.83	0.42
9:I:401:ASN:HD22	9:I:497:GLU:CB	2.23	0.42
2:B:238:SER:HB2	5:E:359:GLY:HA3	2.02	0.42
7:G:45:DC:H2''	7:G:46:DA:C8	2.55	0.42
9:I:323:LYS:HD2	9:I:323:LYS:HA	1.71	0.42
4:D:48:GLY:O	4:D:299:SER:OG	2.31	0.41
9:I:388:ASN:O	9:I:392:LYS:CA	2.68	0.41
9:I:399:ASN:C	9:I:400:ASN:ND2	2.67	0.41
1:A:639:ARG:HA	1:A:639:ARG:HD2	1.75	0.41
9:I:101:SER:OG	9:I:102:ASP:OD2	2.34	0.41
1:A:428:LYS:HA	1:A:428:LYS:HD3	1.88	0.41
3:C:138:ASN:OD1	3:C:138:ASN:N	2.54	0.41
3:C:465:LEU:HD21	6:F:412:LEU:HD11	2.03	0.41
4:D:112:LEU:HD23	4:D:112:LEU:HA	1.89	0.41
5:E:280:GLU:OE1	5:E:284:LEU:N	2.53	0.41
9:I:69:LEU:HG	9:I:70:VAL:HG22	2.02	0.41
1:A:796:ARG:HG2	4:D:279:GLN:HG3	2.02	0.41
8:H:40:DT:H2''	8:H:41:DG:N7	2.36	0.41
1:A:580:TYR:O	1:A:584:ASN:HB2	2.21	0.41
3:C:252:ARG:O	3:C:255:THR:OG1	2.34	0.41
4:D:446:ASN:N	4:D:446:ASN:OD1	2.53	0.41
9:I:211:PRO:HB2	9:I:214:LYS:O	2.21	0.41
2:B:381:ASP:HA	2:B:384:VAL:HG22	2.03	0.41
4:D:241:SER:OG	4:D:242:ARG:N	2.53	0.41
5:E:366:ARG:HD2	8:H:47:DC:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:108:GLY:H	9:I:114:LYS:HZ1	1.69	0.41
1:A:514:ASN:HA	1:A:566:ASP:HB3	2.02	0.41
1:A:879:LEU:HD12	1:A:879:LEU:HA	1.92	0.41
3:C:106:PHE:HD1	3:C:240:ILE:HD11	1.85	0.41
3:C:553:ILE:HA	3:C:556:PHE:HB3	2.02	0.41
1:A:473:THR:OG1	1:A:474:THR:N	2.53	0.41
8:H:80:DA:OP2	8:H:80:DA:H8	2.04	0.41
9:I:433:ILE:HG12	9:I:489:ILE:HD11	2.04	0.40
5:E:215:LEU:HA	5:E:270:VAL:HG11	2.03	0.40
5:E:228:THR:H	5:E:231:GLN:HB2	1.87	0.40
1:A:414:GLN:HA	4:D:208:THR:HG23	2.04	0.40
2:B:374:ASP:OD1	2:B:374:ASP:N	2.54	0.40
3:C:143:LEU:HD22	3:C:222:LEU:HD21	2.03	0.40
3:C:213:PHE:HB3	3:C:251:LEU:HD23	2.02	0.40
9:I:509:LYS:HA	9:I:509:LYS:HD2	1.80	0.40
2:B:238:SER:HA	5:E:357:ILE:HB	2.03	0.40
5:E:286:LYS:HA	5:E:286:LYS:HD2	1.90	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	A	485/914 (53%)	448 (92%)	37 (8%)	0	100	100
2	B	249/620 (40%)	228 (92%)	21 (8%)	0	100	100
3	C	580/616 (94%)	536 (92%)	44 (8%)	0	100	100
4	D	430/529 (81%)	404 (94%)	26 (6%)	0	100	100
5	E	446/479 (93%)	410 (92%)	36 (8%)	0	100	100
6	F	162/435 (37%)	150 (93%)	12 (7%)	0	100	100
9	I	366/513 (71%)	316 (86%)	48 (13%)	2 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2718/4106 (66%)	2492 (92%)	224 (8%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	410	LEU
9	I	211	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	A	437/813 (54%)	434 (99%)	3 (1%)	84	93
2	B	236/573 (41%)	236 (100%)	0	100	100
3	C	545/576 (95%)	544 (100%)	1 (0%)	93	98
4	D	405/488 (83%)	403 (100%)	2 (0%)	88	95
5	E	418/440 (95%)	417 (100%)	1 (0%)	93	98
6	F	157/406 (39%)	157 (100%)	0	100	100
9	I	342/470 (73%)	333 (97%)	9 (3%)	46	74
All	All	2540/3766 (67%)	2524 (99%)	16 (1%)	86	94

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

Mol	Chain	Res	Type
1	A	503	ARG
1	A	509	LEU
1	A	825	ILE
3	C	102	PHE
4	D	331	PHE
4	D	500	ASP
5	E	228	THR
9	I	215	LYS
9	I	216	THR

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Mol	Chain	Res	Type
9	I	389	TYR
9	I	392	LYS
9	I	396	LYS
9	I	403	THR
9	I	409	LYS
9	I	418	LEU
9	I	421	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	ASN
1	A	397	ASN
1	A	771	GLN
1	A	820	GLN
2	B	256	ASN
2	B	284	ASN
2	B	291	GLN
2	B	364	ASN
2	B	425	HIS
3	C	178	ASN
3	C	241	ASN
3	C	331	GLN
3	C	383	ASN
3	C	523	GLN
3	C	536	ASN
4	D	105	GLN
4	D	137	HIS
4	D	240	HIS
4	D	306	ASN
4	D	339	ASN
4	D	409	ASN
4	D	458	ASN
5	E	32	ASN
5	E	52	ASN
5	E	82	GLN
5	E	101	GLN
5	E	139	GLN
5	E	248	HIS
5	E	253	ASN
5	E	391	GLN
5	E	397	GLN

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Mol	Chain	Res	Type
6	F	290	ASN
9	I	99	HIS
9	I	193	ASN
9	I	213	HIS
9	I	313	GLN
9	I	401	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
11	AGS	D	2001	-	26,33,33	1.88	3 (11%)	26,52,52	1.62	4 (15%)
11	AGS	I	601	10	26,33,33	0.72	1 (3%)	26,52,52	1.09	2 (7%)
11	AGS	D	2002	10	26,33,33	0.83	1 (3%)	26,52,52	1.28	2 (7%)
11	AGS	E	2001	10	26,33,33	0.78	0	26,52,52	0.99	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
11	AGS	D	2001	-	-	7/17/38/38	0/3/3/3
11	AGS	I	601	10	-	5/17/38/38	0/3/3/3
11	AGS	D	2002	10	-	3/17/38/38	0/3/3/3
11	AGS	E	2001	10	-	3/17/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2001	AGS	PG-S1G	7.99	2.08	1.90
11	D	2001	AGS	C5-C4	2.42	1.47	1.40
11	D	2002	AGS	PG-S1G	2.12	1.95	1.90
11	D	2001	AGS	PG-O3G	-2.07	1.48	1.54
11	I	601	AGS	PG-S1G	2.04	1.95	1.90

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	2002	AGS	PA-O3A-PB	-5.32	114.58	132.83
11	D	2001	AGS	PA-O3A-PB	-4.17	118.51	132.83
11	I	601	AGS	PA-O3A-PB	-4.14	118.64	132.83
11	E	2001	AGS	PA-O3A-PB	-3.52	120.74	132.83
11	D	2001	AGS	C3'-C2'-C1'	3.38	106.07	100.98
11	D	2001	AGS	N3-C2-N1	-3.18	123.70	128.68
11	D	2001	AGS	C4-C5-N7	-2.59	106.70	109.40
11	D	2002	AGS	C5-C6-N6	2.35	123.92	120.35
11	I	601	AGS	C5-C6-N6	2.23	123.73	120.35
11	E	2001	AGS	C5-C6-N6	2.14	123.60	120.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	2001	AGS	PB-O3B-PG-O2G
11	D	2001	AGS	C5'-O5'-PA-O2A
11	D	2001	AGS	C5'-O5'-PA-O3A
11	D	2002	AGS	O4'-C4'-C5'-O5'
11	D	2002	AGS	C3'-C4'-C5'-O5'
11	I	601	AGS	C5'-O5'-PA-O1A
11	I	601	AGS	C5'-O5'-PA-O2A

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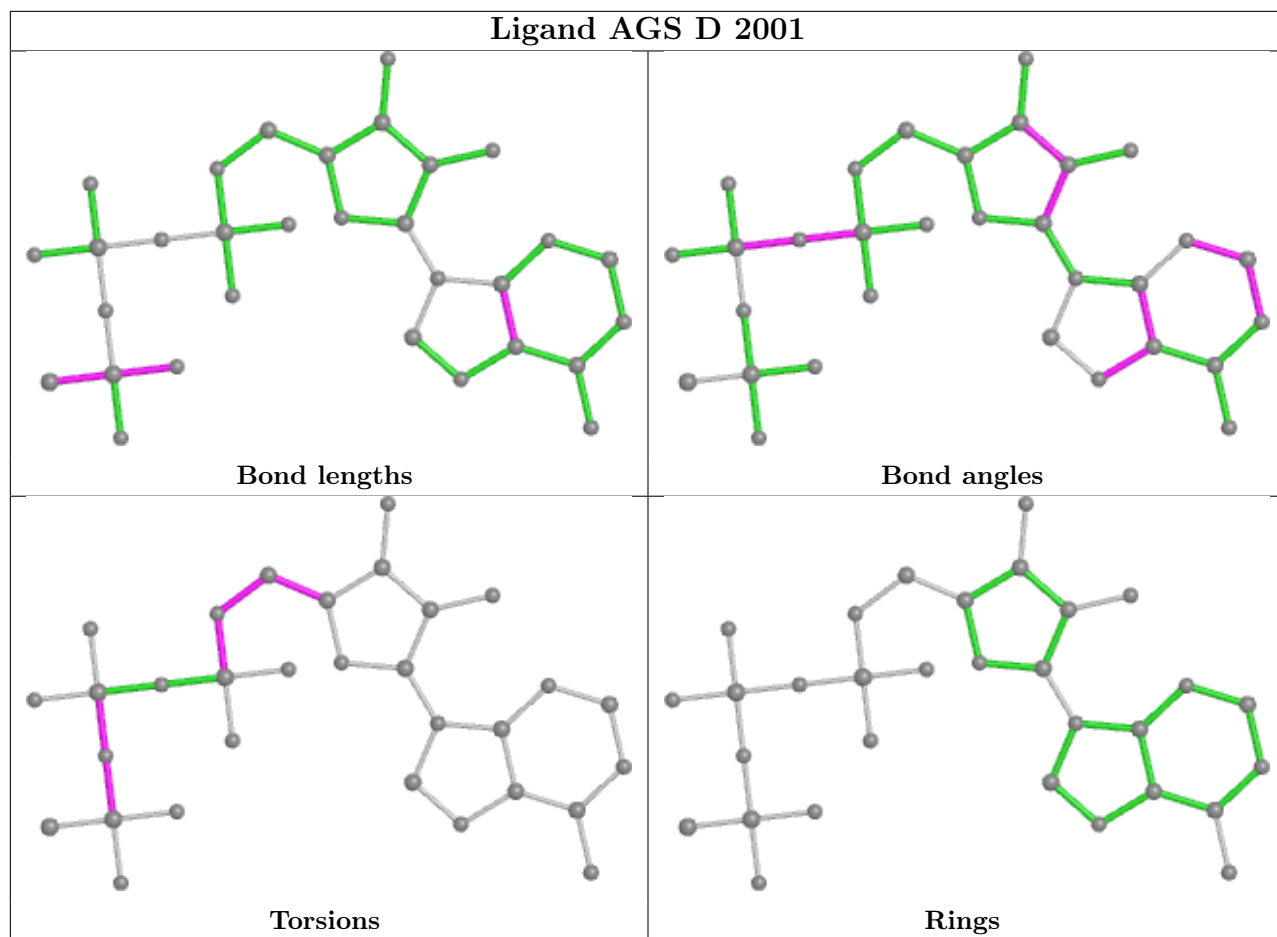
Mol	Chain	Res	Type	Atoms
11	I	601	AGS	C5'-O5'-PA-O3A
11	I	601	AGS	O4'-C4'-C5'-O5'
11	D	2002	AGS	PA-O3A-PB-O2B
11	E	2001	AGS	PB-O3A-PA-O2A
11	D	2001	AGS	PG-O3B-PB-O1B
11	I	601	AGS	C3'-C4'-C5'-O5'
11	D	2001	AGS	C4'-C5'-O5'-PA
11	D	2001	AGS	PG-O3B-PB-O2B
11	E	2001	AGS	O4'-C4'-C5'-O5'
11	E	2001	AGS	PB-O3A-PA-O1A
11	D	2001	AGS	C3'-C4'-C5'-O5'

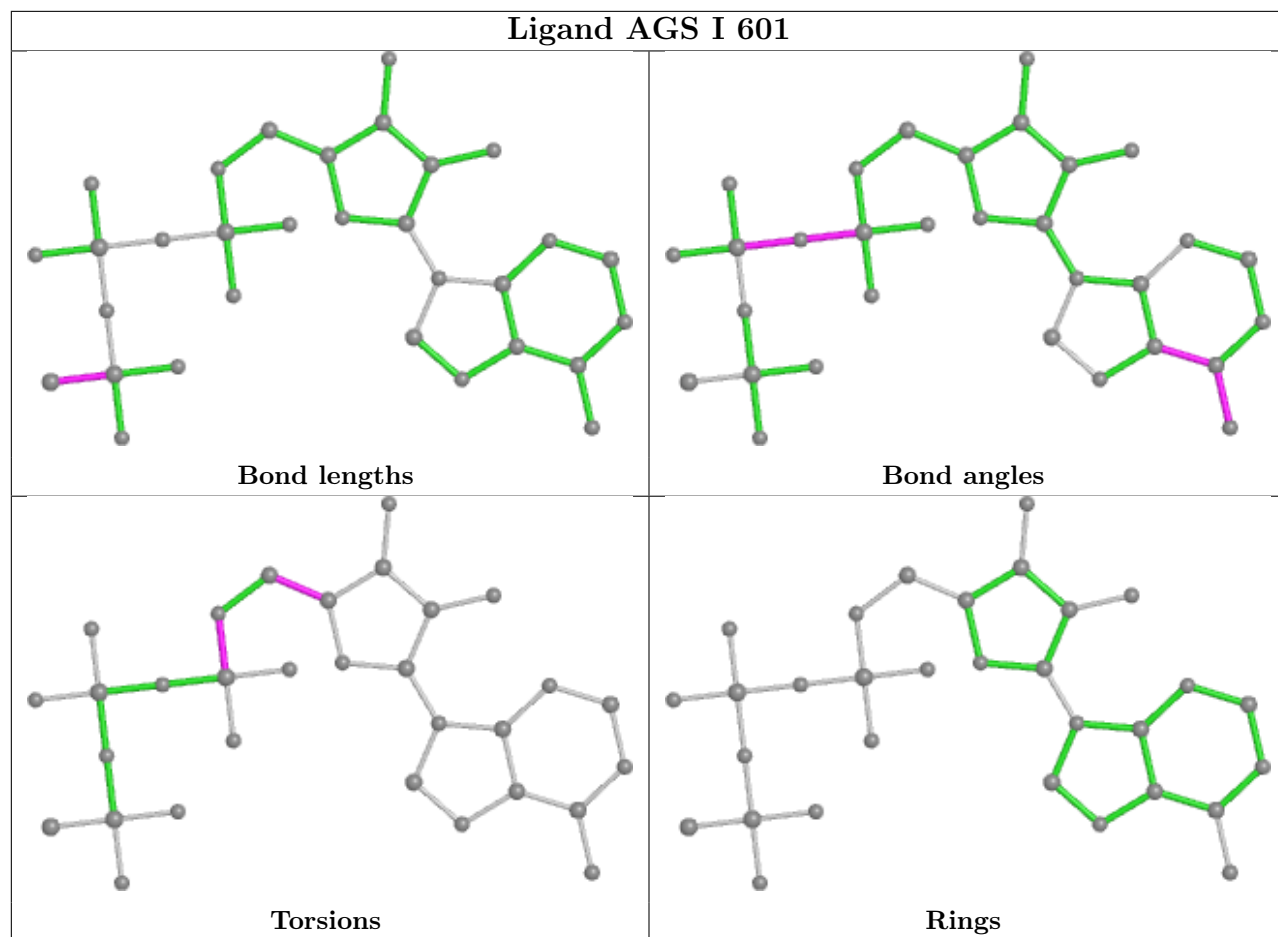
There are no ring outliers.

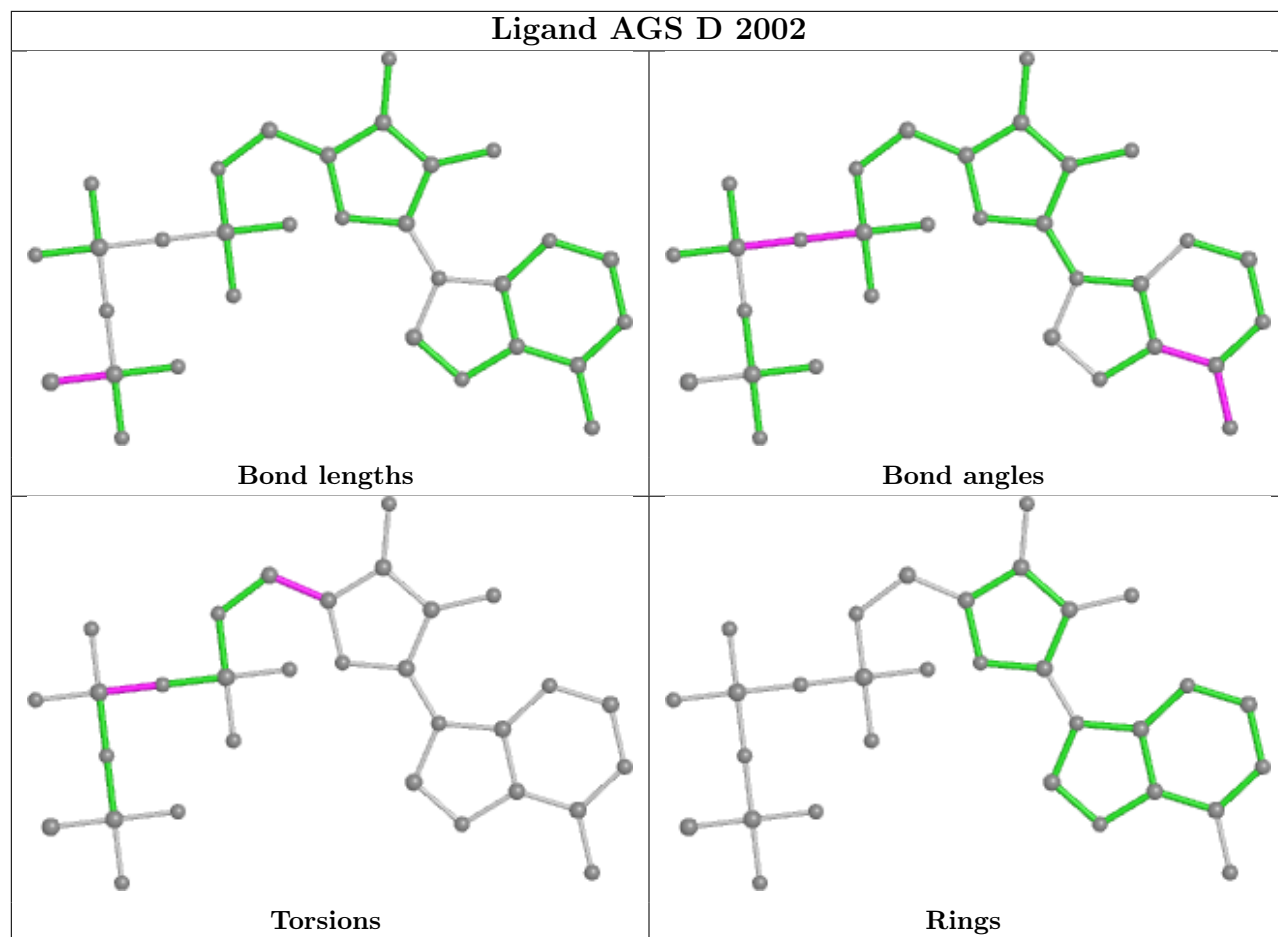
4 monomers are involved in 16 short contacts:

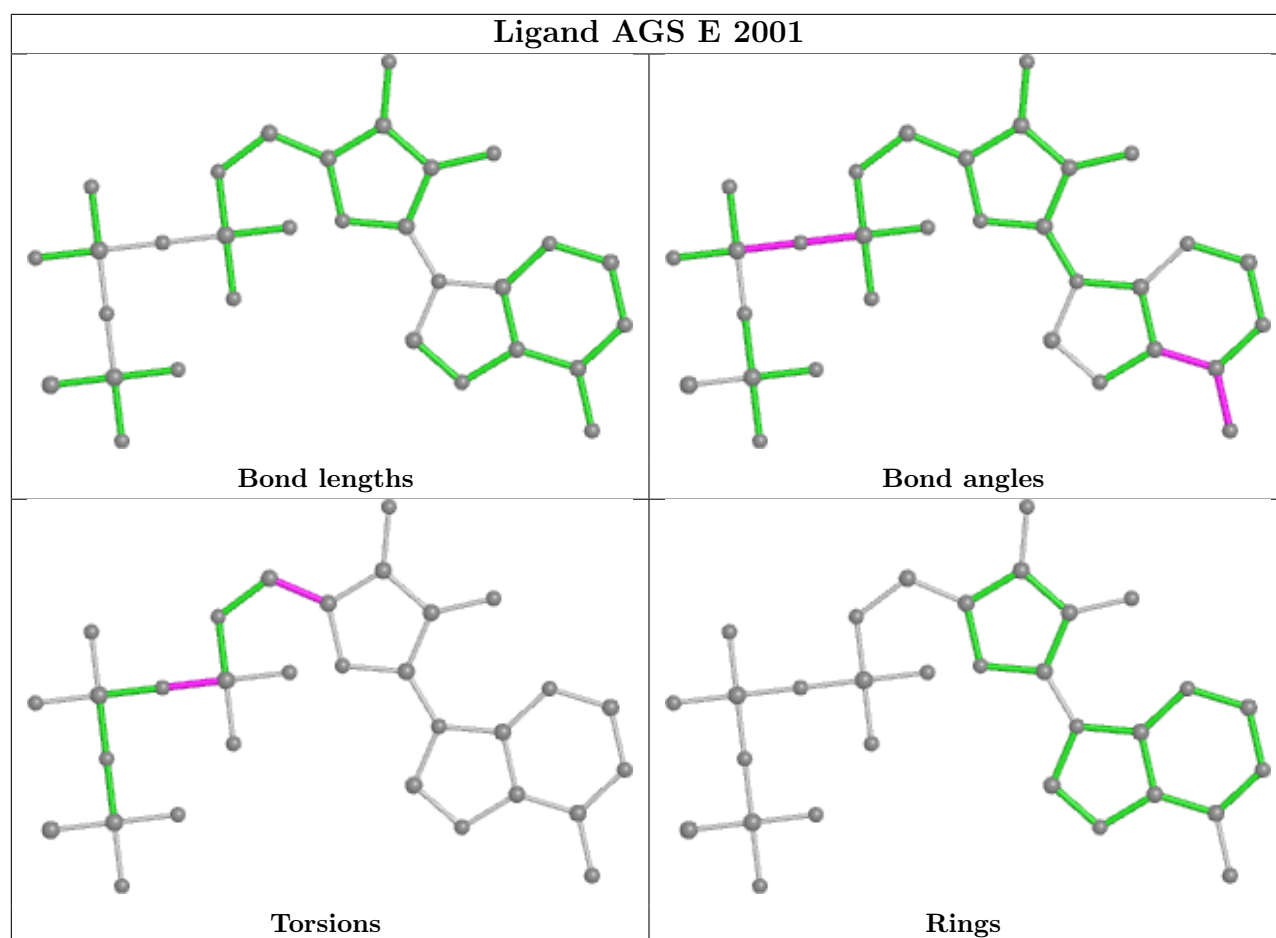
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2001	AGS	10	0
11	I	601	AGS	1	0
11	D	2002	AGS	4	0
11	E	2001	AGS	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

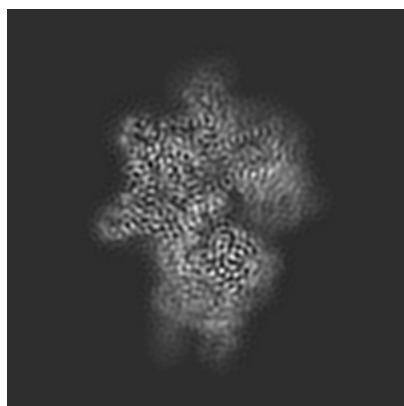
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23755. These allow visual inspection of the internal detail of the map and identification of artifacts.

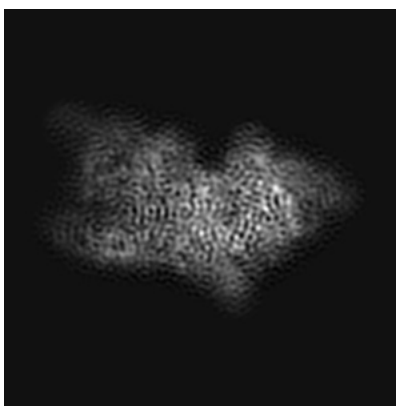
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

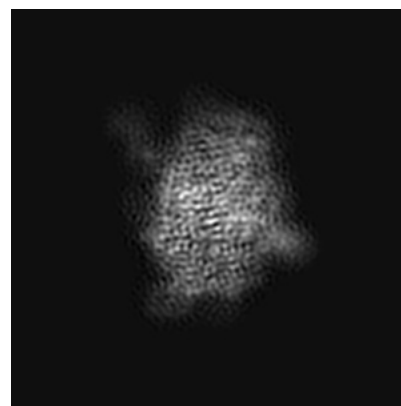
6.1.1 Primary map



X

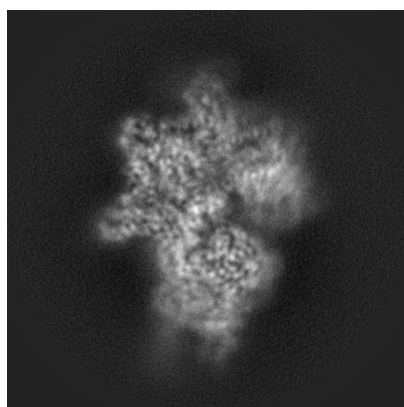


Y

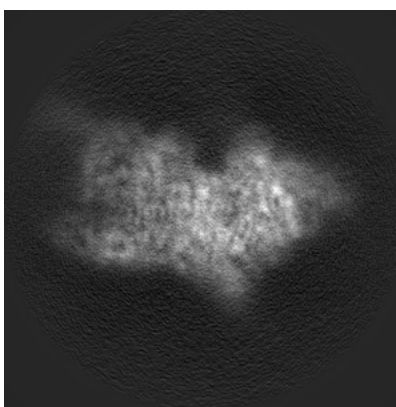


Z

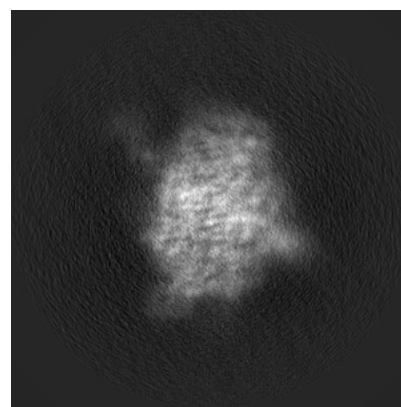
6.1.2 Raw map



X



Y

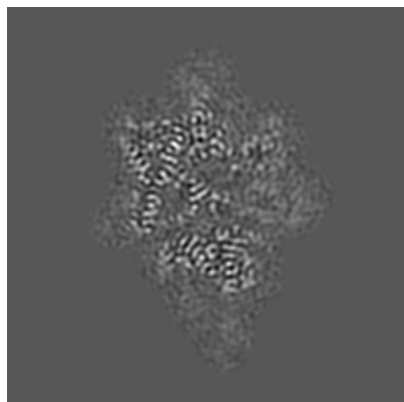


Z

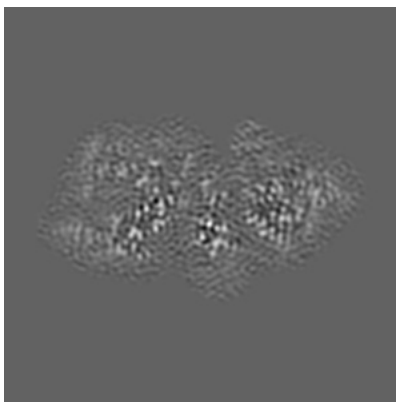
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

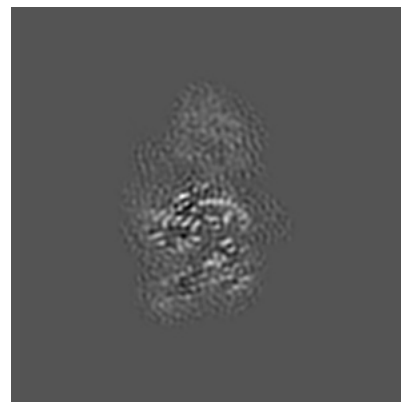
6.2.1 Primary map



X Index: 140

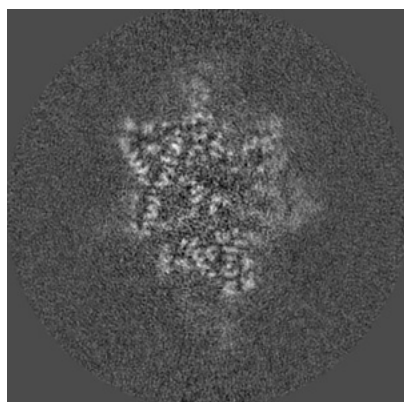


Y Index: 140

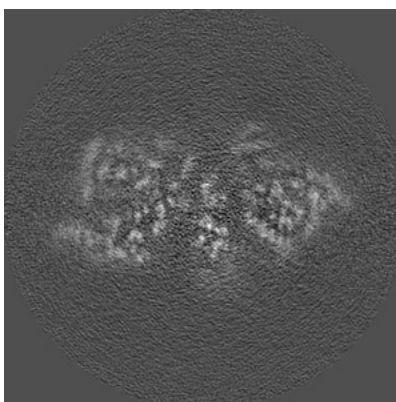


Z Index: 140

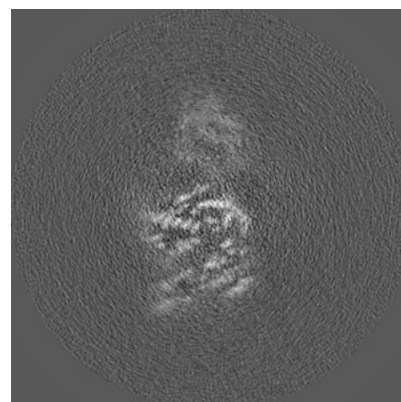
6.2.2 Raw map



X Index: 140



Y Index: 140

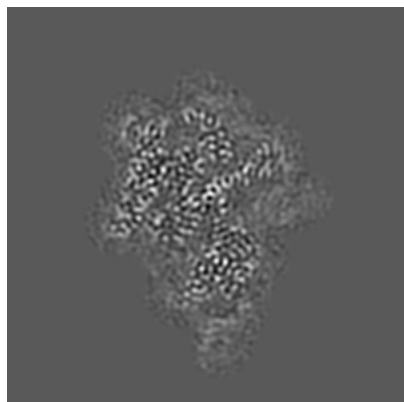


Z Index: 140

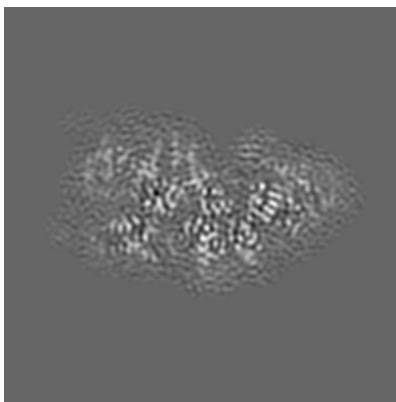
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 125

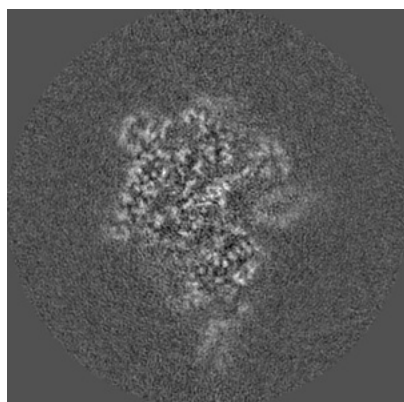


Y Index: 132

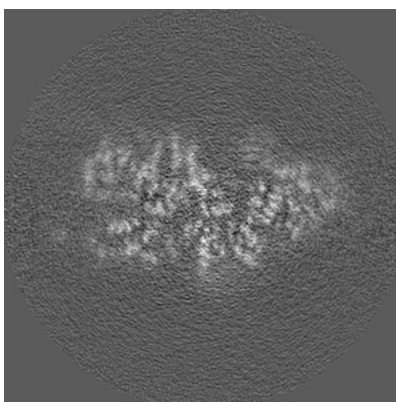


Z Index: 166

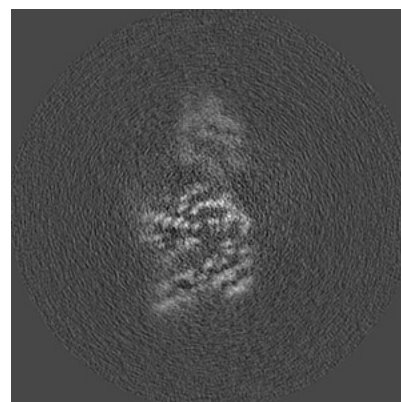
6.3.2 Raw map



X Index: 126



Y Index: 132

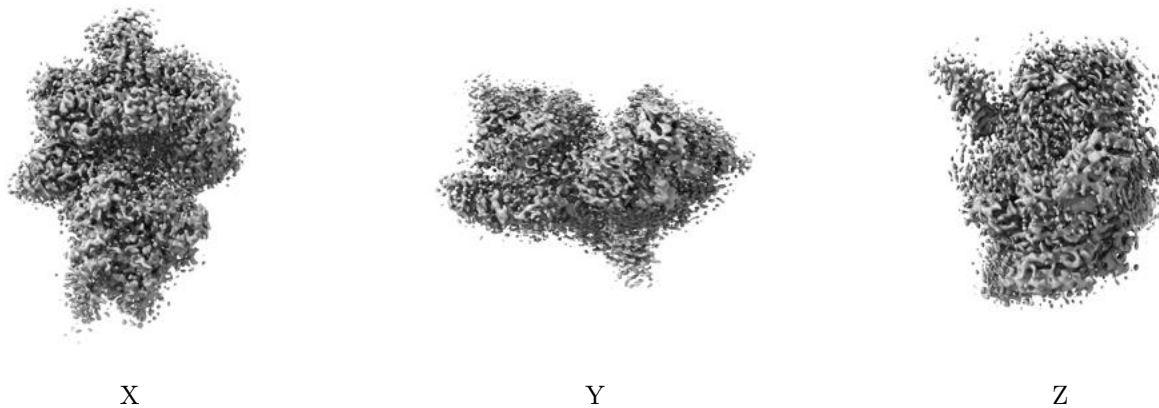


Z Index: 139

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

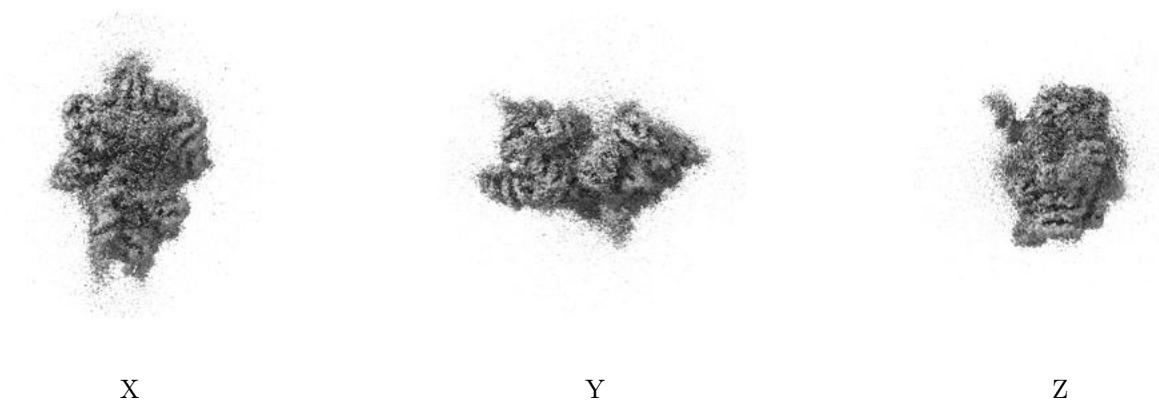
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

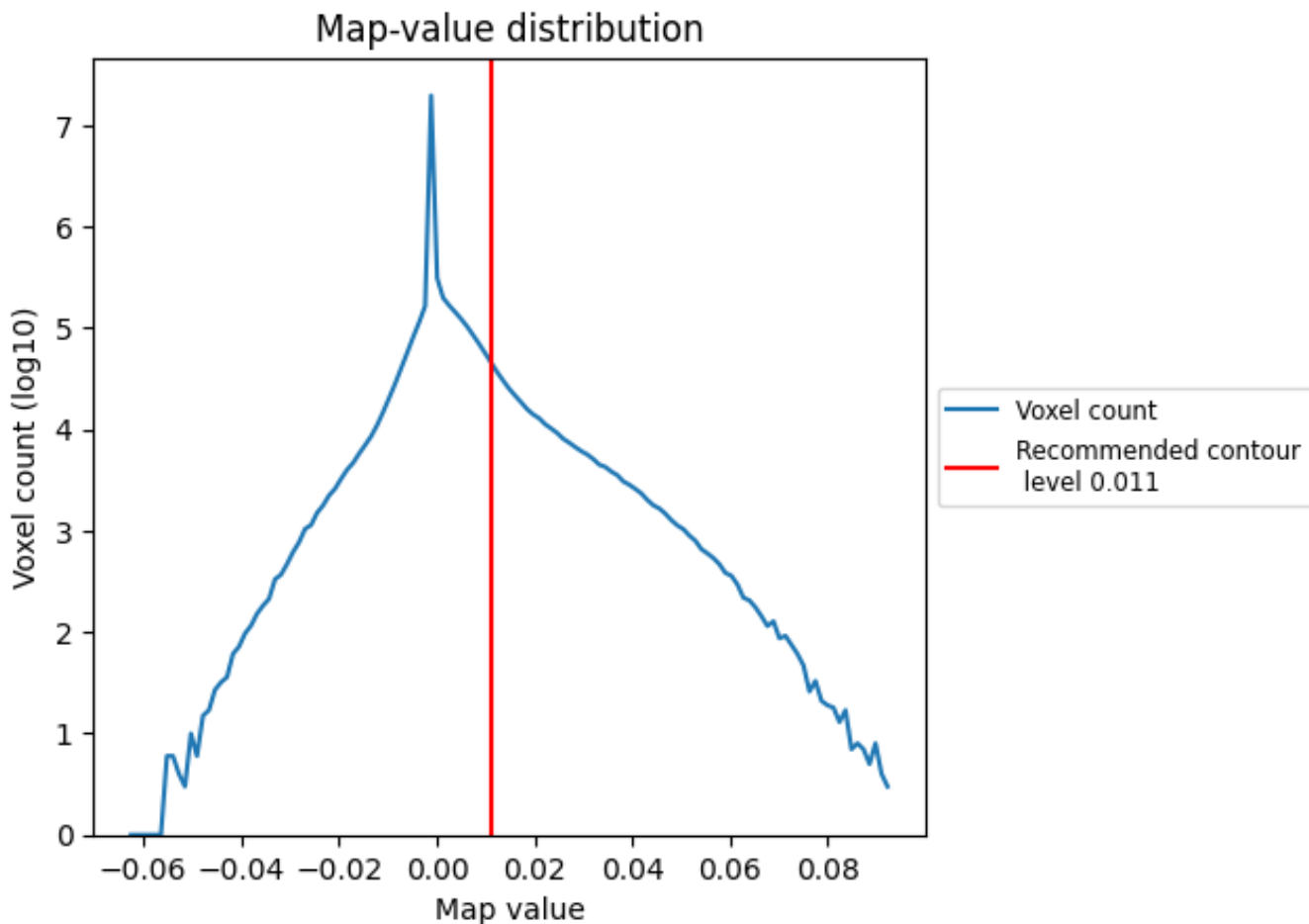
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

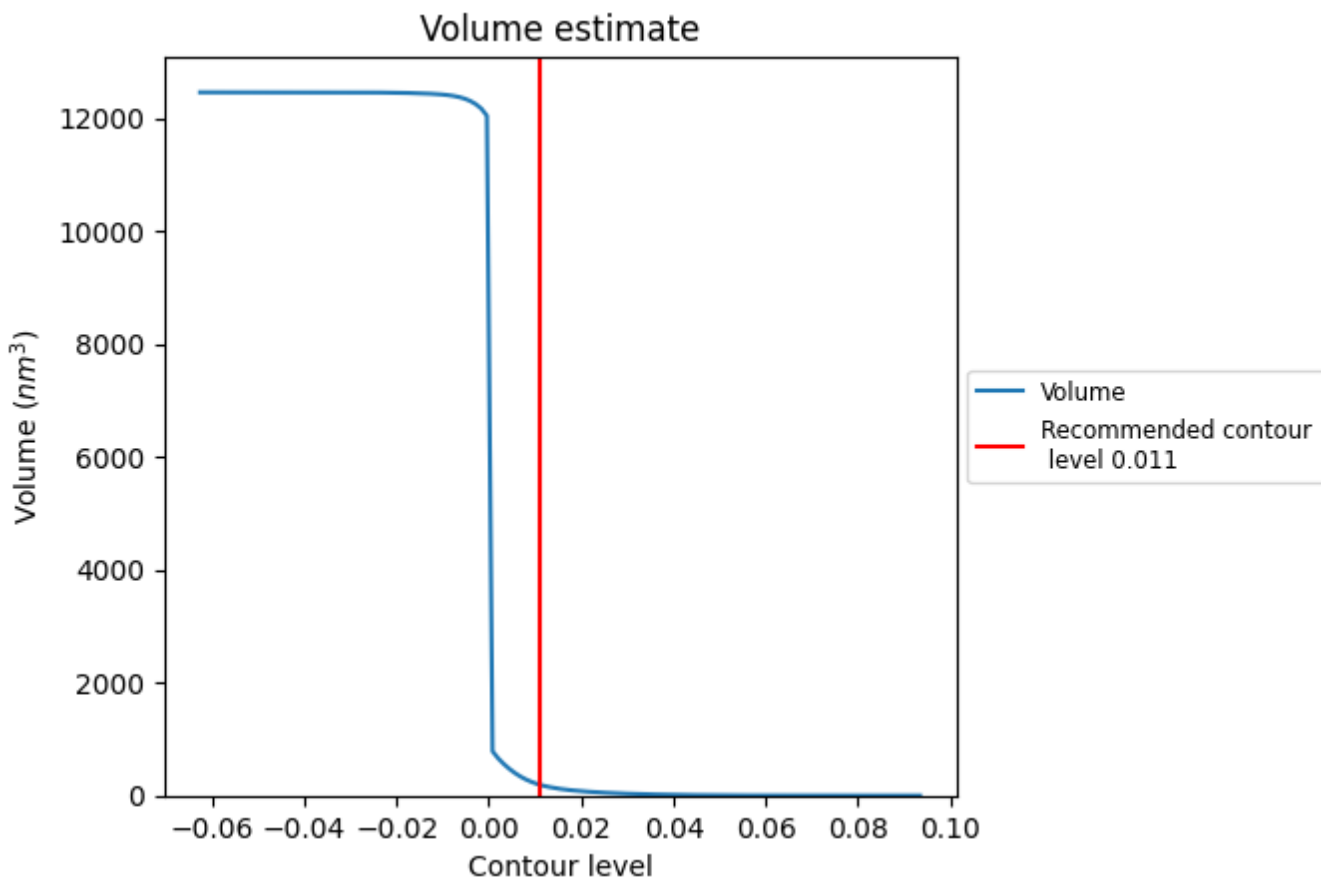
This section contains the results of statistical analysis of the map.

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.

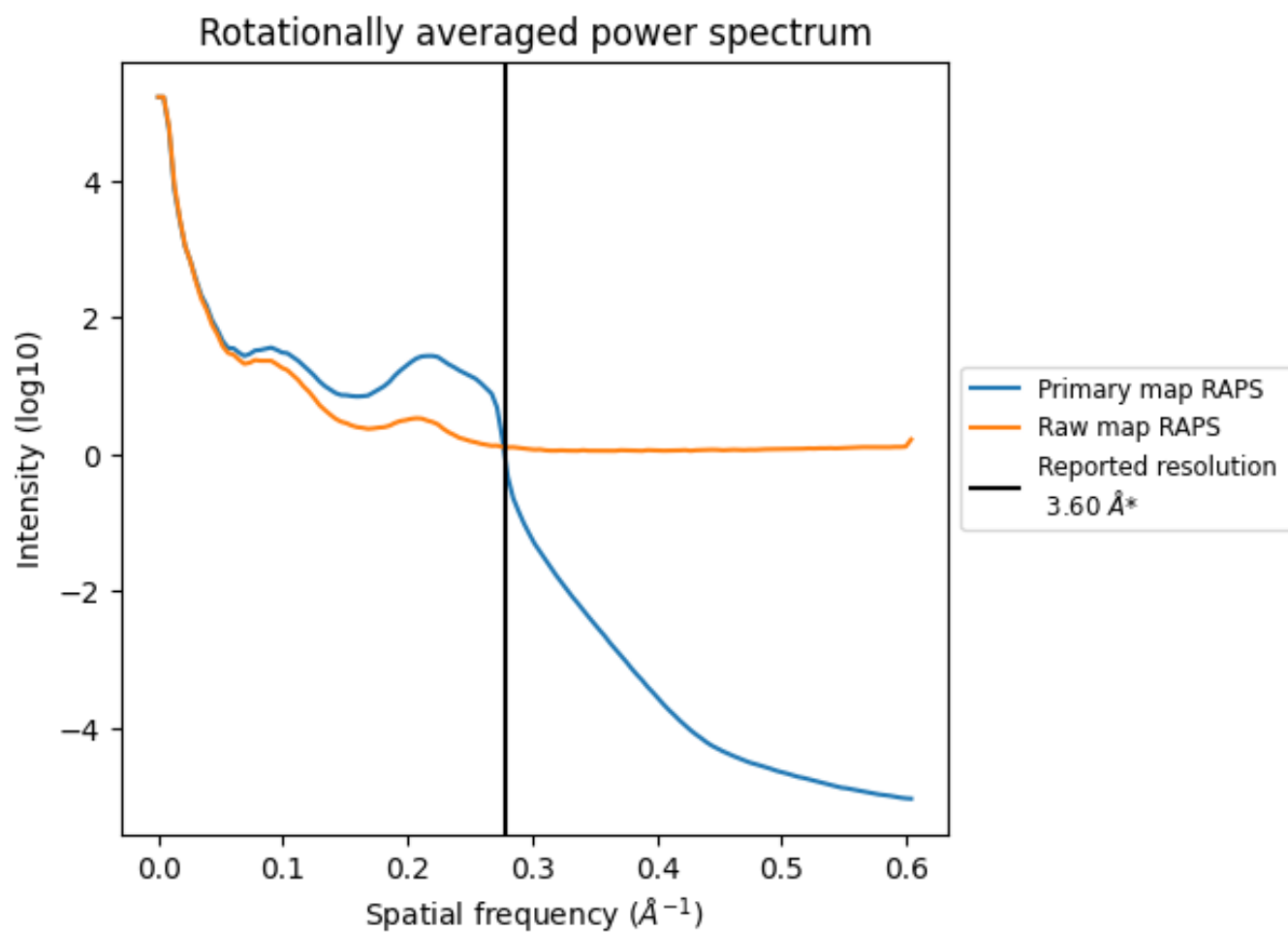
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 175 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](#)

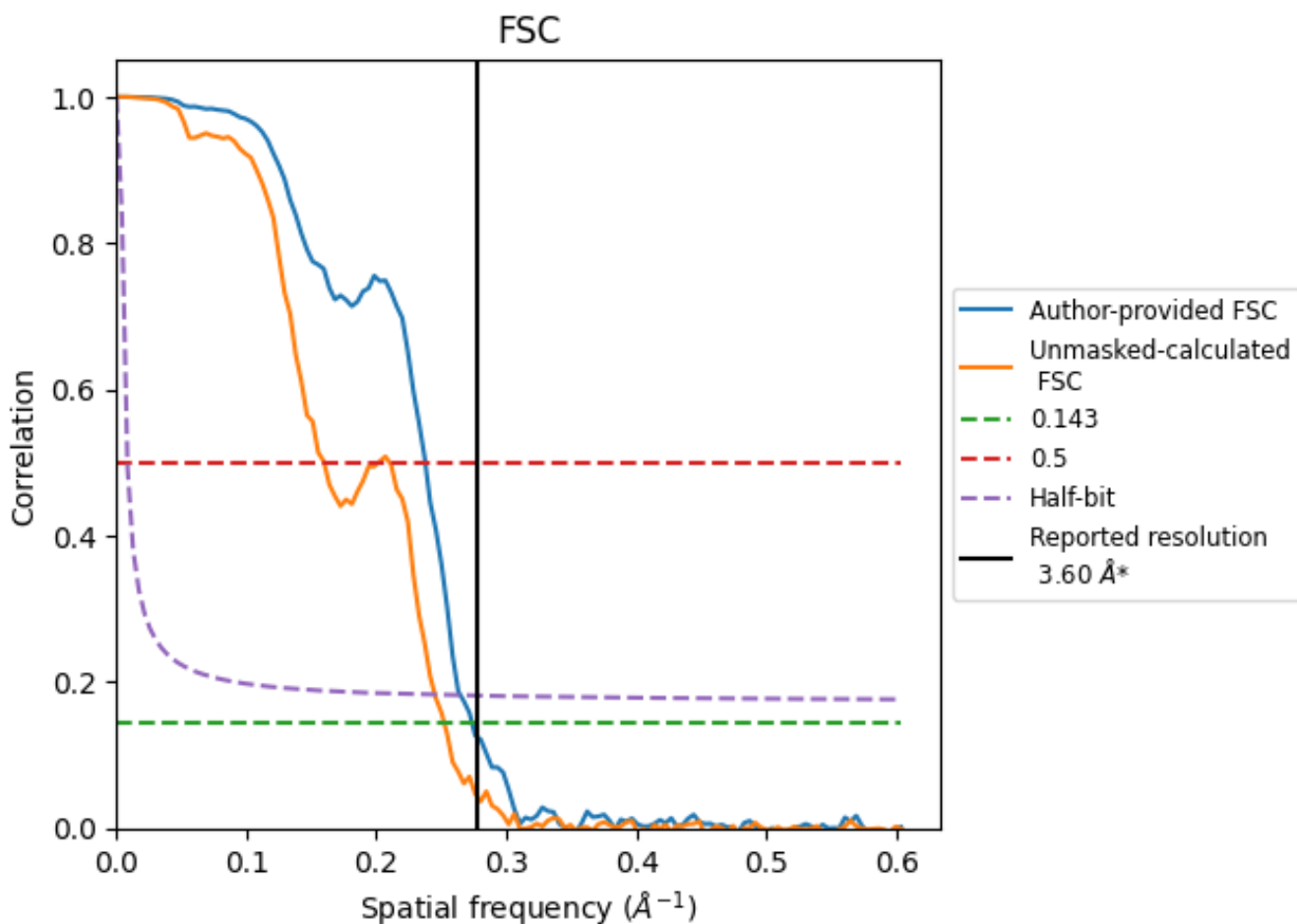


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

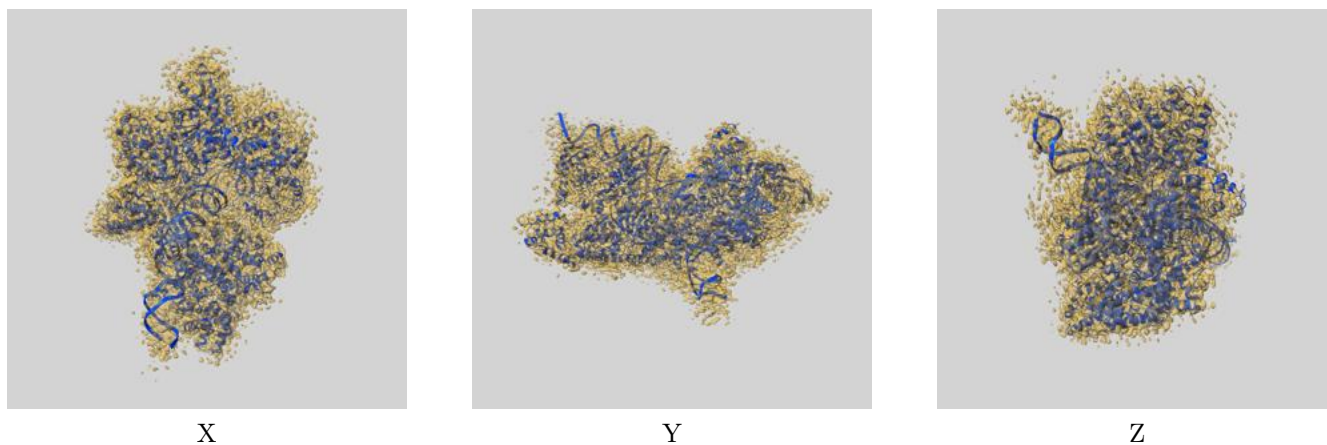
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.65	4.21	3.78
Unmasked-calculated*	3.96	6.26	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

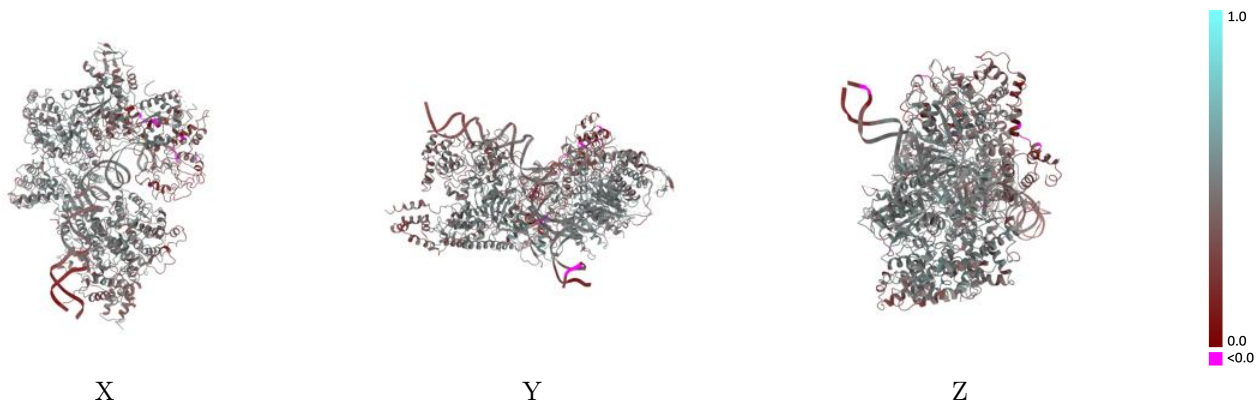
This section contains information regarding the fit between EMDB map EMD-23755 and PDB model 7MCA. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



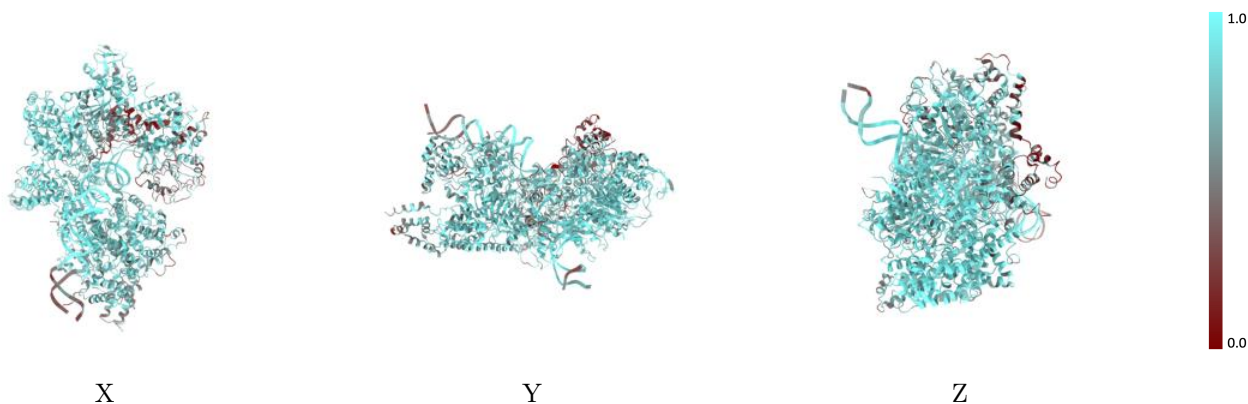
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



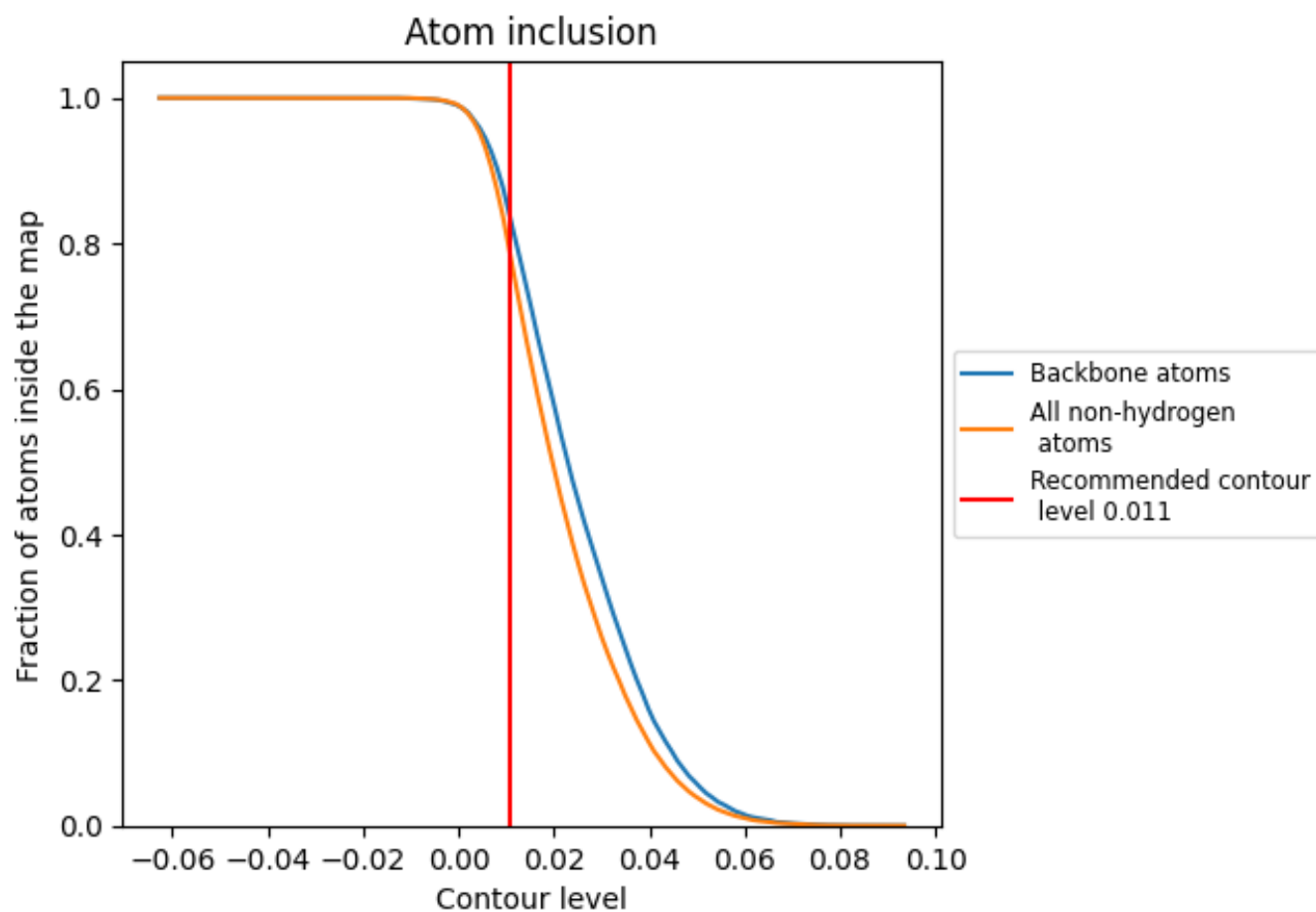
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.011).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7796	 0.4410
A	 0.8292	 0.4670
B	 0.8500	 0.4830
C	 0.7710	 0.4490
D	 0.8788	 0.4950
E	 0.8383	 0.4790
F	 0.7181	 0.4100
G	 0.7967	 0.3640
H	 0.8314	 0.3760
I	 0.4943	 0.3140

