



## Full wwPDB EM Validation Report ⓘ

Apr 17, 2025 – 12:23 PM JST

PDB ID : 9LGO / pdb\_00009lgo  
EMDB ID : EMD-63069  
Title : Cryo-EM structure of the SPATA5-SPATA5L1-CINP-C1orf109 complex  
Authors : Dai, Y.; Zhang, Y.; Gao, N.  
Deposited on : 2025-01-10  
Resolution : 3.51 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

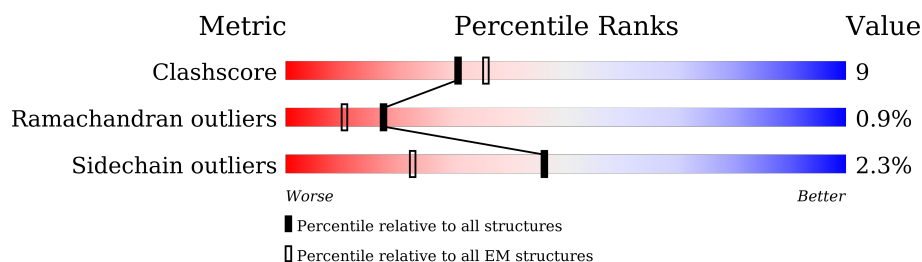
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.51 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	886	
1	B	886	
1	D	886	
1	E	886	
2	I	242	
2	J	242	
3	G	275	
3	H	275	

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Mol	Chain	Length	Quality of chain
4	C	749	<div><div></div><div>78%</div><div>12%</div><div>9%</div></div>
4	F	749	<div><div>6%</div><div>73%</div><div>16%</div><div>7%</div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 38406 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 ATPase family gene 2 protein homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	700	Total	C	N	O	S	0	0
			5418	3444	938	1009	27		
1	E	699	Total	C	N	O	S	0	0
			5377	3420	933	998	26		
1	D	710	Total	C	N	O	S	0	0
			5498	3498	952	1021	27		
1	B	701	Total	C	N	O	S	0	0
			5394	3429	938	1000	27		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	GLN	GLU	conflict	UNP Q8NB90
A	728	GLN	GLU	conflict	UNP Q8NB90
E	454	GLN	GLU	conflict	UNP Q8NB90
E	728	GLN	GLU	conflict	UNP Q8NB90
D	454	GLN	GLU	conflict	UNP Q8NB90
D	728	GLN	GLU	conflict	UNP Q8NB90
B	454	GLN	GLU	conflict	UNP Q8NB90
B	728	GLN	GLU	conflict	UNP Q8NB90

- Molecule 2 is a protein called Cyclin-dependent kinase 2-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	174	Total	C	N	O	S	0	0
			1420	903	241	270	6		
2	I	174	Total	C	N	O	S	0	0
			1420	903	241	270	6		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-29	MET	-	initiating methionine	UNP Q9BW66

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-28	TRP	-	expression tag	UNP Q9BW66
J	-27	SER	-	expression tag	UNP Q9BW66
J	-26	HIS	-	expression tag	UNP Q9BW66
J	-25	PRO	-	expression tag	UNP Q9BW66
J	-24	GLN	-	expression tag	UNP Q9BW66
J	-23	PHE	-	expression tag	UNP Q9BW66
J	-22	GLU	-	expression tag	UNP Q9BW66
J	-21	LYS	-	expression tag	UNP Q9BW66
J	-20	GLY	-	expression tag	UNP Q9BW66
J	-19	GLY	-	expression tag	UNP Q9BW66
J	-18	GLY	-	expression tag	UNP Q9BW66
J	-17	SER	-	expression tag	UNP Q9BW66
J	-16	GLY	-	expression tag	UNP Q9BW66
J	-15	GLY	-	expression tag	UNP Q9BW66
J	-14	GLY	-	expression tag	UNP Q9BW66
J	-13	SER	-	expression tag	UNP Q9BW66
J	-12	GLY	-	expression tag	UNP Q9BW66
J	-11	GLY	-	expression tag	UNP Q9BW66
J	-10	SER	-	expression tag	UNP Q9BW66
J	-9	ALA	-	expression tag	UNP Q9BW66
J	-8	TRP	-	expression tag	UNP Q9BW66
J	-7	SER	-	expression tag	UNP Q9BW66
J	-6	HIS	-	expression tag	UNP Q9BW66
J	-5	PRO	-	expression tag	UNP Q9BW66
J	-4	GLN	-	expression tag	UNP Q9BW66
J	-3	PHE	-	expression tag	UNP Q9BW66
J	-2	GLU	-	expression tag	UNP Q9BW66
J	-1	LYS	-	expression tag	UNP Q9BW66
J	0	GLY	-	expression tag	UNP Q9BW66
I	-29	MET	-	initiating methionine	UNP Q9BW66
I	-28	TRP	-	expression tag	UNP Q9BW66
I	-27	SER	-	expression tag	UNP Q9BW66
I	-26	HIS	-	expression tag	UNP Q9BW66
I	-25	PRO	-	expression tag	UNP Q9BW66
I	-24	GLN	-	expression tag	UNP Q9BW66
I	-23	PHE	-	expression tag	UNP Q9BW66
I	-22	GLU	-	expression tag	UNP Q9BW66
I	-21	LYS	-	expression tag	UNP Q9BW66
I	-20	GLY	-	expression tag	UNP Q9BW66
I	-19	GLY	-	expression tag	UNP Q9BW66
I	-18	GLY	-	expression tag	UNP Q9BW66
I	-17	SER	-	expression tag	UNP Q9BW66

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-16	GLY	-	expression tag	UNP Q9BW66
I	-15	GLY	-	expression tag	UNP Q9BW66
I	-14	GLY	-	expression tag	UNP Q9BW66
I	-13	SER	-	expression tag	UNP Q9BW66
I	-12	GLY	-	expression tag	UNP Q9BW66
I	-11	GLY	-	expression tag	UNP Q9BW66
I	-10	SER	-	expression tag	UNP Q9BW66
I	-9	ALA	-	expression tag	UNP Q9BW66
I	-8	TRP	-	expression tag	UNP Q9BW66
I	-7	SER	-	expression tag	UNP Q9BW66
I	-6	HIS	-	expression tag	UNP Q9BW66
I	-5	PRO	-	expression tag	UNP Q9BW66
I	-4	GLN	-	expression tag	UNP Q9BW66
I	-3	PHE	-	expression tag	UNP Q9BW66
I	-2	GLU	-	expression tag	UNP Q9BW66
I	-1	LYS	-	expression tag	UNP Q9BW66
I	0	GLY	-	expression tag	UNP Q9BW66

- Molecule 3 is a protein called cDNA FLJ55172.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	203	Total	C	N	O	S	0	0
			1647	1046	290	306	5		
3	G	200	Total	C	N	O	S	0	0
			1623	1032	286	301	4		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	MET	-	initiating methionine	UNP B4DRQ5
H	-8	TYR	-	expression tag	UNP B4DRQ5
H	-7	PRO	-	expression tag	UNP B4DRQ5
H	-6	TYR	-	expression tag	UNP B4DRQ5
H	-5	ASP	-	expression tag	UNP B4DRQ5
H	-4	VAL	-	expression tag	UNP B4DRQ5
H	-3	PRO	-	expression tag	UNP B4DRQ5
H	-2	ASP	-	expression tag	UNP B4DRQ5
H	-1	TYR	-	expression tag	UNP B4DRQ5
H	0	ALA	-	expression tag	UNP B4DRQ5
G	-9	MET	-	initiating methionine	UNP B4DRQ5
G	-8	TYR	-	expression tag	UNP B4DRQ5
G	-7	PRO	-	expression tag	UNP B4DRQ5

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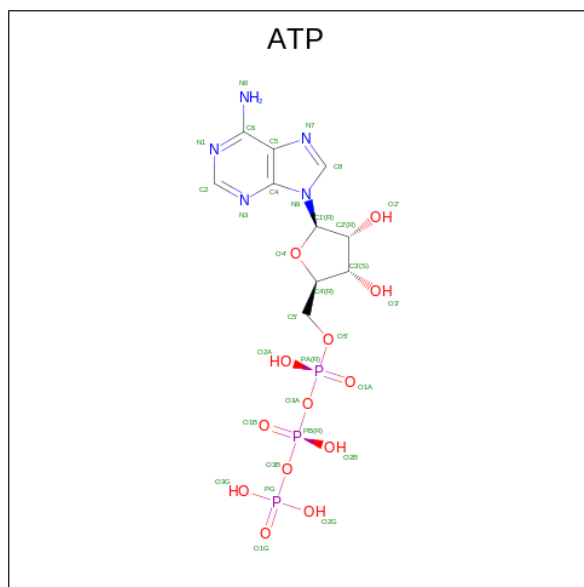
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	TYR	-	expression tag	UNP B4DRQ5
G	-5	ASP	-	expression tag	UNP B4DRQ5
G	-4	VAL	-	expression tag	UNP B4DRQ5
G	-3	PRO	-	expression tag	UNP B4DRQ5
G	-2	ASP	-	expression tag	UNP B4DRQ5
G	-1	TYR	-	expression tag	UNP B4DRQ5
G	0	ALA	-	expression tag	UNP B4DRQ5

- Molecule 4 is a protein called ATPase family gene 2 protein homolog B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	693	Total	C	N	O	S	0	0
			5228	3308	939	959	22		
4	C	681	Total	C	N	O	S	0	0
			5132	3245	925	940	22		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

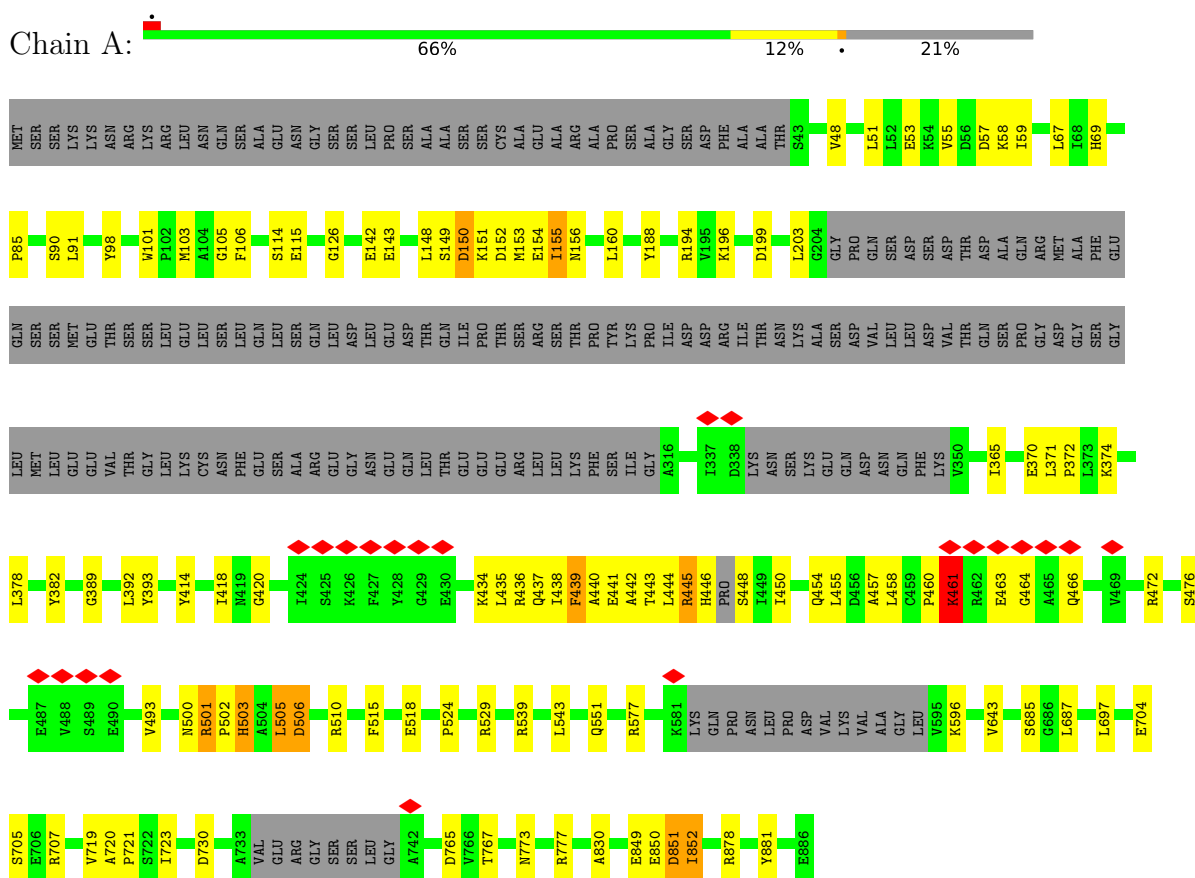
Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total	Mg	0
			1	1	



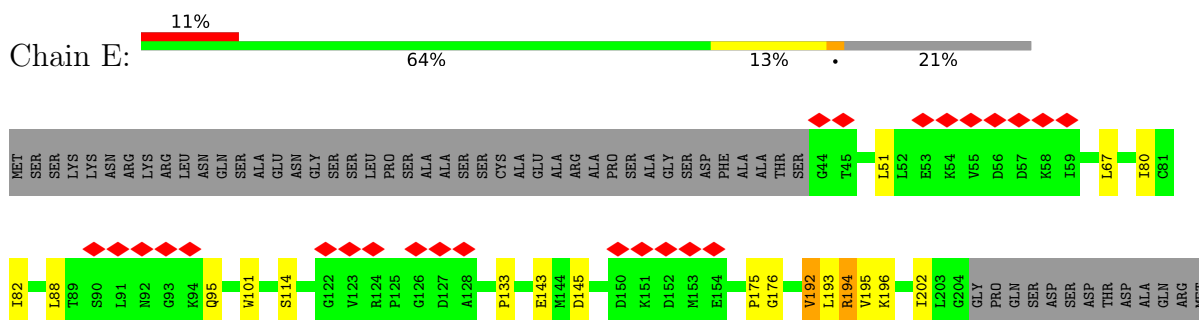
### 3 Residue-property plots

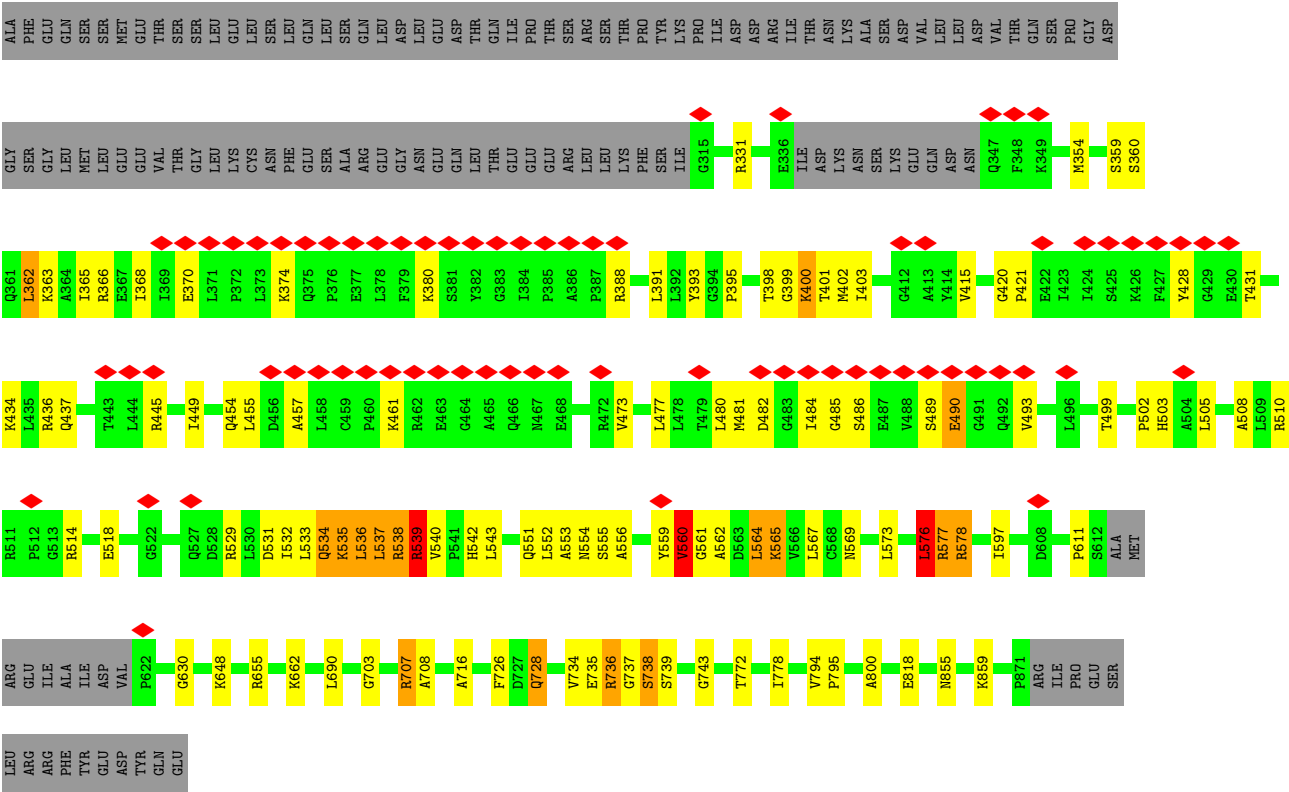
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ATPase family gene 2 protein homolog A

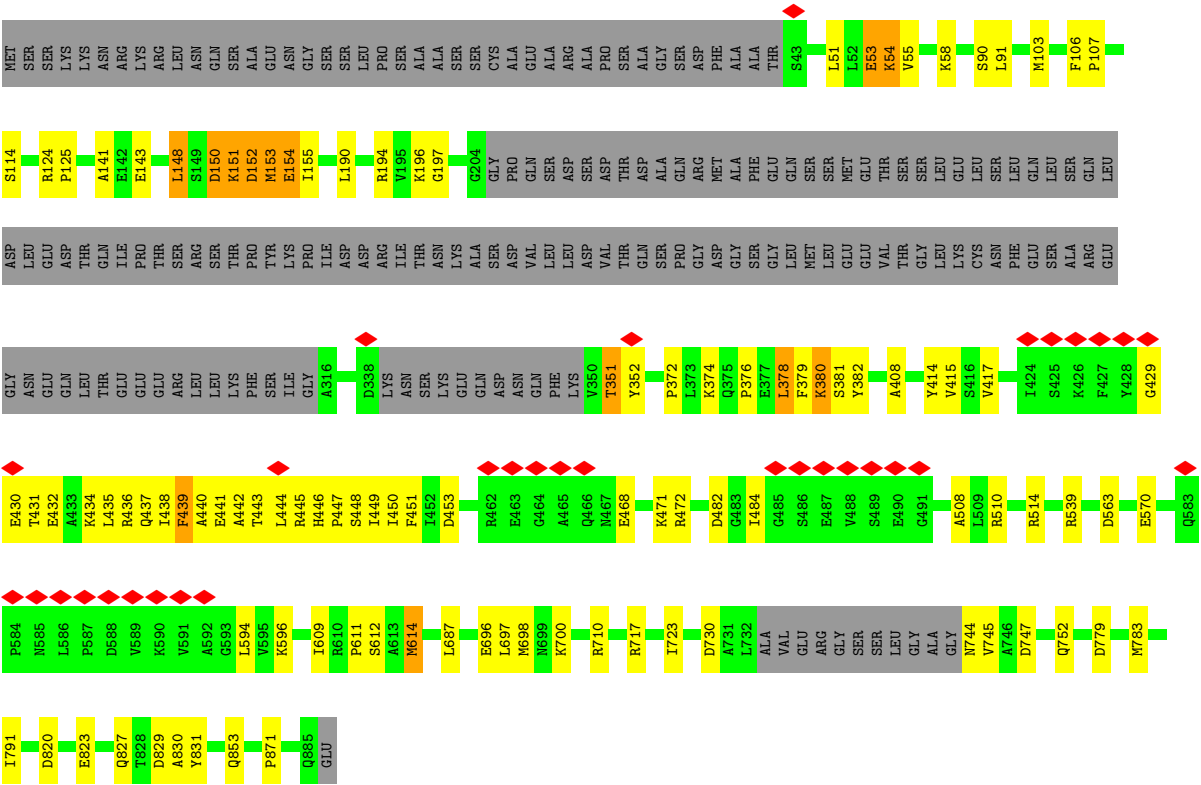


- Molecule 1: ATPase family gene 2 protein homolog A

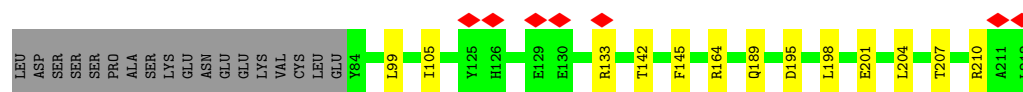




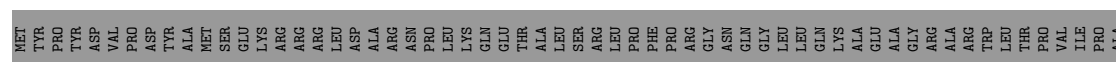
• Molecule 1: ATPase family gene 2 protein homolog A



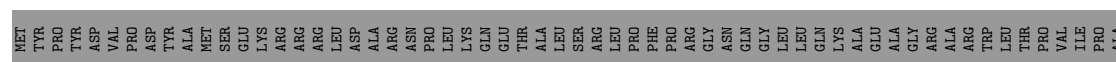




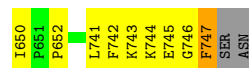
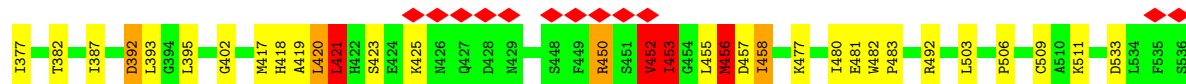
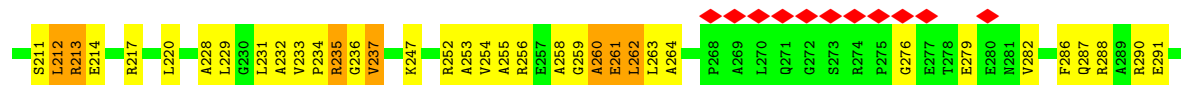
• Molecule 3: cDNA FLJ55172



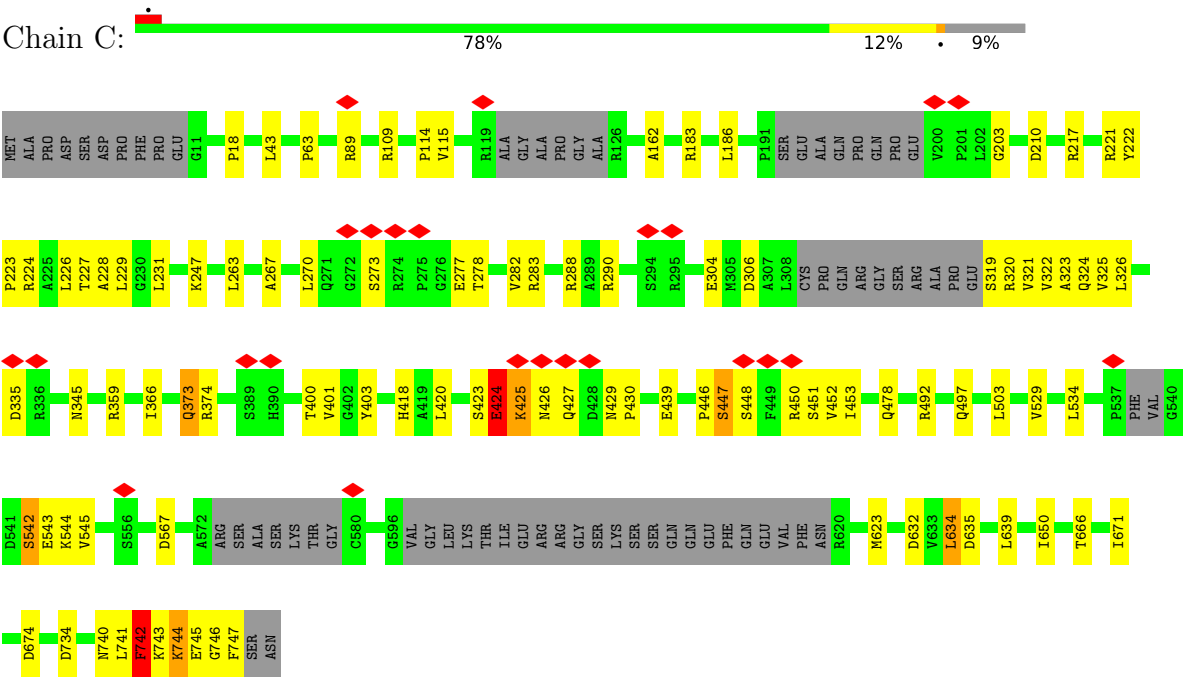
• Molecule 3: cDNA FLJ55172



• Molecule 4: ATPase family gene 2 protein homolog B



• Molecule 4: ATPase family gene 2 protein homolog B



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	194789	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	18.331	Depositor
Minimum map value	-0.442	Depositor
Average map value	0.071	Depositor
Map value standard deviation	0.706	Depositor
Recommended contour level	1	Depositor
Map size ( $\text{\AA}$ )	305.76, 305.76, 305.76	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.092, 1.092, 1.092	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, ATP

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	0.40	0/5502	0.71	1/7439 (0.0%)
1	B	0.34	0/5479	0.69	0/7409
1	D	0.39	0/5587	0.70	0/7560
1	E	0.39	0/5463	0.73	0/7389
2	I	0.38	0/1450	0.60	0/1959
2	J	0.46	0/1450	0.68	0/1959
3	G	0.42	0/1652	0.65	0/2235
3	H	0.46	1/1676 (0.1%)	0.71	0/2267
4	C	0.41	0/5220	0.72	0/7087
4	F	0.47	0/5322	0.74	1/7230 (0.0%)
All	All	0.41	1/38801 (0.0%)	0.70	2/52534 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	67	ARG	C-N	5.04	1.43	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	LEU	N-CA-C	-5.96	94.90	111.00
4	F	235	ARG	N-CA-C	-5.12	97.18	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	5418	0	5581	109	0
1	B	5394	0	5581	64	0
1	D	5498	0	5677	88	0
1	E	5377	0	5562	139	0
2	I	1420	0	1415	8	0
2	J	1420	0	1415	27	0
3	G	1623	0	1646	7	0
3	H	1647	0	1670	8	0
4	C	5132	0	5328	101	0
4	F	5228	0	5418	153	0
5	A	31	0	12	0	0
5	B	31	0	12	0	0
5	C	62	0	24	2	0
5	D	31	0	12	0	0
5	E	31	0	12	2	0
5	F	62	0	24	0	0
6	C	1	0	0	0	0
All	All	38406	0	39389	674	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (674) 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)
4:C:744:LYS:NZ	4:C:745:GLU:HB3	1.37	1.32
1:E:536:LEU:HD13	1:E:537:LEU:CD1	1.65	1.24
4:F:557:THR:HA	4:F:620:ARG:HH12	1.11	1.16
4:C:744:LYS:NZ	4:C:745:GLU:CB	2.08	1.15
1:E:536:LEU:HD13	1:E:537:LEU:HD11	1.31	1.08
4:C:744:LYS:HZ1	4:C:745:GLU:CB	1.67	1.03
4:F:557:THR:CA	4:F:620:ARG:HH12	1.70	1.03
1:E:536:LEU:HD13	1:E:537:LEU:HD13	1.41	1.03
4:F:557:THR:HA	4:F:620:ARG:NH1	1.74	1.00
1:B:530:LEU:HD13	1:B:533:LEU:HD21	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:HD23	1:A:505:LEU:HD11	1.46	0.97
4:C:453:ILE:HD13	4:C:529:VAL:HG22	1.47	0.97
1:E:533:LEU:O	1:E:536:LEU:HB2	1.65	0.96
4:F:557:THR:HB	4:F:558:PRO:HD2	1.46	0.95
4:C:424:GLU:HG2	4:C:426:ASN:H	1.32	0.95
4:C:744:LYS:HZ1	4:C:745:GLU:HB3	0.79	0.93
1:A:155:ILE:HG13	1:A:160:LEU:HD22	1.50	0.91
1:E:529:ARG:HD2	1:E:556:ALA:HB1	1.50	0.91
4:F:323:ALA:HA	4:F:326:LEU:HG	1.53	0.90
1:E:559:TYR:H	1:E:611:PRO:HB2	1.36	0.90
4:C:282:VAL:HG21	4:C:324:GLN:HG3	1.52	0.88
4:F:506:PRO:HG3	4:F:652:PRO:HG3	1.53	0.88
1:A:461:LYS:HZ2	1:A:506:ASP:HA	1.38	0.86
1:D:378:LEU:HG	4:C:420:LEU:HD11	1.57	0.86
1:A:414:TYR:HB3	1:A:445:ARG:HG3	1.57	0.85
1:E:421:PRO:HD3	1:E:454:GLN:HG3	1.60	0.84
1:E:529:ARG:HD2	1:E:556:ALA:CB	2.08	0.83
4:F:304:GLU:C	4:F:306:ASP:H	1.82	0.82
4:C:221:ARG:O	4:C:223:PRO:HD3	1.79	0.82
4:F:52:PRO:HA	4:F:98:ARG:HH22	1.43	0.81
4:F:324:GLN:HA	4:F:327:THR:HG22	1.62	0.81
1:D:440:ALA:HB1	1:D:443:THR:HA	1.60	0.81
1:B:543:LEU:HB3	1:B:597:ILE:O	1.79	0.81
1:E:559:TYR:N	1:E:611:PRO:HB2	1.96	0.80
1:A:414:TYR:CB	1:A:445:ARG:HG3	2.12	0.79
1:E:481:MET:HA	1:E:485:GLY:HA3	1.65	0.78
4:C:744:LYS:HZ2	4:C:745:GLU:CB	1.95	0.78
1:D:153:MET:C	1:D:155:ILE:H	1.87	0.77
1:A:441:GLU:O	1:A:444:LEU:HB2	1.85	0.77
1:A:440:ALA:O	1:A:443:THR:HB	1.85	0.77
4:F:557:THR:HA	4:F:620:ARG:HH22	1.49	0.76
4:F:107:LEU:HD23	4:F:170:PRO:HD2	1.68	0.75
4:F:557:THR:HA	4:F:620:ARG:NH2	2.01	0.75
1:E:735:GLU:HG2	1:E:737:GLY:H	1.52	0.74
1:E:577:ARG:HH21	1:E:578:ARG:HH22	1.33	0.74
4:F:557:THR:HA	4:F:620:ARG:CZ	2.15	0.74
1:A:543:LEU:HD21	1:A:596:LYS:HG3	1.69	0.73
4:C:217:ARG:HB2	4:C:221:ARG:HD2	1.69	0.73
1:D:436:ARG:HH21	1:D:440:ALA:HA	1.53	0.73
1:D:153:MET:O	1:D:155:ILE:N	2.21	0.73
1:D:451:PHE:CE2	1:D:453:ASP:HB2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:GLU:O	1:D:445:ARG:HB2	1.90	0.71
4:F:319:SER:O	4:F:322:VAL:HB	1.89	0.71
1:E:536:LEU:CD1	1:E:537:LEU:HD11	2.14	0.71
1:E:539:ARG:HB2	1:E:539:ARG:NH1	2.06	0.71
1:D:53:GLU:O	1:D:54:LYS:HB3	1.88	0.71
1:E:559:TYR:HB3	1:E:611:PRO:HB2	1.71	0.71
1:D:442:ALA:HB3	1:D:445:ARG:HB2	1.72	0.70
4:F:315:ARG:HB2	4:F:318:GLU:HG3	1.73	0.70
4:F:557:THR:CB	4:F:558:PRO:HD2	2.22	0.70
4:F:503:LEU:HD23	4:F:650:ILE:HD11	1.74	0.69
4:F:321:VAL:O	4:F:325:VAL:N	2.20	0.69
1:A:155:ILE:HG13	1:A:160:LEU:CD2	2.22	0.69
2:J:117:LYS:HE2	2:J:146:TYR:CE2	2.27	0.69
3:G:257:LEU:HD22	1:D:58:LYS:HD3	1.73	0.69
1:D:372:PRO:HG3	1:D:379:PHE:HE2	1.58	0.69
4:F:557:THR:CB	4:F:620:ARG:HH12	2.03	0.69
1:A:851:ASP:O	1:A:852:ILE:C	2.31	0.68
1:A:440:ALA:HA	1:A:443:THR:OG1	1.93	0.68
1:A:393:TYR:CG	1:A:502:PRO:HG3	2.29	0.67
1:D:431:THR:O	1:D:435:LEU:HG	1.95	0.67
4:C:743:LYS:O	4:C:744:LYS:C	2.31	0.67
1:A:53:GLU:O	1:A:55:VAL:HG23	1.95	0.67
4:C:744:LYS:HZ2	4:C:745:GLU:HB2	1.58	0.66
4:F:232:ALA:HB1	4:F:235:ARG:HE	1.60	0.66
4:C:278:THR:HG21	4:C:320:ARG:HD2	1.76	0.66
4:F:52:PRO:HD3	4:F:94:LEU:HD21	1.76	0.66
4:F:323:ALA:O	4:F:326:LEU:HB2	1.95	0.66
1:A:371:LEU:HD21	4:F:420:LEU:HD21	1.77	0.66
1:E:552:LEU:O	1:E:555:SER:HB2	1.96	0.66
1:B:436:ARG:HA	1:B:436:ARG:NE	2.11	0.66
1:A:442:ALA:HB1	1:A:448:SER:OG	1.96	0.66
1:D:414:TYR:O	1:D:449:ILE:N	2.29	0.66
4:F:304:GLU:C	4:F:306:ASP:N	2.49	0.65
1:E:421:PRO:CD	1:E:454:GLN:HG3	2.26	0.65
2:J:121:GLU:HA	2:J:124:ASN:ND2	2.12	0.65
4:F:741:LEU:HG	4:F:746:GLY:O	1.97	0.65
1:E:559:TYR:HB3	1:E:611:PRO:CB	2.27	0.64
1:A:371:LEU:HB3	1:A:372:PRO:HD3	1.78	0.64
4:F:213:ARG:HB2	4:F:213:ARG:CZ	2.26	0.64
1:D:436:ARG:HA	1:D:439:PHE:HB2	1.80	0.64
4:C:319:SER:N	4:C:321:VAL:HG12	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ARG:HH22	1:A:476:SER:HA	1.64	0.63
1:D:153:MET:C	1:D:155:ILE:N	2.49	0.63
1:A:503:HIS:CE1	1:A:707:ARG:HH11	2.16	0.63
1:A:543:LEU:CD2	1:A:596:LYS:HG3	2.28	0.63
4:C:740:ASN:O	4:C:744:LYS:HB2	1.99	0.63
4:C:492:ARG:HH22	1:B:855:ASN:HA	1.64	0.63
4:C:744:LYS:NZ	4:C:745:GLU:HB2	2.07	0.63
1:A:440:ALA:HA	1:A:443:THR:CB	2.28	0.62
4:F:233:VAL:HB	4:F:234:PRO:HD2	1.82	0.62
1:D:153:MET:SD	1:D:153:MET:N	2.71	0.62
1:B:436:ARG:HH21	1:B:439:PHE:HB2	1.64	0.62
1:E:564:LEU:O	1:E:567:LEU:HB2	2.00	0.62
1:E:737:GLY:O	1:E:738:SER:C	2.38	0.62
4:C:224:ARG:HD3	1:B:588:ASP:CB	2.30	0.62
1:E:736:ARG:CZ	1:E:736:ARG:H	2.13	0.62
1:A:436:ARG:NH1	1:A:476:SER:OG	2.33	0.61
4:F:452:VAL:HA	4:F:533:ASP:OD1	1.99	0.61
1:E:480:LEU:HA	1:E:484:ILE:HB	1.81	0.61
4:F:259:GLY:O	4:F:260:ALA:HB3	2.00	0.61
4:F:324:GLN:O	4:F:328:LEU:HB3	2.00	0.61
1:D:148:LEU:HG	1:D:190:LEU:HD23	1.81	0.61
1:E:559:TYR:CG	1:E:560:VAL:N	2.68	0.61
4:F:331:GLY:O	4:F:333:SER:N	2.34	0.61
4:C:224:ARG:HD3	1:B:588:ASP:HB3	1.82	0.61
4:C:217:ARG:CB	4:C:221:ARG:HD2	2.30	0.61
4:C:222:TYR:OH	1:B:580:LEU:HD12	2.01	0.61
1:A:455:LEU:CD2	1:A:505:LEU:HD11	2.26	0.61
1:D:414:TYR:HB3	1:D:448:SER:CB	2.31	0.61
4:C:109:ARG:HH21	4:C:183:ARG:HH21	1.49	0.60
1:E:559:TYR:CB	1:E:611:PRO:HB2	2.31	0.60
1:D:696:GLU:O	1:D:700:LYS:HG3	2.01	0.60
1:D:434:LYS:HA	1:D:437:GLN:CD	2.21	0.60
1:B:431:THR:O	1:B:435:LEU:HG	2.00	0.60
1:E:481:MET:HA	1:E:485:GLY:CA	2.31	0.60
1:E:576:LEU:O	1:E:578:ARG:N	2.34	0.60
1:D:435:LEU:O	1:D:439:PHE:HB2	2.01	0.60
4:F:392:ASP:CG	4:F:395:LEU:HB3	2.22	0.60
1:E:539:ARG:NE	1:E:540:VAL:H	1.99	0.60
4:C:452:VAL:HG22	4:C:453:ILE:HG13	1.84	0.60
1:D:380:LYS:O	1:D:382:TYR:N	2.34	0.60
4:C:666:THR:HG23	4:C:671:ILE:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:557:THR:O	4:F:558:PRO:C	2.39	0.59
4:C:320:ARG:O	4:C:324:GLN:N	2.27	0.59
4:F:231:LEU:HD13	1:E:569:ASN:HA	1.84	0.59
4:F:744:LYS:O	4:F:746:GLY:N	2.36	0.59
4:F:331:GLY:C	4:F:333:SER:H	2.06	0.59
1:E:391:LEU:HD23	1:E:518:GLU:HG3	1.85	0.59
4:C:450:ARG:HG3	4:C:451:SER:H	1.67	0.59
2:J:122:LEU:HG	2:J:126:HIS:CD2	2.37	0.59
1:E:559:TYR:H	1:E:611:PRO:CB	2.13	0.59
3:G:86:GLN:NE2	3:G:163:MET:SD	2.76	0.59
1:E:455:LEU:HG	1:E:505:LEU:HD11	1.84	0.59
1:E:391:LEU:HD22	1:E:510:ARG:NH1	2.18	0.58
4:F:322:VAL:O	4:F:326:LEU:N	2.30	0.58
1:E:145:ASP:O	1:E:193:LEU:HB3	2.02	0.58
1:E:539:ARG:HG3	1:E:540:VAL:HG22	1.85	0.58
1:A:436:ARG:HH22	1:A:476:SER:CA	2.16	0.58
4:C:270:LEU:HD23	4:C:321:VAL:HG23	1.84	0.58
1:B:350:VAL:HB	1:B:409:ASN:HD21	1.68	0.58
4:F:557:THR:HB	4:F:558:PRO:CD	2.26	0.58
1:E:560:VAL:O	1:E:562:ALA:N	2.37	0.58
1:E:481:MET:HG3	1:E:482:ASP:H	1.68	0.58
1:D:152:ASP:O	1:D:153:MET:HB2	2.04	0.58
4:F:329:LEU:HD23	4:F:359:ARG:HB2	1.86	0.57
1:E:552:LEU:O	1:E:556:ALA:N	2.37	0.57
1:A:501:ARG:O	1:A:503:HIS:N	2.37	0.57
4:F:52:PRO:HA	4:F:98:ARG:NH2	2.15	0.57
1:D:143:GLU:HB2	1:D:196:LYS:HB3	1.85	0.57
4:C:403:TYR:CE1	4:C:446:PRO:HB3	2.39	0.57
2:J:124:ASN:OD1	2:J:125:TYR:N	2.37	0.57
4:C:741:LEU:O	4:C:742:PHE:C	2.42	0.57
4:F:326:LEU:HD21	4:F:354:LEU:HD21	1.86	0.57
4:F:262:LEU:HD13	4:F:299:LEU:HB3	1.85	0.57
2:J:117:LYS:O	2:J:120:CYS:HB3	2.04	0.57
1:A:437:GLN:O	1:A:441:GLU:HB2	2.04	0.57
1:D:687:LEU:HD12	1:D:723:ILE:HG13	1.86	0.57
1:A:543:LEU:HD13	1:A:596:LYS:NZ	2.20	0.57
2:I:195:ASP:O	2:I:198:LEU:HB3	2.05	0.56
4:C:452:VAL:HG21	4:C:545:VAL:HG11	1.87	0.56
1:E:391:LEU:HB3	1:E:518:GLU:HA	1.88	0.56
1:D:414:TYR:HB3	1:D:448:SER:HA	1.87	0.56
1:D:451:PHE:CZ	1:D:453:ASP:HB2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:734:VAL:HG21	1:E:743:GLY:HA2	1.88	0.56
1:D:441:GLU:CD	1:D:448:SER:HB2	2.26	0.56
4:F:741:LEU:O	4:F:742:PHE:C	2.43	0.56
4:C:278:THR:HB	4:C:324:GLN:HE22	1.69	0.56
1:A:434:LYS:O	1:A:437:GLN:HG2	2.06	0.56
1:E:577:ARG:NH2	1:E:578:ARG:HH22	2.03	0.56
4:F:52:PRO:HB3	4:F:98:ARG:HH12	1.71	0.56
1:E:455:LEU:HD23	1:E:499:THR:HB	1.88	0.56
1:B:147:ALA:HB3	1:B:191:GLN:HB3	1.88	0.56
2:J:129:GLU:O	2:J:130:GLU:C	2.44	0.56
1:A:466:GLN:HE22	4:F:310:PRO:HB3	1.72	0.55
1:D:446:HIS:HB2	1:D:447:PRO:HD3	1.88	0.55
1:D:829:ASP:O	1:D:830:ALA:HB3	2.06	0.55
1:B:434:LYS:O	1:B:437:GLN:HB3	2.06	0.55
1:A:719:VAL:HG13	1:A:720:ALA:H	1.69	0.55
1:D:150:ASP:CG	1:D:151:LYS:N	2.60	0.55
4:F:402:GLY:HA2	4:F:450:ARG:NH1	2.22	0.55
1:E:67:LEU:HD22	1:E:101:TRP:HB2	1.88	0.55
4:F:96:LEU:O	4:F:96:LEU:HD23	2.07	0.55
4:F:300:LEU:HB3	4:F:340:VAL:HG22	1.89	0.55
4:F:320:ARG:O	4:F:324:GLN:N	2.39	0.55
1:E:145:ASP:HB3	1:E:193:LEU:HD23	1.89	0.55
1:D:378:LEU:CG	4:C:420:LEU:HD11	2.33	0.55
1:A:442:ALA:HA	1:A:445:ARG:NE	2.22	0.54
2:J:127:TYR:CD2	2:J:131:SER:HB2	2.41	0.54
4:F:323:ALA:HA	4:F:326:LEU:CG	2.31	0.54
2:J:111:LYS:O	2:J:115:THR:HG23	2.07	0.54
4:F:324:GLN:CA	4:F:327:THR:HG22	2.36	0.54
4:F:744:LYS:HA	4:F:747:PHE:CE2	2.42	0.54
1:E:196:LYS:HG2	1:E:202:ILE:HD12	1.89	0.54
1:A:434:LYS:HA	1:A:437:GLN:OE1	2.07	0.54
1:E:393:TYR:HE2	1:E:518:GLU:HG3	1.73	0.54
1:D:440:ALA:HB1	1:D:443:THR:CA	2.36	0.54
1:A:440:ALA:HA	1:A:443:THR:HB	1.88	0.54
1:A:500:ASN:HB2	1:A:501:ARG:HD3	1.89	0.54
4:F:420:LEU:O	4:F:420:LEU:HD22	2.08	0.54
1:D:351:THR:OG1	1:D:352:TYR:N	2.40	0.54
2:J:121:GLU:HA	2:J:124:ASN:HD21	1.73	0.53
4:F:321:VAL:O	4:F:325:VAL:HG23	2.08	0.53
1:E:539:ARG:HB2	1:E:539:ARG:HH11	1.74	0.53
4:C:226:LEU:CD2	4:C:231:LEU:HD21	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:424:GLU:HG2	4:C:426:ASN:N	2.14	0.53
1:B:436:ARG:HA	1:B:436:ARG:CZ	2.39	0.53
1:A:372:PRO:C	1:A:374:LYS:H	2.10	0.53
4:F:557:THR:CA	4:F:620:ARG:NH1	2.50	0.53
1:A:389:GLY:HA3	1:A:515:PHE:HA	1.90	0.53
2:J:112:LEU:O	2:J:115:THR:OG1	2.25	0.53
1:B:436:ARG:O	1:B:439:PHE:HB3	2.08	0.53
1:A:152:ASP:O	1:A:153:MET:C	2.47	0.53
4:F:286:PHE:CG	4:F:328:LEU:HD11	2.44	0.53
4:F:315:ARG:N	4:F:315:ARG:HD2	2.23	0.53
4:F:557:THR:CA	4:F:620:ARG:HH22	2.21	0.53
2:J:131:SER:C	2:J:133:ARG:H	2.12	0.53
2:J:205:LEU:HD23	1:E:82:ILE:HD11	1.90	0.53
1:E:143:GLU:OE2	1:E:331:ARG:NH2	2.41	0.53
4:C:425:LYS:HG3	4:C:427:GLN:H	1.72	0.53
1:A:57:ASP:O	1:A:58:LYS:HD2	2.09	0.53
1:A:382:TYR:HE2	4:F:419:ALA:O	1.92	0.53
1:E:480:LEU:O	1:E:485:GLY:N	2.41	0.53
1:D:124:ARG:HE	1:D:125:PRO:HD2	1.73	0.53
4:C:478:GLN:NE2	1:B:849:GLU:OE2	2.42	0.53
1:D:783:MET:HE1	1:D:791:ILE:HD11	1.91	0.53
1:A:443:THR:HG23	1:A:446:HIS:CE1	2.43	0.52
4:F:262:LEU:O	4:F:264:ALA:N	2.41	0.52
1:B:392:LEU:HB2	1:B:498:ALA:HA	1.91	0.52
1:E:508:ALA:O	1:E:514:ARG:NH1	2.42	0.52
4:C:267:ALA:HB2	4:C:304:GLU:O	2.09	0.52
1:A:436:ARG:NH1	1:A:476:SER:O	2.43	0.52
1:E:194:ARG:HG2	1:E:195:VAL:H	1.73	0.52
1:E:454:GLN:HB3	1:E:457:ALA:HB3	1.91	0.52
1:E:565:LYS:HE3	5:E:901:ATP:H1'	1.92	0.52
4:F:320:ARG:O	4:F:323:ALA:HB3	2.10	0.52
1:E:88:LEU:O	1:E:95:GLN:HA	2.09	0.52
2:J:205:LEU:CD2	1:E:82:ILE:HD11	2.40	0.52
4:F:354:LEU:HD23	4:F:359:ARG:CD	2.40	0.52
1:D:54:LYS:HG3	1:D:55:VAL:N	2.25	0.52
1:A:51:LEU:HD22	1:A:69:HIS:CE1	2.45	0.52
4:F:279:GLU:HG2	4:F:321:VAL:HB	1.92	0.52
1:E:534:GLN:OE1	1:E:534:GLN:N	2.43	0.52
1:E:536:LEU:CD1	1:E:537:LEU:HD13	2.29	0.52
1:E:538:ARG:CZ	1:E:538:ARG:HB3	2.39	0.52
4:C:226:LEU:HD22	4:C:231:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:259:GLY:O	4:F:260:ALA:CB	2.58	0.52
4:F:539:VAL:HG13	4:F:545:VAL:HG21	1.90	0.52
1:A:511:LEU:HD22	1:A:69:HIS:ND1	2.25	0.52
1:A:435:LEU:O	1:A:438:ILE:HB	2.09	0.52
1:A:450:ILE:HD13	1:A:493:VAL:HG13	1.91	0.52
1:A:501:ARG:C	1:A:503:HIS:H	2.14	0.52
4:F:382:THR:HG23	4:F:387:ILE:HD12	1.91	0.52
1:E:533:LEU:C	1:E:536:LEU:H	2.13	0.52
1:D:151:LYS:HG3	1:D:153:MET:SD	2.50	0.52
4:C:319:SER:O	4:C:322:VAL:N	2.42	0.52
4:F:417:MET:O	4:F:421:LEU:HB2	2.10	0.51
4:C:270:LEU:HD23	4:C:321:VAL:CG2	2.41	0.51
4:C:453:ILE:HG12	4:C:529:VAL:HA	1.91	0.51
4:F:354:LEU:HD23	4:F:359:ARG:HD3	1.92	0.51
4:F:743:LYS:O	4:F:744:LYS:C	2.47	0.51
1:D:482:ASP:OD2	1:D:514:ARG:NH1	2.43	0.51
4:C:497:GLN:NE2	4:C:623:MET:SD	2.81	0.51
4:F:255:ALA:O	4:F:256:ARG:C	2.46	0.51
1:B:408:ALA:HB1	1:B:415:VAL:HG13	1.92	0.51
4:F:316:ALA:N	4:F:317:PRO:HD2	2.26	0.51
1:A:850:GLU:O	1:A:851:ASP:HB2	2.10	0.51
2:I:33:LEU:HD22	2:I:105:ILE:HG23	1.93	0.51
4:F:420:LEU:HD13	4:F:421:LEU:N	2.26	0.51
1:A:155:ILE:O	1:A:156:ASN:C	2.49	0.51
4:F:511:LYS:HG2	4:F:650:ILE:HD12	1.92	0.51
1:E:559:TYR:CA	1:E:611:PRO:HB2	2.41	0.51
4:C:247:LYS:HG2	4:C:366:ILE:HD11	1.93	0.51
1:A:155:ILE:HG21	1:A:188:TYR:OH	2.10	0.51
1:A:414:TYR:HB2	1:A:445:ARG:HG3	1.92	0.51
4:F:253:ALA:HA	4:F:256:ARG:NH1	2.26	0.51
4:F:328:LEU:HD23	4:F:329:LEU:N	2.25	0.51
4:C:321:VAL:HA	4:C:324:GLN:NE2	2.26	0.51
4:F:323:ALA:CA	4:F:326:LEU:HG	2.34	0.51
1:D:372:PRO:HG3	1:D:379:PHE:CE2	2.42	0.51
4:C:227:THR:O	4:C:229:LEU:N	2.43	0.51
4:F:744:LYS:O	4:F:745:GLU:HB3	2.11	0.50
1:E:565:LYS:CE	5:E:901:ATP:H1'	2.41	0.50
1:D:106:PHE:O	1:D:107:PRO:C	2.49	0.50
2:I:41:ASN:ND2	2:I:189:GLN:OE1	2.45	0.50
4:F:211:SER:O	4:F:214:GLU:HG3	2.11	0.50
4:F:331:GLY:C	4:F:333:SER:N	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:452:VAL:O	4:C:453:ILE:HG13	2.10	0.50
4:F:252:ARG:O	4:F:256:ARG:HG3	2.12	0.50
4:F:744:LYS:HA	4:F:747:PHE:HE2	1.76	0.50
4:C:114:PRO:HG3	4:C:186:LEU:HD11	1.93	0.50
4:C:447:SER:OG	4:C:448:SER:N	2.44	0.50
1:A:463:GLU:HB2	4:F:308:LEU:HD23	1.93	0.50
2:J:121:GLU:O	2:J:122:LEU:C	2.50	0.50
1:D:436:ARG:CZ	1:D:439:PHE:HB3	2.42	0.50
4:C:418:HIS:NE2	4:C:439:GLU:OE1	2.44	0.50
1:E:415:VAL:HA	1:E:449:ILE:HB	1.94	0.50
1:E:735:GLU:HB2	1:E:736:ARG:NH2	2.26	0.50
1:D:90:SER:OG	1:D:91:LEU:N	2.45	0.50
1:E:80:ILE:HG23	1:E:133:PRO:HB3	1.93	0.50
1:E:388:ARG:HH11	1:E:486:SER:HB3	1.77	0.50
1:B:199:ASP:OD1	1:B:199:ASP:N	2.43	0.50
1:B:366:ARG:HH21	1:B:370:GLU:HG3	1.76	0.50
1:A:67:LEU:HD11	1:A:101:TRP:HB2	1.94	0.50
2:J:122:LEU:HG	2:J:126:HIS:HD2	1.76	0.50
1:E:535:LYS:O	1:E:536:LEU:C	2.49	0.49
4:C:320:ARG:HA	4:C:323:ALA:HB3	1.94	0.49
1:A:90:SER:OG	1:A:91:LEU:N	2.45	0.49
4:F:247:LYS:NZ	4:F:345:ASN:OD1	2.42	0.49
1:E:176:GLY:H	1:E:192:VAL:HG13	1.77	0.49
3:H:137:ARG:O	3:H:141:VAL:HG23	2.11	0.49
4:F:326:LEU:N	4:F:326:LEU:HD23	2.28	0.49
1:D:434:LYS:HA	1:D:437:GLN:NE2	2.28	0.49
1:A:371:LEU:CD2	4:F:420:LEU:HD21	2.42	0.49
1:A:55:VAL:HG12	1:A:55:VAL:O	2.12	0.49
4:F:314:SER:HB2	4:F:318:GLU:OE1	2.13	0.49
1:D:779:ASP:OD1	1:D:779:ASP:N	2.46	0.49
4:F:276:GLY:H	4:F:317:PRO:HB3	1.78	0.49
4:C:746:GLY:O	4:C:747:PHE:C	2.51	0.49
1:A:153:MET:O	1:A:154:GLU:C	2.49	0.49
1:E:533:LEU:HG	1:E:536:LEU:HG	1.95	0.49
3:G:130:ASP:N	3:G:130:ASP:OD1	2.46	0.49
1:B:533:LEU:HD12	1:B:534:GLN:N	2.28	0.49
1:B:614:MET:SD	1:B:614:MET:N	2.86	0.49
4:F:741:LEU:HG	4:F:746:GLY:C	2.33	0.48
1:E:503:HIS:HA	1:E:707:ARG:CZ	2.43	0.48
1:A:543:LEU:CD1	1:A:596:LYS:HZ2	2.26	0.48
4:F:567:ASP:N	4:F:567:ASP:OD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:VAL:HA	1:D:451:PHE:HB3	1.94	0.48
4:C:452:VAL:HG13	4:C:453:ILE:N	2.28	0.48
1:A:440:ALA:CA	1:A:443:THR:HB	2.44	0.48
1:A:442:ALA:O	1:A:443:THR:C	2.51	0.48
1:A:445:ARG:HD3	1:A:445:ARG:N	2.29	0.48
1:A:543:LEU:HD13	1:A:596:LYS:HZ2	1.78	0.48
4:C:229:LEU:HD21	4:C:231:LEU:HD23	1.94	0.48
4:C:321:VAL:O	4:C:324:GLN:HG2	2.13	0.48
1:A:510:ARG:NH1	1:A:518:GLU:OE2	2.46	0.48
1:E:400:LYS:HD2	1:E:401:THR:HG23	1.95	0.48
1:D:698:MET:O	1:D:745:VAL:HG11	2.12	0.48
3:G:214:SER:OG	3:G:218:ARG:NH1	2.45	0.48
4:F:235:ARG:NE	4:F:337:GLU:OE1	2.47	0.48
1:A:463:GLU:O	1:A:464:GLY:C	2.52	0.48
4:F:228:ALA:O	4:F:229:LEU:HD13	2.14	0.48
1:D:432:GLU:HA	1:D:435:LEU:HD12	1.96	0.48
1:D:508:ALA:HB1	1:D:514:ARG:HH21	1.77	0.48
4:F:327:THR:HG23	4:F:328:LEU:N	2.29	0.48
4:F:557:THR:CB	4:F:558:PRO:CD	2.89	0.48
1:D:143:GLU:OE1	1:D:194:ARG:NH2	2.45	0.48
1:B:370:GLU:HA	1:B:373:LEU:HB2	1.96	0.48
1:A:436:ARG:NH2	1:A:476:SER:O	2.46	0.47
1:A:643:VAL:HG12	1:A:767:THR:HG21	1.95	0.47
2:J:127:TYR:CE2	2:J:131:SER:HB2	2.49	0.47
1:E:477:LEU:O	1:E:481:MET:HG2	2.14	0.47
1:D:436:ARG:HA	1:D:439:PHE:CB	2.43	0.47
1:D:823:GLU:O	1:D:827:GLN:HG3	2.14	0.47
4:C:635:ASP:OD1	4:C:635:ASP:N	2.44	0.47
3:H:161:ARG:HD2	3:H:212:ARG:HD2	1.95	0.47
1:D:153:MET:O	1:D:155:ILE:HG12	2.14	0.47
1:D:439:PHE:HE1	1:D:484:ILE:HD12	1.80	0.47
1:B:508:ALA:O	1:B:514:ARG:NE	2.45	0.47
1:B:542:HIS:HB2	1:B:543:LEU:H	1.59	0.47
4:F:326:LEU:CD2	4:F:354:LEU:HD21	2.44	0.47
4:F:95:SER:HB2	4:F:97:ASN:OD1	2.14	0.47
4:F:288:ARG:HA	4:F:291:GLU:HB2	1.96	0.47
4:F:556:SER:C	4:F:557:THR:HG23	2.35	0.47
4:F:636:THR:OG1	1:E:738:SER:HB3	2.14	0.47
1:E:370:GLU:HA	1:E:374:LYS:HB2	1.96	0.47
1:E:538:ARG:O	1:E:539:ARG:HB3	2.14	0.47
1:D:570:GLU:HB2	1:D:609:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:320:ARG:O	4:C:321:VAL:C	2.51	0.47
1:B:442:ALA:HB1	1:B:448:SER:HB2	1.97	0.47
1:A:730:ASP:HB2	1:A:777:ARG:HG3	1.97	0.47
4:F:373:GLN:O	4:F:377:ILE:N	2.47	0.47
1:D:380:LYS:C	1:D:382:TYR:N	2.69	0.47
4:C:374:ARG:NH1	4:C:400:THR:O	2.48	0.47
4:F:220:LEU:HD13	4:F:258:ALA:CB	2.44	0.47
1:B:501:ARG:HH11	1:B:504:ALA:HB2	1.79	0.47
4:C:203:GLY:O	5:C:802:ATP:N6	2.46	0.47
1:A:719:VAL:HG13	1:A:720:ALA:N	2.30	0.46
2:J:116:THR:O	2:J:119:ILE:HG22	2.14	0.46
4:F:319:SER:C	4:F:322:VAL:HB	2.36	0.46
1:E:362:LEU:HD12	1:E:363:LYS:N	2.29	0.46
1:D:414:TYR:HB3	1:D:448:SER:CA	2.45	0.46
4:C:43:LEU:HD22	4:C:63:PRO:HD3	1.96	0.46
2:I:142:THR:HA	2:I:145:PHE:HD2	1.81	0.46
4:F:492:ARG:HH22	1:E:855:ASN:HA	1.81	0.46
1:E:505:LEU:O	1:E:707:ARG:NH2	2.48	0.46
1:D:696:GLU:HG2	1:D:697:LEU:N	2.29	0.46
4:C:452:VAL:C	4:C:453:ILE:HG13	2.35	0.46
2:J:120:CYS:O	2:J:124:ASN:ND2	2.49	0.46
4:C:452:VAL:HG21	4:C:545:VAL:CG1	2.45	0.46
1:A:439:PHE:O	1:A:442:ALA:N	2.47	0.46
1:B:600:LYS:HA	1:B:603:LEU:HB2	1.97	0.46
4:F:542:SER:O	4:F:542:SER:OG	2.34	0.46
1:D:440:ALA:CB	1:D:443:THR:H	2.29	0.46
4:C:321:VAL:HG13	4:C:322:VAL:H	1.78	0.46
1:A:155:ILE:HD13	1:A:155:ILE:N	2.30	0.46
4:F:645:ASP:OD1	4:F:645:ASP:N	2.47	0.46
1:E:577:ARG:HH21	1:E:578:ARG:NH2	2.07	0.46
4:C:115:VAL:HB	4:C:162:ALA:HB3	1.97	0.46
4:C:674:ASP:N	4:C:674:ASP:OD1	2.48	0.46
1:A:150:ASP:N	1:A:150:ASP:OD1	2.49	0.46
4:F:557:THR:HB	4:F:620:ARG:HH12	1.79	0.46
1:A:48:VAL:HG23	1:A:126:GLY:H	1.81	0.46
4:F:509:CYS:SG	4:F:652:PRO:HA	2.55	0.46
1:E:455:LEU:HG	1:E:505:LEU:CD1	2.46	0.46
1:E:489:SER:O	1:E:490:GLU:C	2.54	0.46
1:E:502:PRO:O	1:E:707:ARG:NH1	2.48	0.46
4:C:429:ASN:HA	4:C:430:PRO:HD3	1.85	0.46
4:C:567:ASP:OD1	4:C:567:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:213:ARG:HD3	4:F:217:ARG:HB2	1.97	0.45
4:F:346:ARG:HA	4:F:347:PRO:HD3	1.85	0.45
1:E:359:SER:OG	1:E:360:SER:N	2.49	0.45
1:A:85:PRO:HA	1:A:98:TYR:O	2.16	0.45
1:A:105:GLY:O	1:A:106:PHE:C	2.54	0.45
1:E:772:THR:HG21	1:E:778:ILE:HD11	1.98	0.45
4:C:224:ARG:HD3	1:B:588:ASP:HB2	1.97	0.45
4:C:306:ASP:N	4:C:306:ASP:OD1	2.48	0.45
4:C:321:VAL:HG13	4:C:322:VAL:N	2.31	0.45
1:B:797:PRO:O	1:B:802:ARG:NH1	2.49	0.45
1:E:175:PRO:HA	1:E:192:VAL:HG11	1.98	0.45
1:D:148:LEU:HG	1:D:190:LEU:CD2	2.45	0.45
4:C:224:ARG:NH1	1:B:588:ASP:O	2.49	0.45
1:B:563:ASP:OD1	1:B:563:ASP:N	2.47	0.45
4:F:201:PRO:O	4:F:202:LEU:HG	2.17	0.45
1:E:735:GLU:HB2	1:E:736:ARG:HH22	1.82	0.45
1:E:818:GLU:CD	1:E:859:LYS:HZ3	2.19	0.45
1:B:437:GLN:O	1:B:440:ALA:N	2.49	0.45
2:J:195:ASP:O	2:J:198:LEU:HB3	2.17	0.45
4:F:319:SER:CA	4:F:322:VAL:HB	2.46	0.45
4:F:392:ASP:OD1	4:F:395:LEU:N	2.49	0.45
4:C:423:SER:O	4:C:424:GLU:HB3	2.17	0.45
1:E:537:LEU:O	1:E:538:ARG:HB3	2.16	0.45
1:D:710:ARG:NH2	1:D:752:GLN:OE1	2.49	0.45
4:C:282:VAL:HG21	4:C:324:GLN:CG	2.36	0.45
1:B:60:PRO:HB2	1:B:62:THR:H	1.80	0.45
1:B:87:LEU:HD11	1:B:95:GLN:HB3	1.97	0.45
1:B:356:GLY:HA3	1:B:532:ILE:HD13	1.98	0.45
1:B:544:LEU:HD21	1:B:602:PHE:HZ	1.81	0.45
1:A:501:ARG:C	1:A:503:HIS:N	2.70	0.45
1:A:697:LEU:HD22	1:A:705:SER:HB2	1.99	0.45
4:F:317:PRO:O	4:F:321:VAL:HG12	2.16	0.45
1:E:436:ARG:HH22	1:E:473:VAL:HG12	1.82	0.45
1:E:481:MET:HA	1:E:485:GLY:N	2.32	0.45
1:D:730:ASP:OD1	1:D:730:ASP:N	2.46	0.45
1:D:747:ASP:OD1	1:D:747:ASP:N	2.48	0.45
1:B:816:SER:OG	1:B:817:ASN:N	2.50	0.45
1:A:704:GLU:HG3	1:A:707:ARG:HH21	1.82	0.45
2:J:33:LEU:HD22	2:J:105:ILE:HG23	1.97	0.45
2:J:127:TYR:HE2	2:J:134:PRO:HA	1.81	0.45
4:C:203:GLY:H	5:C:802:ATP:HN61	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:282:VAL:CG2	4:C:324:GLN:HG3	2.37	0.45
4:C:632:ASP:OD1	4:C:741:LEU:HD11	2.17	0.45
1:B:428:TYR:OH	1:B:469:VAL:O	2.35	0.45
1:A:463:GLU:OE1	4:F:308:LEU:HD23	2.17	0.45
4:F:213:ARG:NH2	4:F:254:VAL:HG13	2.31	0.45
1:E:485:GLY:HA2	1:E:493:VAL:HG11	1.99	0.45
1:D:408:ALA:HA	1:D:415:VAL:HG21	1.99	0.45
4:C:210:ASP:OD1	4:C:210:ASP:N	2.50	0.45
4:F:279:GLU:HA	4:F:282:VAL:HG12	1.99	0.45
1:E:481:MET:CA	1:E:485:GLY:H	2.29	0.45
1:D:141:ALA:HA	1:D:197:GLY:HA2	1.99	0.45
1:D:444:LEU:O	1:D:445:ARG:C	2.53	0.45
3:G:187:VAL:HG13	3:G:197:VAL:HB	2.00	0.44
1:E:529:ARG:HD2	1:E:556:ALA:HB3	1.97	0.44
4:F:212:LEU:HD23	4:F:364:VAL:HG21	1.99	0.44
4:F:317:PRO:O	4:F:318:GLU:C	2.56	0.44
4:F:585:ARG:HE	4:F:585:ARG:HB2	1.32	0.44
1:B:760:ILE:CG2	1:B:766:VAL:HB	2.46	0.44
1:E:532:ILE:O	1:E:536:LEU:N	2.51	0.44
1:A:503:HIS:CE1	1:A:707:ARG:HD3	2.53	0.44
1:A:773:ASN:O	1:A:881:TYR:OH	2.34	0.44
3:H:86:GLN:HB3	3:H:160:VAL:HG13	1.98	0.44
4:F:228:ALA:CB	4:F:229:LEU:HD22	2.47	0.44
1:E:461:LYS:NZ	1:E:703:GLY:O	2.46	0.44
1:D:468:GLU:HA	1:D:471:LYS:HD3	1.98	0.44
1:D:614:MET:HE2	1:D:614:MET:HB2	1.87	0.44
1:A:524:PRO:O	1:A:529:ARG:NH1	2.50	0.44
2:J:204:LEU:HA	2:J:207:THR:HG22	1.99	0.44
4:F:213:ARG:HH22	4:F:254:VAL:HG13	1.80	0.44
1:D:440:ALA:HB3	1:D:443:THR:H	1.83	0.44
1:A:420:GLY:HA3	1:A:454:GLN:HB3	1.98	0.44
1:A:721:PRO:HA	1:A:765:ASP:O	2.18	0.44
4:F:321:VAL:HA	4:F:324:GLN:HB2	1.99	0.44
1:E:480:LEU:CA	1:E:484:ILE:HB	2.47	0.44
1:D:744:ASN:N	1:D:747:ASP:OD1	2.51	0.44
4:C:283:ARG:HD2	4:C:283:ARG:HA	1.68	0.44
2:I:204:LEU:HD12	2:I:210:ARG:HG2	1.98	0.44
1:E:393:TYR:HE2	1:E:518:GLU:CG	2.31	0.44
1:E:552:LEU:HA	1:E:555:SER:HB2	1.99	0.44
1:D:831:TYR:CE1	1:D:871:PRO:HG3	2.52	0.44
2:J:131:SER:C	2:J:133:ARG:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:69:ASP:OD1	4:F:69:ASP:N	2.45	0.44
1:E:539:ARG:HB2	1:E:539:ARG:CZ	2.45	0.44
4:C:634:LEU:HD13	4:C:639:LEU:HD11	1.99	0.44
4:F:452:VAL:HB	4:F:453:ILE:HG13	1.98	0.44
1:E:573:LEU:O	1:E:576:LEU:HG	2.17	0.44
4:C:319:SER:C	4:C:321:VAL:N	2.68	0.44
4:C:320:ARG:O	4:C:323:ALA:N	2.50	0.44
1:B:144:MET:O	1:B:332:VAL:HA	2.18	0.44
1:B:366:ARG:HA	1:B:370:GLU:HB2	2.00	0.44
4:F:231:LEU:HD22	1:E:569:ASN:HB2	2.00	0.43
4:F:321:VAL:O	4:F:322:VAL:C	2.55	0.43
4:C:322:VAL:O	4:C:326:LEU:N	2.44	0.43
4:F:282:VAL:HG11	4:F:321:VAL:CG2	2.48	0.43
1:A:551:GLN:HG2	1:B:762:GLN:HE22	1.82	0.43
2:I:24:LYS:NZ	2:I:207:THR:O	2.45	0.43
4:F:232:ALA:C	4:F:233:VAL:O	2.55	0.43
1:D:697:LEU:HD23	1:D:697:LEU:HA	1.83	0.43
4:C:423:SER:OG	4:C:424:GLU:N	2.51	0.43
1:A:114:SER:OG	1:A:115:GLU:N	2.51	0.43
3:H:187:VAL:HG13	3:H:197:VAL:HB	1.98	0.43
4:F:287:GLN:HA	4:F:290:ARG:HH11	1.84	0.43
1:E:362:LEU:HD12	1:E:363:LYS:H	1.84	0.43
1:B:662:LYS:HD2	1:B:662:LYS:HA	1.86	0.43
1:E:428:TYR:HA	1:E:431:THR:HG22	2.00	0.43
1:E:565:LYS:HE2	1:E:565:LYS:HB2	1.78	0.43
1:D:53:GLU:O	1:D:54:LYS:CB	2.63	0.43
1:D:374:LYS:HA	1:D:374:LYS:HD3	1.86	0.43
4:C:326:LEU:HD11	4:C:359:ARG:CZ	2.48	0.43
1:A:436:ARG:N	1:A:436:ARG:HD2	2.33	0.43
4:F:213:ARG:O	4:F:213:ARG:HG3	2.17	0.43
1:E:380:LYS:HG3	1:E:490:GLU:HB3	2.01	0.43
1:D:429:GLY:HA2	1:D:472:ARG:CZ	2.48	0.43
4:C:374:ARG:HH12	4:C:401:VAL:HG12	1.84	0.43
1:B:530:LEU:O	1:B:533:LEU:HG	2.19	0.43
2:J:131:SER:O	2:J:133:ARG:N	2.51	0.43
4:F:220:LEU:HD13	4:F:258:ALA:HB1	2.01	0.43
1:E:480:LEU:O	1:E:484:ILE:HB	2.17	0.43
1:D:380:LYS:C	1:D:382:TYR:H	2.21	0.43
1:D:431:THR:OG1	1:D:472:ARG:NH1	2.51	0.43
1:E:736:ARG:O	1:E:739:SER:OG	2.35	0.43
4:C:373:GLN:HE21	4:C:373:GLN:HB3	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ILE:HD11	1:A:392:LEU:HD21	2.01	0.43
1:A:436:ARG:HH22	1:A:476:SER:C	2.22	0.43
1:E:388:ARG:CD	1:E:486:SER:HB3	2.49	0.43
1:E:539:ARG:CZ	1:E:540:VAL:H	2.32	0.43
1:D:51:LEU:HD22	1:D:114:SER:HA	2.01	0.43
1:D:380:LYS:HD3	1:D:380:LYS:HA	1.35	0.43
1:A:194:ARG:HA	1:A:203:LEU:HD11	2.00	0.42
4:F:204:GLY:HA2	4:F:373:GLN:HG3	2.00	0.42
1:E:362:LEU:O	1:E:366:ARG:N	2.52	0.42
1:E:529:ARG:NE	1:E:556:ALA:O	2.50	0.42
4:C:322:VAL:O	4:C:325:VAL:HB	2.19	0.42
1:B:524:PRO:HB3	1:B:529:ARG:HH22	1.84	0.42
1:A:443:THR:O	1:A:446:HIS:CE1	2.72	0.42
4:F:324:GLN:HA	4:F:327:THR:CG2	2.42	0.42
1:E:51:LEU:HD22	1:E:114:SER:HA	2.02	0.42
1:D:563:ASP:OD2	1:D:612:SER:HB3	2.17	0.42
1:B:530:LEU:HA	1:B:533:LEU:CD2	2.48	0.42
1:A:378:LEU:HD23	4:F:420:LEU:HD23	2.01	0.42
1:A:442:ALA:C	1:A:444:LEU:N	2.70	0.42
4:F:482:TRP:N	4:F:483:PRO:CD	2.82	0.42
1:E:655:ARG:HH12	1:D:853:GLN:HA	1.84	0.42
3:H:238:LYS:O	3:H:238:LYS:HG3	2.17	0.42
4:F:319:SER:HA	4:F:322:VAL:HB	2.01	0.42
4:F:418:HIS:O	4:F:418:HIS:CD2	2.72	0.42
1:B:433:ALA:O	1:B:437:GLN:HB2	2.19	0.42
1:E:175:PRO:HA	1:E:192:VAL:CG1	2.50	0.42
1:B:543:LEU:HD23	1:B:598:THR:HG22	2.01	0.42
1:A:445:ARG:HD3	1:A:445:ARG:H	1.85	0.42
4:F:107:LEU:CD2	4:F:170:PRO:HD2	2.45	0.42
4:F:232:ALA:HB1	4:F:235:ARG:NE	2.30	0.42
4:F:370:THR:OG1	4:F:373:GLN:OE1	2.36	0.42
1:E:398:THR:OG1	1:E:399:GLY:N	2.53	0.42
1:D:442:ALA:HB3	1:D:445:ARG:CB	2.43	0.42
4:C:503:LEU:HD22	4:C:650:ILE:HD11	2.01	0.42
1:A:457:ALA:O	1:A:458:LEU:C	2.58	0.42
1:E:690:LEU:HD22	1:E:716:ALA:HB2	2.02	0.42
1:E:543:LEU:HD23	1:E:597:ILE:HG21	2.01	0.42
1:E:553:ALA:O	1:E:556:ALA:HB3	2.19	0.42
4:C:321:VAL:O	4:C:325:VAL:HG23	2.20	0.42
1:A:687:LEU:HD22	1:A:723:ILE:HG13	2.01	0.42
2:J:192:VAL:O	3:H:138:LYS:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:201:GLU:HG3	1:B:59:ILE:HD11	2.02	0.42
4:F:392:ASP:O	4:F:393:LEU:HD13	2.20	0.42
1:E:534:GLN:N	1:E:534:GLN:CD	2.73	0.42
1:D:820:ASP:OD1	1:D:820:ASP:N	2.53	0.42
4:F:556:SER:O	4:F:557:THR:OG1	2.27	0.41
1:B:85:PRO:HA	1:B:98:TYR:O	2.20	0.41
1:B:436:ARG:NE	1:B:436:ARG:CA	2.82	0.41
1:E:707:ARG:HG3	1:E:708:ALA:N	2.35	0.41
1:A:543:LEU:CD2	1:A:596:LYS:HZ2	2.32	0.41
4:F:477:LYS:HG3	4:F:481:GLU:OE1	2.20	0.41
4:F:480:ILE:C	4:F:483:PRO:HD2	2.40	0.41
4:F:582:VAL:O	4:F:586:VAL:HG23	2.20	0.41
1:E:365:ILE:HA	1:E:368:ILE:HD12	2.02	0.41
1:E:388:ARG:HD2	1:E:486:SER:HB3	2.01	0.41
1:E:728:GLN:HE21	1:E:728:GLN:HB3	1.49	0.41
4:C:534:LEU:HG	4:C:542:SER:OG	2.20	0.41
4:F:421:LEU:HD13	4:F:421:LEU:HA	1.74	0.41
1:E:421:PRO:HD3	1:E:454:GLN:CG	2.41	0.41
1:D:431:THR:OG1	1:D:432:GLU:N	2.53	0.41
1:D:510:ARG:HA	1:D:510:ARG:HD2	1.88	0.41
4:C:306:ASP:OD2	4:C:345:ASN:ND2	2.51	0.41
4:F:322:VAL:O	4:F:325:VAL:N	2.53	0.41
1:E:481:MET:HA	1:E:485:GLY:H	1.86	0.41
1:E:662:LYS:HD2	1:E:662:LYS:HA	1.76	0.41
1:B:419:ASN:ND2	1:B:422:GLU:OE1	2.48	0.41
1:A:59:ILE:HG21	1:A:67:LEU:CD2	2.50	0.41
1:A:148:LEU:HD12	1:A:149:SER:H	1.84	0.41
1:A:153:MET:O	1:A:155:ILE:HG23	2.21	0.41
1:A:685:SER:HB2	1:A:687:LEU:HD12	2.01	0.41
1:B:51:LEU:HD22	1:B:114:SER:HA	2.02	0.41
1:B:393:TYR:HE2	1:B:518:GLU:HG2	1.84	0.41
1:B:530:LEU:HA	1:B:533:LEU:HG	2.03	0.41
1:A:393:TYR:CD2	1:A:502:PRO:HG3	2.56	0.41
1:A:543:LEU:N	1:A:543:LEU:HD22	2.35	0.41
1:E:794:VAL:HA	1:E:795:PRO:HD3	1.95	0.41
4:C:320:ARG:O	4:C:324:GLN:HG2	2.21	0.41
1:A:720:ALA:HB1	1:A:721:PRO:HD2	2.02	0.41
3:H:148:ASP:OD1	3:H:149:LYS:N	2.53	0.41
1:E:354:MET:HA	1:E:535:LYS:HZ1	1.85	0.41
1:E:402:MET:O	1:E:403:ILE:C	2.58	0.41
4:C:290:ARG:HH12	4:C:335:ASP:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASP:HB3	1:B:333:ASN:HB2	2.02	0.41
1:B:760:ILE:HG21	1:B:766:VAL:CG1	2.50	0.41
1:A:142:GLU:OE2	4:F:91:ARG:NH2	2.54	0.41
1:A:543:LEU:HD22	1:A:596:LYS:HZ2	1.85	0.41
1:A:830:ALA:HB2	1:A:878:ARG:HH11	1.86	0.41
2:I:99:LEU:HD13	2:I:164:ARG:HD3	2.03	0.41
3:G:68:PRO:HB3	3:G:178:HIS:HB3	2.03	0.41
4:F:455:LEU:HG	4:F:456:MET:O	2.20	0.41
1:E:531:ASP:HA	1:E:534:GLN:OE1	2.21	0.41
1:D:717:ARG:HH22	4:C:446:PRO:HD2	1.86	0.41
4:C:744:LYS:HE3	4:C:744:LYS:HB3	1.91	0.41
2:J:129:GLU:C	2:J:131:SER:N	2.70	0.41
4:F:261:GLU:H	4:F:261:GLU:HG3	1.66	0.41
4:F:324:GLN:HE22	4:F:328:LEU:HD13	1.85	0.41
1:E:551:GLN:HA	1:E:554:ASN:ND2	2.35	0.41
1:E:648:LYS:HE2	1:E:648:LYS:HB3	1.96	0.41
4:C:273:SER:N	4:C:277:GLU:OE2	2.51	0.41
4:C:734:ASP:OD1	4:C:734:ASP:N	2.54	0.41
1:B:61:LYS:HD3	1:B:61:LYS:HA	1.91	0.41
1:B:535:LYS:HB2	1:B:538:ARG:HH21	1.86	0.41
4:F:264:ALA:HA	4:F:301:PHE:HB3	2.02	0.40
1:E:481:MET:HG3	1:E:482:ASP:N	2.33	0.40
4:C:18:PRO:HB3	4:C:89:ARG:HD3	2.03	0.40
4:C:263:LEU:HD21	4:C:288:ARG:HG2	2.02	0.40
4:C:452:VAL:HG13	4:C:453:ILE:H	1.86	0.40
4:C:745:GLU:O	4:C:747:PHE:HD2	2.04	0.40
1:B:361:GLN:HA	1:B:364:ALA:HB3	2.02	0.40
1:B:367:GLU:HA	1:B:371:LEU:HB2	2.02	0.40
4:F:324:GLN:O	4:F:328:LEU:N	2.31	0.40
1:D:430:GLU:O	1:D:431:THR:C	2.59	0.40
1:B:145:ASP:HA	1:B:333:ASN:O	2.21	0.40
1:A:143:GLU:HB3	1:A:196:LYS:HB3	2.03	0.40
1:A:437:GLN:HB2	1:A:441:GLU:OE2	2.22	0.40
4:F:237:VAL:H	4:F:237:VAL:HG23	1.51	0.40
1:E:143:GLU:HB2	1:E:196:LYS:HB3	2.03	0.40
1:E:553:ALA:C	1:E:556:ALA:H	2.25	0.40
1:E:554:ASN:O	1:E:555:SER:C	2.59	0.40
1:B:774:ARG:HE	1:B:777:ARG:HG3	1.86	0.40
1:A:418:ILE:HD11	1:A:438:ILE:HG21	2.02	0.40
1:E:735:GLU:HG2	1:E:736:ARG:N	2.36	0.40
1:D:372:PRO:O	1:D:376:PRO:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ILE:O	1:B:442:ALA:N	2.47	0.40
1:A:199:ASP:OD1	1:A:199:ASP:N	2.53	0.40
1:A:440:ALA:C	1:A:443:THR:HB	2.40	0.40
2:J:185:MET:HE1	3:H:131:LEU:HD13	2.02	0.40
3:G:69:LEU:HD13	3:G:182:VAL:HG11	2.03	0.40
1:E:420:GLY:HA3	1:E:454:GLN:HB2	2.02	0.40
1:E:434:LYS:HA	1:E:437:GLN:HG3	2.02	0.40
1:E:630:GLY:HA3	1:E:800:ALA:HB3	2.02	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	688/886 (78%)	620 (90%)	61 (9%)	7 (1%)	13	45
1	B	693/886 (78%)	621 (90%)	70 (10%)	2 (0%)	37	68
1	D	702/886 (79%)	622 (89%)	76 (11%)	4 (1%)	22	55
1	E	691/886 (78%)	620 (90%)	62 (9%)	9 (1%)	10	40
2	I	170/242 (70%)	167 (98%)	3 (2%)	0	100	100
2	J	170/242 (70%)	156 (92%)	12 (7%)	2 (1%)	11	42
3	G	198/275 (72%)	194 (98%)	4 (2%)	0	100	100
3	H	201/275 (73%)	195 (97%)	6 (3%)	0	100	100
4	C	667/749 (89%)	617 (92%)	45 (7%)	5 (1%)	19	53
4	F	683/749 (91%)	599 (88%)	69 (10%)	15 (2%)	5	30
All	All	4863/6076 (80%)	4411 (91%)	408 (8%)	44 (1%)	17	48

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	LYS
1	A	851	ASP
4	F	308	LEU
4	F	457	ASP
4	F	557	THR
1	E	395	PRO
1	E	561	GLY
4	C	744	LYS
1	A	439	PHE
1	A	460	PRO
1	A	506	ASP
2	J	132	LYS
4	F	202	LEU
4	F	260	ALA
4	F	263	LEU
4	F	332	ALA
4	F	453	ILE
1	E	490	GLU
1	D	154	GLU
1	D	351	THR
1	D	381	SER
4	C	228	ALA
4	C	424	GLU
4	C	447	SER
4	C	742	PHE
1	B	349	LYS
1	A	370	GLU
4	F	421	LEU
4	F	558	PRO
1	E	542	HIS
1	E	577	ARG
4	F	236	GLY
4	F	307	ALA
4	F	456	MET
1	E	539	ARG
1	E	738	SER
1	A	852	ILE
2	J	129	GLU
4	F	452	VAL
1	E	576	LEU
1	D	611	PRO
4	F	458	ILE
1	E	560	VAL

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Mol	Chain	Res	Type
1	B	350	VAL

### 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	586/746 (79%)	574 (98%)	12 (2%)	50	71
1	B	583/746 (78%)	580 (100%)	3 (0%)	86	92
1	D	597/746 (80%)	579 (97%)	18 (3%)	36	63
1	E	582/746 (78%)	562 (97%)	20 (3%)	32	60
2	I	158/213 (74%)	157 (99%)	1 (1%)	84	91
2	J	158/213 (74%)	156 (99%)	2 (1%)	65	81
3	G	178/240 (74%)	178 (100%)	0	100	100
3	H	181/240 (75%)	177 (98%)	4 (2%)	47	69
4	C	557/612 (91%)	549 (99%)	8 (1%)	62	79
4	F	568/612 (93%)	541 (95%)	27 (5%)	21	50
All	All	4148/5114 (81%)	4053 (98%)	95 (2%)	46	69

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	MET
1	A	150	ASP
1	A	151	LYS
1	A	155	ILE
1	A	445	ARG
1	A	461	LYS
1	A	472	ARG
1	A	501	ARG
1	A	503	HIS
1	A	539	ARG
1	A	577	ARG
1	A	849	GLU

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Mol	Chain	Res	Type
2	J	120	CYS
2	J	127	TYR
2	I	133	ARG
3	H	148	ASP
3	H	230	LEU
3	H	236	LEU
3	H	238	LYS
4	F	108	ARG
4	F	202	LEU
4	F	206	SER
4	F	207	GLU
4	F	212	LEU
4	F	213	ARG
4	F	237	VAL
4	F	261	GLU
4	F	262	LEU
4	F	295	ARG
4	F	306	ASP
4	F	308	LEU
4	F	320	ARG
4	F	324	GLN
4	F	328	LEU
4	F	392	ASP
4	F	420	LEU
4	F	421	LEU
4	F	423	SER
4	F	425	LYS
4	F	450	ARG
4	F	452	VAL
4	F	453	ILE
4	F	456	MET
4	F	458	ILE
4	F	594	LEU
4	F	747	PHE
1	E	192	VAL
1	E	194	ARG
1	E	362	LEU
1	E	400	LYS
1	E	445	ARG
1	E	534	GLN
1	E	535	LYS
1	E	536	LEU

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Mol	Chain	Res	Type
1	E	537	LEU
1	E	538	ARG
1	E	539	ARG
1	E	560	VAL
1	E	564	LEU
1	E	565	LYS
1	E	576	LEU
1	E	578	ARG
1	E	707	ARG
1	E	726	PHE
1	E	728	GLN
1	E	736	ARG
1	D	53	GLU
1	D	54	LYS
1	D	103	MET
1	D	148	LEU
1	D	150	ASP
1	D	151	LYS
1	D	152	ASP
1	D	153	MET
1	D	154	GLU
1	D	378	LEU
1	D	380	LYS
1	D	438	ILE
1	D	439	PHE
1	D	450	ILE
1	D	539	ARG
1	D	594	LEU
1	D	596	LYS
1	D	614	MET
4	C	373	GLN
4	C	424	GLU
4	C	425	LYS
4	C	542	SER
4	C	543	GLU
4	C	544	LYS
4	C	634	LEU
4	C	742	PHE
1	B	400	LYS
1	B	855	ASN
1	B	856	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	GLN
1	A	446	HIS
1	A	503	HIS
2	J	126	HIS
2	I	41	ASN
2	I	189	GLN
4	F	311	GLN
4	F	418	HIS
1	E	728	GLN
4	C	426	ASN
1	B	69	HIS
1	B	762	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z  > 2$
5	ATP	B	901	-	26,33,33	0.60	0	31,52,52	0.75	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ATP	F	801	-	26,33,33	0.62	0	31,52,52	0.79	2 (6%)
5	ATP	F	802	-	26,33,33	0.63	0	31,52,52	0.75	1 (3%)
5	ATP	D	901	-	26,33,33	0.62	0	31,52,52	0.83	2 (6%)
5	ATP	E	901	-	26,33,33	0.64	0	31,52,52	0.84	2 (6%)
5	ATP	C	801	-	26,33,33	0.64	0	31,52,52	0.79	1 (3%)
5	ATP	A	901	-	26,33,33	0.63	0	31,52,52	0.88	2 (6%)
5	ATP	C	802	6	26,33,33	0.61	0	31,52,52	0.83	1 (3%)

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
5	ATP	B	901	-	-	6/18/38/38	0/3/3/3
5	ATP	F	801	-	-	3/18/38/38	0/3/3/3
5	ATP	F	802	-	-	7/18/38/38	0/3/3/3
5	ATP	D	901	-	-	0/18/38/38	0/3/3/3
5	ATP	E	901	-	-	10/18/38/38	0/3/3/3
5	ATP	C	801	-	-	5/18/38/38	0/3/3/3
5	ATP	A	901	-	-	6/18/38/38	0/3/3/3
5	ATP	C	802	6	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	ATP	C1'-N9-C4	2.62	131.24	126.64
5	F	802	ATP	C5-C6-N6	2.28	123.81	120.35
5	C	801	ATP	C5-C6-N6	2.25	123.77	120.35
5	B	901	ATP	C5-C6-N6	2.24	123.76	120.35
5	C	802	ATP	C5-C6-N6	2.24	123.75	120.35
5	D	901	ATP	C1'-N9-C4	2.22	130.55	126.64
5	F	801	ATP	C5-C6-N6	2.22	123.72	120.35
5	A	901	ATP	C5-C6-N6	2.18	123.67	120.35
5	E	901	ATP	PB-O3B-PG	2.15	140.20	132.83
5	D	901	ATP	C5-C6-N6	2.14	123.61	120.35
5	E	901	ATP	C5-C6-N6	2.12	123.58	120.35
5	F	801	ATP	PB-O3B-PG	2.04	139.83	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	901	ATP	PB-O3B-PG	2.03	139.79	132.83

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	ATP	C5'-O5'-PA-O1A
5	A	901	ATP	C5'-O5'-PA-O2A
5	F	801	ATP	C5'-O5'-PA-O1A
5	F	802	ATP	C5'-O5'-PA-O1A
5	F	802	ATP	C5'-O5'-PA-O2A
5	F	802	ATP	C3'-C4'-C5'-O5'
5	E	901	ATP	PB-O3B-PG-O3G
5	E	901	ATP	C5'-O5'-PA-O2A
5	E	901	ATP	C5'-O5'-PA-O3A
5	E	901	ATP	O4'-C4'-C5'-O5'
5	E	901	ATP	C3'-C4'-C5'-O5'
5	C	801	ATP	PB-O3B-PG-O3G
5	C	801	ATP	O4'-C4'-C5'-O5'
5	C	801	ATP	C3'-C4'-C5'-O5'
5	B	901	ATP	C5'-O5'-PA-O1A
5	A	901	ATP	C3'-C4'-C5'-O5'
5	F	802	ATP	O4'-C4'-C5'-O5'
5	A	901	ATP	O4'-C4'-C5'-O5'
5	A	901	ATP	C5'-O5'-PA-O3A
5	F	801	ATP	C5'-O5'-PA-O3A
5	B	901	ATP	C5'-O5'-PA-O3A
5	F	802	ATP	PA-O3A-PB-O2B
5	E	901	ATP	PA-O3A-PB-O2B
5	F	801	ATP	C5'-O5'-PA-O2A
5	B	901	ATP	C5'-O5'-PA-O2A
5	B	901	ATP	C4'-C5'-O5'-PA
5	A	901	ATP	PB-O3A-PA-O2A
5	B	901	ATP	PB-O3A-PA-O2A
5	E	901	ATP	PG-O3B-PB-O1B
5	C	801	ATP	PB-O3A-PA-O2A
5	B	901	ATP	PB-O3A-PA-O1A
5	E	901	ATP	PB-O3B-PG-O2G
5	F	802	ATP	C5'-O5'-PA-O3A
5	F	802	ATP	PA-O3A-PB-O1B
5	E	901	ATP	PG-O3B-PB-O2B
5	E	901	ATP	PA-O3A-PB-O1B

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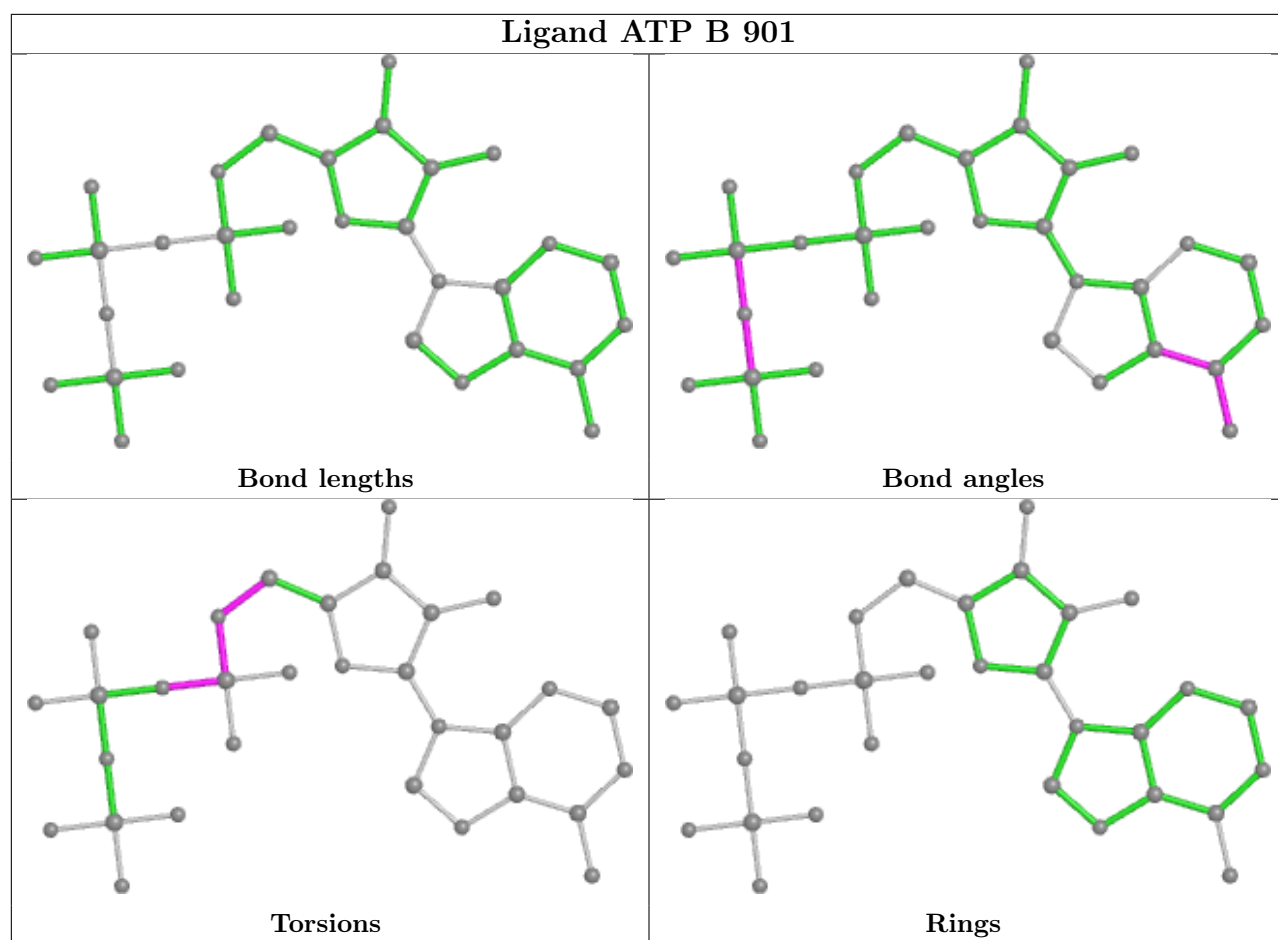
Mol	Chain	Res	Type	Atoms
5	C	802	ATP	PB-O3A-PA-O1A
5	C	802	ATP	PB-O3A-PA-O2A
5	C	801	ATP	C5'-O5'-PA-O1A

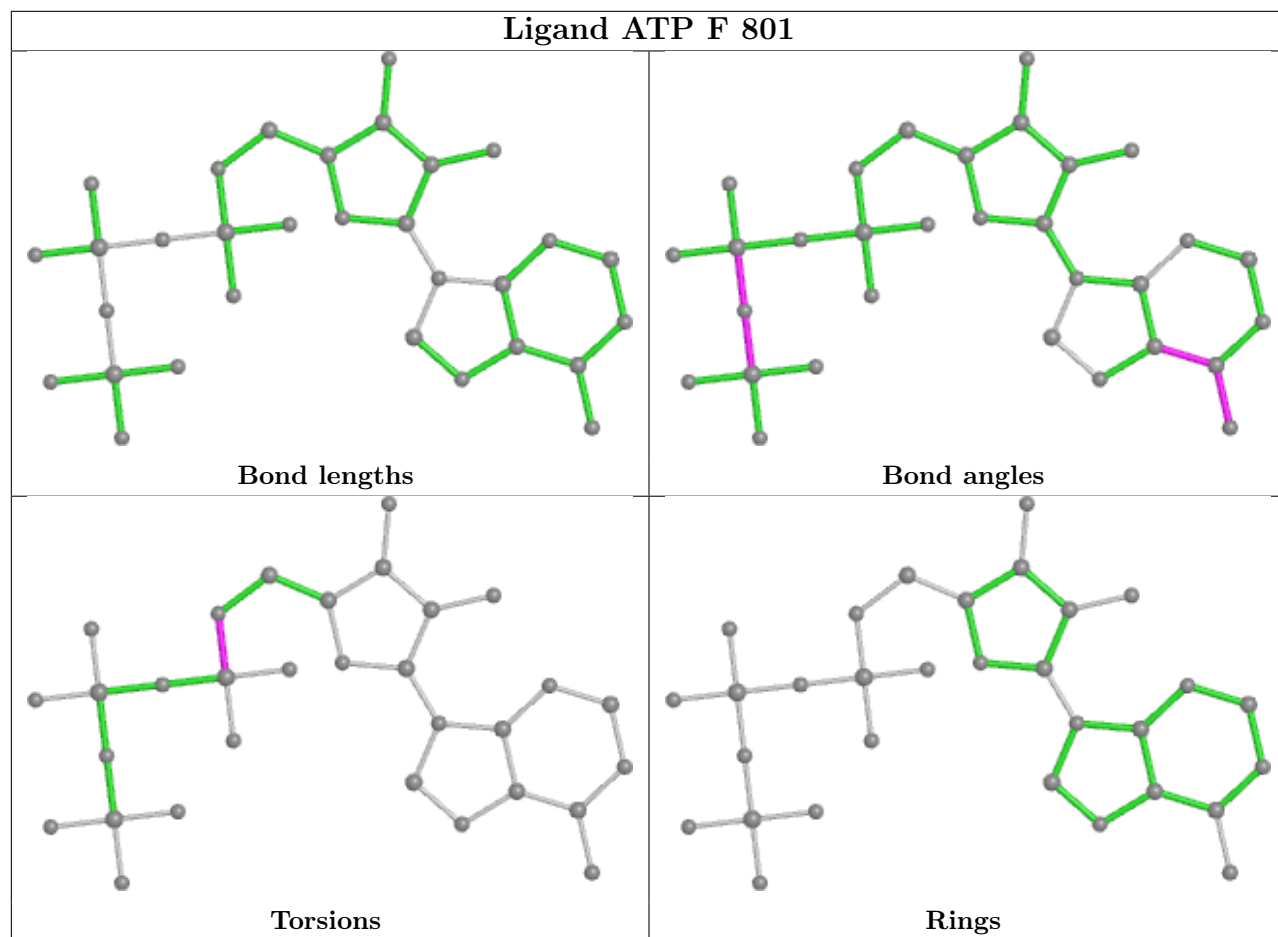
There are no ring outliers.

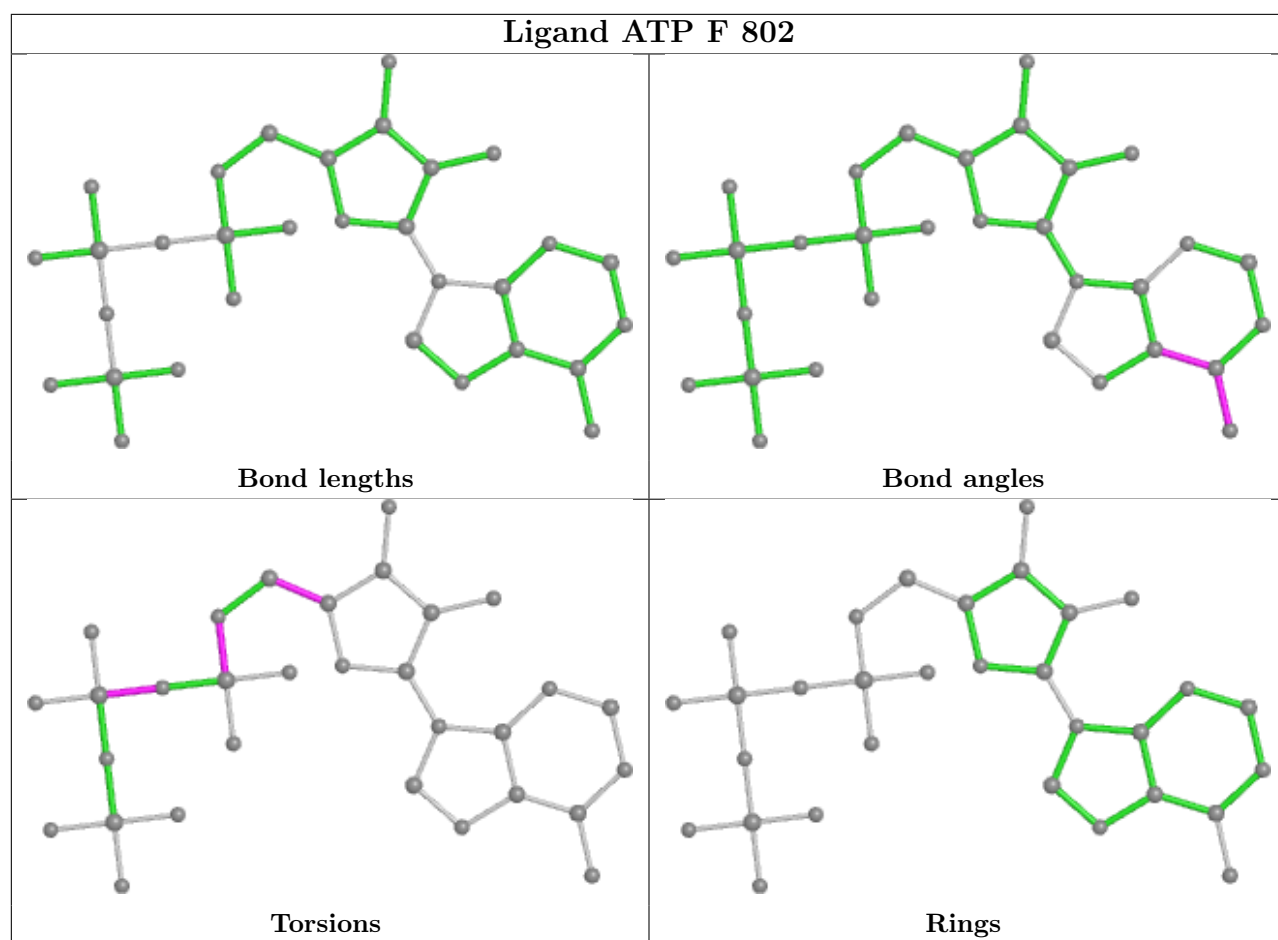
2 monomers are involved in 4 short contacts:

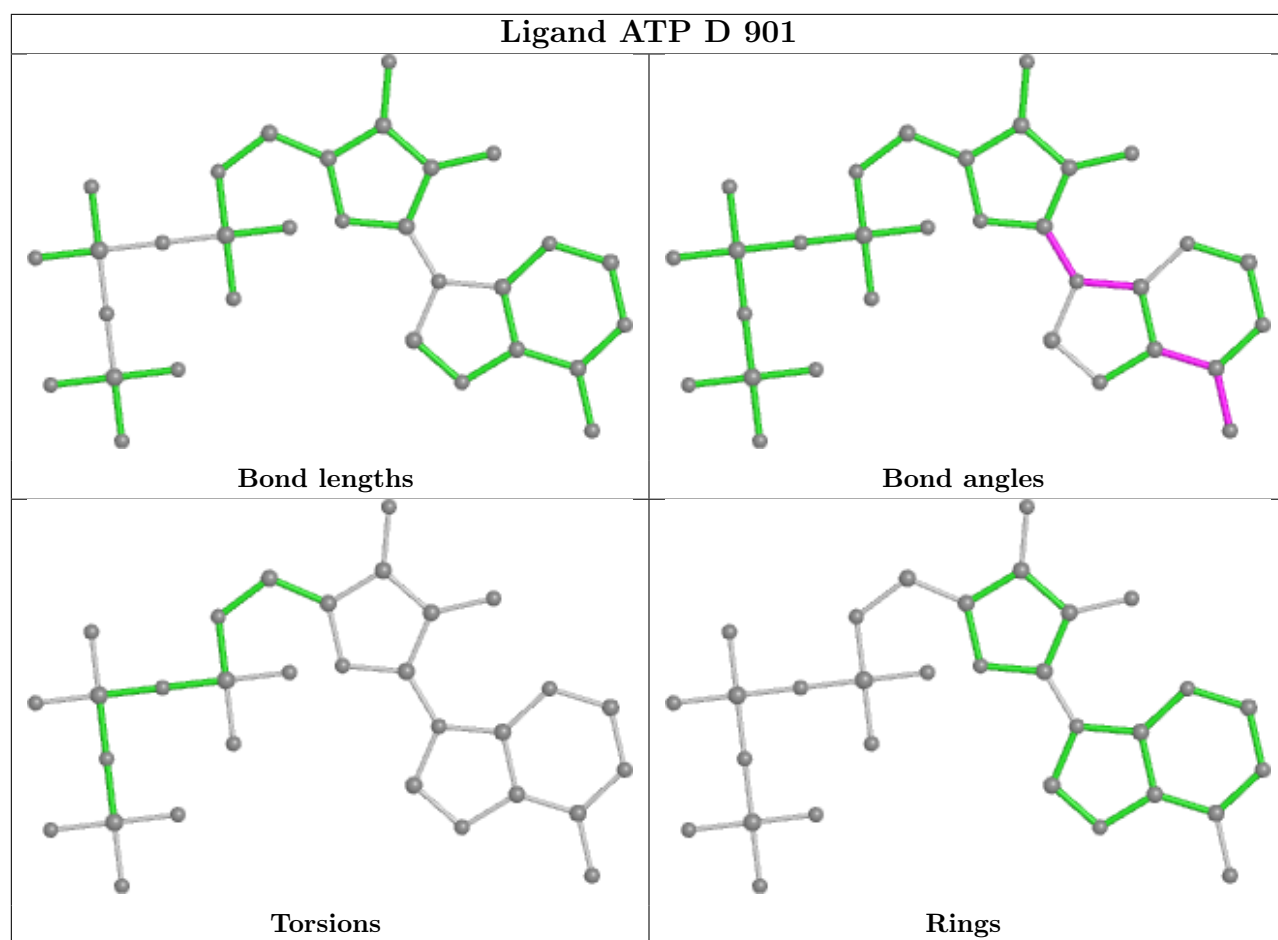
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	901	ATP	2	0
5	C	802	ATP	2	0

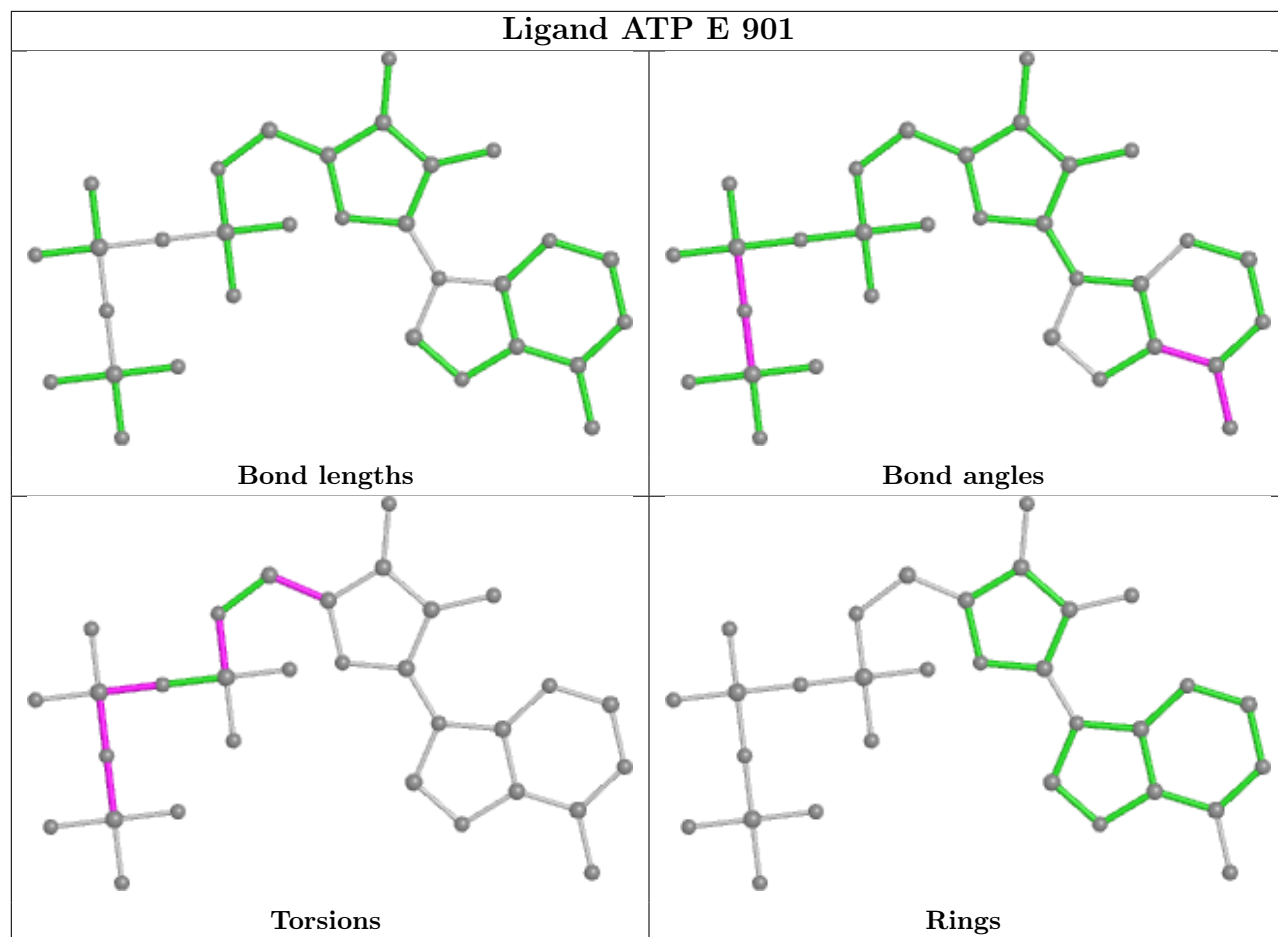
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

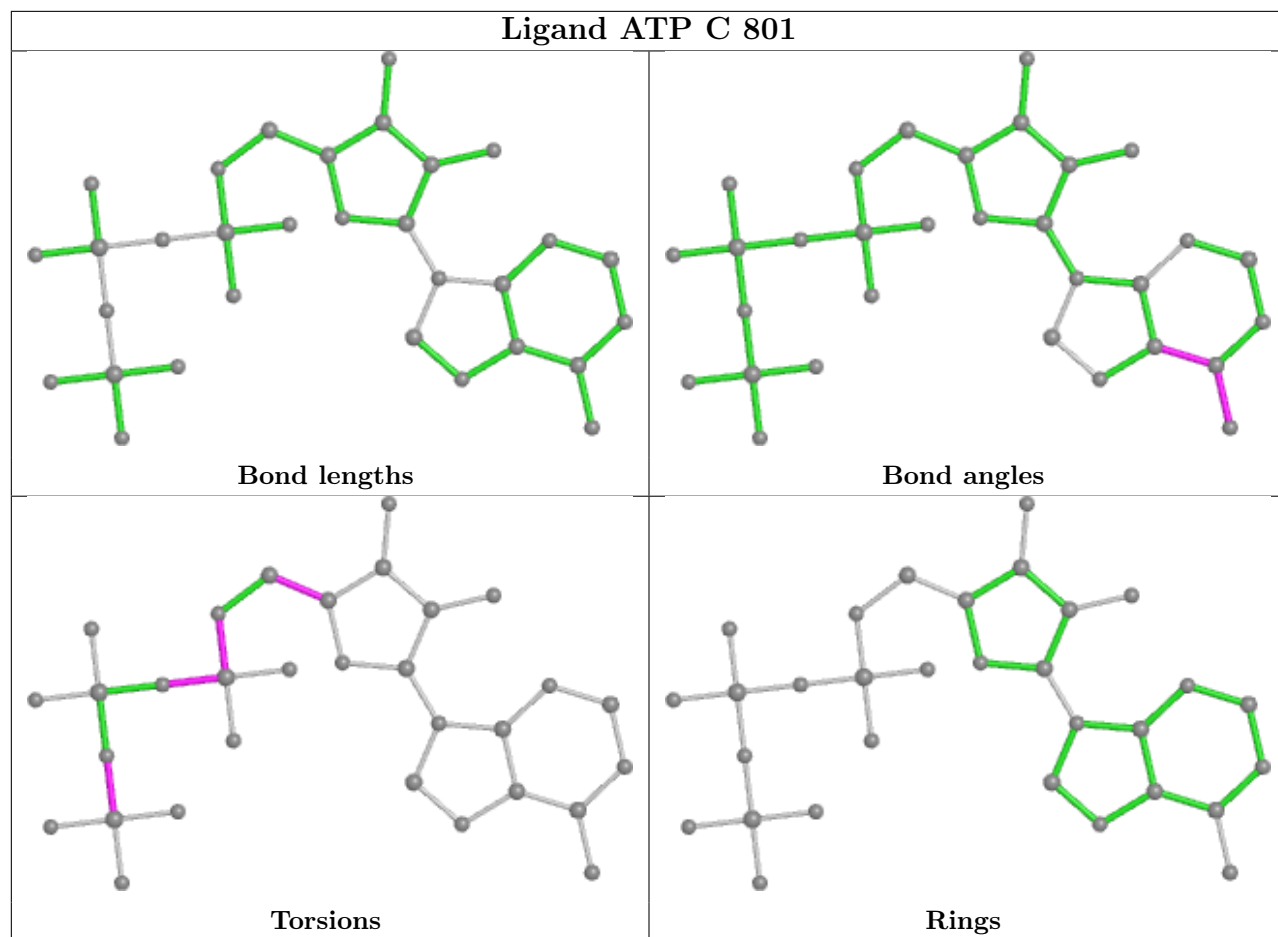


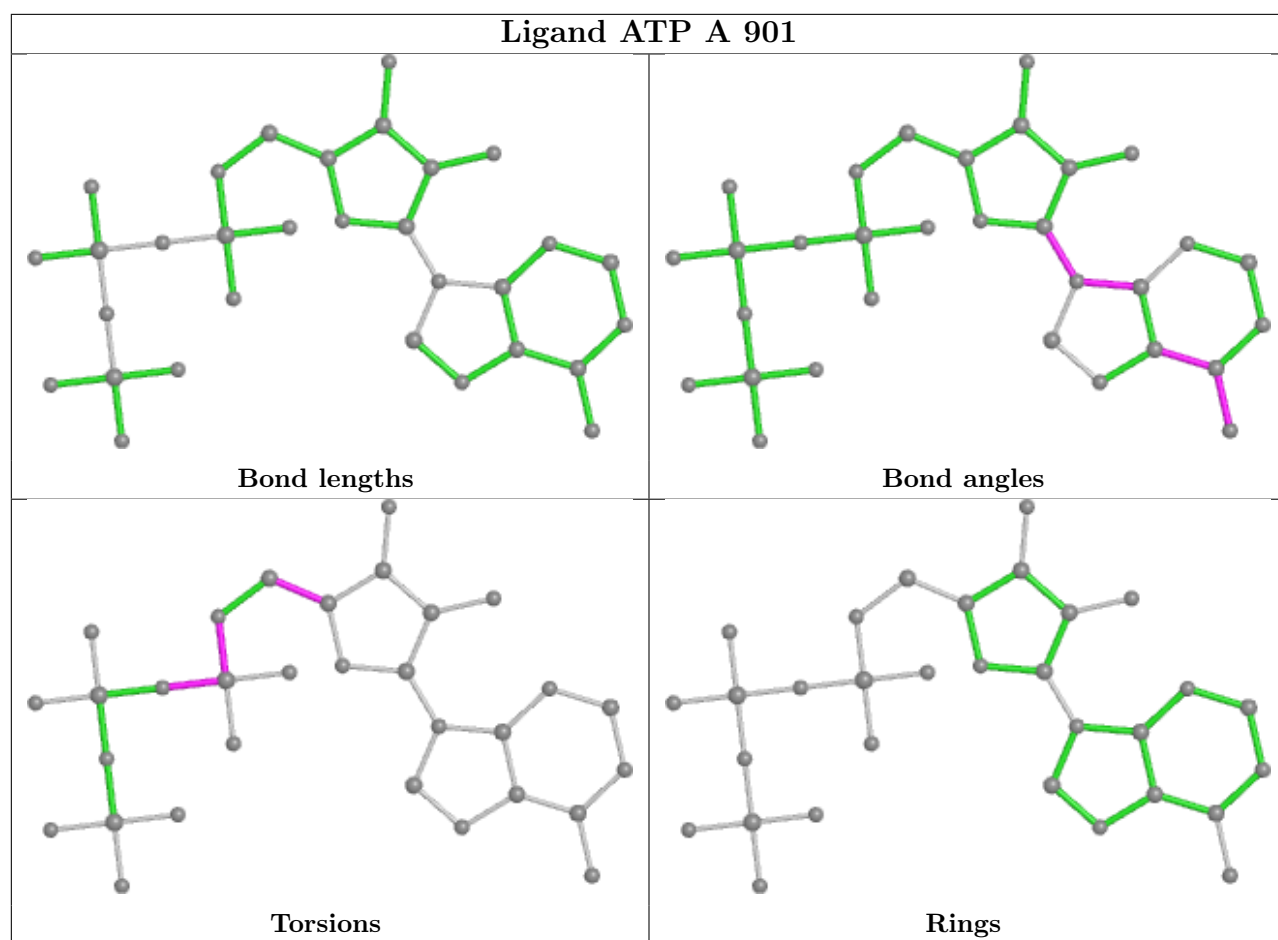




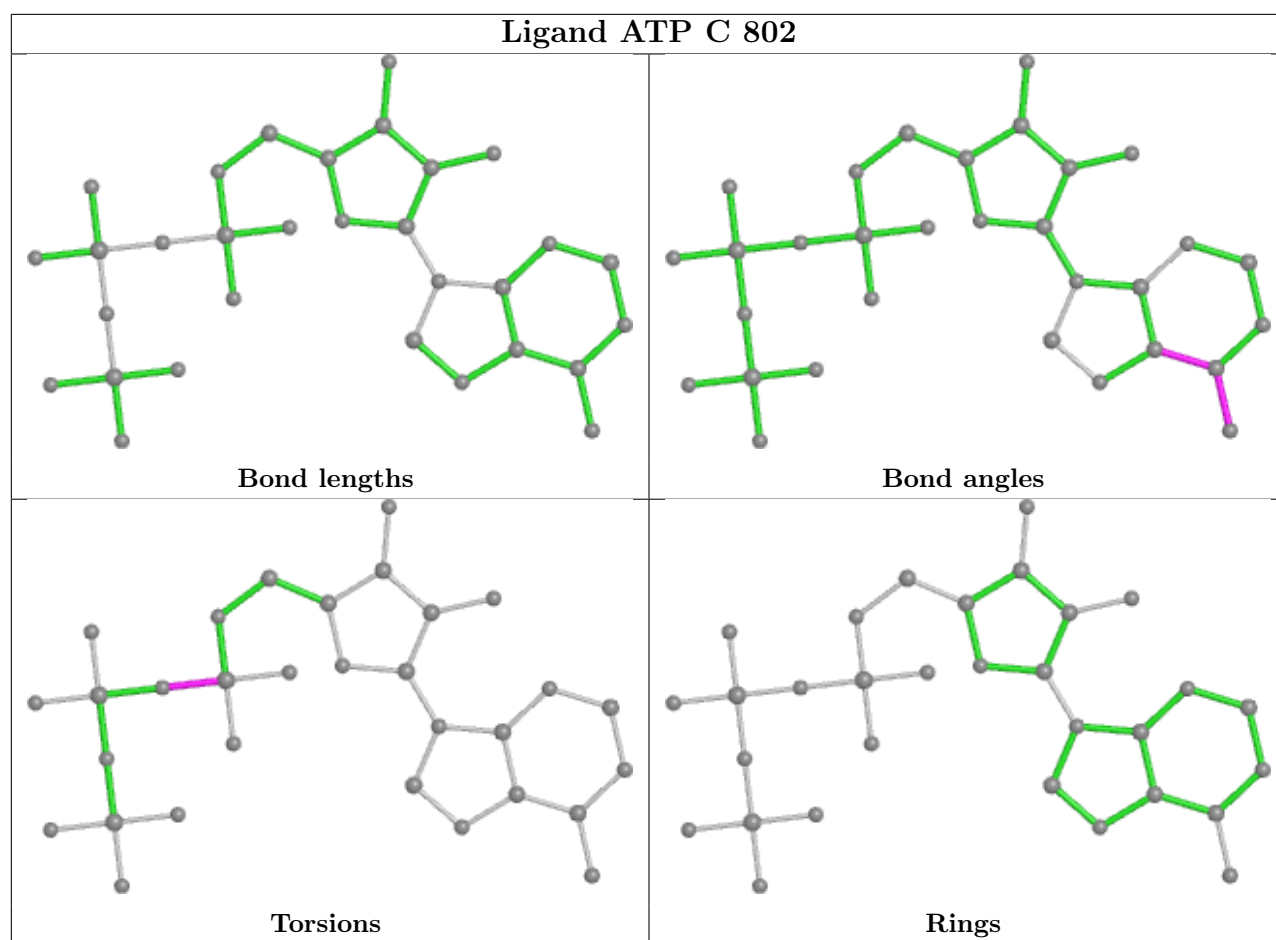












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

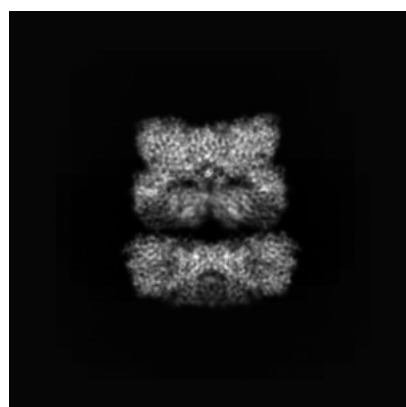
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63069. These allow visual inspection of the internal detail of the map and identification of artifacts.

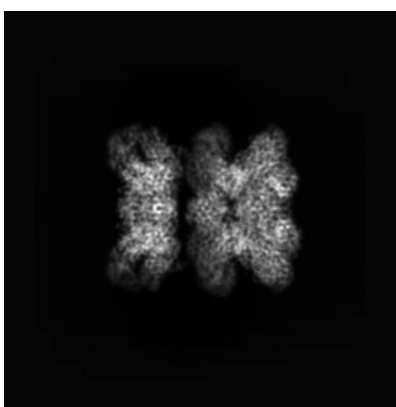
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

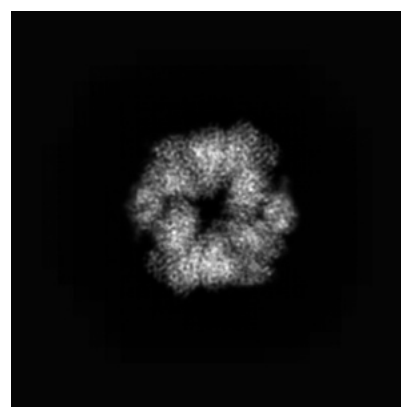
#### 6.1.1 Primary map



X



Y



Z

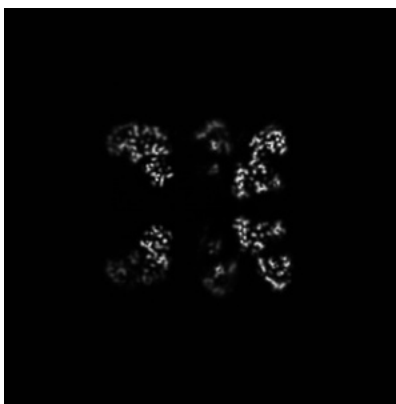
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

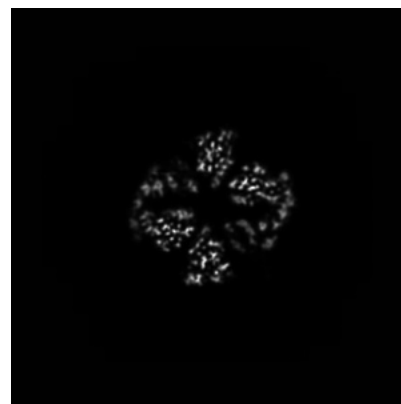
#### 6.2.1 Primary map



X Index: 140



Y Index: 140

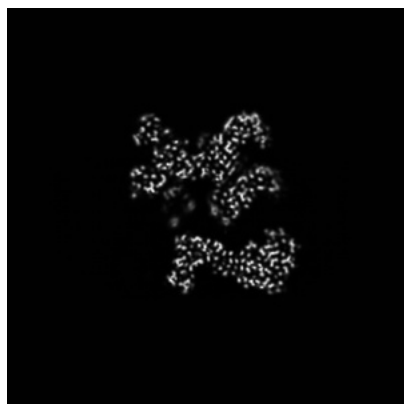


Z Index: 140

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

## 6.3 Largest variance slices [i](#)

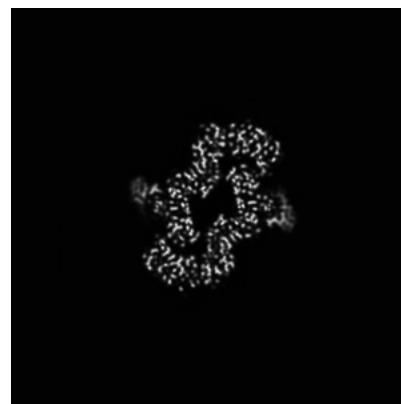
### 6.3.1 Primary map



X Index: 163



Y Index: 99

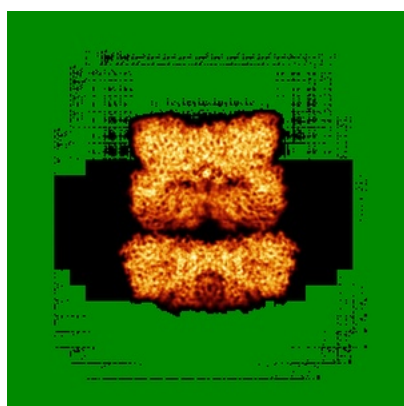


Z Index: 107

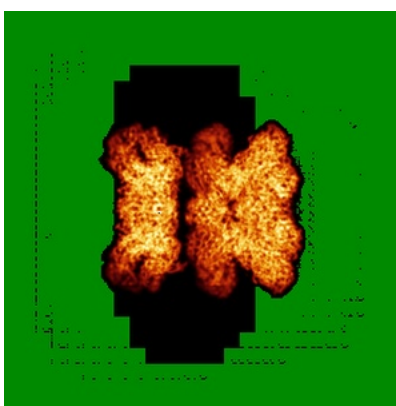
The images above show the largest variance slices of the map in three orthogonal directions.

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

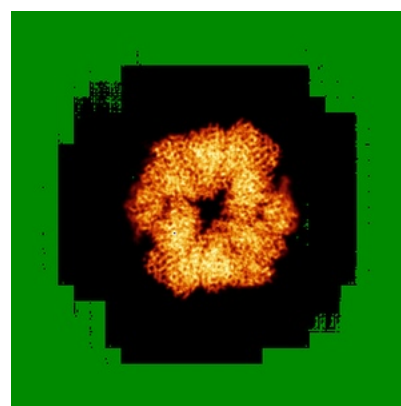
### 6.4.1 Primary map



X



Y

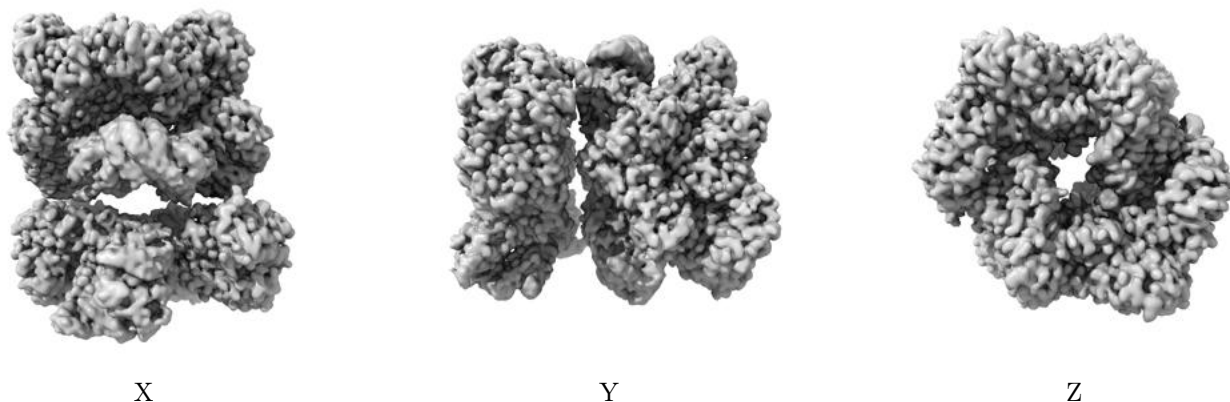


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

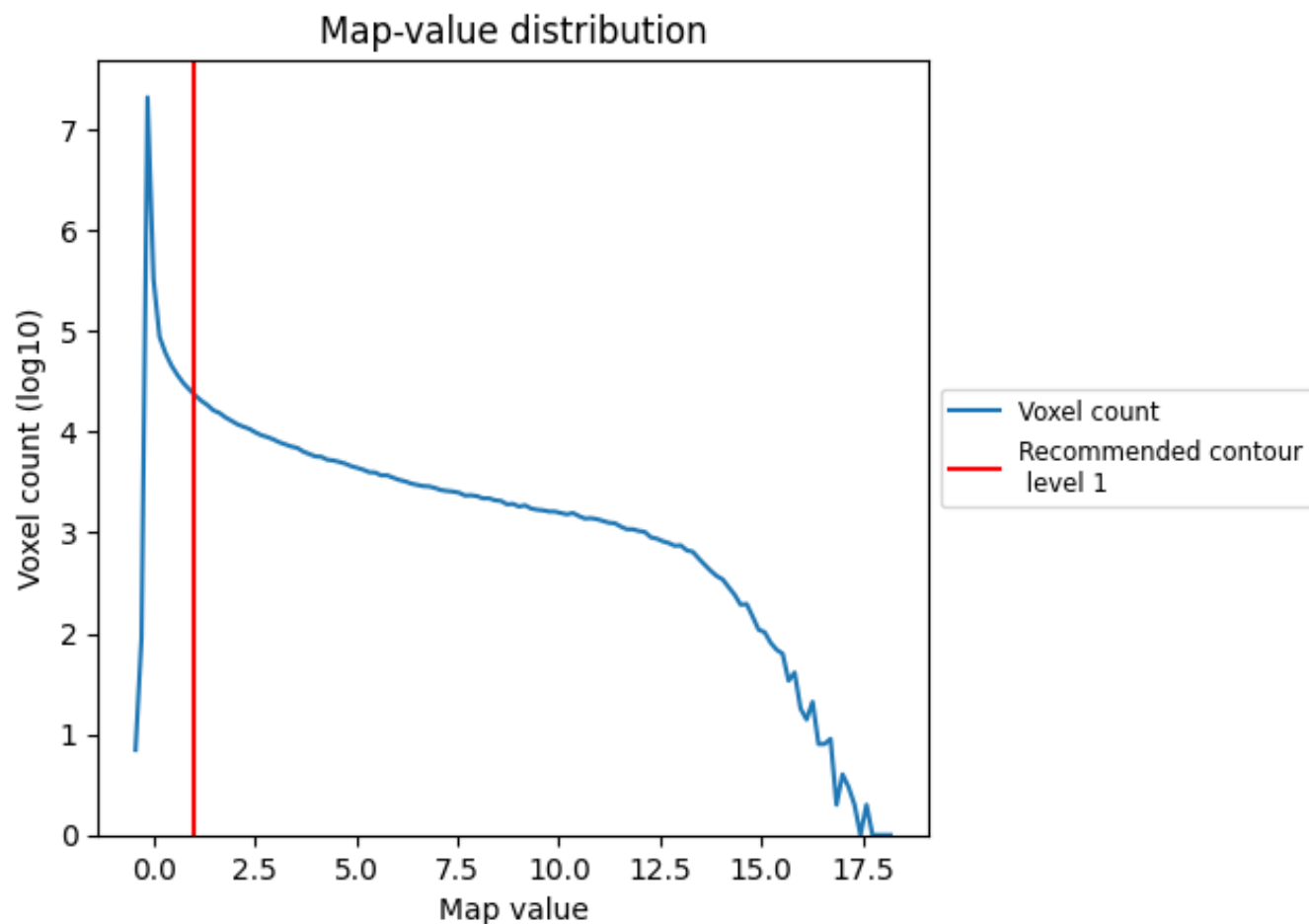
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

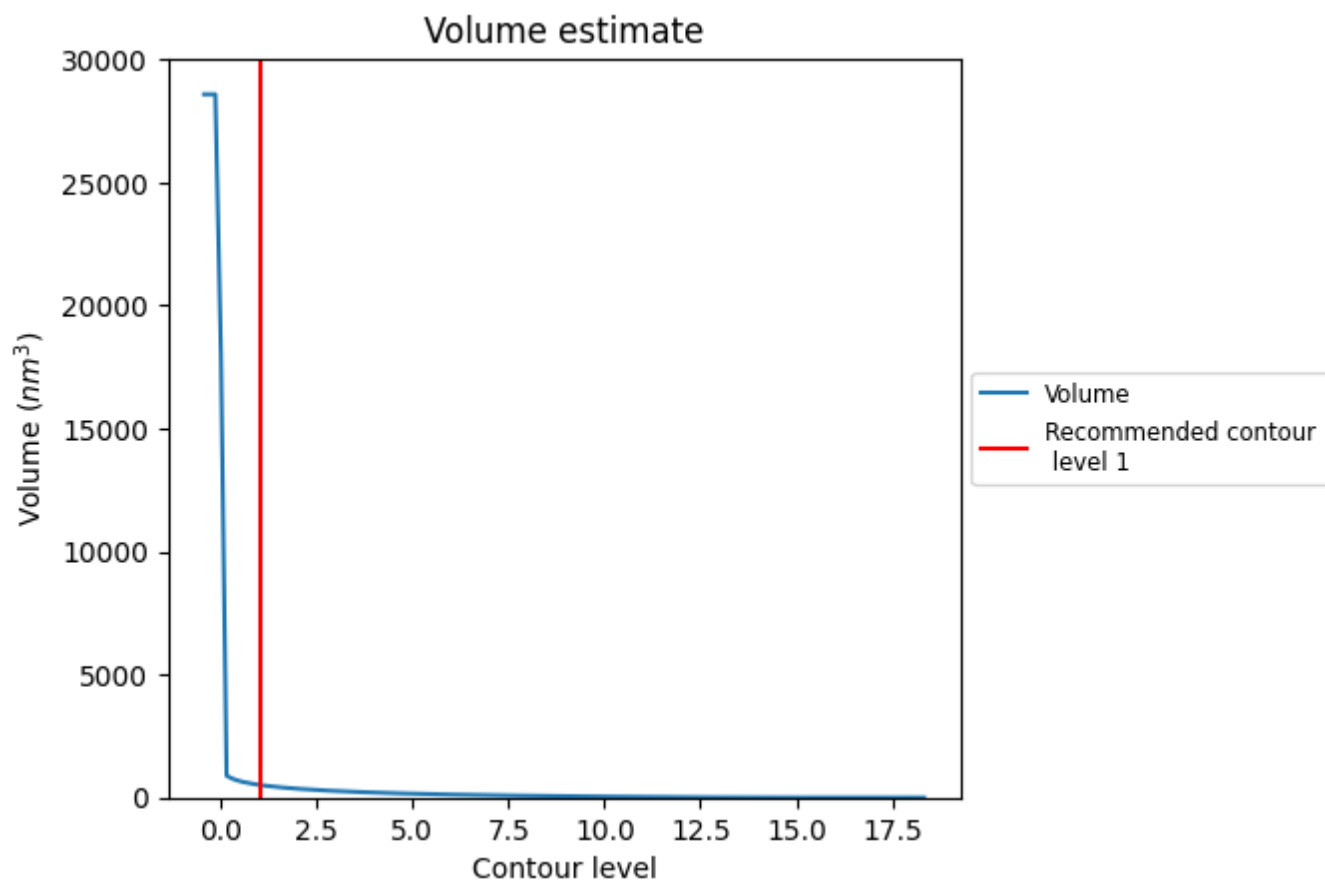
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

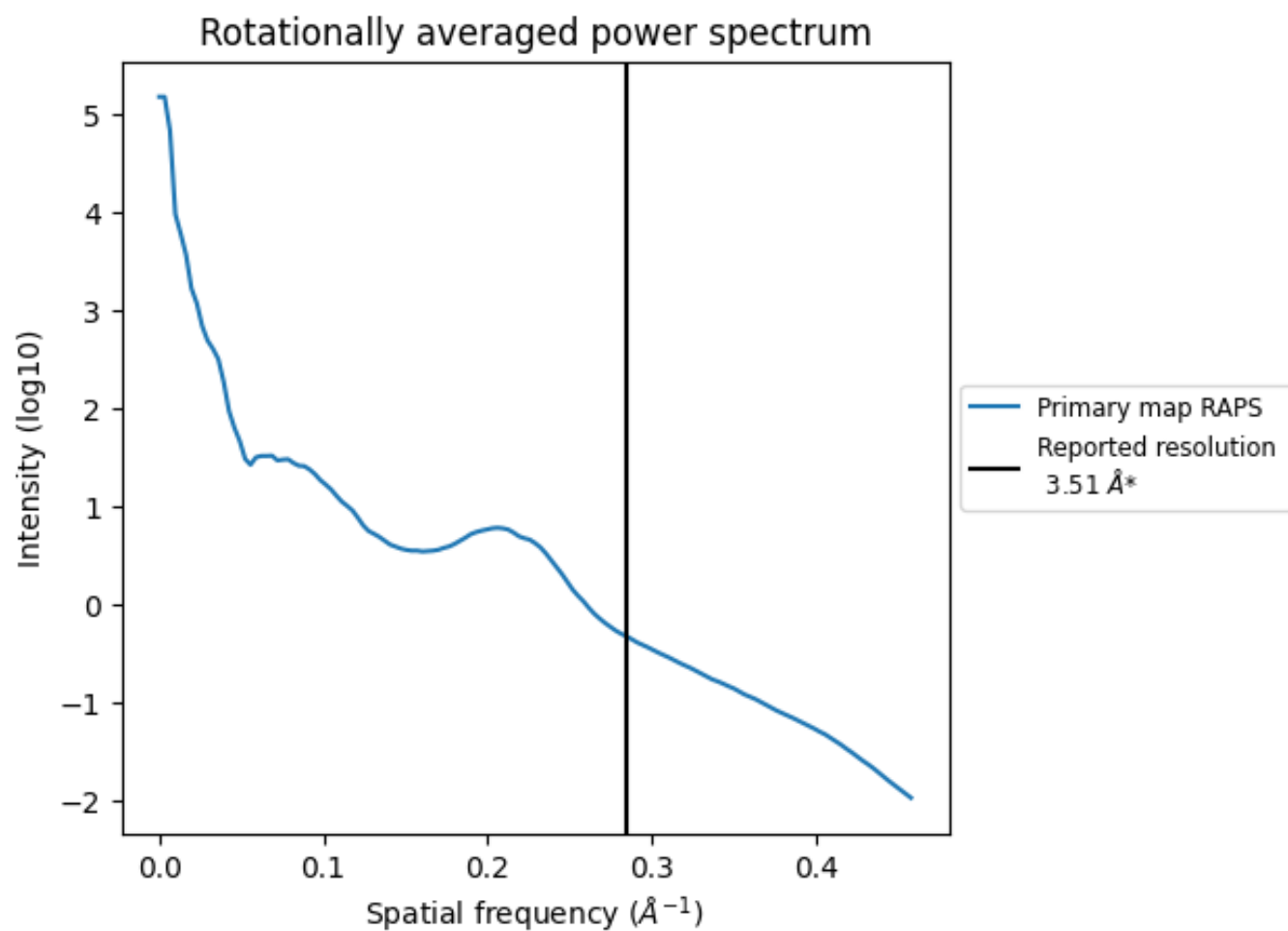
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 515 nm<sup>3</sup>; this corresponds to an approximate mass of 465 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 0.285 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

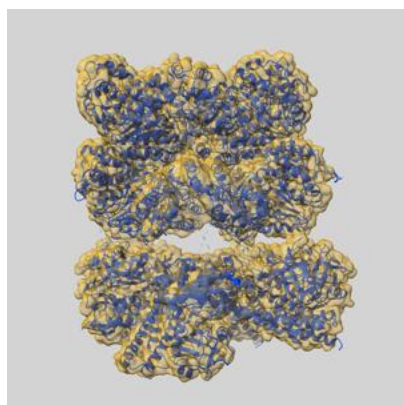
This section was not generated. No FSC curve or half-maps provided.



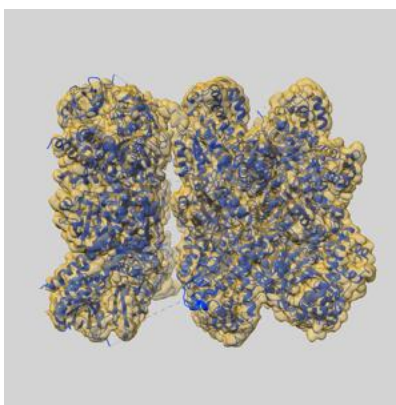
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63069 and PDB model 9LGO. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

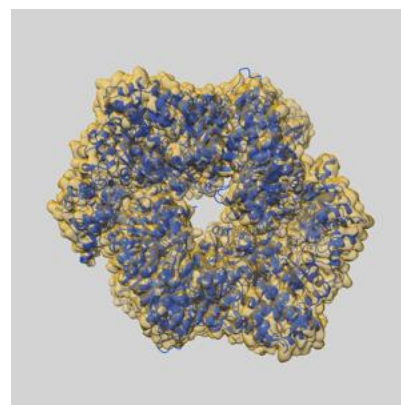
### 9.1 Map-model overlay [i](#)



X



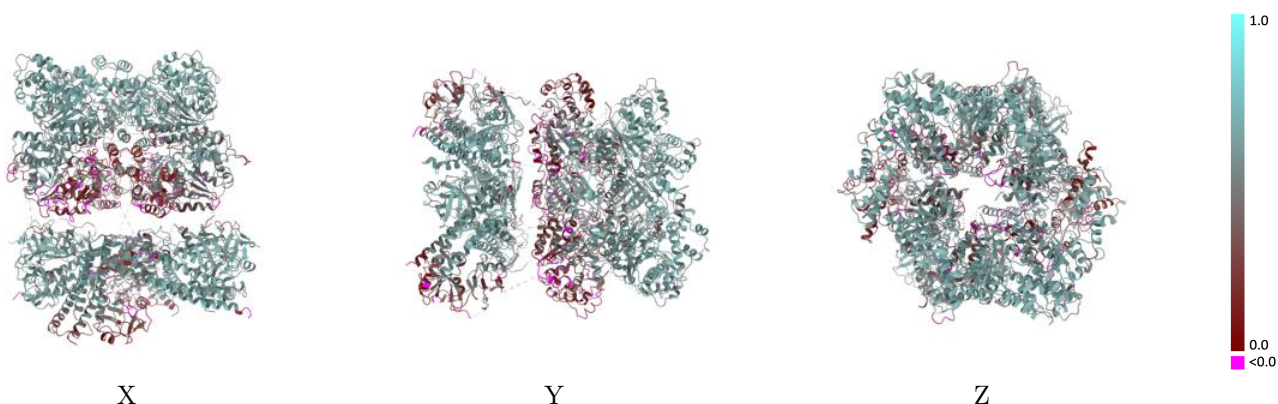
Y



Z

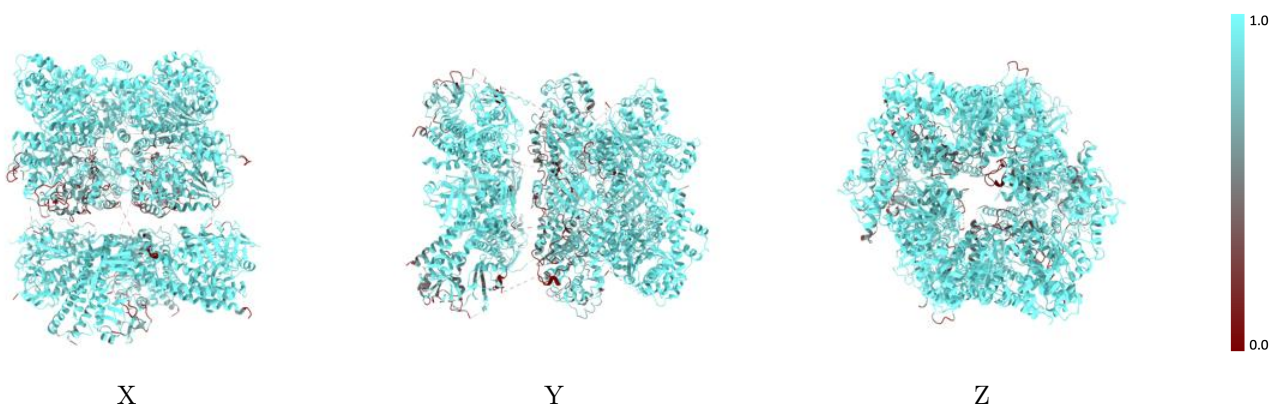
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



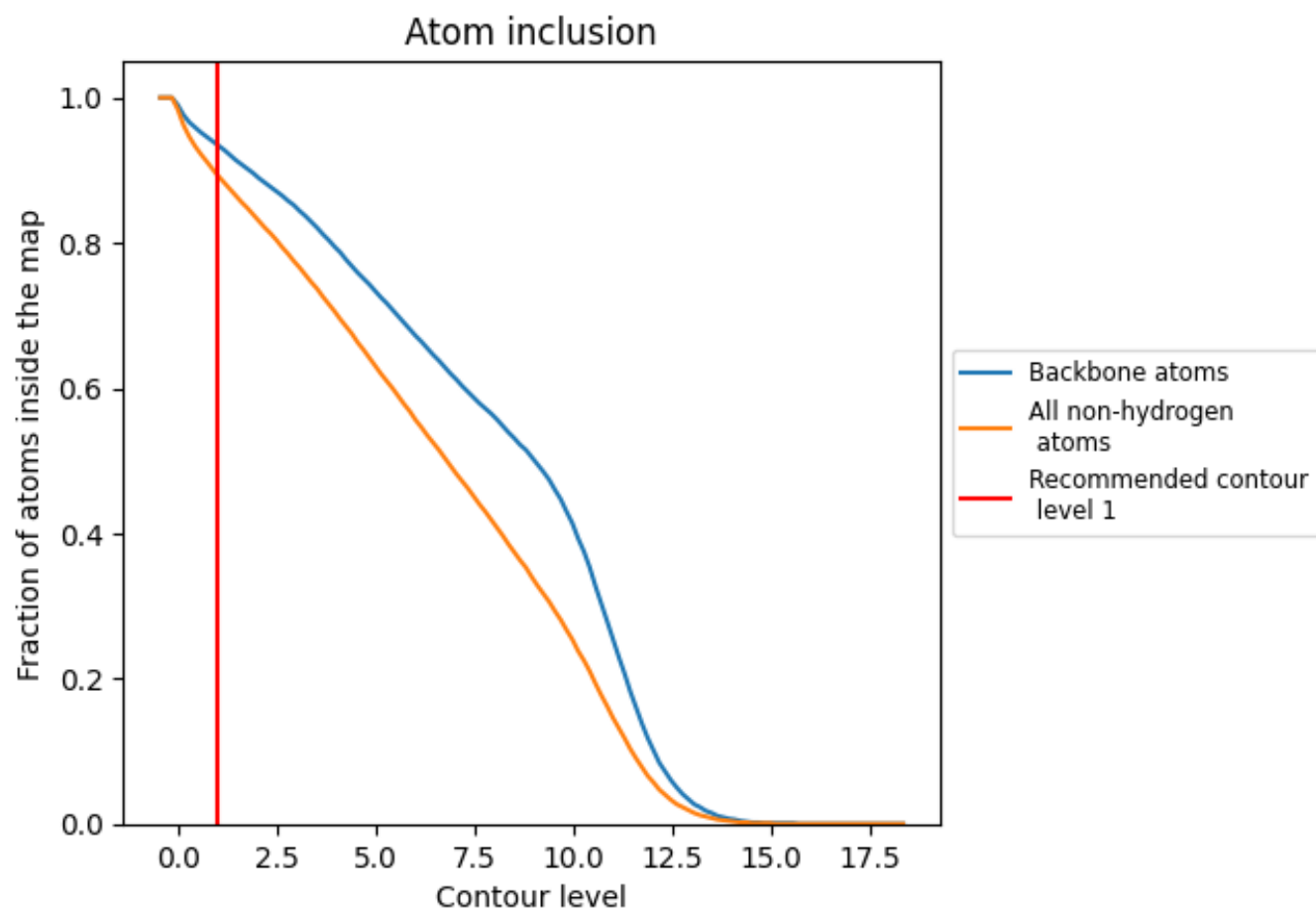
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8930</div>	<div><div></div>0.4790</div>
A	<div><div></div>0.9510</div>	<div><div></div>0.5220</div>
B	<div><div></div>0.7620</div>	<div><div></div>0.3460</div>
C	<div><div></div>0.9410</div>	<div><div></div>0.5190</div>
D	<div><div></div>0.9350</div>	<div><div></div>0.5230</div>
E	<div><div></div>0.7970</div>	<div><div></div>0.3610</div>
F	<div><div></div>0.9040</div>	<div><div></div>0.4990</div>
G	<div><div></div>0.9930</div>	<div><div></div>0.6240</div>
H	<div><div></div>0.9800</div>	<div><div></div>0.6160</div>
I	<div><div></div>0.9000</div>	<div><div></div>0.4990</div>
J	<div><div></div>0.9430</div>	<div><div></div>0.5230</div>

1.0

0.0

<0.0