



## Full wwPDB EM Validation Report ⓘ

Nov 26, 2022 – 03:02 PM EST

PDB ID : 7T0V  
EMDB ID : EMD-25582  
Title : CryoEM structure of the crosslinked Rix7 AAA-ATPase  
Authors : Kocaman, S.; Stanley, R.E.; Lo, Y.H.; Krahn, J.; Dandey, V.P.; Sobhany, M.; Petrovich, M.; Williams, J.G.; Deterding, L.J.; Borgnia, M.J.; Etigunta, S.  
Deposited on : 2021-11-30  
Resolution : 3.67 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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

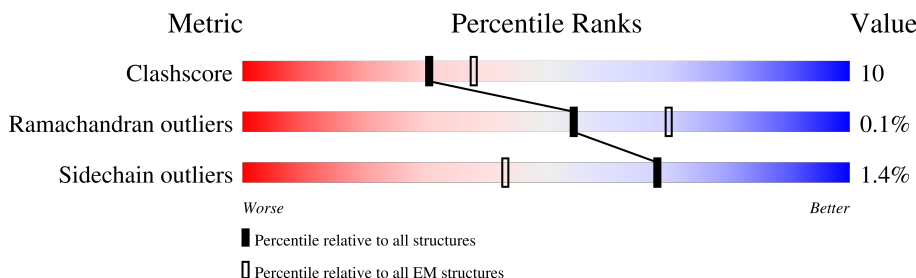
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.67 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	813	
1	B	813	
1	C	813	
1	D	813	
1	E	813	
1	F	813	
2	G	23	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26397 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 Rix7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	568	Total	C	N	O	S	0	0
			4365	2736	780	828	21		
1	B	569	Total	C	N	O	S	0	0
			4387	2750	782	834	21		
1	C	570	Total	C	N	O	S	0	0
			4385	2749	783	832	21		
1	D	570	Total	C	N	O	S	0	0
			4385	2749	783	832	21		
1	E	540	Total	C	N	O	S	0	0
			4121	2590	732	779	20		
1	F	557	Total	C	N	O	S	0	0
			4251	2663	760	808	20		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	GLN	GLU	conflict	UNP G0RZG1
A	602	GLN	GLU	conflict	UNP G0RZG1
A	803	ALA	-	expression tag	UNP G0RZG1
A	804	ALA	-	expression tag	UNP G0RZG1
A	805	ALA	-	expression tag	UNP G0RZG1
A	806	LEU	-	expression tag	UNP G0RZG1
A	807	GLU	-	expression tag	UNP G0RZG1
A	808	HIS	-	expression tag	UNP G0RZG1
A	809	HIS	-	expression tag	UNP G0RZG1
A	810	HIS	-	expression tag	UNP G0RZG1
A	811	HIS	-	expression tag	UNP G0RZG1
A	812	HIS	-	expression tag	UNP G0RZG1
A	813	HIS	-	expression tag	UNP G0RZG1
B	303	GLN	GLU	conflict	UNP G0RZG1
B	602	GLN	GLU	conflict	UNP G0RZG1
B	803	ALA	-	expression tag	UNP G0RZG1
B	804	ALA	-	expression tag	UNP G0RZG1
B	805	ALA	-	expression tag	UNP G0RZG1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	806	LEU	-	expression tag	UNP G0RZG1
B	807	GLU	-	expression tag	UNP G0RZG1
B	808	HIS	-	expression tag	UNP G0RZG1
B	809	HIS	-	expression tag	UNP G0RZG1
B	810	HIS	-	expression tag	UNP G0RZG1
B	811	HIS	-	expression tag	UNP G0RZG1
B	812	HIS	-	expression tag	UNP G0RZG1
B	813	HIS	-	expression tag	UNP G0RZG1
C	303	GLN	GLU	conflict	UNP G0RZG1
C	602	GLN	GLU	conflict	UNP G0RZG1
C	803	ALA	-	expression tag	UNP G0RZG1
C	804	ALA	-	expression tag	UNP G0RZG1
C	805	ALA	-	expression tag	UNP G0RZG1
C	806	LEU	-	expression tag	UNP G0RZG1
C	807	GLU	-	expression tag	UNP G0RZG1
C	808	HIS	-	expression tag	UNP G0RZG1
C	809	HIS	-	expression tag	UNP G0RZG1
C	810	HIS	-	expression tag	UNP G0RZG1
C	811	HIS	-	expression tag	UNP G0RZG1
C	812	HIS	-	expression tag	UNP G0RZG1
C	813	HIS	-	expression tag	UNP G0RZG1
D	303	GLN	GLU	conflict	UNP G0RZG1
D	602	GLN	GLU	conflict	UNP G0RZG1
D	803	ALA	-	expression tag	UNP G0RZG1
D	804	ALA	-	expression tag	UNP G0RZG1
D	805	ALA	-	expression tag	UNP G0RZG1
D	806	LEU	-	expression tag	UNP G0RZG1
D	807	GLU	-	expression tag	UNP G0RZG1
D	808	HIS	-	expression tag	UNP G0RZG1
D	809	HIS	-	expression tag	UNP G0RZG1
D	810	HIS	-	expression tag	UNP G0RZG1
D	811	HIS	-	expression tag	UNP G0RZG1
D	812	HIS	-	expression tag	UNP G0RZG1
D	813	HIS	-	expression tag	UNP G0RZG1
E	303	GLN	GLU	conflict	UNP G0RZG1
E	602	GLN	GLU	conflict	UNP G0RZG1
E	803	ALA	-	expression tag	UNP G0RZG1
E	804	ALA	-	expression tag	UNP G0RZG1
E	805	ALA	-	expression tag	UNP G0RZG1
E	806	LEU	-	expression tag	UNP G0RZG1
E	807	GLU	-	expression tag	UNP G0RZG1
E	808	HIS	-	expression tag	UNP G0RZG1

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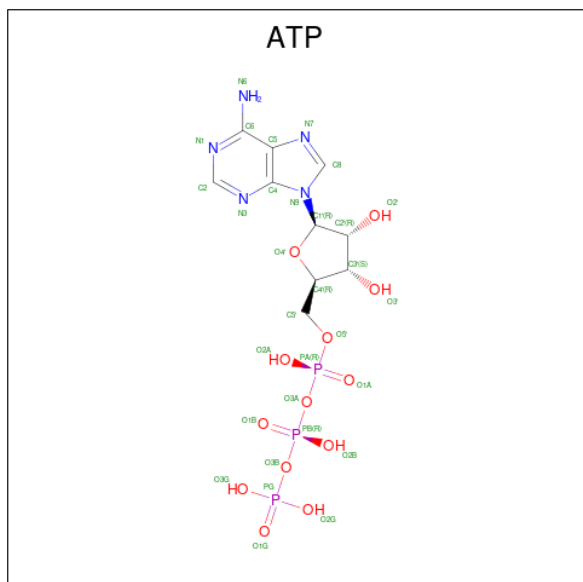
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Chain	Residue	Modelled	Actual	Comment	Reference
E	809	HIS	-	expression tag	UNP G0RZG1
E	810	HIS	-	expression tag	UNP G0RZG1
E	811	HIS	-	expression tag	UNP G0RZG1
E	812	HIS	-	expression tag	UNP G0RZG1
E	813	HIS	-	expression tag	UNP G0RZG1
F	303	GLN	GLU	conflict	UNP G0RZG1
F	602	GLN	GLU	conflict	UNP G0RZG1
F	803	ALA	-	expression tag	UNP G0RZG1
F	804	ALA	-	expression tag	UNP G0RZG1
F	805	ALA	-	expression tag	UNP G0RZG1
F	806	LEU	-	expression tag	UNP G0RZG1
F	807	GLU	-	expression tag	UNP G0RZG1
F	808	HIS	-	expression tag	UNP G0RZG1
F	809	HIS	-	expression tag	UNP G0RZG1
F	810	HIS	-	expression tag	UNP G0RZG1
F	811	HIS	-	expression tag	UNP G0RZG1
F	812	HIS	-	expression tag	UNP G0RZG1
F	813	HIS	-	expression tag	UNP G0RZG1

- Molecule 2 is a protein called polyvaline.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	23	Total	C	N	O	0	0
			161	115	23	23		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

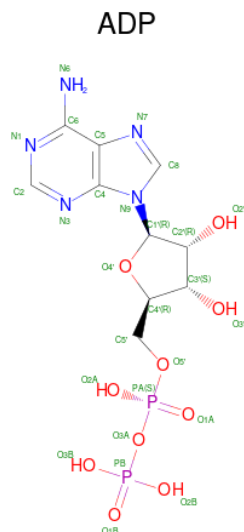


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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	2	Total	Mg	0
			2	2	
4	B	2	Total	Mg	0
			2	2	
4	C	2	Total	Mg	0
			2	2	
4	D	2	Total	Mg	0
			2	2	
4	E	1	Total	Mg	0
			1	1	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



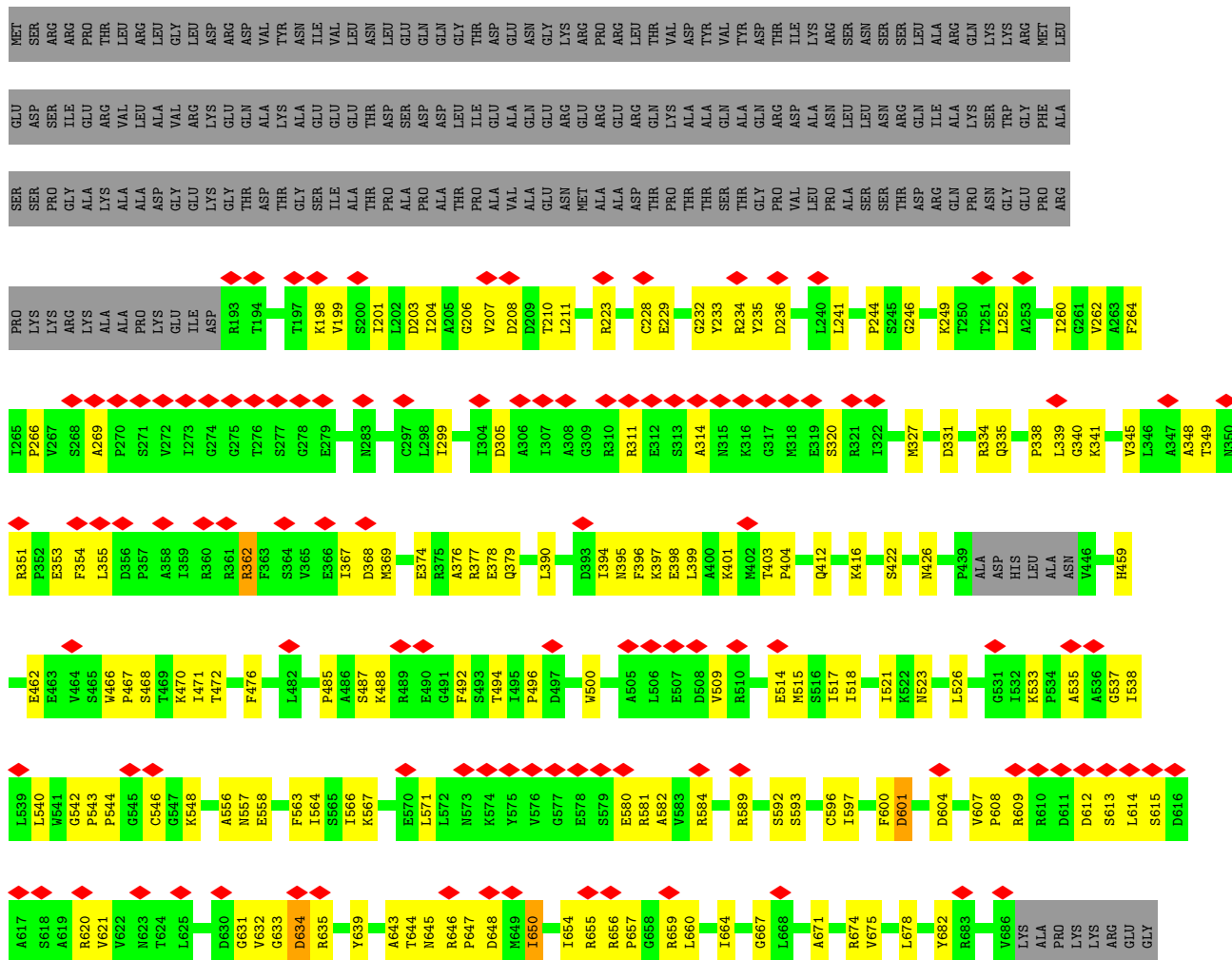
Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total 27	C 10	N 5	O 10	P 2	0
5	F	1	Total 27	C 10	N 5	O 10	P 2	0

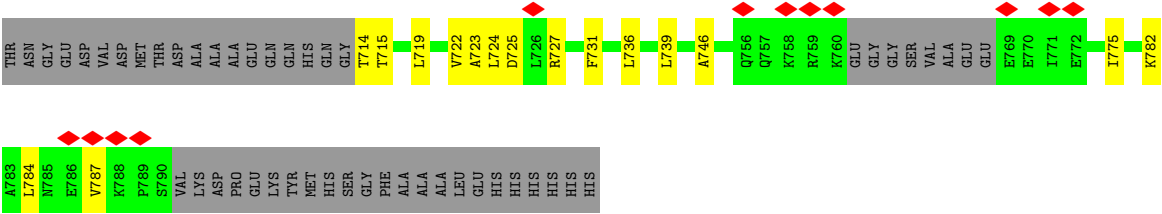




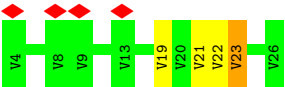
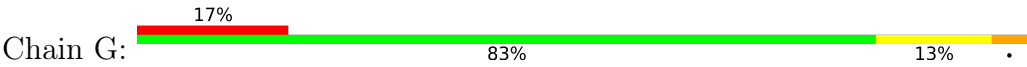


- Molecule 1: Rix7





• Molecule 2: polyvaline



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	201000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.053	Depositor
Minimum map value	-1.124	Depositor
Average map value	0.048	Depositor
Map value standard deviation	0.158	Depositor
Recommended contour level	0.252	Depositor
Map size (Å)	119.03535, 152.15822, 157.33368	wwPDB
Map dimensions	115, 147, 152	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03509, 1.03509, 1.03509	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: ATP, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/4436	0.50	0/5998
1	B	0.28	0/4458	0.51	0/6025
1	C	0.29	0/4456	0.51	0/6023
1	D	0.28	0/4456	0.50	0/6023
1	E	0.27	0/4186	0.54	1/5664 (0.0%)
1	F	0.25	0/4318	0.54	0/5843
2	G	0.23	0/160	0.42	0/227
All	All	0.27	0/26470	0.51	1/35803 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	577	GLY	N-CA-C	5.26	126.26	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4365	0	4414	83	0
1	B	4387	0	4447	84	0
1	C	4385	0	4444	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4385	0	4443	80	0
1	E	4121	0	4178	111	0
1	F	4251	0	4289	129	0
2	G	161	0	206	4	0
3	A	62	0	24	10	0
3	B	62	0	24	10	0
3	C	62	0	24	6	0
3	D	62	0	24	7	0
3	E	31	0	12	6	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
5	E	27	0	12	1	0
5	F	27	0	12	1	0
All	All	26397	0	26553	517	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 10.

All (517) 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:F:535:ALA:HB2	1:F:633:GLY:HA3	1.60	0.82
1:E:669:PRO:HB3	1:E:673:ASP:HB3	1.63	0.81
1:F:674:ARG:NH2	1:F:723:ALA:O	2.19	0.76
1:E:619:ALA:O	1:E:623:ASN:ND2	2.19	0.75
1:F:517:ILE:HG13	1:F:538:ILE:HD13	1.67	0.75
1:E:296:PRO:HD3	1:E:341:LYS:HG2	1.67	0.74
1:E:610:ARG:HA	1:E:614:LEU:HD22	1.68	0.74
1:F:654:ILE:HG23	1:F:660:LEU:HD12	1.69	0.73
1:E:573:ASN:HD22	1:E:578:GLU:HB2	1.54	0.71
1:E:210:THR:HG23	1:E:367:ILE:HG21	1.73	0.71
1:D:416:LYS:NZ	1:E:236:ASP:O	2.21	0.71
1:D:656:ARG:NH1	1:D:657:PRO:O	2.23	0.71
1:F:399:LEU:HD21	1:F:476:PHE:HB3	1.72	0.70
1:E:505:ALA:HB2	1:E:676:LYS:HD2	1.70	0.70
1:A:562:ASN:HD22	1:A:593:SER:HB3	1.56	0.70
1:F:496:PRO:O	1:F:557:ASN:ND2	2.24	0.70
1:D:385:THR:HB	1:D:390:LEU:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:601:ASP:OD1	1:F:601:ASP:N	2.24	0.69
1:E:331:ASP:OD1	1:E:362:ARG:NH1	2.26	0.69
1:F:514:GLU:HA	1:F:518:ILE:HB	1.74	0.68
1:B:203:ASP:OD1	1:B:386:ARG:NH2	2.26	0.68
1:C:311:ARG:NH1	1:C:356:ASP:OD2	2.26	0.68
1:D:409:SER:OG	1:E:361:ARG:NH1	2.27	0.68
1:D:617:ALA:HB2	2:G:23:VAL:HG11	1.75	0.68
1:A:272:VAL:O	1:A:283:ASN:ND2	2.26	0.67
1:F:353:GLU:HA	1:F:581:ARG:HE	1.59	0.67
1:F:398:GLU:HA	1:F:401:LYS:HE2	1.77	0.67
1:F:656:ARG:NH1	1:F:657:PRO:O	2.28	0.67
1:D:281:GLU:OE1	1:D:285:ARG:NH2	2.27	0.67
1:C:203:ASP:OD1	1:C:386:ARG:NH2	2.28	0.66
1:F:236:ASP:OD2	1:F:334:ARG:NH1	2.29	0.66
1:D:378:GLU:OE2	1:D:382:ARG:NE	2.24	0.66
1:E:656:ARG:NH1	1:E:657:PRO:O	2.28	0.66
1:A:645:ASN:OD1	1:B:610:ARG:NH2	2.28	0.66
1:C:404:PRO:HB3	1:C:595:PRO:HD2	1.77	0.66
1:F:727:ARG:HE	1:F:784:LEU:HB3	1.61	0.66
1:F:204:ILE:HG12	1:F:252:LEU:HD13	1.77	0.66
1:F:509:VAL:HG13	1:F:664:ILE:HG21	1.78	0.66
1:B:311:ARG:NH1	1:B:356:ASP:OD2	2.29	0.65
1:C:281:GLU:OE2	1:C:321:ARG:NH1	2.30	0.65
1:F:260:ILE:HG22	1:F:262:VAL:HG23	1.77	0.65
1:D:311:ARG:NH1	1:D:356:ASP:OD2	2.29	0.65
1:D:237:ASN:OD1	1:D:364:SER:OG	2.13	0.65
3:D:902:ATP:O2G	1:E:362:ARG:NH2	2.29	0.65
1:B:248:GLY:N	3:B:902:ATP:O2B	2.30	0.65
1:B:514:GLU:HA	1:B:518:ILE:HB	1.78	0.65
1:E:430:LEU:HD22	1:E:466:TRP:HE1	1.62	0.65
3:B:902:ATP:O3'	1:C:334:ARG:NH2	2.29	0.65
1:D:390:LEU:HB3	1:D:394:ILE:HD12	1.78	0.65
3:A:902:ATP:O2G	1:B:362:ARG:NH2	2.30	0.64
1:C:617:ALA:HB2	2:G:21:VAL:HG11	1.80	0.64
1:D:375:ARG:NH1	1:D:378:GLU:OE1	2.30	0.64
1:C:656:ARG:NH1	1:C:657:PRO:O	2.31	0.64
1:F:229:GLU:HB2	1:F:340:GLY:HA3	1.80	0.64
1:F:338:PRO:HD2	1:F:341:LYS:HB2	1.80	0.64
1:A:398:GLU:HA	1:A:401:LYS:HE2	1.80	0.64
1:D:680:THR:O	1:D:684:ASN:ND2	2.28	0.64
1:D:404:PRO:HB2	1:D:562:ASN:HD21	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:374:GLU:HG2	1:F:377:ARG:HH22	1.64	0.63
1:E:333:ILE:O	1:E:337:THR:OG1	2.10	0.63
1:A:528:THR:OG1	1:A:635:ARG:NH2	2.32	0.63
1:A:219:TRP:HD1	1:A:260:ILE:HG12	1.64	0.63
1:D:213:ARG:NH2	1:D:217:GLU:OE2	2.31	0.63
1:A:541:TRP:HB2	1:A:647:PRO:HG3	1.80	0.63
1:C:310:ARG:NH1	1:C:312:GLU:OE2	2.32	0.63
1:D:489:ARG:HH22	1:E:364:SER:HA	1.63	0.63
1:F:338:PRO:HB2	1:F:341:LYS:HD3	1.79	0.63
1:C:237:ASN:OD1	1:C:364:SER:OG	2.15	0.63
1:D:296:PRO:HD3	1:D:341:LYS:HG2	1.81	0.63
1:D:635:ARG:NH2	1:D:658:GLY:O	2.32	0.62
1:B:205:ALA:HB1	1:B:379:GLN:HG2	1.80	0.62
1:E:390:LEU:HB3	1:E:394:ILE:HD12	1.80	0.62
1:D:610:ARG:HA	1:D:614:LEU:HD22	1.80	0.62
1:D:645:ASN:HB3	1:D:797:TYR:HE1	1.65	0.62
1:E:453:TRP:HB3	1:F:201:ILE:HD13	1.81	0.62
1:E:412:GLN:NE2	3:E:902:ATP:O3'	2.33	0.61
1:F:232:GLY:HA2	1:F:339:LEU:HD21	1.82	0.61
1:E:248:GLY:N	3:E:902:ATP:O2B	2.29	0.61
1:F:542:GLY:O	1:F:645:ASN:ND2	2.33	0.61
1:A:327:MET:O	1:A:362:ARG:NH1	2.34	0.61
1:C:304:ILE:HG23	1:C:355:LEU:HD21	1.83	0.60
1:E:205:ALA:O	3:E:902:ATP:N6	2.27	0.60
1:E:408:GLY:HA3	3:E:902:ATP:C8	2.36	0.60
1:A:195:PRO:HB2	1:A:258:GLY:HA2	1.81	0.60
1:F:368:ASP:OD2	1:F:592:SER:OG	2.18	0.60
1:C:674:ARG:HG2	1:C:736:LEU:HD11	1.82	0.60
1:F:714:THR:HG22	1:F:715:THR:HG23	1.84	0.60
1:A:450:GLN:OE1	1:B:379:GLN:NE2	2.36	0.59
1:E:434:ALA:HB1	1:E:455:LEU:HB3	1.82	0.59
1:E:298:LEU:HD11	1:E:346:LEU:HG	1.84	0.59
1:E:361:ARG:HH11	1:E:361:ARG:HG3	1.67	0.59
1:A:533:LYS:HG2	1:A:634:ASP:HB3	1.85	0.59
1:B:331:ASP:OD1	1:B:362:ARG:NH1	2.35	0.59
1:D:566:ILE:HD13	1:D:600:PHE:CE1	2.37	0.59
1:E:614:LEU:HD23	1:E:619:ALA:HB2	1.84	0.59
1:D:269:ALA:HB1	1:D:307:ILE:HG23	1.85	0.59
1:E:412:GLN:OE1	1:F:334:ARG:NH1	2.32	0.59
1:B:390:LEU:HB3	1:B:394:ILE:HD12	1.84	0.58
1:F:390:LEU:HB3	1:F:394:ILE:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:746:ALA:HB1	1:F:782:LYS:HD2	1.85	0.58
1:A:390:LEU:HB3	1:A:394:ILE:HD12	1.86	0.58
1:A:423:PHE:HA	1:A:426:ASN:HD22	1.67	0.58
1:F:311:ARG:HA	1:F:314:ALA:HB3	1.86	0.58
3:D:901:ATP:O2G	1:E:659:ARG:NH2	2.37	0.57
1:C:450:GLN:NE2	1:D:204:ILE:O	2.37	0.57
1:D:489:ARG:NH1	1:E:366:GLU:OE2	2.36	0.57
1:A:727:ARG:HE	1:A:784:LEU:HB3	1.70	0.57
1:B:738:ASN:HB2	1:C:657:PRO:HB3	1.87	0.57
1:C:269:ALA:HB1	1:C:307:ILE:HG23	1.85	0.57
1:B:674:ARG:NH1	1:B:723:ALA:O	2.38	0.57
1:C:248:GLY:N	3:C:902:ATP:O2B	2.37	0.57
1:A:610:ARG:HA	1:A:614:LEU:HD22	1.86	0.57
1:C:674:ARG:NH1	1:C:723:ALA:O	2.37	0.57
1:A:408:GLY:HA3	3:A:902:ATP:N7	2.20	0.57
1:F:580:GLU:HG2	1:F:620:ARG:HB3	1.87	0.56
1:C:289:ASP:OD1	1:C:332:ARG:NH2	2.38	0.56
1:E:449:PRO:HG2	1:F:208:ASP:HB3	1.86	0.56
1:D:674:ARG:HG2	1:D:736:LEU:HD11	1.86	0.56
1:C:251:THR:HG21	3:C:902:ATP:H2'	1.88	0.56
1:C:338:PRO:O	1:C:340:GLY:N	2.39	0.56
1:F:331:ASP:OD2	1:F:335:GLN:NE2	2.39	0.56
1:B:385:THR:HB	1:B:390:LEU:HD11	1.87	0.56
1:E:203:ASP:OD1	1:E:386:ARG:NH2	2.37	0.56
1:E:251:THR:HG21	3:E:902:ATP:H2'	1.88	0.56
1:F:556:ALA:HA	1:F:597:ILE:HD12	1.88	0.56
1:C:635:ARG:HB2	1:C:638:ILE:HD12	1.88	0.55
1:F:650:ILE:O	1:F:655:ARG:NH2	2.39	0.55
1:A:546:CYS:N	3:A:901:ATP:O2B	2.39	0.55
1:A:614:LEU:HD23	1:A:619:ALA:HB2	1.88	0.55
1:E:214:LEU:HD13	1:E:256:ILE:HD11	1.88	0.55
1:F:311:ARG:NH1	1:F:320:SER:O	2.40	0.55
1:F:580:GLU:OE2	1:F:620:ARG:NH2	2.31	0.55
1:E:670:SER:O	1:E:674:ARG:NH1	2.39	0.55
1:F:327:MET:O	1:F:362:ARG:NH2	2.40	0.55
1:A:228:CYS:O	1:A:232:GLY:N	2.40	0.55
1:B:416:LYS:NZ	1:C:236:ASP:O	2.34	0.55
1:B:733:GLY:HA3	3:B:901:ATP:C8	2.42	0.55
1:C:681:LEU:O	1:C:685:THR:OG1	2.21	0.55
1:F:647:PRO:HA	1:F:650:ILE:HD11	1.88	0.55
1:E:198:LYS:HB3	1:F:335:GLN:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:659:ARG:O	1:F:660:LEU:HD23	2.06	0.55
1:C:541:TRP:CE3	1:C:647:PRO:HG3	2.42	0.55
1:D:270:PRO:HB3	1:E:281:GLU:HG2	1.89	0.55
1:F:376:ALA:HA	1:F:379:GLN:OE1	2.07	0.55
1:E:540:LEU:HD23	1:E:664:ILE:HB	1.88	0.55
1:E:571:LEU:HD22	1:E:582:ALA:HB1	1.89	0.55
1:E:747:CYS:SG	1:E:775:ILE:HG12	2.46	0.55
1:A:449:PRO:HG2	1:B:208:ASP:HB3	1.88	0.54
1:F:731:PHE:HE2	1:F:739:LEU:HD22	1.72	0.54
3:B:901:ATP:O2G	1:C:659:ARG:NH2	2.33	0.54
1:F:634:ASP:N	1:F:634:ASP:OD1	2.39	0.54
1:D:205:ALA:O	3:D:902:ATP:N6	2.27	0.54
1:F:234:ARG:NH1	1:F:334:ARG:O	2.34	0.54
1:F:631:GLY:O	1:F:635:ARG:NE	2.40	0.54
1:E:537:GLY:HA3	1:E:640:VAL:O	2.08	0.54
1:C:409:SER:OG	1:D:361:ARG:NH1	2.41	0.54
1:E:573:ASN:ND2	1:E:578:GLU:HB2	2.22	0.54
1:A:540:LEU:HD23	1:A:664:ILE:HB	1.90	0.54
1:E:245:SER:OG	3:E:902:ATP:O1G	2.25	0.53
1:D:566:ILE:HD13	1:D:600:PHE:HE1	1.71	0.53
1:C:547:GLY:N	3:C:901:ATP:O2B	2.31	0.53
1:C:714:THR:OG1	1:C:775:ILE:O	2.27	0.53
1:C:738:ASN:HB2	1:D:657:PRO:HB3	1.89	0.53
1:E:242:HIS:ND1	1:E:352:PRO:HG3	2.23	0.53
1:F:543:PRO:HG2	1:F:546:CYS:SG	2.49	0.53
1:F:241:LEU:HD23	1:F:367:ILE:HB	1.90	0.53
1:F:374:GLU:HG2	1:F:377:ARG:NH2	2.23	0.53
1:F:338:PRO:O	1:F:340:GLY:N	2.40	0.53
1:B:576:VAL:HG22	2:G:19:VAL:HG22	1.90	0.53
1:C:610:ARG:NH1	1:C:623:ASN:OD1	2.41	0.53
1:E:543:PRO:HG2	1:E:546:CYS:SG	2.49	0.53
1:B:449:PRO:HG2	1:C:208:ASP:HB3	1.91	0.52
1:B:541:TRP:CE3	1:B:647:PRO:HG3	2.44	0.52
1:E:548:LYS:NZ	1:E:645:ASN:OD1	2.42	0.52
1:E:556:ALA:HA	1:E:597:ILE:HD12	1.90	0.52
1:C:234:ARG:NH2	1:C:337:THR:O	2.31	0.52
1:E:752:TYR:HE2	1:F:515:MET:HG3	1.74	0.52
1:D:756:GLN:HG2	1:D:759:ARG:HH21	1.74	0.52
1:F:353:GLU:HG2	1:F:581:ARG:HG2	1.91	0.52
1:C:406:TYR:CE1	1:C:485:PRO:HG3	2.44	0.52
1:D:500:TRP:CD1	1:D:558:GLU:HG3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:647:PRO:HG2	1:D:800:SER:HB3	1.91	0.52
1:D:404:PRO:HB3	1:D:595:PRO:HD2	1.91	0.52
1:D:514:GLU:HA	1:D:518:ILE:HB	1.91	0.52
1:D:793:ASP:N	1:D:793:ASP:OD1	2.43	0.52
1:F:650:ILE:HD12	1:F:655:ARG:HD3	1.91	0.52
1:E:514:GLU:HA	1:E:518:ILE:HB	1.91	0.52
1:F:722:VAL:HG23	1:F:784:LEU:HD21	1.91	0.52
1:D:316:LYS:HG2	1:D:317:GLY:H	1.75	0.51
1:D:459:HIS:O	1:D:461:ASP:N	2.43	0.51
1:E:204:ILE:HG12	1:E:252:LEU:HD13	1.92	0.51
1:E:616:ASP:O	1:E:620:ARG:NH2	2.43	0.51
1:F:714:THR:OG1	1:F:775:ILE:O	2.27	0.51
1:D:248:GLY:N	3:D:902:ATP:O2B	2.44	0.51
1:C:210:THR:HG23	1:C:367:ILE:HG21	1.92	0.51
1:C:546:CYS:N	3:C:901:ATP:O2B	2.44	0.51
1:E:590:ALA:HB2	1:E:598:LEU:HD21	1.92	0.51
1:A:230:LYS:HD3	1:F:468:SER:HB3	1.92	0.51
1:C:268:SER:HG	1:C:271:SER:HG	1.55	0.51
1:C:426:ASN:HB3	1:C:466:TRP:HD1	1.76	0.51
1:F:426:ASN:ND2	1:F:467:PRO:O	2.44	0.51
1:F:492:PHE:HB2	1:F:589:ARG:HH21	1.76	0.51
1:A:738:ASN:HB2	1:B:657:PRO:HB3	1.91	0.51
1:C:607:VAL:HA	1:C:622:VAL:HG22	1.93	0.51
1:D:738:ASN:HB2	1:E:657:PRO:HB3	1.92	0.51
1:E:236:ASP:OD2	1:E:334:ARG:HA	2.10	0.51
1:B:540:LEU:HD23	1:B:664:ILE:HB	1.92	0.51
1:E:538:ILE:HG13	1:E:641:ILE:HG23	1.92	0.51
1:D:457:GLU:HG3	1:D:460:ARG:HH21	1.76	0.50
1:E:496:PRO:O	1:E:557:ASN:ND2	2.40	0.50
1:E:524:PRO:O	1:E:528:THR:OG1	2.15	0.50
1:A:608:PRO:HG2	1:A:614:LEU:HD11	1.92	0.50
1:E:571:LEU:HD13	1:E:583:VAL:HG22	1.92	0.50
1:F:305:ASP:HB3	1:F:355:LEU:HD12	1.91	0.50
1:A:543:PRO:HG2	1:A:546:CYS:SG	2.52	0.50
1:B:399:LEU:HA	1:B:402:MET:HG2	1.94	0.50
1:D:540:LEU:HD23	1:D:664:ILE:HB	1.94	0.50
1:E:398:GLU:HA	1:E:401:LYS:HE2	1.93	0.50
1:A:247:CYS:N	3:A:902:ATP:O2B	2.45	0.50
1:F:566:ILE:HD13	1:F:571:LEU:HD11	1.92	0.50
1:A:205:ALA:O	3:A:902:ATP:N6	2.37	0.50
1:D:399:LEU:HD21	1:D:476:PHE:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:500:TRP:CD1	1:E:558:GLU:HG3	2.47	0.50
1:D:644:THR:HG21	1:D:650:ILE:HD11	1.92	0.50
1:E:644:THR:HG21	1:E:650:ILE:HD13	1.94	0.50
1:F:787:VAL:HG12	1:F:787:VAL:O	2.11	0.50
1:A:214:LEU:HD13	1:A:256:ILE:HD11	1.93	0.50
1:E:659:ARG:O	1:E:661:GLY:N	2.42	0.50
1:F:459:HIS:HB3	1:F:462:GLU:HB2	1.94	0.50
1:E:540:LEU:O	1:E:643:ALA:HA	2.12	0.49
1:F:523:ASN:HB3	1:F:526:LEU:HB3	1.94	0.49
1:F:644:THR:HG21	1:F:650:ILE:HD13	1.93	0.49
1:E:311:ARG:HA	1:E:314:ALA:HB3	1.94	0.49
1:E:714:THR:OG1	1:E:775:ILE:O	2.19	0.49
1:E:377:ARG:NH2	1:E:400:ALA:O	2.31	0.49
1:A:733:GLY:HA3	3:A:901:ATP:C8	2.48	0.49
1:F:593:SER:O	1:F:596:CYS:HB2	2.11	0.49
1:A:478:LYS:HE3	1:A:482:LEU:HD11	1.94	0.49
1:A:562:ASN:ND2	1:A:593:SER:HB3	2.27	0.49
1:B:426:ASN:HD22	1:B:467:PRO:HD2	1.78	0.49
1:A:746:ALA:HB1	1:A:782:LYS:HD2	1.95	0.49
1:C:540:LEU:HD23	1:C:664:ILE:HB	1.95	0.49
1:E:210:THR:HG23	1:E:367:ILE:HD13	1.95	0.49
1:A:754:GLN:HG3	1:A:758:LYS:HE2	1.94	0.49
1:C:256:ILE:HD11	1:C:346:LEU:HD11	1.94	0.49
1:C:485:PRO:HD2	1:C:488:LYS:HB2	1.95	0.49
1:D:371:MET:HG2	1:D:407:VAL:HG12	1.95	0.49
1:E:777:MET:O	1:E:781:GLU:HG3	2.13	0.49
1:E:386:ARG:NH1	1:E:387:ASP:OD1	2.46	0.49
1:F:671:ALA:O	1:F:675:VAL:HG23	2.12	0.48
1:B:648:ASP:N	1:B:648:ASP:OD1	2.46	0.48
1:C:794:PRO:O	1:C:798:MET:N	2.46	0.48
1:B:269:ALA:HB1	1:B:307:ILE:HG23	1.94	0.48
1:C:534:PRO:HG2	1:C:636:SER:HB2	1.94	0.48
1:F:362:ARG:O	1:F:362:ARG:HG3	2.13	0.48
1:F:546:CYS:HB3	1:F:667:GLY:HA2	1.94	0.48
1:D:426:ASN:HB3	1:D:466:TRP:HD1	1.79	0.48
1:A:233:TYR:OH	1:F:416:LYS:HG2	2.14	0.48
1:A:491:GLY:HA3	1:A:589:ARG:HH11	1.78	0.48
1:C:453:TRP:HB3	1:D:201:ILE:HG13	1.95	0.48
1:C:566:ILE:HD13	1:C:600:PHE:CE1	2.49	0.48
1:E:388:LEU:HD21	1:F:233:TYR:HD1	1.78	0.48
1:A:349:THR:HG21	1:A:355:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD12	1:B:215:LEU:HD11	1.95	0.48
1:E:361:ARG:NH1	1:E:361:ARG:HG3	2.28	0.48
1:F:567:LYS:HG3	1:F:601:ASP:HB2	1.96	0.48
1:B:538:ILE:HG12	1:B:662:THR:OG1	2.14	0.48
1:F:353:GLU:OE2	1:F:582:ALA:HA	2.13	0.48
1:F:422:SER:HB2	1:F:471:ILE:HG12	1.94	0.48
1:F:671:ALA:HB1	1:F:724:LEU:HD23	1.95	0.48
1:D:543:PRO:HG2	1:D:546:CYS:SG	2.54	0.48
1:F:492:PHE:HA	1:F:564:ILE:HG12	1.96	0.48
1:B:207:VAL:HG23	1:B:211:LEU:HG	1.96	0.47
1:B:245:SER:OG	3:B:902:ATP:O1G	2.20	0.47
1:B:299:ILE:O	1:B:346:LEU:N	2.42	0.47
1:B:299:ILE:HD12	1:B:345:VAL:HG22	1.96	0.47
1:E:323:VAL:O	1:E:327:MET:HG3	2.14	0.47
1:A:219:TRP:CD1	1:A:260:ILE:HG12	2.48	0.47
1:F:228:CYS:O	1:F:232:GLY:N	2.45	0.47
1:B:605:ALA:HB2	1:C:623:ASN:HD22	1.80	0.47
1:D:509:VAL:HG13	1:D:664:ILE:HG21	1.96	0.47
1:E:733:GLY:HA3	5:E:901:ADP:C8	2.49	0.47
1:F:540:LEU:O	1:F:643:ALA:HA	2.15	0.47
1:B:304:ILE:HG23	1:B:355:LEU:HD21	1.95	0.47
1:E:519:GLY:O	1:E:521:ILE:N	2.42	0.47
1:F:646:ARG:O	1:F:648:ASP:N	2.44	0.47
3:A:901:ATP:O3G	1:B:659:ARG:NH1	2.36	0.47
1:D:682:TYR:CZ	1:D:686:VAL:HG11	2.49	0.47
1:B:644:THR:HG21	1:B:650:ILE:HD11	1.97	0.47
1:A:248:GLY:N	3:A:902:ATP:O2B	2.44	0.47
1:B:311:ARG:HA	1:B:314:ALA:HB3	1.97	0.47
1:B:409:SER:OG	1:C:361:ARG:NH1	2.48	0.47
1:D:657:PRO:HA	1:D:661:GLY:HA3	1.96	0.47
1:A:514:GLU:HA	1:A:518:ILE:HB	1.98	0.46
1:E:518:ILE:HD11	1:E:555:VAL:HG22	1.97	0.46
1:F:656:ARG:HE	1:F:659:ARG:CZ	2.28	0.46
1:F:305:ASP:HB2	1:F:354:PHE:HB2	1.97	0.46
1:D:530:VAL:HG23	1:D:532:ILE:HG13	1.97	0.46
1:E:228:CYS:HA	1:E:231:MET:HG2	1.97	0.46
1:F:207:VAL:HG23	1:F:211:LEU:HG	1.97	0.46
1:F:521:ILE:HG12	1:F:639:TYR:CE1	2.51	0.46
1:F:556:ALA:HB1	1:F:563:PHE:HB2	1.97	0.46
1:B:454:LEU:HD11	1:C:202:LEU:HD21	1.97	0.46
1:A:218:VAL:HG22	1:A:239:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:PRO:HG2	1:B:546:CYS:SG	2.56	0.46
1:A:547:GLY:N	3:A:901:ATP:O2B	2.33	0.46
1:A:583:VAL:HG21	1:A:621:VAL:HG13	1.98	0.46
1:C:356:ASP:O	1:C:359:ILE:HG22	2.15	0.46
1:B:751:VAL:HG21	1:B:773:PRO:HB3	1.96	0.46
1:D:488:LYS:HA	1:D:492:PHE:CD1	2.51	0.46
1:F:395:ASN:O	1:F:397:LYS:N	2.44	0.46
1:E:474:GLU:OE1	1:E:474:GLU:N	2.46	0.46
1:E:493:SER:OG	1:E:494:THR:N	2.40	0.46
1:F:264:PHE:CE2	1:F:266:PRO:HG3	2.51	0.46
1:F:566:ILE:O	1:F:566:ILE:HD12	2.16	0.46
1:F:581:ARG:HG3	1:F:584:ARG:HH21	1.80	0.46
1:A:656:ARG:HH21	1:F:646:ARG:NH2	2.14	0.46
1:E:748:LEU:O	1:E:751:VAL:HG12	2.15	0.46
1:A:329:GLY:HA2	1:A:332:ARG:CZ	2.46	0.46
1:F:349:THR:HG21	1:F:355:LEU:HD11	1.98	0.46
1:F:646:ARG:C	1:F:648:ASP:H	2.20	0.46
1:A:299:ILE:HD12	1:A:345:VAL:HG22	1.97	0.45
1:D:607:VAL:HA	1:D:622:VAL:HG22	1.98	0.45
1:E:221:PRO:HB3	1:E:235:TYR:HB3	1.97	0.45
1:A:614:LEU:O	1:A:615:SER:OG	2.33	0.45
1:B:605:ALA:HB2	1:C:623:ASN:ND2	2.31	0.45
1:D:608:PRO:HB2	1:D:614:LEU:HD11	1.98	0.45
1:F:246:GLY:HA2	5:F:901:ADP:H5'2	1.98	0.45
1:A:677:ILE:HG23	3:A:901:ATP:C2	2.52	0.45
1:B:237:ASN:OD1	1:B:238:GLY:N	2.49	0.45
1:B:657:PRO:HA	1:B:661:GLY:HA2	1.99	0.45
1:A:227:ALA:HB2	1:F:466:TRP:HB2	1.97	0.45
1:A:498:THR:HG23	1:A:502:HIS:HB2	1.98	0.45
1:F:682:TYR:HE1	1:F:775:ILE:HD12	1.81	0.45
1:B:434:ALA:O	1:B:437:LYS:HG2	2.17	0.45
1:B:583:VAL:HG11	1:B:625:LEU:HG	1.99	0.45
1:C:211:LEU:HD23	1:C:211:LEU:HA	1.83	0.45
1:C:485:PRO:HG2	1:C:488:LYS:HG3	1.99	0.45
1:D:546:CYS:N	3:D:901:ATP:O2B	2.50	0.45
1:E:773:PRO:HG3	1:F:526:LEU:HD12	1.98	0.45
1:A:517:ILE:HD11	1:A:538:ILE:HD12	1.99	0.45
1:D:573:ASN:OD1	1:D:574:LYS:N	2.50	0.45
1:F:299:ILE:HB	1:F:345:VAL:HG22	1.99	0.45
1:A:327:MET:HB2	1:A:362:ARG:NE	2.32	0.45
1:B:541:TRP:HE1	1:B:663:SER:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:GLY:N	3:B:901:ATP:O2B	2.28	0.45
1:A:316:LYS:HD2	1:A:319:GLU:HG3	1.99	0.45
1:A:659:ARG:O	1:A:661:GLY:N	2.48	0.44
1:B:608:PRO:HG2	1:B:614:LEU:HD21	1.99	0.44
1:B:646:ARG:NH2	1:B:649:MET:HG3	2.31	0.44
1:D:260:ILE:HG22	1:D:262:VAL:HG13	1.99	0.44
1:E:773:PRO:HG3	1:F:526:LEU:CD1	2.46	0.44
1:F:390:LEU:O	1:F:470:LYS:HD3	2.16	0.44
1:A:546:CYS:SG	1:A:668:LEU:HD23	2.58	0.44
1:C:292:ILE:HD13	1:C:336:ASN:HB2	1.98	0.44
1:C:316:LYS:HB3	1:C:316:LYS:HE2	1.77	0.44
1:C:543:PRO:HG2	1:C:546:CYS:SG	2.57	0.44
3:C:902:ATP:O2G	1:D:362:ARG:NH2	2.51	0.44
1:E:573:ASN:CG	1:F:612:ASP:HB2	2.38	0.44
1:F:244:PRO:O	1:F:249:LYS:NZ	2.50	0.44
1:B:333:ILE:HG23	1:B:343:VAL:HB	1.99	0.44
1:E:602:GLN:OE1	1:E:645:ASN:ND2	2.47	0.44
1:E:305:ASP:OD1	1:E:305:ASP:N	2.50	0.44
1:F:198:LYS:HG3	1:F:199:VAL:HG23	2.00	0.44
1:B:420:SER:HB3	1:C:235:TYR:OH	2.16	0.44
1:F:206:GLY:HA3	1:F:376:ALA:HB2	2.00	0.44
1:F:412:GLN:HG2	1:F:416:LYS:HE3	2.00	0.44
1:B:408:GLY:HA3	3:B:902:ATP:N7	2.33	0.44
1:D:571:LEU:HD11	1:D:586:LEU:HD22	2.00	0.44
1:E:398:GLU:O	1:E:402:MET:HG2	2.18	0.44
1:F:609:ARG:O	1:F:614:LEU:HD11	2.18	0.44
1:F:614:LEU:O	1:F:615:SER:OG	2.31	0.44
1:B:195:PRO:HA	1:B:196:PRO:HD3	1.91	0.44
1:B:727:ARG:HE	1:B:784:LEU:HB3	1.83	0.44
1:D:251:THR:HG21	3:D:902:ATP:H2'	2.00	0.44
1:E:318:MET:O	1:E:322:ILE:HG13	2.18	0.44
1:B:677:ILE:HG23	3:B:901:ATP:C2	2.53	0.43
1:E:297:CYS:SG	1:E:298:LEU:N	2.91	0.43
1:E:517:ILE:HD12	1:E:538:ILE:HD13	2.00	0.43
1:E:739:LEU:HA	1:E:787:VAL:HG21	2.00	0.43
1:A:564:ILE:HB	1:A:598:LEU:HD23	2.00	0.43
1:B:376:ALA:O	1:B:380:ILE:HG13	2.18	0.43
1:B:544:PRO:HB3	1:B:645:ASN:ND2	2.33	0.43
1:E:329:GLY:HA2	1:E:332:ARG:CZ	2.49	0.43
1:E:575:TYR:CE2	1:F:613:SER:HB2	2.53	0.43
1:B:656:ARG:NH1	1:B:657:PRO:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ALA:HB1	1:A:307:ILE:HG23	1.99	0.43
1:C:514:GLU:HA	1:C:518:ILE:HB	2.00	0.43
1:A:193:ARG:N	1:A:264:PHE:O	2.51	0.43
1:A:795:GLU:O	1:A:798:MET:HG2	2.19	0.43
1:C:214:LEU:HD13	1:C:256:ILE:HD13	2.00	0.43
1:C:217:GLU:OE1	1:C:365:VAL:HG11	2.18	0.43
1:C:595:PRO:HA	1:C:637:GLY:O	2.19	0.43
1:D:748:LEU:HD21	1:E:530:VAL:HG21	2.01	0.43
1:A:490:GLU:OE1	1:B:310:ARG:NH2	2.51	0.43
1:B:269:ALA:O	1:B:272:VAL:HG22	2.19	0.43
1:C:426:ASN:HD22	1:C:467:PRO:HD2	1.84	0.43
1:C:644:THR:HG21	1:C:650:ILE:HD11	2.00	0.43
1:C:733:GLY:HA3	3:C:901:ATP:C8	2.53	0.43
1:F:378:GLU:HG3	1:F:396:PHE:O	2.18	0.43
1:F:604:ASP:OD1	1:F:604:ASP:N	2.50	0.43
1:B:539:LEU:HD13	1:B:660:LEU:HD13	2.01	0.43
1:C:319:GLU:OE2	1:D:317:GLY:HA3	2.19	0.43
1:C:371:MET:HG2	1:C:407:VAL:HG12	2.01	0.43
1:D:534:PRO:HG2	1:D:636:SER:HB2	1.99	0.43
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.88	0.43
1:C:490:GLU:HB3	1:D:360:ARG:NH1	2.33	0.43
1:C:567:LYS:HZ3	1:D:633:GLY:H	1.67	0.43
1:D:210:THR:HG23	1:D:367:ILE:HG21	2.00	0.43
1:D:331:ASP:OD1	1:D:362:ARG:NH1	2.52	0.43
1:E:386:ARG:HG3	1:E:387:ASP:OD1	2.19	0.43
1:F:678:LEU:HB2	1:F:736:LEU:HD21	2.01	0.43
1:A:785:ASN:O	1:A:788:LYS:NZ	2.50	0.43
1:C:490:GLU:HB3	1:D:360:ARG:HH12	1.83	0.43
1:D:577:GLY:HA2	1:D:580:GLU:OE1	2.19	0.43
1:E:604:ASP:OD1	1:E:604:ASP:N	2.51	0.43
1:F:580:GLU:HB3	1:F:621:VAL:HG22	2.00	0.43
1:A:331:ASP:CG	1:A:362:ARG:HH12	2.22	0.42
1:B:656:ARG:HE	1:B:659:ARG:NH1	2.17	0.42
1:C:657:PRO:HA	1:C:661:GLY:HA2	2.01	0.42
1:C:750:ARG:NH2	1:C:774:VAL:O	2.51	0.42
1:D:665:TYR:OH	1:D:798:MET:HG2	2.19	0.42
1:B:674:ARG:HG2	1:B:736:LEU:HD11	2.01	0.42
1:E:269:ALA:O	1:E:272:VAL:HG22	2.19	0.42
1:E:316:LYS:HE2	1:E:319:GLU:HG3	2.00	0.42
1:F:377:ARG:NE	1:F:403:THR:O	2.51	0.42
1:F:537:GLY:HA3	1:F:659:ARG:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:PRO:O	1:C:548:LYS:NZ	2.52	0.42
1:A:409:SER:OG	1:B:361:ARG:NH1	2.53	0.42
1:A:523:ASN:HB3	1:A:526:LEU:HB3	2.00	0.42
1:B:569:PRO:HG2	1:C:580:GLU:HG2	2.01	0.42
1:D:434:ALA:HB1	1:D:455:LEU:HB3	2.00	0.42
1:E:211:LEU:HA	1:E:211:LEU:HD23	1.85	0.42
1:E:269:ALA:HB3	1:E:306:ALA:HB3	2.02	0.42
1:B:546:CYS:N	3:B:901:ATP:O2B	2.53	0.42
1:D:408:GLY:HA3	3:D:902:ATP:N7	2.34	0.42
1:D:630:ASP:OD2	1:D:656:ARG:NH2	2.30	0.42
1:C:573:ASN:OD1	1:C:574:LYS:N	2.52	0.42
1:C:646:ARG:CZ	1:C:649:MET:HG3	2.49	0.42
1:C:646:ARG:NH2	1:C:649:MET:HG3	2.35	0.42
1:D:236:ASP:OD2	1:D:334:ARG:HA	2.20	0.42
1:A:210:THR:HG21	1:A:369:MET:HG2	2.01	0.42
1:A:566:ILE:HD13	1:A:600:PHE:CE1	2.54	0.42
1:A:679:LYS:HA	1:A:719:LEU:HD13	2.02	0.42
1:B:371:MET:HG2	1:B:407:VAL:HG12	2.00	0.42
1:B:472:THR:OG1	1:B:475:GLN:HG3	2.20	0.42
1:D:541:TRP:CZ3	1:D:800:SER:HB2	2.55	0.42
1:D:600:PHE:HD2	1:D:603:MET:SD	2.41	0.42
1:B:514:GLU:O	1:B:519:GLY:N	2.51	0.42
1:B:610:ARG:HA	1:B:614:LEU:HD22	2.01	0.42
1:A:634:ASP:N	1:A:634:ASP:OD1	2.53	0.42
1:B:573:ASN:OD1	1:B:574:LYS:N	2.53	0.42
1:E:234:ARG:NE	1:E:337:THR:O	2.52	0.42
1:A:656:ARG:HH21	1:F:646:ARG:HH21	1.66	0.41
1:B:251:THR:HG21	3:B:902:ATP:H2'	2.02	0.41
1:F:487:SER:HB2	1:F:492:PHE:HB3	2.01	0.41
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.90	0.41
1:C:603:MET:HE3	1:C:650:ILE:HD13	2.01	0.41
1:A:491:GLY:HA3	1:A:589:ARG:NH1	2.35	0.41
1:B:388:LEU:HD21	1:C:233:TYR:CD1	2.54	0.41
1:B:507:GLU:OE2	1:B:676:LYS:NZ	2.42	0.41
1:C:751:VAL:HA	1:C:771:ILE:HD11	2.02	0.41
1:F:566:ILE:HD11	1:F:600:PHE:CE1	2.56	0.41
1:F:656:ARG:HE	1:F:659:ARG:NE	2.18	0.41
1:A:466:TRP:CD2	1:B:227:ALA:HB2	2.56	0.41
1:D:538:ILE:HG12	1:D:662:THR:OG1	2.21	0.41
1:A:300:PHE:HA	1:A:346:LEU:O	2.20	0.41
1:B:571:LEU:HD12	1:B:606:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:LYS:HD3	1:B:635:ARG:HA	2.02	0.41
1:C:241:LEU:HD23	1:C:367:ILE:HB	2.02	0.41
1:E:656:ARG:HE	1:E:659:ARG:CZ	2.32	0.41
1:F:210:THR:HG21	1:F:369:MET:SD	2.60	0.41
1:F:500:TRP:NE1	1:F:558:GLU:HG3	2.36	0.41
1:A:423:PHE:CE1	1:B:227:ALA:HB1	2.56	0.41
1:C:795:GLU:HA	1:C:798:MET:HB3	2.02	0.41
1:E:269:ALA:HB1	1:E:307:ILE:HG12	2.03	0.41
1:E:575:TYR:CE2	2:G:22:VAL:HG11	2.55	0.41
1:F:500:TRP:CD1	1:F:558:GLU:HG3	2.55	0.41
1:F:719:LEU:HA	1:F:722:VAL:HG12	2.03	0.41
1:A:385:THR:HB	1:A:390:LEU:HD11	2.01	0.41
1:F:223:ARG:NH2	1:F:262:VAL:HG22	2.36	0.41
1:B:536:ALA:HB3	1:B:639:TYR:HD2	1.85	0.41
1:F:249:LYS:HB3	1:F:348:ALA:HB1	2.02	0.41
1:A:241:LEU:HD23	1:A:367:ILE:HB	2.03	0.41
1:A:505:ALA:HB2	1:A:676:LYS:HB2	2.03	0.41
1:A:607:VAL:HA	1:A:622:VAL:HG22	2.02	0.41
1:A:616:ASP:OD2	1:F:615:SER:OG	2.39	0.41
1:C:213:ARG:NH2	1:C:217:GLU:OE2	2.47	0.41
1:C:448:GLN:HB2	1:C:449:PRO:HD3	2.02	0.41
1:E:195:PRO:HA	1:E:196:PRO:HD3	1.97	0.41
1:E:298:LEU:HD11	1:E:346:LEU:CG	2.51	0.41
1:E:389:SER:HB2	1:E:470:LYS:HG2	2.03	0.41
1:F:305:ASP:OD2	1:F:351:ARG:HB2	2.21	0.41
1:F:613:SER:O	1:F:614:LEU:HD12	2.21	0.41
1:C:716:ASP:O	1:C:720:GLU:HG3	2.21	0.41
1:D:605:ALA:HB2	1:E:623:ASN:ND2	2.36	0.41
1:E:446:VAL:HG12	1:E:451:ARG:HG3	2.03	0.41
1:B:282:LYS:HE2	1:B:282:LYS:HB3	1.92	0.40
1:C:500:TRP:NE1	1:C:558:GLU:HG3	2.36	0.40
1:F:404:PRO:HD2	1:F:494:THR:HG21	2.03	0.40
1:A:303:GLN:NE2	1:B:327:MET:SD	2.94	0.40
1:D:486:ALA:HA	1:D:489:ARG:HG2	2.03	0.40
1:E:530:VAL:HG23	1:E:532:ILE:HG13	2.03	0.40
1:E:752:TYR:CE2	1:F:515:MET:HG3	2.55	0.40
1:F:485:PRO:HG2	1:F:488:LYS:HG3	2.03	0.40
1:A:211:LEU:HD21	1:A:252:LEU:HD11	2.04	0.40
1:E:311:ARG:HH21	1:E:358:ALA:HB2	1.87	0.40
1:A:249:LYS:HG2	1:A:369:MET:SD	2.61	0.40
1:C:280:SER:OG	1:C:322:ILE:HD11	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:LYS:HD2	1:D:562:ASN:OD1	2.21	0.40
1:E:352:PRO:HA	1:E:355:LEU:HD13	2.03	0.40
1:A:388:LEU:HD22	1:B:231:MET:HE2	2.02	0.40
1:B:738:ASN:HB2	1:C:657:PRO:CB	2.51	0.40
1:E:327:MET:SD	1:E:358:ALA:HB1	2.62	0.40
1:F:517:ILE:O	1:F:521:ILE:HG13	2.22	0.40
1:F:544:PRO:HA	1:F:548:LYS:HZ1	1.85	0.40
1:F:566:ILE:H	1:F:566:ILE:HG13	1.75	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	560/813 (69%)	537 (96%)	23 (4%)	0	100	100
1	B	561/813 (69%)	547 (98%)	14 (2%)	0	100	100
1	C	562/813 (69%)	551 (98%)	10 (2%)	1 (0%)	47	78
1	D	562/813 (69%)	545 (97%)	16 (3%)	1 (0%)	47	78
1	E	528/813 (65%)	498 (94%)	29 (6%)	1 (0%)	47	78
1	F	549/813 (68%)	509 (93%)	38 (7%)	2 (0%)	34	69
2	G	21/23 (91%)	17 (81%)	4 (19%)	0	100	100
All	All	3343/4901 (68%)	3204 (96%)	134 (4%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	460	ARG
1	F	269	ALA
1	C	339	LEU

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Mol	Chain	Res	Type
1	E	520	PRO
1	F	608	PRO

### 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	470/671 (70%)	465 (99%)	5 (1%)	73	85
1	B	474/671 (71%)	468 (99%)	6 (1%)	69	83
1	C	473/671 (70%)	468 (99%)	5 (1%)	73	85
1	D	473/671 (70%)	470 (99%)	3 (1%)	86	93
1	E	443/671 (66%)	435 (98%)	8 (2%)	59	77
1	F	455/671 (68%)	444 (98%)	11 (2%)	49	70
2	G	23/23 (100%)	22 (96%)	1 (4%)	29	58
All	All	2811/4049 (69%)	2772 (99%)	39 (1%)	68	82

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	TYR
1	A	337	THR
1	A	354	PHE
1	A	530	VAL
1	A	607	VAL
1	B	235	TYR
1	B	276	THR
1	B	551	VAL
1	B	685	THR
1	B	772	GLU
1	B	796	LYS
1	C	212	GLN
1	C	235	TYR
1	C	276	THR
1	C	635	ARG

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Mol	Chain	Res	Type
1	C	685	THR
1	D	207	VAL
1	D	235	TYR
1	D	361	ARG
1	E	276	THR
1	E	337	THR
1	E	361	ARG
1	E	472	THR
1	E	607	VAL
1	E	625	LEU
1	E	645	ASN
1	E	646	ARG
1	F	203	ASP
1	F	235	TYR
1	F	362	ARG
1	F	472	THR
1	F	533	LYS
1	F	601	ASP
1	F	607	VAL
1	F	632	VAL
1	F	634	ASP
1	F	650	ILE
1	F	725	ASP
2	G	23	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	562	ASN
1	B	379	GLN
1	C	450	GLN
1	D	350	ASN
1	D	562	ASN
1	E	573	ASN
1	F	645	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 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	B	901	4	26,33,33	0.77	0	31,52,52	1.12	2 (6%)
3	ATP	E	902	4	26,33,33	0.71	0	31,52,52	0.94	2 (6%)
3	ATP	C	901	4	26,33,33	0.76	0	31,52,52	1.01	2 (6%)
5	ADP	E	901	-	24,29,29	0.94	1 (4%)	29,45,45	1.48	4 (13%)
3	ATP	B	902	4	26,33,33	0.78	0	31,52,52	1.08	3 (9%)
3	ATP	D	901	4	26,33,33	0.77	0	31,52,52	1.19	3 (9%)
5	ADP	F	901	-	24,29,29	0.97	1 (4%)	29,45,45	1.43	4 (13%)
3	ATP	C	902	4	26,33,33	0.76	0	31,52,52	1.04	3 (9%)
3	ATP	A	901	4	26,33,33	0.75	0	31,52,52	1.06	2 (6%)
3	ATP	D	902	4	26,33,33	0.76	0	31,52,52	1.00	3 (9%)
3	ATP	A	902	4	26,33,33	0.74	0	31,52,52	1.01	3 (9%)

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	B	901	4	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	E	902	4	-	3/18/38/38	0/3/3/3
3	ATP	C	901	4	-	8/18/38/38	0/3/3/3
5	ADP	E	901	-	-	2/12/32/32	0/3/3/3
3	ATP	B	902	4	-	4/18/38/38	0/3/3/3
3	ATP	D	901	4	-	4/18/38/38	0/3/3/3
5	ADP	F	901	-	-	3/12/32/32	0/3/3/3
3	ATP	C	902	4	-	2/18/38/38	0/3/3/3
3	ATP	A	901	4	-	7/18/38/38	0/3/3/3
3	ATP	D	902	4	-	1/18/38/38	0/3/3/3
3	ATP	A	902	4	-	1/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	901	ADP	C5-C4	2.48	1.47	1.40
5	E	901	ADP	C5-C4	2.44	1.47	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	ATP	PA-O3A-PB	-4.15	118.58	132.83
5	E	901	ADP	PA-O3A-PB	-3.72	120.06	132.83
5	F	901	ADP	PA-O3A-PB	-3.49	120.86	132.83
3	D	901	ATP	PA-O3A-PB	-3.40	121.17	132.83
3	A	901	ATP	PA-O3A-PB	-3.38	121.21	132.83
5	E	901	ADP	C3'-C2'-C1'	3.38	106.07	100.98
3	D	901	ATP	PB-O3B-PG	-3.34	121.37	132.83
5	F	901	ADP	N3-C2-N1	-3.16	123.74	128.68
3	C	901	ATP	PA-O3A-PB	-3.15	122.00	132.83
3	A	902	ATP	PA-O3A-PB	-3.15	122.03	132.83
5	F	901	ADP	C3'-C2'-C1'	3.03	105.54	100.98
5	E	901	ADP	N3-C2-N1	-3.00	123.99	128.68
3	D	902	ATP	PA-O3A-PB	-2.94	122.73	132.83
3	B	902	ATP	PB-O3B-PG	-2.86	123.02	132.83
5	E	901	ADP	C4-C5-N7	-2.85	106.43	109.40
3	B	902	ATP	PA-O3A-PB	-2.71	123.54	132.83
5	F	901	ADP	C4-C5-N7	-2.62	106.67	109.40
3	C	902	ATP	PA-O3A-PB	-2.59	123.93	132.83
3	C	902	ATP	PB-O3B-PG	-2.50	124.25	132.83
3	E	902	ATP	PA-O3A-PB	-2.36	124.72	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	ATP	C5-C6-N6	2.21	123.71	120.35
3	E	902	ATP	C5-C6-N6	2.20	123.70	120.35
3	C	901	ATP	C5-C6-N6	2.20	123.70	120.35
3	A	901	ATP	C5-C6-N6	2.19	123.68	120.35
3	A	902	ATP	C5-C6-N6	2.19	123.68	120.35
3	B	902	ATP	C5-C6-N6	2.17	123.65	120.35
3	B	901	ATP	C5-C6-N6	2.17	123.65	120.35
3	D	901	ATP	C5-C6-N6	2.15	123.62	120.35
3	D	902	ATP	C5-C6-N6	2.15	123.61	120.35
3	A	902	ATP	PB-O3B-PG	-2.13	125.52	132.83
3	D	902	ATP	PB-O3B-PG	-2.10	125.62	132.83

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	PB-O3B-PG-O2G
3	A	901	ATP	PB-O3B-PG-O3G
3	A	901	ATP	C5'-O5'-PA-O1A
3	A	901	ATP	C5'-O5'-PA-O3A
3	B	901	ATP	C5'-O5'-PA-O3A
3	B	901	ATP	O4'-C4'-C5'-O5'
3	C	901	ATP	PB-O3B-PG-O2G
3	C	901	ATP	PB-O3B-PG-O3G
3	C	901	ATP	C5'-O5'-PA-O1A
3	C	901	ATP	C5'-O5'-PA-O2A
3	C	901	ATP	C5'-O5'-PA-O3A
3	C	902	ATP	O4'-C4'-C5'-O5'
3	D	901	ATP	C5'-O5'-PA-O1A
3	D	901	ATP	C5'-O5'-PA-O2A
3	D	901	ATP	C5'-O5'-PA-O3A
3	D	901	ATP	O4'-C4'-C5'-O5'
3	E	902	ATP	C5'-O5'-PA-O3A
3	A	901	ATP	O4'-C4'-C5'-O5'
3	B	902	ATP	O4'-C4'-C5'-O5'
3	B	902	ATP	C3'-C4'-C5'-O5'
3	C	901	ATP	O4'-C4'-C5'-O5'
3	C	902	ATP	C3'-C4'-C5'-O5'
3	B	902	ATP	PG-O3B-PB-O1B
3	A	901	ATP	C5'-O5'-PA-O2A
3	B	901	ATP	C5'-O5'-PA-O1A
3	B	901	ATP	C5'-O5'-PA-O2A

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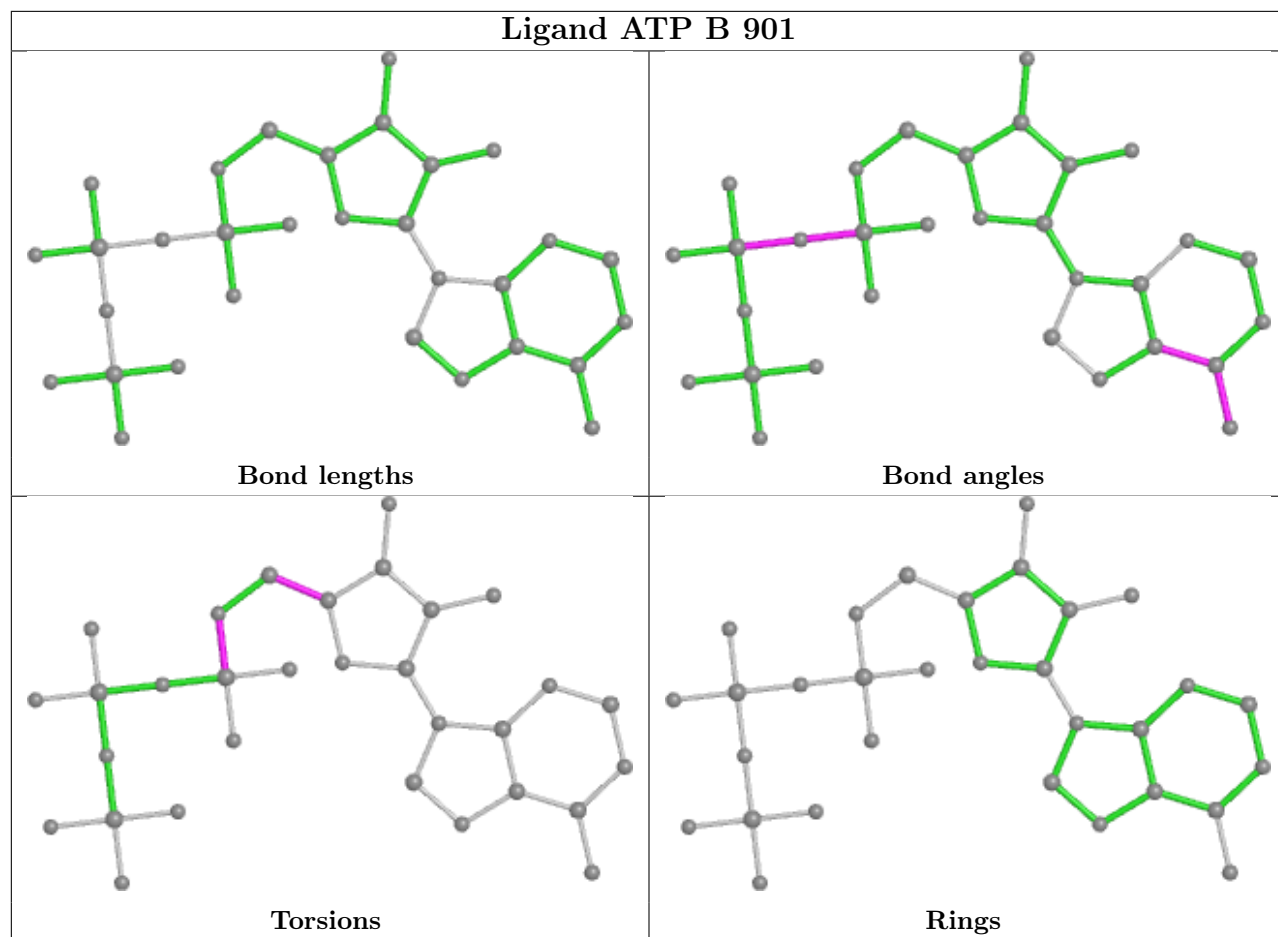
Mol	Chain	Res	Type	Atoms
3	C	901	ATP	C3'-C4'-C5'-O5'
5	E	901	ADP	PB-O3A-PA-O2A
3	A	902	ATP	O4'-C4'-C5'-O5'
5	E	901	ADP	PB-O3A-PA-O1A
3	A	901	ATP	PB-O3B-PG-O1G
3	D	902	ATP	O4'-C4'-C5'-O5'
5	F	901	ADP	O4'-C4'-C5'-O5'
3	B	902	ATP	PG-O3B-PB-O2B
5	F	901	ADP	PB-O3A-PA-O1A
5	F	901	ADP	PB-O3A-PA-O2A
3	E	902	ATP	C5'-O5'-PA-O1A
3	E	902	ATP	O4'-C4'-C5'-O5'
3	C	901	ATP	PB-O3B-PG-O1G

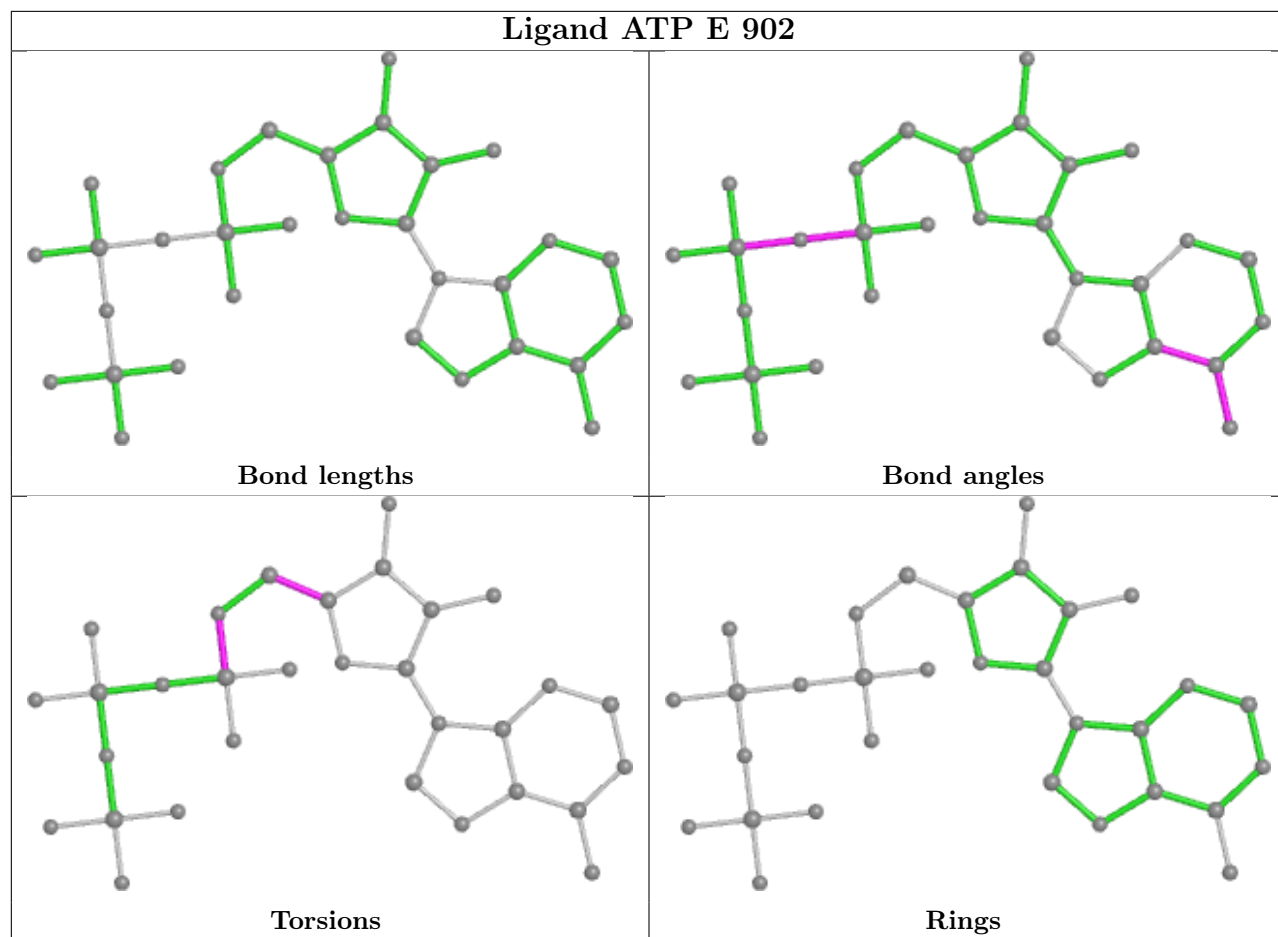
There are no ring outliers.

11 monomers are involved in 41 short contacts:

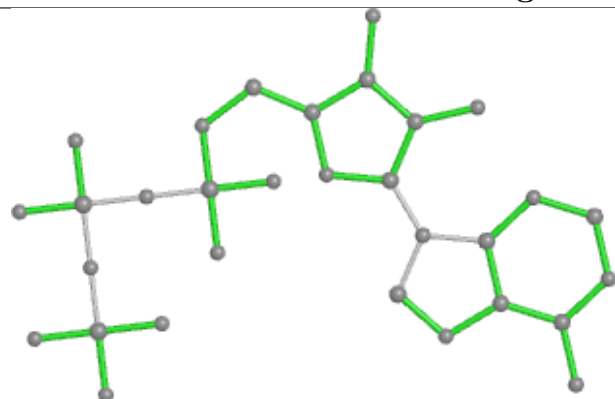
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	ATP	5	0
3	E	902	ATP	6	0
3	C	901	ATP	3	0
5	E	901	ADP	1	0
3	B	902	ATP	5	0
3	D	901	ATP	2	0
5	F	901	ADP	1	0
3	C	902	ATP	3	0
3	A	901	ATP	5	0
3	D	902	ATP	5	0
3	A	902	ATP	5	0

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.

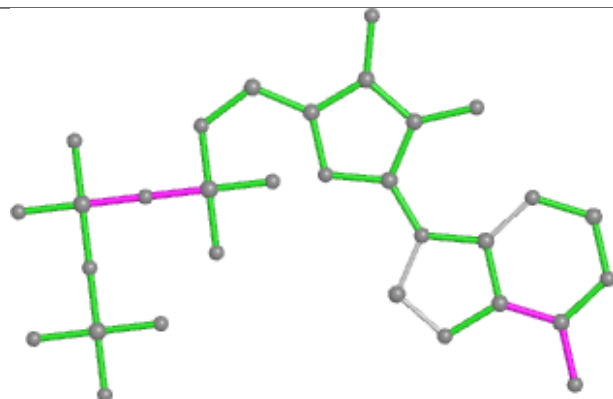




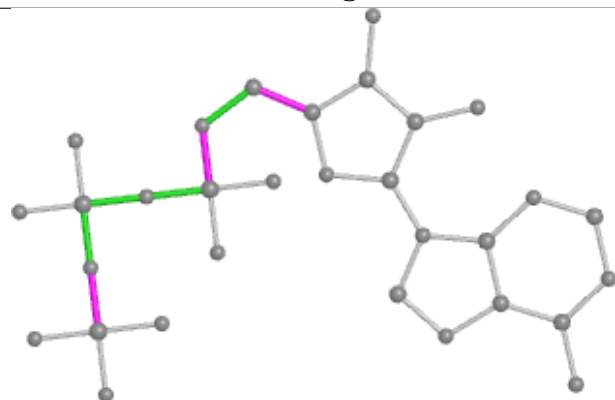
## Ligand ATP C 901



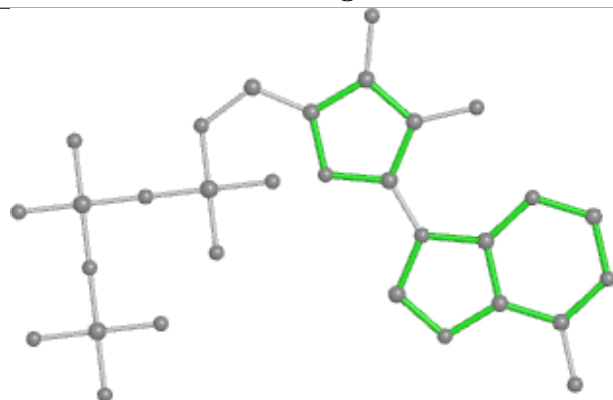
Bond lengths



Bond angles

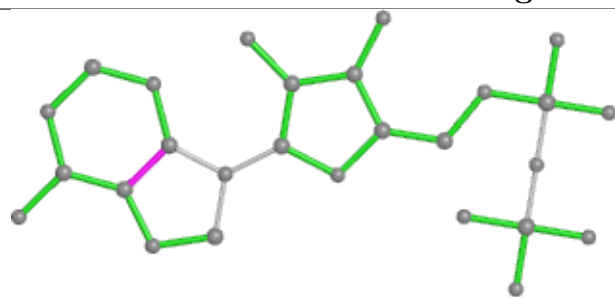


Torsions

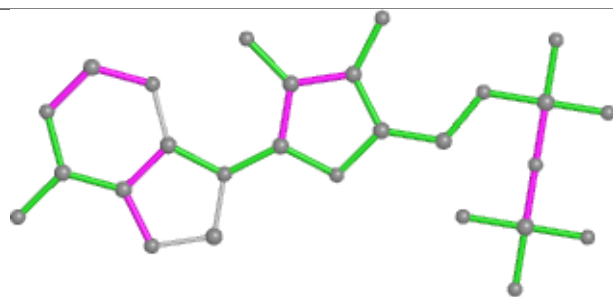


Rings

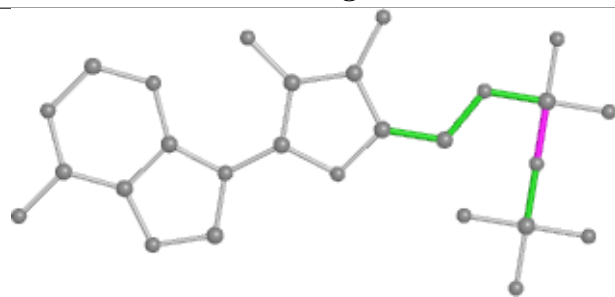
## Ligand ADP E 901



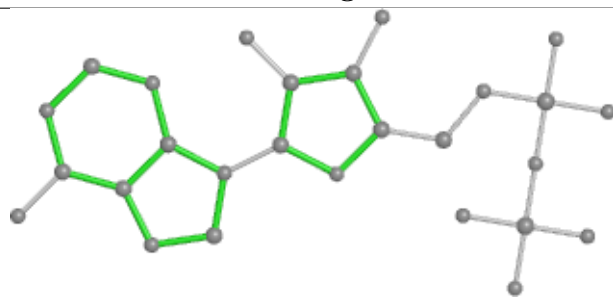
Bond lengths



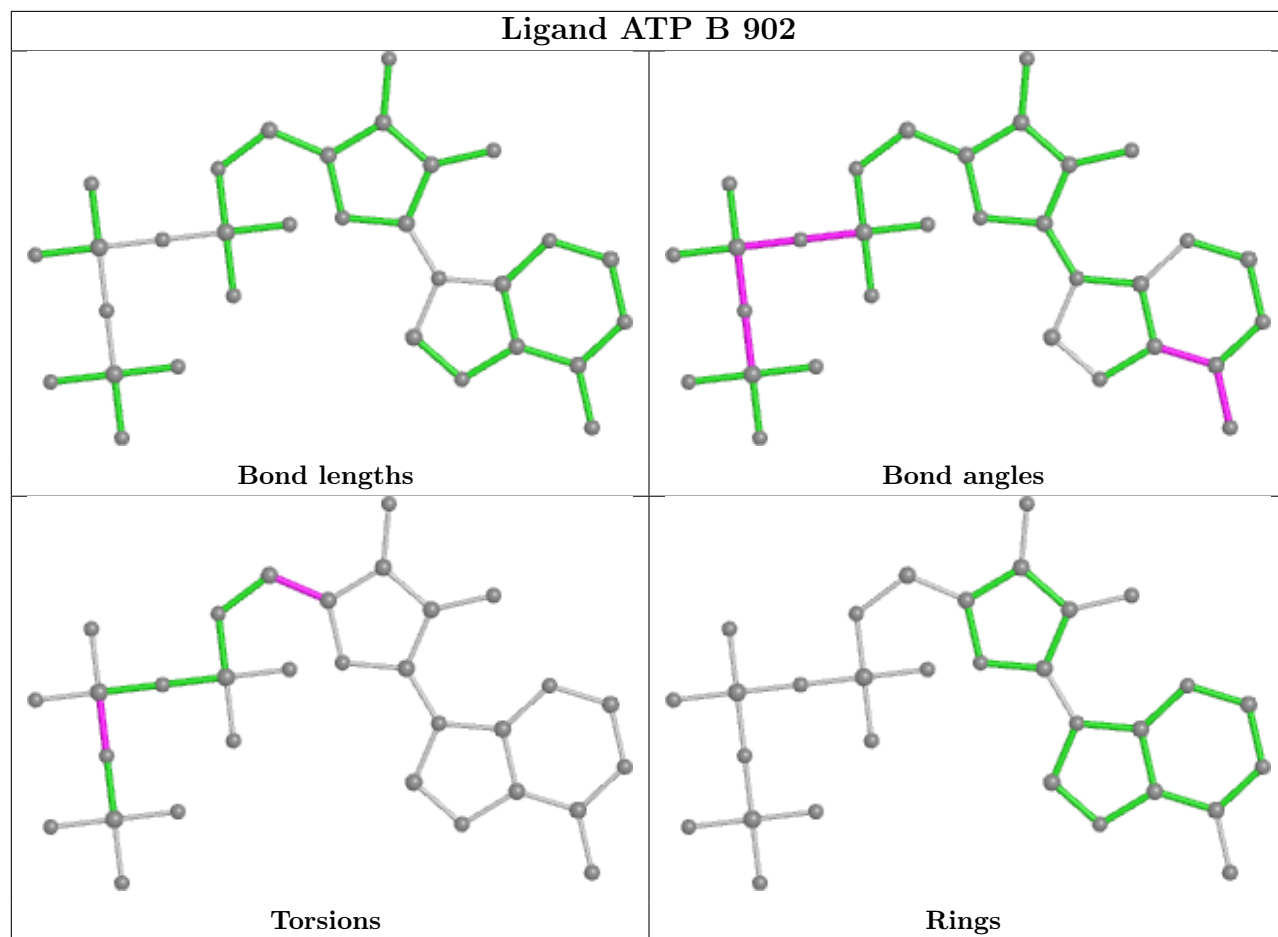
Bond angles

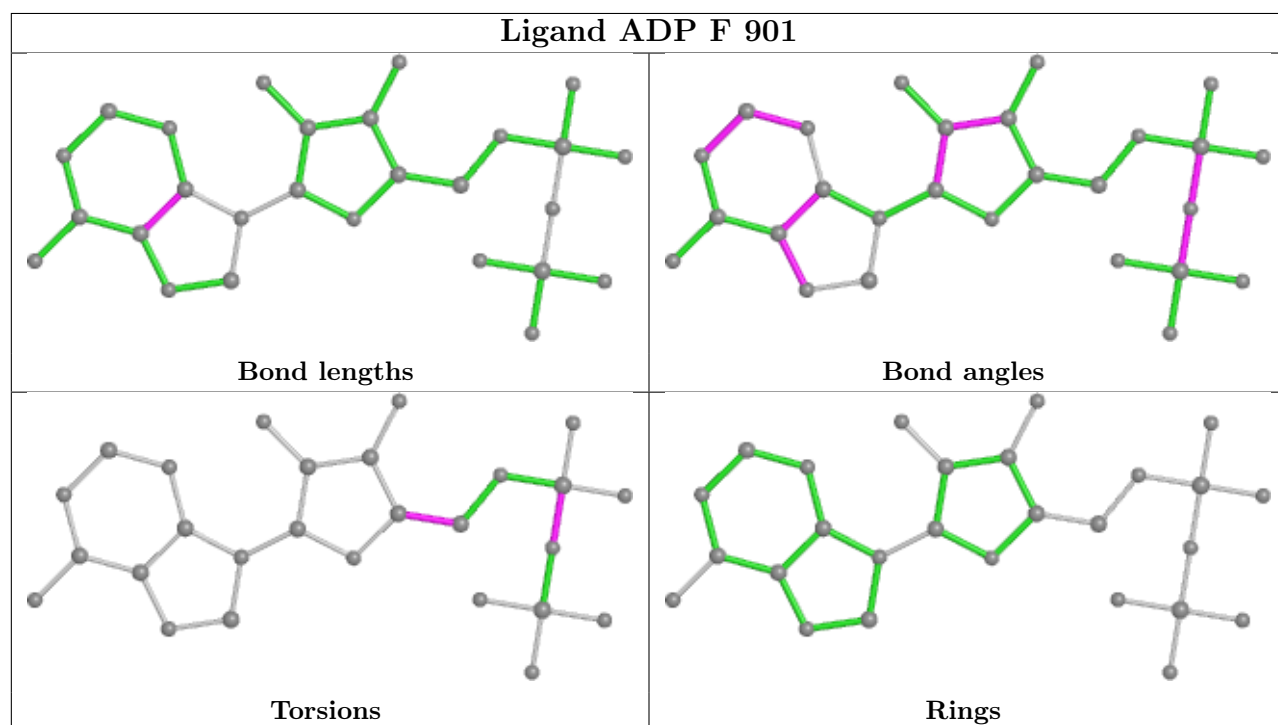
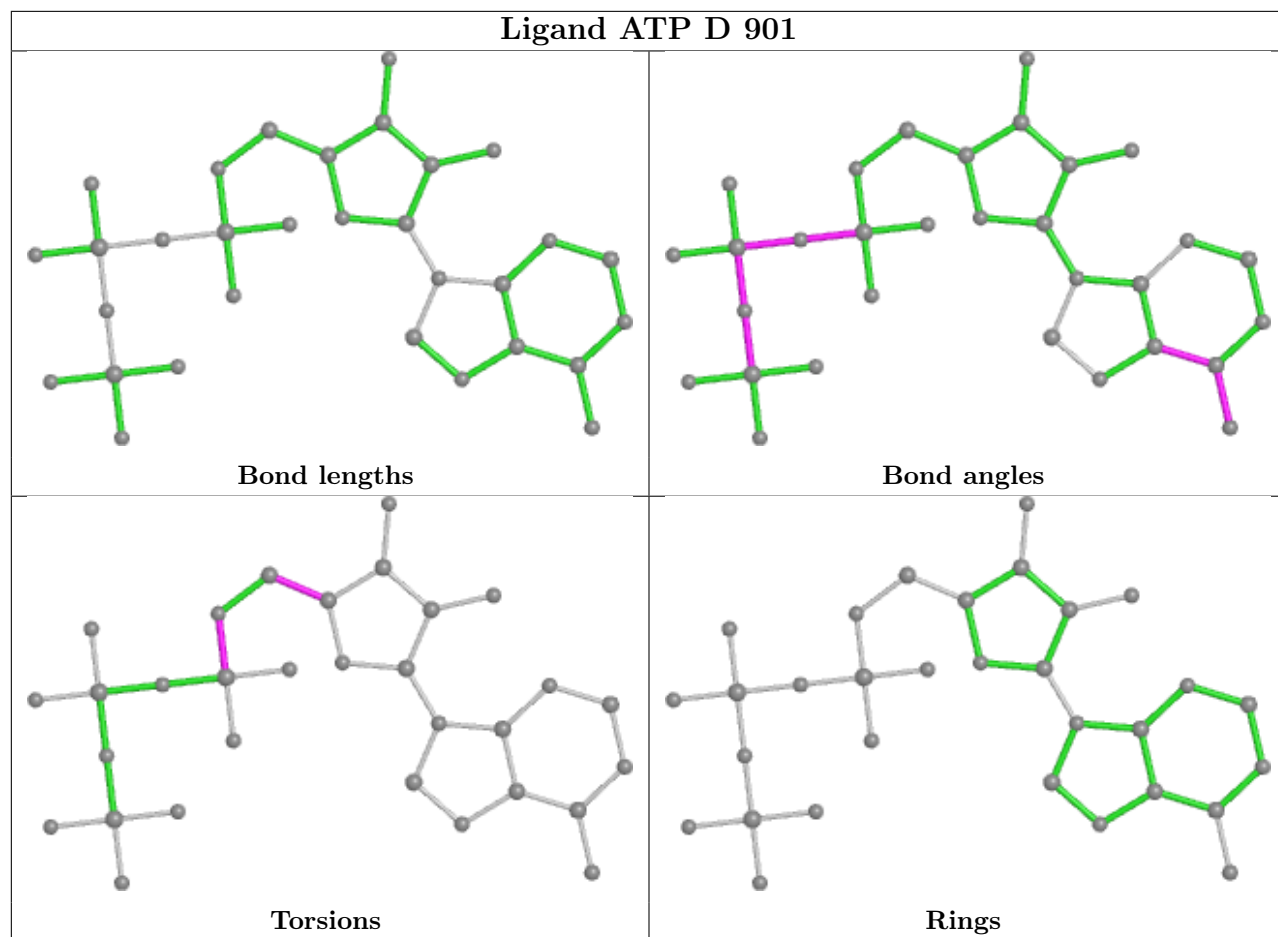


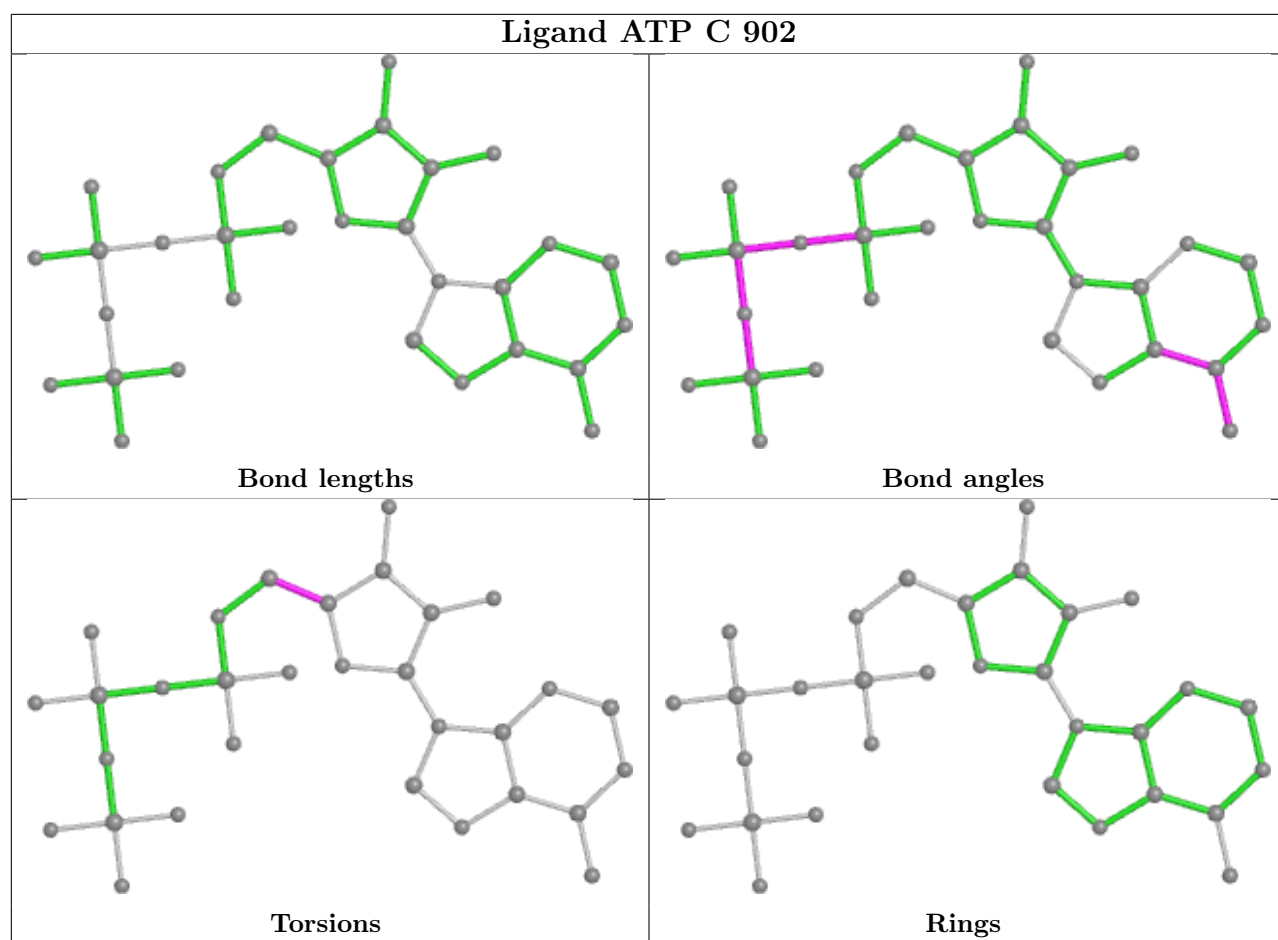
Torsions

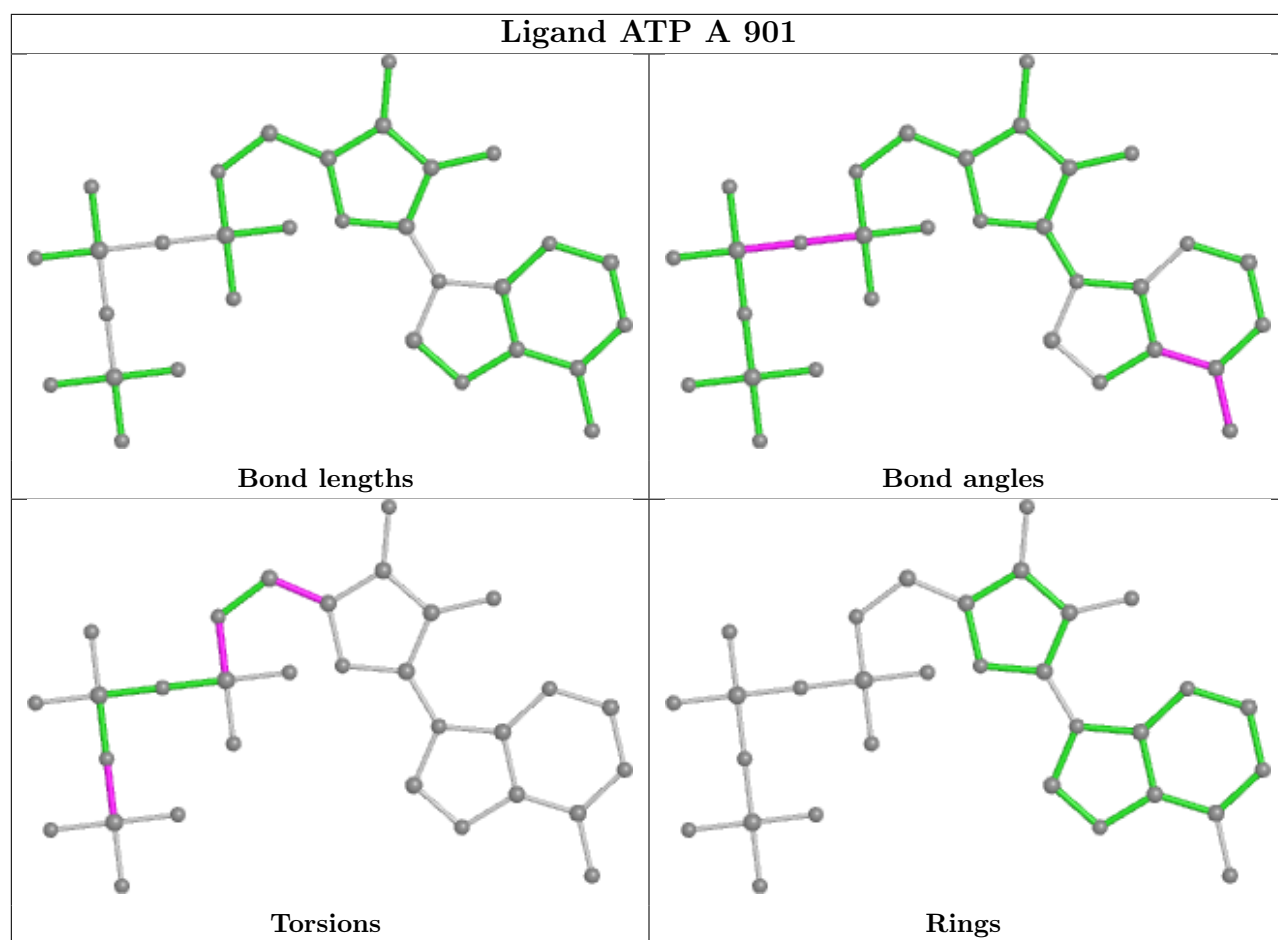


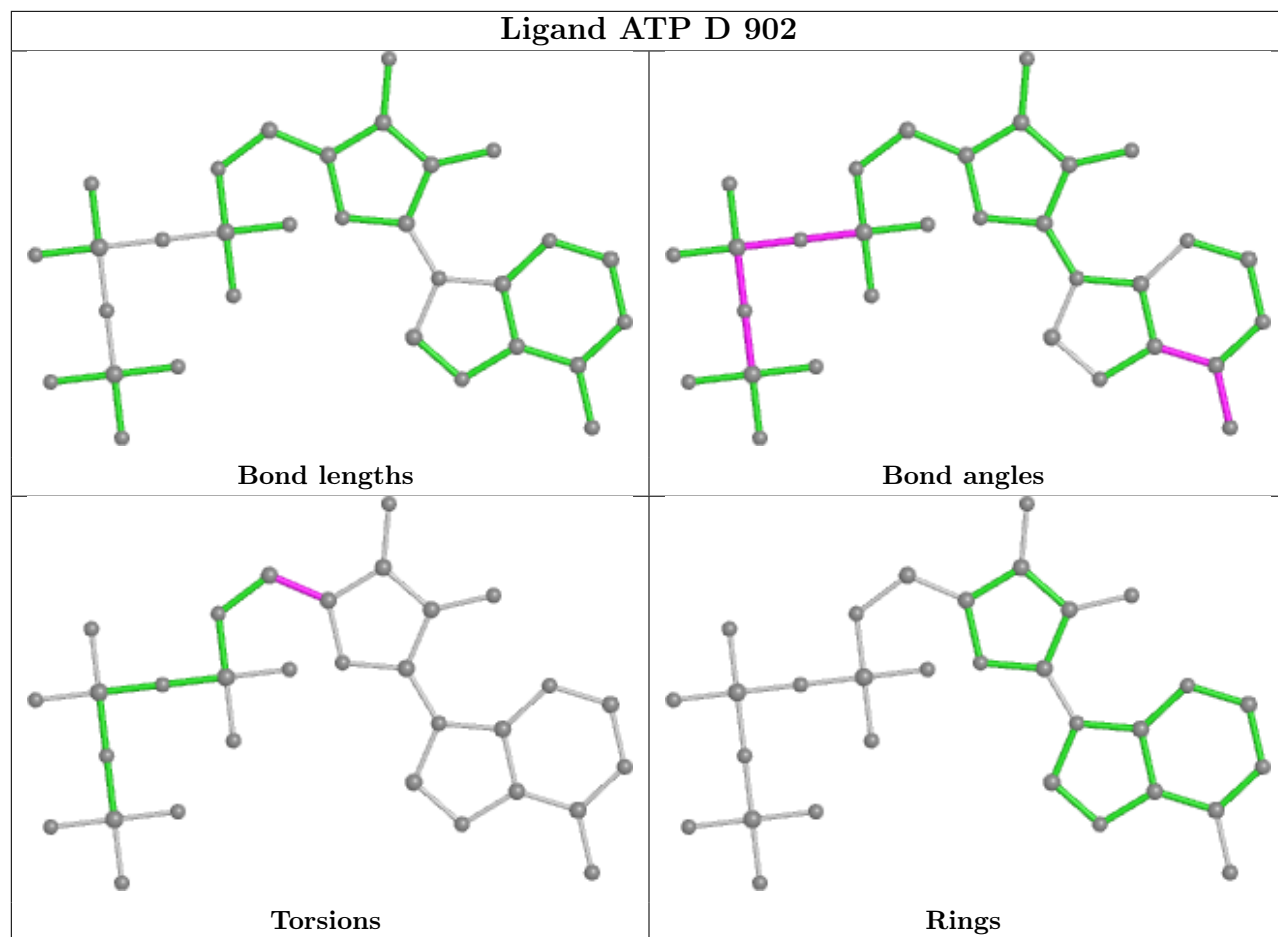
Rings

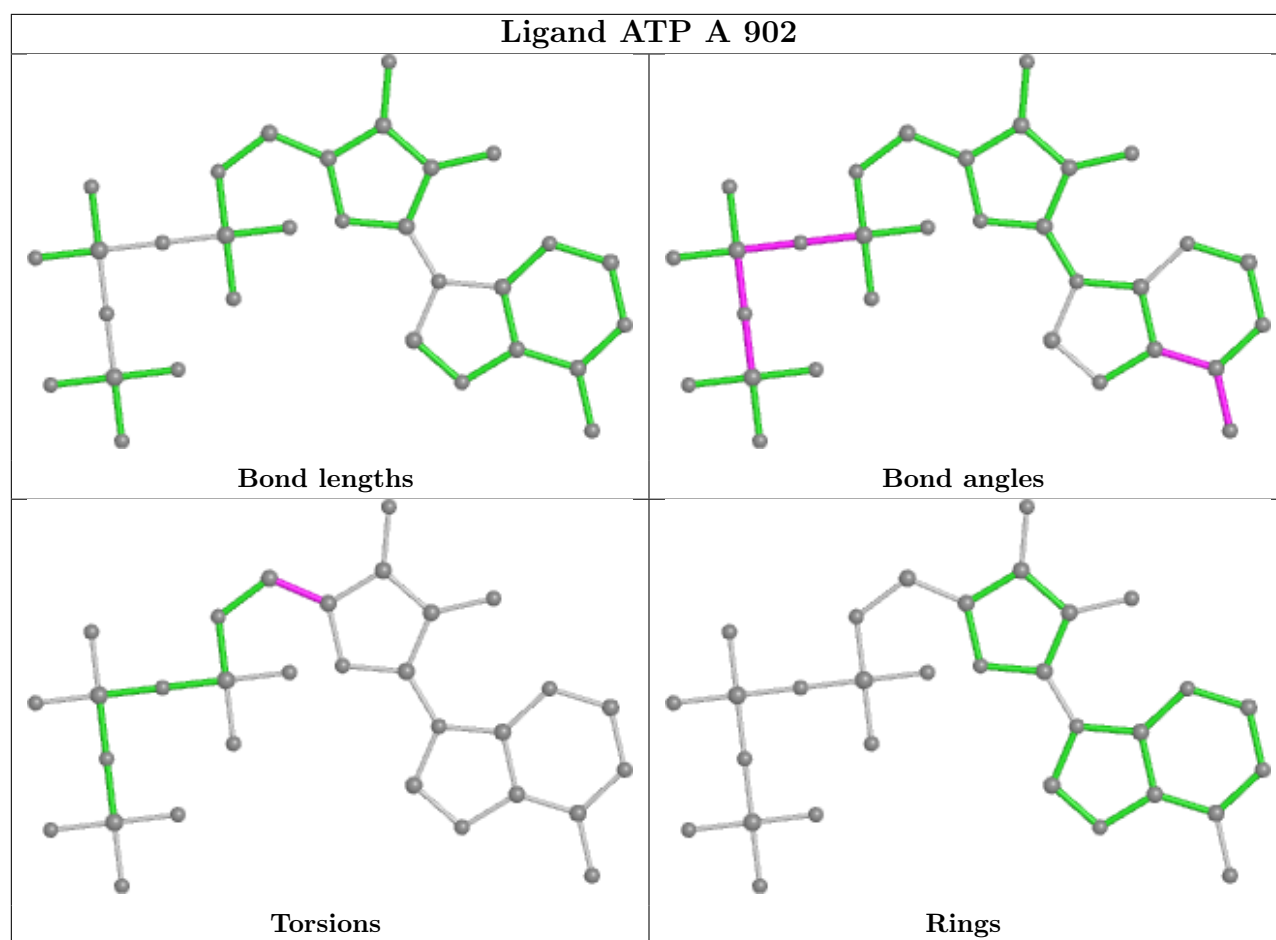












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

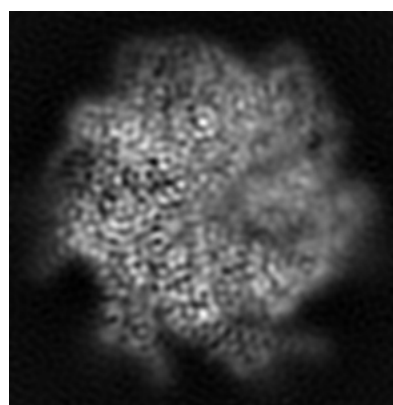
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25582. These allow visual inspection of the internal detail of the map and identification of artifacts.

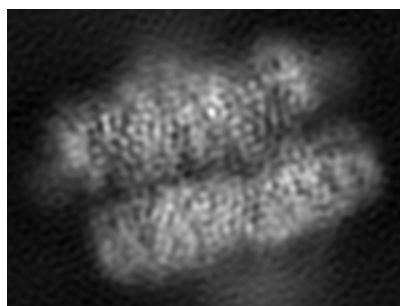
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

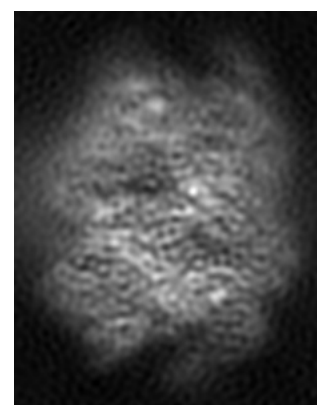
#### 6.1.1 Primary map



X



Y

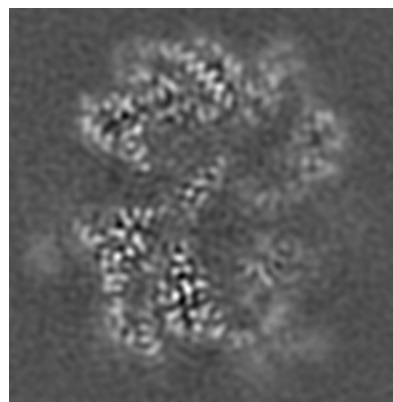


Z

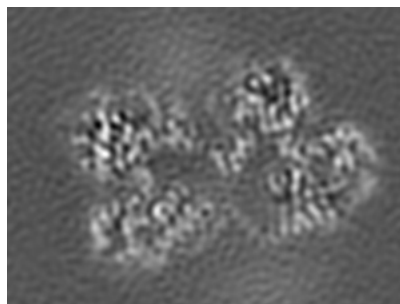
The images above show the map projected in three orthogonal directions.

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

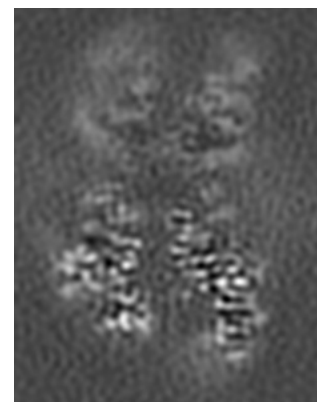
#### 6.2.1 Primary map



X Index: 57



Y Index: 73

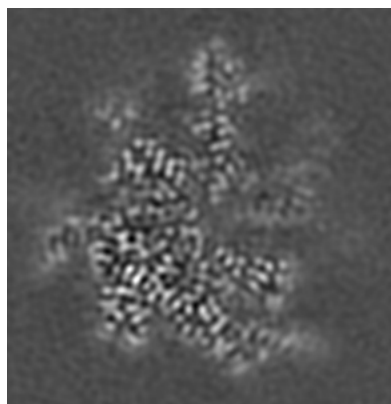


Z Index: 76

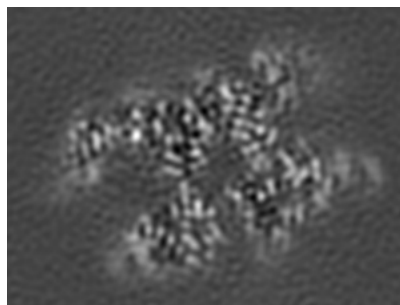
The images above show central slices of the map in three orthogonal directions.

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

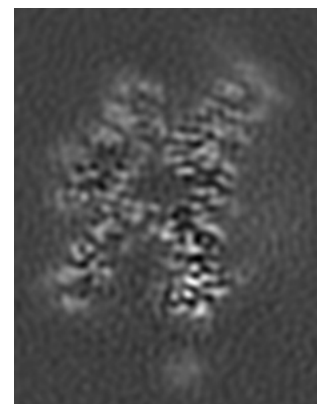
### 6.3.1 Primary map



X Index: 65



Y Index: 49

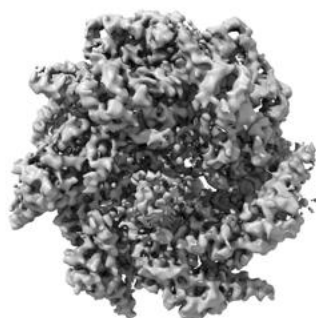


Z Index: 52

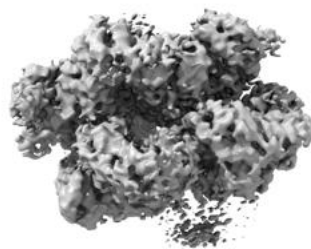
The images above show the largest variance slices of the map in three orthogonal directions.

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

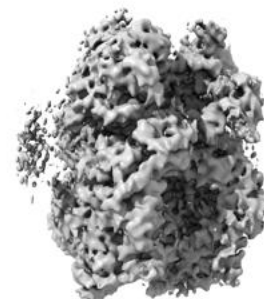
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.252. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

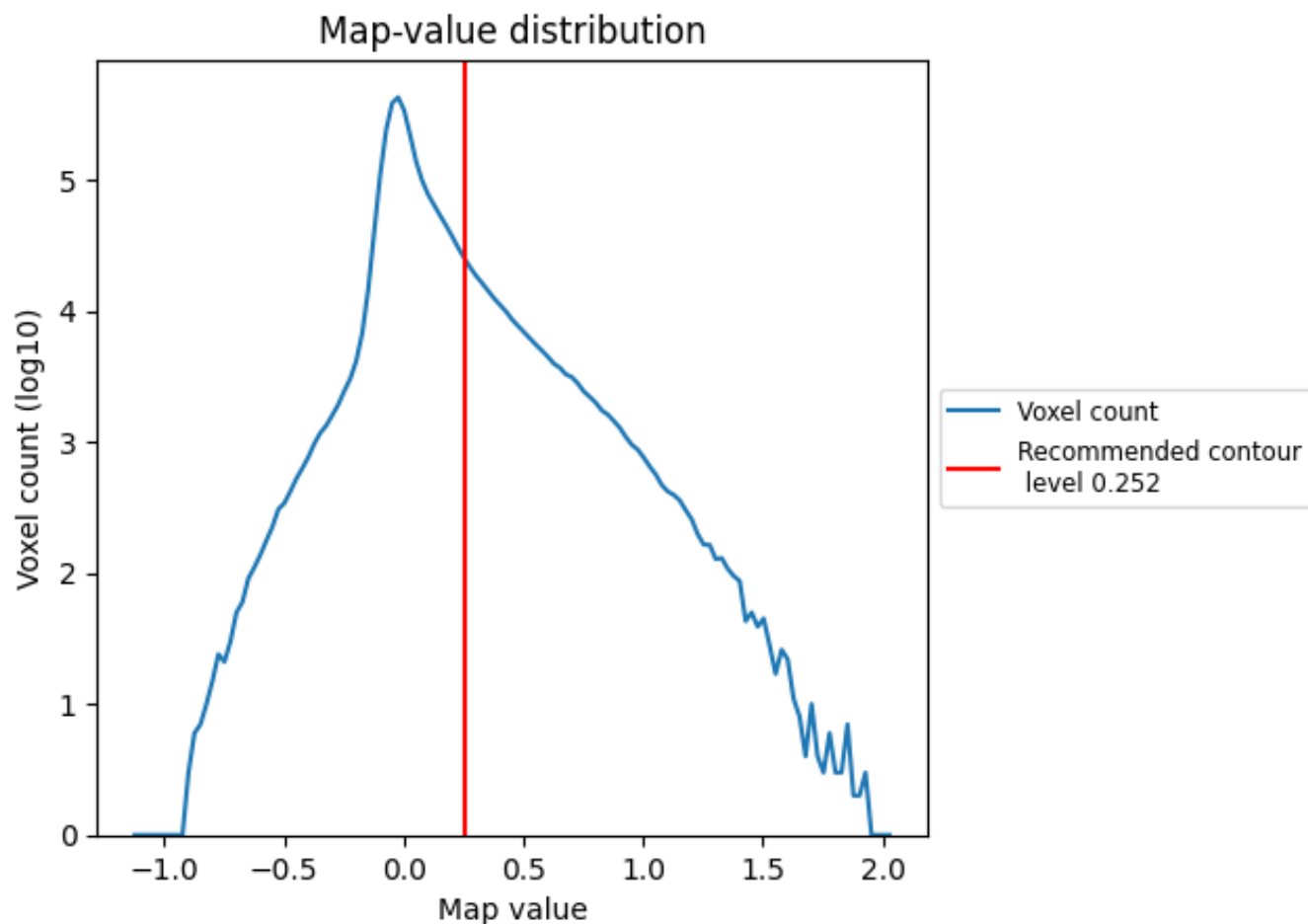
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

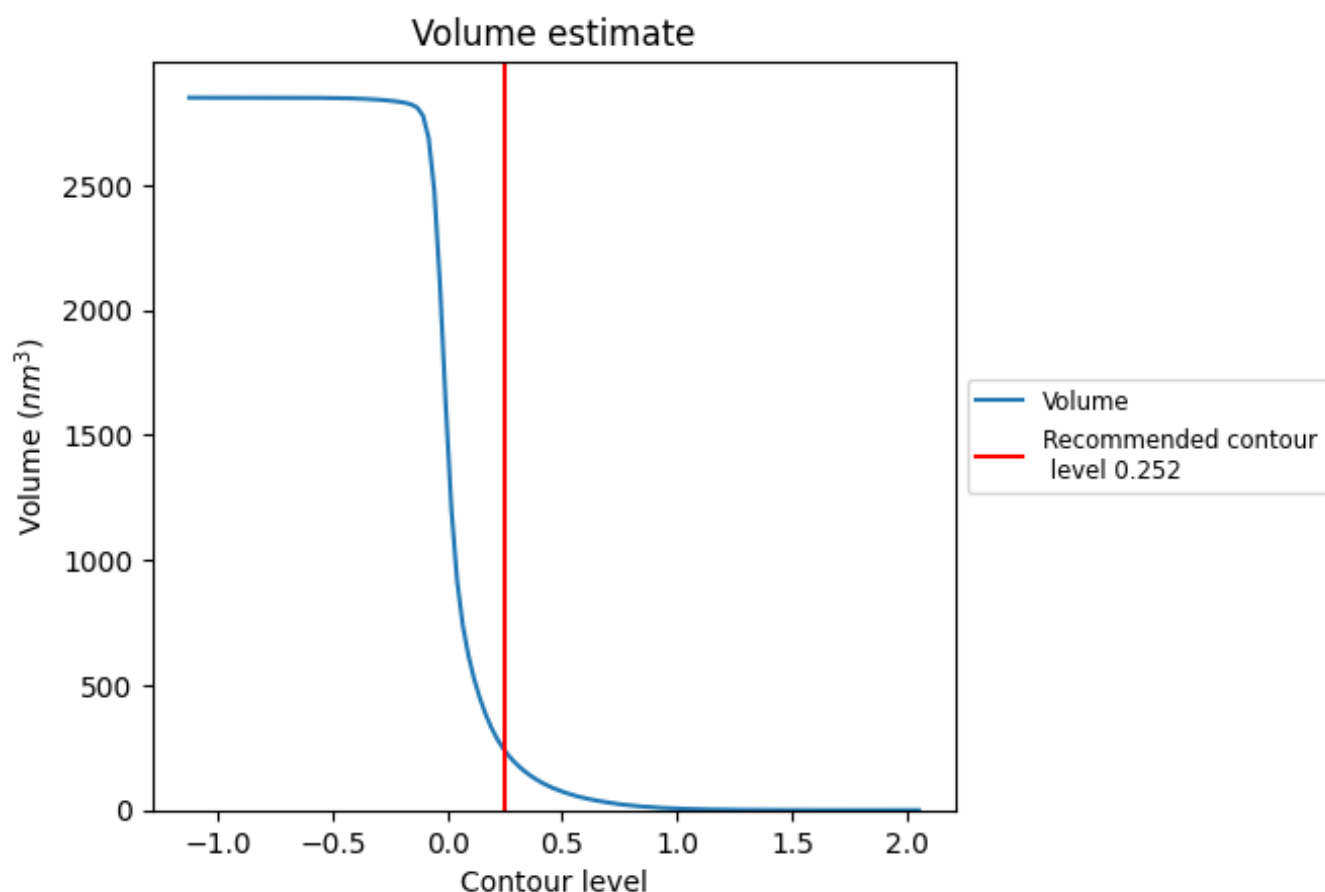
This section contains the results of statistical analysis of the map.

### 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 236 nm<sup>3</sup>; this corresponds to an approximate mass of 214 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

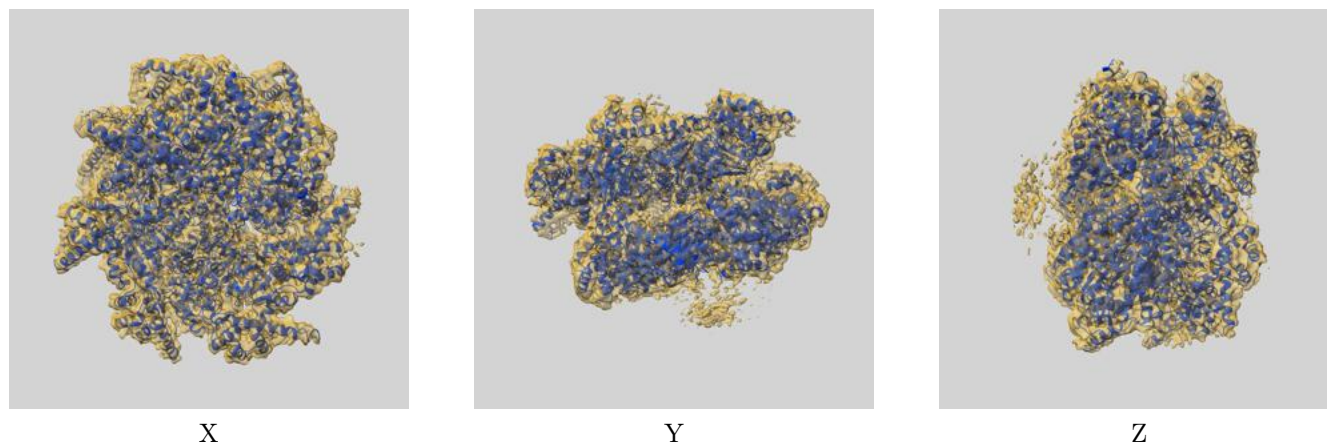
## 8 Fourier-Shell correlation ⓘ

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

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

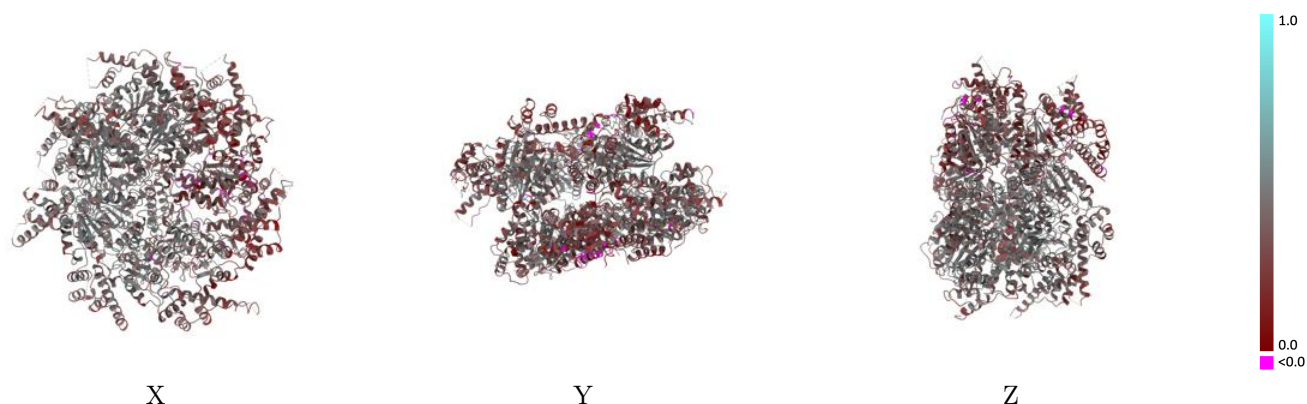
This section contains information regarding the fit between EMDB map EMD-25582 and PDB model 7T0V. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



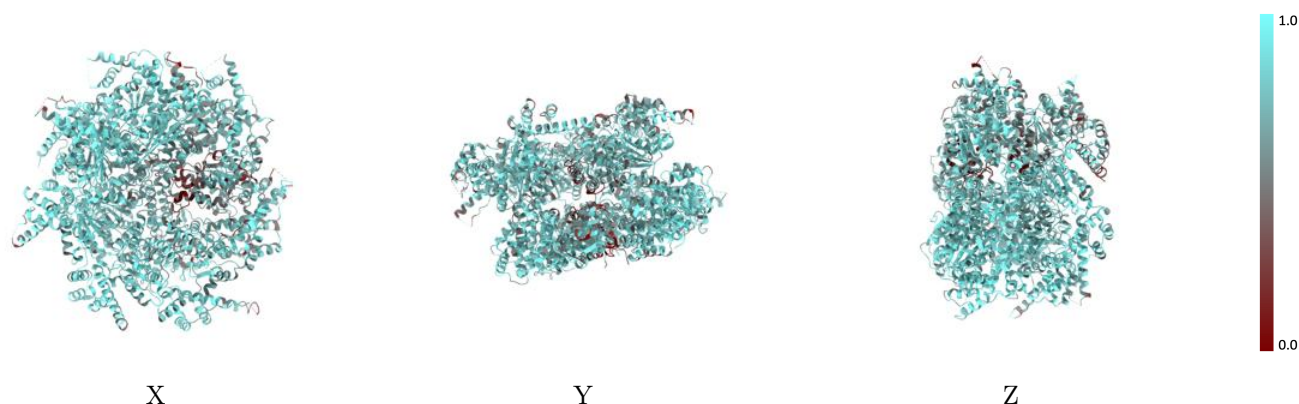
The images above show the 3D surface view of the map at the recommended contour level 0.252 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



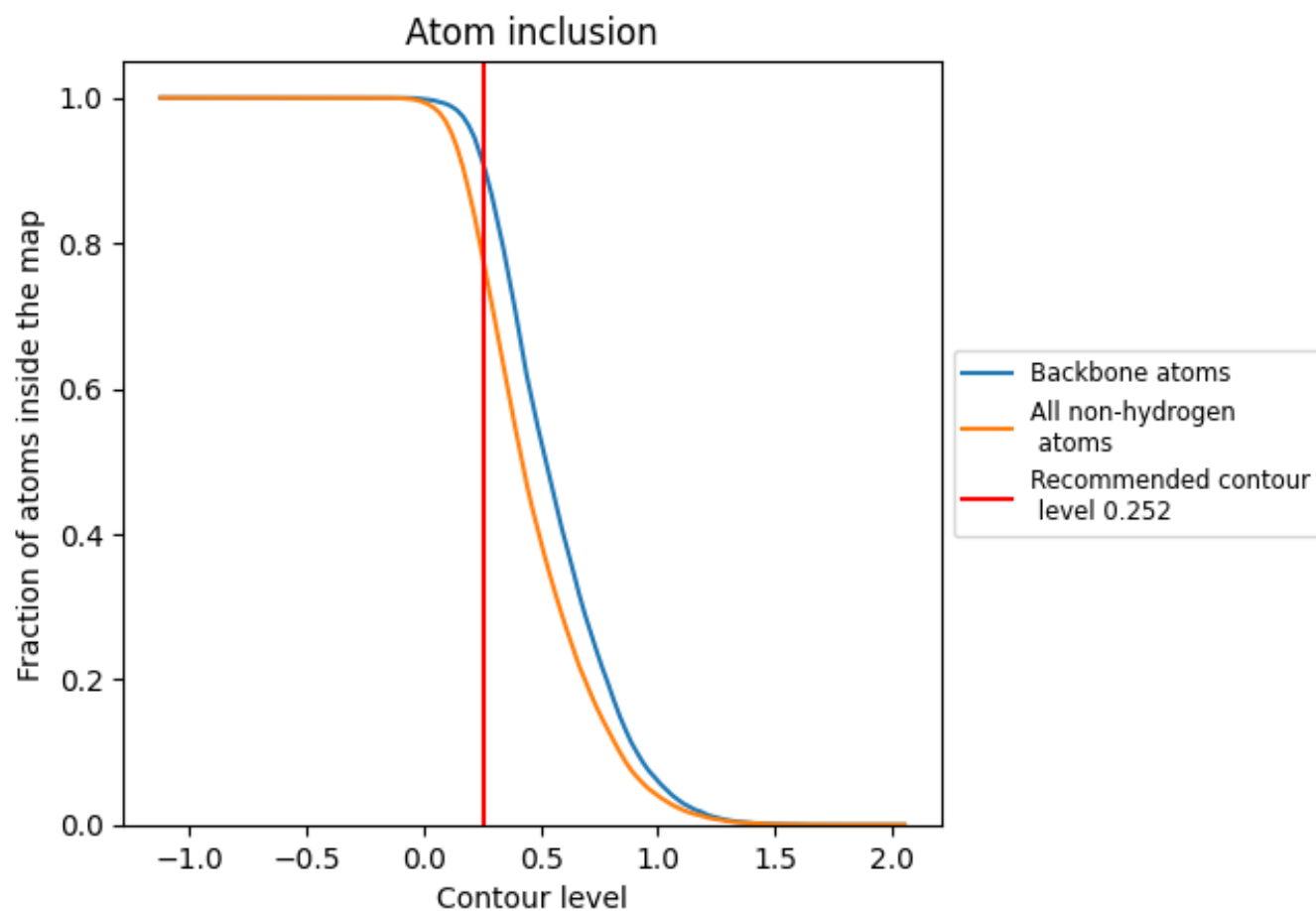
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.252).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.252) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7805	<div><div></div></div> 0.3810
A	<div><div></div></div> 0.8041	<div><div></div></div> 0.3900
B	<div><div></div></div> 0.8439	<div><div></div></div> 0.4320
C	<div><div></div></div> 0.8473	<div><div></div></div> 0.4300
D	<div><div></div></div> 0.8236	<div><div></div></div> 0.4080
E	<div><div></div></div> 0.7510	<div><div></div></div> 0.3530
F	<div><div></div></div> 0.6098	<div><div></div></div> 0.2640
G	<div><div></div></div> 0.6460	<div><div></div></div> 0.4230

1.0

0.0

<0.0