



## Full wwPDB EM Validation Report ⓘ

Jul 7, 2025 – 04:39 PM EDT

PDB ID : 9OA2 / pdb\_00009oa2  
EMDB ID : EMD-70271  
Title : Ecoli DnaB helicase and Phage Lambda loader P with ADP-Mg in a 6:6 stoichiometry ratio.  
Authors : Shatarupa, A.; Brown, D.; Olinares, P.D.B.; Chase, J.; Isiorho, E.; Chait, B.T.; Jeruzalmi, D.  
Deposited on : 2025-04-18  
Resolution : 3.85 Å (reported)  
Based on initial models : ., 1B79, 8V9S

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

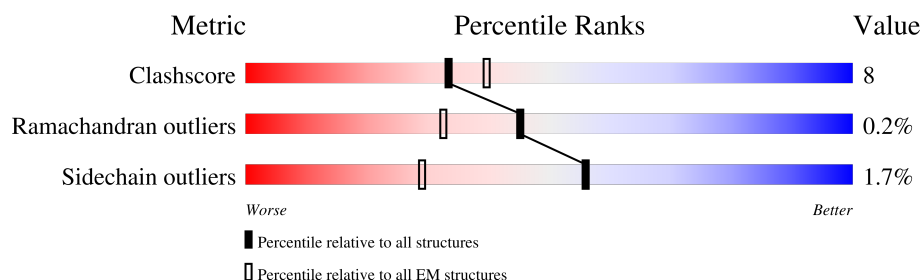
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.85 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	471	<div> <div>26%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>
1	B	471	<div> <div>37%</div> <div>76%</div> <div>18%</div> <div>6%</div> </div>
1	C	471	<div> <div>30%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>
1	D	471	<div> <div>42%</div> <div>74%</div> <div>20%</div> <div>6%</div> </div>
1	E	471	<div> <div>31%</div> <div>73%</div> <div>21%</div> <div>6%</div> </div>
1	F	471	<div> <div>27%</div> <div>76%</div> <div>18%</div> <div>6%</div> </div>
2	U	233	<div> <div>6%</div> <div>9%</div> <div>91%</div> </div>
2	V	233	<div> <div>44%</div> <div>40%</div> <div>9%</div> <div>51%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	W	233	<div><div><div></div><div></div><div></div></div><div>46%42%7%51%</div></div>
2	X	233	<div><div><div></div><div></div><div></div></div><div>7%9%90%</div></div>
2	Y	233	<div><div><div></div><div></div><div></div></div><div>47%38%10%51%</div></div>
2	Z	233	<div><div><div></div><div></div><div></div></div><div>44%41%7%52%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24938 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 Replicative DNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	445	Total	C	N	O	S	0	0
			3474	2158	620	683	13		
1	B	445	Total	C	N	O	S	0	0
			3474	2158	620	683	13		
1	C	445	Total	C	N	O	S	0	0
			3474	2158	620	683	13		
1	D	445	Total	C	N	O	S	0	0
			3474	2158	620	683	13		
1	E	445	Total	C	N	O	S	0	0
			3474	2158	620	683	13		
1	F	445	Total	C	N	O	S	0	0
			3474	2158	620	683	13		

- Molecule 2 is a protein called Helicase loader.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	22	Total	C	N	O		0	0
			160	102	31	27			
2	V	114	Total	C	N	O	S	0	0
			901	570	165	161	5		
2	W	114	Total	C	N	O	S	0	0
			901	570	165	161	5		
2	X	23	Total	C	N	O		0	0
			168	108	32	28			
2	Y	114	Total	C	N	O	S	0	0
			901	570	165	161	5		
2	Z	113	Total	C	N	O	S	0	0
			895	567	164	159	5		

There are 6 discrepancies between the modelled and reference sequences:

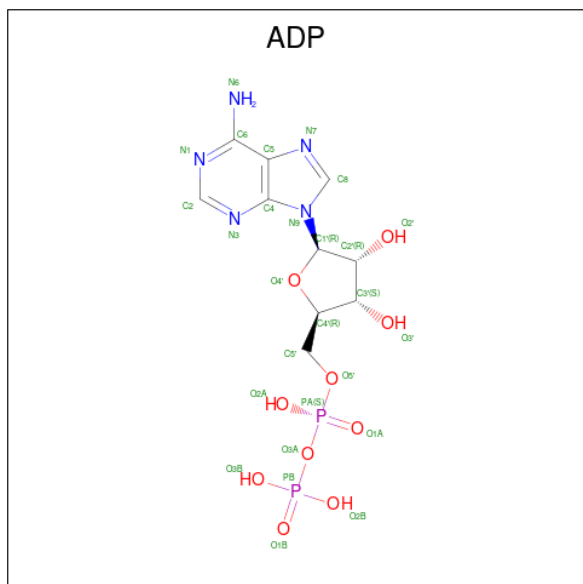
Chain	Residue	Modelled	Actual	Comment	Reference
U	2	GLU	LYS	engineered mutation	UNP P03689
V	2	GLU	LYS	engineered mutation	UNP P03689

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
W	2	GLU	LYS	engineered mutation	UNP P03689
X	2	GLU	LYS	engineered mutation	UNP P03689
Y	2	GLU	LYS	engineered mutation	UNP P03689
Z	2	GLU	LYS	engineered mutation	UNP P03689

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

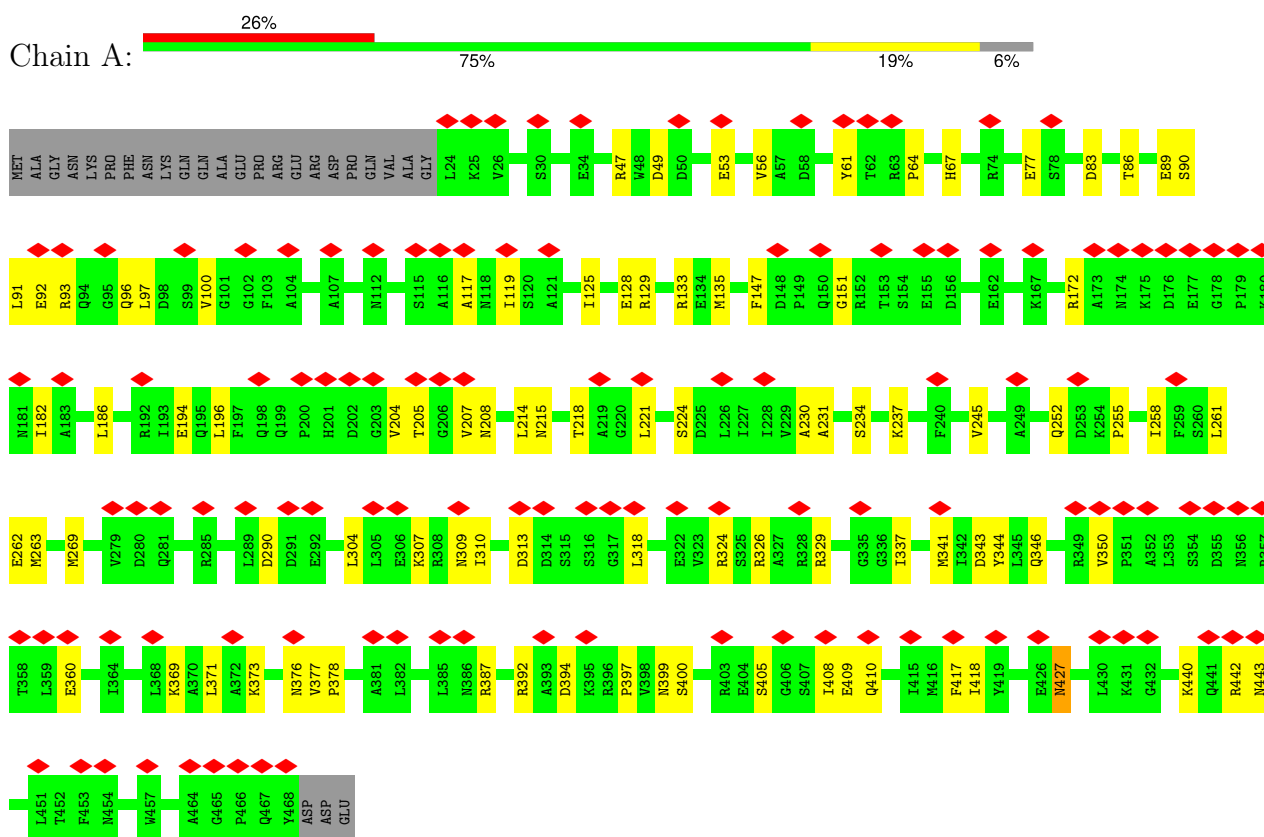
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Mg 1	0
4	B	1	Total 1	Mg 1	0
4	C	1	Total 1	Mg 1	0
4	D	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0

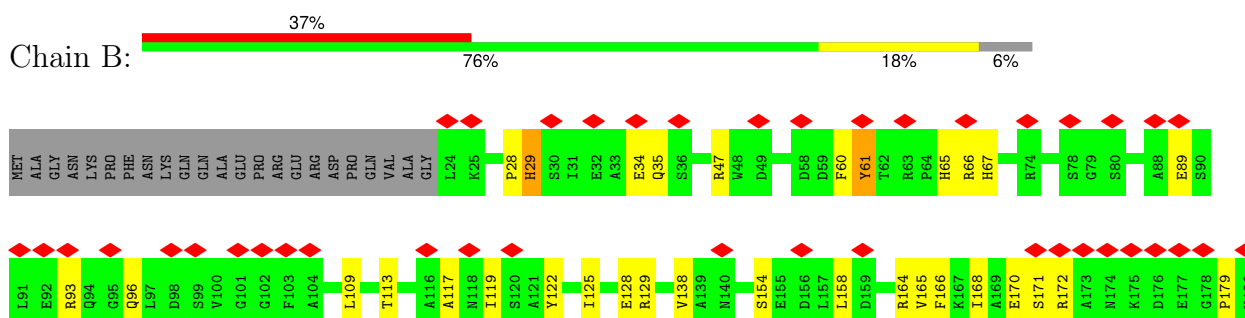
### 3 Residue-property plots

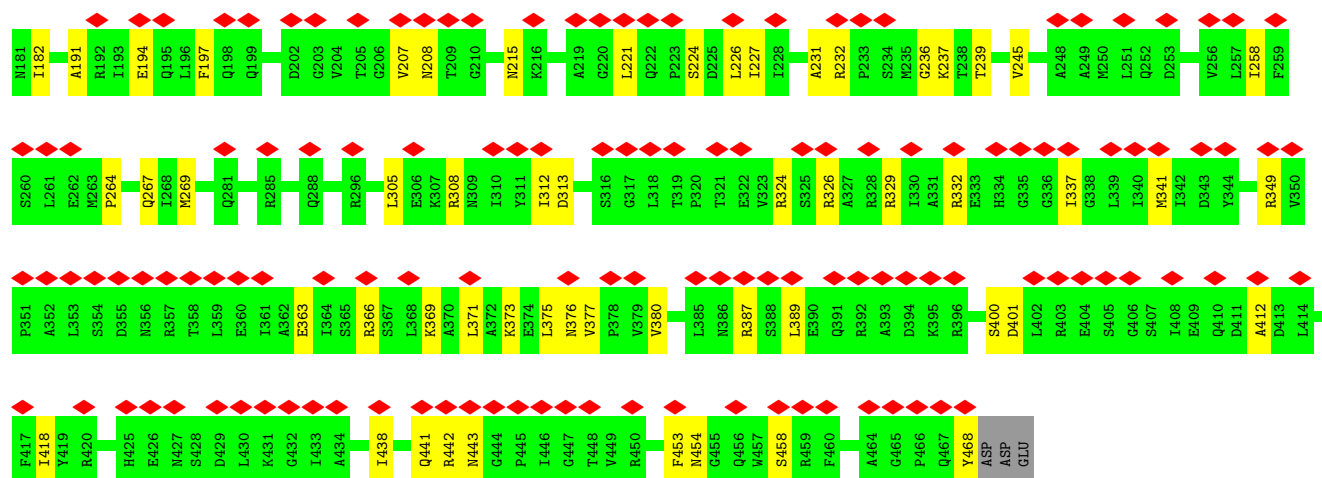
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Replicative DNA helicase

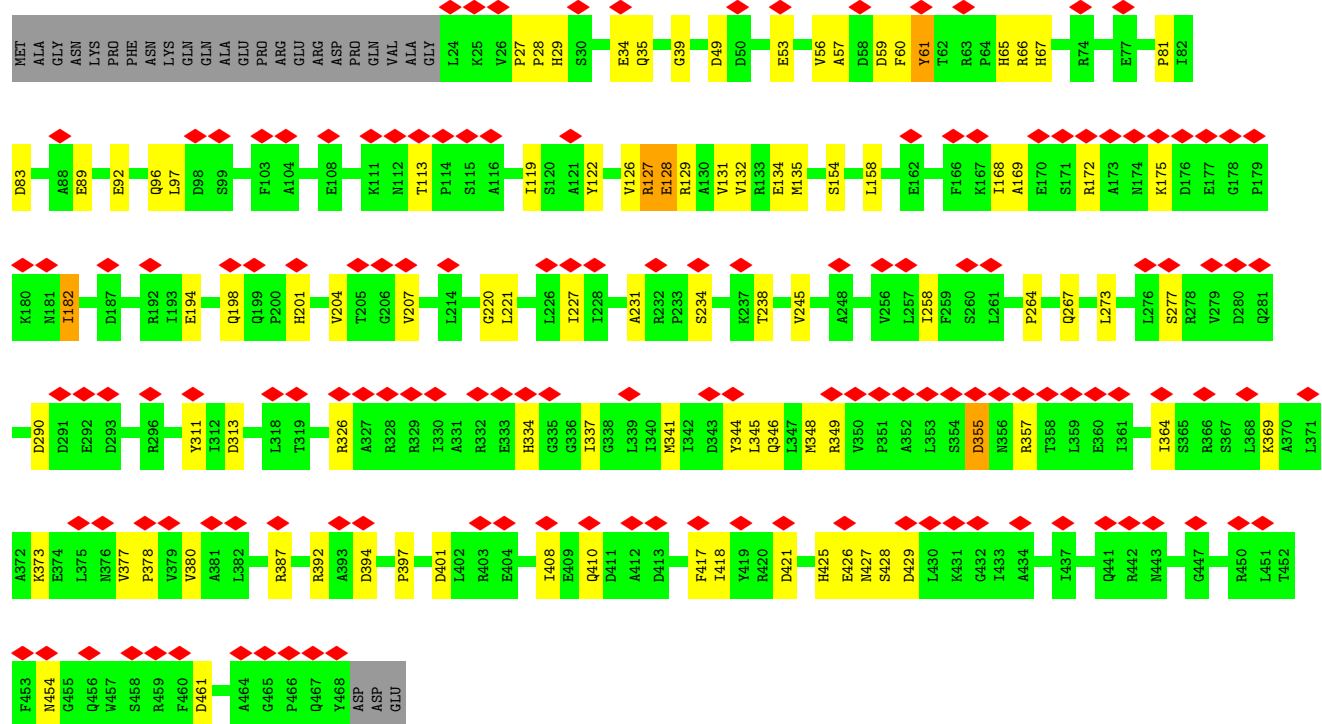
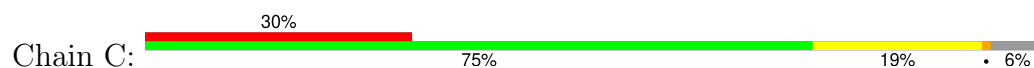


#### • Molecule 1: Replicative DNA helicase

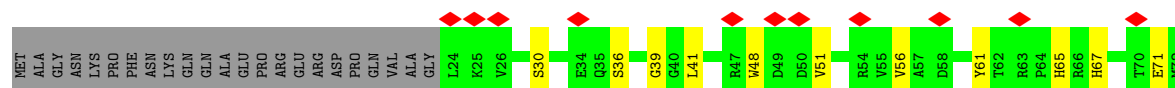
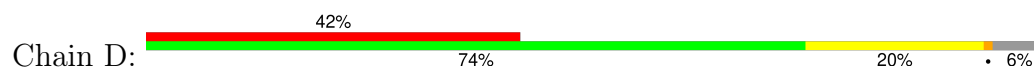




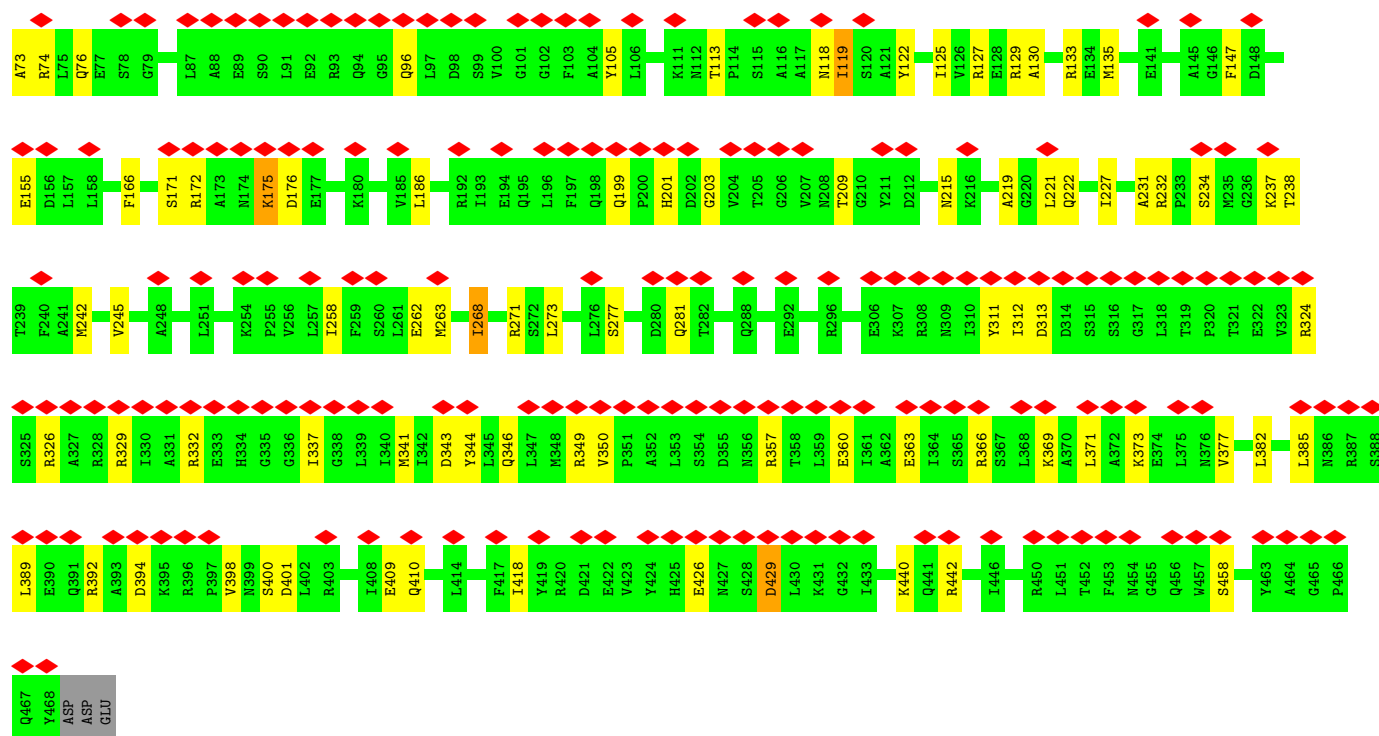
• Molecule 1: Replicative DNA helicase



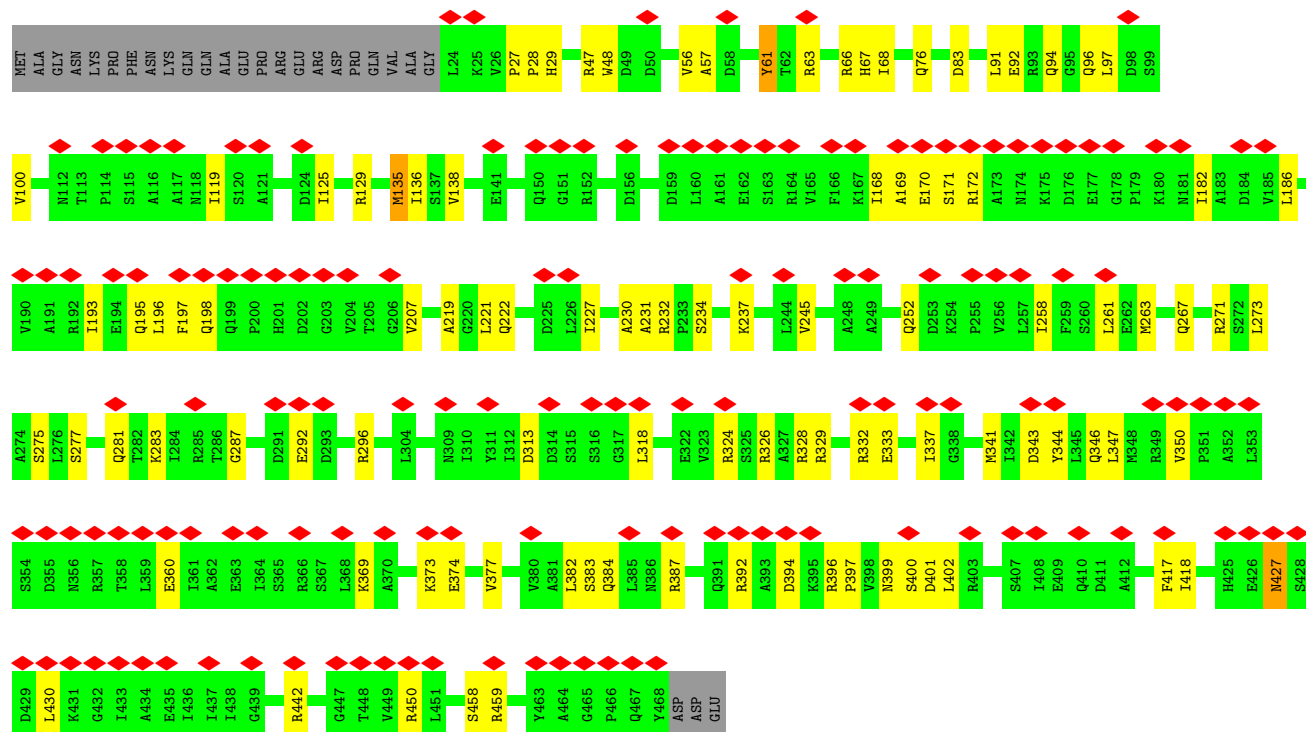
• Molecule 1: Replicative DNA helicase



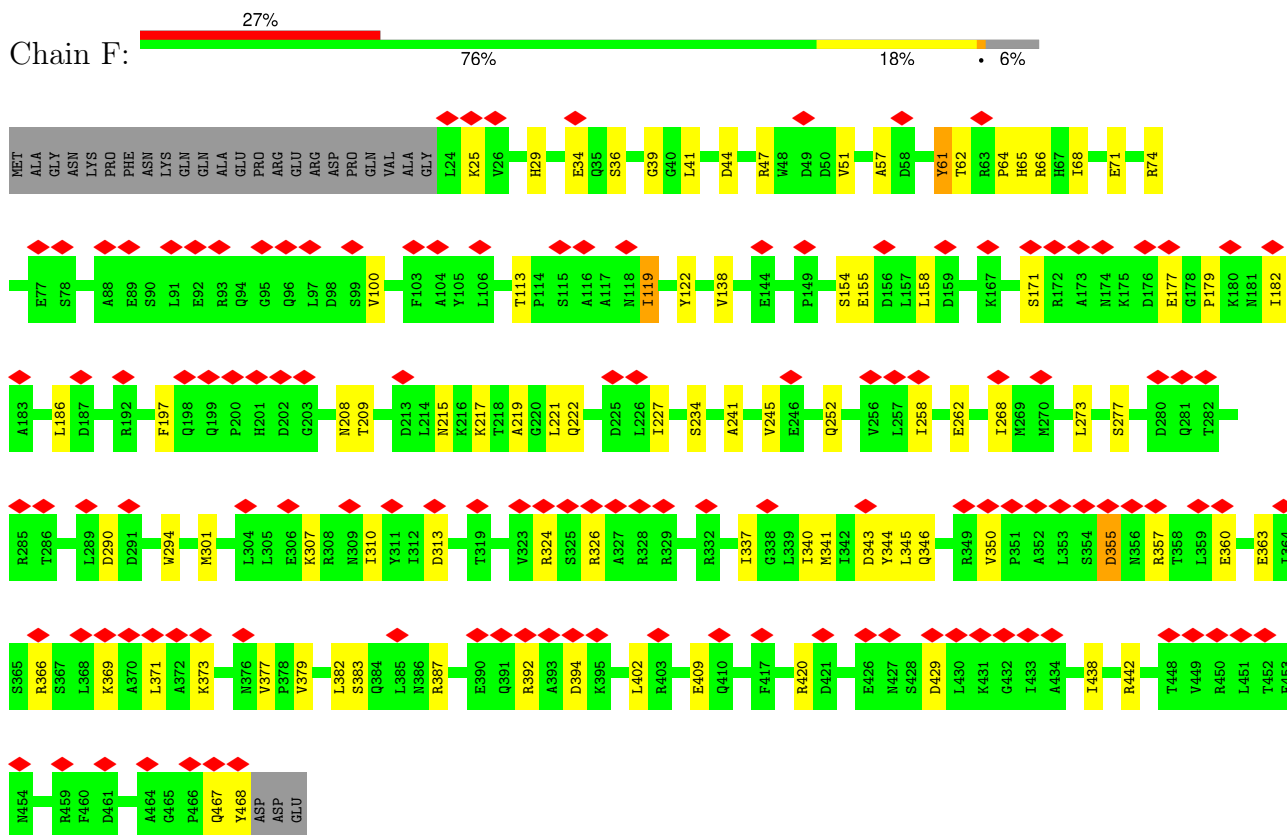




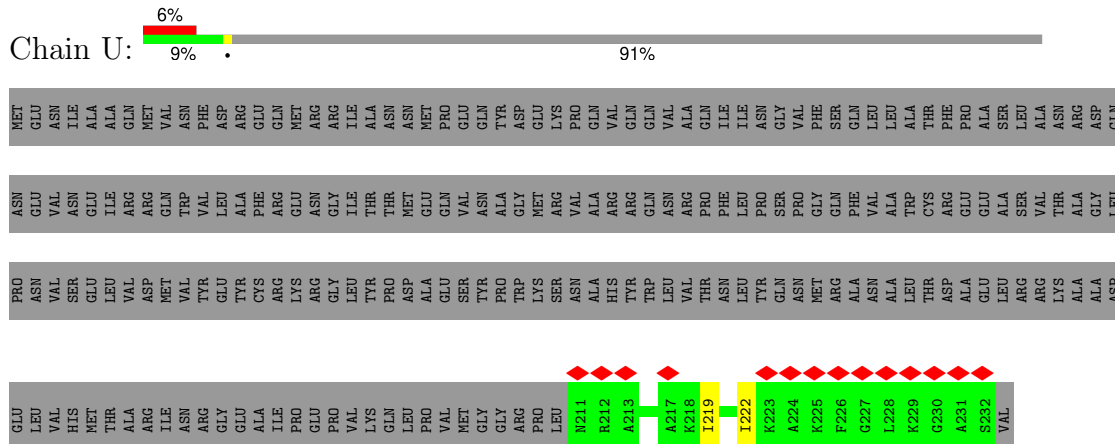
• Molecule 1: Replicative DNA helicase



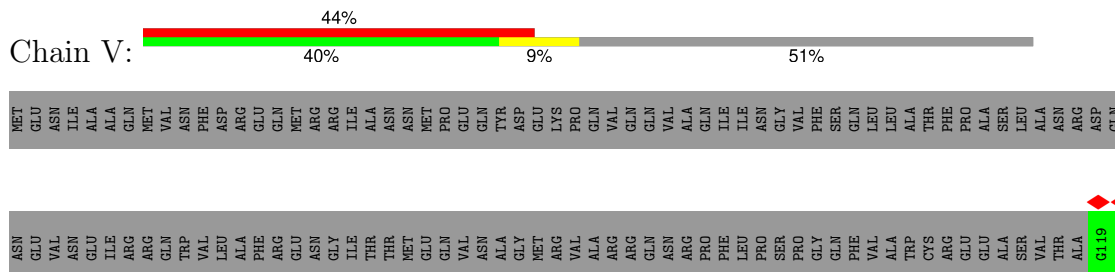
• Molecule 1: Replicative DNA helicase



- Molecule 2: Helicase loader



- Molecule 2: Helicase loader

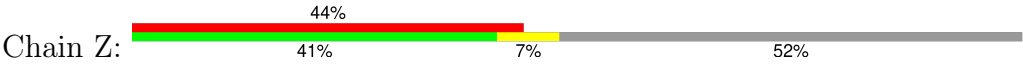




P121	N122	V123	S124	E125	L126	V127	D128	M129	V130	Y131	E132	Y133	C134	R135	K136	R137	G138	L139	Y140	P141	D142	A143	E144	S145	Y146	P147	W148	K149	S150	N151	A152	H153	Y154	W155	L156	V157	T158	N159	L160	Y161	Q162	N163	M164	R165	A166	N167	A168	L169	T170	D171	A172	E173	L174	R175	R176	K177	A178	A179	D180
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

E181	L182	V183	H184	M185	T186	A187	R188	I189	N190	R191	G192	E193	A194	I195	P196	E197	P198	V199	K200	Q201	L202	P203	V204	M205	G206	G207	R208	P209	L210	N211	R212	A213	Q214	A215	L216	A217	K218	I219	A220	E221	I222	K223	A224	K225	F226	G227	L228	K229	G230	A231	S232	VAL
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

• Molecule 2: Helicase loader



MET	GLU	ASN	ILE	ALA	GLN	MET	VAL	ASN	TRP	PHE	ASP	ARG	GLU	GLN	MET	ASN	ARG	ILE	ALA	ASN	MET	PRO	GLU	GLN	TYR	ASP	GLY	LYS	PRO	GLN	VAL	GLN	GLN	VAL	ALA	GLN	ILE	ILE	ASN	GLY	VAL	PHE	SER	GLN	PHE	VAL	LEU	LEU	ALA	ALA	THR	PHE	PRO	GLU	GLU	ALA	SER	LEU	ALA	ASN	ARG	ASP	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASN	GLU	VAL	ASN	GLU	ILE	ARG	GLN	ARG	TRP	VAL	LEU	ALA	PHE	ARG	GLU	GLY	ILE	THR	MET	GLU	GLN	VAL	ASN	ALA	GLY	MET	ARG	VAL	ALA	ARG	ARG	ASN	ARG	PRO	PHE	LEU	PRO	SER	PRO	GLY	GLN	PHE	VAL	ALA	TRP	CYS	ARG	GLU	GLU	ALA	SER	VAL	THR	ALA	G119	L120
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------

P121	N122	S124	E125	L126	V127	D128	M129	V130	Y131	E132	Y133	C134	R135	K136	R137	G138	L139	Y140	P141	D142	A143	E144	S145	Y146	P147	W148	K149	S150	N151	A152	H153	Y154	W155	L156	W157	T158	N159	L160	Y161	Q162	N163	M164	R165	A166	N167	A168	L169	T170	D171	A172	E173	L174	R175	R176	K177	A178	A179	D180
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

E181	L182	V183	H184	M185	T186	A187	R188	I189	N190	R191	G192	E193	A194	I195	P196	E197	P198	V199	K200	Q201	L202	P203	V204	M205	G206	G207	R208	P209	L210	N211	R212	A213	Q214	A215	L216	A217	K218	E221	A224	K225	F226	G227	L228	K229	G230	A231	SER	VAL
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	572557	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51.19	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.380	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.109	Depositor
Map size (Å)	433.19998, 433.19998, 433.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	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: MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.15	0/3524	0.39	0/4765
1	B	0.14	0/3524	0.39	0/4765
1	C	0.14	0/3524	0.42	0/4765
1	D	0.13	0/3524	0.38	0/4765
1	E	0.15	0/3524	0.41	0/4765
1	F	0.15	0/3524	0.39	0/4765
2	U	0.07	0/160	0.26	0/210
2	V	0.12	0/920	0.34	0/1244
2	W	0.12	0/920	0.33	0/1244
2	X	0.08	0/168	0.27	0/221
2	Y	0.11	0/920	0.32	0/1244
2	Z	0.11	0/914	0.33	0/1236
All	All	0.14	0/25146	0.39	0/33989

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	A	3474	0	3468	78	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3474	0	3467	74	0
1	C	3474	0	3468	72	0
1	D	3474	0	3467	71	0
1	E	3474	0	3467	77	0
1	F	3474	0	3468	70	0
2	U	160	0	178	1	0
2	V	901	0	913	14	0
2	W	901	0	913	9	0
2	X	168	0	189	1	0
2	Y	901	0	913	19	0
2	Z	895	0	908	10	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	2	0
3	D	27	0	12	1	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	24938	0	24891	401	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 (401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ARG:HG3	1:A:371:LEU:HD13	1.61	0.82
1:A:262:GLU:O	1:F:442:ARG:NH2	2.12	0.81
1:E:232:ARG:HH22	1:E:387:ARG:HG2	1.45	0.79
1:E:328:ARG:NH1	1:E:374:GLU:OE2	2.17	0.78
1:A:400:SER:H	1:B:387:ARG:NH1	1.86	0.73
1:C:49:ASP:OD2	1:D:332:ARG:NH2	2.21	0.73
1:F:252:GLN:O	1:F:307:LYS:NZ	2.18	0.73
1:D:232:ARG:NH1	1:D:385:LEU:O	2.21	0.72
1:A:329:ARG:HH11	1:F:171:SER:HA	1.53	0.71
1:B:47:ARG:NH1	1:B:117:ALA:O	2.23	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ASP:OD2	1:C:326:ARG:NH1	2.21	0.70
1:B:324:ARG:HG3	1:B:371:LEU:HD13	1.72	0.70
1:E:245:VAL:HG11	1:E:258:ILE:HD11	1.73	0.70
1:A:49:ASP:OD2	1:B:332:ARG:NH2	2.26	0.69
1:A:392:ARG:NH1	1:A:394:ASP:O	2.25	0.69
1:F:313:ASP:OD2	1:F:326:ARG:NH1	2.26	0.69
1:D:337:ILE:HB	1:D:377:VAL:HG11	1.75	0.68
1:D:313:ASP:OD2	1:D:326:ARG:NH1	2.26	0.68
1:D:166:PHE:HE2	1:E:329:ARG:HG3	1.56	0.68
1:F:245:VAL:HG11	1:F:258:ILE:HD11	1.75	0.67
1:C:127:ARG:O	1:C:129:ARG:N	2.28	0.67
1:E:369:LYS:HE3	1:E:373:LYS:HE3	1.75	0.67
1:B:337:ILE:HB	1:B:377:VAL:HG11	1.76	0.66
1:A:442:ARG:O	1:B:267:GLN:NE2	2.29	0.66
1:E:442:ARG:NH2	1:F:262:GLU:O	2.24	0.66
1:E:396:ARG:NH1	2:Y:134:CYS:SG	2.70	0.65
1:B:443:ASN:OD1	1:C:267:GLN:NE2	2.29	0.65
1:F:392:ARG:NH1	1:F:394:ASP:O	2.30	0.65
1:A:53:GLU:OE2	1:B:329:ARG:NH1	2.30	0.64
1:D:61:TYR:HE1	1:D:133:ARG:HD3	1.62	0.64
1:B:207:VAL:HB	1:B:221:LEU:HB2	1.78	0.64
1:A:369:LYS:HE3	1:A:373:LYS:HE3	1.80	0.64
1:D:39:GLY:HA3	1:D:113:THR:HG21	1.79	0.64
1:D:258:ILE:HG23	1:D:341:MET:HE3	1.80	0.63
1:B:245:VAL:HG11	1:B:258:ILE:HD11	1.80	0.63
1:A:83:ASP:OD2	1:B:122:TYR:OH	2.11	0.63
1:B:128:GLU:HG3	1:C:154:SER:HB3	1.79	0.63
1:B:442:ARG:O	1:C:267:GLN:NE2	2.30	0.63
1:E:402:LEU:HB2	1:F:387:ARG:HH22	1.64	0.63
1:E:232:ARG:NH2	1:E:387:ARG:HG2	2.14	0.62
1:A:172:ARG:HH22	1:F:155:GLU:HA	1.64	0.62
1:D:219:ALA:O	1:D:222:GLN:NE2	2.32	0.62
1:A:387:ARG:HH22	1:F:402:LEU:HB2	1.65	0.62
1:C:83:ASP:OD2	1:D:122:TYR:OH	2.14	0.62
1:B:231:ALA:HB2	1:B:418:ILE:HB	1.82	0.62
1:E:263:MET:HE1	1:E:271:ARG:HD2	1.81	0.62
1:D:429:ASP:N	1:D:429:ASP:OD1	2.32	0.61
1:C:245:VAL:HG11	1:C:258:ILE:HD11	1.81	0.61
1:F:34:GLU:OE1	1:F:65:HIS:ND1	2.30	0.61
1:A:207:VAL:HB	1:A:221:LEU:HB2	1.82	0.61
1:B:369:LYS:HE3	1:B:373:LYS:HE3	1.83	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:ALA:O	1:E:172:ARG:HG3	2.00	0.61
1:B:468:TYR:HB3	2:V:138:GLY:HA3	1.82	0.61
1:C:67:HIS:NE2	1:C:96:GLN:OE1	2.33	0.61
1:E:234:SER:O	3:E:500:ADP:O3'	2.19	0.61
1:A:337:ILE:HB	1:A:377:VAL:HG11	1.83	0.60
1:E:92:GLU:HB2	1:E:97:LEU:HD22	1.83	0.60
1:D:61:TYR:CE1	1:D:133:ARG:HD3	2.36	0.60
1:B:194:GLU:OE1	2:V:223:LYS:NZ	2.32	0.60
2:Y:163:ASN:OD1	2:Y:167:ASN:ND2	2.33	0.60
1:C:29:HIS:HB2	1:C:61:TYR:CD2	2.36	0.60
1:A:400:SER:H	1:B:387:ARG:HH12	1.49	0.60
1:F:468:TYR:HB2	2:Z:139:LEU:HB2	1.83	0.60
1:E:450:ARG:NH2	2:Y:135:ARG:O	2.35	0.59
1:B:454:ASN:O	1:B:458:SER:N	2.35	0.59
1:B:400:SER:OG	1:C:387:ARG:NE	2.35	0.59
1:A:252:GLN:O	1:A:307:LYS:NZ	2.27	0.59
1:A:261:LEU:HD21	1:A:318:LEU:HB2	1.83	0.59
1:C:392:ARG:NH1	1:C:394:ASP:O	2.36	0.59
1:D:281:GLN:OE1	1:D:458:SER:OG	2.21	0.58
1:A:313:ASP:OD2	1:A:326:ARG:NH1	2.36	0.58
1:D:324:ARG:HG3	1:D:371:LEU:HD13	1.84	0.58
1:E:29:HIS:HB2	1:E:61:TYR:CD2	2.38	0.58
1:E:399:ASN:O	1:F:387:ARG:NH2	2.36	0.58
1:D:234:SER:O	3:D:500:ADP:O3'	2.14	0.58
1:E:198:GLN:O	2:Y:212:ARG:NH1	2.36	0.58
1:F:420:ARG:NH1	3:F:500:ADP:O3'	2.33	0.58
1:C:346:GLN:O	1:C:357:ARG:NH2	2.35	0.58
1:E:397:PRO:HG2	1:E:417:PHE:HB3	1.85	0.58
1:E:67:HIS:NE2	1:E:96:GLN:OE1	2.29	0.58
1:E:427:ASN:OD1	1:E:427:ASN:N	2.36	0.57
1:D:350:VAL:HB	1:D:360:GLU:HG3	1.85	0.57
2:W:127:VAL:HG21	2:W:175:ARG:HG2	1.85	0.57
2:W:163:ASN:OD1	2:W:167:ASN:ND2	2.38	0.57
1:C:290:ASP:HB3	2:V:208:ARG:HG3	1.86	0.57
1:D:245:VAL:HG11	1:D:258:ILE:HD11	1.85	0.57
1:E:392:ARG:NH2	1:E:401:ASP:OD2	2.37	0.57
1:F:221:LEU:HD22	1:F:227:ILE:HD13	1.86	0.57
1:F:258:ILE:HG23	1:F:341:MET:HE3	1.87	0.57
1:C:194:GLU:HG2	2:W:219:ILE:HG13	1.87	0.57
2:V:163:ASN:OD1	2:V:167:ASN:ND2	2.37	0.57
1:A:350:VAL:HB	1:A:360:GLU:HG3	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:210:LEU:HD22	2:X:214:GLN:HB3	1.87	0.57
1:F:47:ARG:HD3	1:F:119:ILE:HG12	1.87	0.56
1:E:195:GLN:HA	1:E:198:GLN:HG2	1.87	0.56
1:A:186:LEU:HB2	1:B:269:MET:HE2	1.87	0.56
1:A:405:SER:HB3	1:A:408:ILE:HD12	1.87	0.56
1:C:57:ALA:O	1:C:66:ARG:HG2	2.05	0.56
2:Y:156:LEU:HD22	2:Y:181:GLU:HB3	1.87	0.56
1:D:442:ARG:O	1:E:267:GLN:NE2	2.39	0.56
1:A:67:HIS:NE2	1:A:96:GLN:OE1	2.39	0.56
2:Z:163:ASN:OD1	2:Z:167:ASN:ND2	2.39	0.55
1:A:326:ARG:NH2	1:F:177:GLU:O	2.40	0.55
1:D:30:SER:HB2	1:D:129:ARG:HH21	1.72	0.55
1:D:155:GLU:HG2	1:E:172:ARG:HH22	1.72	0.55
1:D:392:ARG:NH1	1:D:394:ASP:O	2.39	0.55
1:A:224:SER:OG	1:A:376:ASN:OD1	2.23	0.55
1:C:234:SER:O	3:C:500:ADP:O3'	2.20	0.55
1:D:175:LYS:HD2	1:D:176:ASP:H	1.72	0.55
1:A:128:GLU:HG3	1:F:154:SER:HB3	1.88	0.55
1:E:292:GLU:OE2	1:E:296:ARG:NH2	2.39	0.55
1:F:36:SER:HA	1:F:113:THR:HG22	1.88	0.54
1:B:28:PRO:HB3	1:B:129:ARG:NH2	2.23	0.54
1:B:208:ASN:OD1	1:B:215:ASN:ND2	2.41	0.54
1:C:201:HIS:O	1:C:201:HIS:ND1	2.38	0.54
1:C:207:VAL:HB	1:C:221:LEU:HB2	1.89	0.54
1:E:258:ILE:HG23	1:E:341:MET:SD	2.47	0.54
1:F:68:ILE:HD11	1:F:100:VAL:HG13	1.90	0.54
1:C:311:TYR:OH	1:C:334:HIS:NE2	2.39	0.54
1:F:355:ASP:OD1	1:F:355:ASP:N	2.40	0.54
1:F:357:ARG:NH1	1:F:360:GLU:OE1	2.41	0.54
1:E:313:ASP:OD2	1:E:326:ARG:NH1	2.39	0.54
1:F:39:GLY:HA3	1:F:113:THR:HG21	1.89	0.54
1:B:231:ALA:HB3	1:B:237:LYS:HB2	1.90	0.54
1:B:363:GLU:OE1	1:B:366:ARG:NH2	2.33	0.54
1:D:273:LEU:O	1:D:277:SER:OG	2.21	0.54
1:A:151:GLY:HA2	1:E:94:GLN:HG2	1.91	0.53
1:A:214:LEU:O	1:A:218:THR:OG1	2.16	0.53
1:B:232:ARG:NH2	1:B:387:ARG:HG2	2.24	0.53
1:C:122:TYR:O	1:C:126:VAL:HG23	2.09	0.53
1:C:410:GLN:OE1	1:D:349:ARG:NH2	2.42	0.53
1:A:245:VAL:HG11	1:A:258:ILE:HD11	1.90	0.53
1:E:273:LEU:O	1:E:277:SER:OG	2.20	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:HD2	1:B:129:ARG:HD3	1.90	0.53
1:F:324:ARG:HG3	1:F:371:LEU:HD13	1.91	0.53
1:E:350:VAL:HB	1:E:360:GLU:HG3	1.89	0.52
1:A:204:VAL:HG22	1:A:215:ASN:HB3	1.90	0.52
1:A:313:ASP:HB2	1:F:179:PRO:HB3	1.91	0.52
1:C:369:LYS:HE3	1:C:373:LYS:HE3	1.91	0.52
1:B:258:ILE:HB	1:B:312:ILE:HG12	1.92	0.52
1:D:41:LEU:HD11	1:D:51:VAL:HG11	1.92	0.52
1:D:203:GLY:HA2	1:D:219:ALA:HA	1.92	0.52
1:E:221:LEU:HD22	1:E:227:ILE:HD13	1.90	0.52
1:C:131:VAL:HG11	1:C:172:ARG:NE	2.25	0.52
1:B:313:ASP:OD2	1:B:326:ARG:NH1	2.43	0.52
1:C:273:LEU:O	1:C:277:SER:OG	2.27	0.52
1:C:34:GLU:OE1	1:C:65:HIS:ND1	2.33	0.52
1:C:337:ILE:HB	1:C:377:VAL:HG11	1.91	0.52
1:A:91:LEU:HD13	1:A:100:VAL:HG21	1.91	0.51
1:A:290:ASP:HB3	2:Z:208:ARG:HG2	1.92	0.51
1:D:130:ALA:HA	1:D:133:ARG:NH1	2.25	0.51
1:E:281:GLN:OE1	1:E:458:SER:OG	2.28	0.51
2:Y:148:TRP:CG	2:Y:154:TYR:HB2	2.46	0.51
1:E:91:LEU:HD13	1:E:100:VAL:HG21	1.92	0.51
1:E:193:ILE:HA	1:E:196:LEU:HD12	1.92	0.51
1:E:237:LYS:HG2	1:E:382:LEU:HD23	1.92	0.51
1:A:194:GLU:HG2	2:U:219:ILE:HG12	1.92	0.51
2:V:156:LEU:HD22	2:V:181:GLU:HB3	1.92	0.51
2:Y:229:LYS:HD2	2:Y:230:GLY:H	1.76	0.51
1:A:207:VAL:HG21	1:A:378:PRO:HG3	1.93	0.50
1:E:47:ARG:HD3	1:E:119:ILE:HG12	1.93	0.50
1:C:221:LEU:HD22	1:C:227:ILE:HD13	1.92	0.50
1:F:467:GLN:HG3	2:Z:139:LEU:HD23	1.93	0.50
1:F:350:VAL:HB	1:F:360:GLU:HG3	1.94	0.50
1:C:53:GLU:OE2	1:D:329:ARG:NH1	2.44	0.50
1:B:67:HIS:NE2	1:B:96:GLN:OE1	2.44	0.50
1:C:258:ILE:HG23	1:C:341:MET:HE3	1.93	0.50
1:E:396:ARG:HH22	2:Y:135:ARG:HA	1.75	0.50
1:F:219:ALA:O	1:F:222:GLN:NE2	2.45	0.50
1:A:231:ALA:HB2	1:A:418:ILE:HB	1.93	0.50
1:B:154:SER:HB2	1:C:172:ARG:NH2	2.27	0.50
2:V:127:VAL:HG21	2:V:175:ARG:HG2	1.94	0.50
1:A:89:GLU:O	1:A:93:ARG:HG3	2.12	0.49
1:B:221:LEU:HD22	1:B:227:ILE:HD13	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:MET:HE2	1:D:268:ILE:HG23	1.93	0.49
2:V:126:LEU:HD23	2:V:178:ALA:HB1	1.94	0.49
2:Z:127:VAL:HG21	2:Z:175:ARG:HG2	1.94	0.49
1:C:81:PRO:HG3	1:D:118:ASN:HD22	1.77	0.49
1:D:67:HIS:NE2	1:D:96:GLN:OE1	2.45	0.49
1:D:147:PHE:CE1	1:E:136:ILE:HD13	2.47	0.49
1:F:337:ILE:HB	1:F:377:VAL:HG11	1.95	0.49
1:C:397:PRO:HG2	1:C:417:PHE:HB3	1.93	0.49
1:E:275:SER:O	1:E:459:ARG:NH1	2.45	0.49
2:W:148:TRP:CG	2:W:154:TYR:HB2	2.48	0.49
1:A:262:GLU:C	1:F:442:ARG:HH22	2.13	0.49
1:B:179:PRO:HB3	1:C:313:ASP:HB2	1.93	0.49
1:F:429:ASP:HA	2:Y:199:VAL:HG21	1.95	0.49
1:F:41:LEU:HD11	1:F:51:VAL:HG11	1.94	0.49
2:Z:148:TRP:CG	2:Z:154:TYR:HB2	2.48	0.49
1:D:221:LEU:HD22	1:D:227:ILE:HD13	1.95	0.49
1:D:258:ILE:HD12	1:D:312:ILE:HG12	1.95	0.49
1:B:28:PRO:HB3	1:B:129:ARG:HH21	1.78	0.49
1:B:191:ALA:HA	2:V:223:LYS:HZ1	1.78	0.49
1:B:305:LEU:HD22	1:B:308:ARG:HH21	1.77	0.49
1:E:67:HIS:CE1	1:E:96:GLN:HB3	2.48	0.49
1:B:337:ILE:HD12	1:B:375:LEU:HD13	1.95	0.48
1:D:127:ARG:HH21	1:D:172:ARG:HG2	1.78	0.48
1:E:125:ILE:O	1:E:129:ARG:HG2	2.13	0.48
2:V:148:TRP:CG	2:V:154:TYR:HB2	2.48	0.48
1:D:209:THR:HG22	1:D:221:LEU:HG	1.96	0.48
1:A:409:GLU:O	1:A:440:LYS:NZ	2.34	0.48
1:E:344:TYR:CD2	1:E:346:GLN:HB2	2.48	0.48
1:F:344:TYR:CD2	1:F:346:GLN:HB2	2.48	0.48
1:B:227:ILE:HB	1:B:380:VAL:HG22	1.96	0.48
1:D:426:GLU:HG3	2:W:165:ARG:HH22	1.78	0.48
2:W:126:LEU:HD23	2:W:178:ALA:HB1	1.95	0.48
1:C:134:GLU:CD	1:C:168:ILE:HG13	2.39	0.48
1:D:231:ALA:HB2	1:D:418:ILE:HB	1.96	0.48
1:E:83:ASP:OD2	1:F:122:TYR:OH	2.14	0.48
1:E:230:ALA:O	1:E:417:PHE:HA	2.14	0.48
1:A:86:THR:HG23	1:B:125:ILE:HD11	1.96	0.47
1:A:326:ARG:HD3	1:F:179:PRO:HD3	1.94	0.47
1:B:158:LEU:HD11	1:C:172:ARG:HD2	1.96	0.47
1:F:241:ALA:HB2	1:F:382:LEU:HD11	1.96	0.47
1:A:77:GLU:OE1	1:B:324:ARG:NH2	2.47	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:GLN:HE22	1:B:349:ARG:NH2	2.11	0.47
1:F:29:HIS:HB2	1:F:61:TYR:CD2	2.49	0.47
1:F:468:TYR:HE2	2:Z:136:LYS:HD2	1.79	0.47
2:Z:126:LEU:HD23	2:Z:178:ALA:HB1	1.96	0.47
1:A:258:ILE:HG23	1:A:341:MET:SD	2.55	0.47
1:E:392:ARG:NH1	1:E:394:ASP:O	2.48	0.47
2:Y:223:LYS:HG2	2:Y:229:LYS:HG2	1.96	0.47
1:C:169:ALA:HA	1:C:172:ARG:HG3	1.96	0.47
1:C:421:ASP:OD2	1:C:428:SER:OG	2.28	0.47
1:D:400:SER:H	1:E:387:ARG:NH1	2.13	0.47
1:E:237:LYS:HA	1:E:418:ILE:HD12	1.97	0.47
1:B:236:GLY:H	3:B:500:ADP:H5'1	1.80	0.47
1:C:427:ASN:HB2	2:V:162:GLN:HG3	1.96	0.47
1:E:337:ILE:HB	1:E:377:VAL:HG11	1.97	0.47
1:B:226:LEU:HB3	1:B:412:ALA:HA	1.97	0.47
1:B:109:LEU:O	1:B:113:THR:OG1	2.26	0.47
1:E:48:TRP:CD1	1:E:76:GLN:HG2	2.49	0.47
1:F:57:ALA:O	1:F:66:ARG:HG2	2.15	0.47
1:A:208:ASN:OD1	1:A:215:ASN:ND2	2.45	0.47
1:B:29:HIS:HB2	1:B:61:TYR:CD2	2.50	0.47
2:W:156:LEU:HD22	2:W:181:GLU:HB3	1.97	0.46
1:E:57:ALA:O	1:E:66:ARG:HG2	2.16	0.46
1:F:369:LYS:HE3	1:F:373:LYS:HE3	1.97	0.46
1:A:269:MET:HE2	1:F:186:LEU:HD13	1.97	0.46
1:C:454:ASN:ND2	1:C:461:ASP:OD2	2.48	0.46
1:D:363:GLU:OE1	1:D:366:ARG:NH2	2.48	0.46
1:A:344:TYR:CD2	1:A:346:GLN:HB2	2.50	0.46
1:C:131:VAL:HG11	1:C:172:ARG:CZ	2.45	0.46
2:Y:126:LEU:HD23	2:Y:178:ALA:HB1	1.98	0.46
1:B:237:LYS:HA	1:B:418:ILE:HD12	1.98	0.46
1:B:264:PRO:HG2	1:B:267:GLN:HG3	1.96	0.46
1:D:36:SER:HA	1:D:113:THR:HG22	1.97	0.46
1:D:369:LYS:HE3	1:D:373:LYS:HE3	1.97	0.46
1:E:197:PHE:HE2	1:F:294:TRP:HE1	1.63	0.46
1:B:438:ILE:HG21	1:B:441:GLN:HB2	1.97	0.46
1:C:39:GLY:HA3	1:C:113:THR:OG1	2.15	0.46
1:C:227:ILE:HB	1:C:380:VAL:HG22	1.97	0.46
1:F:217:LYS:HD3	1:F:438:ILE:HD12	1.98	0.46
1:C:92:GLU:HB2	1:C:97:LEU:HD22	1.98	0.45
1:C:344:TYR:CD2	1:C:346:GLN:HB2	2.51	0.45
1:C:425:HIS:HB2	1:C:428:SER:HB2	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:ARG:HD2	1:E:328:ARG:HH21	1.80	0.45
1:D:262:GLU:HG2	1:D:263:MET:HG3	1.98	0.45
1:E:396:ARG:NH2	2:Y:135:ARG:HA	2.31	0.45
1:A:92:GLU:HB2	1:A:97:LEU:HD22	1.97	0.45
1:C:81:PRO:HG3	1:D:118:ASN:ND2	2.32	0.45
1:C:355:ASP:OD1	1:C:355:ASP:N	2.49	0.45
1:D:263:MET:HE1	1:D:271:ARG:HD2	1.97	0.45
1:C:60:PHE:HB2	1:C:66:ARG:HG3	1.97	0.45
1:F:290:ASP:HA	2:Y:210:LEU:HG	1.99	0.45
1:D:119:ILE:H	1:D:119:ILE:HG13	1.48	0.45
2:Y:146:TYR:HB3	2:Y:148:TRP:NE1	2.32	0.45
1:B:158:LEU:HG	1:C:172:ARG:NH2	2.32	0.45
1:C:392:ARG:NH2	1:C:401:ASP:OD2	2.47	0.45
1:E:261:LEU:HD21	1:E:318:LEU:HB2	1.98	0.45
1:F:345:LEU:HD21	1:F:383:SER:HB2	1.99	0.45
1:A:387:ARG:NH2	1:F:409:GLU:OE1	2.36	0.45
1:B:35:GLN:O	1:B:113:THR:HG21	2.17	0.45
1:B:164:ARG:O	1:B:168:ILE:HG13	2.16	0.45
1:B:197:PHE:O	2:V:212:ARG:NH2	2.41	0.45
1:C:264:PRO:HG2	1:C:267:GLN:HG3	1.99	0.45
1:D:48:TRP:CD1	1:D:76:GLN:HG2	2.52	0.45
1:F:71:GLU:OE2	1:F:74:ARG:NH1	2.50	0.45
1:B:258:ILE:HG23	1:B:341:MET:SD	2.57	0.44
1:F:44:ASP:HB3	1:F:47:ARG:HD2	1.98	0.44
1:E:343:ASP:HA	1:E:344:TYR:HA	1.72	0.44
1:A:234:SER:O	3:A:500:ADP:O3'	2.33	0.44
1:B:34:GLU:HB3	1:B:65:HIS:ND1	2.32	0.44
1:C:198:GLN:HG2	2:W:216:LEU:HD22	2.00	0.44
1:C:344:TYR:CE2	1:C:346:GLN:HB2	2.51	0.44
1:D:398:VAL:HB	1:E:387:ARG:NH1	2.32	0.44
1:F:208:ASN:OD1	1:F:215:ASN:ND2	2.47	0.44
1:A:125:ILE:O	1:A:129:ARG:HG2	2.18	0.44
1:A:147:PHE:CZ	1:F:25:LYS:HB3	2.53	0.44
1:B:239:THR:HG21	1:B:453:PHE:HE1	1.83	0.44
1:C:128:GLU:O	1:C:132:VAL:HG23	2.18	0.44
1:E:231:ALA:HB2	1:E:418:ILE:HB	2.00	0.44
1:F:234:SER:O	3:F:500:ADP:O3'	2.23	0.44
1:F:340:ILE:HB	1:F:379:VAL:HG22	2.00	0.44
1:A:427:ASN:ND2	2:Z:158:THR:O	2.48	0.44
1:C:204:VAL:HG13	1:C:220:GLY:HA3	1.99	0.44
1:E:219:ALA:O	1:E:222:GLN:NE2	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ARG:HH22	1:B:387:ARG:NE	2.16	0.43
1:D:357:ARG:NH1	1:D:360:GLU:OE1	2.51	0.43
1:C:238:THR:OG1	3:C:500:ADP:O3B	2.31	0.43
1:C:426:GLU:OE1	2:V:137:ARG:NH2	2.47	0.43
1:E:186:LEU:HD11	1:F:301:MET:HG2	2.00	0.43
1:D:237:LYS:HA	1:D:418:ILE:HD12	2.00	0.43
1:E:186:LEU:HG	1:F:301:MET:HE3	2.01	0.43
1:A:443:ASN:HA	1:B:267:GLN:NE2	2.33	0.43
1:D:48:TRP:CZ2	1:D:73:ALA:HA	2.53	0.43
1:D:237:LYS:HG2	1:D:382:LEU:HG	2.01	0.43
1:D:343:ASP:HA	1:D:344:TYR:HA	1.74	0.43
1:D:409:GLU:O	1:D:440:LYS:NZ	2.39	0.43
1:E:27:PRO:HA	1:E:28:PRO:HD3	1.93	0.43
1:E:283:LYS:O	1:E:287:GLY:N	2.51	0.43
1:A:304:LEU:HB3	1:F:182:ILE:HD11	2.01	0.43
1:A:61:TYR:CE1	1:A:133:ARG:HD3	2.54	0.43
1:A:207:VAL:HG13	1:A:252:GLN:OE1	2.18	0.43
1:A:255:PRO:HA	1:A:309:ASN:HB2	2.01	0.43
1:E:346:GLN:OE1	1:E:383:SER:HA	2.18	0.43
1:F:273:LEU:O	1:F:277:SER:OG	2.29	0.43
1:D:199:GLN:HB3	1:D:201:HIS:NE2	2.33	0.43
1:A:90:SER:HA	1:A:93:ARG:CZ	2.49	0.43
1:E:68:ILE:HD11	1:E:100:VAL:HG13	2.00	0.43
1:F:209:THR:OG1	1:F:215:ASN:OD1	2.24	0.43
1:A:61:TYR:OH	1:A:129:ARG:HB3	2.19	0.42
1:B:232:ARG:CZ	1:B:387:ARG:HG2	2.49	0.42
1:C:59:ASP:CG	1:C:127:ARG:HH11	2.26	0.42
1:D:127:ARG:NH2	1:D:172:ARG:HA	2.34	0.42
2:Y:162:GLN:HE22	2:Y:165:ARG:HH21	1.67	0.42
1:A:135:MET:HE2	1:F:158:LEU:HD23	2.02	0.42
1:D:344:TYR:CD2	1:D:346:GLN:HB2	2.54	0.42
1:A:64:PRO:HB3	1:A:100:VAL:HA	2.01	0.42
1:B:89:GLU:HG2	1:B:93:ARG:HH11	1.83	0.42
1:B:400:SER:CB	1:C:387:ARG:HE	2.31	0.42
1:E:207:VAL:HG22	1:E:252:GLN:HE22	1.84	0.42
1:E:430:LEU:HD11	2:Y:135:ARG:HB3	2.00	0.42
2:Y:130:VAL:HA	2:Y:157:VAL:HG13	2.01	0.42
1:A:397:PRO:HG2	1:A:417:PHE:HB3	2.02	0.42
1:B:138:VAL:HG11	1:B:168:ILE:HD11	2.00	0.42
1:C:89:GLU:OE1	1:D:125:ILE:HG21	2.18	0.42
1:D:65:HIS:NE2	1:D:105:TYR:OH	2.41	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:LEU:HD12	1:D:401:ASP:OD2	2.19	0.42
1:F:41:LEU:HD23	1:F:41:LEU:HA	1.88	0.42
1:A:237:LYS:HA	1:A:418:ILE:HD12	2.01	0.42
1:B:166:PHE:O	1:B:170:GLU:HB2	2.20	0.42
1:C:158:LEU:HD23	1:C:158:LEU:HA	1.88	0.42
1:A:399:ASN:HB3	1:A:409:GLU:OE2	2.19	0.42
1:C:27:PRO:HA	1:C:28:PRO:HD3	1.92	0.42
1:D:135:MET:HE3	1:D:135:MET:HB2	1.91	0.42
1:C:348:MET:HB2	1:C:364:ILE:HD13	2.02	0.42
1:B:60:PHE:HB2	1:B:66:ARG:HG2	2.02	0.41
1:B:227:ILE:O	1:B:380:VAL:HA	2.20	0.41
1:C:349:ARG:HD3	1:C:349:ARG:HA	1.92	0.41
2:V:134:CYS:HA	2:V:137:ARG:HD2	2.02	0.41
1:D:166:PHE:HZ	1:E:333:GLU:HG3	1.86	0.41
1:D:410:GLN:HG2	1:E:347:LEU:CD2	2.50	0.41
1:E:230:ALA:HB3	1:E:417:PHE:CD1	2.55	0.41
2:Y:223:LYS:O	2:Y:227:GLY:N	2.54	0.41
1:A:196:LEU:HD22	1:A:205:THR:HG21	2.01	0.41
1:A:310:ILE:O	1:F:182:ILE:HB	2.21	0.41
1:F:344:TYR:CE2	1:F:346:GLN:HB2	2.56	0.41
1:A:47:ARG:NH1	1:A:117:ALA:O	2.51	0.41
1:C:345:LEU:HD11	1:C:408:ILE:HD11	2.01	0.41
1:F:343:ASP:HA	1:F:344:TYR:HA	1.73	0.41
1:A:172:ARG:CZ	1:F:158:LEU:HD12	2.51	0.41
1:A:262:GLU:HG2	1:F:442:ARG:NH2	2.35	0.41
1:A:427:ASN:OD1	1:A:427:ASN:N	2.53	0.41
1:C:127:ARG:HG2	1:C:175:LYS:NZ	2.36	0.41
1:D:238:THR:HG21	1:D:263:MET:SD	2.61	0.41
1:E:182:ILE:HB	1:F:310:ILE:O	2.21	0.41
1:F:363:GLU:OE1	1:F:366:ARG:NH2	2.53	0.41
2:V:146:TYR:HB3	2:V:148:TRP:CE2	2.56	0.41
1:B:158:LEU:HG	1:C:172:ARG:CZ	2.51	0.41
1:D:203:GLY:HA3	1:D:215:ASN:HB3	2.02	0.41
1:A:89:GLU:OE2	1:B:125:ILE:HG21	2.20	0.41
1:A:399:ASN:HB2	1:B:387:ARG:HH22	1.86	0.41
1:B:224:SER:OG	1:B:376:ASN:HA	2.21	0.41
1:C:35:GLN:O	1:C:113:THR:HG21	2.21	0.41
1:C:182:ILE:HD12	1:D:311:TYR:HA	2.02	0.41
1:C:231:ALA:HB2	1:C:418:ILE:HB	2.03	0.41
1:D:71:GLU:OE2	1:D:74:ARG:NH1	2.54	0.41
1:D:237:LYS:HE2	1:D:237:LYS:HB3	1.80	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:216:LEU:HA	2:Y:219:ILE:HD12	2.02	0.41
1:A:343:ASP:HA	1:A:344:TYR:HA	1.74	0.41
1:B:349:ARG:HA	1:B:349:ARG:HD3	1.91	0.41
1:D:147:PHE:CD1	1:E:136:ILE:HD13	2.56	0.41
1:E:135:MET:HE3	1:E:135:MET:HB3	1.79	0.41
1:E:170:GLU:O	1:E:171:SER:OG	2.31	0.41
1:F:62:THR:HB	1:F:64:PRO:HD2	2.03	0.41
2:Z:146:TYR:HB3	2:Z:148:TRP:CE2	2.56	0.41
1:B:35:GLN:C	1:B:113:THR:HG21	2.46	0.40
1:B:171:SER:OG	1:B:172:ARG:N	2.50	0.40
1:A:67:HIS:CE1	1:A:96:GLN:HB3	2.56	0.40
1:A:263:MET:HG2	1:F:442:ARG:NH2	2.36	0.40
1:A:129:ARG:HD3	1:A:129:ARG:HA	1.83	0.40
1:A:230:ALA:O	1:A:417:PHE:HA	2.21	0.40
1:B:165:VAL:O	1:B:168:ILE:HB	2.20	0.40
1:C:207:VAL:HG21	1:C:378:PRO:HG3	2.03	0.40
1:D:166:PHE:CG	1:E:332:ARG:HD2	2.56	0.40
1:D:186:LEU:HD11	1:E:273:LEU:HD11	2.03	0.40
1:E:344:TYR:HD2	1:E:346:GLN:HB2	1.85	0.40
1:B:389:LEU:HD12	1:B:401:ASP:OD2	2.20	0.40
1:E:400:SER:HA	1:F:387:ARG:CZ	2.52	0.40
2:W:212:ARG:O	2:W:216:LEU:HG	2.22	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	443/471 (94%)	438 (99%)	5 (1%)	0	100	100
1	B	443/471 (94%)	433 (98%)	10 (2%)	0	100	100
1	C	443/471 (94%)	429 (97%)	12 (3%)	2 (0%)	25	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	443/471 (94%)	434 (98%)	8 (2%)	1 (0%)	44	75
1	E	443/471 (94%)	436 (98%)	7 (2%)	0	100	100
1	F	443/471 (94%)	434 (98%)	9 (2%)	0	100	100
2	U	20/233 (9%)	18 (90%)	2 (10%)	0	100	100
2	V	112/233 (48%)	101 (90%)	10 (9%)	1 (1%)	14	48
2	W	112/233 (48%)	105 (94%)	6 (5%)	1 (1%)	14	48
2	X	21/233 (9%)	20 (95%)	1 (5%)	0	100	100
2	Y	112/233 (48%)	103 (92%)	8 (7%)	1 (1%)	14	48
2	Z	111/233 (48%)	102 (92%)	8 (7%)	1 (1%)	14	48
All	All	3146/4224 (74%)	3053 (97%)	86 (3%)	7 (0%)	45	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	198	PRO
2	W	198	PRO
2	Y	198	PRO
2	Z	198	PRO
1	C	128	GLU
1	C	127	ARG
1	D	171	SER

### 5.3.2 Protein sidechains ⓘ

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	377/398 (95%)	373 (99%)	4 (1%)	70	79
1	B	377/398 (95%)	373 (99%)	4 (1%)	70	79
1	C	377/398 (95%)	370 (98%)	7 (2%)	52	70
1	D	377/398 (95%)	372 (99%)	5 (1%)	65	76
1	E	377/398 (95%)	369 (98%)	8 (2%)	48	67

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	377/398 (95%)	371 (98%)	6 (2%)	58	73
2	U	14/194 (7%)	13 (93%)	1 (7%)	12	36
2	V	92/194 (47%)	91 (99%)	1 (1%)	70	79
2	W	92/194 (47%)	91 (99%)	1 (1%)	70	79
2	X	15/194 (8%)	14 (93%)	1 (7%)	13	39
2	Y	92/194 (47%)	88 (96%)	4 (4%)	25	49
2	Z	91/194 (47%)	88 (97%)	3 (3%)	33	56
All	All	2658/3552 (75%)	2613 (98%)	45 (2%)	56	72

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	119	ILE
1	A	182	ILE
1	A	427	ASN
1	B	29	HIS
1	B	61	TYR
1	B	119	ILE
1	B	182	ILE
1	C	56	VAL
1	C	61	TYR
1	C	119	ILE
1	C	135	MET
1	C	182	ILE
1	C	355	ASP
1	C	429	ASP
1	D	56	VAL
1	D	119	ILE
1	D	175	LYS
1	D	268	ILE
1	D	429	ASP
1	E	56	VAL
1	E	61	TYR
1	E	63	ARG
1	E	135	MET
1	E	138	VAL
1	E	168	ILE
1	E	384	GLN
1	E	427	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	61	TYR
1	F	119	ILE
1	F	138	VAL
1	F	197	PHE
1	F	268	ILE
1	F	355	ASP
2	U	222	ILE
2	V	193	GLU
2	W	210	LEU
2	X	228	LEU
2	Y	134	CYS
2	Y	210	LEU
2	Y	228	LEU
2	Y	229	LYS
2	Z	162	GLN
2	Z	210	LEU
2	Z	228	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	C	94	GLN
1	C	454	ASN
1	E	94	GLN
1	E	201	HIS
1	E	441	GLN
1	F	118	ASN
1	F	443	ASN
2	V	159	ASN
2	W	159	ASN
2	Y	159	ASN
2	Y	162	GLN
2	Z	159	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	ADP	D	500	4	24,29,29	0.92	1 (4%)	29,45,45	1.26	3 (10%)
3	ADP	E	500	4	24,29,29	0.91	0	29,45,45	1.34	3 (10%)
3	ADP	C	500	4	24,29,29	0.91	0	29,45,45	1.30	3 (10%)
3	ADP	B	500	4	24,29,29	0.90	0	29,45,45	1.16	2 (6%)
3	ADP	A	500	4	24,29,29	0.90	0	29,45,45	1.28	3 (10%)
3	ADP	F	500	4	24,29,29	0.91	1 (4%)	29,45,45	1.22	3 (10%)

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
3	ADP	D	500	4	-	7/12/32/32	0/3/3/3
3	ADP	E	500	4	-	5/12/32/32	0/3/3/3
3	ADP	C	500	4	-	4/12/32/32	0/3/3/3
3	ADP	B	500	4	-	7/12/32/32	0/3/3/3
3	ADP	A	500	4	-	2/12/32/32	0/3/3/3
3	ADP	F	500	4	-	4/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	500	ADP	O4'-C1'	2.02	1.43	1.40
3	D	500	ADP	O4'-C1'	2.00	1.43	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	500	ADP	N3-C2-N1	-3.74	123.59	128.67
3	F	500	ADP	N3-C2-N1	-3.72	123.62	128.67
3	C	500	ADP	N3-C2-N1	-3.71	123.64	128.67
3	A	500	ADP	N3-C2-N1	-3.70	123.65	128.67
3	D	500	ADP	N3-C2-N1	-3.69	123.66	128.67
3	B	500	ADP	N3-C2-N1	-3.65	123.72	128.67
3	E	500	ADP	O4'-C1'-N9	2.89	112.57	108.75
3	E	500	ADP	C4-C5-N7	-2.70	106.48	109.34
3	D	500	ADP	C4-C5-N7	-2.69	106.49	109.34
3	C	500	ADP	C4-C5-N7	-2.68	106.51	109.34
3	A	500	ADP	C4-C5-N7	-2.63	106.56	109.34
3	C	500	ADP	O4'-C1'-N9	2.62	112.21	108.75
3	F	500	ADP	C4-C5-N7	-2.59	106.60	109.34
3	B	500	ADP	C4-C5-N7	-2.56	106.64	109.34
3	A	500	ADP	O4'-C1'-N9	2.34	111.85	108.75
3	D	500	ADP	O4'-C1'-N9	2.31	111.81	108.75
3	F	500	ADP	O4'-C1'-N9	2.22	111.69	108.75

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	500	ADP	C5'-O5'-PA-O2A
3	B	500	ADP	O4'-C4'-C5'-O5'
3	C	500	ADP	O4'-C4'-C5'-O5'
3	D	500	ADP	C5'-O5'-PA-O2A
3	D	500	ADP	O4'-C4'-C5'-O5'
3	E	500	ADP	O4'-C4'-C5'-O5'
3	E	500	ADP	C3'-C4'-C5'-O5'
3	B	500	ADP	C3'-C4'-C5'-O5'
3	C	500	ADP	C3'-C4'-C5'-O5'
3	D	500	ADP	C3'-C4'-C5'-O5'
3	F	500	ADP	O4'-C4'-C5'-O5'
3	F	500	ADP	C3'-C4'-C5'-O5'
3	B	500	ADP	PB-O3A-PA-O1A

*Continued on next page...*

*Continued from previous page...*

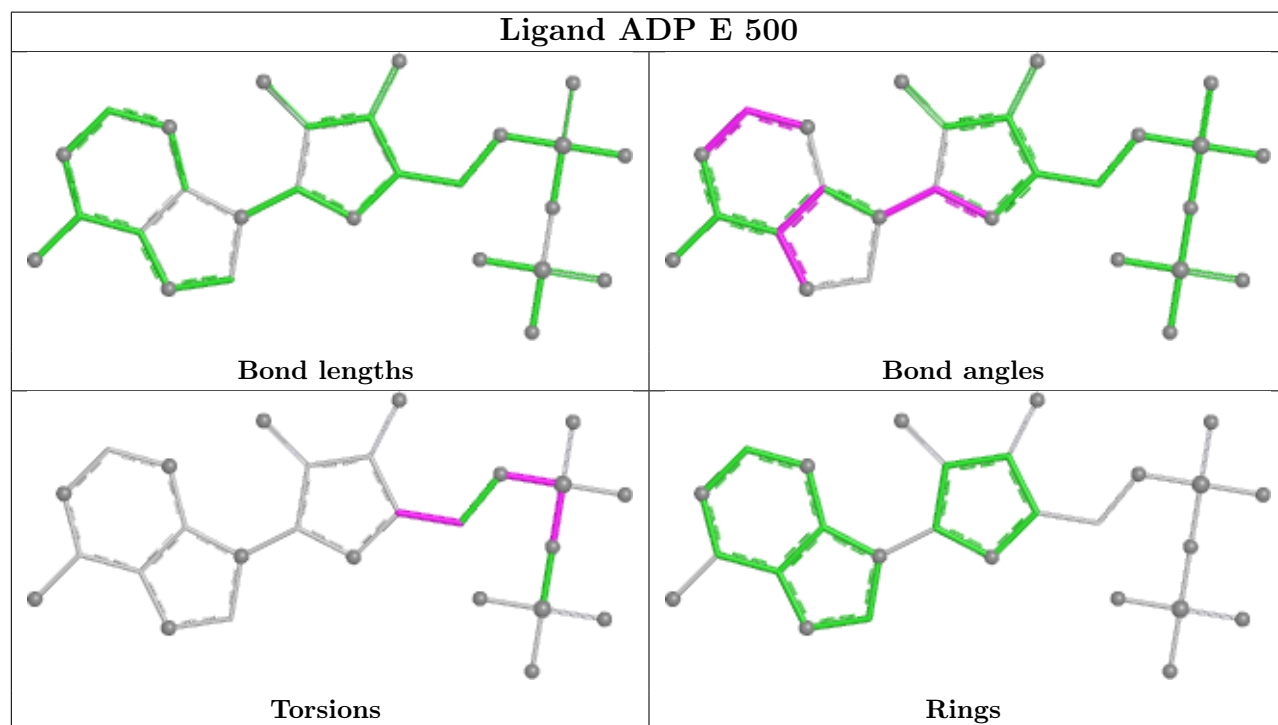
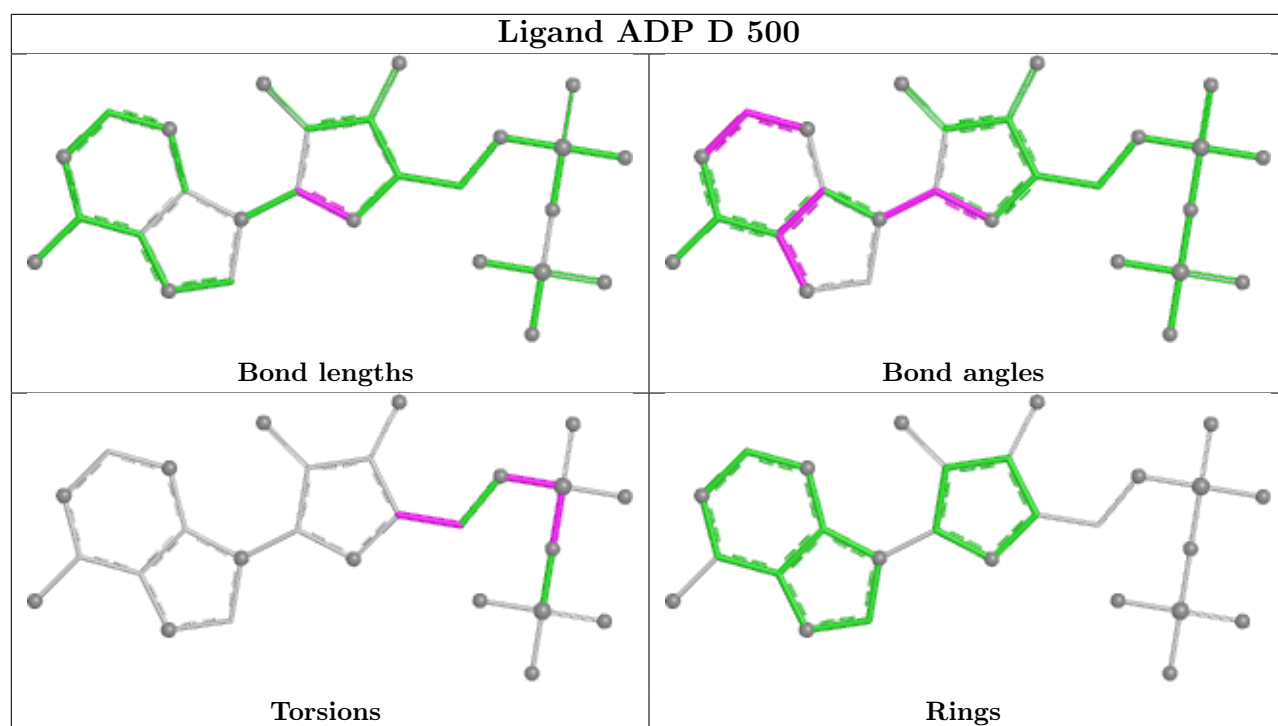
Mol	Chain	Res	Type	Atoms
3	A	500	ADP	PB-O3A-PA-O2A
3	C	500	ADP	PB-O3A-PA-O2A
3	E	500	ADP	PB-O3A-PA-O2A
3	F	500	ADP	PB-O3A-PA-O2A
3	B	500	ADP	C5'-O5'-PA-O1A
3	B	500	ADP	C5'-O5'-PA-O3A
3	D	500	ADP	C5'-O5'-PA-O1A
3	D	500	ADP	C5'-O5'-PA-O3A
3	E	500	ADP	C5'-O5'-PA-O3A
3	B	500	ADP	PB-O3A-PA-O2A
3	D	500	ADP	PB-O3A-PA-O1A
3	D	500	ADP	PB-O3A-PA-O2A
3	C	500	ADP	PB-O3A-PA-O1A
3	F	500	ADP	PB-O3A-PA-O1A
3	A	500	ADP	PB-O3A-PA-O1A
3	E	500	ADP	PB-O3A-PA-O1A

There are no ring outliers.

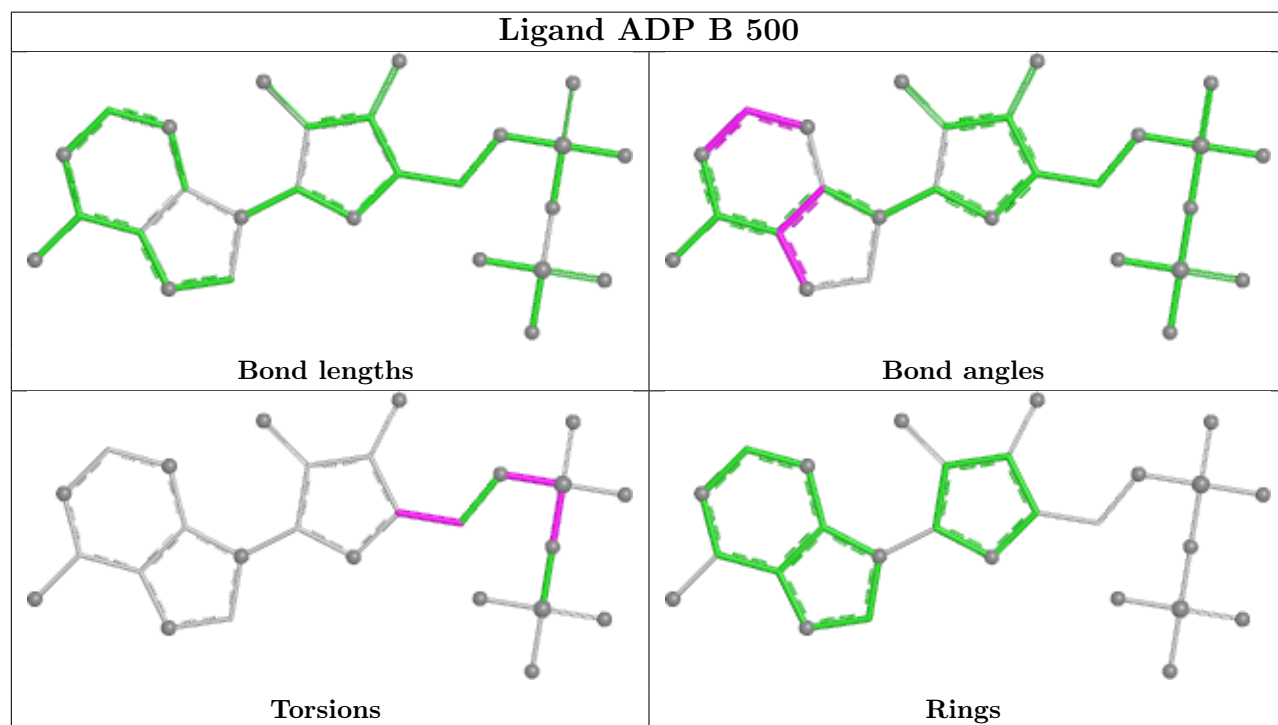
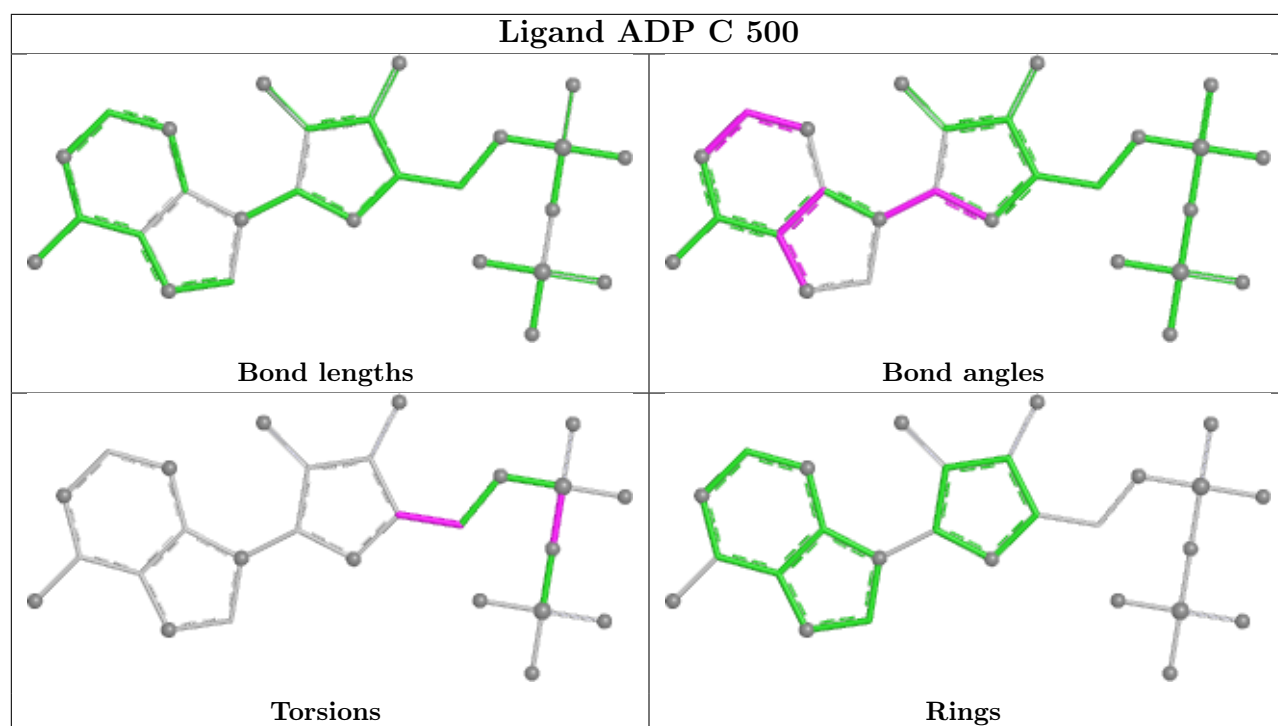
6 monomers are involved in 8 short contacts:

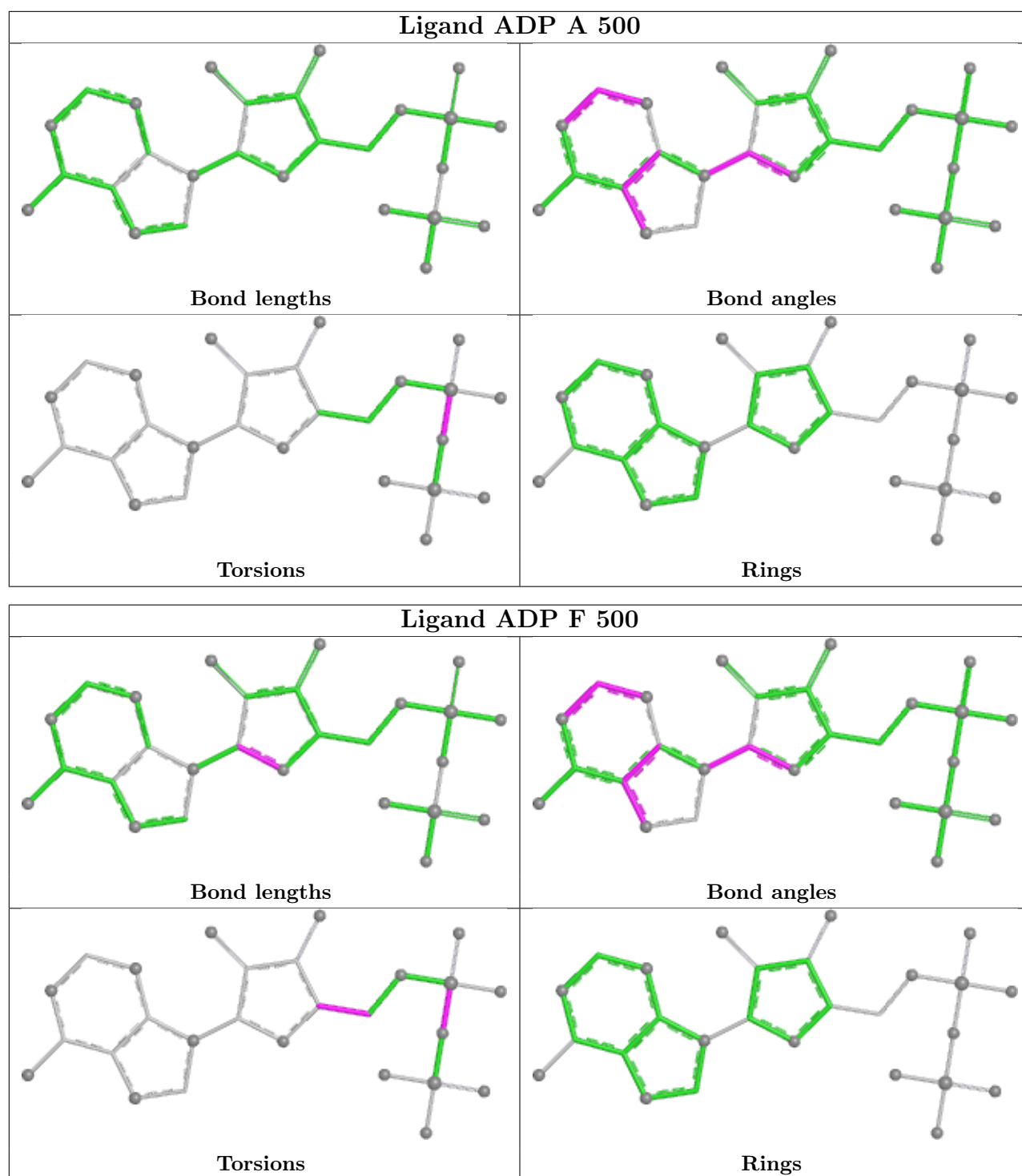
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	500	ADP	1	0
3	E	500	ADP	1	0
3	C	500	ADP	2	0
3	B	500	ADP	1	0
3	A	500	ADP	1	0
3	F	500	ADP	2	0

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

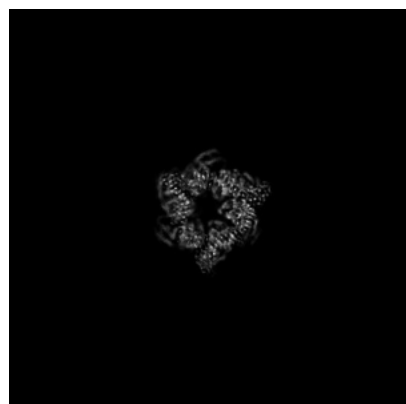
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70271. These allow visual inspection of the internal detail of the map and identification of artifacts.

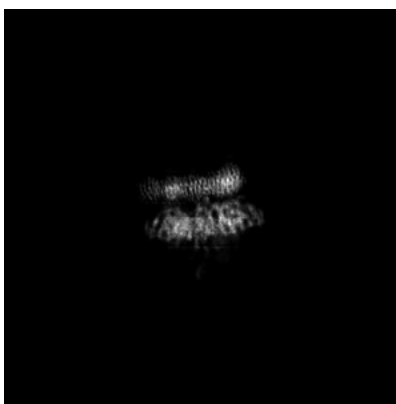
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

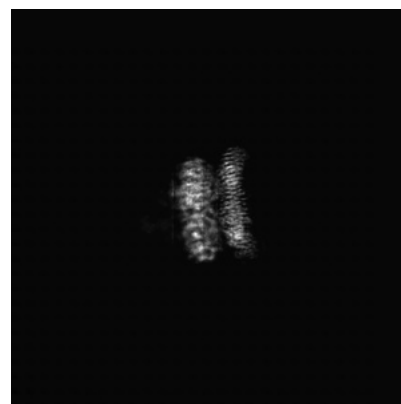
#### 6.1.1 Primary map



X

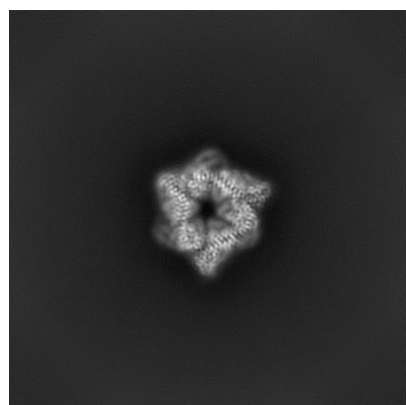


Y

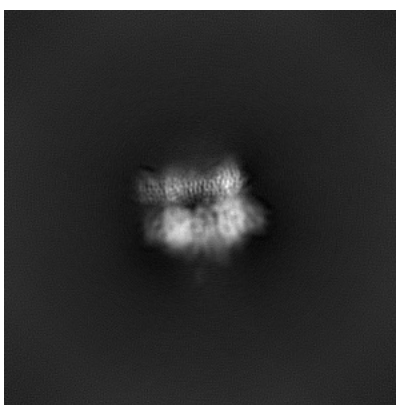


Z

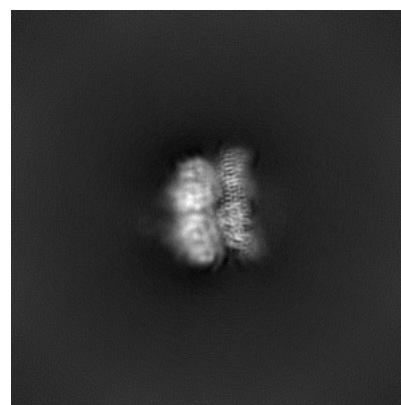
#### 6.1.2 Raw map



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: 200

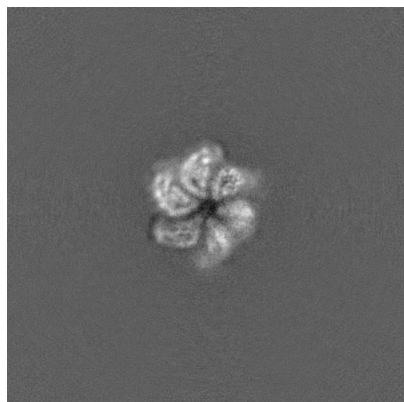


Y Index: 200

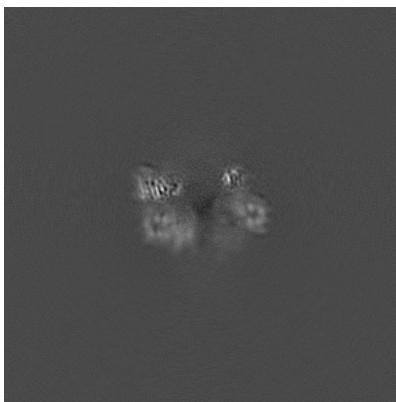


Z Index: 200

### 6.2.2 Raw map



X Index: 200



Y Index: 200

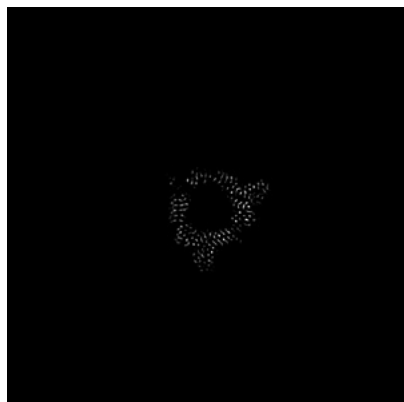


Z Index: 200

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: 220

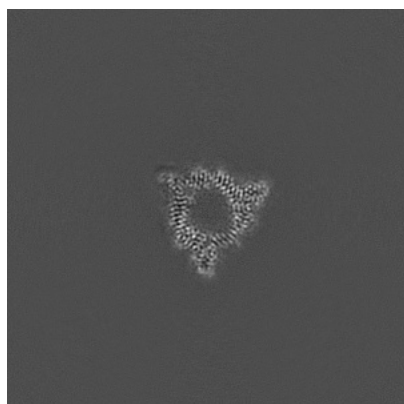


Y Index: 174



Z Index: 218

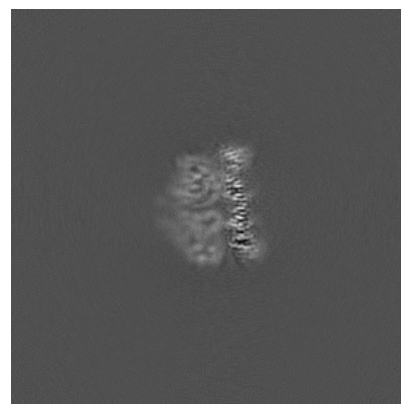
### 6.3.2 Raw map



X Index: 223



Y Index: 174

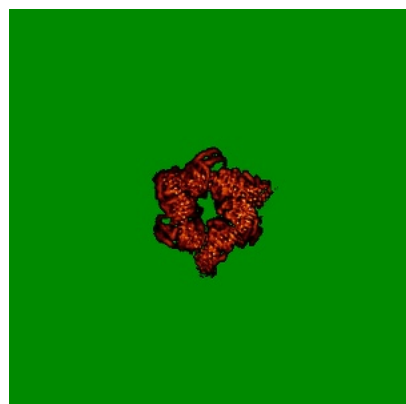


Z Index: 223

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

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

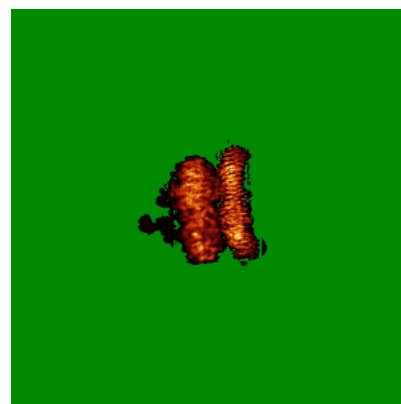
### 6.4.1 Primary map



X

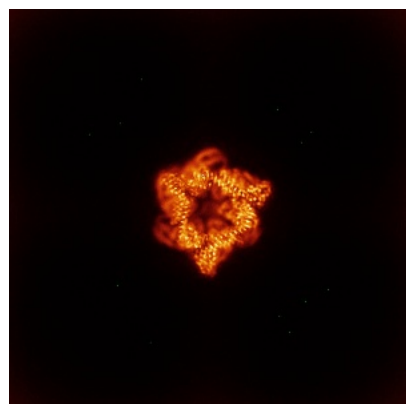


Y

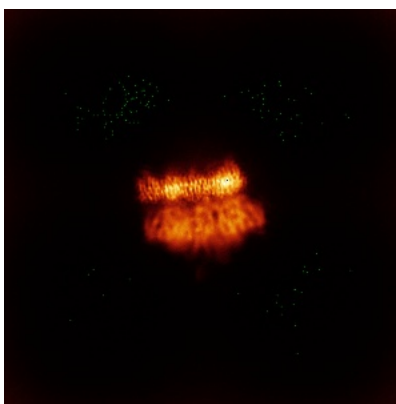


Z

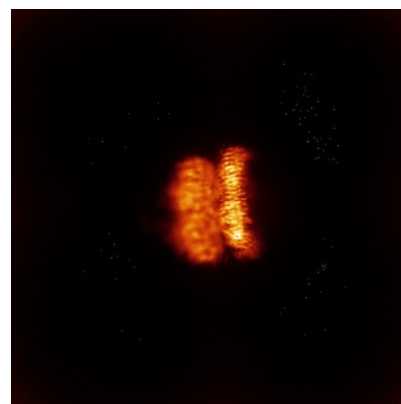
### 6.4.2 Raw map



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.

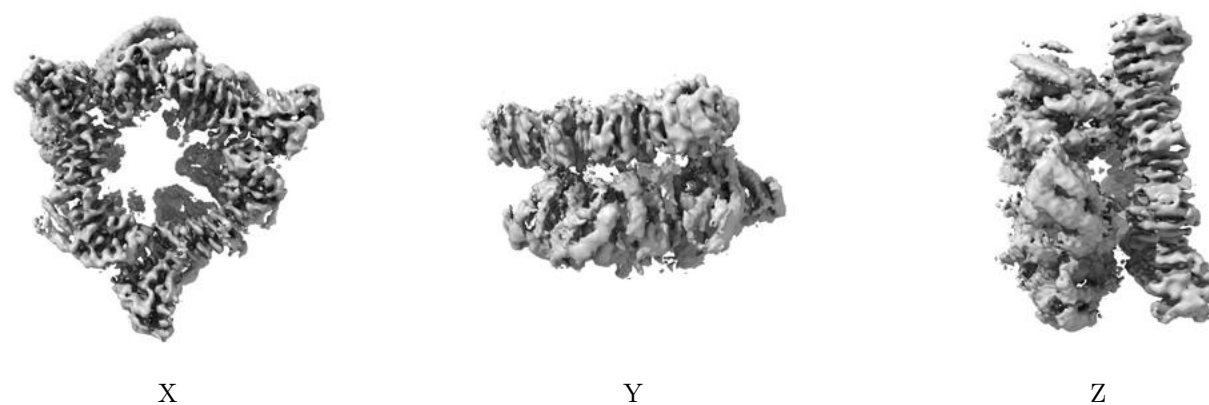
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.109. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 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.

## 6.6 Mask visualisation [i](#)

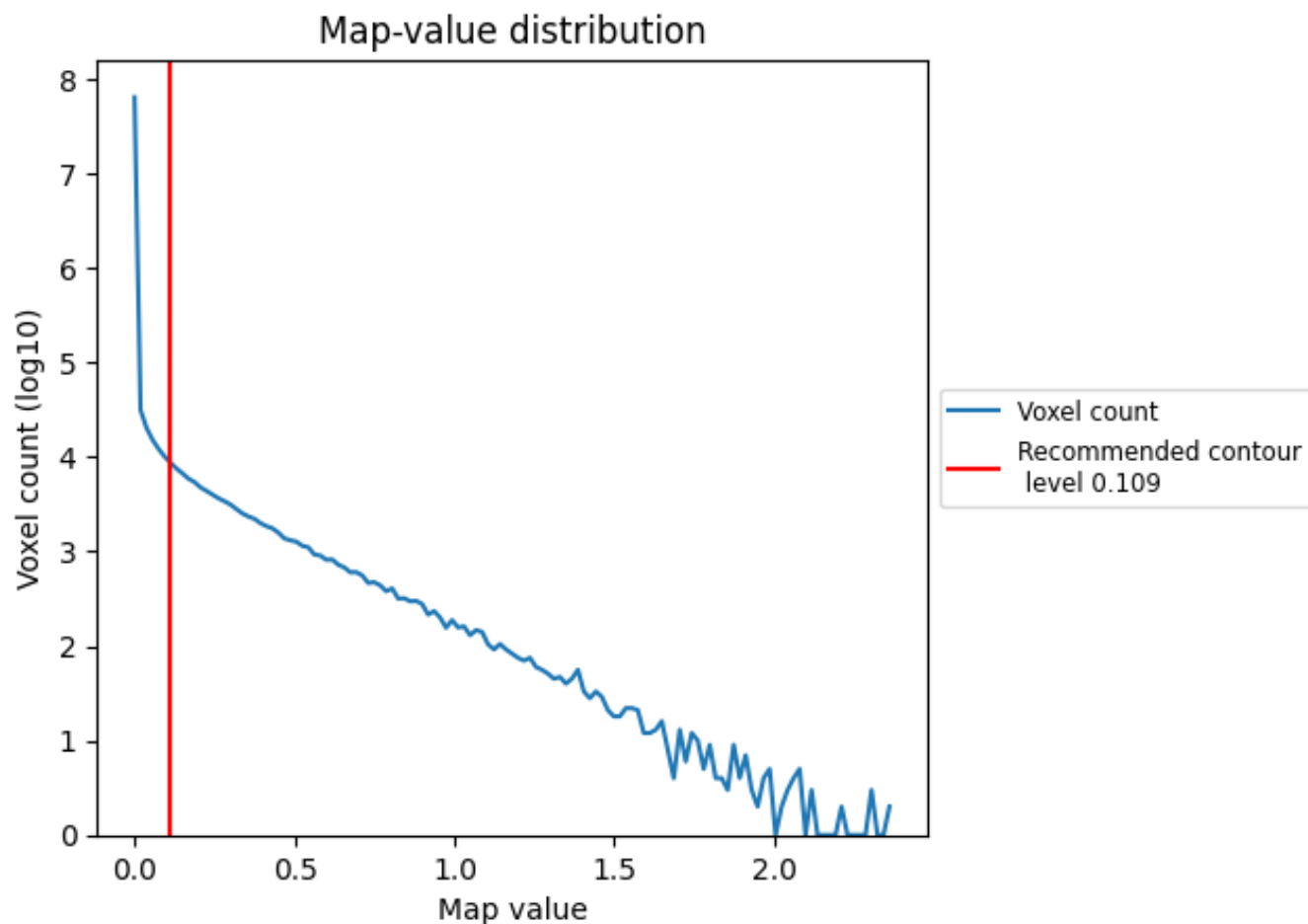
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

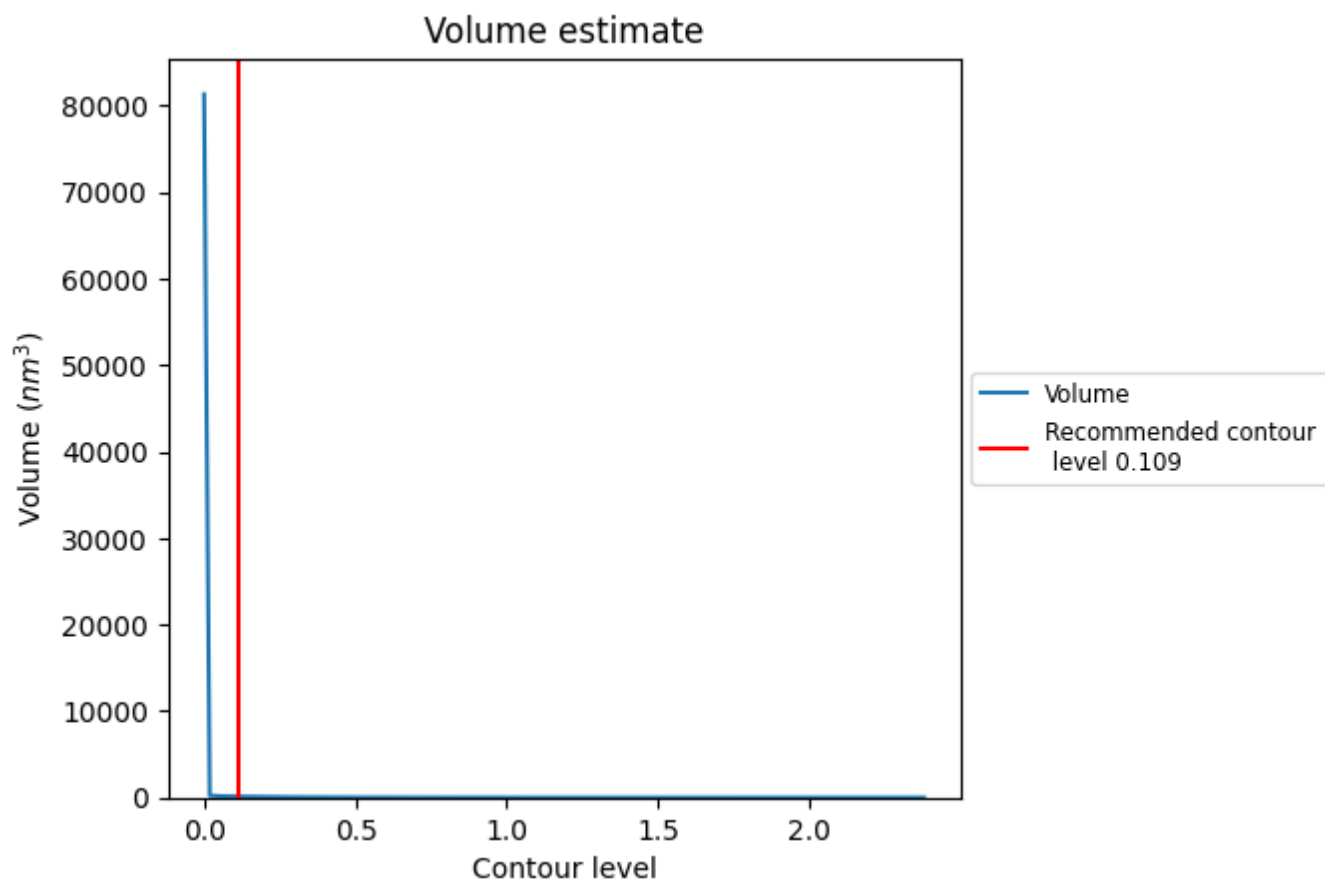
This section contains the results of statistical analysis of the map.

### 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.

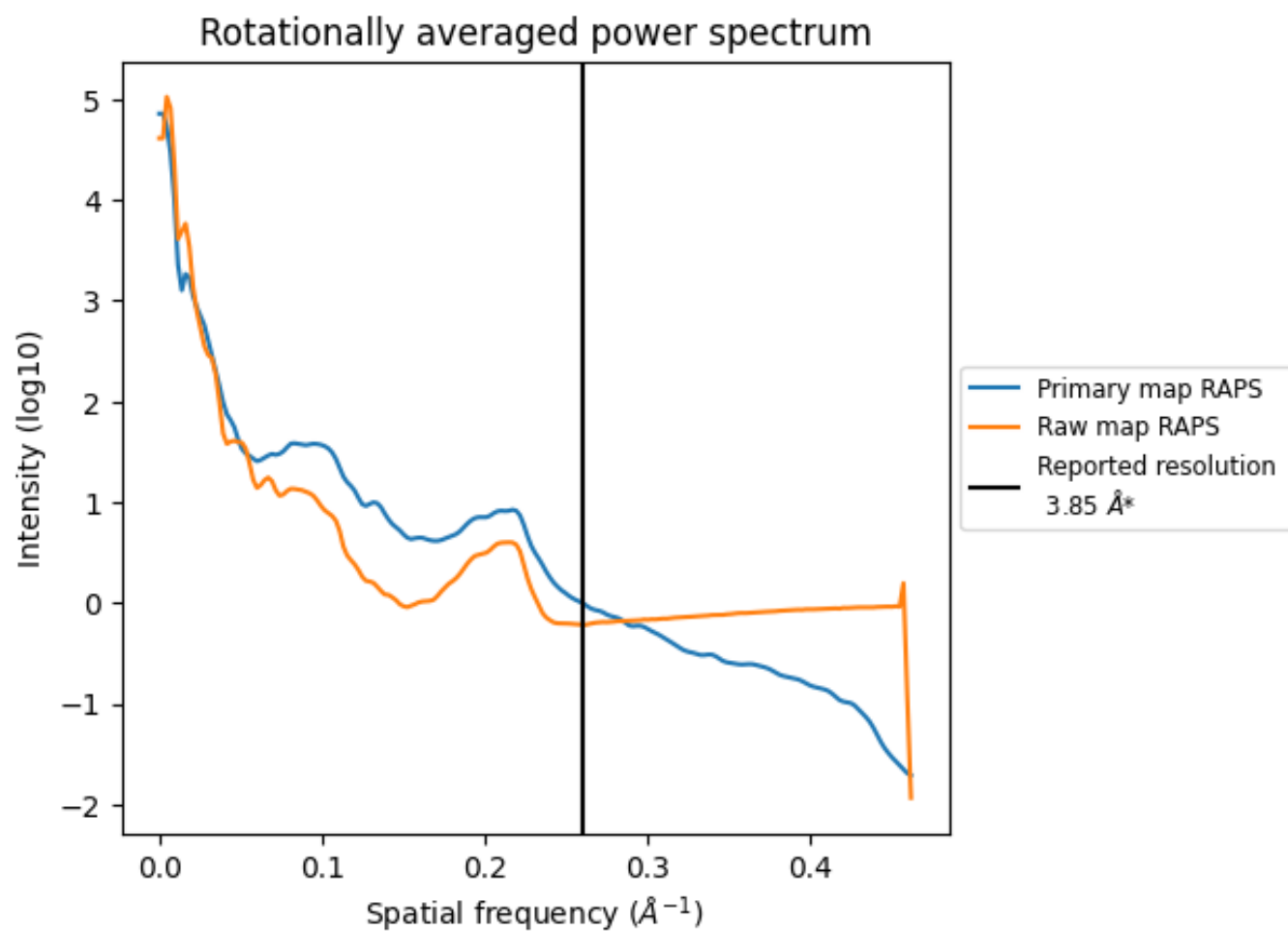
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121 nm<sup>3</sup>; this corresponds to an approximate mass of 109 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 ⓘ

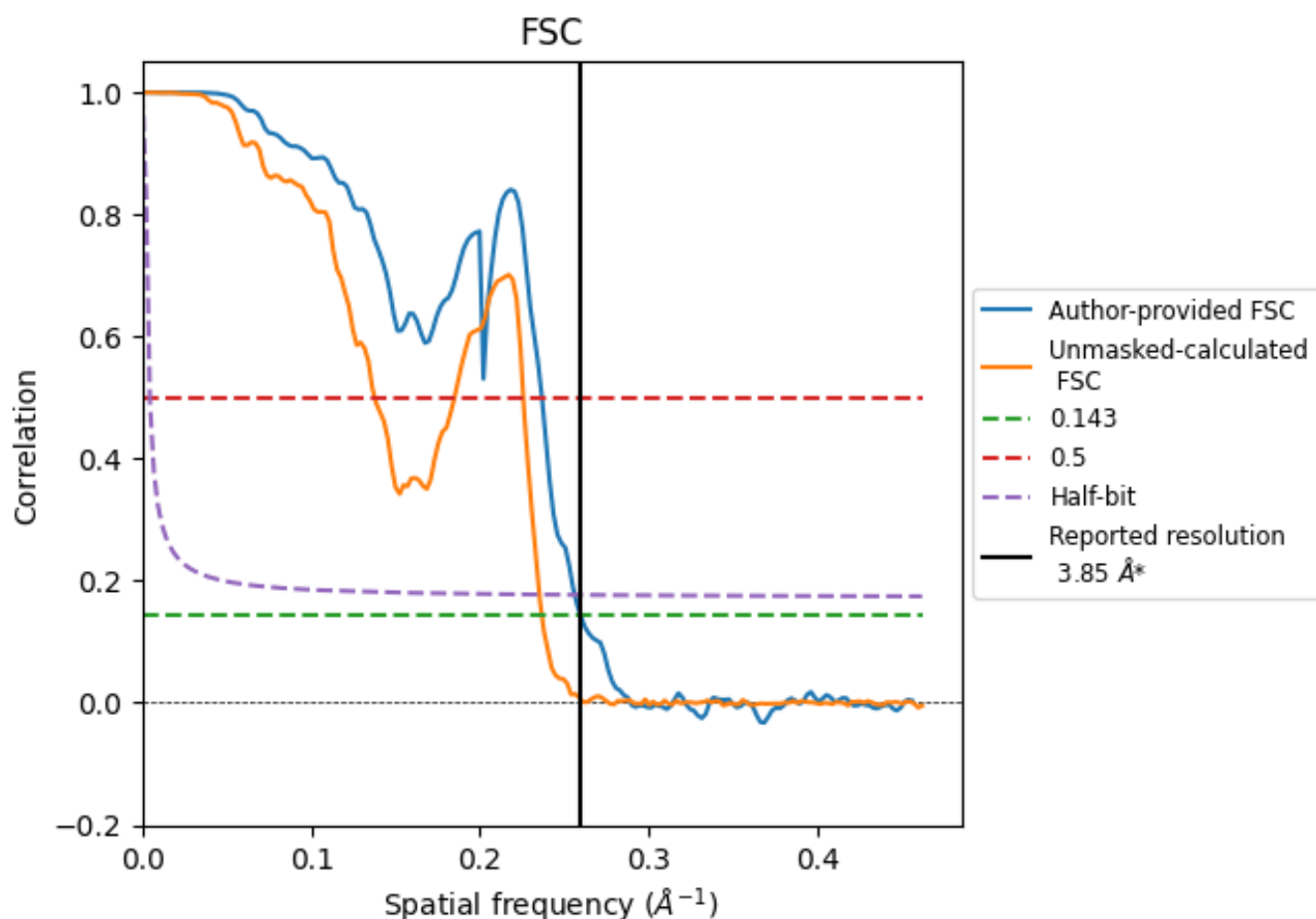


\*Reported resolution corresponds to spatial frequency of 0.260 Å<sup>-1</sup>

## 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 0.260  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

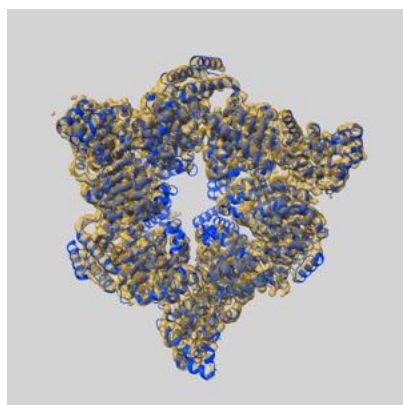
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	3.85	4.22	3.91
Unmasked-calculated*	4.23	7.26	4.25

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

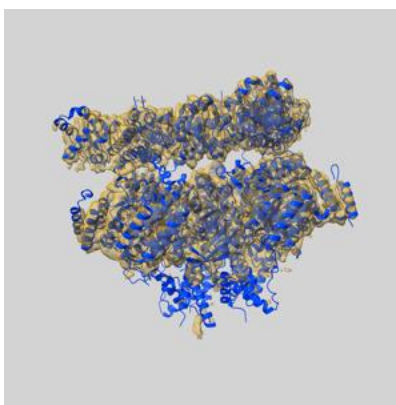
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70271 and PDB model 9OA2. Per-residue inclusion information can be found in section [3](#) on page [7](#).

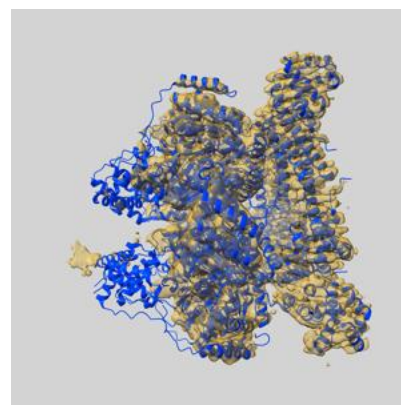
### 9.1 Map-model overlay [i](#)



X



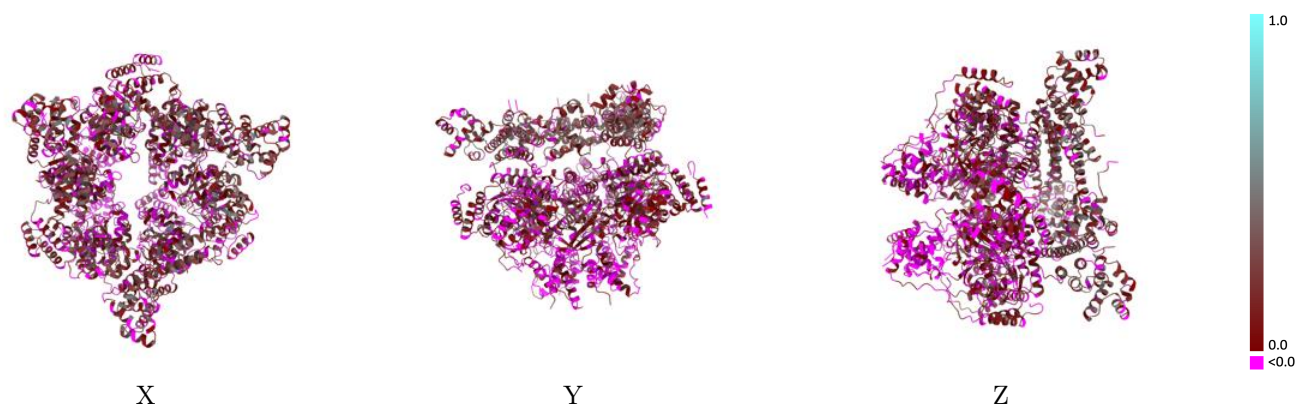
Y



Z

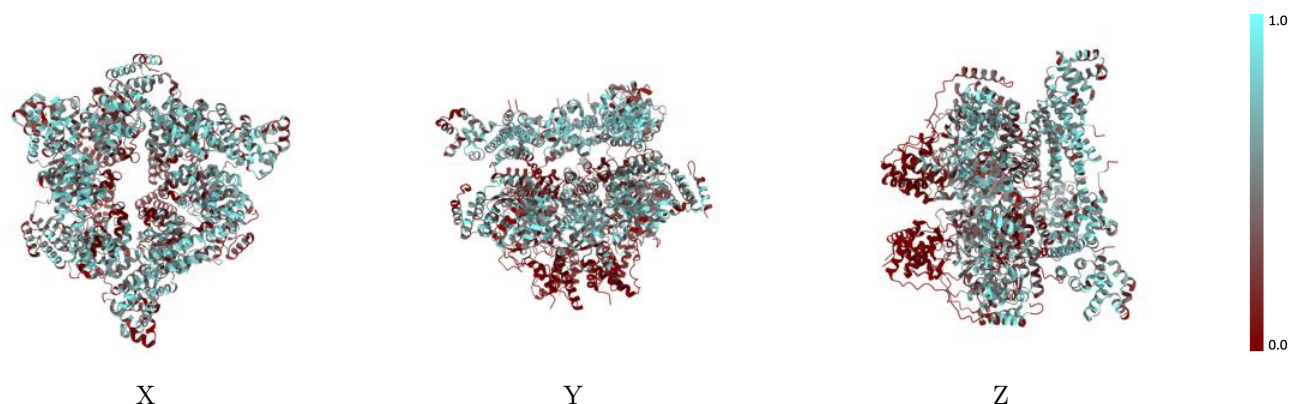
The images above show the 3D surface view of the map at the recommended contour level 0.109 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



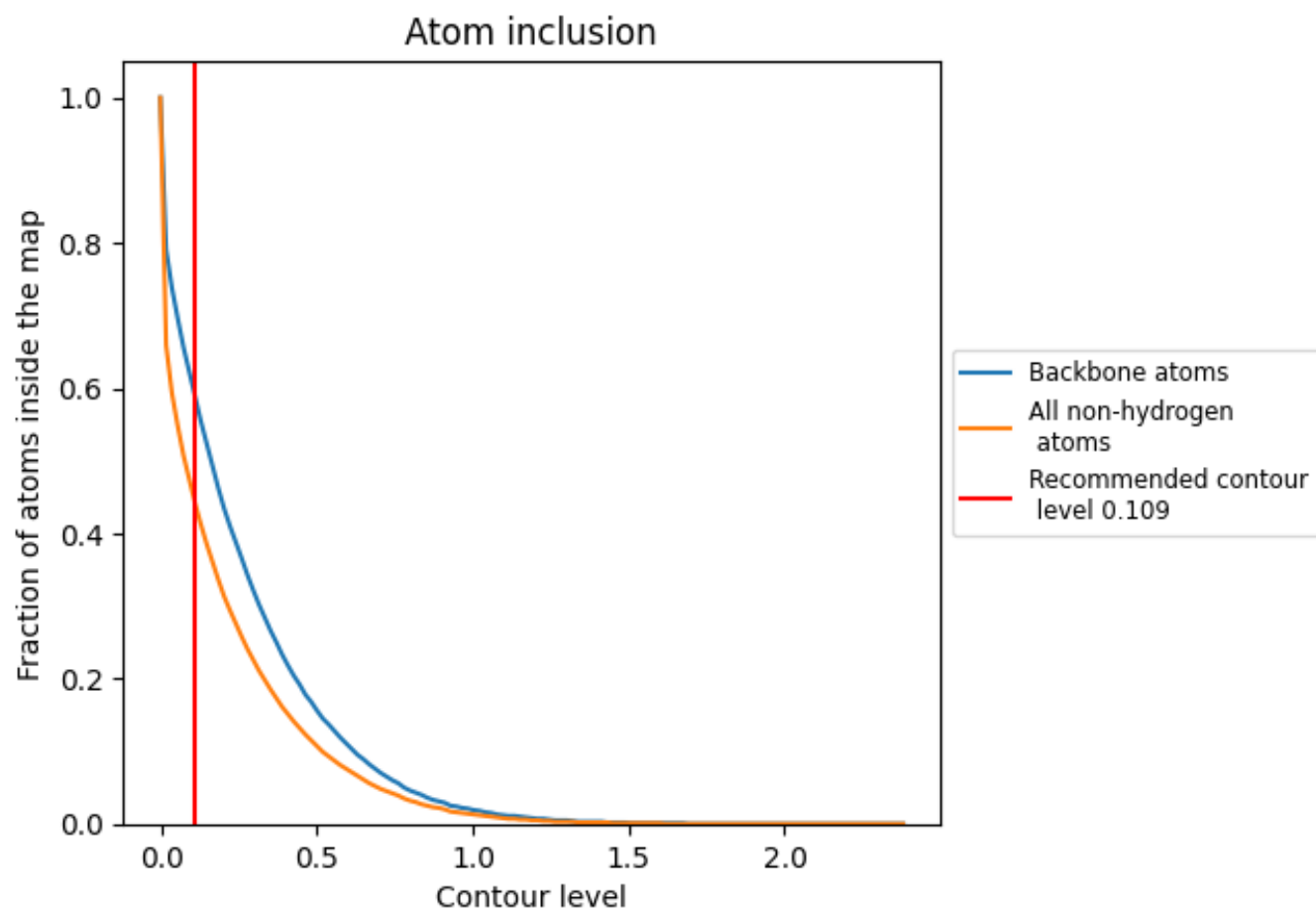
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.109).

## 9.4 Atom inclusion [i](#)





























At the recommended contour level, 59% of all backbone atoms, 44% 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 (0.109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4420	 0.1030
A	 0.5520	 0.1570
B	 0.4770	 0.0990
C	 0.5190	 0.1180
D	 0.4290	 0.0900
E	 0.5220	 0.1230
F	 0.5450	 0.1460
U	 0.3290	 0.0380
V	 0.0720	 -0.0310
W	 0.0560	 -0.0010
X	 0.2530	 0.0320
Y	 0.0420	 -0.0030
Z	 0.1240	 0.0180

