



## Full wwPDB EM Validation Report ⓘ

Dec 14, 2024 – 01:07 PM EST

PDB ID : 9C77  
EMDB ID : EMD-45277  
Title : cryoEM structure of CRISPR associated effector, CARF-Adenosine deaminase 1, Cad1, in cA4 bound form with ATP.  
Authors : Majumder, P.; Patel, D.J.  
Deposited on : 2024-06-10  
Resolution : 3.20 Å(reported)  
Based on initial model : .

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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
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) : 2.40

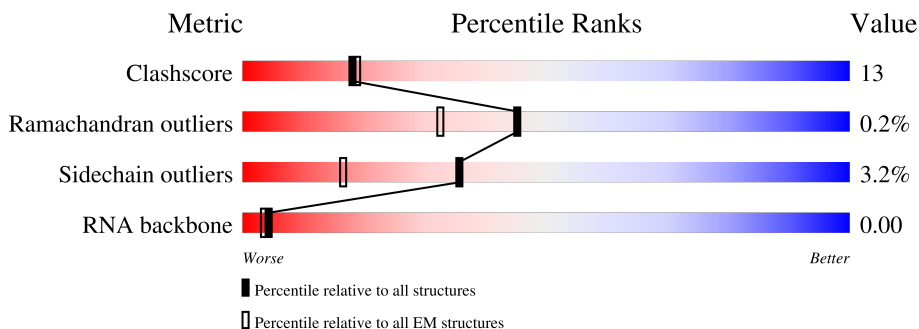
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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
RNA backbone	6643	2191

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	600	
1	B	600	
1	C	600	
1	D	600	
1	E	600	
1	F	600	
2	G	4	

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Mol	Chain	Length	Quality of chain
2	H	4	<div><div></div><div>75%</div><div>25%</div></div>
2	I	4	<div><div>25%</div><div>25%</div><div>50%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28792 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 Adenosine deaminase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	592	Total	C	N	O	S	0	0
			4666	2973	804	863	26		
1	B	600	Total	C	N	O	S	0	0
			4720	3005	813	874	28		
1	C	592	Total	C	N	O	S	0	0
			4666	2973	804	863	26		
1	D	599	Total	C	N	O	S	0	0
			4712	3001	812	871	28		
1	E	592	Total	C	N	O	S	0	0
			4666	2973	804	863	26		
1	F	600	Total	C	N	O	S	0	0
			4720	3005	813	874	28		

- Molecule 2 is a RNA chain called RNA (5'-R(P\*AP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	4	Total	C	N	O	P	0	0
			88	40	20	24	4		
2	H	4	Total	C	N	O	P	0	0
			88	40	20	24	4		
2	I	4	Total	C	N	O	P	0	0
			88	40	20	24	4		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

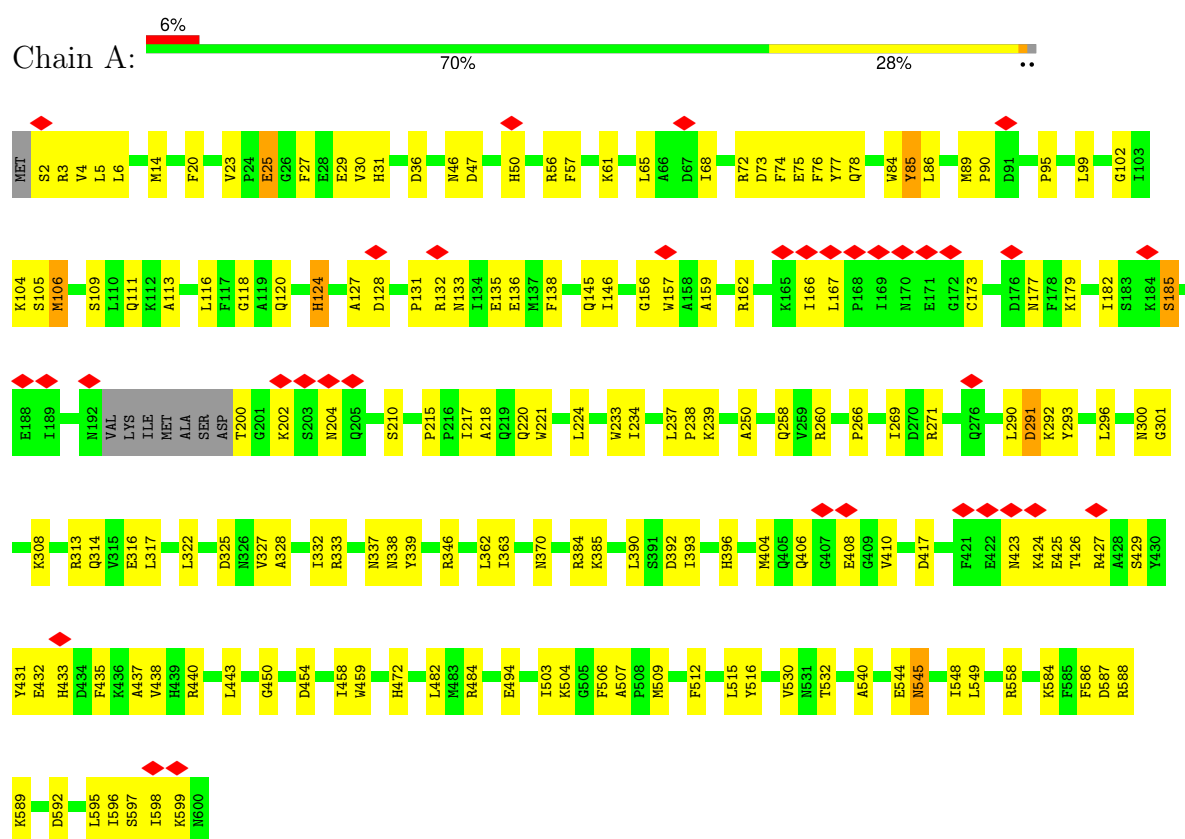
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

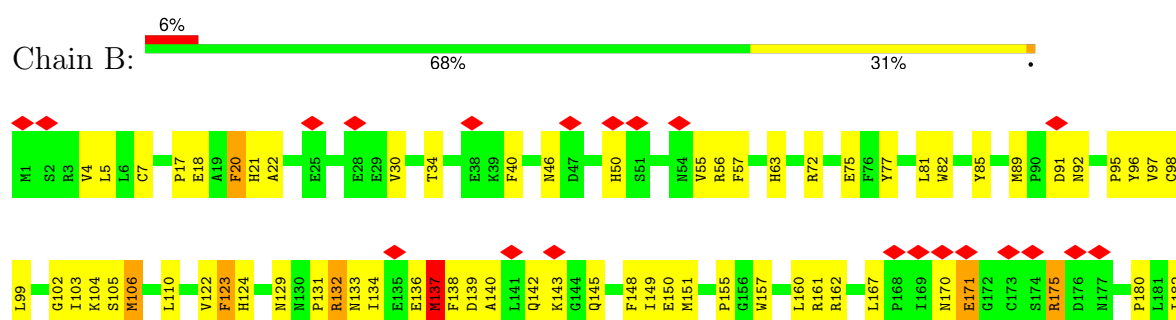
### 3 Residue-property plots

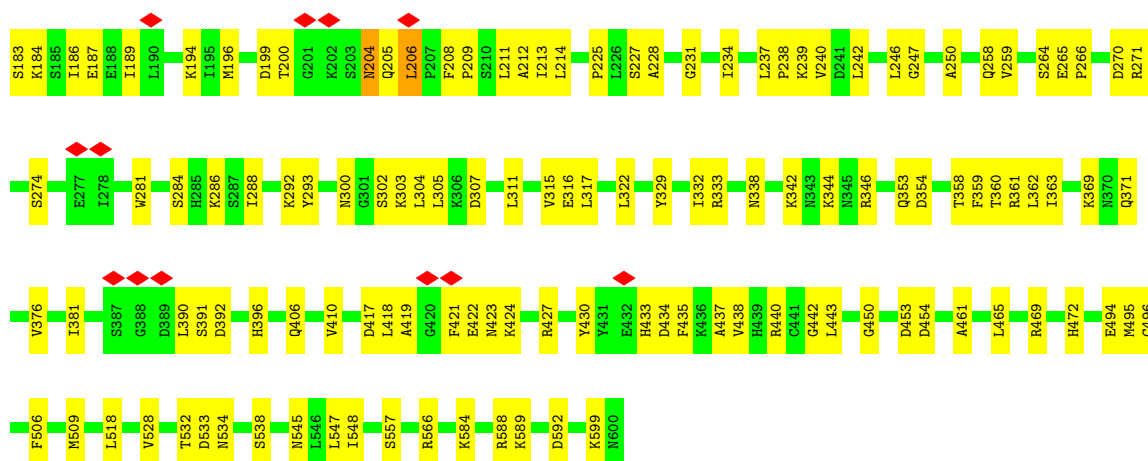
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

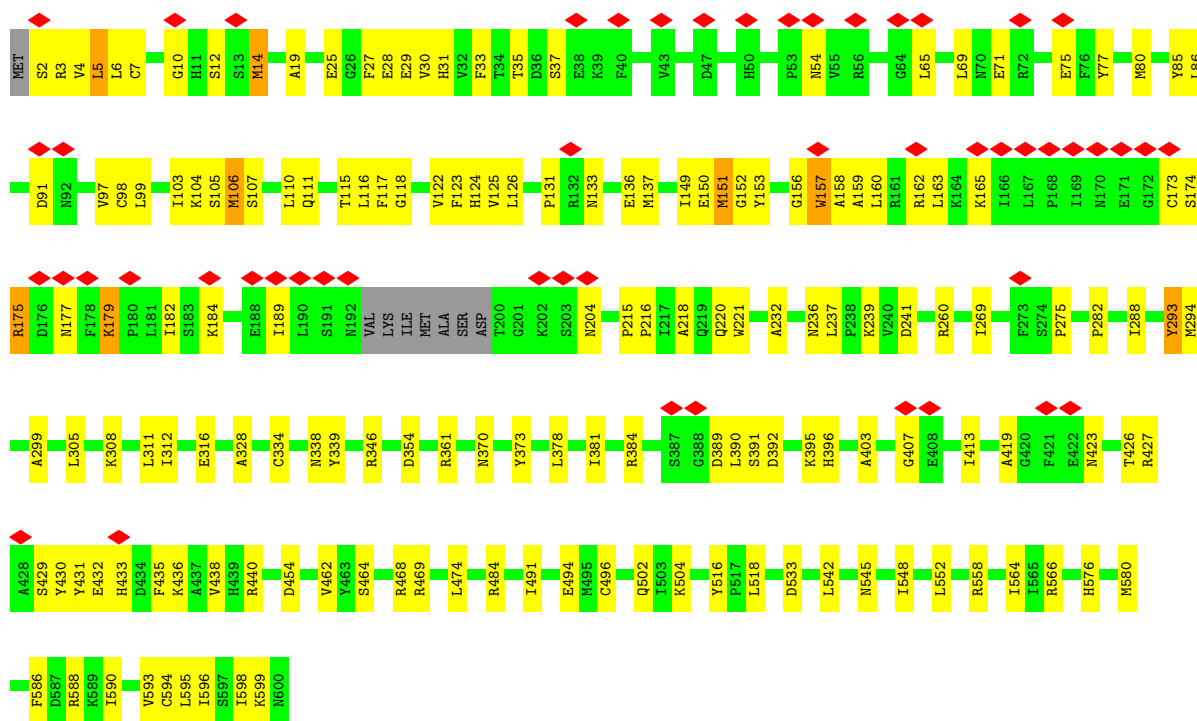


- Molecule 1: Adenosine deaminase domain-containing protein

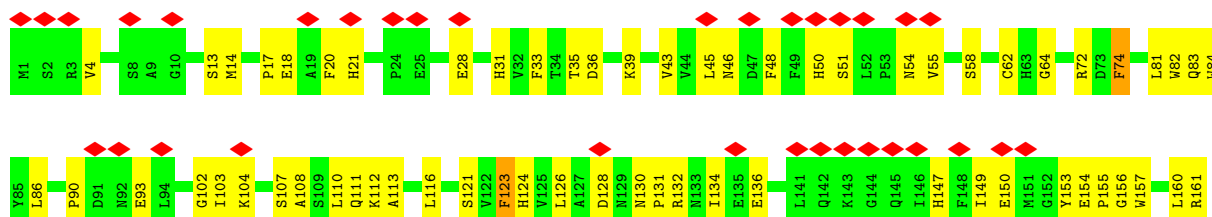




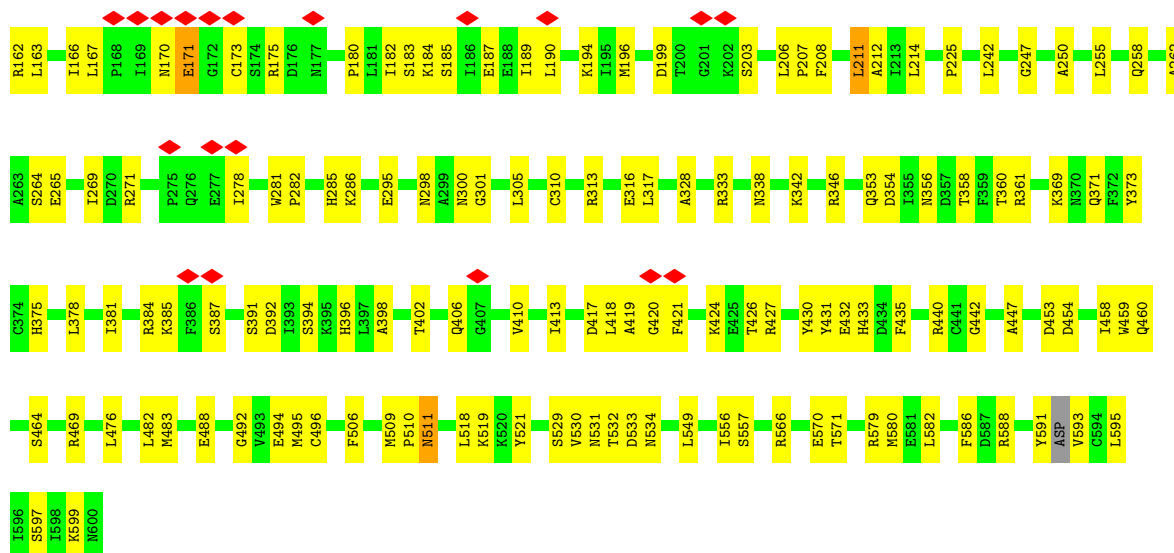
• Molecule 1: Adenosine deaminase domain-containing protein



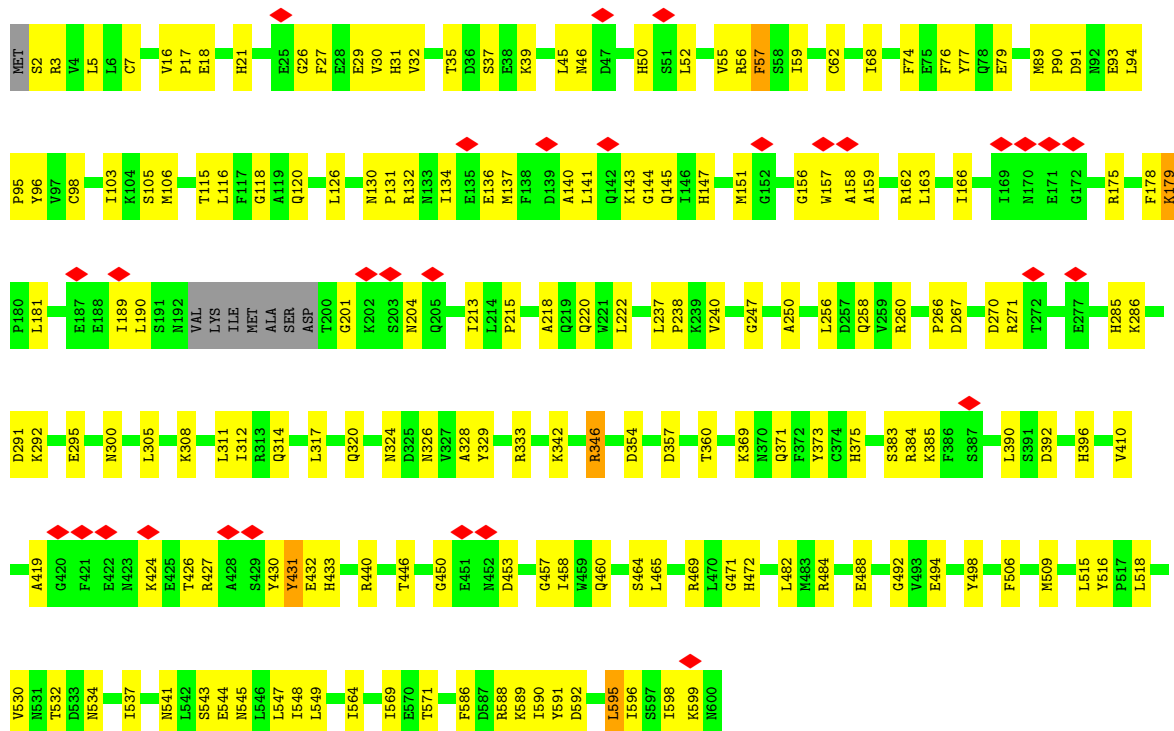
• Molecule 1: Adenosine deaminase domain-containing protein



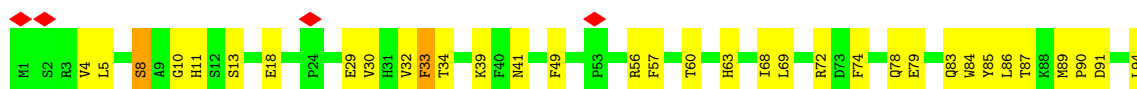


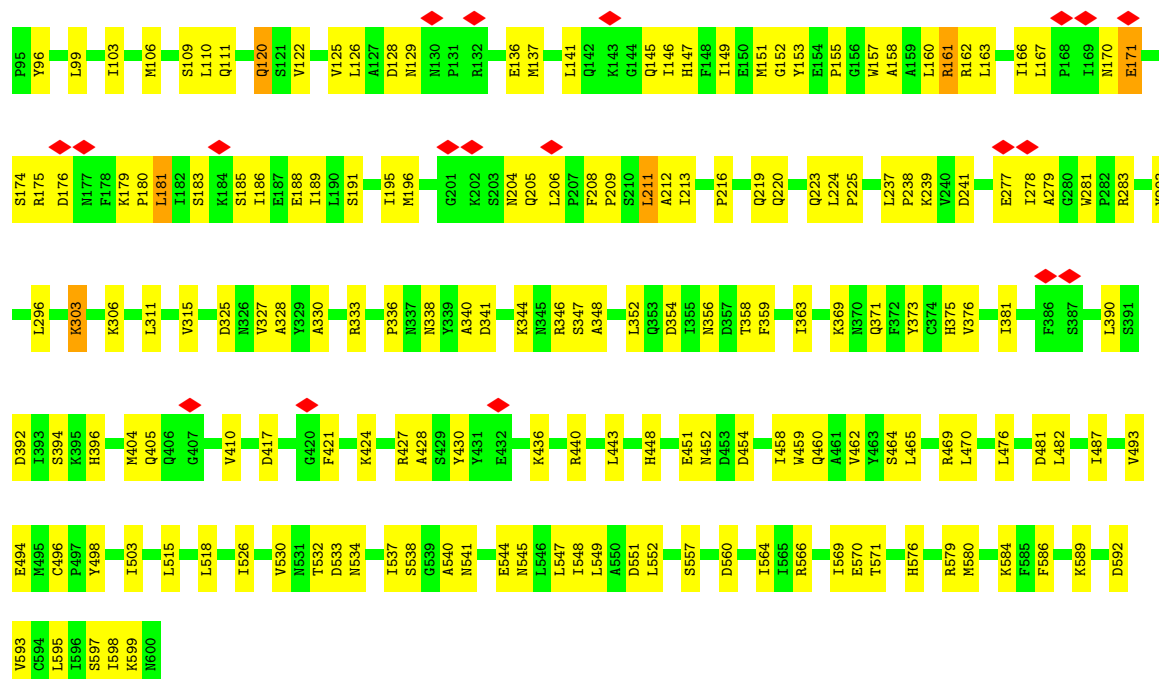


• Molecule 1: Adenosine deaminase domain-containing protein




• Molecule 1: Adenosine deaminase domain-containing protein






- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*A)-3')

Chain G:  50%



- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*A)-3')

Chain H:  75%



- Molecule 2: RNA (5'-R(P\*AP\*AP\*AP\*A)-3')

Chain I:  25%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	27.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.431	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.065	Depositor
Map size ( $\text{\AA}$ )	371.2, 371.2, 371.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.725, 0.725, 0.725	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.26	0/4770	0.48	0/6462
1	B	0.25	0/4824	0.48	1/6535 (0.0%)
1	C	0.25	0/4770	0.46	0/6462
1	D	0.25	0/4815	0.49	1/6521 (0.0%)
1	E	0.25	0/4770	0.48	0/6462
1	F	0.26	0/4824	0.51	1/6535 (0.0%)
2	G	0.32	0/99	0.87	0/152
2	H	0.18	0/99	0.69	0/152
2	I	0.14	0/99	0.62	0/152
All	All	0.25	0/29070	0.49	3/39433 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	LEU	CA-CB-CG	5.65	128.30	115.30
1	F	211	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	137	MET	CA-CB-CG	5.24	122.20	113.30

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	4666	0	4635	122	0
1	B	4720	0	4696	143	0
1	C	4666	0	4635	121	0
1	D	4712	0	4690	136	0
1	E	4666	0	4634	128	0
1	F	4720	0	4698	140	0
2	G	88	0	45	4	0
2	H	88	0	45	3	0
2	I	88	0	45	2	0
3	A	62	0	20	3	0
3	B	62	0	19	3	0
3	C	62	0	22	5	0
3	D	62	0	22	5	0
3	E	62	0	22	5	0
3	F	62	0	22	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	28792	0	28250	744	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 13.

All (744) 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:D:338:ASN:ND2	3:D:702:ATP:O2A	1.61	1.32
1:C:338:ASN:ND2	3:C:702:ATP:O2A	1.76	1.17
1:D:211:LEU:HD13	1:D:214:LEU:HD13	1.53	0.89
1:A:162:ARG:H	1:A:599:LYS:HG2	1.40	0.85
1:D:247:GLY:HA3	3:D:702:ATP:O1B	1.77	0.84
1:F:166:ILE:HG12	1:F:181:LEU:HD12	1.64	0.79
1:E:189:ILE:HD13	1:F:155:PRO:HD3	1.64	0.79
1:E:131:PRO:HB3	1:E:136:GLU:HB3	1.67	0.76
1:C:157:TRP:CE3	1:C:215:PRO:HB3	2.21	0.76
1:C:162:ARG:H	1:C:599:LYS:HG2	1.48	0.76
1:C:162:ARG:HD3	1:C:599:LYS:HB3	1.68	0.76
1:F:211:LEU:HD12	1:F:212:ALA:H	1.49	0.75
1:C:427:ARG:HH21	1:C:429:SER:HB3	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ASN:O	1:A:50:HIS:ND1	2.18	0.74
1:F:204:ASN:OD1	1:F:205:GLN:N	2.21	0.73
1:A:406:GLN:O	1:D:342:LYS:NZ	2.22	0.72
1:E:159:ALA:HB3	1:E:598:ILE:HG13	1.72	0.72
1:C:99:LEU:HB3	1:C:110:LEU:HD22	1.72	0.72
1:E:118:GLY:HA2	1:E:156:GLY:HA3	1.74	0.70
1:A:89:MET:HE3	1:A:95:PRO:HD3	1.75	0.69
1:C:12:SER:OG	1:C:14:MET:SD	2.51	0.68
1:D:72:ARG:HH22	1:D:175:ARG:HE	1.39	0.68
1:D:469:ARG:NH1	1:D:494:GLU:OE1	2.25	0.68
1:B:422:GLU:HB3	1:B:427:ARG:HH22	1.58	0.68
1:F:315:VAL:HG11	1:F:358:THR:HG21	1.75	0.68
1:B:214:LEU:HD12	1:B:214:LEU:H	1.59	0.68
1:D:167:LEU:O	1:D:170:ASN:ND2	2.26	0.68
1:C:588:ARG:NH2	1:D:199:ASP:O	2.27	0.68
1:B:17:PRO:O	1:B:21:HIS:ND1	2.27	0.68
1:E:373:TYR:O	3:E:701:ATP:N6	2.27	0.68
1:E:29:GLU:HA	1:E:55:VAL:HG23	1.75	0.67
1:E:134:ILE:HA	1:E:137:MET:HG2	1.74	0.67
1:B:333:ARG:NH1	1:B:417:ASP:OD2	2.27	0.67
1:E:130:ASN:OD1	2:I:10:A:O2'	2.12	0.67
1:C:384:ARG:NH1	1:C:426:THR:O	2.28	0.67
1:B:469:ARG:NH1	1:B:494:GLU:OE2	2.28	0.67
1:D:510:PRO:O	1:D:511:ASN:ND2	2.28	0.66
1:C:2:SER:OG	1:C:3:ARG:N	2.29	0.66
1:B:97:VAL:HB	1:B:122:VAL:HG22	1.78	0.66
1:C:151:MET:SD	1:C:151:MET:N	2.67	0.66
1:F:373:TYR:O	3:F:701:ATP:N6	2.29	0.66
1:C:474:LEU:HD12	1:C:504:LYS:HD2	1.78	0.66
1:C:158:ALA:HB3	1:C:595:LEU:HD21	1.78	0.65
1:D:333:ARG:NH1	1:D:417:ASP:OD2	2.29	0.65
1:B:288:ILE:HD11	1:B:292:LYS:HB2	1.78	0.65
1:C:381:ILE:HG21	3:C:702:ATP:O2'	1.96	0.65
1:D:18:GLU:OE2	2:H:4:A:N6	2.30	0.65
1:F:157:TRP:HB2	1:F:160:LEU:HB3	1.78	0.65
1:D:419:ALA:HB1	3:D:702:ATP:N3	2.11	0.65
1:D:155:PRO:O	1:D:161:ARG:NH2	2.30	0.64
1:C:126:LEU:HB2	1:C:149:ILE:HD11	1.79	0.64
1:C:373:TYR:O	3:C:701:ATP:N6	2.30	0.64
1:E:384:ARG:HD3	1:E:431:TYR:HE2	1.63	0.64
1:C:391:SER:OG	1:C:395:LYS:NZ	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:ILE:HG22	1:F:106:MET:HG2	1.79	0.64
1:F:469:ARG:NH1	1:F:494:GLU:OE2	2.30	0.64
1:C:588:ARG:NH2	1:D:196:MET:O	2.30	0.64
1:C:103:ILE:HG13	1:C:105:SER:H	1.62	0.64
1:F:155:PRO:O	1:F:161:ARG:NH2	2.31	0.64
1:F:191:SER:O	1:F:195:ILE:HG12	1.98	0.64
1:F:63:HIS:O	1:F:175:ARG:NH2	2.31	0.64
1:F:162:ARG:NH2	1:F:592:ASP:OD2	2.29	0.64
1:C:118:GLY:HA2	1:C:156:GLY:HA3	1.79	0.64
1:F:333:ARG:NH1	1:F:417:ASP:OD2	2.29	0.64
1:A:118:GLY:HA2	1:A:156:GLY:HA3	1.78	0.63
1:B:225:PRO:HA	1:B:557:SER:HA	1.80	0.63
1:C:232:ALA:O	1:C:236:ASN:ND2	2.28	0.63
1:D:333:ARG:NH2	1:D:494:GLU:OE2	2.31	0.63
1:D:373:TYR:O	3:D:701:ATP:N6	2.31	0.63
1:C:3:ARG:NH1	1:C:25:GLU:OE2	2.32	0.63
1:B:91:ASP:OD1	1:B:92:ASN:N	2.32	0.62
1:B:131:PRO:HB2	1:B:137:MET:HB3	1.81	0.62
1:B:363:ILE:HD11	1:B:376:VAL:HG22	1.80	0.62
1:A:440:ARG:HH21	1:D:391:SER:H	1.47	0.62
1:B:238:PRO:HG3	1:B:589:LYS:HB3	1.81	0.62
1:C:204:ASN:ND2	1:D:580:MET:O	2.33	0.62
1:B:160:LEU:HD11	1:B:189:ILE:HD13	1.82	0.62
1:D:31:HIS:ND1	1:D:58:SER:OG	2.33	0.62
1:A:339:TYR:OH	3:A:702:ATP:O1B	2.17	0.62
1:B:124:HIS:HB2	1:B:149:ILE:HB	1.82	0.61
1:E:392:ASP:O	1:E:396:HIS:ND1	2.33	0.61
1:F:126:LEU:N	1:F:147:HIS:O	2.29	0.61
1:F:211:LEU:HD12	1:F:212:ALA:N	2.15	0.61
1:A:2:SER:OG	1:A:3:ARG:N	2.29	0.61
1:F:208:PHE:O	1:F:566:ARG:NH1	2.33	0.61
1:F:363:ILE:HD11	1:F:376:VAL:HG12	1.82	0.61
1:D:82:TRP:HB3	1:D:182:ILE:HG21	1.81	0.61
1:A:237:LEU:O	1:A:239:LYS:NZ	2.32	0.61
1:C:111:GLN:HE22	1:D:108:ALA:HA	1.64	0.61
1:A:433:HIS:HB2	1:D:433:HIS:HB2	1.83	0.61
1:C:518:LEU:HD21	1:C:564:ILE:HD11	1.81	0.61
1:A:157:TRP:CD1	1:A:217:ILE:HG21	2.35	0.61
1:F:238:PRO:HG3	1:F:589:LYS:HB3	1.82	0.61
1:B:209:PRO:HG2	1:B:211:LEU:HD22	1.83	0.60
1:D:353:GLN:OE1	1:D:406:GLN:NE2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PRO:HB3	1:A:136:GLU:HB3	1.82	0.60
1:F:428:ALA:HB1	1:F:465:LEU:HG	1.83	0.60
1:A:540:ALA:HB1	1:A:544:GLU:HG3	1.83	0.60
1:C:288:ILE:HD11	1:C:293:TYR:HD1	1.66	0.60
1:B:424:LYS:HD2	1:B:427:ARG:HG3	1.83	0.60
1:C:6:LEU:HB2	1:C:97:VAL:HG23	1.82	0.60
1:C:111:GLN:NE2	1:D:111:GLN:OE1	2.30	0.60
1:F:8:SER:OG	1:F:33:PHE:O	2.16	0.60
1:B:250:ALA:O	1:B:300:ASN:ND2	2.35	0.60
1:E:218:ALA:HB2	1:E:598:ILE:HD13	1.83	0.60
1:D:131:PRO:HB3	1:D:136:GLU:HG3	1.84	0.60
1:D:162:ARG:HH21	1:D:588:ARG:HD2	1.66	0.60
1:A:338:ASN:ND2	3:A:702:ATP:O2A	2.35	0.60
1:D:316:GLU:OE2	1:D:361:ARG:NH2	2.31	0.60
1:A:72:ARG:NH2	1:A:73:ASP:OD1	2.35	0.59
1:B:18:GLU:OE2	2:G:0:A:N6	2.35	0.59
1:C:150:GLU:OE2	1:C:152:GLY:N	2.32	0.59
1:E:375:HIS:NE2	1:E:410:VAL:O	2.34	0.59
1:E:588:ARG:NH1	1:E:592:ASP:OD1	2.35	0.59
1:A:5:LEU:HG	1:A:27:PHE:CE2	2.37	0.59
1:C:419:ALA:HB1	3:C:702:ATP:C2	2.37	0.59
1:E:204:ASN:HD21	1:F:584:LYS:HE3	1.66	0.59
1:F:128:ASP:HB2	1:F:145:GLN:HE21	1.67	0.59
1:E:2:SER:OG	1:E:3:ARG:N	2.36	0.59
1:A:6:LEU:HB3	1:A:84:TRP:HH2	1.68	0.59
1:A:404:MET:SD	1:A:443:LEU:HG	2.43	0.59
1:A:47:ASP:HA	1:A:50:HIS:CE1	2.38	0.58
1:B:392:ASP:O	1:B:396:HIS:ND1	2.36	0.58
1:D:281:TRP:HE3	1:D:282:PRO:HA	1.68	0.58
1:F:237:LEU:O	1:F:239:LYS:NZ	2.36	0.58
1:B:211:LEU:HG	1:B:212:ALA:H	1.67	0.58
1:A:363:ILE:HG21	1:A:410:VAL:HG11	1.86	0.58
1:B:103:ILE:HG22	1:B:106:MET:HG2	1.84	0.58
1:E:115:THR:O	1:E:157:TRP:NE1	2.37	0.58
1:A:291:ASP:OD1	1:A:291:ASP:N	2.35	0.58
1:B:454:ASP:OD1	1:B:454:ASP:N	2.37	0.58
1:D:20:PHE:HE2	1:D:55:VAL:HG11	1.69	0.58
1:D:346:ARG:NH2	1:D:354:ASP:OD2	2.31	0.57
1:C:116:LEU:HA	1:C:157:TRP:NE1	2.19	0.57
1:D:385:LYS:NZ	1:D:387:SER:OG	2.30	0.57
1:C:218:ALA:HB2	1:C:598:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:460:GLN:O	1:F:464:SER:OG	2.17	0.57
1:A:5:LEU:HD11	1:A:20:PHE:HA	1.87	0.57
1:E:256:LEU:HG	1:E:260:ARG:HD2	1.85	0.57
1:E:384:ARG:NH1	1:E:426:THR:O	2.37	0.57
1:D:392:ASP:O	1:D:396:HIS:ND1	2.38	0.57
1:E:157:TRP:CE3	1:E:215:PRO:HB3	2.40	0.57
1:F:167:LEU:O	1:F:170:ASN:ND2	2.37	0.57
1:B:422:GLU:O	1:B:427:ARG:NH1	2.37	0.57
1:C:484:ARG:HH12	1:D:442:GLY:HA3	1.70	0.57
1:D:154:GLU:OE1	1:D:156:GLY:N	2.30	0.57
1:E:266:PRO:HB3	1:E:271:ARG:HH22	1.70	0.57
1:F:225:PRO:HA	1:F:557:SER:HA	1.87	0.57
1:D:398:ALA:O	1:D:402:THR:HG23	2.05	0.57
1:D:420:GLY:H	3:D:702:ATP:H2	1.53	0.57
1:F:338:ASN:ND2	3:F:702:ATP:O2A	2.37	0.57
1:A:384:ARG:NH1	1:A:426:THR:O	2.38	0.57
1:E:140:ALA:O	1:E:144:GLY:N	2.38	0.57
1:D:418:LEU:HB2	1:D:447:ALA:HA	1.86	0.57
1:E:162:ARG:H	1:E:599:LYS:HG2	1.70	0.56
1:C:33:PHE:HZ	1:C:80:MET:HG3	1.70	0.56
1:E:162:ARG:HD2	1:E:599:LYS:HB3	1.88	0.56
1:E:267:ASP:OD1	1:E:267:ASP:N	2.36	0.56
1:E:79:GLU:HG2	1:E:178:PHE:HD1	1.70	0.56
1:A:162:ARG:HB2	1:A:599:LYS:HB3	1.87	0.56
1:B:381:ILE:HG12	1:B:417:ASP:HB3	1.87	0.56
1:F:208:PHE:HB2	1:F:209:PRO:HD3	1.88	0.56
1:D:48:PHE:O	1:D:51:SER:OG	2.23	0.56
1:A:23:VAL:HG23	1:A:25:GLU:H	1.71	0.56
1:B:293:TYR:OH	1:B:538:SER:OG	2.22	0.56
1:E:427:ARG:HD2	1:E:457:GLY:HA3	1.88	0.56
1:B:5:LEU:HB2	1:B:30:VAL:HG22	1.87	0.55
1:D:112:LYS:O	1:D:116:LEU:HD12	2.06	0.55
1:A:458:ILE:HB	1:A:482:LEU:HD21	1.87	0.55
1:E:132:ARG:O	1:E:132:ARG:NH1	2.39	0.55
1:B:360:THR:HG23	1:B:410:VAL:HG22	1.87	0.55
1:B:418:LEU:HD21	1:B:435:PHE:CE2	2.41	0.55
1:F:163:LEU:O	1:F:166:ILE:HG22	2.05	0.55
1:A:392:ASP:O	1:A:396:HIS:ND1	2.40	0.55
1:B:461:ALA:HA	1:B:465:LEU:HB2	1.87	0.55
3:B:701:ATP:O3A	3:B:701:ATP:H4'	2.07	0.55
1:F:72:ARG:HH22	1:F:175:ARG:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:LYS:NZ	1:D:430:TYR:OH	2.39	0.55
1:D:225:PRO:HA	1:D:557:SER:HA	1.88	0.55
1:D:458:ILE:HB	1:D:482:LEU:HD21	1.87	0.55
1:B:316:GLU:OE2	1:B:361:ARG:NH2	2.37	0.55
1:C:237:LEU:O	1:C:239:LYS:NZ	2.39	0.55
1:C:162:ARG:HG2	1:C:165:LYS:HE3	1.89	0.55
1:A:220:GLN:HE22	1:B:155:PRO:HG3	1.72	0.54
1:B:99:LEU:HD21	1:B:110:LEU:HB3	1.90	0.54
1:B:342:LYS:NZ	1:F:405:GLN:O	2.34	0.54
1:E:453:ASP:HB3	1:E:458:ILE:HD11	1.88	0.54
1:E:541:ASN:OD1	1:E:543:SER:OG	2.20	0.54
1:F:94:LEU:HB2	1:F:120:GLN:HG2	1.88	0.54
1:F:216:PRO:O	1:F:220:GLN:HG2	2.07	0.54
1:A:65:LEU:HD11	1:A:76:PHE:HD1	1.73	0.54
1:D:360:THR:HG23	1:D:410:VAL:HG22	1.89	0.54
1:E:419:ALA:HB1	3:E:702:ATP:N3	2.22	0.54
1:B:346:ARG:NH2	1:B:354:ASP:OD2	2.33	0.54
1:C:346:ARG:NH2	1:C:354:ASP:OD2	2.36	0.54
1:D:269:ILE:HG13	1:D:271:ARG:HH22	1.73	0.54
1:C:116:LEU:HA	1:C:157:TRP:HE1	1.73	0.54
1:B:72:ARG:HH22	1:B:175:ARG:HE	1.54	0.54
1:B:167:LEU:O	1:B:170:ASN:ND2	2.40	0.54
1:D:81:LEU:HD11	1:D:110:LEU:HD13	1.90	0.54
1:E:46:ASN:O	1:E:50:HIS:ND1	2.40	0.54
1:F:346:ARG:NH2	1:F:354:ASP:OD2	2.38	0.54
1:F:18:GLU:HB3	1:F:125:VAL:HG21	1.89	0.54
1:A:157:TRP:CE3	1:A:215:PRO:HB3	2.42	0.54
1:F:392:ASP:O	1:F:396:HIS:ND1	2.40	0.54
1:D:28:GLU:OE1	1:D:28:GLU:N	2.41	0.54
1:F:5:LEU:HD22	1:F:96:TYR:HB2	1.88	0.54
1:B:237:LEU:O	1:B:239:LYS:NZ	2.37	0.54
1:F:541:ASN:O	1:F:545:ASN:ND2	2.40	0.54
1:A:221:TRP:O	1:A:558:ARG:NH1	2.38	0.53
1:B:85:TYR:O	1:B:89:MET:HG2	2.08	0.53
1:B:208:PHE:O	1:B:566:ARG:NH1	2.40	0.53
1:C:468:ARG:NH1	1:D:488:GLU:OE1	2.41	0.53
1:D:72:ARG:HH22	1:D:175:ARG:NE	2.06	0.53
1:F:341:ASP:OD2	1:F:344:LYS:NZ	2.36	0.53
1:F:534:ASN:HB3	1:F:537:ILE:HD12	1.89	0.53
1:A:384:ARG:HG2	1:A:393:ILE:HD12	1.90	0.53
1:A:408:GLU:H	1:D:342:LYS:HZ1	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:VAL:HA	1:D:46:ASN:HD21	1.73	0.53
1:C:99:LEU:HD13	1:C:111:GLN:HB2	1.90	0.53
1:D:48:PHE:HB2	1:D:134:ILE:HD13	1.90	0.53
1:E:45:LEU:HD12	1:E:45:LEU:H	1.73	0.53
1:A:454:ASP:N	1:A:454:ASP:OD1	2.42	0.53
1:B:518:LEU:HD13	1:B:528:VAL:HG11	1.91	0.53
1:C:14:MET:HB2	1:C:137:MET:HE1	1.91	0.53
1:F:498:TYR:CE2	1:F:548:ILE:HG13	2.43	0.53
1:C:316:GLU:OE2	1:C:361:ARG:NH2	2.39	0.53
1:C:124:HIS:HB2	1:C:149:ILE:HB	1.90	0.53
1:D:86:LEU:HB3	1:D:167:LEU:HD11	1.88	0.53
1:B:353:GLN:OE1	1:B:406:GLN:NE2	2.42	0.53
1:D:384:ARG:HD3	1:D:426:THR:HB	1.90	0.53
1:D:418:LEU:HD21	1:D:435:PHE:CE2	2.44	0.53
1:E:116:LEU:HA	1:E:157:TRP:CD1	2.44	0.53
1:C:103:ILE:N	1:C:106:MET:SD	2.82	0.53
1:E:518:LEU:HD11	1:E:564:ILE:HD11	1.89	0.53
1:F:454:ASP:N	1:F:454:ASP:OD1	2.42	0.53
1:B:186:ILE:HG13	1:B:187:GLU:N	2.24	0.52
1:B:211:LEU:HD12	1:B:214:LEU:HD11	1.92	0.52
1:B:4:VAL:HG13	1:B:95:PRO:HB3	1.91	0.52
1:C:174:SER:OG	1:C:175:ARG:NH1	2.43	0.52
1:E:159:ALA:HB2	1:E:596:ILE:HA	1.91	0.52
1:F:86:LEU:HD21	1:F:163:LEU:HD12	1.90	0.52
1:F:277:GLU:C	1:F:279:ALA:H	2.13	0.52
1:A:132:ARG:O	1:A:132:ARG:NH1	2.37	0.52
1:A:127:ALA:HB2	1:A:146:ILE:HG12	1.90	0.52
1:C:77:TYR:OH	1:C:106:MET:HB2	2.09	0.52
1:E:189:ILE:HG12	1:E:220:GLN:HG2	1.91	0.52
1:E:143:LYS:HE2	1:E:145:GLN:NE2	2.25	0.52
1:C:4:VAL:HG22	1:C:29:GLU:HG3	1.91	0.52
1:C:403:ALA:HB1	1:C:413:ILE:HD13	1.91	0.52
1:B:246:LEU:HD11	1:B:315:VAL:HG22	1.91	0.52
1:C:221:TRP:O	1:C:558:ARG:NH1	2.41	0.52
1:A:133:ASN:OD1	1:A:136:GLU:N	2.43	0.52
1:F:283:ARG:NH2	1:F:551:ASP:OD2	2.41	0.52
1:A:116:LEU:HA	1:A:157:TRP:CD1	2.45	0.51
1:C:3:ARG:HB3	1:C:28:GLU:HB2	1.91	0.51
1:F:296:LEU:HD22	1:F:537:ILE:HG23	1.92	0.51
1:A:89:MET:HE3	1:A:90:PRO:HD2	1.93	0.51
1:A:234:ILE:O	1:A:239:LYS:NZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:HB2	1:D:440:ARG:HH21	1.76	0.51
1:C:103:ILE:HD11	1:C:105:SER:HB3	1.92	0.51
1:D:529:SER:O	1:D:531:ASN:ND2	2.43	0.51
1:A:162:ARG:HD3	1:A:599:LYS:HB3	1.92	0.51
1:E:103:ILE:HG22	1:E:105:SER:H	1.74	0.51
1:F:137:MET:SD	1:F:137:MET:N	2.83	0.51
1:E:56:ARG:HD2	1:E:57:PHE:N	2.25	0.51
1:A:437:ALA:HB1	1:D:394:SER:HB3	1.92	0.51
1:B:496:CYS:SG	1:B:533:ASP:HB2	2.51	0.51
1:C:392:ASP:O	1:C:396:HIS:ND1	2.43	0.51
1:D:476:LEU:HB3	1:D:483:MET:HG3	1.93	0.51
1:E:21:HIS:CD2	1:E:141:LEU:HD11	2.45	0.51
1:A:509:MET:HB3	1:A:512:PHE:HB2	1.92	0.51
1:E:237:LEU:HD22	1:E:590:ILE:HD13	1.93	0.51
1:A:77:TYR:CE2	1:A:106:MET:HB2	2.45	0.51
1:A:503:ILE:HG22	1:A:504:LYS:HD3	1.92	0.51
1:D:211:LEU:HD12	1:D:212:ALA:N	2.25	0.51
1:D:460:GLN:O	1:D:464:SER:OG	2.22	0.51
1:E:260:ARG:NH2	1:E:270:ASP:O	2.43	0.51
1:A:532:THR:HG22	1:A:545:ASN:HD22	1.75	0.50
1:F:91:ASP:OD1	1:F:91:ASP:N	2.43	0.50
1:B:264:SER:OG	1:B:265:GLU:OE1	2.28	0.50
1:C:588:ARG:NE	1:D:203:SER:OG	2.44	0.50
1:F:186:ILE:HA	1:F:189:ILE:HG22	1.92	0.50
1:B:533:ASP:OD2	1:B:534:ASN:ND2	2.45	0.50
1:D:381:ILE:HG12	1:D:417:ASP:HB3	1.94	0.50
1:E:151:MET:N	1:E:151:MET:SD	2.83	0.50
1:B:183:SER:HA	1:B:186:ILE:HG12	1.94	0.50
1:B:237:LEU:HD12	1:B:238:PRO:HD2	1.93	0.50
1:E:5:LEU:HG	1:E:27:PHE:CZ	2.47	0.50
1:D:17:PRO:O	1:D:21:HIS:ND1	2.45	0.50
1:C:431:TYR:HB2	1:C:435:PHE:HE2	1.76	0.50
1:E:424:LYS:H	1:E:427:ARG:NH2	2.09	0.50
1:A:308:LYS:HD3	1:A:346:ARG:HH12	1.77	0.50
1:E:204:ASN:ND2	1:F:584:LYS:HE3	2.27	0.50
1:A:588:ARG:NH1	1:A:592:ASP:OD1	2.44	0.50
1:F:341:ASP:N	1:F:346:ARG:O	2.32	0.50
1:B:20:PHE:HZ	1:B:55:VAL:HG21	1.76	0.50
1:B:160:LEU:HD21	1:B:189:ILE:HG21	1.94	0.50
1:C:103:ILE:HG22	2:H:7:A:H2'	1.94	0.50
1:A:116:LEU:HA	1:A:157:TRP:NE1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ALA:H	1:A:314:GLN:HE22	1.59	0.49
1:C:596:ILE:O	1:C:599:LYS:HB2	2.12	0.49
1:A:105:SER:OG	1:A:106:MET:N	2.45	0.49
1:B:180:PRO:HB2	1:B:183:SER:HB2	1.94	0.49
1:F:375:HIS:NE2	1:F:410:VAL:O	2.46	0.49
1:A:293:TYR:HA	1:A:296:LEU:HD12	1.93	0.49
1:C:431:TYR:HB2	1:C:435:PHE:CE2	2.47	0.49
1:D:495:MET:SD	1:D:518:LEU:HD13	2.53	0.49
1:E:5:LEU:HD23	1:E:96:TYR:HB2	1.94	0.49
1:F:8:SER:HA	1:F:32:VAL:HG13	1.95	0.49
1:C:173:CYS:HB2	1:C:177:ASN:HD21	1.77	0.49
1:D:130:ASN:OD1	1:D:132:ARG:NH2	2.46	0.49
1:E:140:ALA:HA	1:E:145:GLN:NE2	2.27	0.49
1:C:131:PRO:HB3	1:C:136:GLU:HB3	1.94	0.49
1:C:260:ARG:HG2	1:C:269:ILE:HD11	1.94	0.49
1:D:13:SER:O	1:D:45:LEU:HD21	2.13	0.49
1:D:250:ALA:O	1:D:300:ASN:ND2	2.45	0.49
1:E:7:CYS:HB3	1:E:98:CYS:SG	2.52	0.49
1:E:137:MET:O	1:E:141:LEU:HD23	2.13	0.49
1:B:63:HIS:O	1:B:175:ARG:NH1	2.45	0.49
1:B:129:ASN:HD21	1:B:140:ALA:HB2	1.77	0.49
1:D:86:LEU:HD23	1:D:167:LEU:HD21	1.95	0.49
1:D:356:ASN:ND2	1:D:406:GLN:OE1	2.45	0.49
1:E:492:GLY:HA3	1:E:571:THR:HG21	1.95	0.49
1:E:258:GLN:HG3	1:E:317:LEU:HD11	1.95	0.49
1:E:440:ARG:HA	1:F:459:TRP:CZ2	2.48	0.49
1:A:432:GLU:H	1:A:432:GLU:CD	2.15	0.49
1:E:333:ARG:NH2	1:E:494:GLU:OE2	2.44	0.49
1:B:56:ARG:HD2	1:B:57:PHE:N	2.27	0.49
1:B:300:ASN:HB2	1:B:304:LEU:HD23	1.94	0.49
1:D:36:ASP:OD2	1:D:64:GLY:N	2.45	0.49
1:D:126:LEU:O	1:D:147:HIS:N	2.40	0.49
1:D:184:LYS:O	1:D:187:GLU:HG3	2.12	0.49
1:E:383:SER:OG	3:E:702:ATP:O2'	2.19	0.49
1:D:163:LEU:HD13	1:D:166:ILE:HD11	1.95	0.48
1:E:424:LYS:NZ	1:E:430:TYR:OH	2.45	0.48
1:F:83:GLN:O	1:F:87:THR:HG23	2.13	0.48
1:F:487:ILE:HD11	1:F:526:ILE:HG12	1.95	0.48
1:F:496:CYS:SG	1:F:533:ASP:HB2	2.53	0.48
1:B:438:VAL:HG22	1:B:443:LEU:HB2	1.95	0.48
1:D:262:ALA:HB3	1:D:313:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:496:CYS:SG	1:D:533:ASP:HB2	2.53	0.48
1:A:333:ARG:NH2	1:A:494:GLU:OE2	2.45	0.48
1:C:435:PHE:HD1	1:C:438:VAL:HG11	1.79	0.48
1:D:570:GLU:O	1:D:579:ARG:NH1	2.46	0.48
1:D:591:TYR:O	1:D:593:VAL:N	2.47	0.48
1:E:74:PHE:HZ	1:F:151:MET:HB3	1.78	0.48
1:F:424:LYS:HA	1:F:427:ARG:HG2	1.95	0.48
1:A:104:LYS:NZ	1:B:102:GLY:O	2.34	0.48
1:A:210:SER:HB2	1:A:587:ASP:OD1	2.13	0.48
1:B:258:GLN:HG3	1:B:317:LEU:HD11	1.96	0.48
1:E:308:LYS:O	1:E:312:ILE:HG12	2.13	0.48
1:A:588:ARG:NH2	1:B:199:ASP:O	2.43	0.48
1:B:82:TRP:HB3	1:B:182:ILE:HG21	1.96	0.48
1:B:234:ILE:O	1:B:239:LYS:NZ	2.45	0.48
1:B:354:ASP:O	1:B:358:THR:HG22	2.14	0.48
1:D:258:GLN:HG3	1:D:317:LEU:HD11	1.95	0.48
1:E:460:GLN:O	1:E:464:SER:OG	2.22	0.48
1:F:354:ASP:O	1:F:358:THR:HG22	2.13	0.48
1:A:173:CYS:HB2	1:A:177:ASN:HD21	1.77	0.48
1:D:124:HIS:HB2	1:D:149:ILE:HB	1.96	0.48
1:D:185:SER:O	1:D:189:ILE:HG23	2.13	0.48
1:A:220:GLN:NE2	1:B:155:PRO:HG3	2.29	0.48
1:A:507:ALA:HA	1:A:509:MET:H	1.79	0.48
1:E:247:GLY:HA3	3:E:702:ATP:O1B	2.13	0.48
1:C:10:GLY:HA3	2:H:7:A:N7	2.29	0.48
1:F:306:LYS:NZ	1:F:340:ALA:O	2.36	0.48
1:B:211:LEU:CD1	1:B:214:LEU:HD11	2.44	0.48
1:C:159:ALA:HB3	1:C:595:LEU:O	2.14	0.48
1:F:548:ILE:HG22	1:F:552:LEU:HG	1.94	0.48
1:A:47:ASP:HA	1:A:50:HIS:HE1	1.77	0.47
1:A:159:ALA:HB1	1:A:599:LYS:HG3	1.96	0.47
1:E:162:ARG:O	1:E:166:ILE:HG23	2.14	0.47
1:B:532:THR:HG22	1:B:545:ASN:HD22	1.79	0.47
1:F:68:ILE:HD13	1:F:74:PHE:HD1	1.79	0.47
1:F:311:LEU:O	1:F:315:VAL:HG12	2.12	0.47
1:C:133:ASN:OD1	1:C:136:GLU:N	2.40	0.47
1:C:216:PRO:O	1:C:220:GLN:HG3	2.13	0.47
1:D:162:ARG:O	1:D:162:ARG:HD3	2.14	0.47
1:E:126:LEU:HD21	1:E:147:HIS:HB2	1.95	0.47
1:E:357:ASP:HA	1:E:360:THR:HG22	1.97	0.47
1:A:293:TYR:CG	1:A:503:ILE:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:PHE:O	1:A:509:MET:HB2	2.14	0.47
1:C:4:VAL:HG13	1:C:31:HIS:HD2	1.79	0.47
1:D:33:PHE:HB2	1:D:84:TRP:CZ3	2.49	0.47
1:E:151:MET:HB2	1:F:78:GLN:HE22	1.80	0.47
1:F:237:LEU:HD12	1:F:593:VAL:HG21	1.96	0.47
1:E:163:LEU:HA	1:E:166:ILE:HG12	1.95	0.47
1:F:122:VAL:HB	1:F:152:GLY:HA3	1.97	0.47
1:F:540:ALA:HB1	1:F:544:GLU:HB2	1.97	0.47
1:B:205:GLN:O	1:B:206:LEU:HB2	2.13	0.47
1:B:369:LYS:HG3	1:B:371:GLN:HG2	1.97	0.47
1:C:576:HIS:O	1:C:580:MET:HG2	2.14	0.47
1:E:569:ILE:HD11	1:E:586:PHE:CG	2.50	0.47
1:A:78:GLN:OE1	1:A:109:SER:OG	2.31	0.47
1:A:116:LEU:HD21	1:A:182:ILE:HG21	1.96	0.47
1:B:134:ILE:O	1:B:138:PHE:HD1	1.98	0.47
1:B:162:ARG:HD2	1:B:592:ASP:OD1	2.13	0.47
1:C:116:LEU:HD23	1:C:182:ILE:HD13	1.97	0.47
1:C:151:MET:HB3	1:D:74:PHE:HZ	1.80	0.47
1:C:220:GLN:HE22	1:D:155:PRO:HG2	1.79	0.47
1:C:328:ALA:HB3	1:C:586:PHE:CZ	2.48	0.47
1:C:594:CYS:O	1:C:598:ILE:HG23	2.14	0.47
1:E:3:ARG:NH2	1:E:26:GLY:O	2.48	0.47
1:A:258:GLN:HG3	1:A:317:LEU:HD11	1.97	0.47
1:D:103:ILE:HG13	1:D:104:LYS:H	1.80	0.47
1:D:295:GLU:OE1	1:D:298:ASN:ND2	2.38	0.47
1:F:13:SER:OG	1:F:41:ASN:OD1	2.33	0.47
1:F:60:THR:HG21	1:F:84:TRP:CD1	2.50	0.47
1:B:170:ASN:O	1:B:171:GLU:HG3	2.15	0.47
1:B:333:ARG:HH22	1:B:494:GLU:CD	2.19	0.47
1:E:158:ALA:HB3	1:E:595:LEU:HD22	1.97	0.47
1:D:255:LEU:HD22	1:D:317:LEU:HD13	1.96	0.47
1:F:576:HIS:O	1:F:580:MET:HG2	2.15	0.47
1:A:30:VAL:O	1:A:57:PHE:HA	2.16	0.46
1:A:313:ARG:NH1	1:A:316:GLU:OE1	2.48	0.46
1:B:103:ILE:HG23	1:B:105:SER:H	1.80	0.46
1:C:294:MET:SD	1:C:294:MET:N	2.88	0.46
1:D:54:ASN:OD1	1:D:54:ASN:N	2.47	0.46
1:B:46:ASN:O	1:B:50:HIS:ND1	2.49	0.46
1:B:138:PHE:O	1:B:142:GLN:HG2	2.16	0.46
1:C:14:MET:HB2	1:C:137:MET:CE	2.45	0.46
1:D:354:ASP:O	1:D:358:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:SER:HB2	1:E:39:LYS:HG2	1.98	0.46
1:E:530:VAL:HG21	1:E:549:LEU:HD11	1.97	0.46
1:F:347:SER:OG	1:F:348:ALA:N	2.48	0.46
1:A:68:ILE:HD11	1:A:74:PHE:HA	1.96	0.46
1:B:124:HIS:N	1:B:149:ILE:O	2.47	0.46
1:D:189:ILE:HG13	1:D:190:LEU:N	2.30	0.46
1:D:432:GLU:OE1	1:D:432:GLU:N	2.27	0.46
1:B:194:LYS:HA	1:B:194:LYS:HD2	1.63	0.46
1:C:378:LEU:HB2	1:C:413:ILE:HG13	1.98	0.46
1:B:240:VAL:HG13	1:B:329:TYR:HD2	1.81	0.46
1:C:282:PRO:O	1:C:502:GLN:NE2	2.38	0.46
1:D:43:VAL:HA	1:D:46:ASN:ND2	2.31	0.46
1:E:74:PHE:CZ	1:F:151:MET:HB3	2.50	0.46
1:E:446:THR:HG23	1:E:469:ARG:HB2	1.97	0.46
1:F:11:HIS:HB3	1:F:39:LYS:HG3	1.96	0.46
1:D:4:VAL:HG23	1:D:90:PRO:HG3	1.97	0.46
1:E:2:SER:HB3	1:E:93:GLU:HB3	1.98	0.46
1:E:145:GLN:OE1	1:E:145:GLN:N	2.49	0.46
1:F:277:GLU:O	1:F:279:ALA:N	2.47	0.46
1:F:303:LYS:C	1:F:303:LYS:HD2	2.35	0.46
1:D:532:THR:O	1:D:534:ASN:N	2.48	0.46
1:C:104:LYS:NZ	1:D:102:GLY:O	2.40	0.46
1:C:122:VAL:HG23	1:C:151:MET:SD	2.56	0.46
1:C:179:LYS:HD2	1:C:179:LYS:O	2.16	0.46
1:E:76:PHE:HE2	1:E:175:ARG:HG2	1.81	0.46
1:C:389:ASP:HB2	1:E:440:ARG:HH12	1.80	0.46
1:E:76:PHE:CE2	1:E:175:ARG:HG2	2.50	0.46
1:C:184:LYS:HB3	1:C:184:LYS:HE3	1.82	0.46
1:C:462:VAL:HG22	1:C:491:ILE:HD13	1.98	0.46
1:E:458:ILE:HB	1:E:482:LEU:HD21	1.96	0.46
1:A:300:ASN:OD1	1:A:301:GLY:N	2.47	0.45
1:A:333:ARG:NE	1:A:417:ASP:OD2	2.49	0.45
1:D:519:LYS:HD3	1:D:556:ILE:HD12	1.98	0.45
1:E:5:LEU:HB2	1:E:30:VAL:HG13	1.98	0.45
2:G:1:A:N3	2:G:1:A:H2'	2.30	0.45
1:D:180:PRO:HB2	1:D:183:SER:HB2	1.99	0.45
1:D:492:GLY:HA3	1:D:571:THR:HG21	1.98	0.45
1:A:85:TYR:HD2	1:A:113:ALA:HB1	1.81	0.45
1:A:459:TRP:CE2	1:B:440:ARG:HD2	2.50	0.45
1:B:5:LEU:HD22	1:B:96:TYR:HB2	1.99	0.45
1:B:453:ASP:OD1	1:B:453:ASP:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:N	1:A:202:LYS:HZ2	2.15	0.45
1:C:275:PRO:HG3	1:C:299:ALA:HB2	1.98	0.45
1:E:56:ARG:HD2	1:E:56:ARG:C	2.37	0.45
1:E:95:PRO:O	1:E:120:GLN:N	2.43	0.45
1:E:484:ARG:O	1:E:488:GLU:HG3	2.17	0.45
3:E:702:ATP:O2A	3:E:702:ATP:H4'	2.15	0.45
1:A:5:LEU:HB2	1:A:30:VAL:HG22	1.97	0.45
1:A:260:ARG:HD3	1:A:271:ARG:HG3	1.97	0.45
1:A:292:LYS:HE2	1:A:292:LYS:HB2	1.65	0.45
1:A:484:ARG:HH22	1:B:442:GLY:HA3	1.81	0.45
1:B:72:ARG:O	1:B:75:GLU:HG3	2.16	0.45
1:D:93:GLU:N	1:D:93:GLU:OE2	2.50	0.45
1:E:189:ILE:HA	1:E:220:GLN:HG2	1.97	0.45
1:F:293:TYR:CG	1:F:503:ILE:HD11	2.51	0.45
1:F:381:ILE:HA	1:F:417:ASP:HB3	1.98	0.45
1:D:208:PHE:O	1:D:566:ARG:NH1	2.49	0.45
1:D:369:LYS:HG3	1:D:371:GLN:HG2	1.99	0.45
1:F:293:TYR:OH	1:F:538:SER:OG	2.23	0.45
1:A:99:LEU:HG	1:A:124:HIS:NE2	2.32	0.45
1:A:166:ILE:HG23	1:A:167:LEU:HD22	1.97	0.45
1:D:495:MET:HE1	1:D:521:TYR:CE2	2.51	0.45
1:B:22:ALA:HA	1:B:148:PHE:CZ	2.52	0.45
1:B:423:ASN:OD1	1:B:423:ASN:N	2.49	0.45
1:C:305:LEU:HD22	1:C:311:LEU:HA	1.99	0.45
1:F:86:LEU:HA	1:F:89:MET:HE3	1.98	0.45
1:F:179:LYS:HA	1:F:179:LYS:HD3	1.78	0.45
1:A:4:VAL:HG22	1:A:29:GLU:HB2	1.98	0.45
1:B:247:GLY:HA3	3:B:702:ATP:O1B	2.17	0.45
1:C:99:LEU:HG	1:C:124:HIS:NE2	2.31	0.45
1:E:32:VAL:HB	1:E:59:ILE:HD13	1.99	0.45
1:E:385:LYS:HD2	1:E:385:LYS:HA	1.67	0.45
1:A:328:ALA:HB3	1:A:586:PHE:CZ	2.51	0.45
1:D:170:ASN:O	1:D:171:GLU:HG3	2.17	0.45
1:E:147:HIS:ND1	1:F:69:LEU:O	2.50	0.45
1:F:220:GLN:O	1:F:224:LEU:HG	2.17	0.45
1:A:99:LEU:HD13	1:A:111:GLN:HB2	2.00	0.44
1:A:300:ASN:ND2	1:A:314:GLN:OE1	2.44	0.44
1:A:435:PHE:O	1:A:438:VAL:HG12	2.18	0.44
1:B:123:PHE:HB3	1:B:150:GLU:HG2	2.00	0.44
1:D:83:GLN:HG3	1:D:167:LEU:HD22	1.98	0.44
1:D:595:LEU:O	1:D:599:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:436:LYS:HD2	1:F:440:ARG:HG3	1.99	0.44
1:C:454:ASP:OD1	1:C:454:ASP:N	2.49	0.44
1:C:590:ILE:HA	1:C:593:VAL:HG12	1.99	0.44
1:D:163:LEU:HD12	1:D:163:LEU:O	2.17	0.44
1:E:131:PRO:HB2	1:E:137:MET:SD	2.58	0.44
1:E:179:LYS:HB2	1:E:181:LEU:HG	2.00	0.44
1:D:162:ARG:NH2	1:D:588:ARG:HD2	2.32	0.44
1:E:213:ILE:HG21	1:F:196:MET:HG2	1.98	0.44
1:F:79:GLU:HG2	1:F:180:PRO:HA	1.98	0.44
1:F:99:LEU:HD21	1:F:111:GLN:HB2	1.99	0.44
1:F:458:ILE:HB	1:F:482:LEU:HD21	1.99	0.44
1:E:591:TYR:CE2	1:F:196:MET:HG3	2.53	0.44
1:F:170:ASN:O	1:F:171:GLU:HG3	2.17	0.44
1:C:548:ILE:HG23	1:C:552:LEU:HD12	2.00	0.44
1:D:378:LEU:HB2	1:D:413:ILE:HD13	1.99	0.44
1:F:60:THR:HG21	1:F:84:TRP:HD1	1.83	0.44
1:F:369:LYS:HG3	1:F:371:GLN:HG2	1.99	0.44
1:F:404:MET:SD	1:F:443:LEU:HG	2.58	0.44
1:A:316:GLU:HG2	1:A:362:LEU:HD11	1.99	0.44
1:A:431:TYR:O	1:A:435:PHE:HD1	2.01	0.44
1:B:162:ARG:NH2	1:B:588:ARG:HD3	2.33	0.44
1:B:390:LEU:HB3	1:F:440:ARG:CZ	2.47	0.44
1:C:334:CYS:SG	1:C:378:LEU:HD12	2.58	0.44
1:D:533:ASP:OD2	1:D:534:ASN:ND2	2.51	0.44
1:F:166:ILE:HD11	1:F:599:LYS:HG3	1.99	0.44
1:F:325:ASP:HB3	1:F:327:VAL:HG23	2.00	0.44
1:B:103:ILE:HG13	1:B:104:LYS:H	1.82	0.44
1:B:259:VAL:HG23	1:B:317:LEU:HD12	1.99	0.44
1:B:437:ALA:HB1	1:F:394:SER:HB3	2.00	0.44
1:C:160:LEU:HA	1:C:599:LYS:HA	2.00	0.44
1:D:375:HIS:NE2	1:D:410:VAL:O	2.51	0.44
1:E:18:GLU:HA	1:E:21:HIS:CE1	2.53	0.44
1:B:132:ARG:H	1:B:136:GLU:CD	2.21	0.44
1:B:182:ILE:O	1:B:186:ILE:HG23	2.18	0.44
1:B:227:SER:OG	1:B:228:ALA:N	2.51	0.44
1:B:302:SER:HB3	1:B:338:ASN:HB3	2.00	0.44
1:D:123:PHE:HB3	1:D:150:GLU:HG2	1.99	0.44
1:F:5:LEU:HB2	1:F:30:VAL:HG22	1.99	0.44
1:F:41:ASN:OD1	1:F:41:ASN:N	2.48	0.44
1:F:158:ALA:O	1:F:162:ARG:HG2	2.17	0.44
1:F:532:THR:O	1:F:534:ASN:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:HA	1:A:61:LYS:HD3	2.00	0.43
1:F:176:ASP:OD1	1:F:176:ASP:N	2.51	0.43
1:F:185:SER:O	1:F:188:GLU:HB3	2.18	0.43
1:F:336:PRO:HG3	1:F:352:LEU:HD13	2.00	0.43
1:A:459:TRP:CZ2	1:B:440:ARG:HA	2.53	0.43
1:B:271:ARG:HA	1:B:271:ARG:HD3	1.84	0.43
1:C:436:LYS:NZ	1:C:440:ARG:HD2	2.34	0.43
1:D:431:TYR:HA	1:D:433:HIS:CE1	2.53	0.43
1:E:116:LEU:HA	1:E:157:TRP:NE1	2.33	0.43
1:C:149:ILE:HG22	1:D:74:PHE:CD2	2.53	0.43
1:D:328:ALA:HB3	1:D:586:PHE:CZ	2.53	0.43
1:E:328:ALA:HB3	1:E:586:PHE:CZ	2.53	0.43
1:F:451:GLU:HG2	1:F:452:ASN:ND2	2.33	0.43
1:F:595:LEU:HD23	1:F:595:LEU:HA	1.88	0.43
1:B:162:ARG:HE	1:B:162:ARG:HB2	1.56	0.43
1:C:432:GLU:HG2	1:C:464:SER:HB2	1.99	0.43
1:D:242:LEU:HB3	1:D:469:ARG:NH1	2.33	0.43
1:E:471:GLY:HA2	1:E:494:GLU:HG3	1.99	0.43
1:F:120:GLN:HE21	1:F:120:GLN:HB3	1.61	0.43
1:F:469:ARG:HD3	1:F:571:THR:HB	2.00	0.43
1:B:231:GLY:HA2	1:B:547:LEU:HD11	2.00	0.43
1:B:242:LEU:HB3	1:B:469:ARG:NH1	2.33	0.43
1:C:5:LEU:HB2	1:C:30:VAL:HG22	2.00	0.43
1:C:7:CYS:SG	1:C:98:CYS:HB3	2.57	0.43
1:D:207:PRO:HB3	1:D:211:LEU:HG	2.01	0.43
1:A:102:GLY:HA3	1:A:106:MET:SD	2.59	0.43
1:B:305:LEU:HD22	1:B:311:LEU:HA	1.99	0.43
1:C:390:LEU:HD23	1:C:390:LEU:HA	1.82	0.43
1:E:77:TYR:OH	1:E:106:MET:HB3	2.18	0.43
1:F:49:PHE:HD2	1:F:57:PHE:CG	2.36	0.43
1:F:149:ILE:HD13	1:F:149:ILE:HA	1.86	0.43
1:A:322:LEU:HD11	1:A:332:ILE:HD11	1.99	0.43
1:B:34:THR:HG21	1:B:40:PHE:CD2	2.54	0.43
1:B:81:LEU:HD11	1:B:110:LEU:HD13	2.01	0.43
1:B:391:SER:HB3	1:F:440:ARG:HE	1.84	0.43
1:F:211:LEU:O	1:F:213:ILE:HG12	2.19	0.43
1:A:6:LEU:HA	1:A:31:HIS:O	2.18	0.43
1:A:233:TRP:HD1	1:A:597:SER:HB3	1.83	0.43
1:B:270:ASP:OD1	1:B:270:ASP:N	2.49	0.43
1:B:303:LYS:HE3	1:B:303:LYS:HB2	1.86	0.43
1:C:19:ALA:HA	1:C:125:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ASP:HB2	1:C:542:LEU:HD22	2.01	0.43
1:D:506:PHE:O	1:D:509:MET:HB3	2.19	0.43
1:F:328:ALA:HB3	1:F:586:PHE:CZ	2.54	0.43
1:A:385:LYS:HA	1:A:385:LYS:HD2	1.70	0.43
1:B:344:LYS:H	1:B:344:LYS:HG2	1.70	0.43
1:C:433:HIS:NE2	1:E:433:HIS:HA	2.33	0.43
1:D:157:TRP:CG	1:D:160:LEU:HD12	2.54	0.43
1:E:94:LEU:HD13	1:E:94:LEU:HA	1.92	0.43
1:E:250:ALA:H	1:E:314:GLN:HE22	1.66	0.43
1:A:429:SER:O	1:A:429:SER:OG	2.37	0.43
1:A:135:GLU:HA	1:A:138:PHE:HB2	2.01	0.42
1:A:584:LYS:HB3	1:B:204:ASN:HB3	2.00	0.42
1:E:305:LEU:HD23	1:E:311:LEU:HA	2.00	0.42
1:F:29:GLU:HB3	1:F:56:ARG:HB3	2.01	0.42
1:B:200:THR:O	1:B:204:ASN:ND2	2.53	0.42
1:C:162:ARG:HB2	1:C:599:LYS:HB3	2.01	0.42
1:C:435:PHE:O	1:C:438:VAL:HG12	2.19	0.42
1:F:183:SER:HA	1:F:186:ILE:HG12	2.01	0.42
1:A:423:ASN:O	1:A:425:GLU:N	2.51	0.42
1:B:184:LYS:HA	1:B:187:GLU:HG2	2.00	0.42
1:C:151:MET:HB3	1:D:74:PHE:CZ	2.54	0.42
1:E:21:HIS:NE2	1:E:141:LEU:HD11	2.33	0.42
1:E:240:VAL:HG13	1:E:329:TYR:HD2	1.84	0.42
1:F:530:VAL:HG21	1:F:549:LEU:HD11	2.01	0.42
1:A:204:ASN:HB2	1:B:584:LYS:HD3	2.01	0.42
1:A:440:ARG:HH21	1:D:391:SER:N	2.15	0.42
1:A:530:VAL:HG21	1:A:549:LEU:HD11	2.02	0.42
1:B:5:LEU:HD11	1:B:123:PHE:HZ	1.84	0.42
1:D:427:ARG:HD2	1:D:427:ARG:HA	1.92	0.42
1:E:5:LEU:HG	1:E:27:PHE:CE2	2.55	0.42
1:E:450:GLY:HA3	1:E:472:HIS:HB2	2.02	0.42
1:B:322:LEU:HD11	1:B:332:ILE:HD11	2.00	0.42
1:B:506:PHE:O	1:B:509:MET:HB3	2.20	0.42
1:C:5:LEU:HD21	1:C:123:PHE:HE1	1.85	0.42
1:C:308:LYS:O	1:C:312:ILE:HG12	2.20	0.42
1:D:35:THR:HA	1:D:62:CYS:HB3	2.01	0.42
1:A:128:ASP:N	1:A:145:GLN:OE1	2.51	0.42
1:A:290:LEU:HA	1:A:290:LEU:HD23	1.82	0.42
1:A:584:LYS:HG2	1:B:205:GLN:HB3	2.02	0.42
1:B:157:TRP:O	1:B:161:ARG:HG3	2.19	0.42
1:B:545:ASN:O	1:B:548:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LYS:NZ	1:D:107:SER:HB2	2.35	0.42
1:D:264:SER:OG	1:D:265:GLU:N	2.50	0.42
1:D:453:ASP:OD1	1:D:453:ASP:N	2.37	0.42
1:E:286:LYS:HB2	1:E:286:LYS:HE2	1.88	0.42
1:E:432:GLU:HA	1:E:465:LEU:HD21	2.01	0.42
1:A:238:PRO:HG3	1:A:589:LYS:HB3	2.02	0.42
1:A:595:LEU:HD23	1:A:595:LEU:HA	1.79	0.42
1:B:133:ASN:O	1:B:137:MET:HG3	2.20	0.42
1:B:184:LYS:HA	1:B:184:LYS:HD3	1.82	0.42
1:E:427:ARG:NE	1:E:453:ASP:OD1	2.52	0.42
1:E:498:TYR:CZ	1:E:548:ILE:HD12	2.55	0.42
1:F:196:MET:HE2	1:F:196:MET:HA	2.02	0.42
1:F:470:LEU:HB2	1:F:493:VAL:HG12	2.01	0.42
1:A:266:PRO:O	1:A:269:ILE:HG12	2.19	0.42
1:E:369:LYS:HD2	1:E:371:GLN:NE2	2.34	0.42
1:B:316:GLU:HG2	1:B:362:LEU:HD11	2.02	0.42
1:E:320:GLN:NE2	1:E:324:ASN:OD1	2.53	0.42
1:E:346:ARG:NH2	1:E:354:ASP:OD2	2.36	0.42
1:E:506:PHE:O	1:E:509:MET:HB3	2.20	0.42
1:F:533:ASP:OD2	1:F:534:ASN:ND2	2.53	0.42
1:F:547:LEU:HD23	1:F:547:LEU:HA	1.89	0.42
1:F:557:SER:OG	1:F:560:ASP:OD2	2.27	0.42
1:C:35:THR:HG23	1:C:37:SER:H	1.84	0.42
1:C:189:ILE:HG23	1:C:220:GLN:OE1	2.19	0.42
1:C:440:ARG:HG2	1:D:459:TRP:CZ2	2.55	0.42
1:E:222:LEU:HD12	1:E:222:LEU:HA	1.88	0.42
1:F:476:LEU:HD23	1:F:476:LEU:HA	1.90	0.42
1:A:72:ARG:O	1:A:75:GLU:HG3	2.20	0.41
1:C:86:LEU:HD13	1:C:163:LEU:HB2	2.02	0.41
1:D:582:LEU:HD12	1:D:582:LEU:HA	1.94	0.41
1:E:16:VAL:HB	1:E:17:PRO:HD3	2.02	0.41
1:E:52:LEU:O	1:E:55:VAL:HG12	2.19	0.41
1:E:238:PRO:HG3	1:E:589:LYS:HB3	2.02	0.41
1:E:300:ASN:ND2	1:E:314:GLN:OE1	2.53	0.41
1:C:159:ALA:C	1:C:599:LYS:HG3	2.40	0.41
1:C:427:ARG:NH1	1:C:430:TYR:OH	2.52	0.41
1:F:166:ILE:CD1	1:F:599:LYS:HG3	2.49	0.41
1:A:6:LEU:HB3	1:A:84:TRP:CH2	2.52	0.41
1:A:548:ILE:HD12	1:A:548:ILE:HA	1.92	0.41
1:B:419:ALA:HB1	3:B:702:ATP:N3	2.35	0.41
1:C:54:ASN:N	1:C:54:ASN:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ILE:HD12	1:C:220:GLN:OE1	2.20	0.41
1:C:496:CYS:SG	1:C:533:ASP:HB2	2.60	0.41
1:D:82:TRP:CD1	1:D:113:ALA:HB2	2.55	0.41
1:E:532:THR:HA	1:E:545:ASN:ND2	2.35	0.41
1:B:211:LEU:HD23	1:B:211:LEU:H	1.85	0.41
1:B:213:ILE:HG22	1:B:213:ILE:O	2.19	0.41
1:B:599:LYS:HA	1:B:599:LYS:HD2	1.72	0.41
1:F:518:LEU:HD21	1:F:564:ILE:HD11	2.03	0.41
1:A:95:PRO:O	1:A:120:GLN:N	2.43	0.41
1:B:433:HIS:ND1	1:B:434:ASP:OD1	2.53	0.41
1:C:429:SER:HA	1:C:432:GLU:OE2	2.19	0.41
1:F:598:ILE:HD13	1:F:598:ILE:HA	1.81	0.41
1:A:325:ASP:HB3	1:A:327:VAL:HG23	2.02	0.41
1:B:77:TYR:CE2	1:B:106:MET:HB3	2.56	0.41
1:B:450:GLY:HA2	1:B:472:HIS:HB2	2.03	0.41
1:E:291:ASP:O	1:E:295:GLU:HG2	2.21	0.41
1:F:219:GLN:O	1:F:223:GLN:HG2	2.21	0.41
1:F:241:ASP:O	1:F:330:ALA:HA	2.20	0.41
1:B:532:THR:O	1:B:534:ASN:N	2.52	0.41
1:C:35:THR:OG1	1:C:65:LEU:O	2.38	0.41
1:D:190:LEU:HB3	1:D:194:LYS:NZ	2.35	0.41
1:D:530:VAL:HG21	1:D:549:LEU:HD11	2.01	0.41
1:E:145:GLN:CD	1:E:145:GLN:H	2.24	0.41
1:A:185:SER:HA	1:A:224:LEU:HD11	2.03	0.41
1:B:137:MET:SD	1:B:138:PHE:CD1	3.14	0.41
1:B:143:LYS:NZ	1:B:145:GLN:HG3	2.36	0.41
1:D:157:TRP:HB2	1:D:160:LEU:HB2	2.02	0.41
1:F:33:PHE:HD1	1:F:34:THR:H	1.69	0.41
1:C:71:GLU:O	1:C:75:GLU:HG2	2.21	0.41
1:C:469:ARG:NE	1:C:494:GLU:OE1	2.43	0.41
1:D:454:ASP:N	1:D:454:ASP:OD1	2.54	0.41
1:E:29:GLU:OE2	1:E:31:HIS:NE2	2.46	0.41
1:E:35:THR:HA	1:E:62:CYS:HB3	2.01	0.41
1:E:534:ASN:HB2	1:E:537:ILE:HB	2.03	0.41
1:F:110:LEU:HD12	1:F:110:LEU:O	2.20	0.41
1:A:450:GLY:HA3	1:A:472:HIS:HB2	2.02	0.41
1:B:7:CYS:SG	1:B:98:CYS:HB3	2.61	0.41
1:C:407:GLY:HA3	1:E:342:LYS:NZ	2.36	0.41
1:F:10:GLY:HA3	2:I:9:A:N7	2.35	0.41
1:F:129:ASN:ND2	1:F:136:GLU:OE2	2.54	0.41
1:F:141:LEU:HA	1:F:146:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ALA:HB2	1:A:598:ILE:HD13	2.04	0.40
1:B:103:ILE:HA	2:G:2:A:OP2	2.21	0.40
1:B:134:ILE:HG23	1:B:138:PHE:CE1	2.56	0.40
1:B:211:LEU:O	1:B:213:ILE:HG12	2.21	0.40
1:D:103:ILE:HG13	1:D:104:LYS:N	2.36	0.40
1:E:89:MET:CE	1:E:90:PRO:HD2	2.51	0.40
1:E:292:LYS:HA	1:E:292:LYS:HD2	1.89	0.40
1:E:544:GLU:H	1:E:544:GLU:HG2	1.61	0.40
1:F:569:ILE:HD11	1:F:586:PHE:CG	2.56	0.40
1:F:570:GLU:O	1:F:579:ARG:NH1	2.54	0.40
3:A:701:ATP:O3B	3:A:701:ATP:H4'	2.22	0.40
1:B:34:THR:HG21	1:B:40:PHE:CE2	2.56	0.40
1:C:115:THR:HG22	1:C:157:TRP:CZ2	2.56	0.40
1:D:301:GLY:O	1:D:305:LEU:HB2	2.21	0.40
1:F:72:ARG:NH2	1:F:175:ARG:HD2	2.34	0.40
1:F:78:GLN:OE1	1:F:109:SER:OG	2.26	0.40
1:B:103:ILE:HD12	2:G:1:A:H3'	2.04	0.40
1:B:136:GLU:HA	1:B:139:ASP:OD2	2.22	0.40
1:D:116:LEU:HB3	1:D:160:LEU:HD13	2.02	0.40
1:D:599:LYS:HA	1:D:599:LYS:HD2	1.85	0.40
1:F:4:VAL:HG23	1:F:90:PRO:HG3	2.03	0.40
1:F:458:ILE:O	1:F:462:VAL:HG13	2.21	0.40
1:A:3:ARG:NH1	1:A:25:GLU:OE2	2.54	0.40
1:A:56:ARG:NH1	1:A:57:PHE:O	2.55	0.40
1:A:159:ALA:CB	1:A:596:ILE:HA	2.52	0.40
1:B:440:ARG:CZ	1:F:390:LEU:HB3	2.51	0.40
1:B:495:MET:HE2	1:B:495:MET:HB3	1.95	0.40
3:C:701:ATP:O3A	3:C:701:ATP:H4'	2.21	0.40
1:E:201:GLY:HA2	1:E:204:ASN:OD1	2.22	0.40
1:A:74:PHE:HZ	1:B:151:MET:HG3	1.86	0.40
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.82	0.40
1:B:284:SER:OG	1:B:286:LYS:O	2.38	0.40
1:C:33:PHE:CZ	1:C:80:MET:HG3	2.54	0.40
1:E:390:LEU:HD23	1:E:390:LEU:HA	1.94	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	588/600 (98%)	551 (94%)	36 (6%)	1 (0%)	44	75
1	B	598/600 (100%)	564 (94%)	33 (6%)	1 (0%)	44	75
1	C	588/600 (98%)	556 (95%)	32 (5%)	0	100	100
1	D	595/600 (99%)	561 (94%)	32 (5%)	2 (0%)	37	69
1	E	588/600 (98%)	560 (95%)	27 (5%)	1 (0%)	44	75
1	F	598/600 (100%)	568 (95%)	28 (5%)	2 (0%)	37	69
All	All	3555/3600 (99%)	3360 (94%)	188 (5%)	7 (0%)	45	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	206	LEU
1	D	206	LEU
1	F	206	LEU
1	F	278	ILE
1	A	424	LYS
1	E	68	ILE
1	D	278	ILE

### 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	510/517 (99%)	496 (97%)	14 (3%)	40	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	516/517 (100%)	500 (97%)	16 (3%)	35	66
1	C	510/517 (99%)	489 (96%)	21 (4%)	26	59
1	D	515/517 (100%)	499 (97%)	16 (3%)	35	66
1	E	510/517 (99%)	498 (98%)	12 (2%)	44	71
1	F	516/517 (100%)	497 (96%)	19 (4%)	29	62
All	All	3077/3102 (99%)	2979 (97%)	98 (3%)	36	65

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	MET
1	A	25	GLU
1	A	85	TYR
1	A	106	MET
1	A	124	HIS
1	A	179	LYS
1	A	185	SER
1	A	291	ASP
1	A	337	ASN
1	A	370	ASN
1	A	427	ARG
1	A	515	LEU
1	A	516	TYR
1	A	545	ASN
1	B	20	PHE
1	B	106	MET
1	B	123	PHE
1	B	132	ARG
1	B	137	MET
1	B	171	GLU
1	B	175	ARG
1	B	196	MET
1	B	204	ASN
1	B	266	PRO
1	B	274	SER
1	B	281	TRP
1	B	307	ASP
1	B	359	PHE
1	B	421	PHE
1	B	430	TYR

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Mol	Chain	Res	Type
1	C	5	LEU
1	C	14	MET
1	C	27	PHE
1	C	69	LEU
1	C	85	TYR
1	C	91	ASP
1	C	106	MET
1	C	107	SER
1	C	117	PHE
1	C	151	MET
1	C	153	TYR
1	C	157	TRP
1	C	175	ARG
1	C	179	LYS
1	C	293	TYR
1	C	339	TYR
1	C	370	ASN
1	C	423	ASN
1	C	516	TYR
1	C	545	ASN
1	C	566	ARG
1	D	14	MET
1	D	39	LYS
1	D	50	HIS
1	D	74	PHE
1	D	121	SER
1	D	123	PHE
1	D	128	ASP
1	D	153	TYR
1	D	171	GLU
1	D	173	CYS
1	D	285	HIS
1	D	286	LYS
1	D	310	CYS
1	D	421	PHE
1	D	511	ASN
1	D	597	SER
1	E	57	PHE
1	E	91	ASP
1	E	179	LYS
1	E	190	LEU
1	E	285	HIS

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Mol	Chain	Res	Type
1	E	326	ASN
1	E	346	ARG
1	E	431	TYR
1	E	515	LEU
1	E	516	TYR
1	E	547	LEU
1	E	595	LEU
1	F	8	SER
1	F	33	PHE
1	F	85	TYR
1	F	120	GLN
1	F	153	TYR
1	F	161	ARG
1	F	171	GLU
1	F	174	SER
1	F	181	LEU
1	F	281	TRP
1	F	303	LYS
1	F	356	ASN
1	F	359	PHE
1	F	421	PHE
1	F	430	TYR
1	F	448	HIS
1	F	481	ASP
1	F	515	LEU
1	F	597	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	300	ASN
1	B	353	GLN
1	B	356	ASN
1	B	406	GLN
1	C	204	ASN
1	D	353	GLN
1	D	356	ASN
1	D	377	ASN
1	D	406	GLN
1	E	204	ASN
1	F	31	HIS
1	F	83	GLN

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Mol	Chain	Res	Type
1	F	353	GLN
1	F	356	ASN
1	F	406	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	3/4 (75%)	3 (100%)	0
2	H	3/4 (75%)	3 (100%)	0
2	I	3/4 (75%)	3 (100%)	0
All	All	9/12 (75%)	9 (100%)	0

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	1	A
2	G	2	A
2	G	3	A
2	H	5	A
2	H	6	A
2	H	7	A
2	I	9	A
2	I	10	A
2	I	11	A

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ATP	C	701	-	28,33,33	4.11	9 (32%)	34,52,52	1.32	2 (5%)
3	ATP	F	702	-	28,33,33	4.15	9 (32%)	34,52,52	1.37	2 (5%)
3	ATP	D	702	-	28,33,33	4.15	9 (32%)	34,52,52	1.40	2 (5%)
3	ATP	E	701	-	28,33,33	4.10	9 (32%)	34,52,52	1.31	2 (5%)
3	ATP	A	702	-	28,33,33	4.13	9 (32%)	34,52,52	1.27	2 (5%)
3	ATP	B	701	-	28,33,33	4.13	9 (32%)	34,52,52	1.32	2 (5%)
3	ATP	C	702	-	28,33,33	4.15	9 (32%)	34,52,52	1.37	3 (8%)
3	ATP	F	701	-	28,33,33	4.11	9 (32%)	34,52,52	1.33	2 (5%)
3	ATP	E	702	-	28,33,33	4.12	9 (32%)	34,52,52	1.41	3 (8%)
3	ATP	D	701	-	28,33,33	4.11	9 (32%)	34,52,52	1.32	2 (5%)
3	ATP	A	701	-	28,33,33	4.10	9 (32%)	34,52,52	1.28	2 (5%)
3	ATP	B	702	-	28,33,33	4.12	9 (32%)	34,52,52	1.41	2 (5%)

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	ATP	C	701	-	-	5/18/38/38	0/3/3/3
3	ATP	F	702	-	-	7/18/38/38	0/3/3/3
3	ATP	D	702	-	-	9/18/38/38	0/3/3/3
3	ATP	E	701	-	-	6/18/38/38	0/3/3/3
3	ATP	A	702	-	-	10/18/38/38	0/3/3/3
3	ATP	B	701	-	-	4/18/38/38	0/3/3/3
3	ATP	C	702	-	-	9/18/38/38	0/3/3/3
3	ATP	F	701	-	-	8/18/38/38	0/3/3/3
3	ATP	E	702	-	-	7/18/38/38	0/3/3/3
3	ATP	D	701	-	-	8/18/38/38	0/3/3/3
3	ATP	A	701	-	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	702	-	-	9/18/38/38	0/3/3/3

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	ATP	O4'-C1'	16.90	1.63	1.40
3	F	702	ATP	O4'-C1'	16.90	1.63	1.40
3	D	701	ATP	O4'-C1'	16.84	1.63	1.40
3	B	702	ATP	O4'-C1'	16.84	1.63	1.40
3	F	701	ATP	O4'-C1'	16.84	1.63	1.40
3	E	702	ATP	O4'-C1'	16.81	1.62	1.40
3	C	701	ATP	O4'-C1'	16.80	1.62	1.40
3	E	701	ATP	O4'-C1'	16.78	1.62	1.40
3	A	702	ATP	O4'-C1'	16.77	1.62	1.40
3	B	701	ATP	O4'-C1'	16.75	1.62	1.40
3	A	701	ATP	O4'-C1'	16.74	1.62	1.40
3	C	702	ATP	O4'-C1'	16.73	1.62	1.40
3	D	702	ATP	O4'-C4'	-7.71	1.27	1.45
3	F	702	ATP	O4'-C4'	-7.71	1.27	1.45
3	E	702	ATP	O4'-C4'	-7.70	1.27	1.45
3	C	702	ATP	O4'-C4'	-7.70	1.27	1.45
3	C	701	ATP	O4'-C4'	-7.67	1.27	1.45
3	F	701	ATP	O4'-C4'	-7.67	1.28	1.45
3	A	702	ATP	O4'-C4'	-7.66	1.28	1.45
3	B	701	ATP	O4'-C4'	-7.65	1.28	1.45
3	E	701	ATP	O4'-C4'	-7.65	1.28	1.45
3	B	702	ATP	O4'-C4'	-7.64	1.28	1.45
3	D	701	ATP	O4'-C4'	-7.63	1.28	1.45
3	A	701	ATP	O4'-C4'	-7.59	1.28	1.45
3	C	702	ATP	PB-O3A	5.75	1.65	1.59
3	C	702	ATP	PA-O3A	5.71	1.65	1.59
3	B	701	ATP	PA-O3A	5.59	1.65	1.59
3	D	702	ATP	PB-O3B	5.51	1.65	1.59
3	A	702	ATP	PB-O3A	5.50	1.65	1.59
3	F	702	ATP	PA-O3A	5.49	1.65	1.59
3	E	702	ATP	PB-O3B	5.47	1.65	1.59
3	F	702	ATP	PB-O3B	5.43	1.65	1.59
3	F	702	ATP	PB-O3A	5.36	1.65	1.59
3	A	702	ATP	PB-O3B	5.35	1.65	1.59
3	B	702	ATP	PB-O3B	5.33	1.65	1.59
3	B	701	ATP	PB-O3A	5.32	1.65	1.59
3	D	702	ATP	PB-O3A	5.31	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ATP	PB-O3A	5.29	1.65	1.59
3	B	702	ATP	PB-O3A	5.29	1.65	1.59
3	D	702	ATP	PA-O3A	5.28	1.65	1.59
3	C	702	ATP	PB-O3B	5.26	1.65	1.59
3	E	702	ATP	PB-O3A	5.25	1.65	1.59
3	E	701	ATP	PB-O3A	5.25	1.65	1.59
3	C	701	ATP	PB-O3A	5.25	1.65	1.59
3	A	702	ATP	PA-O3A	5.25	1.65	1.59
3	B	701	ATP	PB-O3B	5.25	1.65	1.59
3	C	701	ATP	PB-O3B	5.24	1.65	1.59
3	D	701	ATP	PB-O3B	5.22	1.65	1.59
3	A	701	ATP	PB-O3B	5.21	1.65	1.59
3	F	701	ATP	PB-O3B	5.21	1.65	1.59
3	D	701	ATP	PB-O3A	5.20	1.65	1.59
3	F	701	ATP	PA-O3A	5.18	1.65	1.59
3	D	701	ATP	PA-O3A	5.18	1.65	1.59
3	B	702	ATP	PA-O3A	5.17	1.65	1.59
3	E	701	ATP	PB-O3B	5.16	1.65	1.59
3	A	701	ATP	PA-O3A	5.16	1.65	1.59
3	F	701	ATP	PB-O3A	5.14	1.65	1.59
3	C	701	ATP	PA-O3A	5.11	1.65	1.59
3	E	701	ATP	PA-O3A	5.10	1.65	1.59
3	E	702	ATP	PA-O3A	5.10	1.65	1.59
3	C	702	ATP	O2'-C2'	3.34	1.51	1.43
3	D	702	ATP	O2'-C2'	3.31	1.51	1.43
3	F	702	ATP	O2'-C2'	3.30	1.51	1.43
3	D	701	ATP	O2'-C2'	3.30	1.51	1.43
3	A	701	ATP	O2'-C2'	3.29	1.51	1.43
3	B	701	ATP	O2'-C2'	3.29	1.51	1.43
3	A	702	ATP	O2'-C2'	3.29	1.51	1.43
3	F	701	ATP	O2'-C2'	3.28	1.51	1.43
3	C	701	ATP	O2'-C2'	3.27	1.51	1.43
3	E	701	ATP	O2'-C2'	3.26	1.51	1.43
3	B	702	ATP	O2'-C2'	3.25	1.51	1.43
3	E	702	ATP	O2'-C2'	3.24	1.51	1.43
3	F	702	ATP	C6-N6	3.24	1.45	1.34
3	C	702	ATP	C6-N6	3.23	1.45	1.34
3	A	702	ATP	C6-N6	3.23	1.45	1.34
3	A	701	ATP	C6-N6	3.23	1.45	1.34
3	B	702	ATP	C6-N6	3.21	1.45	1.34
3	D	702	ATP	C6-N6	3.21	1.45	1.34
3	E	702	ATP	C6-N6	3.20	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	ATP	C6-N6	3.17	1.45	1.34
3	E	701	ATP	C6-N6	3.15	1.45	1.34
3	C	701	ATP	C6-N6	3.15	1.45	1.34
3	D	701	ATP	C6-N6	3.15	1.45	1.34
3	F	701	ATP	C6-N6	3.14	1.45	1.34
3	D	702	ATP	O3'-C3'	-2.73	1.36	1.43
3	E	701	ATP	O3'-C3'	-2.68	1.36	1.43
3	C	701	ATP	O3'-C3'	-2.68	1.36	1.43
3	B	702	ATP	O3'-C3'	-2.67	1.36	1.43
3	E	702	ATP	O3'-C3'	-2.66	1.36	1.43
3	D	701	ATP	O3'-C3'	-2.66	1.36	1.43
3	A	701	ATP	O3'-C3'	-2.65	1.36	1.43
3	A	702	ATP	O3'-C3'	-2.65	1.36	1.43
3	F	701	ATP	O3'-C3'	-2.64	1.36	1.43
3	F	702	ATP	O3'-C3'	-2.64	1.36	1.43
3	B	701	ATP	O3'-C3'	-2.62	1.36	1.43
3	C	702	ATP	O3'-C3'	-2.54	1.36	1.43
3	B	701	ATP	C1'-N9	-2.35	1.44	1.49
3	E	701	ATP	C1'-N9	-2.26	1.44	1.49
3	A	701	ATP	C1'-N9	-2.25	1.44	1.49
3	E	702	ATP	C1'-N9	-2.20	1.44	1.49
3	A	702	ATP	C1'-N9	-2.20	1.44	1.49
3	C	701	ATP	C1'-N9	-2.19	1.44	1.49
3	F	702	ATP	C1'-N9	-2.19	1.44	1.49
3	F	701	ATP	C1'-N9	-2.17	1.44	1.49
3	D	702	ATP	C1'-N9	-2.16	1.44	1.49
3	B	702	ATP	C1'-N9	-2.15	1.44	1.49
3	D	701	ATP	C1'-N9	-2.15	1.44	1.49
3	C	702	ATP	C1'-N9	-2.11	1.44	1.49

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	ATP	N3-C2-N1	-6.12	120.37	128.67
3	F	701	ATP	N3-C2-N1	-5.79	120.81	128.67
3	B	701	ATP	N3-C2-N1	-5.77	120.84	128.67
3	D	701	ATP	N3-C2-N1	-5.74	120.88	128.67
3	C	701	ATP	N3-C2-N1	-5.72	120.90	128.67
3	E	701	ATP	N3-C2-N1	-5.69	120.95	128.67
3	A	701	ATP	N3-C2-N1	-5.69	120.95	128.67
3	C	702	ATP	N3-C2-N1	-5.68	120.96	128.67
3	A	702	ATP	N3-C2-N1	-5.64	121.01	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	702	ATP	N3-C2-N1	-5.64	121.02	128.67
3	F	702	ATP	N3-C2-N1	-5.59	121.09	128.67
3	D	702	ATP	N3-C2-N1	-5.56	121.12	128.67
3	D	702	ATP	C4'-O4'-C1'	-3.95	106.31	109.92
3	F	702	ATP	C4'-O4'-C1'	-3.74	106.50	109.92
3	E	702	ATP	C4'-O4'-C1'	-3.53	106.69	109.92
3	B	702	ATP	C4'-O4'-C1'	-3.42	106.79	109.92
3	C	702	ATP	C4'-O4'-C1'	-3.35	106.86	109.92
3	B	701	ATP	C4'-O4'-C1'	-3.26	106.94	109.92
3	C	701	ATP	C4'-O4'-C1'	-2.88	107.29	109.92
3	E	701	ATP	C4'-O4'-C1'	-2.82	107.34	109.92
3	D	701	ATP	C4'-O4'-C1'	-2.79	107.37	109.92
3	F	701	ATP	C4'-O4'-C1'	-2.74	107.42	109.92
3	A	702	ATP	C4'-O4'-C1'	-2.59	107.56	109.92
3	A	701	ATP	C4'-O4'-C1'	-2.49	107.65	109.92
3	C	702	ATP	O3G-PG-O3B	2.18	111.95	104.64
3	E	702	ATP	C5'-C4'-C3'	-2.14	107.50	115.21

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	ATP	PB-O3A-PA-O5'
3	A	701	ATP	C4'-C5'-O5'-PA
3	A	702	ATP	PB-O3B-PG-O2G
3	A	702	ATP	PB-O3A-PA-O5'
3	A	702	ATP	C5'-O5'-PA-O1A
3	A	702	ATP	C5'-O5'-PA-O2A
3	A	702	ATP	C5'-O5'-PA-O3A
3	A	702	ATP	C4'-C5'-O5'-PA
3	B	701	ATP	C4'-C5'-O5'-PA
3	B	702	ATP	PB-O3B-PG-O2G
3	B	702	ATP	C4'-C5'-O5'-PA
3	C	701	ATP	C4'-C5'-O5'-PA
3	C	701	ATP	O4'-C4'-C5'-O5'
3	C	701	ATP	C3'-C4'-C5'-O5'
3	C	702	ATP	PB-O3B-PG-O2G
3	C	702	ATP	C4'-C5'-O5'-PA
3	D	701	ATP	PB-O3A-PA-O5'
3	D	701	ATP	C4'-C5'-O5'-PA
3	D	701	ATP	C3'-C4'-C5'-O5'
3	D	702	ATP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
3	D	702	ATP	C4'-C5'-O5'-PA
3	E	701	ATP	C4'-C5'-O5'-PA
3	E	701	ATP	O4'-C4'-C5'-O5'
3	E	701	ATP	C3'-C4'-C5'-O5'
3	E	702	ATP	PB-O3B-PG-O2G
3	E	702	ATP	PB-O3A-PA-O5'
3	E	702	ATP	C4'-C5'-O5'-PA
3	E	702	ATP	O4'-C4'-C5'-O5'
3	E	702	ATP	C3'-C4'-C5'-O5'
3	F	701	ATP	PB-O3A-PA-O5'
3	F	701	ATP	C4'-C5'-O5'-PA
3	F	701	ATP	C3'-C4'-C5'-O5'
3	F	702	ATP	PB-O3B-PG-O2G
3	F	702	ATP	C4'-C5'-O5'-PA
3	A	701	ATP	O4'-C4'-C5'-O5'
3	A	701	ATP	C3'-C4'-C5'-O5'
3	B	702	ATP	C3'-C4'-C5'-O5'
3	A	702	ATP	C3'-C4'-C5'-O5'
3	B	702	ATP	O4'-C4'-C5'-O5'
3	D	701	ATP	O4'-C4'-C5'-O5'
3	F	701	ATP	O4'-C4'-C5'-O5'
3	C	702	ATP	C3'-C4'-C5'-O5'
3	D	702	ATP	C3'-C4'-C5'-O5'
3	A	702	ATP	O4'-C4'-C5'-O5'
3	C	702	ATP	O4'-C4'-C5'-O5'
3	D	702	ATP	O4'-C4'-C5'-O5'
3	B	701	ATP	C3'-C4'-C5'-O5'
3	D	702	ATP	PA-O3A-PB-O1B
3	C	701	ATP	PB-O3A-PA-O5'
3	C	702	ATP	PB-O3A-PA-O5'
3	D	702	ATP	PB-O3A-PA-O5'
3	E	701	ATP	PB-O3A-PA-O5'
3	F	702	ATP	PB-O3A-PA-O5'
3	F	702	ATP	PB-O3B-PG-O3G
3	D	701	ATP	C5'-O5'-PA-O1A
3	D	701	ATP	C5'-O5'-PA-O3A
3	E	701	ATP	C5'-O5'-PA-O1A
3	F	701	ATP	C5'-O5'-PA-O1A
3	F	701	ATP	C5'-O5'-PA-O3A
3	D	701	ATP	PG-O3B-PB-O1B
3	B	702	ATP	PA-O3A-PB-O3B
3	B	701	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	A	701	ATP	PG-O3B-PB-O1B
3	C	702	ATP	PA-O3A-PB-O1B
3	F	701	ATP	PG-O3B-PB-O1B
3	F	702	ATP	PA-O3A-PB-O1B
3	B	702	ATP	PB-O3A-PA-O5'
3	A	702	ATP	PB-O3B-PG-O1G
3	C	702	ATP	PB-O3B-PG-O1G
3	F	702	ATP	PB-O3B-PG-O1G
3	B	702	ATP	PB-O3B-PG-O3G
3	D	702	ATP	PB-O3B-PG-O3G
3	E	702	ATP	PB-O3B-PG-O3G
3	F	702	ATP	PA-O3A-PB-O3B
3	B	701	ATP	PA-O3A-PB-O2B
3	B	702	ATP	PA-O3A-PB-O1B
3	C	701	ATP	PG-O3B-PB-O1B
3	E	701	ATP	PG-O3B-PB-O1B
3	E	702	ATP	PB-O3A-PA-O1A
3	F	701	ATP	PG-O3B-PB-O2B
3	D	702	ATP	PB-O3B-PG-O1G
3	A	701	ATP	PG-O3B-PB-O2B
3	A	701	ATP	PA-O3A-PB-O2B
3	A	702	ATP	PB-O3A-PA-O2A
3	B	702	ATP	PB-O3A-PA-O2A
3	C	702	ATP	PB-O3A-PA-O1A
3	C	702	ATP	PB-O3A-PA-O2A
3	D	701	ATP	PG-O3B-PB-O2B
3	D	702	ATP	PB-O3A-PA-O2A

There are no ring outliers.

12 monomers are involved in 23 short contacts:

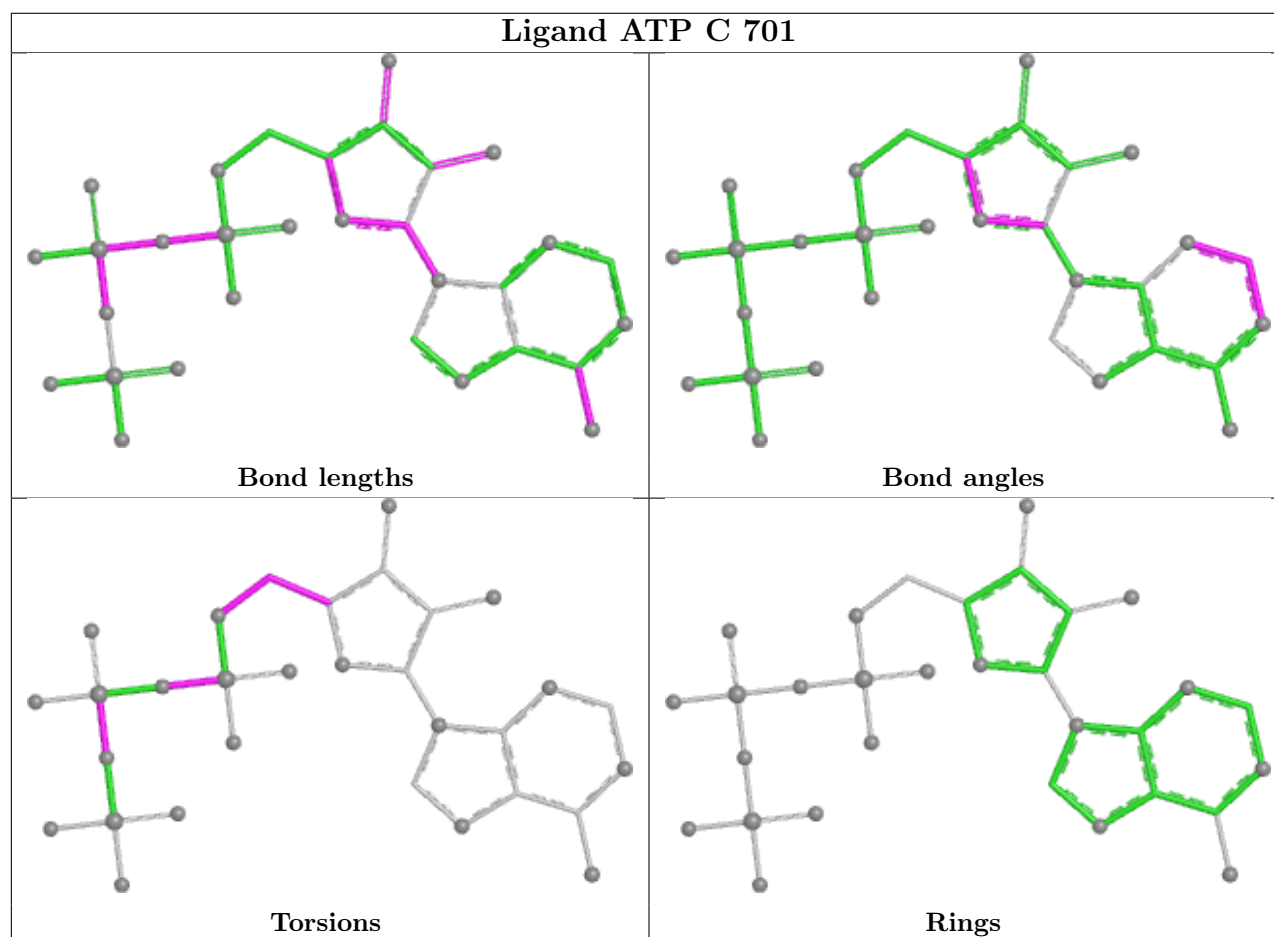
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	ATP	2	0
3	F	702	ATP	1	0
3	D	702	ATP	4	0
3	E	701	ATP	1	0
3	A	702	ATP	2	0
3	B	701	ATP	1	0
3	C	702	ATP	3	0
3	F	701	ATP	1	0
3	E	702	ATP	4	0
3	D	701	ATP	1	0

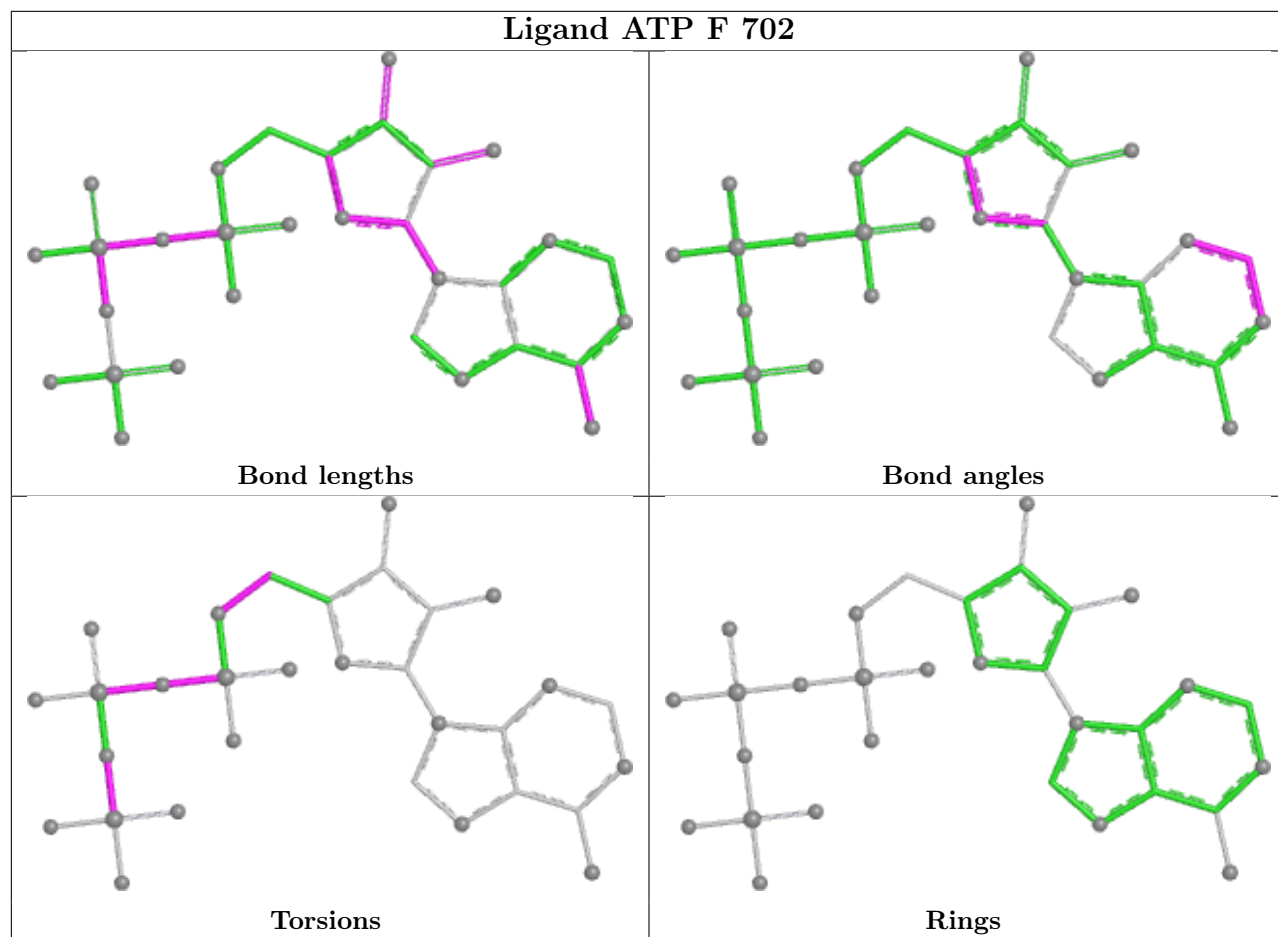
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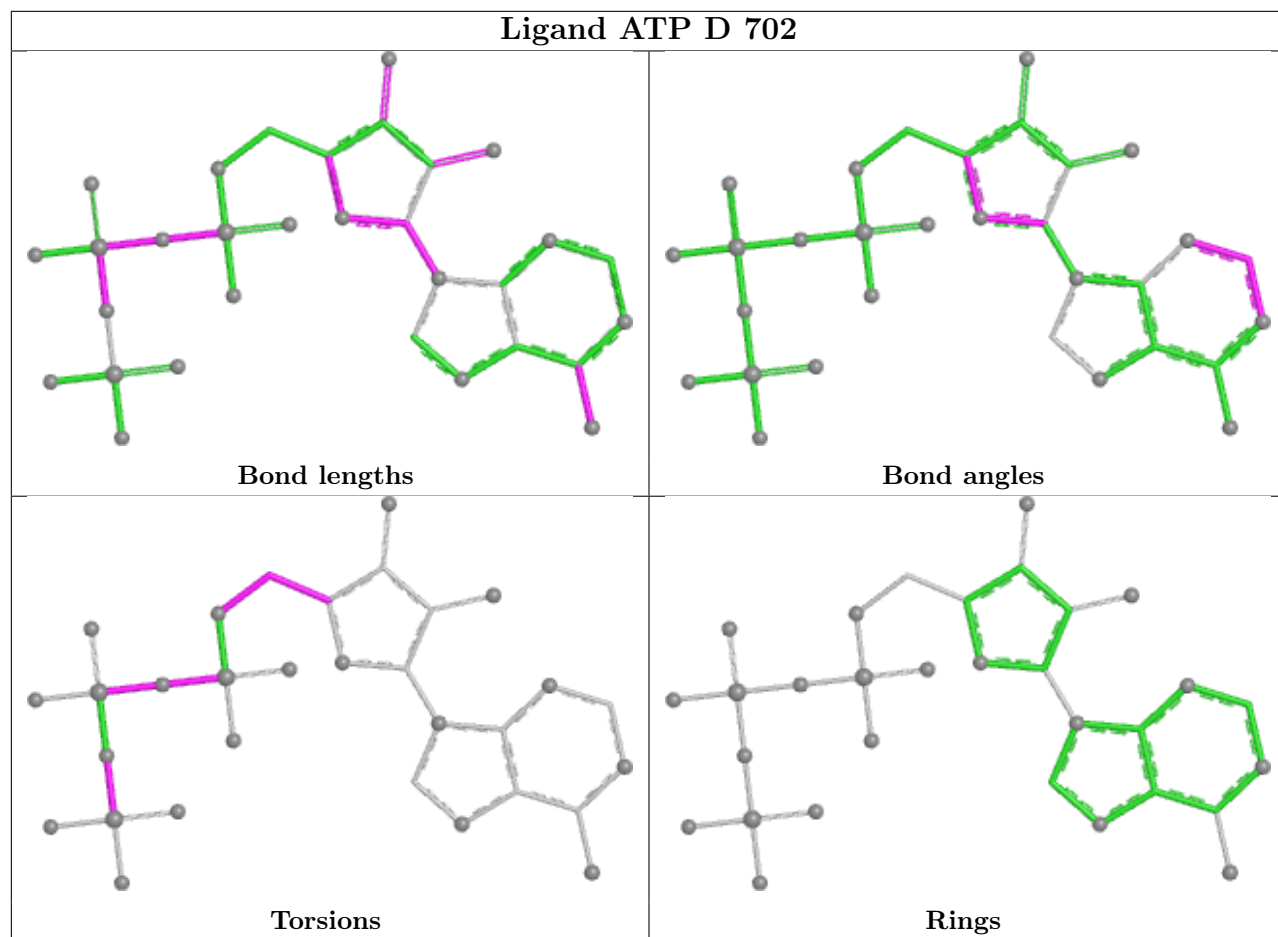
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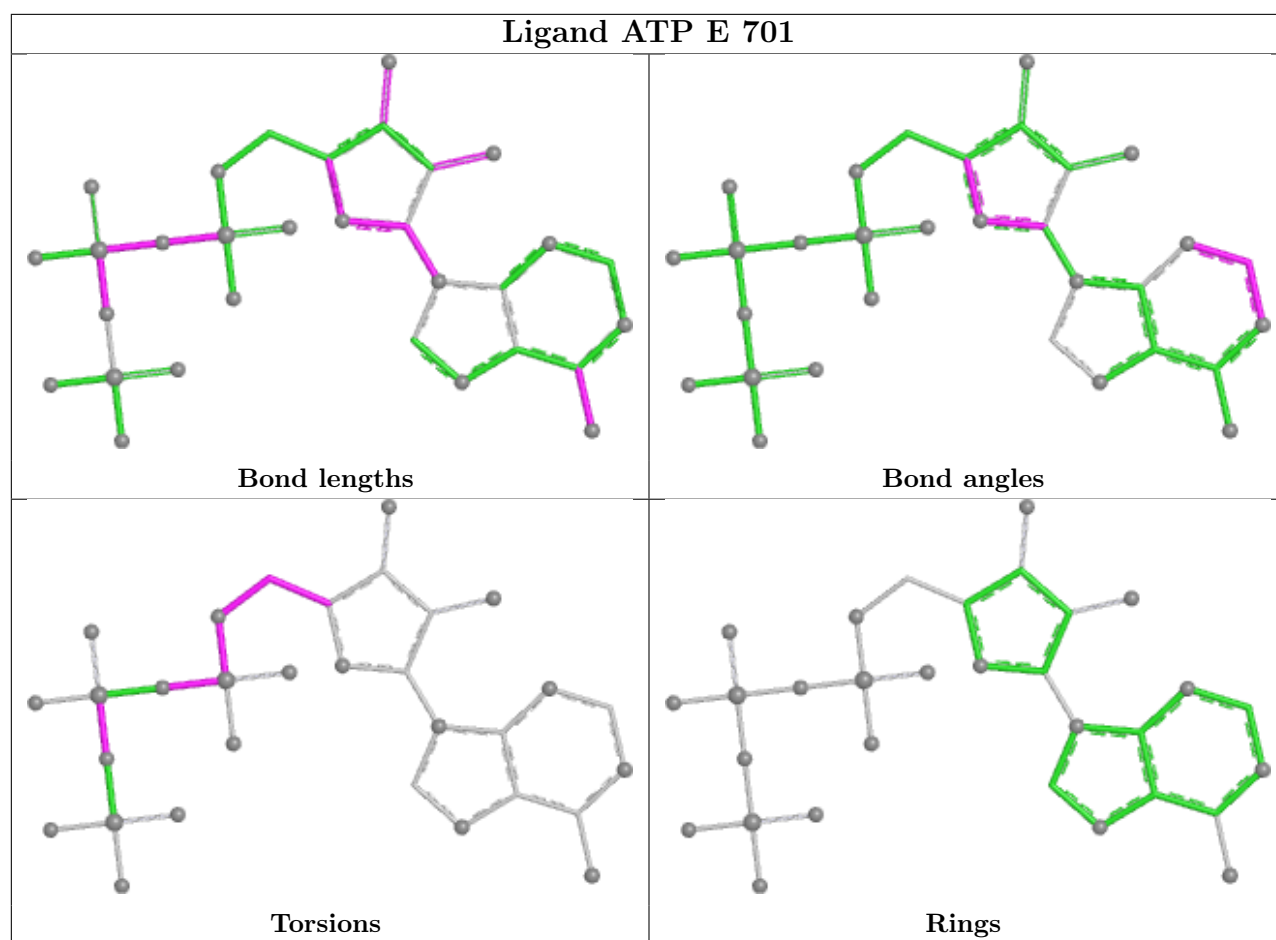
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	ATP	1	0
3	B	702	ATP	2	0

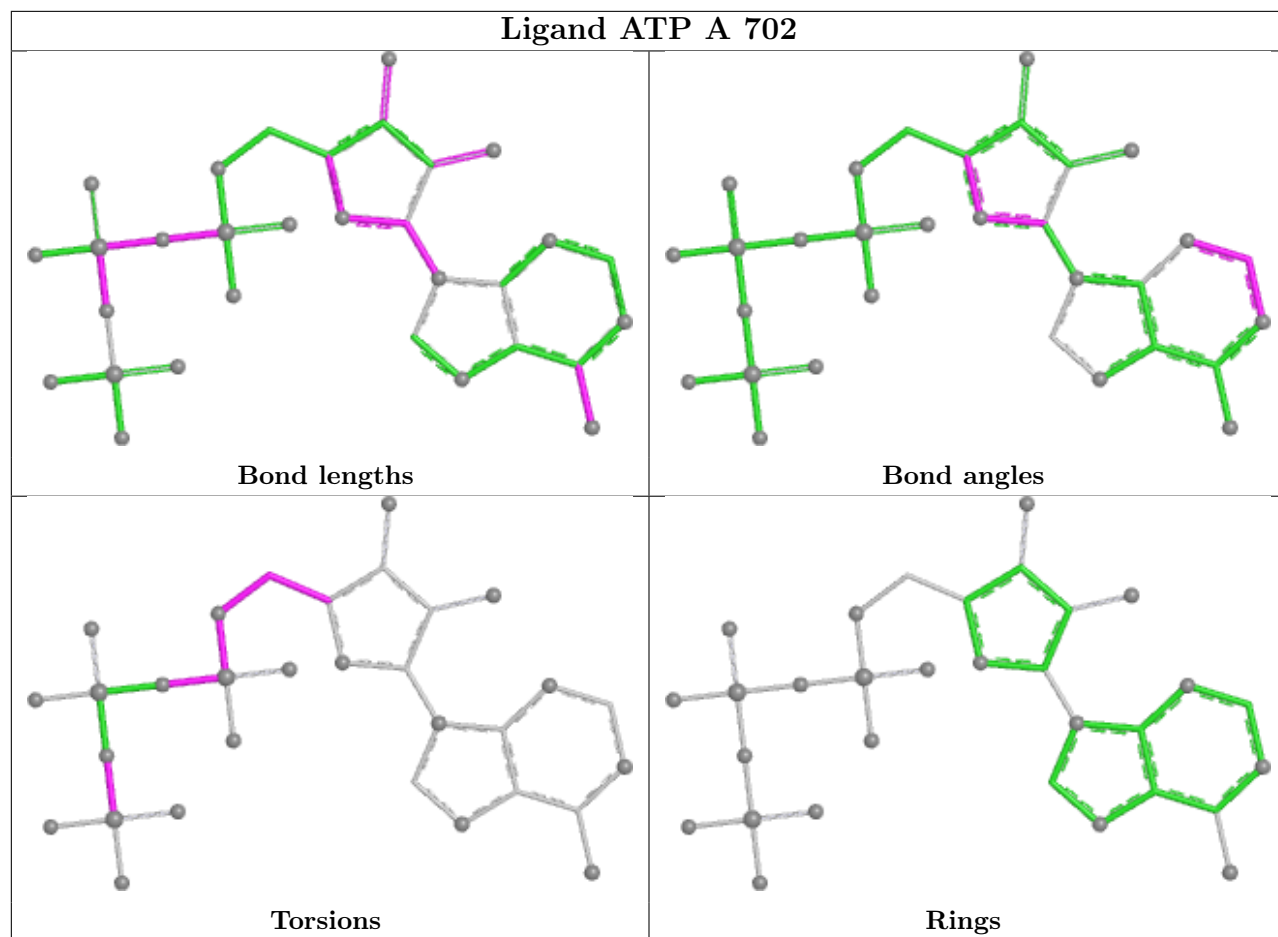
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



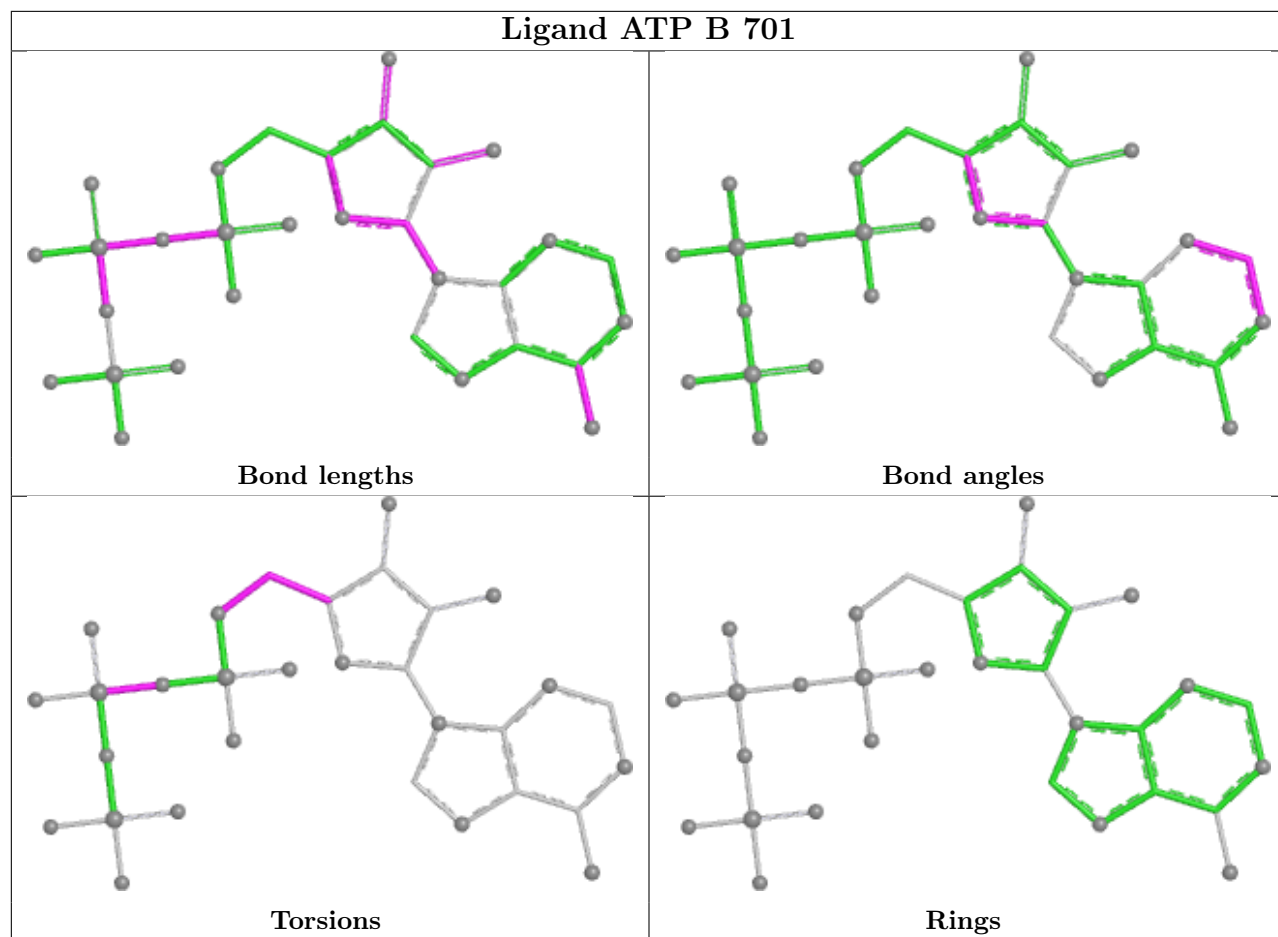


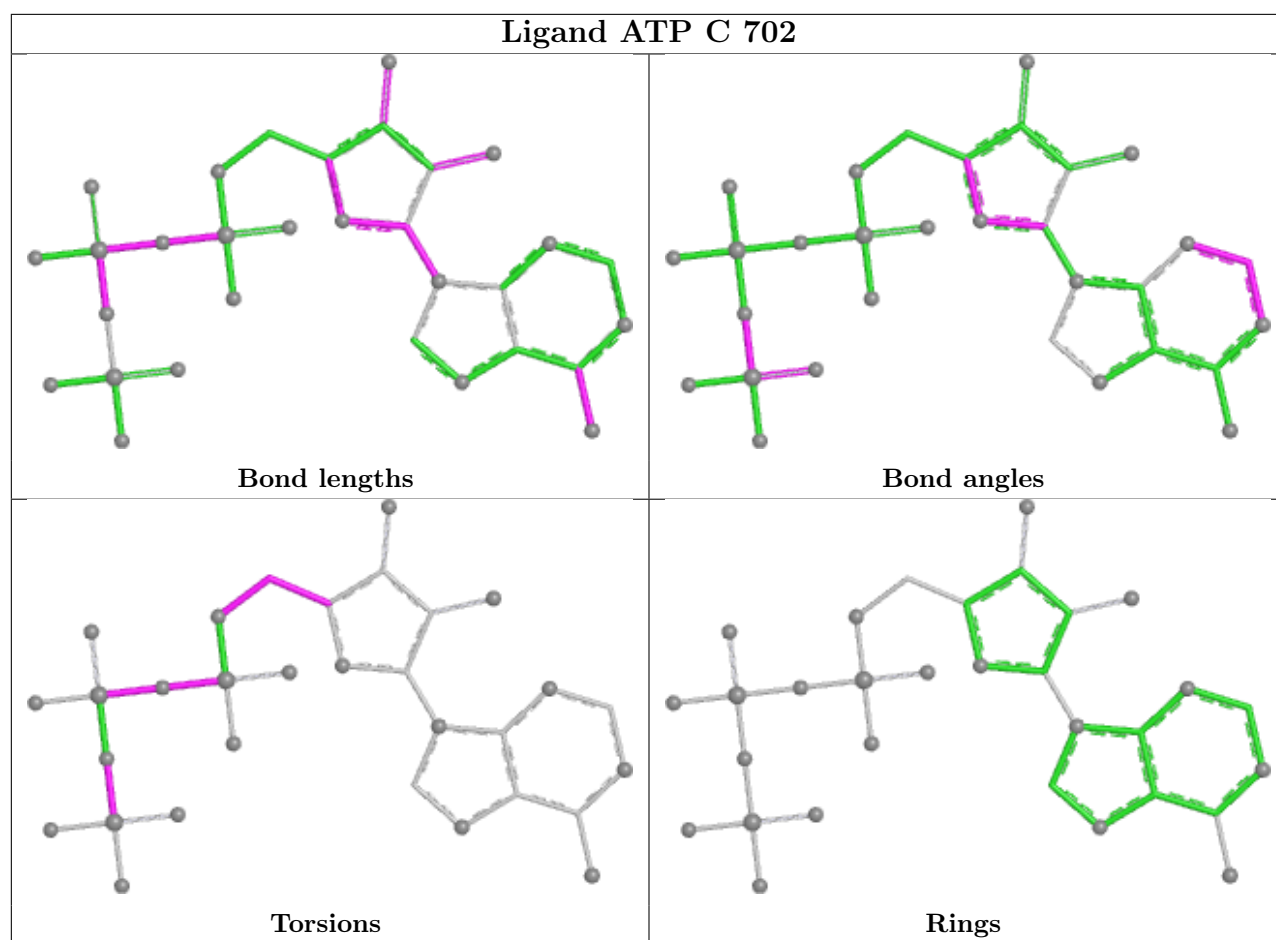


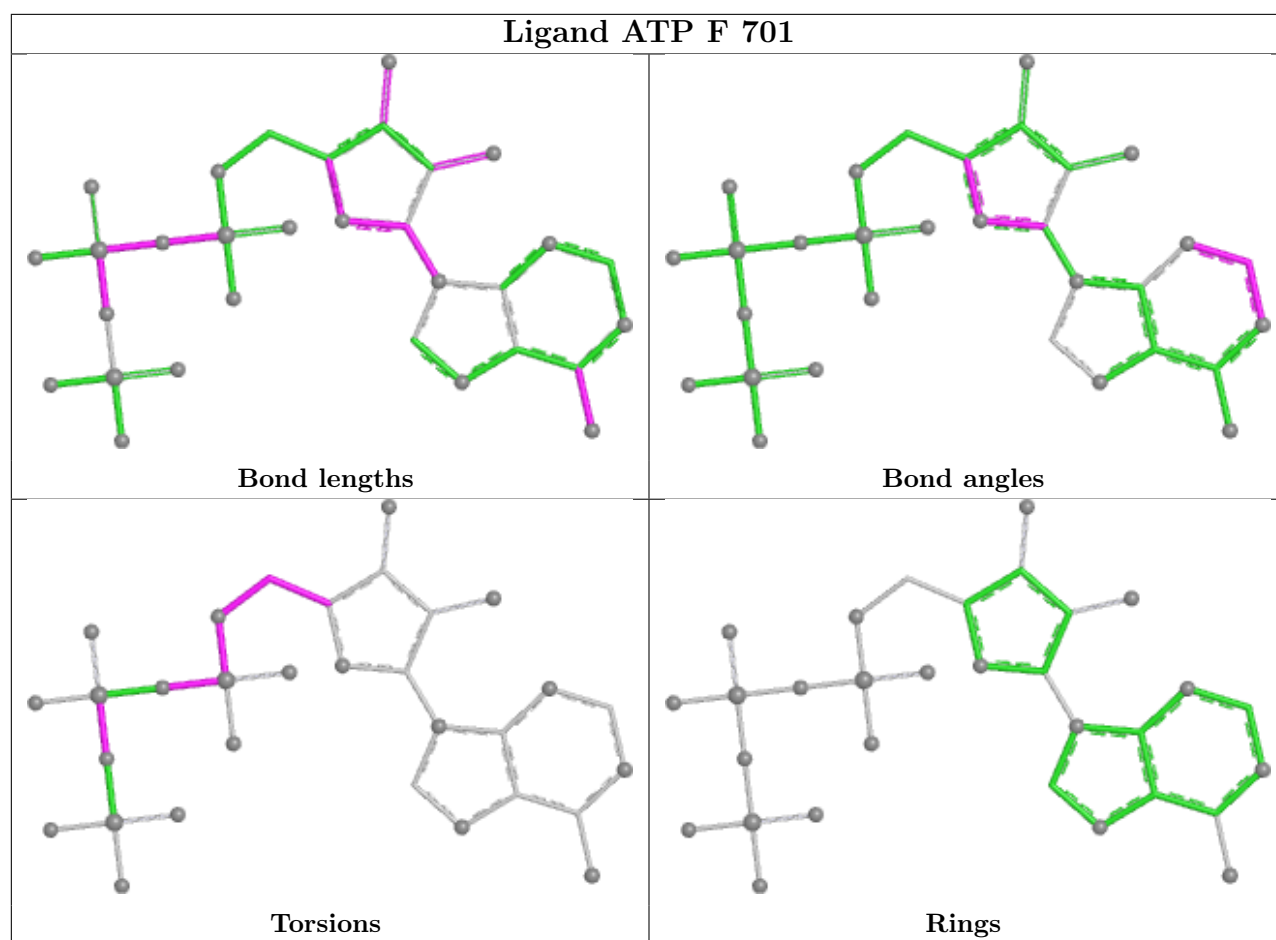


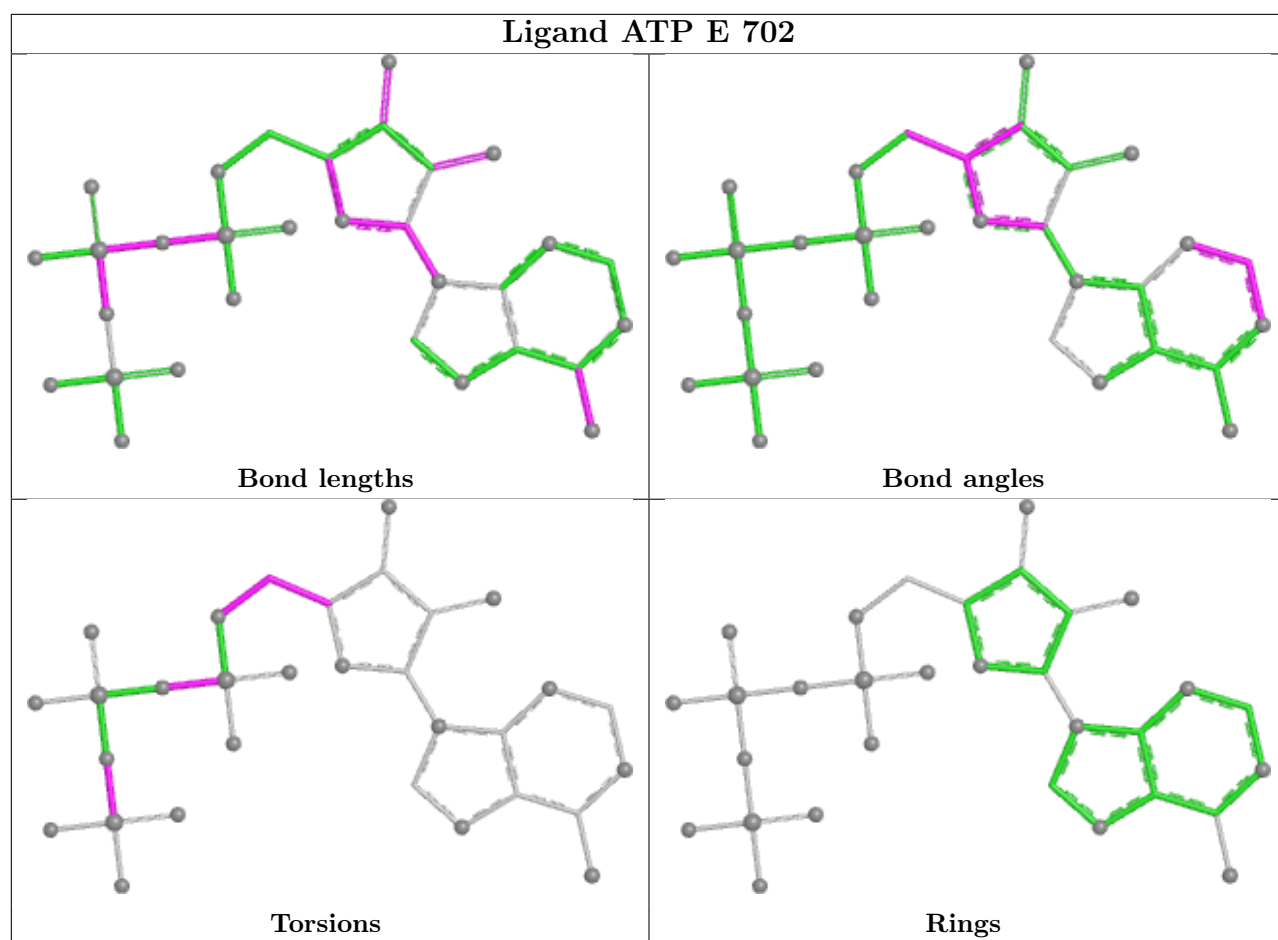


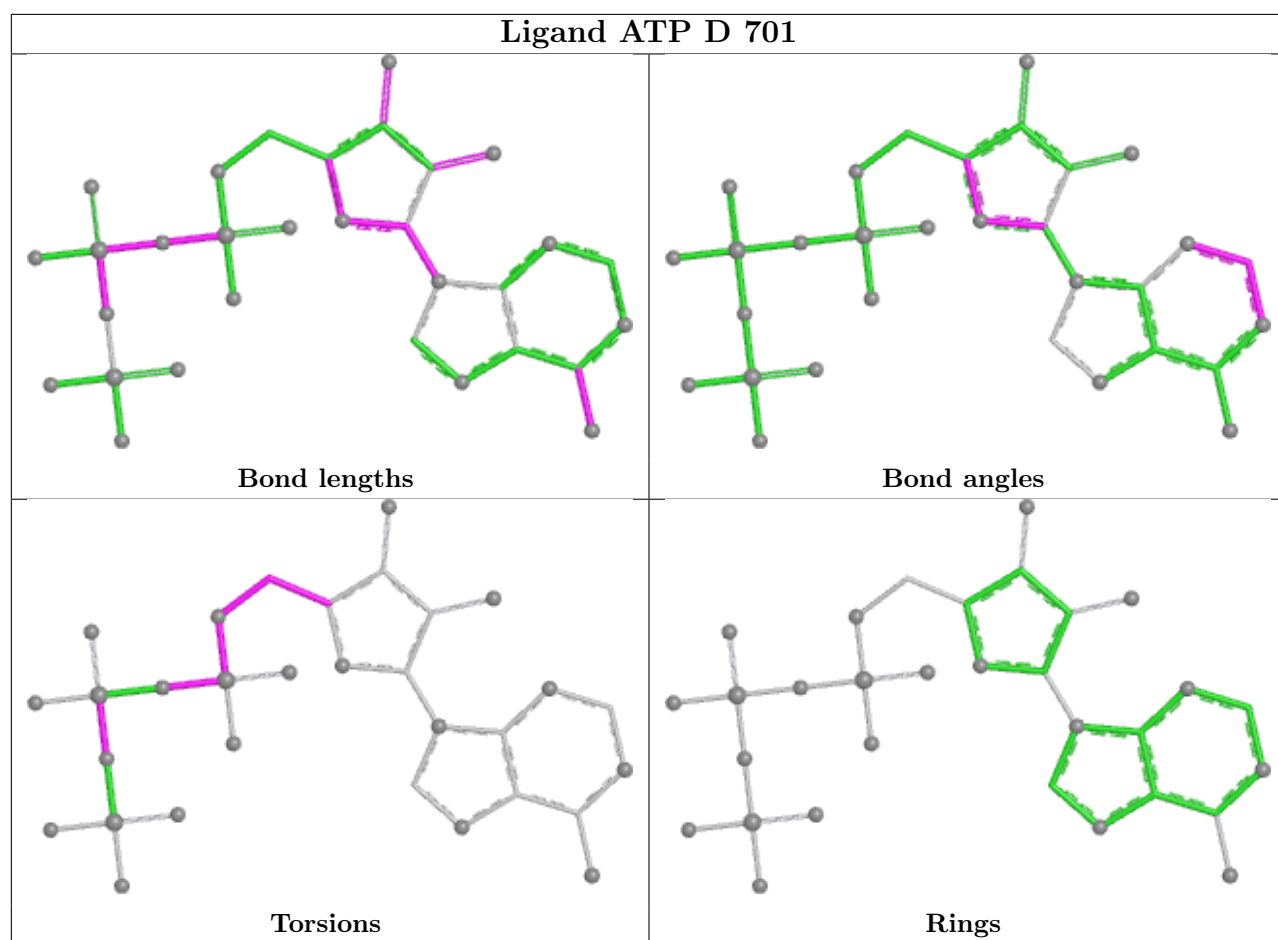


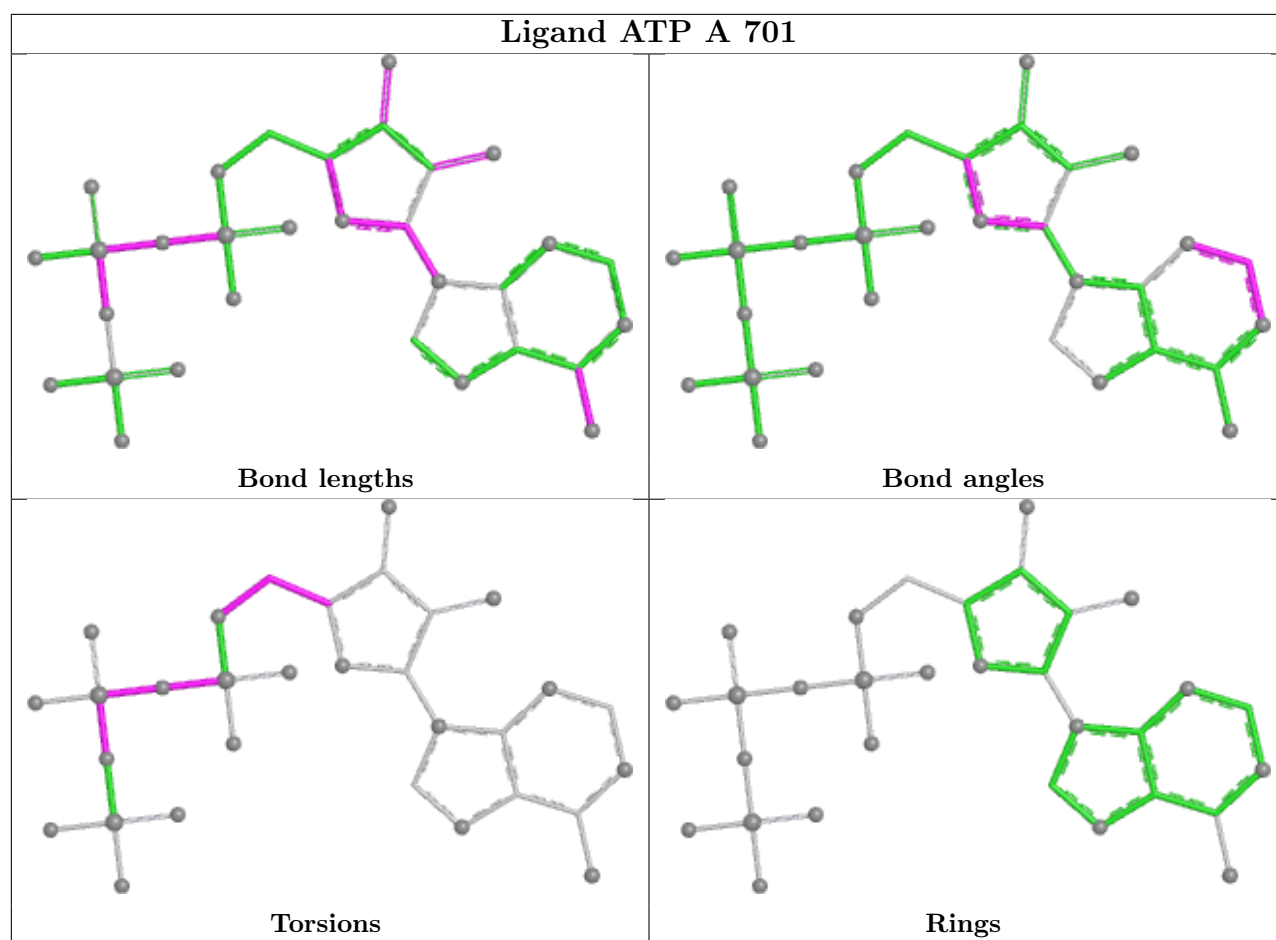


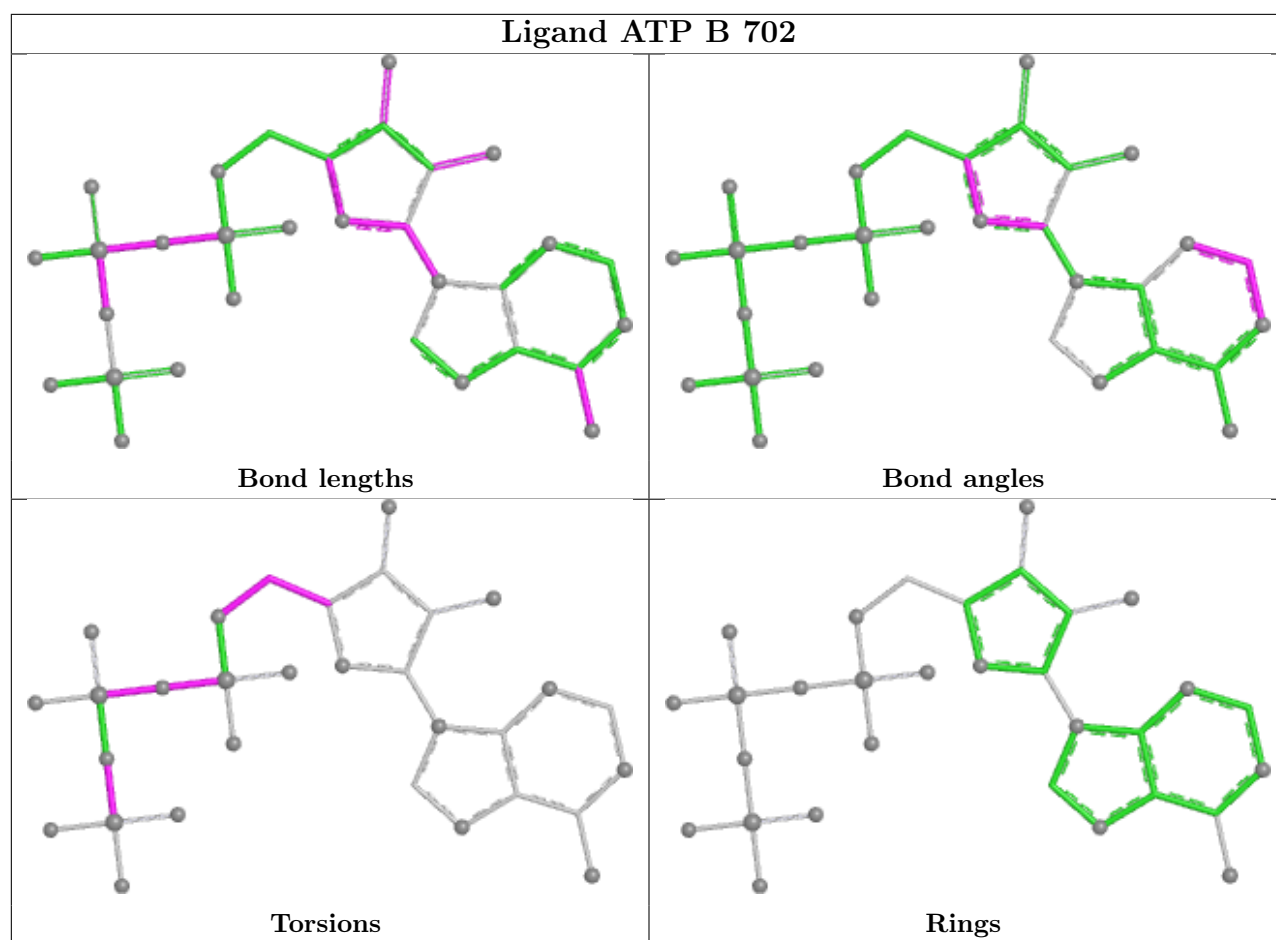












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

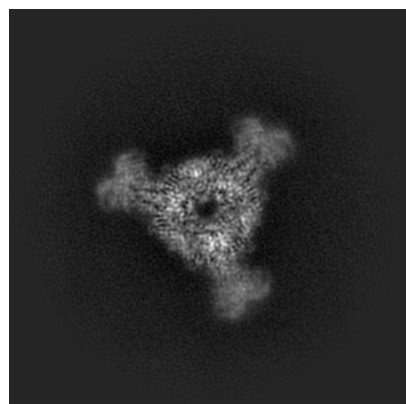
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45277. These allow visual inspection of the internal detail of the map and identification of artifacts.

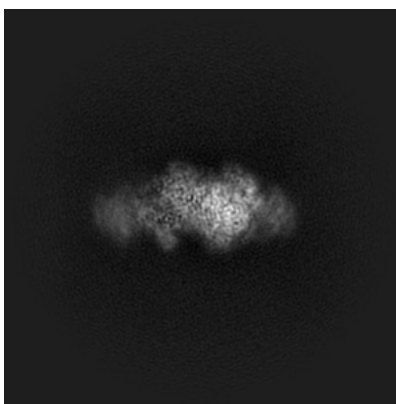
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

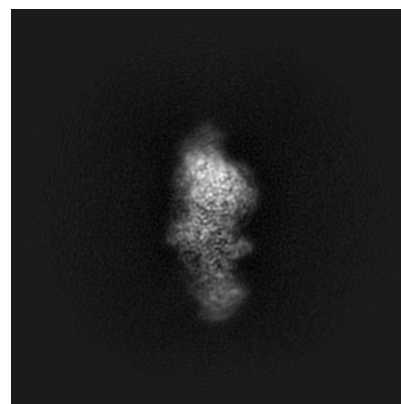
#### 6.1.1 Primary map



X

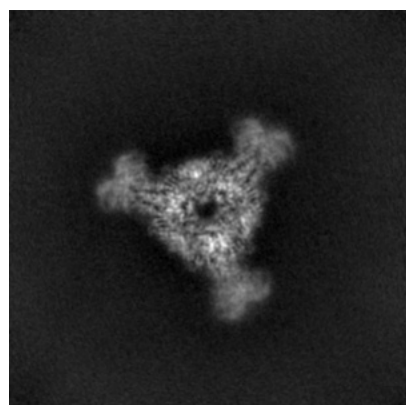


Y

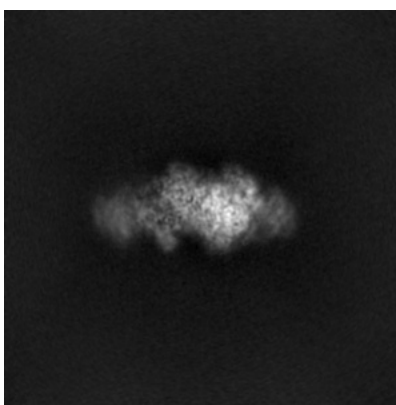


Z

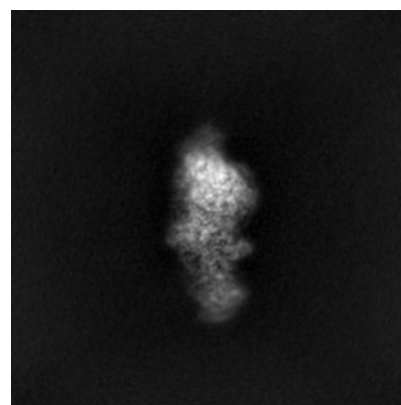
#### 6.1.2 Raw map



X



Y



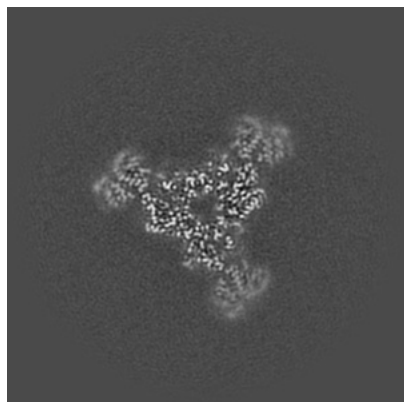
Z

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

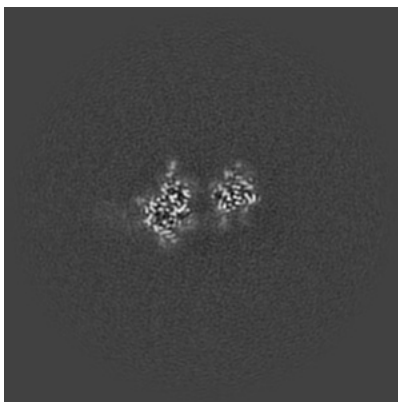


## 6.2 Central slices [i](#)

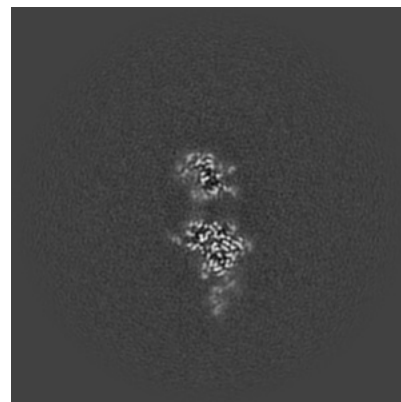
### 6.2.1 Primary map



X Index: 256

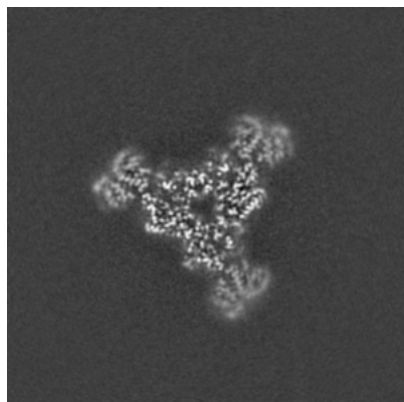


Y Index: 256

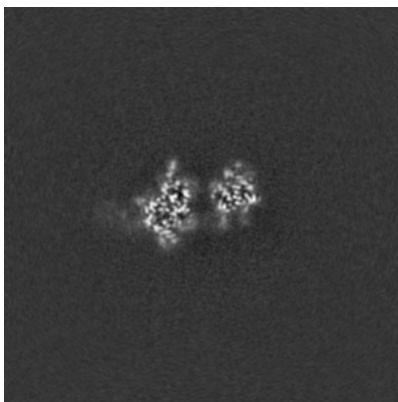


Z Index: 256

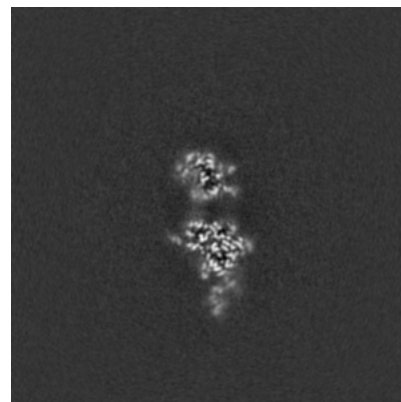
### 6.2.2 Raw map



X Index: 256



Y Index: 256

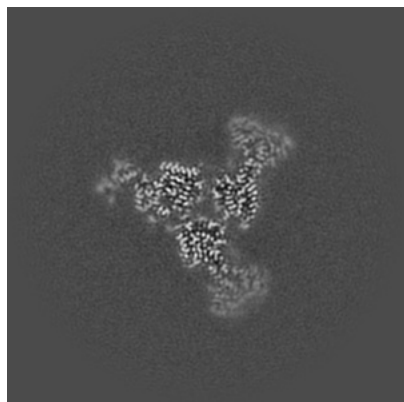


Z Index: 256

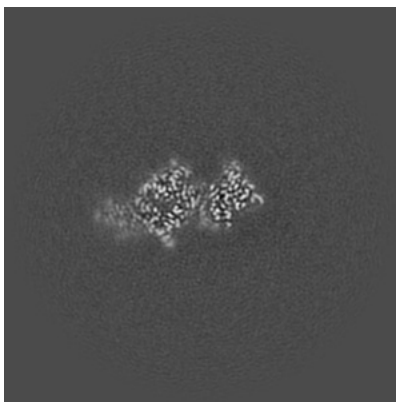
The images above show central slices of the map in three orthogonal directions.

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

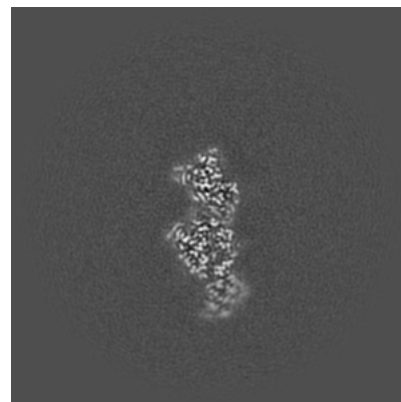
### 6.3.1 Primary map



X Index: 246

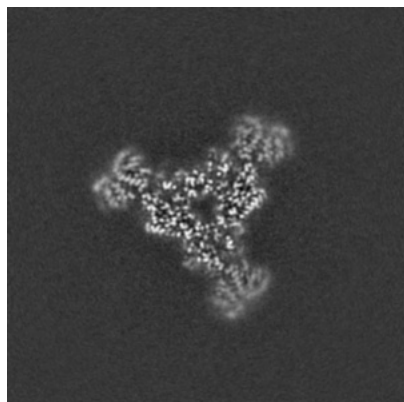


Y Index: 271

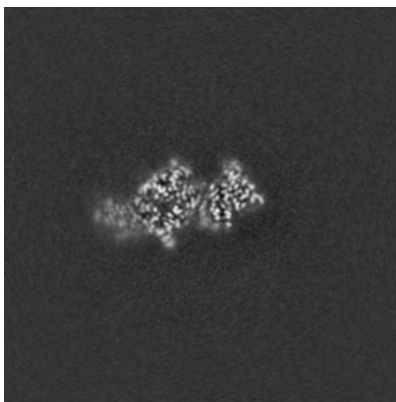


Z Index: 274

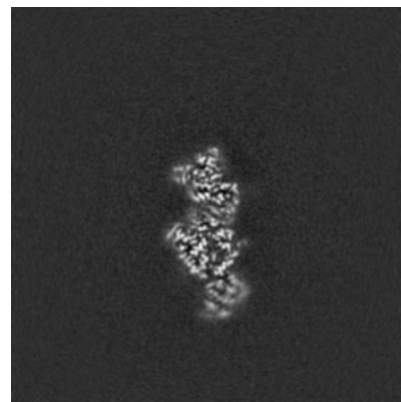
### 6.3.2 Raw map



X Index: 257



Y Index: 271

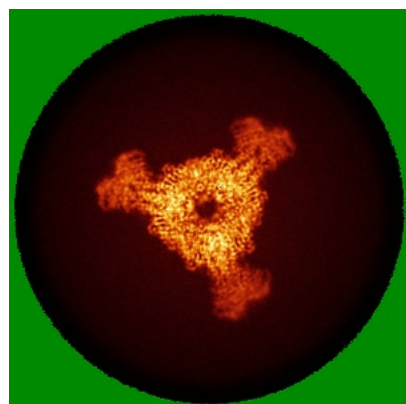


Z Index: 273

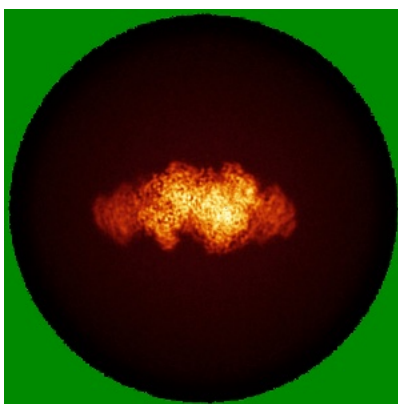
The images above show the largest variance slices of the map in three orthogonal directions.

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

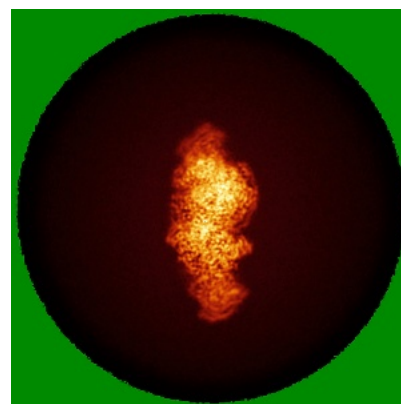
### 6.4.1 Primary map



X



Y

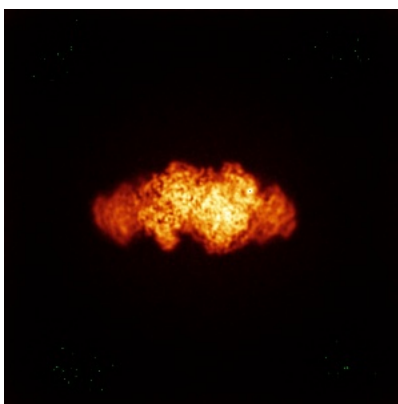


Z

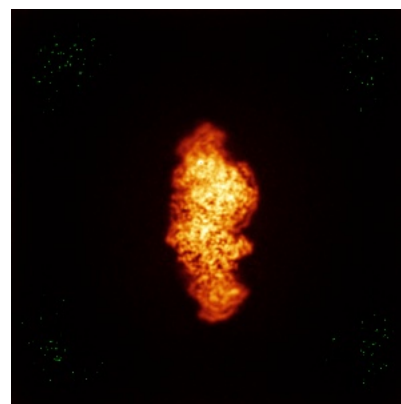
### 6.4.2 Raw map



X



Y

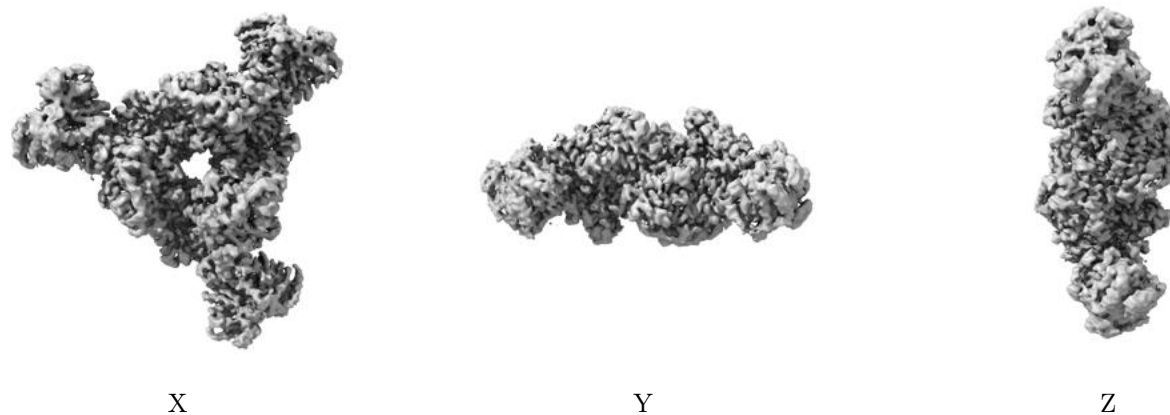


Z

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.

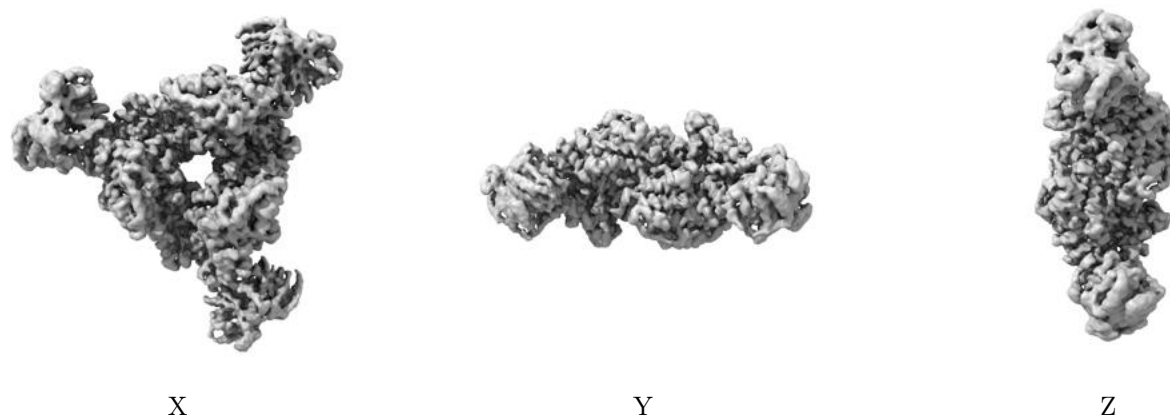
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. 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.

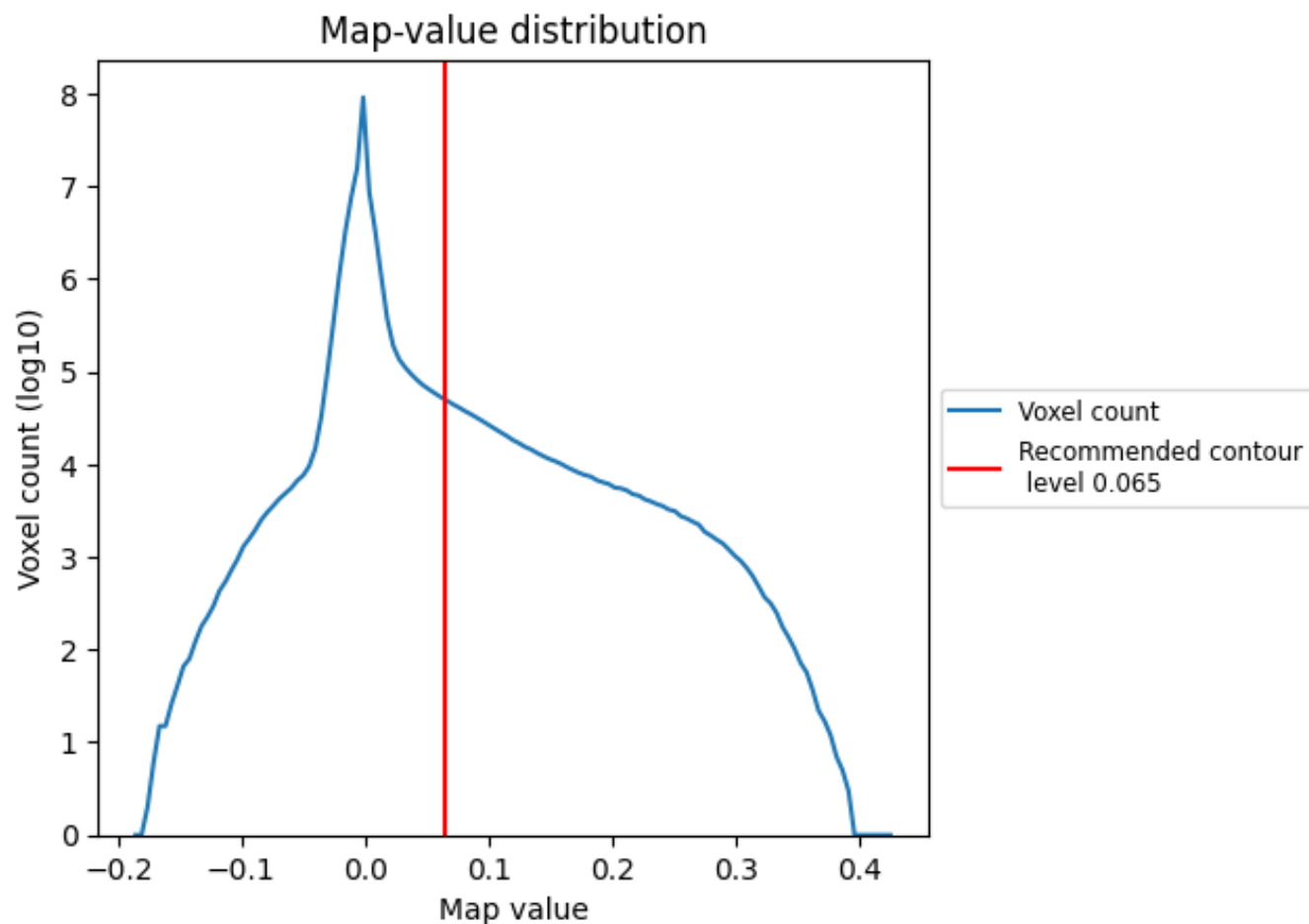
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

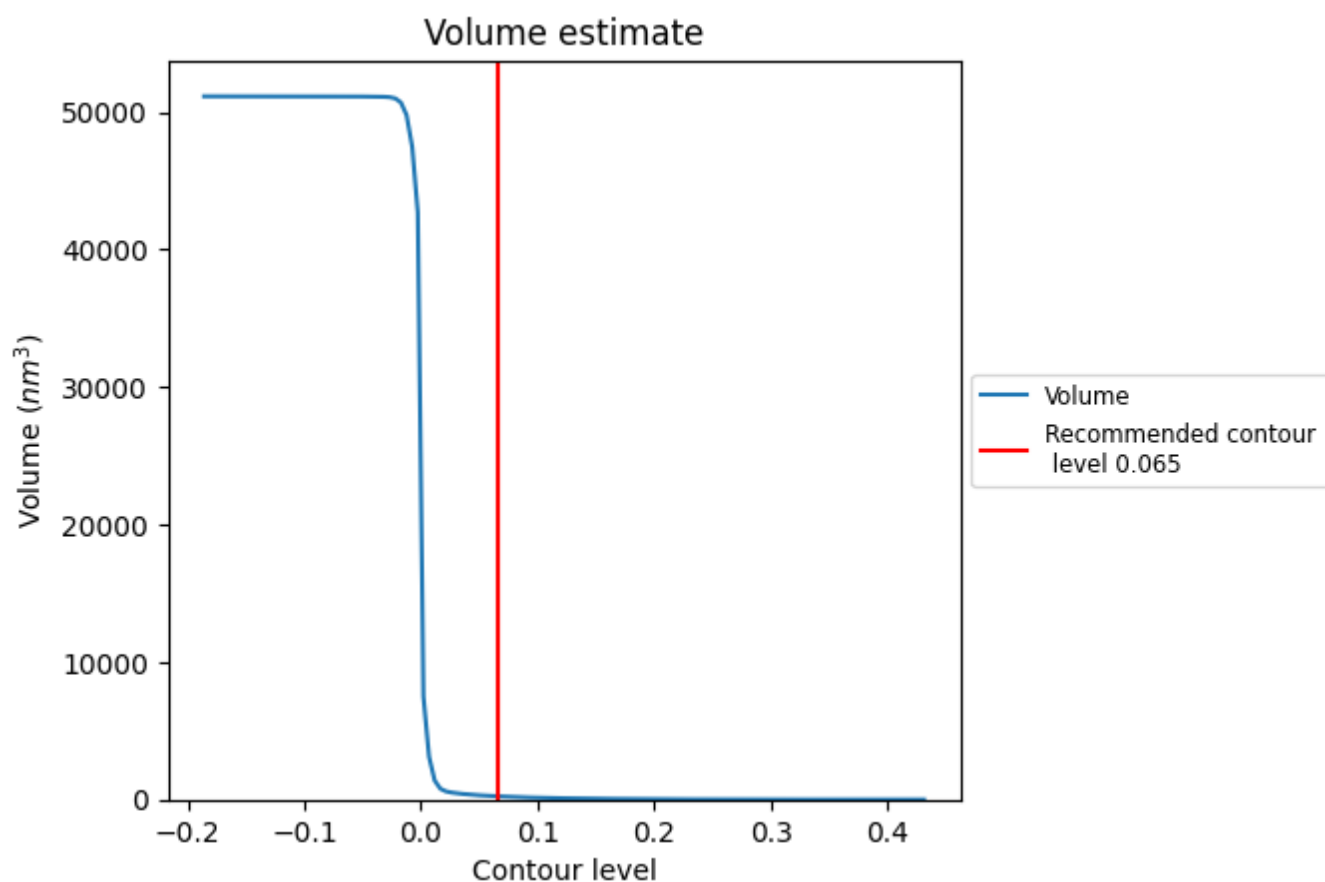
This section contains the results of statistical analysis of the map.

### 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.

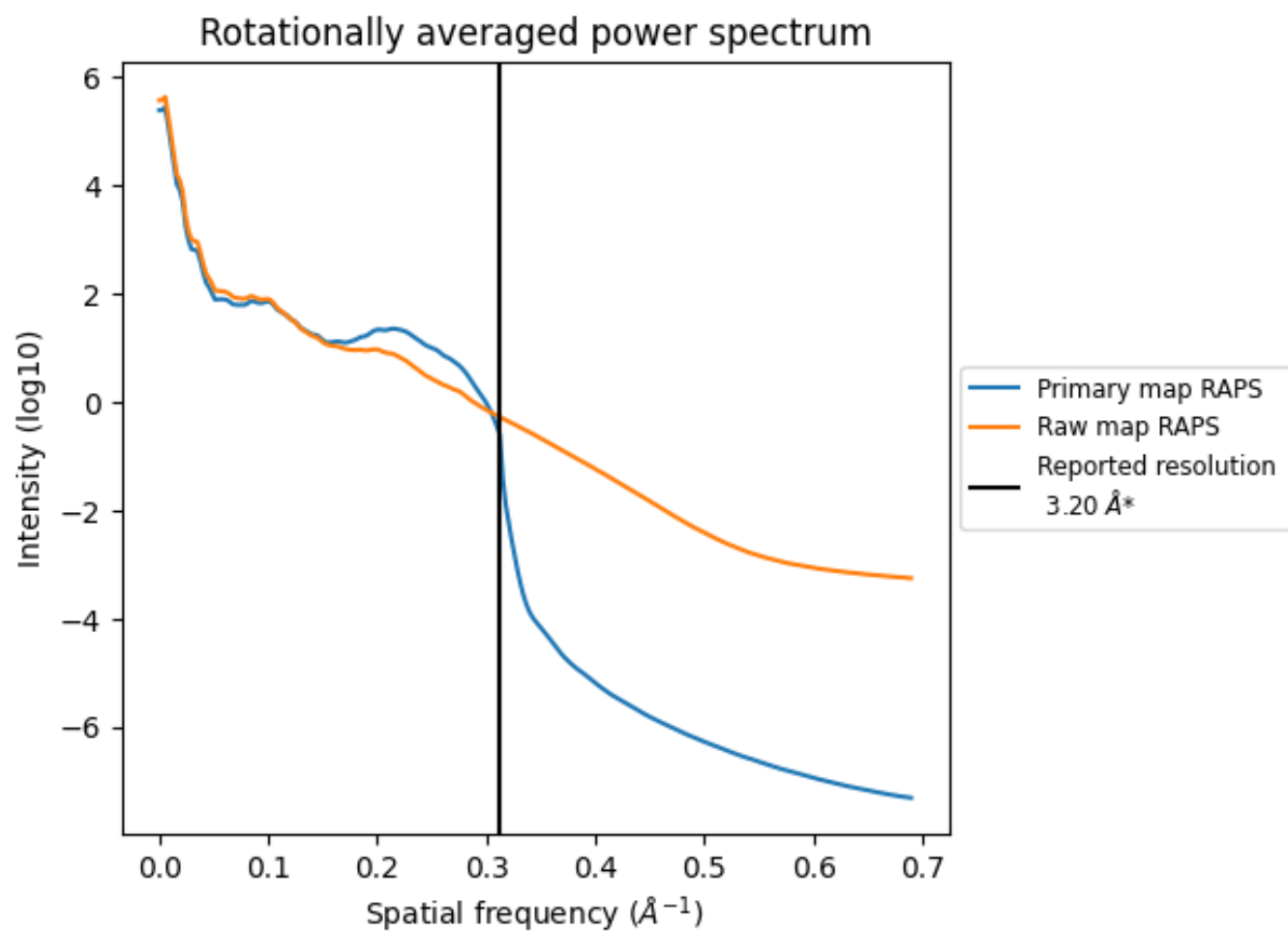
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 240 nm<sup>3</sup>; this corresponds to an approximate mass of 217 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 ⓘ

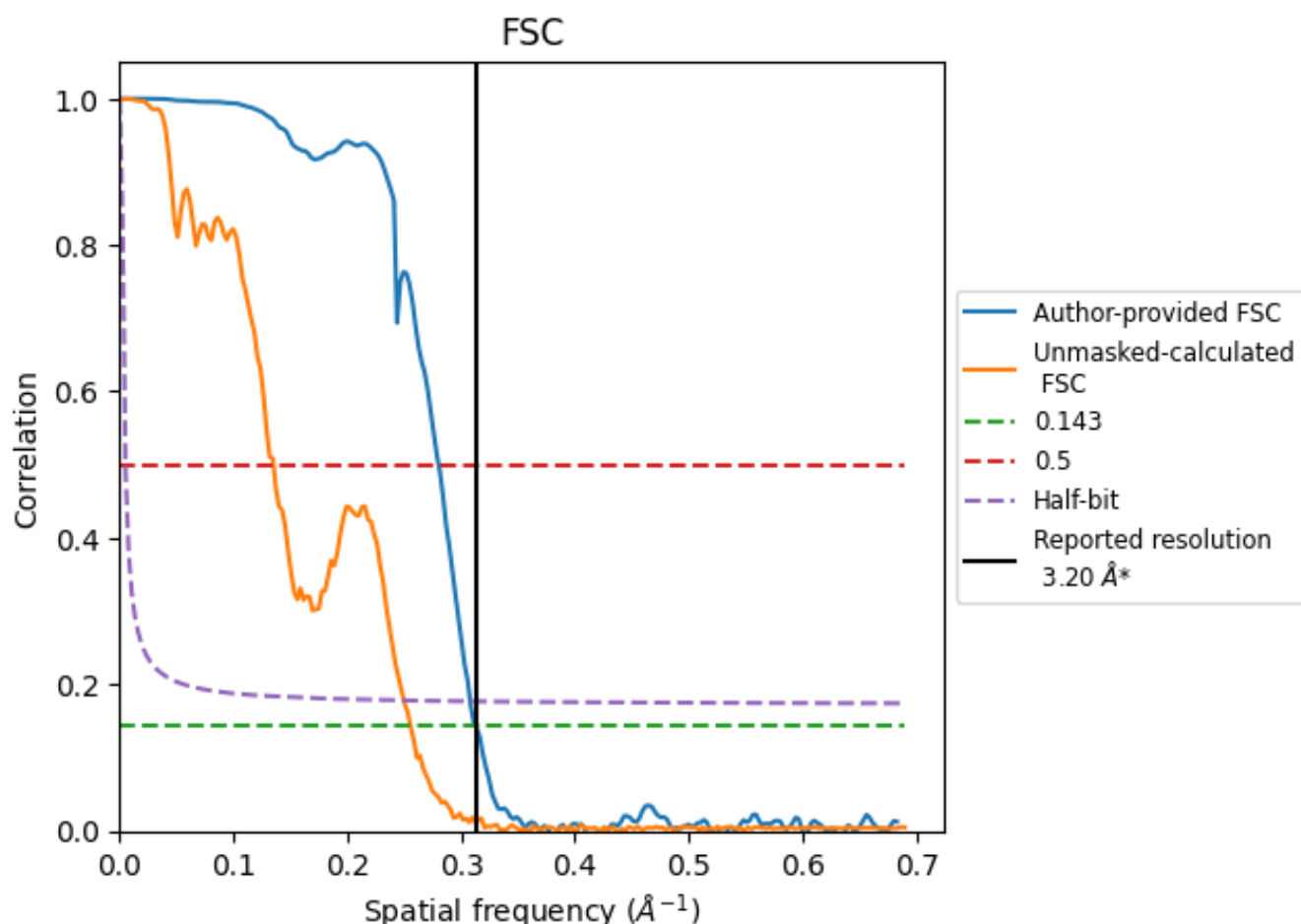


\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

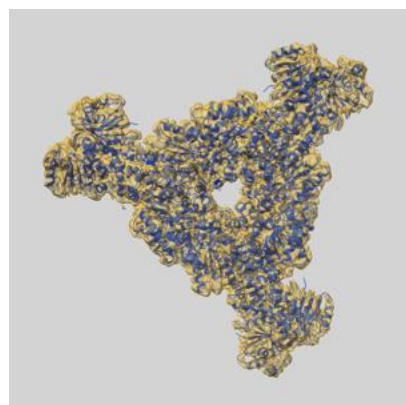
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.57	3.25
Unmasked-calculated*	3.91	7.40	4.00

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.2 by more than 10 %

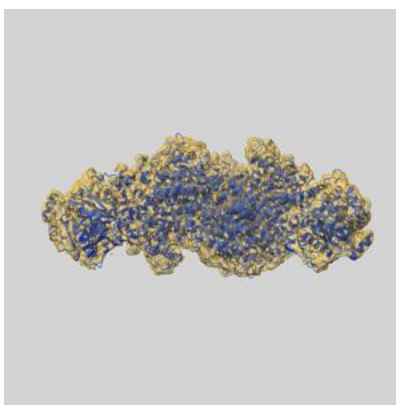
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45277 and PDB model 9C77. Per-residue inclusion information can be found in section [3](#) on page [7](#).

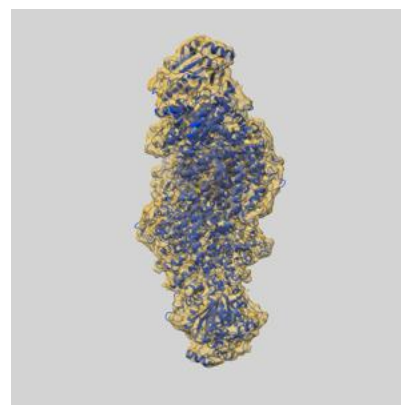
### 9.1 Map-model overlay [i](#)



X



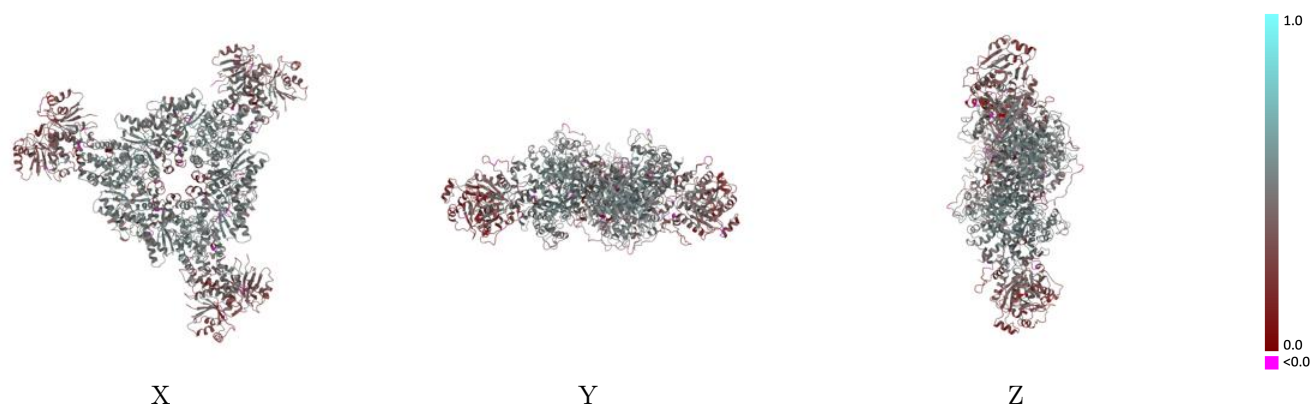
Y



Z

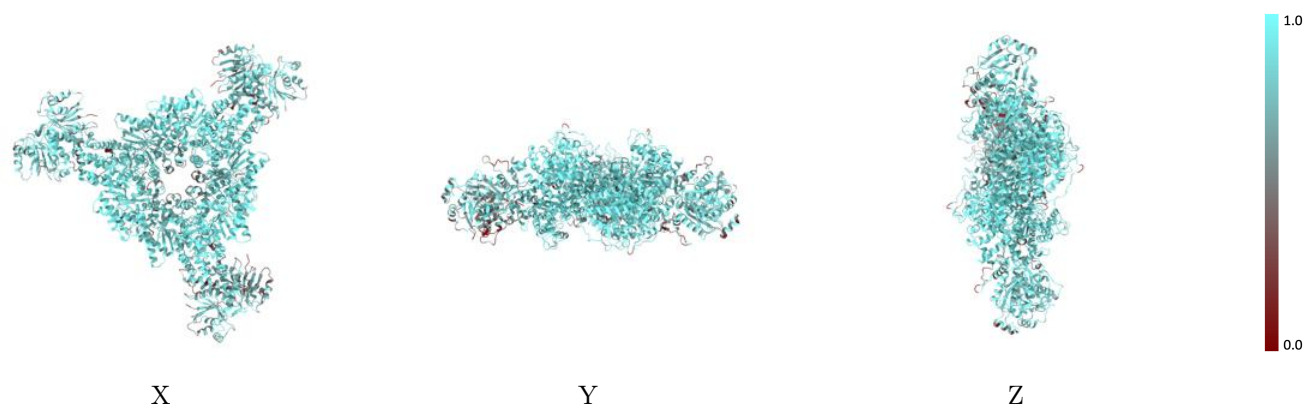
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



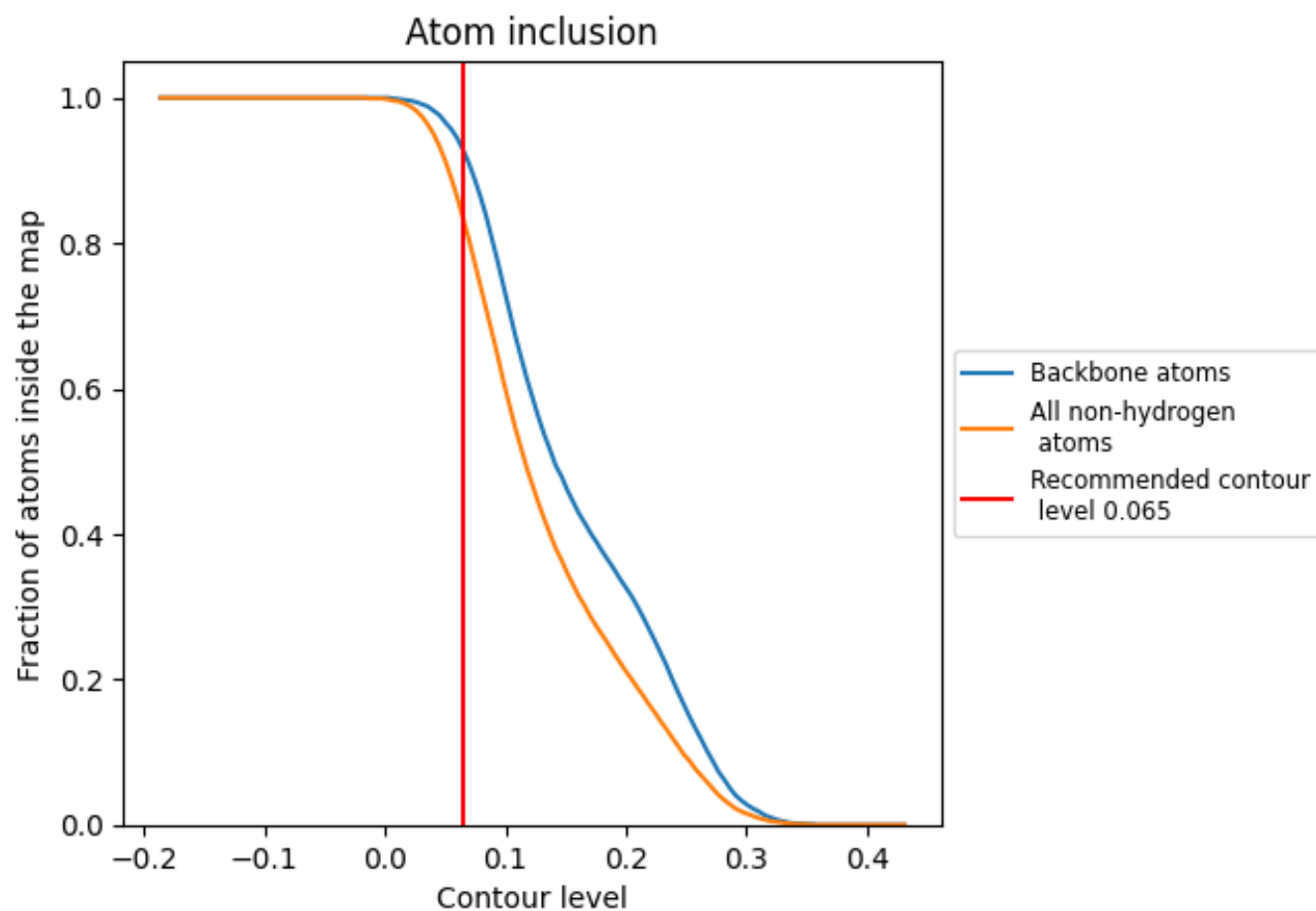
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 83% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8340</div>	<div><div></div>0.4260</div>
A	<div><div></div>0.8360</div>	<div><div></div>0.4250</div>
B	<div><div></div>0.8410</div>	<div><div></div>0.4400</div>
C	<div><div></div>0.8020</div>	<div><div></div>0.4110</div>
D	<div><div></div>0.8150</div>	<div><div></div>0.4310</div>
E	<div><div></div>0.8620</div>	<div><div></div>0.4280</div>
F	<div><div></div>0.8490</div>	<div><div></div>0.4270</div>
G	<div><div></div>0.8640</div>	<div><div></div>0.3390</div>
H	<div><div></div>0.8640</div>	<div><div></div>0.3060</div>
I	<div><div></div>0.7840</div>	<div><div></div>0.2550</div>

1.0

0.0

<0.0