



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 05:37 PM EST

PDB ID : 6OA9  
EMDB ID : EMD-0665  
Title : Cdc48-Npl4 complex processing poly-ubiquitinated substrate in the presence of ATP  
Authors : Twomey, E.C.; Ji, Z.; Wales, T.E.; Bodnar, N.O.; Engen, J.R.; Rapoport, T.A.  
Deposited on : 2019-03-15  
Resolution : 3.90 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

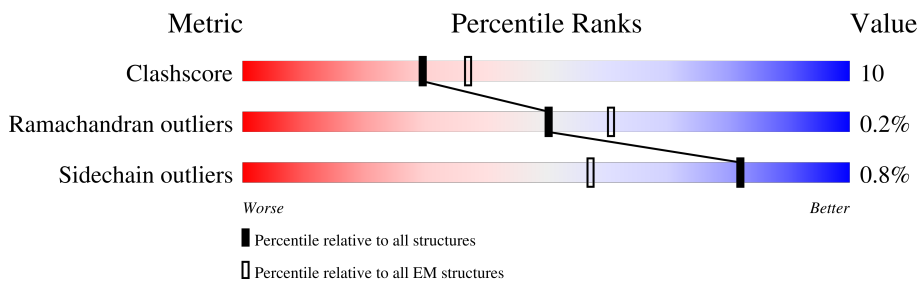
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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	835	
1	B	835	
1	C	835	
1	D	835	
1	E	835	
1	F	835	
2	H	76	
2	J	76	

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Mol	Chain	Length	Quality of chain
2	K	76	
3	G	580	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	A	901	-	-	X	-
4	ATP	C	1001	-	-	X	-
4	ATP	C	1003	-	-	X	-
4	ATP	D	901	-	-	X	-
4	ATP	D	902	-	-	X	-
4	ATP	E	902	-	-	X	-
4	ATP	F	901	-	-	X	-
5	ADP	E	901	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29006 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 Cell division control protein 48.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	547	Total	C	N	O	S	0	0
			4206	2641	732	814	19		
1	B	493	Total	C	N	O	S	0	0
			3767	2369	657	724	17		
1	C	492	Total	C	N	O	S	0	0
			3759	2363	656	723	17		
1	D	489	Total	C	N	O	S	0	0
			3747	2354	659	717	17		
1	E	496	Total	C	N	O	S	0	0
			3786	2380	660	729	17		
1	F	533	Total	C	N	O	S	0	0
			4093	2567	720	787	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	588	GLN	GLU	conflict	UNP P25694
B	588	GLN	GLU	conflict	UNP P25694
C	588	GLN	GLU	conflict	UNP P25694
D	588	GLN	GLU	conflict	UNP P25694
E	588	GLN	GLU	conflict	UNP P25694
F	588	GLN	GLU	conflict	UNP P25694

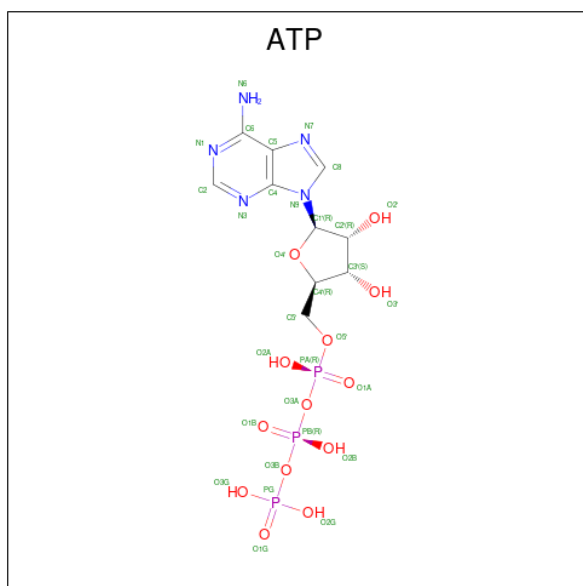
- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	48	Total	C	N	O		0	0
			376	237	63	76			
2	H	76	Total	C	N	O	S	0	0
			601	375	105	120	1		
2	J	76	Total	C	N	O	S	0	0
			601	375	105	120	1		

- Molecule 3 is a protein called Nuclear protein localization protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	468	Total	C	N	O	S	0	0
			3762	2381	628	732	21		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



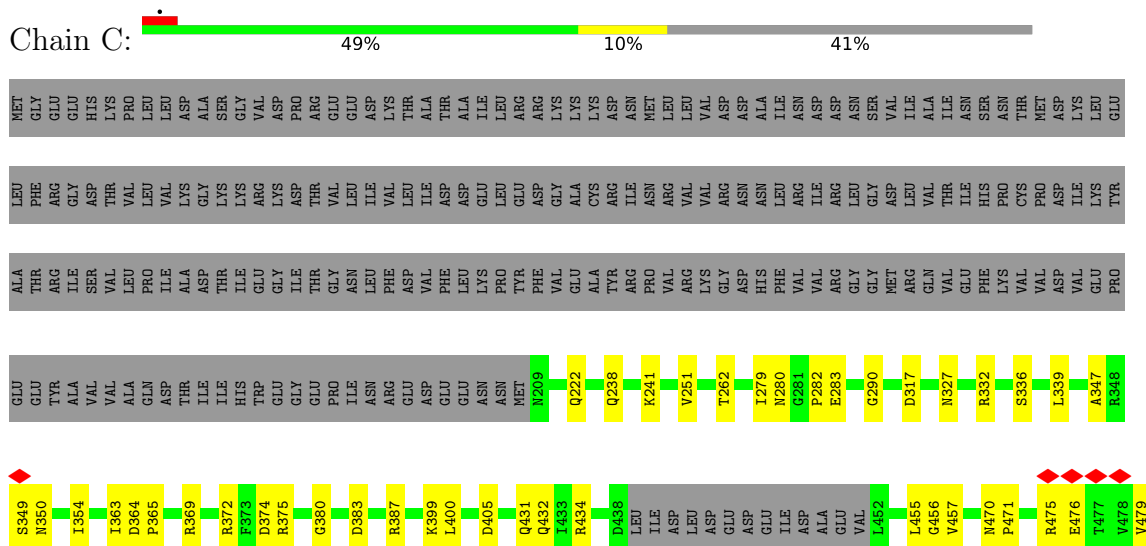
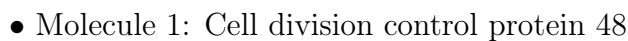


Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

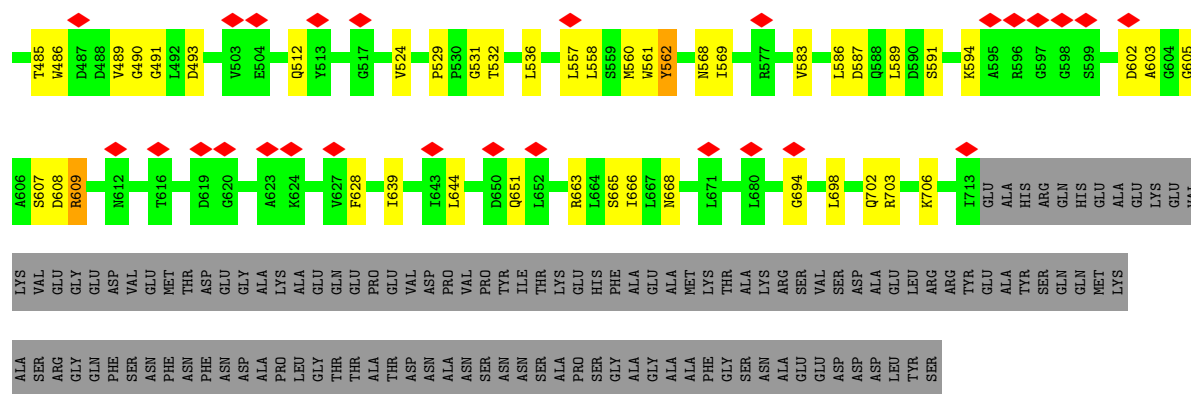
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	G	2	Total	Zn	0
			2	2	

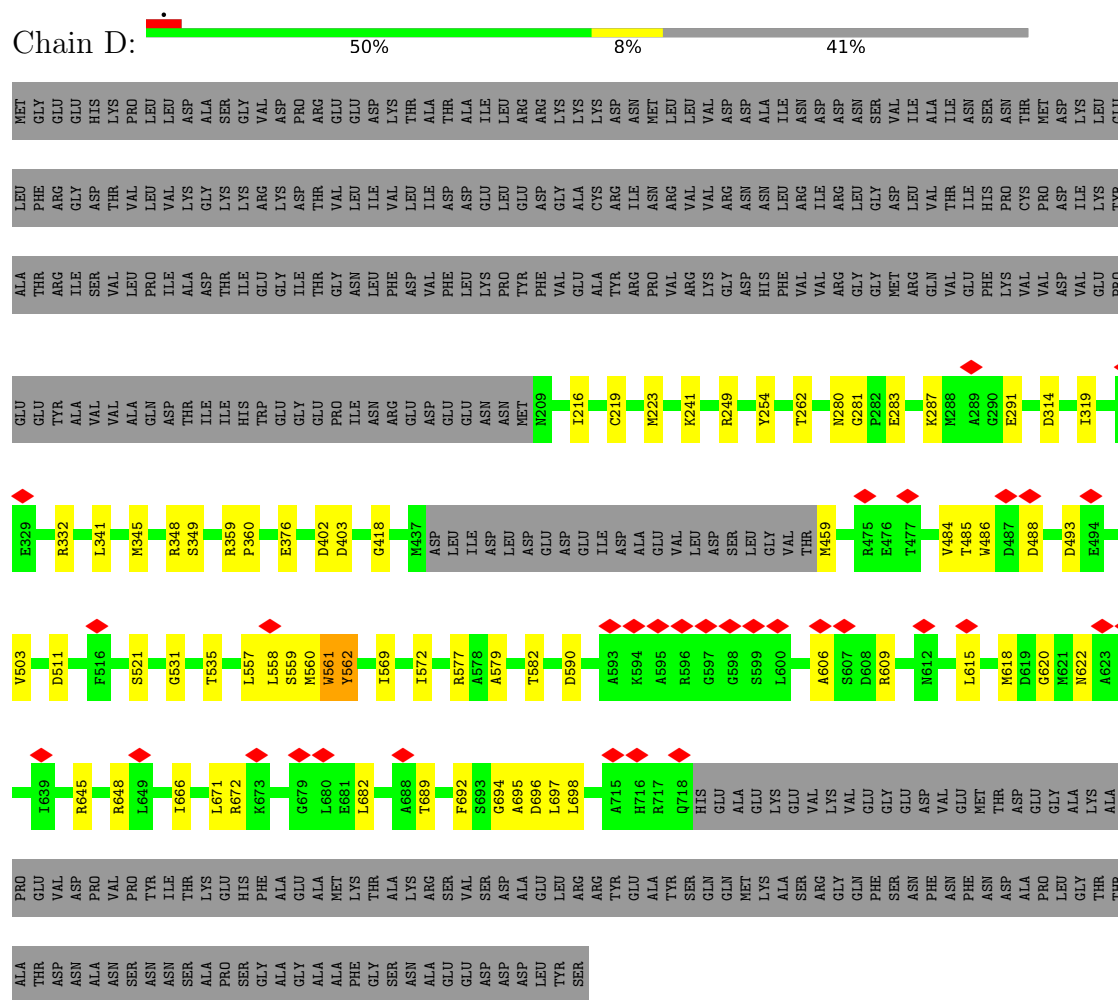




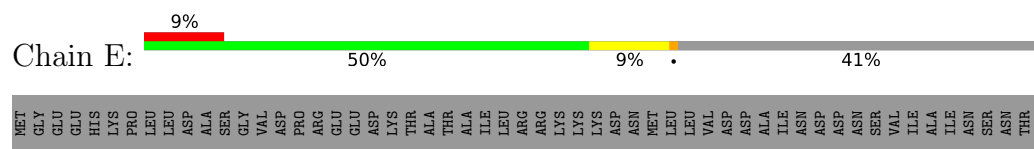




• Molecule 1: Cell division control protein 48



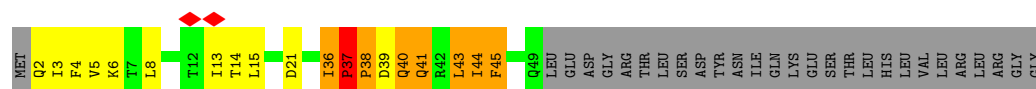
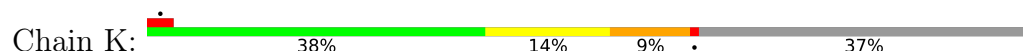
• Molecule 1: Cell division control protein 48



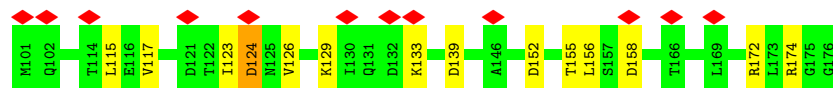
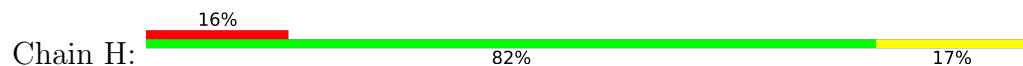




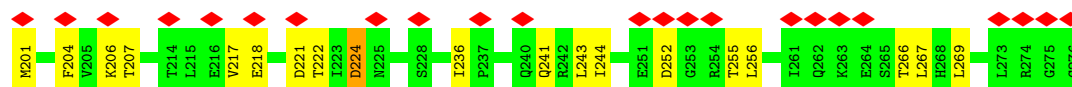
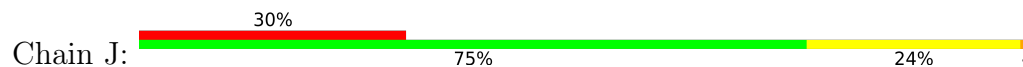
- Molecule 2: Ubiquitin



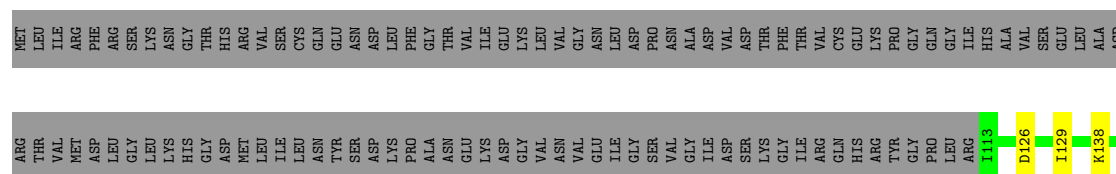
- Molecule 2: Ubiquitin

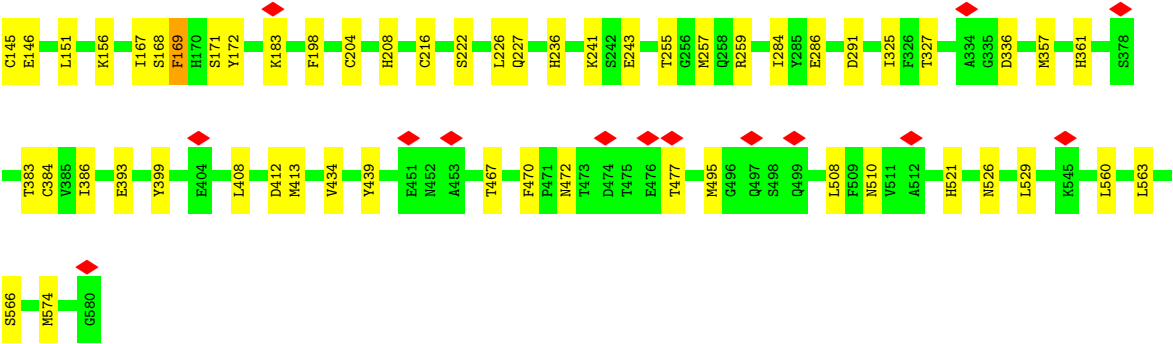


- Molecule 2: Ubiquitin



- Molecule 3: Nuclear protein localization protein 4





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127261	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	54.9	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	3.203	Depositor
Minimum map value	-1.441	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.45	Depositor
Map size ( $\text{\AA}$ )	270.0, 270.0, 270.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.35, 1.35, 1.35	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: ADP, ZN, 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	0.25	0/4273	0.47	0/5775
1	B	0.25	0/3827	0.47	1/5176 (0.0%)
1	C	0.25	0/3819	0.49	0/5165
1	D	0.26	0/3808	0.48	0/5148
1	E	0.27	0/3846	0.48	0/5202
1	F	0.25	0/4158	0.46	2/5614 (0.0%)
2	H	0.24	0/606	0.52	1/812 (0.1%)
2	J	0.24	0/606	0.48	1/812 (0.1%)
2	K	0.47	0/379	1.45	4/509 (0.8%)
3	G	0.26	0/3851	0.49	1/5201 (0.0%)
All	All	0.26	0/29173	0.50	10/39414 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	36	ILE	C-N-CD	-22.66	70.76	120.60
2	K	37	PRO	C-N-CD	-14.16	89.45	120.60
1	B	239	LEU	CA-CB-CG	6.94	131.27	115.30
2	K	43	LEU	N-CA-C	6.78	129.31	111.00
1	F	492	LEU	CA-CB-CG	6.22	129.60	115.30
2	K	43	LEU	CA-CB-CG	-5.90	101.74	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	508	LEU	CA-CB-CG	5.52	128.00	115.30
2	H	124	ASP	CB-CG-OD2	5.24	123.01	118.30
2	J	224	ASP	CB-CG-OD2	5.17	122.95	118.30
1	F	652	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	510	ASN	Peptide

## 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	4206	0	4232	60	0
1	B	3767	0	3811	81	0
1	C	3759	0	3798	85	0
1	D	3747	0	3784	120	0
1	E	3786	0	3827	129	0
1	F	4093	0	4121	65	0
2	H	601	0	622	8	0
2	J	601	0	622	11	0
2	K	376	0	392	60	0
3	G	3762	0	3638	46	0
4	A	31	0	12	24	0
4	B	31	0	12	2	0
4	C	93	0	32	63	0
4	D	62	0	22	45	0
4	E	31	0	10	15	0
4	F	31	0	12	18	0
5	E	27	0	11	25	0
6	G	2	0	0	0	0
All	All	29006	0	28958	587	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 (587) 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:E:536:LEU:HD22	5:E:901:ADP:C5'	1.23	1.63
1:E:536:LEU:CD2	5:E:901:ADP:H3'	1.14	1.60
1:E:536:LEU:CD2	5:E:901:ADP:C3'	1.85	1.55
1:D:559:SER:CB	1:E:562:TYR:HE2	1.18	1.52
1:D:216:ILE:HG22	4:D:902:ATP:N6	1.19	1.47
1:E:536:LEU:CD2	5:E:901:ADP:H5'2	1.45	1.43
1:D:559:SER:CB	1:E:562:TYR:CE2	2.03	1.42
1:B:489:VAL:HG13	4:C:1001:ATP:N6	1.39	1.35
1:D:562:TYR:CE2	1:D:609:ARG:NH2	1.92	1.34
1:D:216:ILE:CG2	4:D:902:ATP:HN61	1.43	1.32
4:C:1003:ATP:O1B	1:D:645:ARG:NH1	1.61	1.32
4:C:1003:ATP:O1B	1:D:645:ARG:CZ	1.78	1.31
1:E:418:GLY:O	4:E:902:ATP:N3	1.62	1.31
1:D:561:TRP:CD1	2:K:4:PHE:HB2	1.65	1.31
2:H:124:ASP:OD1	2:H:152:ASP:HB2	1.27	1.29
1:D:559:SER:OG	1:E:562:TYR:CE2	1.86	1.28
1:D:531:GLY:HA2	4:D:901:ATP:O1B	1.11	1.28
1:D:559:SER:HB2	1:E:562:TYR:CE2	1.64	1.25
1:D:216:ILE:CG2	4:D:902:ATP:N6	1.97	1.23
1:C:558:LEU:HD11	1:D:562:TYR:CZ	1.74	1.22
1:E:536:LEU:HD22	5:E:901:ADP:C4'	1.69	1.22
1:D:216:ILE:HG22	4:D:902:ATP:C6	1.74	1.21
1:B:531:GLY:O	4:C:1001:ATP:O5'	1.58	1.20
1:E:536:LEU:CD2	5:E:901:ADP:C5'	1.98	1.20
2:K:36:ILE:CG2	2:K:40:GLN:HB3	1.71	1.19
4:D:902:ATP:O1B	1:E:369:ARG:NH1	1.76	1.19
1:C:536:LEU:HD11	4:C:1003:ATP:C8	1.78	1.18
1:D:634:ASN:ND2	4:D:901:ATP:O3G	1.78	1.15
2:K:39:ASP:HB2	3:G:472:ASN:HB2	1.19	1.15
2:K:37:PRO:CB	2:K:38:PRO:HD2	1.76	1.14
1:B:489:VAL:CG1	4:C:1001:ATP:N6	2.09	1.13
1:F:263:LEU:HD22	4:F:901:ATP:C2'	1.77	1.13
1:D:531:GLY:CA	4:D:901:ATP:O1B	1.98	1.12
1:B:532:THR:CG2	4:C:1001:ATP:N3	2.12	1.12
1:F:263:LEU:HD22	4:F:901:ATP:H2'	1.24	1.12
2:K:36:ILE:HG21	2:K:40:GLN:HB3	1.15	1.11
1:C:558:LEU:HD11	1:D:562:TYR:OH	1.48	1.10
1:A:216:ILE:CA	4:A:901:ATP:HN61	1.65	1.09
1:E:536:LEU:CD2	5:E:901:ADP:C4'	2.28	1.09
1:C:262:THR:CG2	4:C:1002:ATP:O3G	2.00	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:THR:HG23	4:C:1002:ATP:O3G	1.51	1.09
1:A:216:ILE:HA	4:A:901:ATP:HN61	1.01	1.08
1:B:532:THR:CG2	4:C:1001:ATP:C2	2.35	1.08
1:A:217:GLY:H	4:A:901:ATP:N6	1.52	1.07
1:D:562:TYR:CD2	1:D:609:ARG:NH2	2.15	1.07
1:B:532:THR:HG21	4:C:1001:ATP:C2	1.89	1.07
1:E:536:LEU:HD21	5:E:901:ADP:C3'	1.66	1.07
1:E:536:LEU:HD22	5:E:901:ADP:H5'1	1.29	1.06
1:E:536:LEU:HB2	5:E:901:ADP:H5'2	1.37	1.06
1:D:606:ALA:HB1	1:E:562:TYR:OH	1.56	1.05
1:E:536:LEU:CB	5:E:901:ADP:H5'2	1.85	1.05
2:K:39:ASP:CB	3:G:472:ASN:HB2	1.87	1.04
1:D:562:TYR:HE2	1:D:609:ARG:CZ	1.70	1.03
1:D:561:TRP:HD1	2:K:4:PHE:CB	1.70	1.02
1:C:558:LEU:CD1	1:D:562:TYR:OH	2.06	1.01
1:D:562:TYR:HE2	1:D:609:ARG:NH2	1.41	1.01
1:E:536:LEU:HD23	5:E:901:ADP:C3'	1.89	1.01
1:C:694:GLY:HA3	4:C:1003:ATP:H2	1.23	1.00
1:E:536:LEU:HB2	5:E:901:ADP:C5'	1.91	0.99
1:D:262:THR:CG2	4:D:902:ATP:O3G	2.11	0.98
1:B:532:THR:HG23	4:C:1001:ATP:N3	1.79	0.97
2:K:37:PRO:CB	2:K:38:PRO:CD	2.40	0.97
1:A:217:GLY:H	4:A:901:ATP:HN62	1.09	0.97
2:K:36:ILE:CG2	2:K:40:GLN:CB	2.41	0.97
1:D:606:ALA:CB	1:E:562:TYR:CZ	2.48	0.97
1:D:606:ALA:HB3	1:E:562:TYR:CZ	2.00	0.96
1:E:261:LYS:O	1:E:263:LEU:N	1.99	0.96
1:D:561:TRP:HD1	2:K:4:PHE:HB2	0.78	0.95
1:D:606:ALA:CB	1:E:562:TYR:OH	2.15	0.94
1:B:489:VAL:HA	4:C:1001:ATP:HN61	1.33	0.94
2:K:37:PRO:HB3	2:K:38:PRO:HD2	1.48	0.94
1:E:536:LEU:CG	5:E:901:ADP:H5'2	1.96	0.94
1:D:559:SER:HB2	1:E:562:TYR:HE2	0.77	0.93
1:E:261:LYS:H	1:E:261:LYS:HD3	1.34	0.92
1:C:694:GLY:HA3	4:C:1003:ATP:C2	2.05	0.91
1:E:536:LEU:HD23	5:E:901:ADP:H5'2	1.53	0.91
2:K:44:ILE:HD13	3:G:393:GLU:OE1	1.70	0.91
1:D:562:TYR:HE2	1:D:609:ARG:NH1	1.69	0.90
1:A:260:GLY:CA	4:A:901:ATP:H5'2	2.01	0.90
1:D:262:THR:HG23	4:D:902:ATP:O3B	1.72	0.89
1:D:262:THR:HG22	4:D:902:ATP:O3G	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:562:TYR:CZ	1:E:609:ARG:NH1	2.40	0.89
1:D:666:ILE:HD13	4:D:901:ATP:C6	2.06	0.89
1:A:216:ILE:CA	4:A:901:ATP:N6	2.35	0.89
1:A:216:ILE:HA	4:A:901:ATP:N6	1.86	0.89
1:E:262:THR:HG22	4:E:902:ATP:O2A	1.73	0.89
1:B:532:THR:HG23	4:C:1001:ATP:C2	2.06	0.89
1:A:260:GLY:HA2	4:A:901:ATP:H5'2	1.55	0.88
1:B:532:THR:O	4:C:1001:ATP:O2B	1.91	0.88
1:D:216:ILE:HG22	4:D:902:ATP:C5	2.09	0.88
2:K:39:ASP:OD1	3:G:472:ASN:ND2	2.07	0.88
4:D:902:ATP:PB	1:E:369:ARG:HH12	1.97	0.88
1:C:536:LEU:CD1	4:C:1003:ATP:C8	2.57	0.87
2:K:37:PRO:HB2	2:K:38:PRO:HD2	1.55	0.87
1:B:532:THR:HA	4:C:1001:ATP:H5'2	1.57	0.87
2:K:44:ILE:O	2:K:45:PHE:HB2	1.75	0.87
1:A:217:GLY:N	4:A:901:ATP:N6	2.21	0.86
2:K:39:ASP:HB3	3:G:472:ASN:CG	1.96	0.86
1:B:532:THR:CG2	4:C:1001:ATP:C4	2.60	0.85
1:C:698:LEU:HD13	4:C:1003:ATP:O2'	1.75	0.85
1:E:562:TYR:OH	1:E:609:ARG:NH2	2.10	0.84
1:D:216:ILE:CB	4:D:902:ATP:HN61	1.90	0.83
1:D:561:TRP:HE1	2:K:5:VAL:H	1.24	0.83
1:B:558:LEU:CD1	1:C:562:TYR:OH	2.27	0.83
1:D:418:GLY:HA3	4:D:902:ATP:C2	2.14	0.83
2:K:37:PRO:HG2	2:K:40:GLN:OE1	1.79	0.83
1:B:489:VAL:CG1	4:C:1001:ATP:HN62	1.90	0.82
1:B:418:GLY:HA3	4:B:901:ATP:C2	2.15	0.82
1:E:263:LEU:O	1:E:266:ARG:N	2.12	0.82
1:A:262:THR:CG2	4:A:901:ATP:O3G	2.29	0.81
1:D:606:ALA:HB3	1:E:562:TYR:CE1	2.16	0.81
1:B:489:VAL:HG13	4:C:1001:ATP:C6	2.16	0.81
1:A:216:ILE:HB	4:A:901:ATP:N6	1.94	0.81
1:E:260:GLY:HA2	4:E:902:ATP:O2A	1.81	0.80
2:K:36:ILE:HG22	2:K:40:GLN:CB	2.11	0.80
1:B:558:LEU:HD22	1:C:562:TYR:CZ	2.17	0.80
1:D:216:ILE:CB	4:D:902:ATP:N6	2.45	0.80
1:A:260:GLY:HA2	4:A:901:ATP:C5'	2.12	0.80
2:K:39:ASP:CB	3:G:472:ASN:CB	2.59	0.79
1:D:606:ALA:HB1	1:E:562:TYR:HH	1.45	0.79
1:D:666:ILE:CD1	4:D:901:ATP:C6	2.66	0.79
1:F:263:LEU:CD2	4:F:901:ATP:C2'	2.60	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:TRP:CD1	2:K:4:PHE:CB	2.55	0.78
2:J:224:ASP:OD1	2:J:252:ASP:O	2.02	0.78
1:D:216:ILE:CG2	4:D:902:ATP:C6	2.58	0.78
1:E:261:LYS:O	1:E:262:THR:C	2.20	0.78
2:K:40:GLN:HA	3:G:470:PHE:O	1.83	0.78
1:D:560:MET:HG3	1:D:561:TRP:CE3	2.19	0.78
1:F:263:LEU:CD2	4:F:901:ATP:O2'	2.32	0.77
1:A:217:GLY:N	4:A:901:ATP:HN62	1.82	0.77
2:K:36:ILE:HG22	2:K:40:GLN:HB2	1.67	0.76
1:C:536:LEU:CD1	4:C:1003:ATP:N7	2.50	0.75
1:D:216:ILE:HG22	4:D:902:ATP:HN61	0.76	0.75
1:F:258:GLY:N	4:F:901:ATP:O1B	2.20	0.75
2:K:40:GLN:O	2:K:41:GLN:O	2.05	0.74
1:D:634:ASN:HD21	4:D:901:ATP:PG	2.10	0.74
1:A:216:ILE:CB	4:A:901:ATP:N6	2.51	0.74
1:C:561:TRP:CD2	2:K:8:LEU:HD11	2.24	0.73
1:F:258:GLY:O	4:F:901:ATP:H2	1.70	0.73
1:D:262:THR:CG2	4:D:902:ATP:PG	2.77	0.73
1:C:698:LEU:HD22	4:C:1003:ATP:O2'	1.89	0.73
2:K:36:ILE:CG2	2:K:37:PRO:HD2	2.16	0.72
1:B:489:VAL:CA	4:C:1001:ATP:HN61	2.03	0.72
1:B:558:LEU:HD13	1:C:562:TYR:OH	1.89	0.71
1:B:531:GLY:O	4:C:1001:ATP:PA	2.49	0.71
1:D:562:TYR:HD2	1:D:609:ARG:NH2	1.87	0.71
1:D:562:TYR:CE2	1:D:609:ARG:NH1	2.56	0.71
1:E:262:THR:CG2	4:E:902:ATP:O2A	2.39	0.71
1:D:262:THR:CG2	4:D:902:ATP:O3B	2.39	0.70
1:D:216:ILE:CG2	4:D:902:ATP:C5	2.75	0.69
1:E:262:THR:CG2	4:E:902:ATP:PA	2.80	0.69
1:B:532:THR:HA	4:C:1001:ATP:C5'	2.23	0.69
1:E:536:LEU:HD22	5:E:901:ADP:C3'	1.79	0.69
1:E:536:LEU:HD23	5:E:901:ADP:C2'	2.22	0.69
1:E:536:LEU:HD21	5:E:901:ADP:H3'	0.69	0.69
1:B:532:THR:HG22	4:C:1001:ATP:C4	2.26	0.68
1:D:694:GLY:HA3	4:D:901:ATP:C2	2.29	0.68
1:B:536:LEU:CD1	4:C:1001:ATP:C8	2.77	0.67
1:B:558:LEU:CD2	1:C:562:TYR:OH	2.42	0.67
2:K:39:ASP:CB	3:G:472:ASN:CG	2.63	0.66
1:F:394:HIS:HE1	4:F:901:ATP:H1'	1.60	0.66
1:D:535:THR:OG1	4:D:901:ATP:O2A	2.08	0.66
1:D:561:TRP:NE1	2:K:5:VAL:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:THR:HG21	4:C:1002:ATP:O3G	1.95	0.66
1:D:634:ASN:ND2	4:D:901:ATP:PG	2.67	0.66
1:D:666:ILE:HD11	4:D:901:ATP:N6	2.11	0.66
1:E:536:LEU:CD2	5:E:901:ADP:C2'	2.72	0.65
1:E:261:LYS:HD3	1:E:261:LYS:N	2.08	0.65
2:K:43:LEU:HD22	2:K:43:LEU:H	1.62	0.65
2:K:39:ASP:HB3	3:G:472:ASN:CB	2.26	0.65
1:B:489:VAL:HG12	4:C:1001:ATP:HN62	1.60	0.65
4:D:902:ATP:O1B	1:E:369:ARG:CZ	2.44	0.64
1:D:560:MET:HG3	1:D:561:TRP:CZ3	2.33	0.64
4:F:901:ATP:H3'	4:F:901:ATP:O2A	1.97	0.63
1:F:394:HIS:CE1	4:F:901:ATP:H1'	2.33	0.63
1:E:216:ILE:HG13	4:E:902:ATP:N7	2.14	0.63
4:C:1003:ATP:O1B	1:D:645:ARG:NH2	2.28	0.63
2:J:218:GLU:HB2	2:J:221:ASP:HB2	1.81	0.62
1:B:489:VAL:HG13	4:C:1001:ATP:HN61	1.56	0.62
1:D:418:GLY:HA3	4:D:902:ATP:H2	1.59	0.62
1:E:314:ASP:OD2	4:E:902:ATP:O3G	2.17	0.62
1:B:532:THR:HG21	4:C:1001:ATP:N1	2.15	0.62
1:B:536:LEU:HD11	4:C:1001:ATP:N7	2.15	0.61
2:K:39:ASP:HB2	3:G:472:ASN:CB	2.10	0.61
1:E:418:GLY:O	4:E:902:ATP:C2	2.47	0.61
2:K:44:ILE:O	2:K:45:PHE:CB	2.45	0.61
1:C:698:LEU:CD1	4:C:1003:ATP:O2'	2.47	0.61
1:D:561:TRP:HE1	2:K:5:VAL:N	1.96	0.61
1:F:583:VAL:HG23	1:F:628:PHE:HB3	1.83	0.61
1:E:560:MET:CE	1:E:561:TRP:HE1	2.13	0.60
1:E:553:LYS:HB3	1:E:556:GLU:HB2	1.84	0.60
1:C:531:GLY:N	4:C:1003:ATP:O2B	2.32	0.60
1:D:618:MET:HB3	1:D:648:ARG:HH21	1.66	0.60
1:B:536:LEU:CD1	4:C:1001:ATP:N7	2.65	0.60
1:E:560:MET:HE3	1:E:561:TRP:HE1	1.66	0.60
2:K:36:ILE:HG22	2:K:36:ILE:O	2.01	0.60
1:B:536:LEU:HD11	4:C:1001:ATP:C8	2.35	0.60
1:B:489:VAL:CG1	4:C:1001:ATP:HN61	2.13	0.59
1:E:536:LEU:HD23	5:E:901:ADP:C5'	2.15	0.59
1:C:222:GLN:HE22	1:C:380:GLY:H	1.50	0.58
1:C:524:VAL:HG23	1:C:651:GLN:HB2	1.83	0.58
1:D:666:ILE:CD1	4:D:901:ATP:N6	2.66	0.58
2:K:43:LEU:HD22	2:K:43:LEU:N	2.18	0.58
1:F:263:LEU:HD22	4:F:901:ATP:O2'	1.97	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:GLY:CA	4:C:1003:ATP:C2	2.83	0.57
1:C:347:ALA:HB1	1:C:350:ASN:HD22	1.69	0.57
1:C:561:TRP:CZ3	2:K:8:LEU:HD12	2.40	0.56
1:E:431:GLN:HB3	1:E:461:ASN:HD21	1.70	0.56
1:E:561:TRP:CD1	1:E:561:TRP:N	2.72	0.56
1:A:315:GLU:OE2	4:A:901:ATP:PG	2.64	0.56
1:E:261:LYS:O	1:E:264:MET:N	2.38	0.56
1:E:562:TYR:OH	1:E:609:ARG:CZ	2.53	0.56
1:B:558:LEU:HD22	1:C:562:TYR:OH	2.05	0.56
1:C:557:LEU:O	1:C:568:ASN:ND2	2.38	0.56
1:A:663:ARG:HG3	1:A:666:ILE:HD12	1.87	0.56
1:D:216:ILE:CG2	4:D:902:ATP:N7	2.68	0.56
1:E:428:ALA:O	1:E:461:ASN:ND2	2.39	0.56
1:F:419:ALA:HB2	4:F:901:ATP:H5'2	1.88	0.56
3:G:145:CYS:SG	3:G:146:GLU:N	2.79	0.56
1:D:280:ASN:HB3	1:D:283:GLU:HB2	1.88	0.56
1:D:484:VAL:HG13	1:D:488:ASP:HB2	1.88	0.56
2:K:37:PRO:HB2	2:K:38:PRO:CD	2.19	0.55
1:B:262:THR:OG1	4:B:901:ATP:O1A	2.25	0.55
1:B:558:LEU:HD11	1:C:562:TYR:OH	2.05	0.55
1:B:534:LYS:HG2	1:B:535:THR:HG23	1.87	0.55
1:E:261:LYS:H	1:E:261:LYS:CD	2.14	0.55
1:F:337:GLN:HE21	1:F:341:LEU:HD23	1.71	0.55
1:A:697:LEU:HD23	1:A:700:ILE:HD13	1.88	0.55
1:E:536:LEU:HD23	5:E:901:ADP:C4'	2.21	0.55
2:K:43:LEU:N	2:K:43:LEU:CD2	2.69	0.55
1:B:589:LEU:HB3	1:B:639:ILE:HD13	1.88	0.55
1:D:262:THR:HG23	4:D:902:ATP:PG	2.46	0.55
1:C:262:THR:HG23	4:C:1002:ATP:PG	2.48	0.54
1:C:639:ILE:HD12	1:C:644:LEU:HD21	1.89	0.54
1:E:562:TYR:CE1	1:E:609:ARG:NH1	2.75	0.54
2:J:204:PHE:HB2	2:J:266:THR:HA	1.90	0.54
1:B:400:LEU:HD12	1:B:404:VAL:HG21	1.89	0.54
1:B:493:ASP:OD1	1:B:493:ASP:N	2.41	0.54
1:D:577:ARG:HD2	1:D:625:LYS:HD3	1.90	0.53
1:E:262:THR:HG22	4:E:902:ATP:PA	2.48	0.53
1:D:561:TRP:CG	2:K:6:LYS:HD3	2.43	0.53
1:E:562:TYR:HH	1:E:609:ARG:NH2	2.07	0.53
1:A:513:TYR:HE2	1:A:520:PRO:HA	1.73	0.53
1:A:281:GLY:HA3	1:A:315:GLU:HB2	1.90	0.53
3:G:226:LEU:HD12	3:G:439:TYR:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:HB	4:A:901:ATP:HN62	1.74	0.53
1:B:490:GLY:H	4:C:1001:ATP:N6	2.06	0.53
1:B:591:SER:HB2	1:C:609:ARG:HG3	1.91	0.53
1:F:245:ILE:O	1:F:348:ARG:NH2	2.41	0.53
1:D:531:GLY:H	4:D:901:ATP:PB	2.31	0.52
1:D:559:SER:OG	1:E:562:TYR:CD2	2.32	0.52
1:E:340:THR:HG23	3:G:138:LYS:HB3	1.90	0.52
1:E:663:ARG:NH2	1:E:693:SER:O	2.41	0.52
2:J:201:MET:N	2:J:217:VAL:O	2.42	0.52
1:A:439:LEU:HD23	1:A:440:ILE:HG12	1.92	0.52
1:C:605:GLY:HA2	1:C:609:ARG:HH22	1.74	0.52
1:E:464:PHE:O	1:E:468:ASN:ND2	2.42	0.52
1:A:525:LEU:HD21	1:A:652:LEU:HD13	1.91	0.52
1:B:535:THR:HB	1:B:539:LYS:HE2	1.90	0.52
1:B:600:LEU:HD12	1:C:602:ASP:HB2	1.91	0.52
1:C:665:SER:HA	1:C:668:ASN:HB2	1.91	0.52
1:E:479:VAL:O	1:E:548:ASN:ND2	2.43	0.52
1:C:698:LEU:CD2	4:C:1003:ATP:O2'	2.57	0.52
1:E:261:LYS:N	1:E:261:LYS:CD	2.70	0.52
1:F:525:LEU:HD11	1:F:649:LEU:HD23	1.91	0.52
1:C:432:GLN:HG3	1:C:455:LEU:HD12	1.92	0.52
1:E:291:GLU:O	1:E:295:ASN:ND2	2.43	0.52
1:E:286:SER:HB2	1:F:333:ARG:HD2	1.90	0.52
1:E:479:VAL:HB	1:E:548:ASN:HD21	1.73	0.52
2:J:236:ILE:O	2:J:241:GLN:NE2	2.42	0.52
1:B:532:THR:C	4:C:1001:ATP:O2A	2.48	0.52
1:B:532:THR:CA	4:C:1001:ATP:H5'2	2.37	0.52
1:F:558:LEU:HG	1:F:606:ALA:HB1	1.91	0.52
1:B:261:LYS:NZ	1:B:358:ASN:OD1	2.44	0.51
1:B:536:LEU:HD11	4:C:1001:ATP:C5	2.44	0.51
1:B:532:THR:HG21	4:C:1001:ATP:C4	2.40	0.51
1:C:470:ASN:ND2	1:C:471:PRO:O	2.44	0.51
1:D:341:LEU:HD23	3:G:183:LYS:HG2	1.91	0.51
1:F:301:GLU:O	1:F:305:LYS:NZ	2.43	0.51
1:C:561:TRP:CE3	2:K:8:LEU:HD12	2.45	0.51
3:G:357:MET:O	3:G:361:HIS:ND1	2.44	0.51
1:A:260:GLY:HA2	4:A:901:ATP:O2A	2.11	0.51
1:E:399:LYS:HE2	1:E:452:LEU:HD13	1.92	0.51
1:E:562:TYR:HB3	2:K:2:GLN:HA	1.93	0.51
1:C:557:LEU:HD21	1:C:569:ILE:HG12	1.93	0.51
1:D:502:THR:HG23	1:D:503:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:902:ATP:PB	1:E:369:ARG:NH1	2.70	0.51
1:C:703:ARG:HD2	1:C:706:LYS:HE2	1.92	0.51
1:D:281:GLY:HA2	1:D:319:ILE:HD11	1.93	0.51
3:G:412:ASP:OD1	3:G:412:ASP:N	2.43	0.51
1:B:534:LYS:HB2	4:C:1001:ATP:O3B	2.11	0.51
1:F:663:ARG:NH2	1:F:689:THR:OG1	2.44	0.51
1:C:431:GLN:OE1	1:C:434:ARG:NH2	2.44	0.50
1:D:671:LEU:HD21	1:D:682:LEU:HD11	1.93	0.50
1:A:464:PHE:O	1:A:468:ASN:ND2	2.44	0.50
1:A:616:THR:OG1	1:F:475:ARG:NH2	2.44	0.50
1:D:558:LEU:HD12	1:D:560:MET:H	1.77	0.50
1:E:536:LEU:HD23	5:E:901:ADP:H8	1.77	0.50
1:C:405:ASP:OD1	1:C:405:ASP:N	2.44	0.50
2:K:13:ILE:HG22	2:K:14:THR:HG22	1.94	0.50
1:B:664:LEU:O	1:B:668:ASN:ND2	2.45	0.50
1:B:698:LEU:HD12	4:C:1001:ATP:O2'	2.12	0.50
1:C:251:VAL:HB	1:C:354:ILE:HG22	1.92	0.50
1:B:558:LEU:CD2	1:C:562:TYR:CZ	2.92	0.50
1:D:216:ILE:HB	4:D:902:ATP:N6	2.25	0.50
1:E:300:PHE:HE1	1:E:311:ILE:HG21	1.77	0.50
1:E:562:TYR:CD2	1:E:562:TYR:C	2.85	0.50
1:D:216:ILE:CA	4:D:902:ATP:HN61	2.25	0.50
1:B:283:GLU:O	1:B:287:LYS:NZ	2.41	0.49
1:F:522:LYS:HD2	1:F:648:ARG:HG3	1.94	0.49
1:F:393:ILE:HA	1:F:396:LYS:HE3	1.94	0.49
1:C:586:LEU:HD13	1:C:589:LEU:HD13	1.94	0.49
1:D:280:ASN:ND2	1:D:283:GLU:OE1	2.45	0.49
1:E:669:ALA:O	1:E:672:ARG:NH1	2.45	0.49
1:E:696:ASP:OD1	1:F:645:ARG:NH1	2.45	0.49
2:K:40:GLN:O	2:K:41:GLN:C	2.51	0.49
2:K:40:GLN:C	2:K:41:GLN:O	2.49	0.49
1:C:561:TRP:CE3	2:K:8:LEU:CD1	2.95	0.49
1:F:336:SER:HA	1:F:339:LEU:HD12	1.95	0.49
3:G:126:ASP:OD1	3:G:126:ASP:N	2.46	0.49
1:A:500:LYS:HD2	1:A:504:GLU:HG2	1.95	0.49
1:D:511:ASP:OD1	1:D:511:ASP:N	2.46	0.49
2:K:40:GLN:CA	3:G:470:PHE:O	2.57	0.49
1:E:560:MET:CE	1:E:561:TRP:NE1	2.75	0.49
1:F:525:LEU:HB2	1:F:652:LEU:HA	1.94	0.49
1:B:560:MET:HB3	1:B:564:GLU:HB2	1.95	0.49
1:E:216:ILE:C	4:E:902:ATP:N6	2.62	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:561:TRP:H	1:E:561:TRP:HD1	1.58	0.49
1:A:317:ASP:OD1	1:A:317:ASP:N	2.46	0.49
1:A:549:PHE:HE1	1:A:585:PHE:HB3	1.77	0.49
1:B:382:PRO:O	1:B:387:ARG:NH1	2.45	0.49
1:E:536:LEU:HD23	5:E:901:ADP:C8	2.48	0.49
1:E:222:GLN:HE21	1:E:379:ILE:HG22	1.78	0.49
1:E:263:LEU:HD12	1:E:266:ARG:HB3	1.95	0.49
1:E:663:ARG:HD3	1:E:686:ALA:HB1	1.94	0.49
1:F:693:SER:OG	1:F:694:GLY:N	2.45	0.49
1:A:485:THR:HA	1:A:543:THR:HG21	1.93	0.48
1:D:561:TRP:NE1	2:K:5:VAL:N	2.56	0.48
1:B:658:PRO:O	1:B:663:ARG:NH1	2.46	0.48
1:C:238:GLN:HA	1:C:241:LYS:HE2	1.95	0.48
1:F:493:ASP:HA	1:F:496:LYS:HE2	1.94	0.48
2:J:244:ILE:HD13	3:G:574:MET:HG3	1.95	0.48
1:B:534:LYS:HB2	4:C:1001:ATP:O3G	2.13	0.48
3:G:167:ILE:O	3:G:171:SER:OG	2.30	0.48
1:D:287:LYS:HD3	1:D:291:GLU:HB2	1.96	0.48
1:D:314:ASP:OD1	1:D:314:ASP:N	2.47	0.48
1:D:403:ASP:OD2	1:D:459:MET:N	2.47	0.48
1:E:261:LYS:C	1:E:263:LEU:N	2.65	0.48
1:B:671:LEU:HD23	1:B:676:LEU:HD22	1.96	0.48
3:G:259:ARG:NH2	3:G:286:GLU:OE1	2.46	0.48
3:G:383:THR:OG1	3:G:399:TYR:O	2.32	0.48
1:F:263:LEU:HD13	4:F:901:ATP:O2A	2.13	0.48
1:E:369:ARG:HB2	1:E:372:ARG:HD2	1.96	0.48
2:H:117:VAL:HG11	2:H:126:VAL:HG22	1.96	0.48
1:C:558:LEU:HD11	1:D:562:TYR:CE2	2.38	0.48
1:F:258:GLY:O	4:F:901:ATP:C2	2.61	0.48
3:G:236:HIS:ND1	3:G:467:THR:O	2.47	0.48
1:D:241:LYS:HG3	1:D:348:ARG:HH12	1.79	0.47
1:A:343:ASP:OD2	1:A:372:ARG:NH2	2.47	0.47
1:D:254:TYR:HE1	1:D:376:GLU:HB2	1.78	0.47
1:D:560:MET:CG	1:D:561:TRP:CZ3	2.97	0.47
1:E:339:LEU:HD22	1:E:372:ARG:HD3	1.96	0.47
1:F:234:LEU:HD22	1:F:308:PRO:HB3	1.95	0.47
1:A:399:LYS:NZ	1:B:242:ALA:O	2.46	0.47
1:D:531:GLY:N	4:D:901:ATP:O1B	2.46	0.47
1:D:615:LEU:O	1:D:648:ARG:NH1	2.48	0.47
2:K:39:ASP:CG	3:G:472:ASN:ND2	2.67	0.47
3:G:521:HIS:HD2	3:G:560:LEU:HD13	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ARG:NH1	1:B:342:MET:O	2.48	0.47
1:B:489:VAL:CA	4:C:1001:ATP:N6	2.74	0.47
1:C:591:SER:O	1:C:594:LYS:NZ	2.45	0.47
1:F:614:LEU:O	1:F:648:ARG:NH2	2.47	0.47
1:D:216:ILE:HA	4:D:902:ATP:HN61	1.80	0.47
1:C:349:SER:O	1:C:349:SER:OG	2.32	0.47
1:C:493:ASP:OD1	1:C:493:ASP:N	2.47	0.47
1:E:499:LEU:HD11	1:E:524:VAL:HG11	1.97	0.47
1:C:369:ARG:HH21	1:C:372:ARG:HH22	1.63	0.47
1:E:430:MET:SD	1:F:375:ARG:NH2	2.87	0.47
3:G:198:PHE:H	3:G:408:LEU:HD22	1.80	0.47
1:C:374:ASP:OD1	1:C:374:ASP:N	2.44	0.46
2:H:123:ILE:HB	2:H:152:ASP:HA	1.97	0.46
1:A:246:LYS:HD3	1:A:247:PRO:HD2	1.97	0.46
1:F:317:ASP:OD1	1:F:317:ASP:N	2.48	0.46
1:A:262:THR:HG23	4:A:901:ATP:O3B	2.15	0.46
1:C:698:LEU:HD13	4:C:1003:ATP:HO2'	1.80	0.46
1:D:694:GLY:HA2	1:D:697:LEU:HD12	1.97	0.46
4:D:901:ATP:O1B	1:E:645:ARG:NH2	2.48	0.46
1:E:650:ASP:OD1	1:E:650:ASP:N	2.47	0.46
1:F:495:ILE:HD11	1:F:653:ILE:HD12	1.97	0.46
3:G:168:SER:OG	3:G:171:SER:OG	2.30	0.46
1:A:687:LYS:O	1:A:690:GLN:NE2	2.48	0.46
3:G:336:ASP:N	3:G:336:ASP:OD1	2.45	0.46
1:C:603:ALA:HB2	2:K:3:ILE:HB	1.96	0.46
1:E:452:LEU:HA	1:E:455:LEU:HD23	1.97	0.46
1:E:536:LEU:CG	5:E:901:ADP:C5'	2.75	0.46
3:G:526:ASN:HB3	3:G:529:LEU:HB3	1.97	0.46
1:C:536:LEU:HD12	4:C:1003:ATP:N7	2.29	0.46
1:E:261:LYS:NZ	4:E:902:ATP:O1G	2.48	0.46
2:J:207:THR:HA	2:J:269:LEU:HB3	1.97	0.46
1:F:260:GLY:HA2	4:F:901:ATP:O2A	2.16	0.46
1:D:694:GLY:HA3	4:D:901:ATP:N3	2.30	0.46
1:B:430:MET:HG2	1:C:375:ARG:HH12	1.81	0.46
1:D:493:ASP:N	1:D:493:ASP:OD1	2.48	0.46
1:F:622:ASN:O	1:F:624:LYS:NZ	2.42	0.46
1:A:432:GLN:OE1	1:A:461:ASN:ND2	2.49	0.46
1:C:383:ASP:O	1:C:387:ARG:NH2	2.49	0.46
1:F:647:GLY:H	1:F:650:ASP:HB3	1.81	0.46
3:G:291:ASP:OD1	3:G:291:ASP:N	2.48	0.46
1:B:709:ILE:HG23	1:C:512:GLN:HE21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:PRO:HB3	1:D:332:ARG:HG2	1.98	0.45
1:E:259:THR:HG23	1:E:261:LYS:HD2	1.97	0.45
1:C:280:ASN:HB3	1:C:283:GLU:HB2	1.97	0.45
1:D:562:TYR:CD2	1:D:562:TYR:O	2.69	0.45
1:B:532:THR:HG21	4:C:1001:ATP:C6	2.51	0.45
2:H:115:LEU:HD11	2:H:129:LYS:HB3	1.98	0.45
1:A:316:ILE:HD13	1:A:355:ALA:HB1	1.99	0.45
1:C:336:SER:HA	1:C:339:LEU:HG	1.99	0.45
1:E:481:SER:HB2	1:E:543:THR:HG22	1.97	0.45
2:K:44:ILE:HG22	2:K:45:PHE:N	2.32	0.45
3:G:168:SER:OG	3:G:168:SER:O	2.34	0.45
1:A:219:CYS:HB2	1:A:222:GLN:HB2	1.99	0.45
1:B:317:ASP:N	1:B:317:ASP:OD1	2.45	0.45
1:B:536:LEU:HD13	4:C:1001:ATP:C8	2.50	0.45
1:C:485:THR:OG1	1:C:486:TRP:N	2.48	0.45
1:D:695:ALA:HA	1:D:698:LEU:HD12	1.96	0.45
1:F:671:LEU:HD13	1:F:676:LEU:HD22	1.99	0.45
1:B:286:SER:OG	1:C:290:GLY:O	2.33	0.45
1:B:534:LYS:HB2	4:C:1001:ATP:PG	2.56	0.45
1:E:535:THR:OG1	5:E:901:ADP:O3A	2.35	0.45
1:F:390:VAL:HA	1:F:393:ILE:HD12	1.99	0.45
2:H:158:ASP:OD1	2:H:158:ASP:N	2.46	0.45
1:E:562:TYR:CZ	1:E:609:ARG:CZ	2.99	0.45
1:F:263:LEU:HD22	4:F:901:ATP:C3'	2.43	0.45
2:K:36:ILE:HG23	2:K:37:PRO:HD2	1.98	0.45
1:B:291:GLU:OE1	3:G:222:SER:OG	2.35	0.45
1:F:680:LEU:HG	1:F:755:LYS:HG3	1.98	0.45
4:F:901:ATP:N3	4:F:901:ATP:H5'1	2.32	0.45
1:A:216:ILE:C	4:A:901:ATP:N6	2.68	0.45
1:E:562:TYR:CD2	1:E:562:TYR:O	2.70	0.45
1:F:222:GLN:HE21	1:F:379:ILE:HD13	1.82	0.45
1:F:321:PRO:HD2	1:F:323:ARG:HH12	1.82	0.45
1:F:436:LYS:HA	1:F:436:LYS:HD3	1.79	0.45
1:C:400:LEU:HA	1:C:457:VAL:HG22	1.99	0.44
1:C:594:LYS:HE3	1:C:607:SER:HB3	1.99	0.44
1:F:527:TYR:HB3	1:F:633:THR:HG23	1.98	0.44
1:C:561:TRP:CE2	2:K:8:LEU:HD11	2.52	0.44
1:C:587:ASP:OD1	1:C:587:ASP:N	2.51	0.44
4:D:902:ATP:O1B	1:E:369:ARG:NH2	2.50	0.44
1:F:387:ARG:HA	1:F:390:VAL:HG22	1.98	0.44
1:F:605:GLY:HA2	1:F:609:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:255:THR:HG23	3:G:257:MET:H	1.82	0.44
1:A:590:ASP:OD1	1:A:590:ASP:N	2.48	0.44
1:D:622:ASN:HB3	1:D:625:LYS:HD2	1.99	0.44
1:E:571:ASP:O	1:E:575:LYS:NZ	2.47	0.44
3:G:413:MET:HG3	3:G:434:VAL:HG11	2.00	0.44
1:B:677:GLU:HG3	1:B:679:GLY:H	1.82	0.44
1:C:702:GLN:NE2	1:D:521:SER:OG	2.50	0.44
2:J:243:LEU:HD11	2:J:267:LEU:HB3	1.99	0.44
1:A:262:THR:HG21	4:A:901:ATP:O3G	2.16	0.44
1:E:262:THR:CG2	4:E:902:ATP:O1A	2.66	0.44
3:G:325:ILE:HG22	3:G:384:CYS:HB3	2.00	0.44
1:B:531:GLY:HA2	1:B:695:ALA:HB2	2.00	0.43
1:D:249:ARG:NH1	1:D:349:SER:O	2.49	0.43
3:G:327:THR:HG22	3:G:386:ILE:HD12	2.00	0.43
3:G:495:MET:SD	3:G:495:MET:N	2.91	0.43
1:D:531:GLY:CA	4:D:901:ATP:PB	3.02	0.43
1:D:561:TRP:CD1	2:K:5:VAL:N	2.85	0.43
1:A:624:LYS:HE3	1:F:464:PHE:HA	2.00	0.43
1:D:262:THR:HG21	4:D:902:ATP:PG	2.54	0.43
1:A:262:THR:HG22	4:A:901:ATP:O3G	2.17	0.43
1:A:530:PRO:HB3	1:A:634:ASN:HB3	2.00	0.43
1:B:328:GLY:HA3	2:K:15:LEU:HD23	2.00	0.43
1:D:561:TRP:CD1	2:K:6:LYS:HD3	2.54	0.43
1:D:689:THR:HB	1:D:692:PHE:HB2	2.00	0.43
1:E:561:TRP:CD1	1:E:564:GLU:HG3	2.54	0.43
1:E:574:ASP:OD1	1:E:574:ASP:N	2.47	0.43
1:A:490:GLY:H	1:A:666:ILE:HG12	1.83	0.43
1:A:677:GLU:HG2	1:A:679:GLY:H	1.84	0.43
1:D:590:ASP:OD1	1:D:590:ASP:N	2.44	0.43
1:F:258:GLY:CA	4:F:901:ATP:O1B	2.66	0.43
2:H:172:ARG:O	2:H:174:ARG:NH2	2.51	0.43
1:D:359:ARG:HD2	1:D:360:PRO:HD2	2.01	0.43
1:D:485:THR:OG1	1:D:486:TRP:N	2.51	0.43
1:E:560:MET:HE2	1:E:561:TRP:NE1	2.34	0.43
2:J:206:LYS:HB3	2:J:206:LYS:HE2	1.87	0.43
1:B:587:ASP:N	1:B:587:ASP:OD1	2.52	0.43
1:C:317:ASP:HA	1:C:363:ILE:HD13	2.00	0.43
1:C:327:ASN:OD1	1:C:332:ARG:NH1	2.51	0.43
1:D:557:LEU:HD21	1:D:569:ILE:HD12	1.99	0.43
1:E:562:TYR:CB	2:K:2:GLN:HA	2.48	0.43
1:A:260:GLY:HA3	4:A:901:ATP:H5'2	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:LEU:HA	1:B:649:LEU:HD12	2.00	0.43
1:C:561:TRP:CD2	2:K:8:LEU:CD1	2.98	0.43
2:J:255:THR:OG1	2:J:256:LEU:N	2.52	0.43
1:C:706:LYS:HB2	1:D:501:GLU:HG2	2.00	0.43
1:E:217:GLY:N	4:E:902:ATP:N6	2.66	0.43
1:A:663:ARG:HD2	1:A:686:ALA:HB1	2.00	0.42
1:C:663:ARG:HG2	1:C:666:ILE:HD12	2.00	0.42
1:F:504:GLU:HB3	1:F:545:VAL:HG12	2.00	0.42
1:F:529:PRO:HA	1:F:530:PRO:HD3	1.85	0.42
3:G:208:HIS:NE2	3:G:216:CYS:SG	2.91	0.42
1:A:239:LEU:HD13	1:F:433:ILE:HD13	2.01	0.42
1:C:583:VAL:HG13	1:C:628:PHE:HZ	1.84	0.42
1:D:666:ILE:CD1	4:D:901:ATP:N1	2.82	0.42
1:E:301:GLU:O	1:E:305:LYS:NZ	2.49	0.42
1:F:263:LEU:CD2	4:F:901:ATP:H2'	2.18	0.42
1:F:343:ASP:OD1	1:F:343:ASP:N	2.45	0.42
1:A:431:GLN:HA	1:A:434:ARG:HG2	2.02	0.42
1:E:262:THR:HG21	4:E:902:ATP:O1A	2.18	0.42
1:F:511:ASP:OD1	1:F:511:ASP:N	2.51	0.42
2:H:139:ASP:O	2:H:174:ARG:NH1	2.52	0.42
1:B:532:THR:C	4:C:1001:ATP:O2B	2.56	0.42
1:F:564:GLU:OE1	1:F:568:ASN:ND2	2.42	0.42
1:A:314:ASP:OD2	4:A:901:ATP:O3G	2.38	0.42
1:C:489:VAL:CG2	4:C:1003:ATP:N6	2.83	0.42
1:D:488:ASP:OD1	1:D:672:ARG:NH1	2.52	0.42
1:D:696:ASP:HA	1:E:646:PRO:HG2	2.00	0.42
1:E:259:THR:CG2	1:E:261:LYS:HD2	2.49	0.42
1:E:529:PRO:O	1:E:534:LYS:NZ	2.51	0.42
1:F:648:ARG:HG2	1:F:649:LEU:HD12	2.01	0.42
2:K:39:ASP:O	3:G:472:ASN:N	2.53	0.42
1:B:275:PHE:HE1	1:B:277:PHE:HD1	1.67	0.42
1:D:345:MET:O	1:D:349:SER:OG	2.35	0.42
1:A:387:ARG:NH1	1:A:413:THR:O	2.52	0.42
1:A:777:TYR:HA	1:A:780:TYR:HB2	2.02	0.42
1:E:466:LEU:HA	1:E:469:SER:HB3	2.02	0.42
1:D:577:ARG:NH2	1:D:620:GLY:O	2.45	0.42
1:F:364:ASP:HA	1:F:365:PRO:HD3	1.94	0.42
1:F:417:VAL:HG13	1:F:419:ALA:H	1.85	0.42
2:H:155:THR:OG1	2:H:156:LEU:N	2.50	0.42
3:G:241:LYS:HG3	3:G:243:GLU:H	1.83	0.42
1:A:391:LEU:HD13	1:A:409:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:LEU:HD23	1:B:495:ILE:HD12	2.02	0.42
1:C:476:GLU:HG3	1:C:479:VAL:HB	2.02	0.42
1:E:391:LEU:HD13	1:E:406:LEU:HB3	2.02	0.42
3:G:129:ILE:HB	3:G:151:LEU:HB3	2.02	0.42
1:A:279:ILE:HB	1:A:313:ILE:HG22	2.01	0.41
1:A:311:ILE:HB	1:A:353:VAL:HG12	2.02	0.41
1:B:432:GLN:NE2	1:B:456:GLY:O	2.54	0.41
1:E:325:LYS:HD3	1:E:325:LYS:HA	1.84	0.41
1:F:477:THR:HG21	1:F:550:ILE:HG23	2.02	0.41
1:A:415:GLY:HA3	1:A:474:LEU:HD11	2.02	0.41
1:D:219:CYS:O	1:D:223:MET:N	2.51	0.41
1:C:529:PRO:HG2	1:C:532:THR:HG21	2.02	0.41
1:F:413:THR:HB	1:F:416:TYR:HB2	2.02	0.41
3:G:169:PHE:HA	3:G:172:TYR:HB3	2.01	0.41
1:C:560:MET:O	2:K:6:LYS:NZ	2.50	0.41
3:G:284:ILE:HG21	3:G:325:ILE:HD11	2.02	0.41
1:B:666:ILE:HD13	4:C:1001:ATP:C2	2.55	0.41
1:E:640:ASP:HA	1:E:641:PRO:HD3	1.95	0.41
1:A:470:ASN:N	1:A:470:ASN:OD1	2.53	0.41
1:C:279:ILE:HD13	1:C:279:ILE:HA	1.97	0.41
1:E:551:SER:HA	1:E:585:PHE:HB3	2.02	0.41
1:F:689:THR:HA	1:F:692:PHE:HD1	1.86	0.41
1:D:572:ILE:HD12	1:D:572:ILE:HA	1.95	0.41
1:D:579:ALA:O	1:D:582:THR:OG1	2.32	0.41
1:E:261:LYS:HG3	1:E:379:ILE:HD11	2.03	0.41
1:A:262:THR:HG23	4:A:901:ATP:O3G	2.16	0.41
1:A:296:LEU:HD21	1:A:338:LEU:HD13	2.02	0.41
1:C:490:GLY:HA3	1:C:666:ILE:HG12	2.02	0.41
1:C:608:ASP:N	1:C:608:ASP:OD1	2.54	0.41
1:E:399:LYS:NZ	1:F:241:LYS:O	2.43	0.41
1:B:533:GLY:N	4:C:1001:ATP:O2A	2.54	0.41
4:C:1003:ATP:PB	1:D:645:ARG:CZ	3.00	0.41
1:E:278:LEU:HD23	1:E:278:LEU:HA	1.94	0.41
2:K:21:ASP:OD2	3:G:227:GLN:NE2	2.43	0.41
2:J:222:THR:HA	2:J:255:THR:HA	2.02	0.41
1:B:387:ARG:NE	1:B:413:THR:O	2.54	0.41
1:C:491:GLY:N	1:C:665:SER:OG	2.54	0.41
1:E:209:ASN:N	1:E:209:ASN:OD1	2.53	0.41
1:E:625:LYS:HA	1:E:625:LYS:HD3	1.86	0.41
1:F:383:ASP:N	1:F:383:ASP:OD1	2.45	0.41
3:G:168:SER:O	3:G:171:SER:OG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:ASP:HA	1:C:365:PRO:HD3	1.96	0.40
1:D:562:TYR:CE2	1:D:609:ARG:CZ	2.59	0.40
1:F:663:ARG:HD2	1:F:697:LEU:HD12	2.04	0.40
1:B:417:VAL:HG23	1:B:419:ALA:H	1.86	0.40
1:E:256:PRO:HA	1:E:257:PRO:HD3	1.96	0.40
1:E:314:ASP:HA	1:E:356:ALA:HB3	2.03	0.40
1:E:357:THR:OG1	1:E:358:ASN:N	2.53	0.40
1:A:706:LYS:HD2	1:A:706:LYS:HA	1.94	0.40
1:E:263:LEU:O	1:E:264:MET:C	2.59	0.40
1:F:637:ASP:N	1:F:637:ASP:OD1	2.54	0.40
1:E:418:GLY:O	4:E:902:ATP:C4	2.60	0.40
3:G:563:LEU:O	3:G:566:SER:OG	2.36	0.40
1:C:399:LYS:HG3	1:C:456:GLY:HA2	2.04	0.40
1:D:402:ASP:OD1	1:D:402:ASP:N	2.48	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	543/835 (65%)	522 (96%)	21 (4%)	0	100	100
1	B	489/835 (59%)	454 (93%)	35 (7%)	0	100	100
1	C	488/835 (58%)	447 (92%)	41 (8%)	0	100	100
1	D	485/835 (58%)	449 (93%)	36 (7%)	0	100	100
1	E	492/835 (59%)	463 (94%)	27 (6%)	2 (0%)	34	71
1	F	527/835 (63%)	501 (95%)	26 (5%)	0	100	100
2	H	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	J	74/76 (97%)	74 (100%)	0	0	100	100
2	K	46/76 (60%)	31 (67%)	10 (22%)	5 (11%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	466/580 (80%)	421 (90%)	44 (9%)	1 (0%)	47	79
All	All	3684/5818 (63%)	3435 (93%)	241 (6%)	8 (0%)	50	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	561	TRP
2	K	37	PRO
2	K	38	PRO
2	K	41	GLN
1	E	262	THR
2	K	45	PHE
3	G	169	PHE
2	K	44	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	448/695 (64%)	446 (100%)	2 (0%)	91	94
1	B	402/695 (58%)	399 (99%)	3 (1%)	84	90
1	C	401/695 (58%)	398 (99%)	3 (1%)	84	90
1	D	398/695 (57%)	396 (100%)	2 (0%)	88	93
1	E	403/695 (58%)	397 (98%)	6 (2%)	65	80
1	F	434/695 (62%)	431 (99%)	3 (1%)	84	90
2	H	69/69 (100%)	68 (99%)	1 (1%)	67	81
2	J	69/69 (100%)	69 (100%)	0	100	100
2	K	44/69 (64%)	43 (98%)	1 (2%)	50	71
3	G	420/516 (81%)	417 (99%)	3 (1%)	84	90
All	All	3088/4893 (63%)	3064 (99%)	24 (1%)	82	89

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	755	LYS
1	A	763	LYS
1	B	368	ARG
1	B	392	ARG
1	B	437	MET
1	C	475	ARG
1	C	562	TYR
1	C	609	ARG
1	D	561	TRP
1	D	562	TYR
1	E	261	LYS
1	E	262	THR
1	E	263	LEU
1	E	359	ARG
1	E	562	TYR
1	E	672	ARG
1	F	249	ARG
1	F	325	LYS
1	F	359	ARG
2	K	40	GLN
2	H	133	LYS
3	G	156	LYS
3	G	204	CYS
3	G	477	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	588	GLN
1	B	238	GLN
1	B	270	ASN
1	B	394	HIS
1	C	337	GLN
1	C	350	ASN
1	C	461	ASN
1	C	470	ASN
1	C	512	GLN
1	C	702	GLN
1	D	295	ASN
1	D	337	GLN
1	E	209	ASN
1	E	461	ASN
1	E	468	ASN

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Mol	Chain	Res	Type
1	E	548	ASN
1	F	337	GLN
1	F	394	HIS
2	K	25	ASN
2	K	31	GLN
3	G	179	ASN
3	G	181	ASN
3	G	491	ASN
3	G	521	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z  > 2$
4	ATP	D	902	-	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)
5	ADP	E	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)
4	ATP	E	902	-	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)
4	ATP	F	901	-	26,33,33	0.94	1 (3%)	31,52,52	1.61	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ATP	B	901	-	26,33,33	0.93	1 (3%)	31,52,52	1.62	5 (16%)
4	ATP	D	901	-	26,33,33	0.93	1 (3%)	31,52,52	1.62	5 (16%)
4	ATP	C	1003	-	26,33,33	0.94	1 (3%)	31,52,52	1.61	5 (16%)
4	ATP	A	901	-	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)
4	ATP	C	1002	-	26,33,33	0.94	1 (3%)	31,52,52	1.61	5 (16%)
4	ATP	C	1001	-	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)

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
4	ATP	D	902	-	-	5/18/38/38	0/3/3/3
5	ADP	E	901	-	-	3/12/32/32	0/3/3/3
4	ATP	E	902	-	-	4/18/38/38	0/3/3/3
4	ATP	F	901	-	-	2/18/38/38	0/3/3/3
4	ATP	B	901	-	-	4/18/38/38	0/3/3/3
4	ATP	D	901	-	-	4/18/38/38	0/3/3/3
4	ATP	C	1003	-	-	5/18/38/38	0/3/3/3
4	ATP	A	901	-	-	5/18/38/38	0/3/3/3
4	ATP	C	1002	-	-	5/18/38/38	0/3/3/3
4	ATP	C	1001	-	-	5/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	902	ATP	C5-C4	2.53	1.47	1.40
4	C	1003	ATP	C5-C4	2.52	1.47	1.40
4	D	901	ATP	C5-C4	2.52	1.47	1.40
4	C	1002	ATP	C5-C4	2.52	1.47	1.40
5	E	901	ADP	C5-C4	2.52	1.47	1.40
4	B	901	ATP	C5-C4	2.50	1.47	1.40
4	F	901	ATP	C5-C4	2.50	1.47	1.40
4	A	901	ATP	C5-C4	2.49	1.47	1.40
4	C	1001	ATP	C5-C4	2.49	1.47	1.40
4	E	902	ATP	C5-C4	2.48	1.47	1.40

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	ATP	PB-O3B-PG	-3.60	120.46	132.83
4	E	902	ATP	PA-O3A-PB	-3.60	120.47	132.83
4	C	1002	ATP	PB-O3B-PG	-3.60	120.47	132.83
4	C	1003	ATP	PB-O3B-PG	-3.60	120.47	132.83
5	E	901	ADP	PA-O3A-PB	-3.60	120.47	132.83
4	A	901	ATP	PB-O3B-PG	-3.59	120.49	132.83
4	A	901	ATP	PA-O3A-PB	-3.59	120.49	132.83
4	C	1001	ATP	PA-O3A-PB	-3.59	120.50	132.83
4	C	1001	ATP	PB-O3B-PG	-3.59	120.50	132.83
4	D	901	ATP	PA-O3A-PB	-3.59	120.51	132.83
4	B	901	ATP	PA-O3A-PB	-3.59	120.51	132.83
4	F	901	ATP	PA-O3A-PB	-3.59	120.51	132.83
4	B	901	ATP	PB-O3B-PG	-3.59	120.51	132.83
4	F	901	ATP	PB-O3B-PG	-3.59	120.52	132.83
4	D	902	ATP	PB-O3B-PG	-3.59	120.52	132.83
4	D	902	ATP	PA-O3A-PB	-3.59	120.52	132.83
4	C	1002	ATP	PA-O3A-PB	-3.58	120.54	132.83
4	E	902	ATP	PB-O3B-PG	-3.58	120.55	132.83
4	C	1003	ATP	PA-O3A-PB	-3.57	120.56	132.83
5	E	901	ADP	C3'-C2'-C1'	3.41	106.11	100.98
4	D	901	ATP	C3'-C2'-C1'	3.40	106.10	100.98
4	D	902	ATP	C3'-C2'-C1'	3.40	106.10	100.98
4	F	901	ATP	C3'-C2'-C1'	3.39	106.08	100.98
4	E	902	ATP	C3'-C2'-C1'	3.39	106.08	100.98
4	C	1003	ATP	C3'-C2'-C1'	3.39	106.08	100.98
4	C	1002	ATP	C3'-C2'-C1'	3.38	106.07	100.98
4	A	901	ATP	C3'-C2'-C1'	3.38	106.07	100.98
4	C	1001	ATP	C3'-C2'-C1'	3.37	106.06	100.98
4	B	901	ATP	C3'-C2'-C1'	3.37	106.05	100.98
4	D	901	ATP	N3-C2-N1	-3.20	123.67	128.68
4	B	901	ATP	N3-C2-N1	-3.20	123.68	128.68
4	C	1002	ATP	N3-C2-N1	-3.20	123.68	128.68
4	E	902	ATP	N3-C2-N1	-3.18	123.70	128.68
4	A	901	ATP	N3-C2-N1	-3.17	123.73	128.68
4	D	902	ATP	N3-C2-N1	-3.17	123.73	128.68
5	E	901	ADP	N3-C2-N1	-3.16	123.74	128.68
4	C	1003	ATP	N3-C2-N1	-3.16	123.74	128.68
4	F	901	ATP	N3-C2-N1	-3.16	123.75	128.68
4	C	1001	ATP	N3-C2-N1	-3.15	123.76	128.68
4	B	901	ATP	C4-C5-N7	-2.71	106.57	109.40
4	C	1001	ATP	C4-C5-N7	-2.71	106.58	109.40
4	A	901	ATP	C4-C5-N7	-2.70	106.58	109.40
4	D	902	ATP	C4-C5-N7	-2.70	106.58	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1003	ATP	C4-C5-N7	-2.70	106.58	109.40
4	C	1002	ATP	C4-C5-N7	-2.70	106.59	109.40
4	F	901	ATP	C4-C5-N7	-2.70	106.59	109.40
4	D	901	ATP	C4-C5-N7	-2.68	106.61	109.40
4	E	902	ATP	C4-C5-N7	-2.68	106.61	109.40
5	E	901	ADP	C4-C5-N7	-2.67	106.62	109.40

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	ATP	O4'-C4'-C5'-O5'
4	A	901	ATP	C3'-C4'-C5'-O5'
4	C	1001	ATP	O4'-C4'-C5'-O5'
4	C	1001	ATP	C3'-C4'-C5'-O5'
4	C	1002	ATP	O4'-C4'-C5'-O5'
4	C	1002	ATP	C3'-C4'-C5'-O5'
4	C	1003	ATP	O4'-C4'-C5'-O5'
4	C	1003	ATP	C3'-C4'-C5'-O5'
4	D	901	ATP	O4'-C4'-C5'-O5'
4	D	901	ATP	C3'-C4'-C5'-O5'
4	D	902	ATP	O4'-C4'-C5'-O5'
4	D	902	ATP	C3'-C4'-C5'-O5'
4	E	902	ATP	O4'-C4'-C5'-O5'
4	E	902	ATP	C3'-C4'-C5'-O5'
5	E	901	ADP	C5'-O5'-PA-O3A
5	E	901	ADP	C4'-C5'-O5'-PA
4	A	901	ATP	PB-O3A-PA-O2A
4	B	901	ATP	PB-O3A-PA-O2A
4	C	1002	ATP	PB-O3A-PA-O2A
4	D	901	ATP	PG-O3B-PB-O2B
4	D	902	ATP	PB-O3A-PA-O2A
4	E	902	ATP	PB-O3A-PA-O2A
4	B	901	ATP	C5'-O5'-PA-O2A
5	E	901	ADP	C5'-O5'-PA-O1A
4	F	901	ATP	C4'-C5'-O5'-PA
4	C	1001	ATP	PB-O3A-PA-O2A
4	C	1003	ATP	PB-O3A-PA-O2A
4	D	901	ATP	PG-O3B-PB-O1B
4	B	901	ATP	C5'-O5'-PA-O3A
4	A	901	ATP	PB-O3A-PA-O1A
4	B	901	ATP	PB-O3A-PA-O1A

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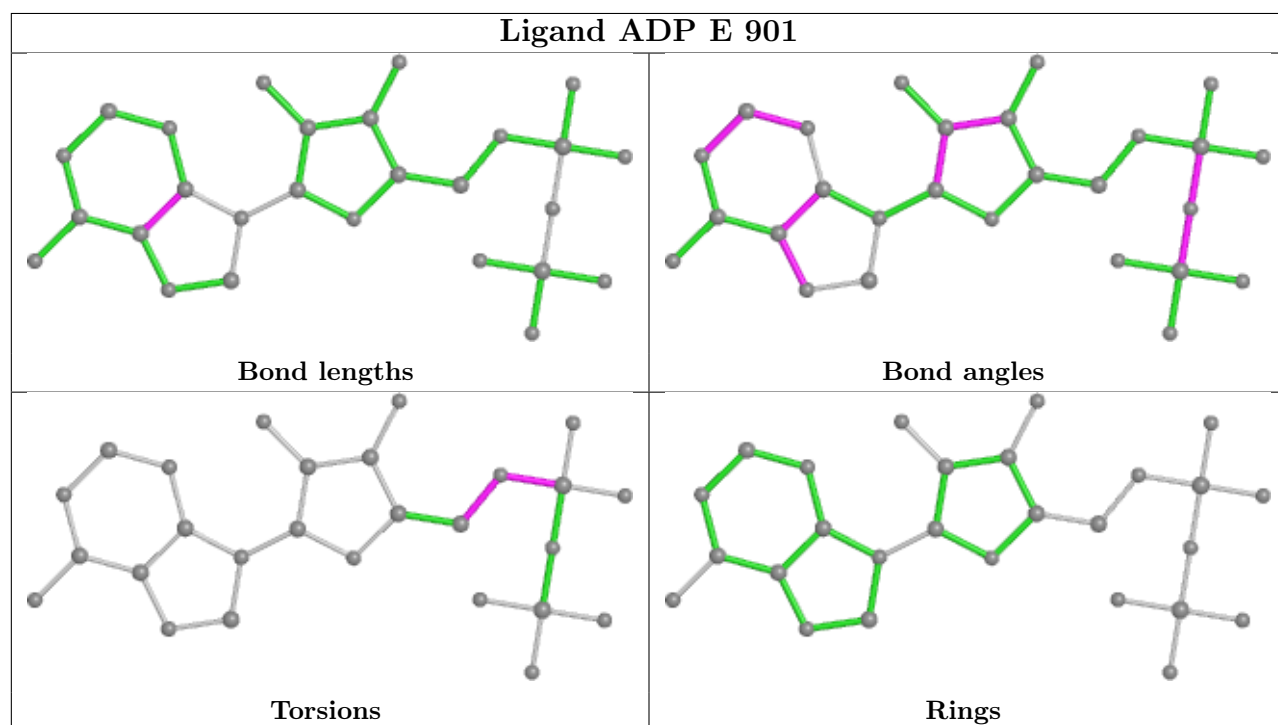
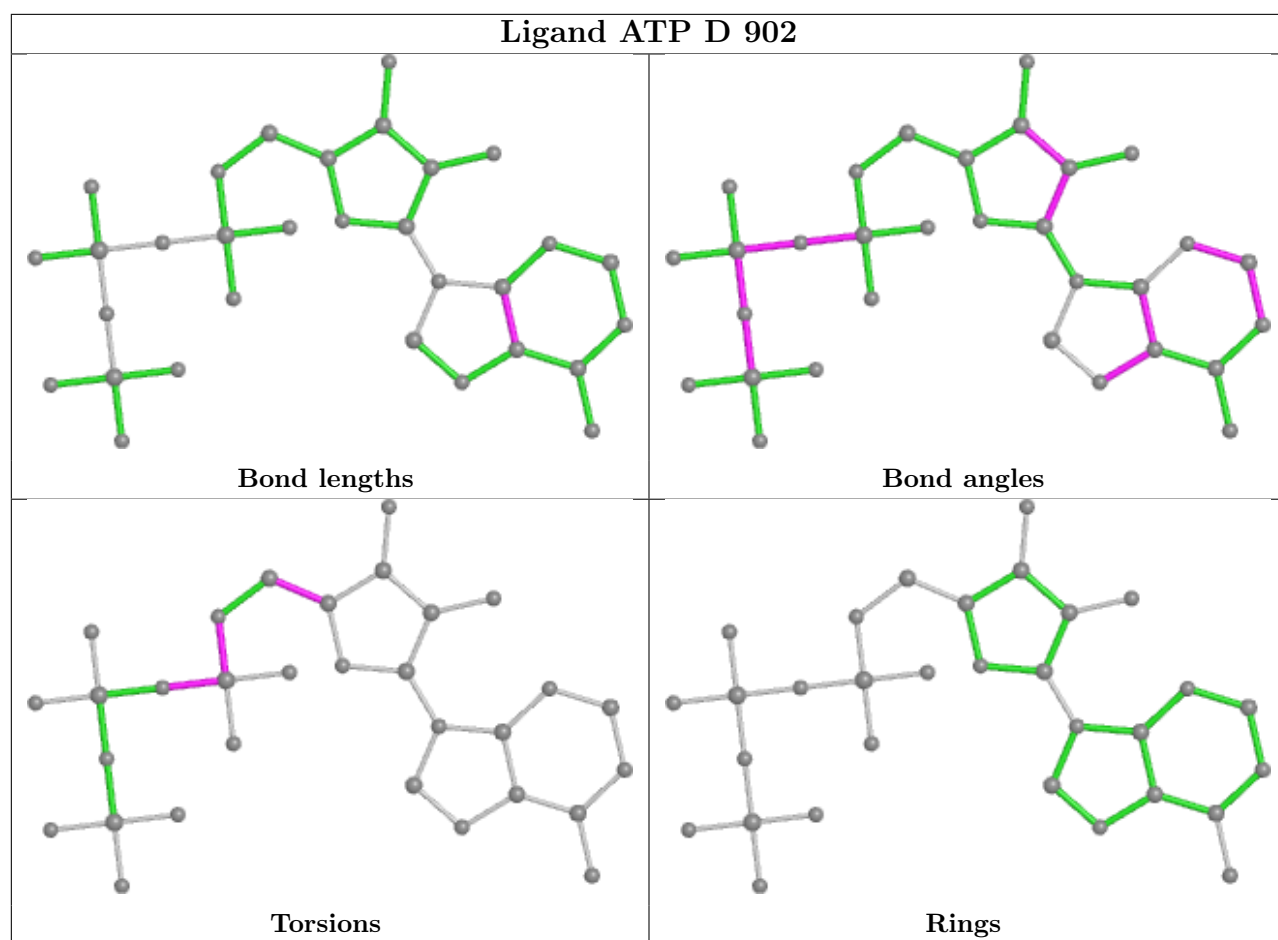
Mol	Chain	Res	Type	Atoms
4	C	1001	ATP	PB-O3A-PA-O1A
4	C	1002	ATP	PB-O3A-PA-O1A
4	C	1003	ATP	PB-O3A-PA-O1A
4	D	902	ATP	PB-O3A-PA-O1A
4	E	902	ATP	PB-O3A-PA-O1A
4	A	901	ATP	C5'-O5'-PA-O1A
4	C	1001	ATP	C5'-O5'-PA-O1A
4	C	1002	ATP	C5'-O5'-PA-O1A
4	C	1003	ATP	C5'-O5'-PA-O1A
4	D	902	ATP	C5'-O5'-PA-O1A
4	F	901	ATP	O4'-C4'-C5'-O5'

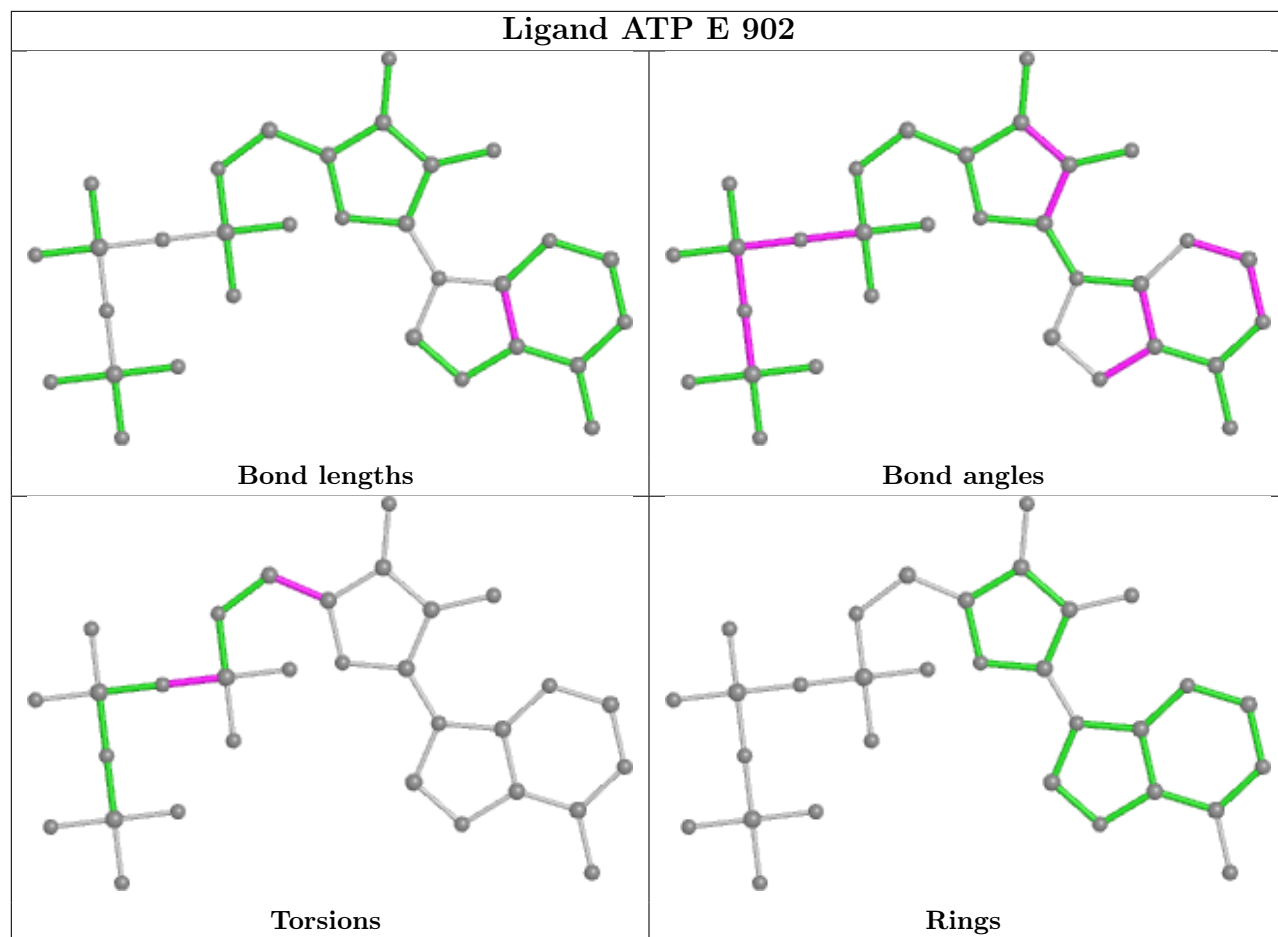
There are no ring outliers.

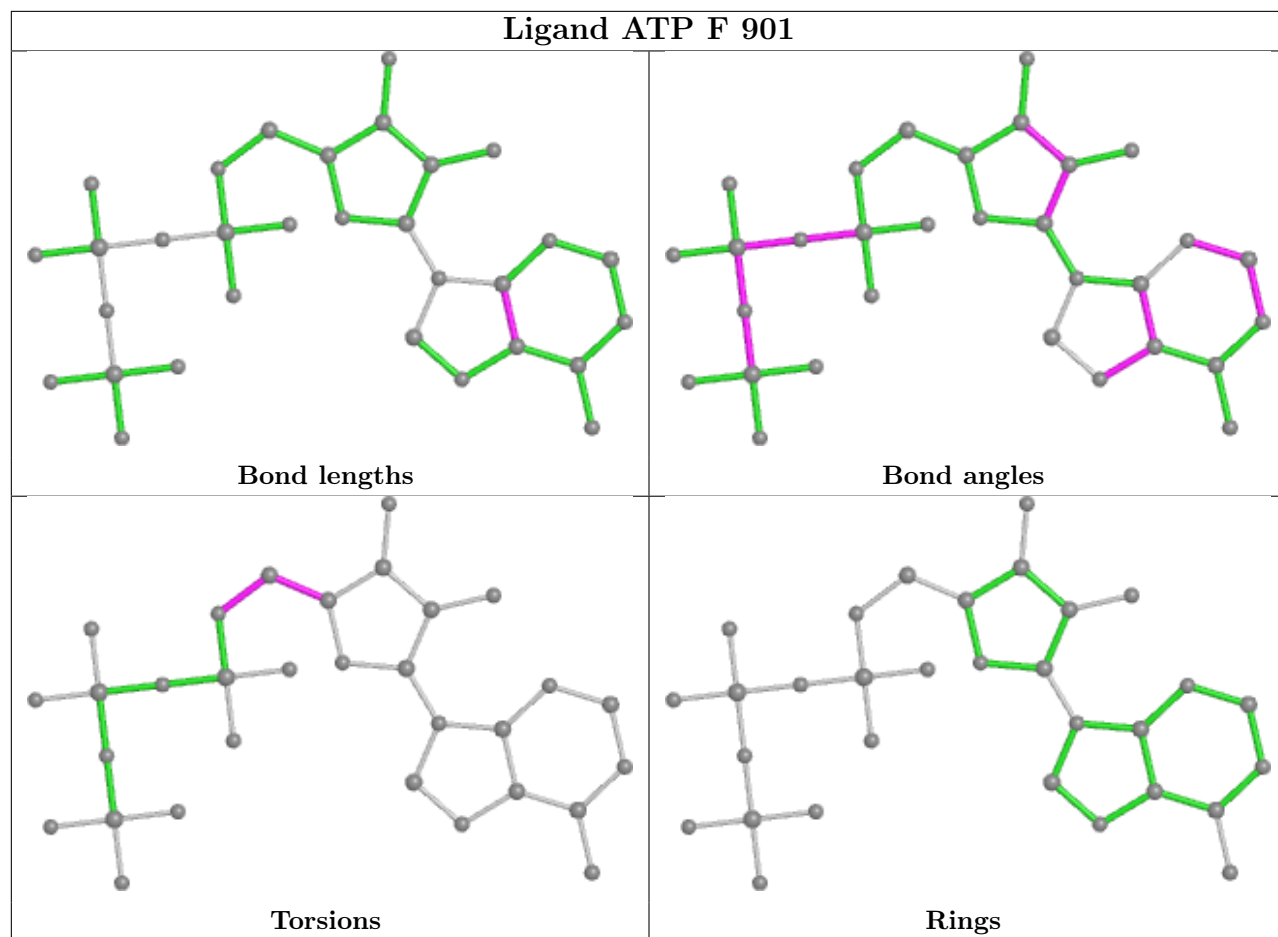
10 monomers are involved in 192 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	902	ATP	28	0
5	E	901	ADP	25	0
4	E	902	ATP	15	0
4	F	901	ATP	18	0
4	B	901	ATP	2	0
4	D	901	ATP	17	0
4	C	1003	ATP	18	0
4	A	901	ATP	24	0
4	C	1002	ATP	4	0
4	C	1001	ATP	41	0

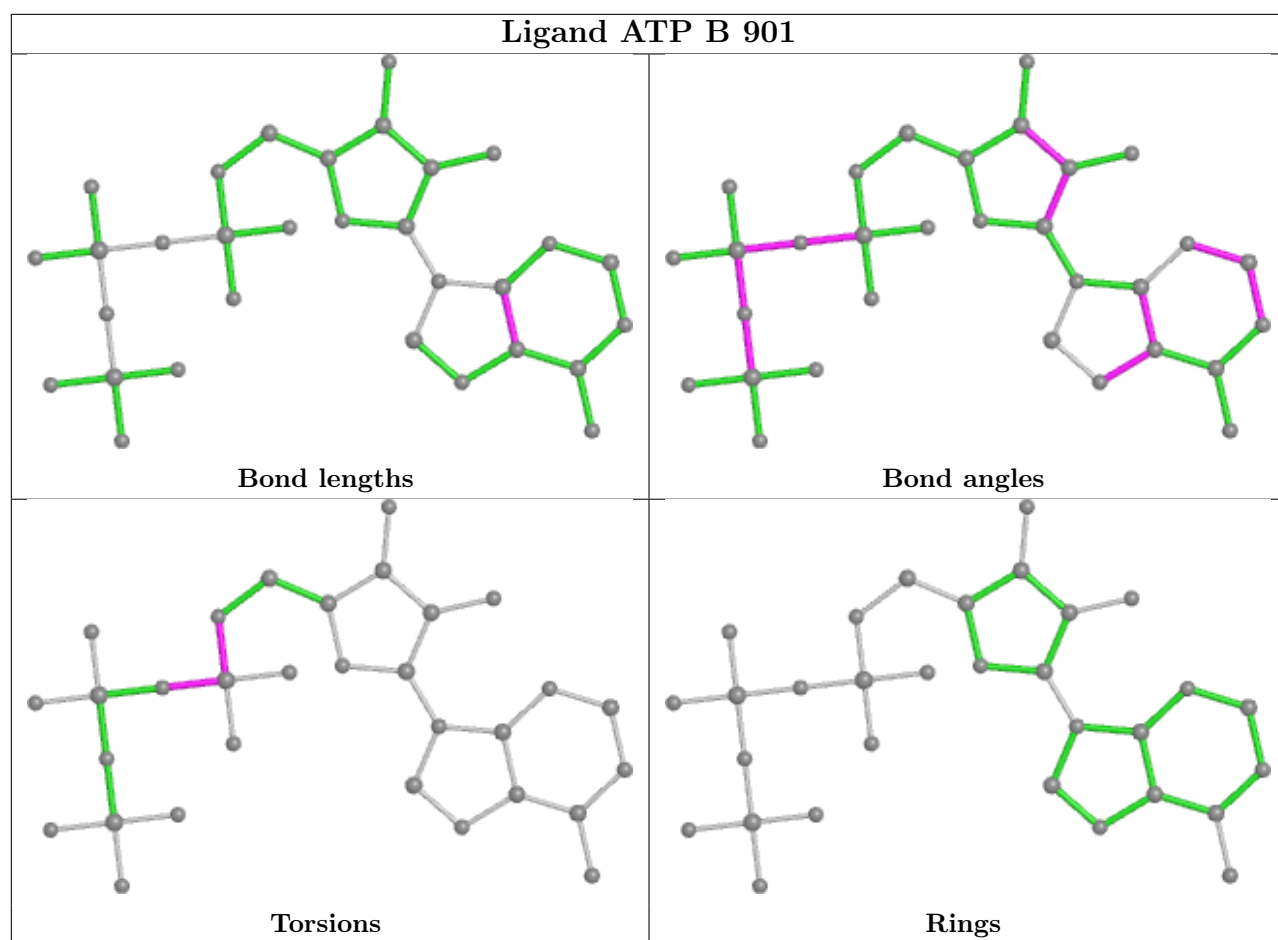
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

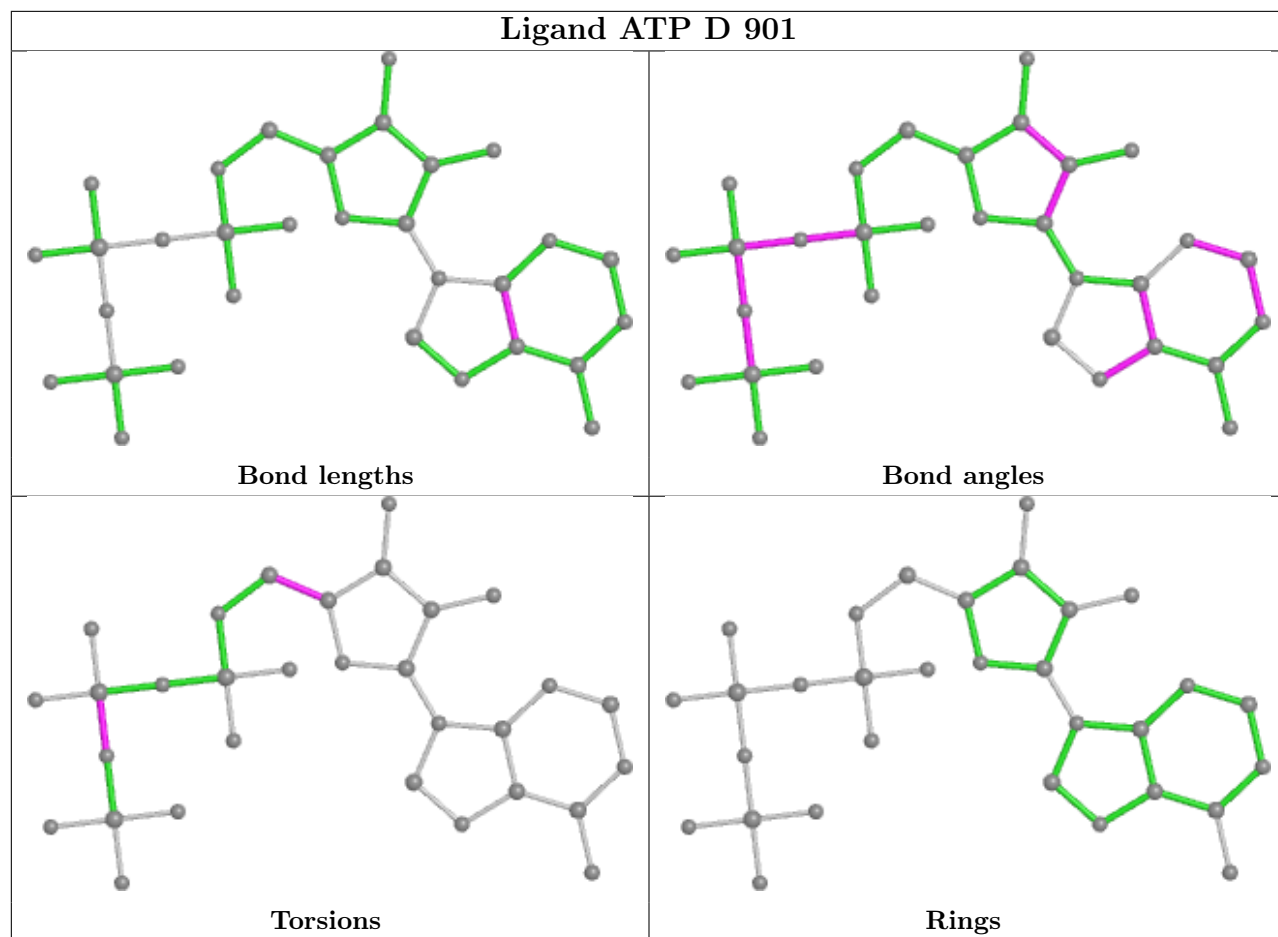


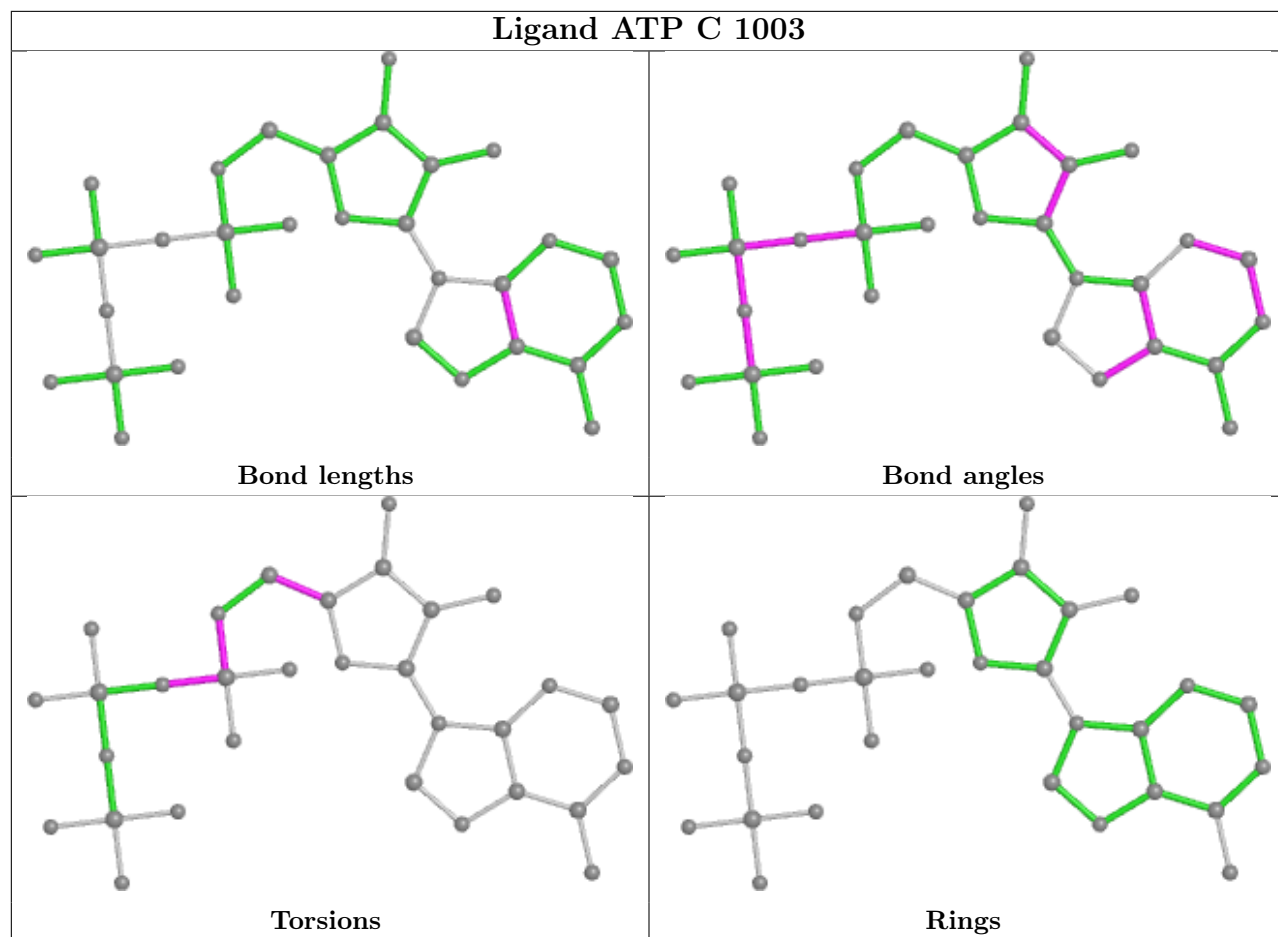


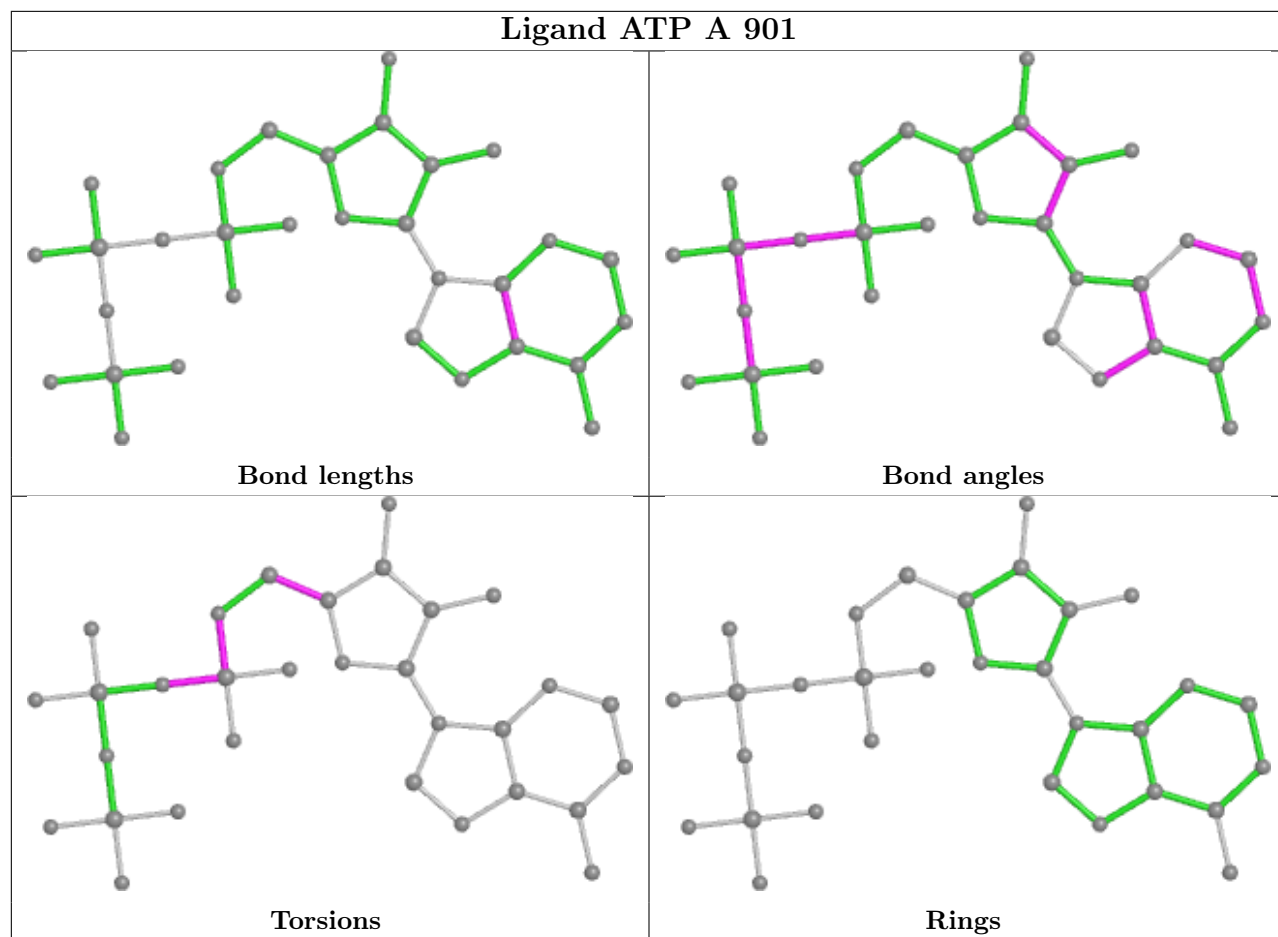


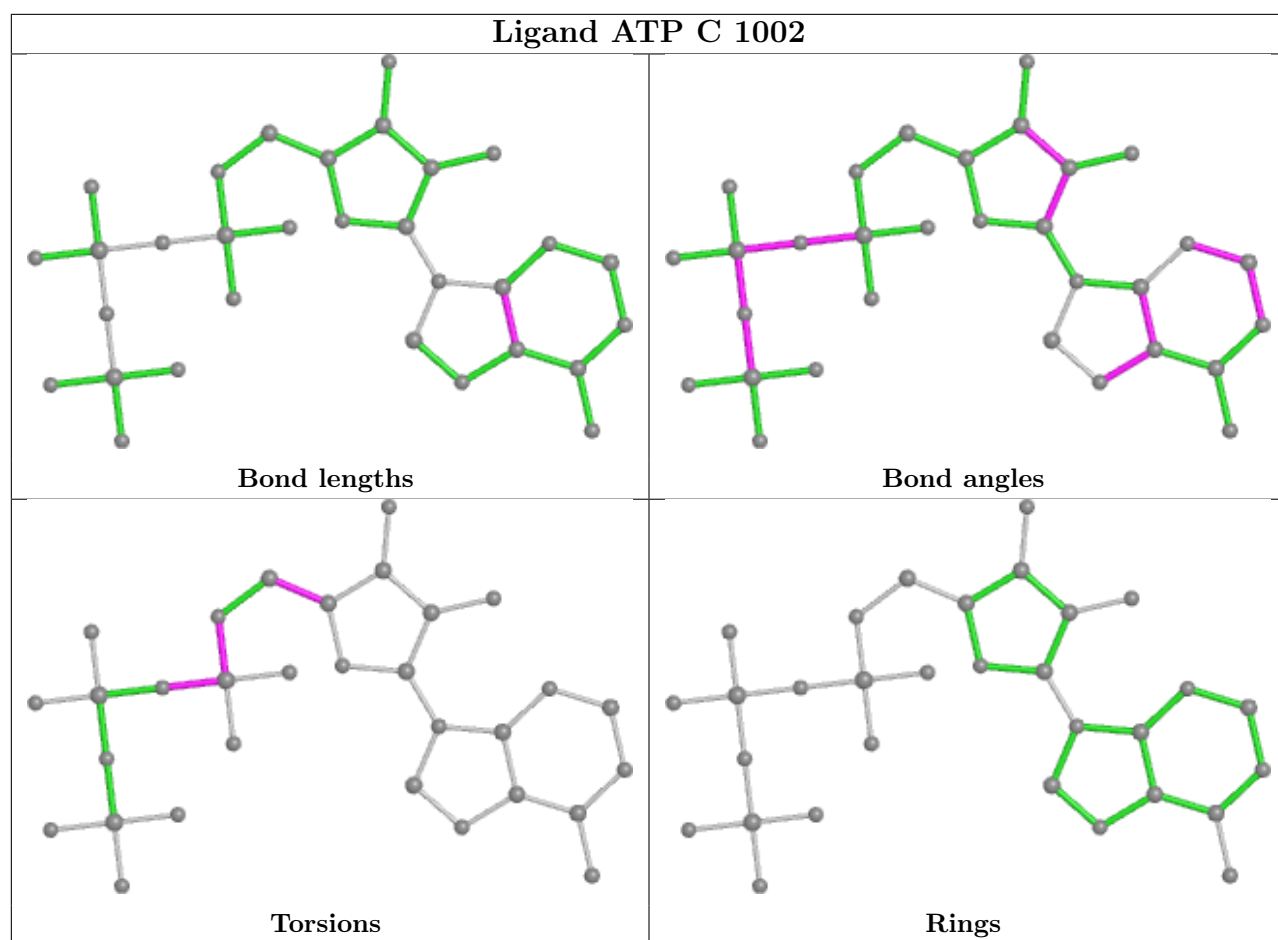


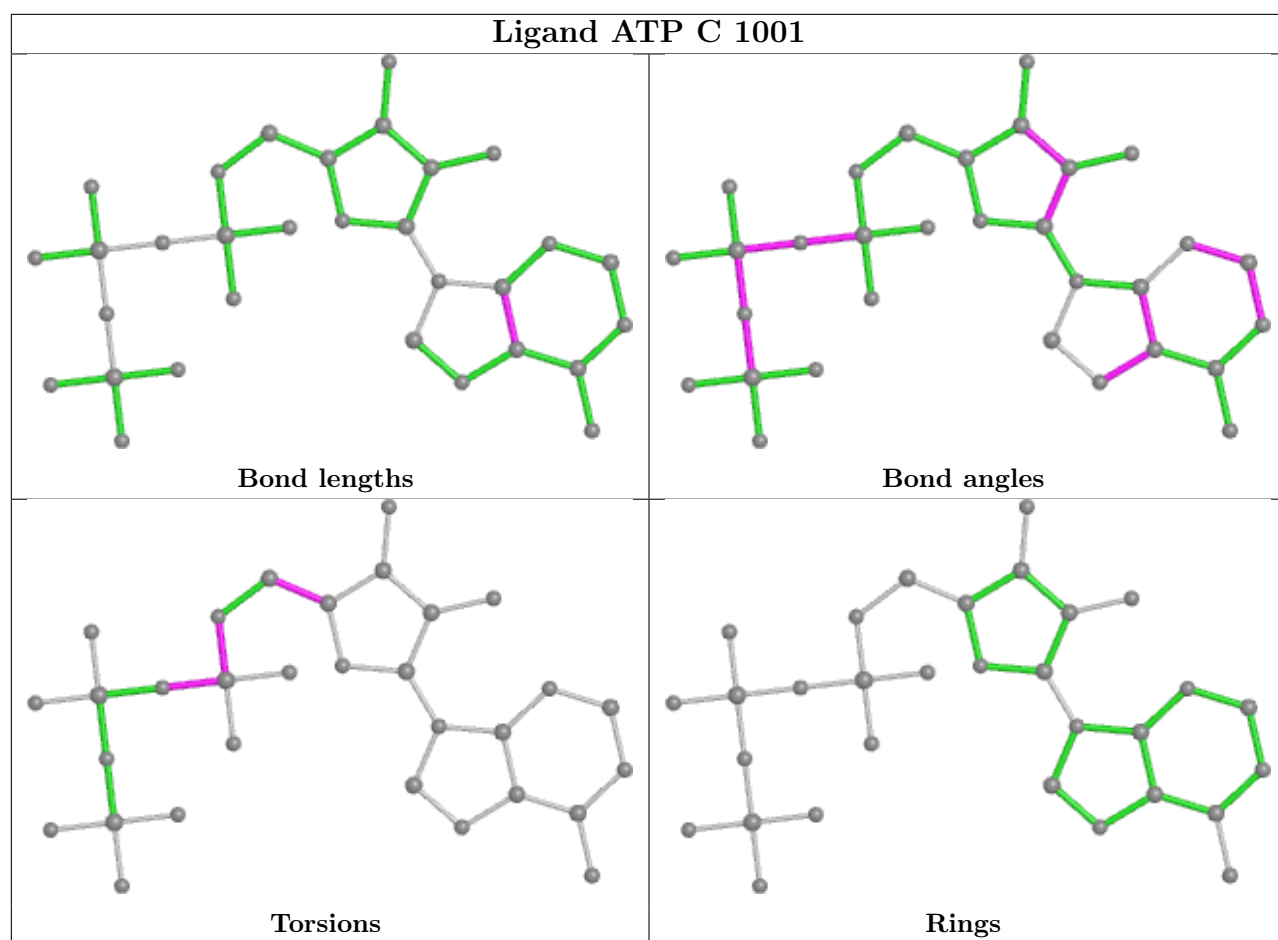












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

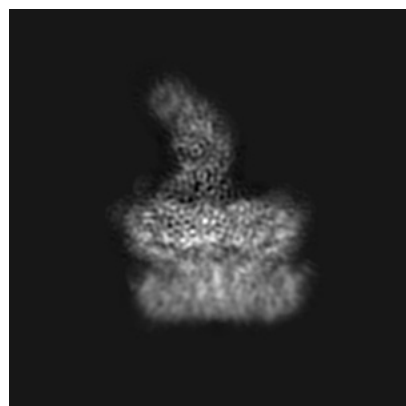
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0665. These allow visual inspection of the internal detail of the map and identification of artifacts.

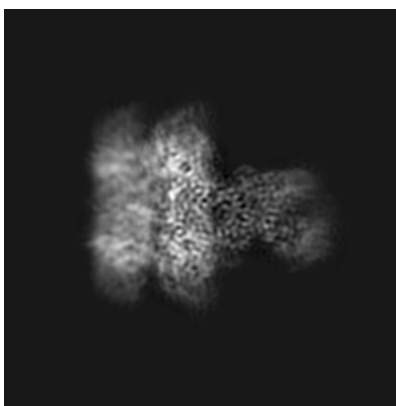
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

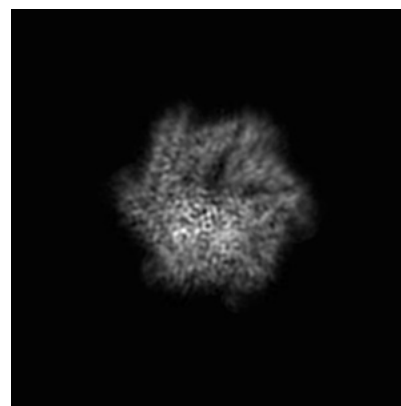
#### 6.1.1 Primary map



X

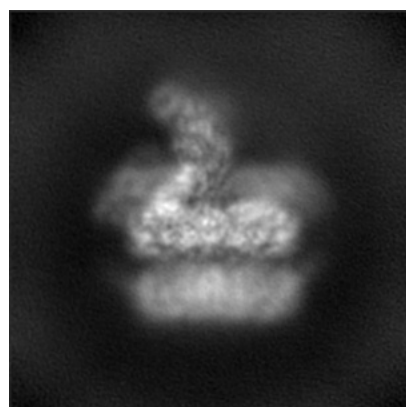


Y

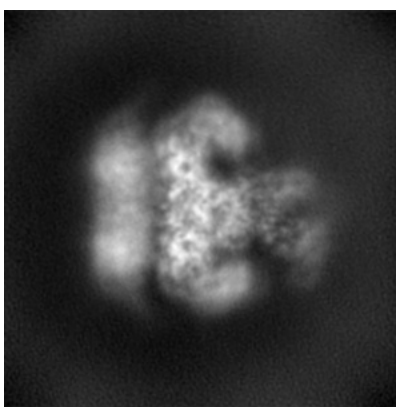


Z

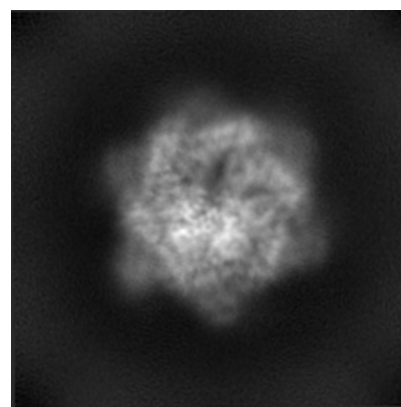
#### 6.1.2 Raw map



X



Y

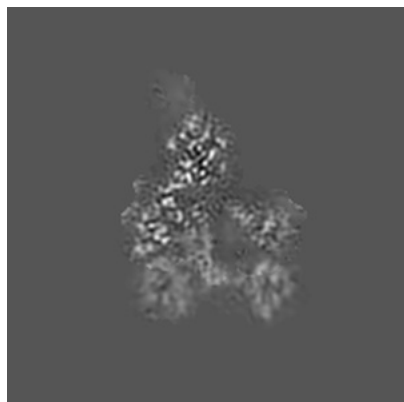


Z

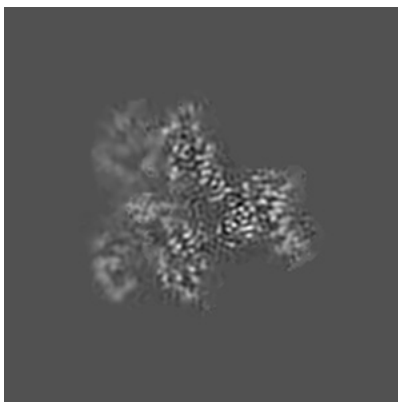
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

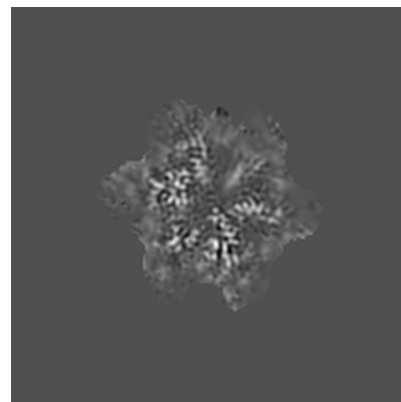
### 6.2.1 Primary map



X Index: 100

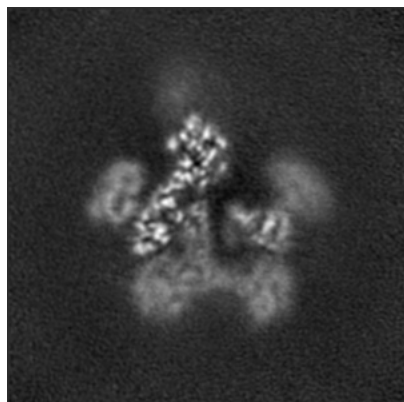


Y Index: 100

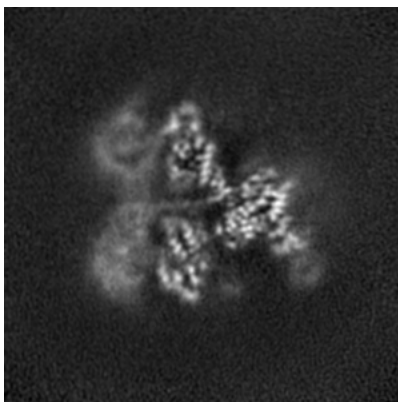


Z Index: 100

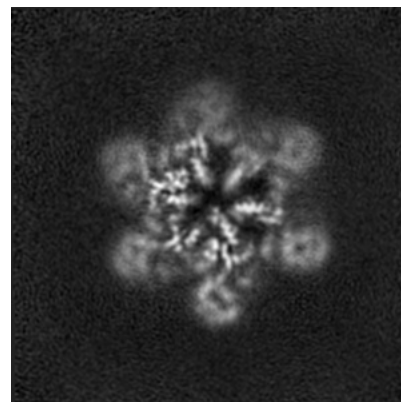
### 6.2.2 Raw map



X Index: 100



Y Index: 100



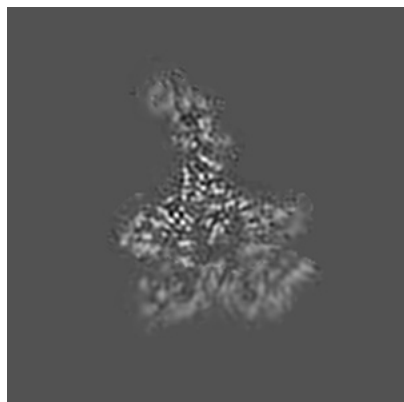
Z Index: 100

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

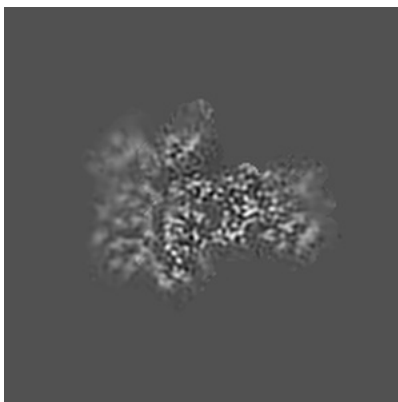


## 6.3 Largest variance slices [i](#)

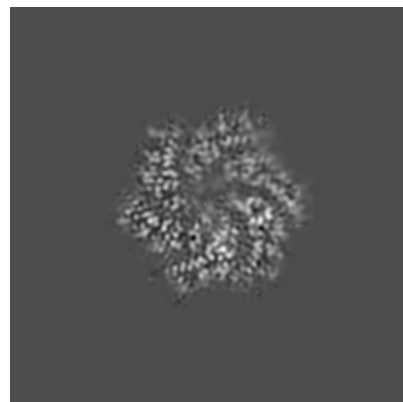
### 6.3.1 Primary map



X Index: 86

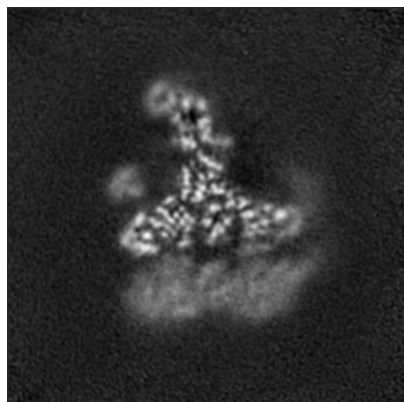


Y Index: 89

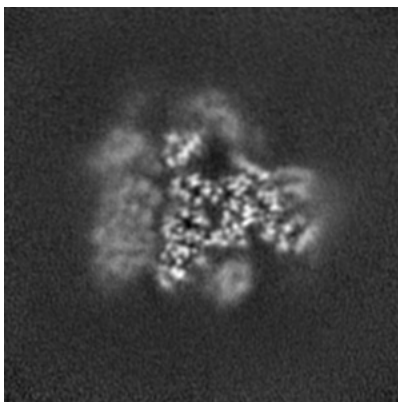


Z Index: 84

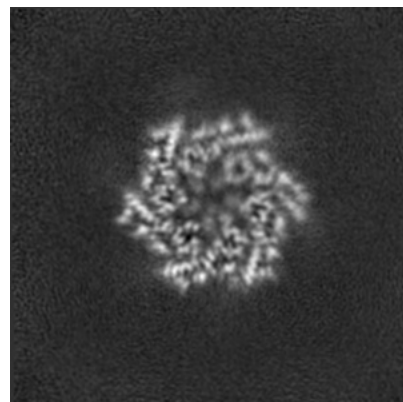
### 6.3.2 Raw map



X Index: 86



Y Index: 88

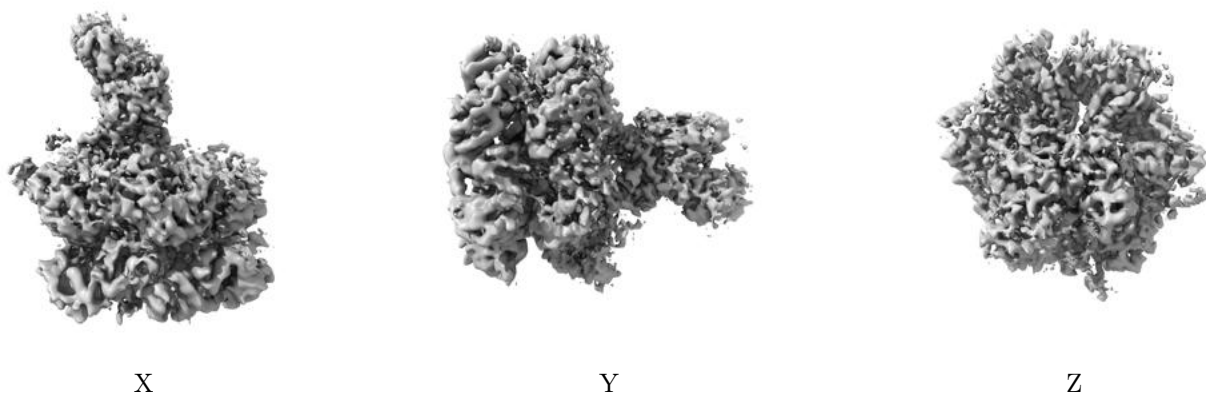


Z Index: 86

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

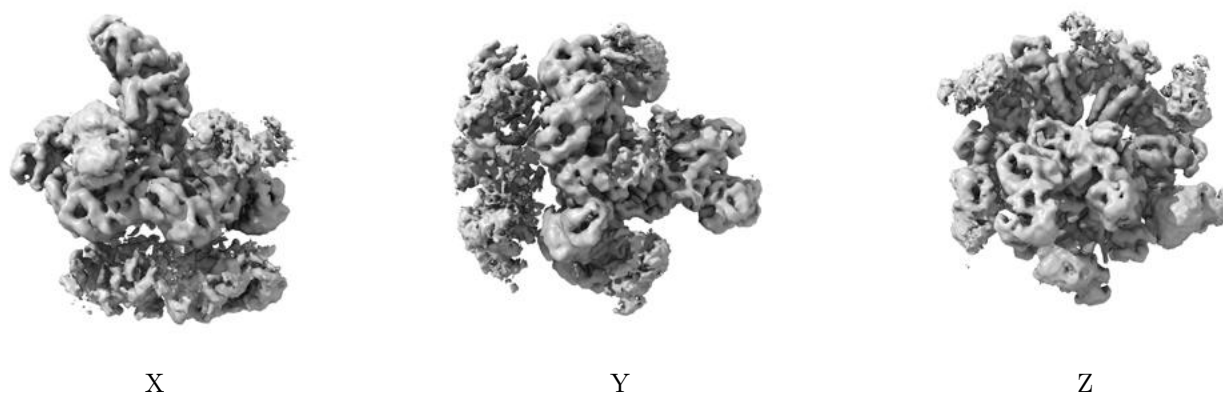
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

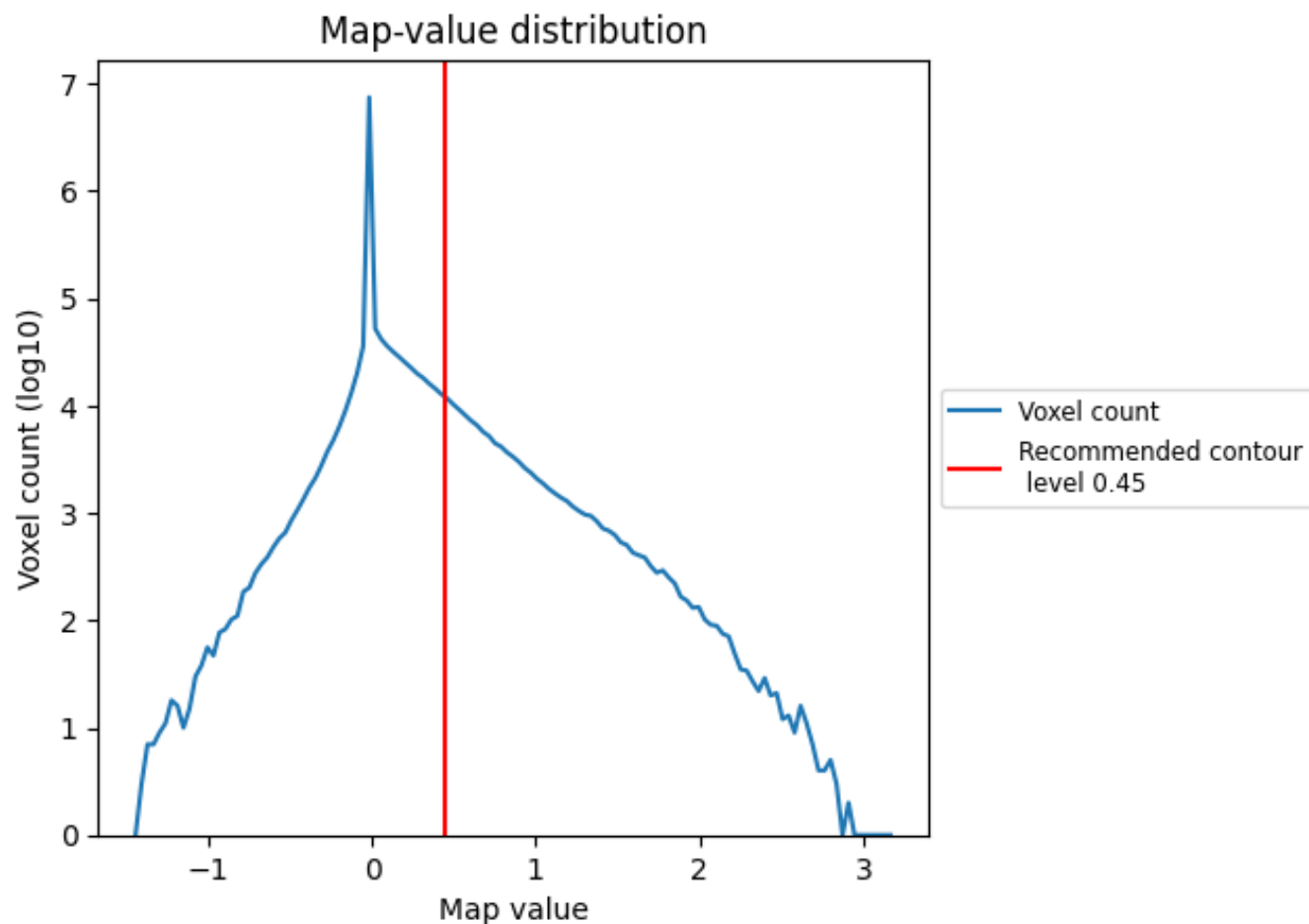
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

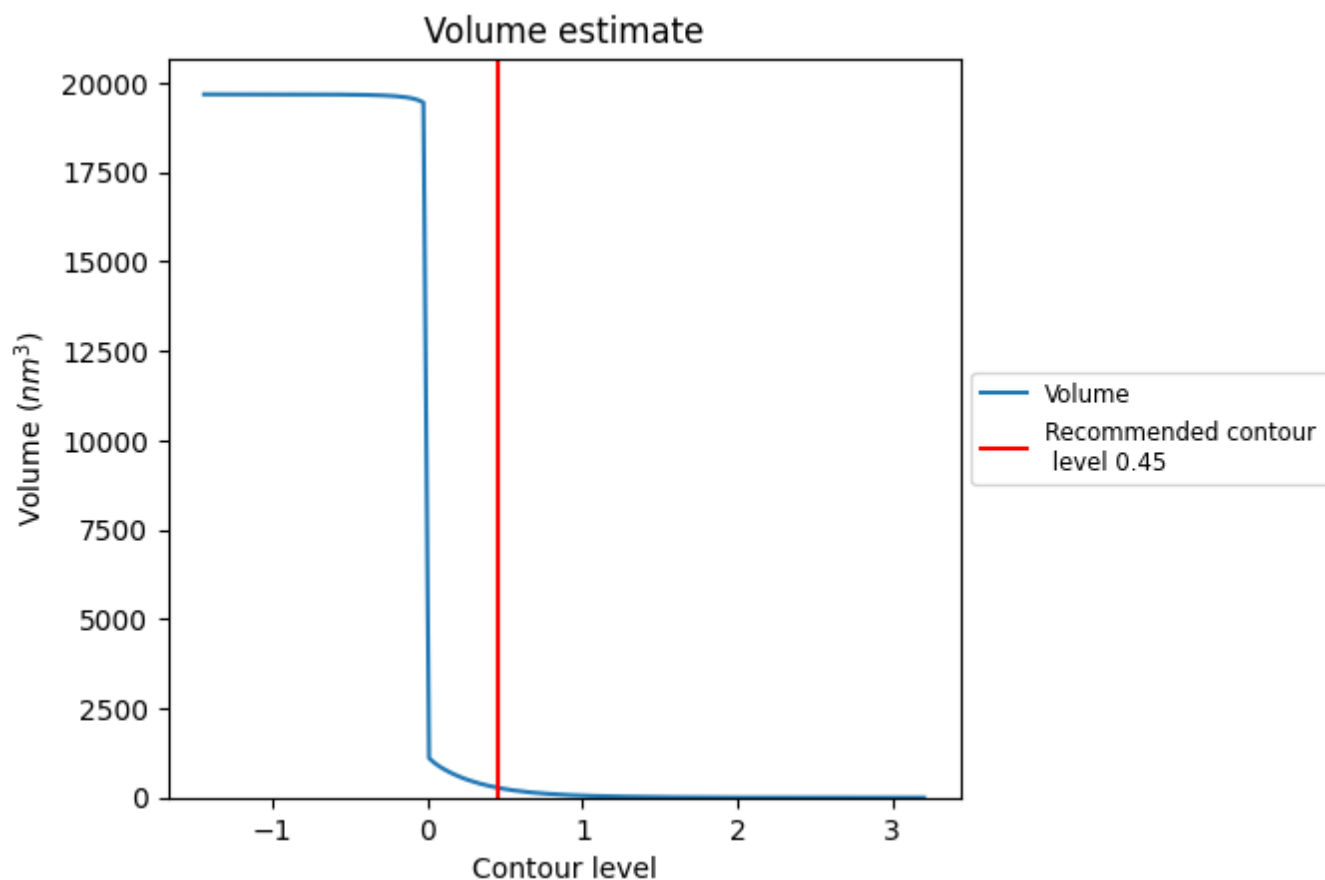
This section contains the results of statistical analysis of the map.

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



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

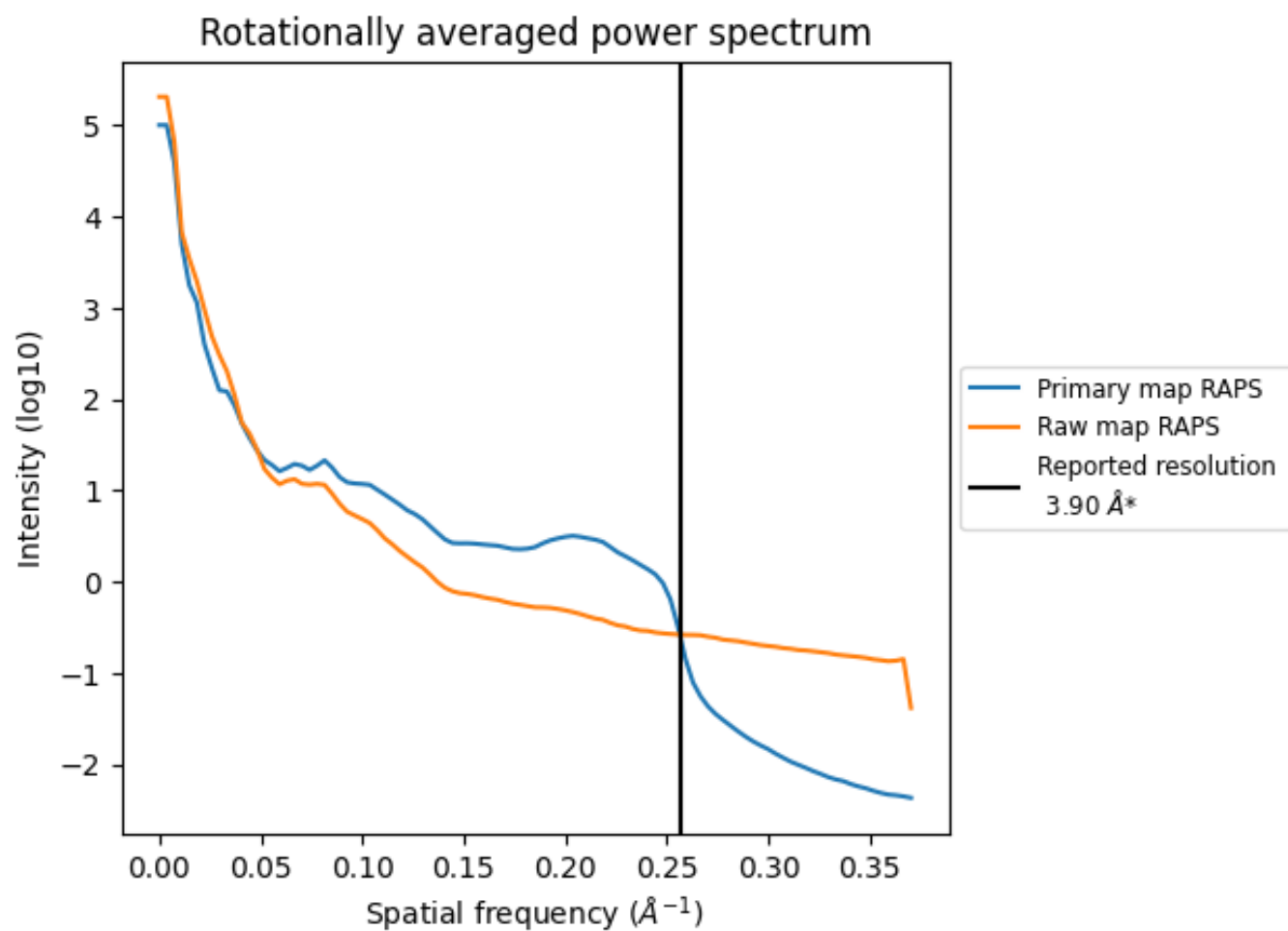
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 278  $\text{nm}^3$ ; this corresponds to an approximate mass of 251 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 ⓘ

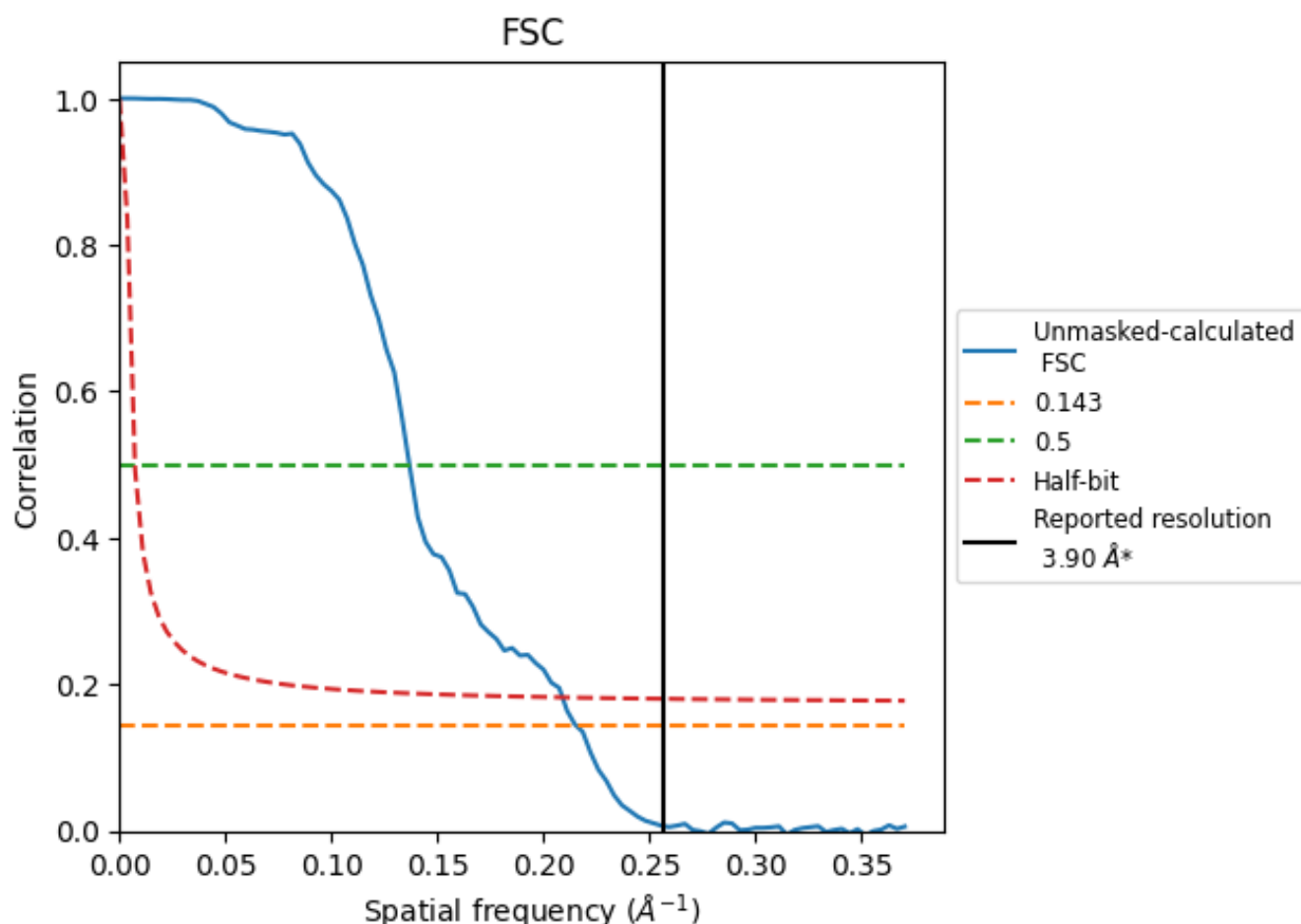


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

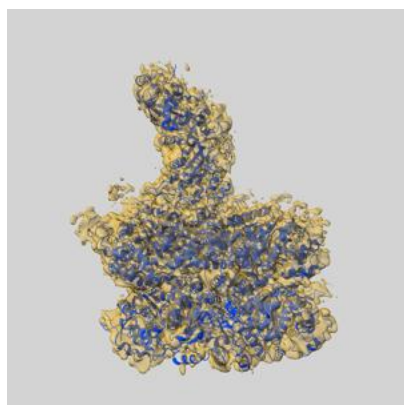
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.64	7.31	4.78

\*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 4.64 differs from the reported value 3.9 by more than 10 %

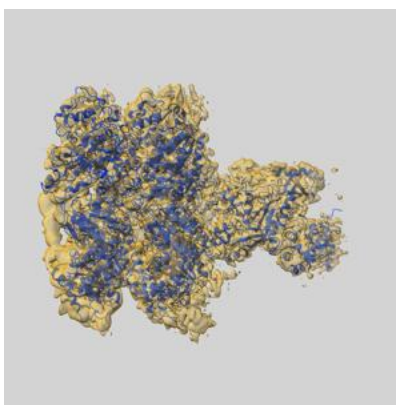
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0665 and PDB model 6OA9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

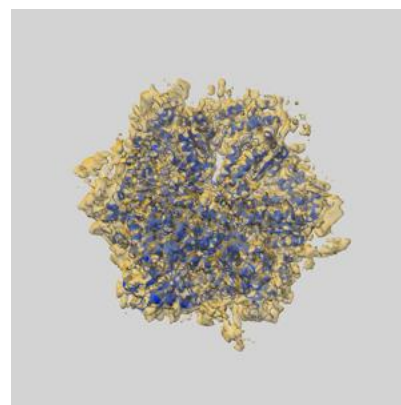
### 9.1 Map-model overlay [i](#)



X



Y

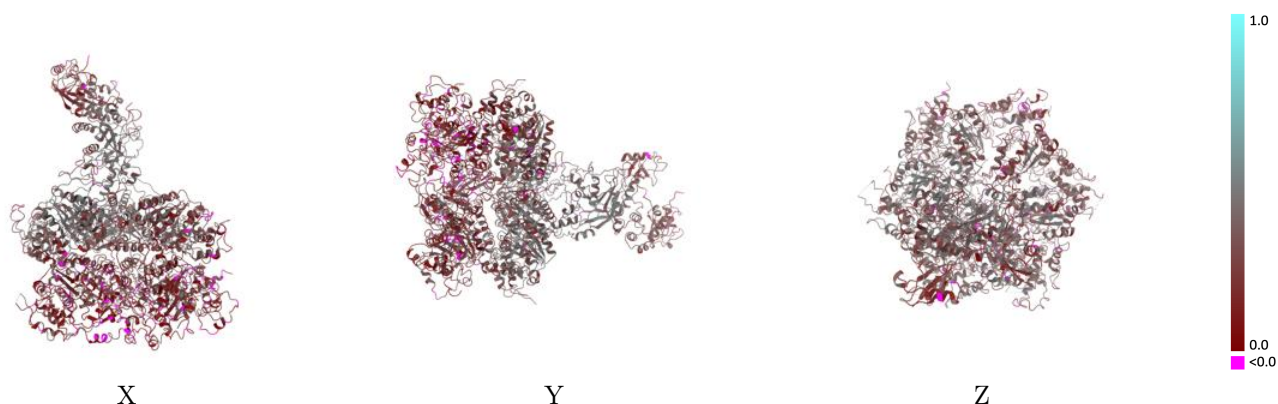


Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 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.

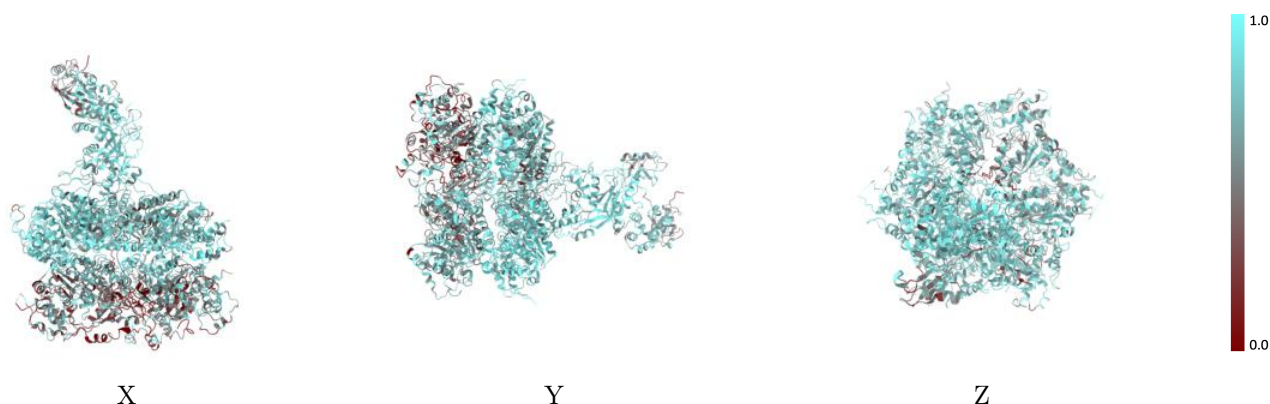


## 9.2 Q-score mapped to coordinate model [i](#)



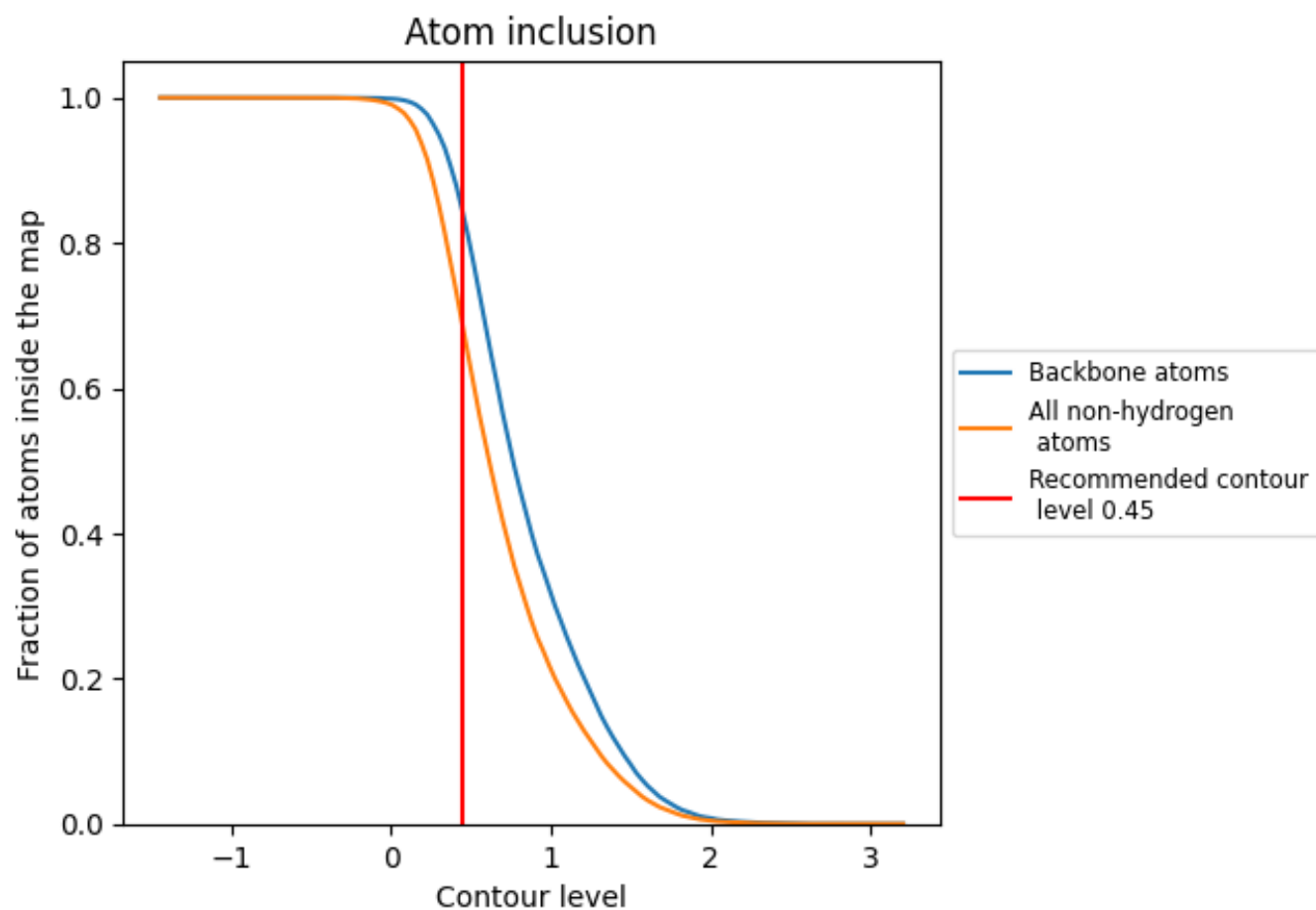
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 68% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6840	<div></div> 0.2820
A	<div></div> 0.5992	<div></div> 0.2470
B	<div></div> 0.7050	<div></div> 0.2940
C	<div></div> 0.7492	<div></div> 0.3090
D	<div></div> 0.7382	<div></div> 0.3030
E	<div></div> 0.6845	<div></div> 0.2680
F	<div></div> 0.5789	<div></div> 0.2100
G	<div></div> 0.7837	<div></div> 0.3660
H	<div></div> 0.6216	<div></div> 0.2480
J	<div></div> 0.4882	<div></div> 0.2200
K	<div></div> 0.7701	<div></div> 0.3290

1.0  
0.0  
<0.0