



Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 08:45 PM EST

PDB ID : 8DAV
EMDB ID : EMD-27277
Title : Saccharomyces cerevisiae Ufd1/Npl4/Cdc48 complex bound to two ubiquitin moieties and one unfolded ubiquitin in presence of SUMO-ubiquitin(K48poly Ub)-mEOS and ATP, state 2 (uC)
Authors : Lee, H.G.; Lima, C.D.
Deposited on : 2022-06-14
Resolution : 3.50 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

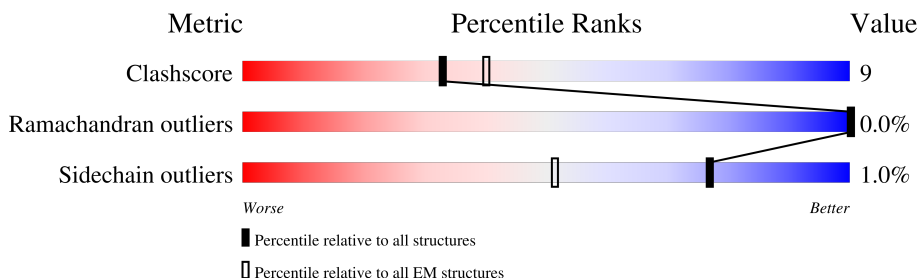
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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 ≥ 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	838	<div> <div>24%</div> <div>66%</div> <div>18%</div> <div>•</div> <div>15%</div> </div>
1	B	838	<div> <div>27%</div> <div>65%</div> <div>20%</div> <div>•</div> <div>14%</div> </div>
1	C	838	<div> <div>16%</div> <div>54%</div> <div>12%</div> <div></div> <div>34%</div> </div>
1	D	838	<div> <div>16%</div> <div>51%</div> <div>14%</div> <div></div> <div>35%</div> </div>
1	E	838	<div> <div>13%</div> <div>51%</div> <div>12%</div> <div>•</div> <div>37%</div> </div>
1	F	838	<div> <div>10%</div> <div>53%</div> <div>13%</div> <div></div> <div>34%</div> </div>
2	G	583	<div> <div>•</div> <div>62%</div> <div>19%</div> <div></div> <div>19%</div> </div>
3	H	363	<div> <div>•</div> <div>14%</div> <div>•</div> <div>83%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	I	76	<div> <div>5%</div> <div>39%</div> <div>9%</div> <div>50%</div> </div>
4	J	76	<div> <div>78%</div> <div>17%</div> <div>5%</div> </div>
4	K	76	<div> <div>7%</div> <div>64%</div> <div>32%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34248 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	712	Total	C	N	O	S	0	0
			5555	3492	963	1075	25		
1	B	718	Total	C	N	O	S	0	0
			5599	3523	978	1073	25		
1	C	555	Total	C	N	O	S	0	0
			4311	2703	759	829	20		
1	D	547	Total	C	N	O	S	0	0
			4240	2662	745	813	20		
1	E	532	Total	C	N	O	S	0	0
			4113	2587	715	791	20		
1	F	551	Total	C	N	O	S	0	0
			4284	2688	755	821	20		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P25694
A	-1	SER	-	expression tag	UNP P25694
A	0	HIS	-	expression tag	UNP P25694
B	-2	GLY	-	expression tag	UNP P25694
B	-1	SER	-	expression tag	UNP P25694
B	0	HIS	-	expression tag	UNP P25694
C	-2	GLY	-	expression tag	UNP P25694
C	-1	SER	-	expression tag	UNP P25694
C	0	HIS	-	expression tag	UNP P25694
D	-2	GLY	-	expression tag	UNP P25694
D	-1	SER	-	expression tag	UNP P25694
D	0	HIS	-	expression tag	UNP P25694
E	-2	GLY	-	expression tag	UNP P25694
E	-1	SER	-	expression tag	UNP P25694
E	0	HIS	-	expression tag	UNP P25694
F	-2	GLY	-	expression tag	UNP P25694
F	-1	SER	-	expression tag	UNP P25694
F	0	HIS	-	expression tag	UNP P25694

- Molecule 2 is a protein called Nuclear protein localization protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	475	Total	C	N	O	S	0	0
			3825	2421	643	740	21		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	GLY	-	expression tag	UNP P33755
G	-1	SER	-	expression tag	UNP P33755
G	0	HIS	-	expression tag	UNP P33755

- Molecule 3 is a protein called Ubiquitin fusion degradation protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	62	Total	C	N	O	S	0	0
			477	306	77	91	3		

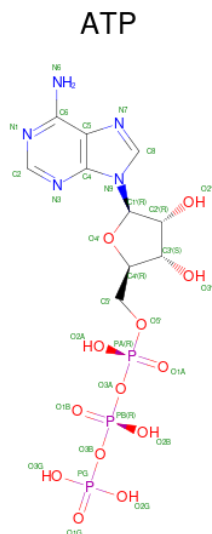
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	expression tag	UNP P53044
H	0	SER	-	expression tag	UNP P53044

- Molecule 4 is a protein called Ubiquitin.

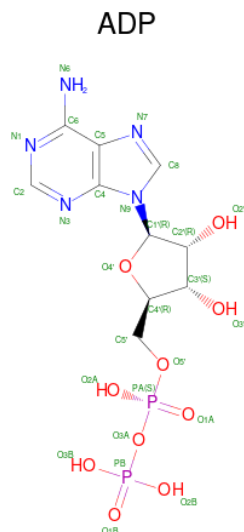
Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	38	Total	C	N	O		0	0
			298	186	50	62			
4	J	76	Total	C	N	O	S	0	0
			600	375	105	119	1		
4	K	76	Total	C	N	O	S	0	0
			600	375	105	119	1		

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



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

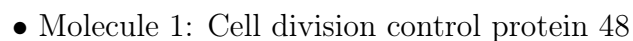
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).

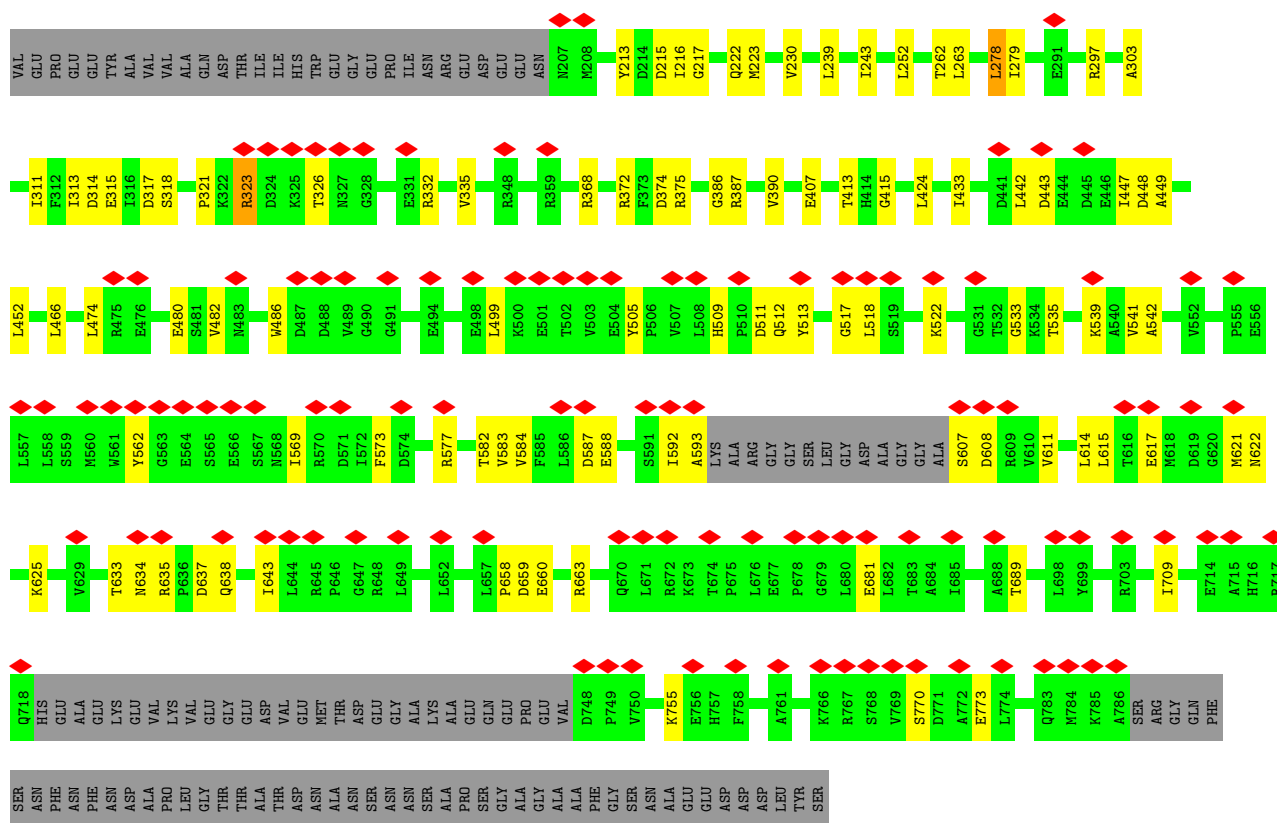


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total 27	C 10	N 5	O 10	P 2	0
6	B	1	Total 27	C 10	N 5	O 10	P 2	0
6	C	1	Total 27	C 10	N 5	O 10	P 2	0
6	D	1	Total 27	C 10	N 5	O 10	P 2	0
6	E	1	Total 54	C 20	N 10	O 20	P 4	0
6	E	1	Total 54	C 20	N 10	O 20	P 4	0
6	F	1	Total 27	C 10	N 5	O 10	P 2	0

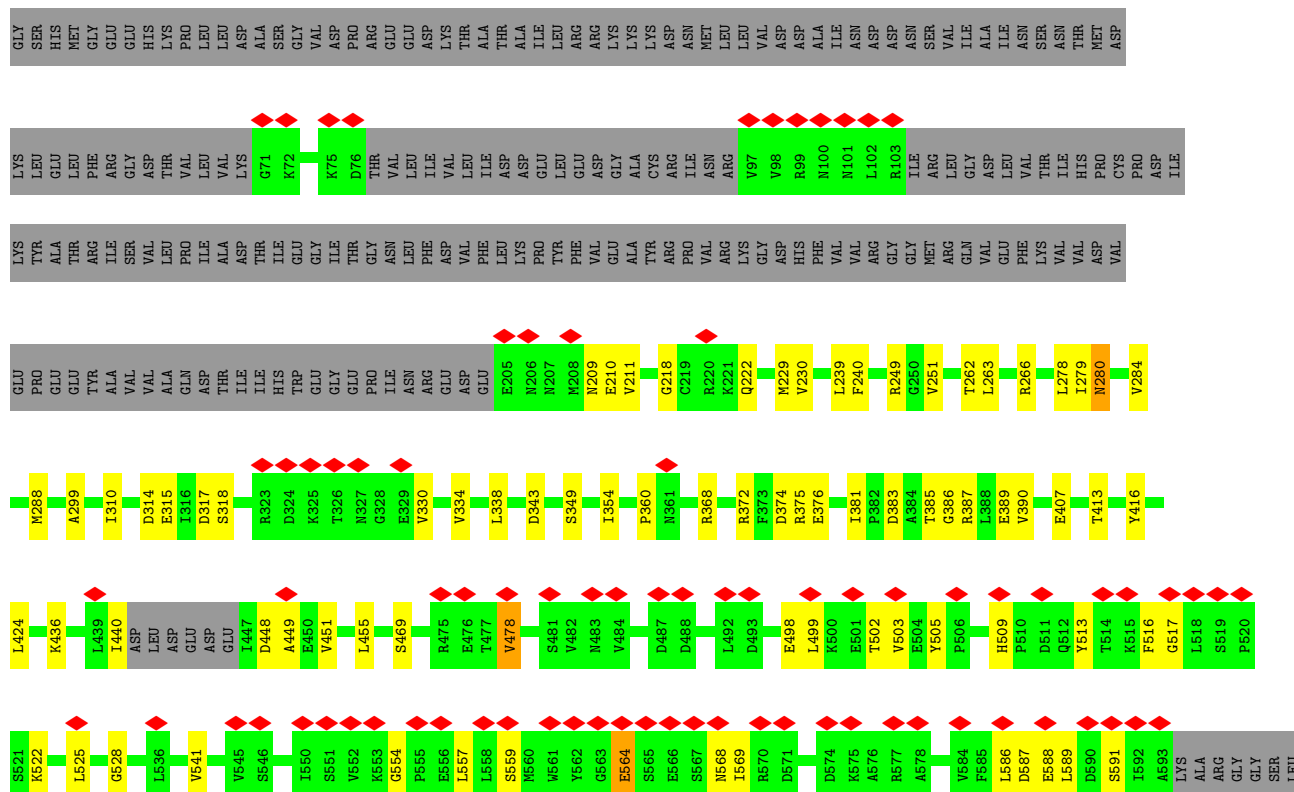
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

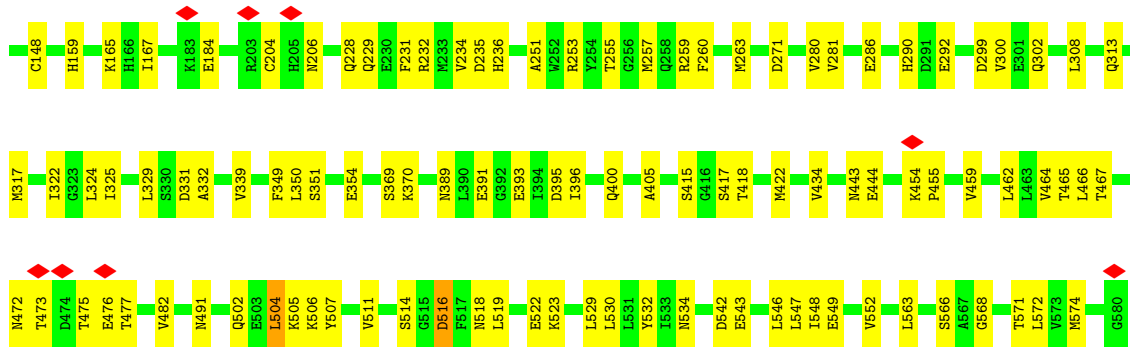




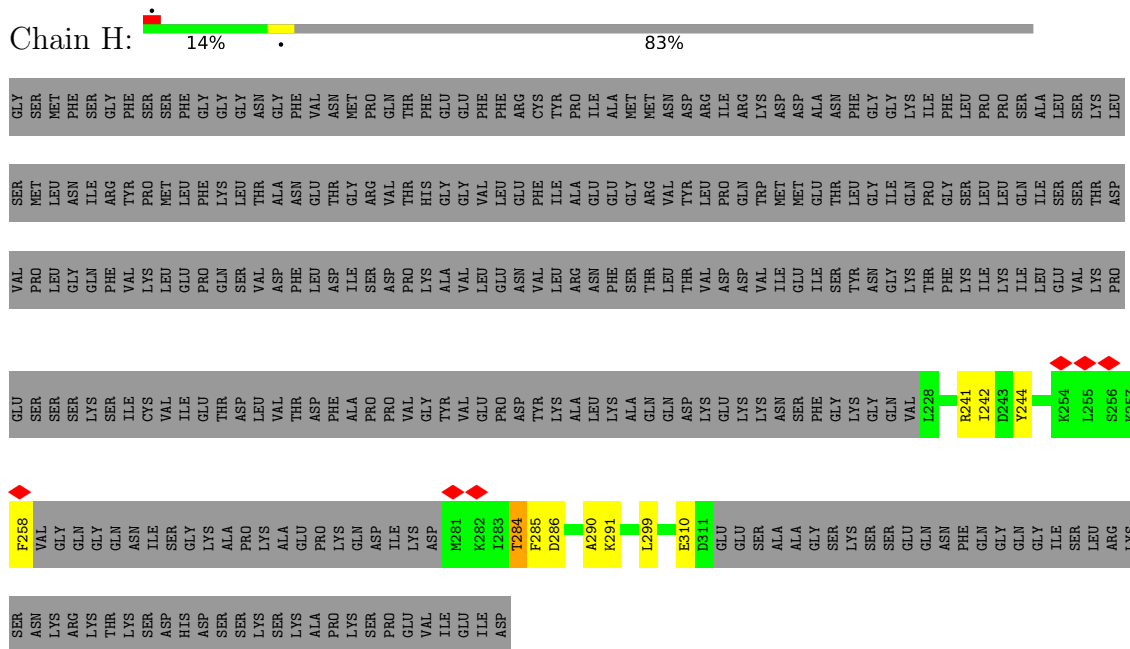
• Molecule 1: Cell division control protein 48



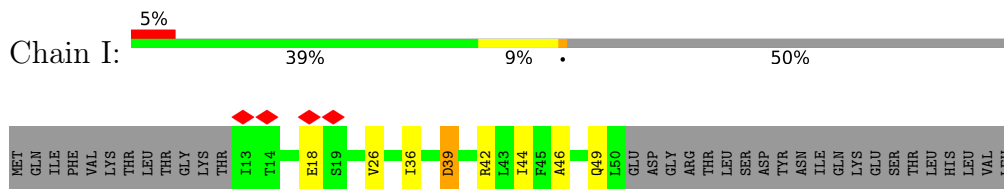




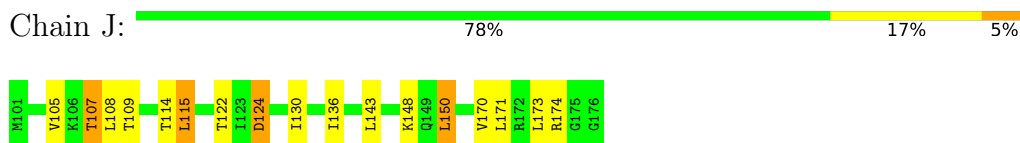
- Molecule 3: Ubiquitin fusion degradation protein 1



- Molecule 4: Ubiquitin



- Molecule 4: Ubiquitin



- Molecule 4: Ubiquitin





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48941	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 ($e^-/\text{\AA}^2$)	70.577	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	66.074	Depositor
Minimum map value	-25.924	Depositor
Average map value	-0.017	Depositor
Map value standard deviation	1.081	Depositor
Recommended contour level	9.0	Depositor
Map size (\AA)	408.576, 408.576, 408.576	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.064, 1.064, 1.064	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP, 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	0/5644	0.54	12/7639 (0.2%)
1	B	0.26	0/5687	0.73	30/7692 (0.4%)
1	C	0.25	0/4376	0.48	2/5908 (0.0%)
1	D	0.25	0/4304	0.58	6/5810 (0.1%)
1	E	0.26	0/4179	0.71	19/5649 (0.3%)
1	F	0.25	0/4348	0.57	9/5868 (0.2%)
2	G	0.30	0/3917	0.47	0/5290
3	H	0.28	0/486	0.45	0/651
4	I	0.26	0/300	0.44	0/403
4	J	0.27	0/605	0.70	6/812 (0.7%)
4	K	0.27	0/605	0.74	4/812 (0.5%)
All	All	0.26	0/34451	0.60	88/46534 (0.2%)

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
1	F	0	1

There are no bond length outliers.

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	639	ILE	C-N-CA	11.48	150.41	121.70
1	E	248	PRO	C-N-CA	9.12	144.50	121.70
1	B	370	PHE	C-N-CA	7.98	139.06	122.30
1	B	314	ASP	C-N-CA	7.49	140.42	121.70
1	E	331	GLU	C-N-CA	7.37	140.12	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	367	LEU	C-N-CA	7.36	140.09	121.70
1	D	284	VAL	CG1-CB-CG2	7.06	122.20	110.90
1	E	245	ILE	CG1-CB-CG2	6.93	126.65	111.40
1	B	112	ILE	CG1-CB-CG2	6.89	126.56	111.40
1	B	156	VAL	CG1-CB-CG2	6.83	121.82	110.90
1	E	552	VAL	CG1-CB-CG2	6.83	121.82	110.90
1	B	552	VAL	CG1-CB-CG2	6.82	121.81	110.90
1	B	42	ILE	CG1-CB-CG2	6.79	126.34	111.40
1	B	230	VAL	CG1-CB-CG2	6.79	121.75	110.90
1	E	319	ILE	CG1-CB-CG2	6.76	126.28	111.40
1	A	351	VAL	CG1-CB-CG2	6.75	121.71	110.90
1	E	550	ILE	CG1-CB-CG2	6.75	126.24	111.40
1	B	268	VAL	CG1-CB-CG2	6.72	121.65	110.90
1	B	81	VAL	CG1-CB-CG2	6.69	121.60	110.90
1	E	335	VAL	CG1-CB-CG2	6.67	121.56	110.90
1	D	478	VAL	CG1-CB-CG2	6.66	121.55	110.90
4	K	223	ILE	CG1-CB-CG2	6.65	126.04	111.40
1	B	98	VAL	CG1-CB-CG2	6.64	121.53	110.90
1	A	750	VAL	CG1-CB-CG2	6.64	121.52	110.90
1	B	83	ILE	CG1-CB-CG2	6.59	125.89	111.40
1	B	226	ILE	CG1-CB-CG2	6.59	125.89	111.40
1	D	280	ASN	C-N-CA	6.51	135.97	122.30
1	B	94	ILE	C-N-CA	6.50	137.96	121.70
1	F	611	VAL	CG1-CB-CG2	6.49	121.28	110.90
4	K	236	ILE	CG1-CB-CG2	6.47	125.64	111.40
1	B	186	VAL	C-N-CA	6.46	137.86	121.70
1	B	672	ARG	C-N-CA	6.42	137.75	121.70
1	D	685	ILE	CG1-CB-CG2	6.42	125.51	111.40
1	B	363	ILE	CG1-CB-CG2	6.38	125.44	111.40
1	B	229	MET	C-N-CA	6.27	137.37	121.70
1	C	278	LEU	CB-CG-CD2	6.21	121.55	111.00
1	B	36	LEU	C-N-CA	6.14	137.04	121.70
1	E	234	LEU	CB-CG-CD2	6.12	121.41	111.00
1	D	589	LEU	CB-CG-CD2	6.10	121.36	111.00
1	B	92	CYS	C-N-CA	6.06	136.84	121.70
1	B	87	LEU	CB-CG-CD2	6.00	121.20	111.00
1	B	589	LEU	CB-CG-CD2	5.98	121.17	111.00
1	B	280	ASN	C-N-CA	5.97	134.84	122.30
4	K	256	LEU	CB-CG-CD2	5.92	121.06	111.00
4	J	150	LEU	CB-CG-CD1	5.90	121.03	111.00
4	J	115	LEU	CB-CG-CD2	5.89	121.01	111.00
1	A	644	LEU	CB-CG-CD2	5.82	120.89	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	LEU	CB-CG-CD2	5.80	120.86	111.00
1	E	339	LEU	CB-CG-CD1	5.78	120.82	111.00
1	E	367	LEU	CB-CG-CD1	5.77	120.81	111.00
1	F	558	LEU	CB-CG-CD1	5.77	120.80	111.00
4	J	108	LEU	CB-CG-CD2	5.74	120.76	111.00
1	F	697	LEU	CB-CG-CD2	5.69	120.68	111.00
1	A	61	LEU	CB-CG-CD2	5.68	120.66	111.00
1	B	774	LEU	CB-CG-CD1	5.68	120.66	111.00
1	A	79	LEU	CB-CG-CD1	5.67	120.63	111.00
1	E	586	LEU	CB-CG-CD2	5.66	120.62	111.00
1	A	239	LEU	CB-CG-CD2	5.63	120.57	111.00
1	B	37	LEU	CB-CG-CD1	5.63	120.57	111.00
1	B	50	ALA	C-N-CA	5.60	135.69	121.70
1	A	79	LEU	CB-CG-CD2	5.58	120.49	111.00
1	E	339	LEU	CB-CG-CD2	5.58	120.49	111.00
1	E	586	LEU	CB-CG-CD1	5.57	120.47	111.00
1	F	649	LEU	CB-CG-CD2	5.57	120.47	111.00
1	F	649	LEU	CB-CG-CD1	5.56	120.46	111.00
1	F	589	LEU	CB-CG-CD2	5.55	120.44	111.00
1	A	239	LEU	CB-CG-CD1	5.55	120.43	111.00
1	E	649	LEU	CB-CG-CD1	5.54	120.43	111.00
1	F	697	LEU	CB-CG-CD1	5.54	120.42	111.00
1	A	61	LEU	CB-CG-CD1	5.54	120.42	111.00
4	K	256	LEU	CB-CG-CD1	5.50	120.36	111.00
1	B	86	GLU	C-N-CA	5.50	135.44	121.70
1	F	589	LEU	CB-CG-CD1	5.49	120.33	111.00
4	J	150	LEU	CB-CG-CD2	5.48	120.31	111.00
1	F	558	LEU	CB-CG-CD2	5.47	120.30	111.00
1	B	37	LEU	CB-CG-CD2	5.46	120.29	111.00
1	B	774	LEU	CB-CG-CD2	5.46	120.28	111.00
1	A	644	LEU	CB-CG-CD1	5.45	120.27	111.00
1	E	367	LEU	CB-CG-CD2	5.45	120.27	111.00
4	J	108	LEU	CB-CG-CD1	5.45	120.27	111.00
1	A	127	LEU	CB-CG-CD1	5.42	120.22	111.00
4	J	115	LEU	CB-CG-CD1	5.38	120.14	111.00
1	E	649	LEU	CB-CG-CD2	5.34	120.08	111.00
1	D	589	LEU	CB-CG-CD1	5.27	119.96	111.00
1	B	90	GLY	C-N-CA	5.26	134.86	121.70
1	E	234	LEU	CB-CG-CD1	5.25	119.93	111.00
1	B	589	LEU	CB-CG-CD1	5.25	119.92	111.00
1	C	278	LEU	CB-CG-CD1	5.16	119.76	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	307	ALA	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	5555	0	5575	107	0
1	B	5599	0	5652	115	0
1	C	4311	0	4347	81	0
1	D	4240	0	4280	86	0
1	E	4113	0	4143	68	0
1	F	4284	0	4326	66	0
2	G	3825	0	3695	89	0
3	H	477	0	476	9	0
4	I	298	0	303	8	0
4	J	600	0	620	11	0
4	K	600	0	622	25	0
5	A	31	0	12	2	0
5	B	31	0	12	2	0
5	C	31	0	12	1	0
5	D	31	0	12	1	0
5	F	31	0	12	0	0
6	A	27	0	12	1	0
6	B	27	0	12	0	0
6	C	27	0	12	1	0
6	D	27	0	12	1	0
6	E	54	0	24	0	0
6	F	27	0	12	0	0
7	G	2	0	0	0	0
All	All	34248	0	34183	628	0

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

All (628) 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)
2:G:281:VAL:HG12	2:G:322:ILE:HD11	1.55	0.88
1:D:559:SER:OG	1:D:564:GLU:O	1.93	0.86
1:D:754:THR:OG1	1:D:756:GLU:OE1	1.94	0.85
1:A:94:ILE:O	1:A:99:ARG:NH1	2.13	0.82
2:G:232:ARG:NE	2:G:235:ASP:OD1	2.11	0.82
2:G:292:GLU:OE2	3:H:241:ARG:NH2	2.11	0.82
1:B:293:GLU:OE1	1:B:293:GLU:N	2.13	0.81
1:A:345:MET:CE	1:A:351:VAL:HB	2.11	0.81
1:B:480:GLU:N	1:B:480:GLU:OE1	2.14	0.80
4:K:217:VAL:O	4:K:263:LYS:NZ	2.15	0.80
1:A:480:GLU:N	1:A:480:GLU:OE1	2.15	0.80
1:B:66:THR:OG1	1:B:115:CYS:O	1.99	0.80
1:F:668:ASN:O	1:F:672:ARG:NE	2.14	0.80
1:B:286:SER:OG	1:B:291:GLU:OE1	1.99	0.80
1:D:310:ILE:HD11	1:D:354:ILE:HD12	1.62	0.80
1:E:412:GLU:OE1	1:E:463:ARG:NH1	2.16	0.79
1:E:634:ASN:O	1:E:777:TYR:OH	2.01	0.79
1:D:262:THR:OG1	5:D:901:ATP:O2G	2.00	0.78
1:B:262:THR:OG1	5:B:901:ATP:O2G	2.01	0.77
1:A:131:ASP:OD2	1:A:201:ARG:NH1	2.18	0.77
1:D:693:SER:OG	1:D:768:SER:OG	2.02	0.77
1:E:431:GLN:OE1	1:E:434:ARG:NH1	2.18	0.76
2:G:443:ASN:OD1	2:G:444:GLU:N	2.18	0.76
1:D:773:GLU:OE2	1:D:776:ARG:NH2	2.18	0.76
1:E:522:LYS:NZ	1:E:625:LYS:O	2.19	0.76
1:B:391:LEU:O	1:B:395:THR:HG22	1.84	0.76
4:K:241:GLN:N	4:K:241:GLN:OE1	2.18	0.76
1:A:205:GLU:N	1:A:205:GLU:OE1	2.19	0.76
1:F:209:ASN:OD1	1:F:266:ARG:NH2	2.18	0.76
1:F:301:GLU:OE1	1:F:305:LYS:NZ	2.19	0.75
1:A:262:THR:OG1	5:A:901:ATP:O3G	2.04	0.75
1:A:666:ILE:HG22	1:A:670:GLN:HE22	1.50	0.75
1:A:121:ALA:O	1:A:190:THR:OG1	2.03	0.75
1:B:525:LEU:HD21	1:B:649:LEU:HD23	1.67	0.75
1:A:434:ARG:NE	1:B:228:GLU:OE2	2.19	0.75
2:G:115:GLU:N	2:G:115:GLU:OE1	2.21	0.74
2:G:331:ASP:OD1	2:G:332:ALA:N	2.20	0.74
1:C:522:LYS:NZ	1:C:625:LYS:O	2.18	0.74
1:B:209:ASN:ND2	2:G:206:ASN:O	2.21	0.74
1:B:329:GLU:OE1	1:B:332:ARG:NH2	2.21	0.74
1:C:323:ARG:NH2	1:C:326:THR:O	2.20	0.73
1:E:658:PRO:O	1:E:663:ARG:NH1	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLN:N	1:B:222:GLN:OE1	2.21	0.73
1:B:231:GLU:OE1	1:B:272:THR:HG22	1.89	0.72
1:F:283:GLU:O	1:F:286:SER:OG	2.03	0.72
1:D:705:ALA:HB3	1:E:518:LEU:HD21	1.71	0.72
1:A:193:HIS:ND1	3:H:258:PHE:O	2.22	0.72
2:G:502:GLN:N	2:G:502:GLN:OE1	2.23	0.72
2:G:417:SER:OG	2:G:422:MET:O	2.07	0.72
4:K:202:GLN:O	4:K:264:GLU:N	2.22	0.72
1:B:287:LYS:NZ	4:I:18:GLU:OE2	2.21	0.71
1:B:56:MET:O	1:B:60:GLU:N	2.24	0.71
2:G:351:SER:OG	2:G:354:GLU:OE1	2.07	0.71
1:E:539:LYS:O	1:E:543:THR:HG23	1.90	0.71
1:C:681:GLU:OE1	1:C:755:LYS:NZ	2.22	0.70
1:A:303:ALA:HB2	1:A:311:ILE:HD11	1.73	0.70
1:F:489:VAL:HG12	1:F:536:LEU:HD23	1.72	0.70
4:K:202:GLN:OE1	4:K:202:GLN:N	2.24	0.70
1:A:52:ASN:O	1:A:55:THR:OG1	2.06	0.70
1:E:703:ARG:NH2	1:E:761:ALA:O	2.24	0.70
1:C:562:TYR:OH	1:D:608:ASP:OD2	2.06	0.70
1:B:261:LYS:NZ	5:B:901:ATP:O2B	2.20	0.70
1:A:149:PHE:O	1:A:188:GLN:NE2	2.26	0.69
1:C:262:THR:OG1	5:C:901:ATP:O1G	2.10	0.69
1:C:407:GLU:N	1:C:407:GLU:OE1	2.25	0.69
2:G:391:GLU:N	2:G:391:GLU:OE1	2.26	0.69
1:B:148:TYR:CE1	1:B:164:VAL:HG13	2.28	0.69
1:F:479:VAL:HG12	1:F:550:ILE:HD12	1.75	0.69
1:B:564:GLU:N	1:B:564:GLU:OE1	2.26	0.69
1:C:321:PRO:CG	1:C:326:THR:HG21	2.23	0.68
1:B:210:GLU:N	1:B:210:GLU:OE1	2.26	0.68
1:F:522:LYS:NZ	1:F:625:LYS:O	2.26	0.68
2:G:475:THR:O	2:G:477:THR:N	2.27	0.68
1:D:619:ASP:OD2	1:D:648:ARG:NH2	2.27	0.68
1:E:523:GLY:HA3	1:E:649:LEU:HA	1.76	0.68
1:E:393:ILE:O	1:E:396:LYS:NZ	2.20	0.67
1:A:315:GLU:N	1:A:315:GLU:OE1	2.27	0.67
1:C:482:VAL:HG11	1:C:539:LYS:HE3	1.76	0.67
4:J:105:VAL:HG21	4:J:130:ILE:HD11	1.76	0.67
1:E:222:GLN:OE1	1:E:222:GLN:N	2.28	0.67
1:C:663:ARG:NH2	1:C:689:THR:O	2.27	0.67
1:D:658:PRO:O	1:D:663:ARG:NH1	2.28	0.67
1:B:48:VAL:HG22	1:B:80:ILE:HB	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:LYS:NZ	1:F:103:ARG:O	2.18	0.67
4:I:39:ASP:N	4:I:39:ASP:OD1	2.28	0.67
1:B:709:ILE:HD12	1:C:518:LEU:HD12	1.76	0.67
1:D:407:GLU:OE1	1:D:407:GLU:N	2.26	0.67
1:E:256:PRO:O	1:E:259:THR:OG1	2.09	0.67
1:F:480:GLU:OE1	1:F:480:GLU:N	2.28	0.66
1:F:570:ARG:NE	1:F:617:GLU:OE2	2.28	0.66
4:K:227:LYS:NZ	4:K:241:GLN:O	2.26	0.66
1:A:387:ARG:NE	1:A:413:THR:O	2.28	0.66
1:B:539:LYS:O	1:B:543:THR:HG23	1.94	0.66
1:C:482:VAL:HG11	1:C:539:LYS:CE	2.26	0.66
1:F:293:GLU:N	1:F:293:GLU:OE1	2.29	0.66
1:A:163:VAL:HG12	1:A:172:GLU:HB3	1.77	0.66
1:B:235:ARG:O	1:B:236:HIS:ND1	2.29	0.66
1:A:562:TYR:OH	1:B:608:ASP:OD2	2.13	0.66
1:D:387:ARG:NE	1:D:413:THR:O	2.28	0.66
1:A:124:ILE:HG22	1:A:178:VAL:HG13	1.77	0.66
1:D:528:GLY:O	1:D:634:ASN:ND2	2.28	0.66
1:D:659:ASP:OD1	1:D:660:GLU:N	2.30	0.65
1:F:566:GLU:N	1:F:566:GLU:OE1	2.29	0.65
2:G:393:GLU:OE1	4:I:44:ILE:HD11	1.96	0.65
1:D:554:GLY:N	1:D:588:GLU:OE2	2.30	0.65
1:D:210:GLU:OE1	1:D:210:GLU:N	2.30	0.65
1:D:499:LEU:O	1:D:503:VAL:HG12	1.97	0.65
1:B:144:PHE:HB3	1:B:164:VAL:HG11	1.79	0.65
1:E:499:LEU:HD21	1:E:541:VAL:HG21	1.79	0.65
1:D:343:ASP:OD2	1:D:372:ARG:NH2	2.30	0.65
2:G:236:HIS:ND1	2:G:467:THR:O	2.29	0.65
1:B:486:TRP:NE1	1:B:544:GLU:OE1	2.30	0.64
1:E:387:ARG:NE	1:E:413:THR:O	2.30	0.64
2:G:405:ALA:HB2	2:G:462:LEU:HD13	1.79	0.64
1:A:303:ALA:CB	1:A:311:ILE:HD11	2.27	0.64
1:E:331:GLU:O	1:E:335:VAL:HG23	1.98	0.64
1:F:222:GLN:N	1:F:222:GLN:OE1	2.30	0.64
1:B:407:GLU:OE1	1:B:407:GLU:N	2.30	0.64
2:G:516:ASP:N	2:G:516:ASP:OD1	2.26	0.64
2:G:106:HIS:HB3	2:G:108:TYR:CE2	2.33	0.64
1:D:222:GLN:N	1:D:222:GLN:OE1	2.30	0.64
4:J:124:ASP:N	4:J:124:ASP:OD1	2.27	0.64
1:D:767:ARG:NE	1:D:769:VAL:O	2.31	0.64
4:K:221:ASP:OD2	4:K:229:LYS:NZ	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLU:HB3	1:A:182:GLU:HA	1.79	0.64
1:A:203:ASP:OD1	1:A:204:GLU:N	2.30	0.64
1:A:278:LEU:HD21	1:A:280:ASN:OD1	1.98	0.64
1:C:222:GLN:N	1:C:222:GLN:OE1	2.31	0.64
2:G:514:SER:OG	2:G:516:ASP:OD1	2.07	0.64
1:B:705:ALA:HB1	1:C:518:LEU:HD11	1.79	0.63
1:F:409:LEU:O	1:F:413:THR:HG22	1.99	0.63
1:E:360:PRO:O	1:E:368:ARG:NH2	2.31	0.63
1:C:592:ILE:O	1:C:607:SER:N	2.31	0.63
1:F:254:TYR:OH	1:F:376:GLU:OE1	2.10	0.63
2:G:260:PHE:CE2	2:G:324:LEU:HD12	2.33	0.63
1:B:283:GLU:OE1	1:C:297:ARG:NH1	2.32	0.63
1:C:321:PRO:HG2	1:C:326:THR:HG21	1.79	0.63
1:F:278:LEU:HD23	1:F:279:ILE:N	2.14	0.63
1:A:222:GLN:N	1:A:222:GLN:OE1	2.31	0.63
1:B:206:ASN:OD1	1:B:207:ASN:N	2.32	0.63
1:B:303:ALA:CB	1:B:311:ILE:HD11	2.28	0.63
1:E:301:GLU:OE1	1:E:305:LYS:NZ	2.32	0.63
1:F:486:TRP:O	1:F:496:LYS:NZ	2.23	0.63
1:F:661:ASN:OD1	1:F:662:ALA:N	2.32	0.63
1:F:696:ASP:OD1	1:F:768:SER:OG	2.10	0.63
1:A:345:MET:HE3	1:A:351:VAL:HB	1.79	0.62
1:B:458:THR:OG1	1:B:460:ASP:OD1	2.17	0.62
1:C:323:ARG:NE	1:C:323:ARG:O	2.32	0.62
2:G:511:VAL:HG21	2:G:523:LYS:CD	2.29	0.62
4:K:215:LEU:HD23	4:K:216:GLU:N	2.14	0.62
1:F:407:GLU:N	1:F:407:GLU:OE1	2.32	0.62
1:A:407:GLU:N	1:A:407:GLU:OE1	2.32	0.62
1:B:303:ALA:HB3	1:B:311:ILE:HD11	1.81	0.62
1:E:525:LEU:HD12	1:E:649:LEU:HD21	1.82	0.62
4:I:49:GLN:N	4:I:49:GLN:OE1	2.32	0.62
1:B:35:MET:O	1:B:36:LEU:HD23	1.99	0.62
1:C:480:GLU:N	1:C:480:GLU:OE1	2.32	0.62
1:B:440:ILE:HD11	1:B:451:VAL:HG21	1.81	0.61
2:G:144:MET:SD	2:G:144:MET:N	2.73	0.61
2:G:299:ASP:OD1	2:G:300:VAL:N	2.33	0.61
1:C:387:ARG:NE	1:C:413:THR:O	2.33	0.61
1:A:202:GLU:OE1	1:A:206:ASN:ND2	2.33	0.61
1:A:560:MET:SD	1:A:569:ILE:N	2.74	0.61
1:A:416:TYR:OH	1:A:469:SER:OG	2.10	0.61
1:A:359:ARG:NE	1:A:571:ASP:OD2	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:ASP:OD1	1:D:315:GLU:N	2.34	0.60
1:E:458:THR:OG1	1:E:461:ASN:OD1	2.18	0.60
1:A:625:LYS:HG3	1:A:627:VAL:HG23	1.83	0.60
1:D:209:ASN:OD1	1:D:266:ARG:NH2	2.34	0.60
1:E:705:ALA:HB3	1:F:518:LEU:HD21	1.81	0.60
2:G:260:PHE:HE2	2:G:324:LEU:HD12	1.66	0.60
1:C:622:ASN:O	1:C:625:LYS:N	2.32	0.60
1:E:278:LEU:HD23	1:E:279:ILE:N	2.16	0.60
4:K:219:SER:HA	4:K:256:LEU:HD12	1.83	0.60
1:D:310:ILE:HD11	1:D:354:ILE:CD1	2.32	0.60
1:D:568:ASN:OD1	1:D:569:ILE:N	2.32	0.60
2:G:263:MET:CE	2:G:281:VAL:HG11	2.31	0.60
4:J:143:LEU:O	4:J:150:LEU:HD13	2.02	0.60
1:D:709:ILE:HD11	1:E:516:PHE:CB	2.32	0.59
1:D:693:SER:N	1:D:696:ASP:OD2	2.35	0.59
1:B:409:LEU:O	1:B:413:THR:HG22	2.01	0.59
1:D:317:ASP:OD1	1:D:318:SER:N	2.35	0.59
4:I:36:ILE:HD11	4:I:42:ARG:NH2	2.18	0.59
1:E:480:GLU:N	1:E:480:GLU:OE1	2.36	0.59
1:C:569:ILE:HG23	1:C:617:GLU:OE2	2.02	0.59
2:G:395:ASP:OD1	2:G:396:ILE:N	2.35	0.59
1:B:203:ASP:OD1	1:B:206:ASN:ND2	2.35	0.59
1:B:702:GLN:OE1	1:B:706:LYS:NZ	2.36	0.59
1:C:615:LEU:HD21	1:C:643:ILE:HD13	1.85	0.59
1:E:484:VAL:N	1:E:543:THR:HG21	2.17	0.59
1:F:306:ASN:O	1:F:306:ASN:ND2	2.36	0.59
3:H:284:THR:OG1	3:H:285:PHE:N	2.34	0.59
1:A:490:GLY:H	6:A:902:ADP:HN61	1.51	0.59
1:D:279:ILE:HD11	1:D:299:ALA:CB	2.32	0.59
1:E:234:LEU:HD21	1:E:352:VAL:HG23	1.85	0.59
2:G:302:GLN:NE2	4:J:109:THR:O	2.36	0.59
1:D:249:ARG:NH2	1:D:349:SER:O	2.36	0.58
1:E:359:ARG:HH22	1:E:567:SER:HA	1.69	0.58
2:G:354:GLU:OE1	2:G:354:GLU:N	2.36	0.58
1:D:383:ASP:OD1	1:D:385:THR:N	2.36	0.58
1:F:207:ASN:OD1	1:F:209:ASN:ND2	2.37	0.58
1:B:484:VAL:N	1:B:543:THR:HG21	2.19	0.58
1:D:699:TYR:OH	1:D:703:ARG:NH1	2.37	0.58
2:G:229:GLN:NE2	2:G:231:PHE:O	2.37	0.58
1:B:151:GLU:OE1	1:B:151:GLU:N	2.36	0.58
1:D:436:LYS:HG3	1:D:455:LEU:HD23	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:402:ASP:OD1	1:F:403:ASP:N	2.37	0.58
1:B:447:ILE:HD12	1:B:452:LEU:HD21	1.85	0.57
1:B:525:LEU:CD2	1:B:649:LEU:HD23	2.34	0.57
2:G:571:THR:HG22	4:K:247:GLY:H	1.70	0.57
1:B:36:LEU:HD22	1:B:90:GLY:HA2	1.86	0.57
1:B:484:VAL:H	1:B:543:THR:HG21	1.69	0.57
1:F:493:ASP:OD1	1:F:494:GLU:N	2.37	0.57
4:J:173:LEU:HD23	4:J:174:ARG:N	2.18	0.57
1:C:317:ASP:OD1	1:C:318:SER:N	2.38	0.57
1:D:635:ARG:NH2	1:D:637:ASP:OD2	2.37	0.57
1:D:522:LYS:NZ	1:D:622:ASN:O	2.25	0.56
2:G:349:PHE:O	2:G:350:LEU:HD12	2.06	0.56
1:D:525:LEU:HD11	1:D:633:THR:HG22	1.86	0.56
1:B:513:TYR:O	1:B:517:GLY:N	2.38	0.56
2:G:281:VAL:HG12	2:G:322:ILE:CD1	2.33	0.56
3:H:242:ILE:O	3:H:244:TYR:N	2.39	0.56
2:G:511:VAL:HG21	2:G:523:LYS:HD2	1.88	0.56
1:E:407:GLU:OE1	1:E:407:GLU:N	2.37	0.56
1:F:211:VAL:HG23	1:F:211:VAL:O	2.05	0.56
1:A:177:ASP:OD1	1:A:178:VAL:N	2.39	0.55
1:B:153:TYR:HA	1:B:186:VAL:O	2.05	0.55
1:B:413:THR:HG23	1:B:413:THR:O	2.05	0.55
1:A:121:ALA:N	1:A:185:VAL:O	2.36	0.55
1:C:433:ILE:HD12	1:D:239:LEU:HD13	1.86	0.55
2:G:507:TYR:O	2:G:511:VAL:HG23	2.06	0.55
1:C:511:ASP:OD1	1:C:512:GLN:N	2.39	0.55
1:D:505:TYR:O	1:D:509:HIS:N	2.38	0.55
2:G:400:GLN:O	2:G:464:VAL:HG22	2.06	0.55
3:H:310:GLU:N	3:H:310:GLU:OE1	2.40	0.55
1:C:663:ARG:NE	1:C:689:THR:OG1	2.34	0.55
1:E:782:GLN:N	1:E:782:GLN:OE1	2.39	0.55
1:A:466:LEU:O	1:A:466:LEU:HD23	2.06	0.55
1:B:150:VAL:HA	1:B:188:GLN:HB2	1.88	0.55
1:C:659:ASP:OD1	1:C:660:GLU:N	2.39	0.55
2:G:165:LYS:NZ	2:G:465:THR:HG21	2.22	0.55
1:C:770:SER:N	1:C:773:GLU:OE2	2.40	0.54
1:D:607:SER:OG	1:D:608:ASP:N	2.41	0.54
1:B:343:ASP:OD2	1:B:372:ARG:NH2	2.41	0.54
2:G:263:MET:HE2	2:G:281:VAL:HG11	1.88	0.54
1:A:56:MET:O	1:A:60:GLU:N	2.40	0.54
1:F:335:VAL:O	1:F:339:LEU:HD13	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:LEU:C	1:B:653:ILE:HD12	2.28	0.54
1:C:569:ILE:HD11	1:C:573:PHE:CE2	2.42	0.54
2:G:126:ASP:OD1	2:G:126:ASP:N	2.40	0.54
2:G:234:VAL:O	2:G:466:LEU:HD22	2.07	0.54
2:G:259:ARG:NE	2:G:286:GLU:OE1	2.41	0.54
2:G:159:HIS:ND1	2:G:167:ILE:HG22	2.23	0.54
1:F:522:LYS:NZ	1:F:623:ALA:O	2.37	0.54
1:A:504:GLU:OE2	1:A:508:LEU:HD12	2.08	0.54
1:D:498:GLU:O	1:D:502:THR:HG23	2.08	0.54
1:B:144:PHE:CB	1:B:164:VAL:HG11	2.38	0.53
1:C:709:ILE:HD11	1:D:516:PHE:CG	2.43	0.53
1:A:515:LYS:NZ	1:F:748:ASP:OD2	2.39	0.53
1:A:61:LEU:HG	1:A:62:PHE:N	2.22	0.53
1:A:96:ARG:NH2	1:A:104:ILE:O	2.41	0.53
1:D:288:MET:SD	1:D:288:MET:N	2.80	0.53
1:B:34:ASN:ND2	1:B:111:THR:HG22	2.23	0.53
1:C:637:ASP:OD1	1:C:638:GLN:N	2.42	0.53
1:B:240:PHE:HA	1:B:243:ILE:HG22	1.89	0.53
2:G:511:VAL:HG21	2:G:523:LYS:HD3	1.89	0.53
1:A:709:ILE:HG21	1:B:513:TYR:CE1	2.44	0.53
1:D:440:ILE:HD11	1:D:451:VAL:HG11	1.90	0.53
2:G:263:MET:HE3	2:G:325:ILE:HD11	1.91	0.53
2:G:459:VAL:HG23	2:G:462:LEU:HD12	1.90	0.53
2:G:511:VAL:HG13	2:G:519:LEU:HD22	1.91	0.53
1:B:95:ASN:OD1	1:B:98:VAL:HG23	2.09	0.53
1:C:513:TYR:O	1:C:517:GLY:N	2.42	0.53
1:E:649:LEU:HG	1:E:649:LEU:O	2.09	0.53
1:D:697:LEU:O	1:D:701:VAL:HG23	2.09	0.53
1:F:284:VAL:O	1:F:292:SER:OG	2.17	0.53
2:G:317:MET:CE	2:G:530:LEU:HD11	2.38	0.53
1:D:239:LEU:HD12	1:D:240:PHE:N	2.24	0.53
1:E:317:ASP:OD1	1:E:318:SER:N	2.41	0.53
1:F:413:THR:O	1:F:413:THR:HG23	2.09	0.53
1:A:671:LEU:HD13	1:A:676:LEU:HD11	1.91	0.52
1:E:479:VAL:HG12	1:E:550:ILE:CD1	2.39	0.52
1:C:569:ILE:HD11	1:C:573:PHE:HE2	1.74	0.52
2:G:482:VAL:HG11	2:G:522:GLU:HG2	1.91	0.52
1:F:317:ASP:HA	1:F:363:ILE:HG22	1.91	0.52
2:G:107:ARG:HG2	2:G:109:GLY:H	1.73	0.52
2:G:329:LEU:N	2:G:329:LEU:HD12	2.25	0.52
1:A:150:VAL:HG13	1:A:150:VAL:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ARG:NE	1:B:413:THR:O	2.43	0.52
1:D:279:ILE:HD11	1:D:299:ALA:HB1	1.91	0.52
4:K:227:LYS:NZ	4:K:238:PRO:O	2.34	0.52
1:B:52:ASN:OD1	1:B:53:SER:N	2.42	0.52
1:F:331:GLU:O	1:F:335:VAL:HG22	2.09	0.52
2:G:393:GLU:CD	4:I:44:ILE:HD11	2.29	0.52
1:A:168:MET:CE	1:A:168:MET:HA	2.40	0.52
1:B:499:LEU:CD2	1:B:541:VAL:HG21	2.40	0.52
1:A:288:MET:SD	1:A:288:MET:N	2.82	0.52
1:A:330:VAL:O	1:A:334:VAL:HG23	2.10	0.52
1:E:619:ASP:OD1	1:E:648:ARG:NE	2.42	0.52
1:C:542:ALA:HA	1:C:583:VAL:HG21	1.92	0.51
2:G:518:ASN:OD1	2:G:519:LEU:N	2.44	0.51
2:G:259:ARG:NH2	2:G:286:GLU:OE1	2.42	0.51
1:C:505:TYR:O	1:C:509:HIS:N	2.42	0.51
2:G:286:GLU:O	2:G:491:ASN:ND2	2.43	0.51
1:D:424:LEU:C	1:D:424:LEU:HD23	2.30	0.51
1:D:607:SER:O	1:D:611:VAL:HG23	2.11	0.51
1:F:303:ALA:O	1:F:307:ALA:HB2	2.10	0.51
1:D:218:GLY:N	1:D:389:GLU:OE1	2.44	0.51
2:G:529:LEU:HD23	2:G:529:LEU:C	2.31	0.51
1:C:583:VAL:HG12	1:C:583:VAL:O	2.11	0.51
1:B:268:VAL:O	1:B:272:THR:HG23	2.10	0.51
2:G:106:HIS:CG	2:G:107:ARG:H	2.27	0.51
2:G:251:ALA:O	2:G:255:THR:HG22	2.11	0.51
1:D:374:ASP:OD1	1:D:375:ARG:N	2.44	0.51
2:G:472:ASN:OD1	2:G:473:THR:N	2.45	0.50
1:A:438:ASP:OD1	1:A:439:LEU:N	2.43	0.50
1:B:37:LEU:HG	1:B:38:VAL:N	2.26	0.50
2:G:548:ILE:O	2:G:552:VAL:HG12	2.11	0.50
1:A:182:GLU:N	1:A:182:GLU:OE1	2.44	0.50
1:B:608:ASP:OD1	1:B:609:ARG:N	2.44	0.50
1:E:499:LEU:O	1:E:503:VAL:HG12	2.12	0.50
1:B:105:ARG:N	1:B:108:ASP:OD2	2.43	0.50
2:G:519:LEU:HD23	2:G:519:LEU:O	2.11	0.50
1:E:291:GLU:OE1	1:E:291:GLU:N	2.39	0.50
1:E:489:VAL:O	1:E:496:LYS:NZ	2.40	0.50
1:B:750:VAL:HG13	1:B:750:VAL:O	2.11	0.50
1:E:718:GLN:N	1:E:718:GLN:OE1	2.45	0.50
1:B:424:LEU:HD23	1:B:424:LEU:C	2.31	0.50
1:B:499:LEU:HD21	1:B:541:VAL:HG21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TYR:CE2	1:A:164:VAL:HG22	2.46	0.49
1:A:569:ILE:HG23	1:A:617:GLU:OE2	2.12	0.49
1:B:460:ASP:OD1	1:B:461:ASN:N	2.45	0.49
1:B:499:LEU:O	1:B:503:VAL:HG12	2.11	0.49
1:A:123:ARG:NH2	1:A:179:GLU:OE1	2.42	0.49
2:G:546:LEU:HD11	2:G:563:LEU:HD13	1.94	0.49
4:K:262:GLN:NE2	4:K:263:LYS:O	2.46	0.49
1:A:748:ASP:OD2	1:B:515:LYS:NZ	2.40	0.49
1:F:511:ASP:OD1	1:F:512:GLN:N	2.46	0.49
1:D:706:LYS:HG2	1:E:518:LEU:HD22	1.93	0.49
1:B:54:ASN:OD1	1:B:58:LYS:NZ	2.46	0.49
1:E:303:ALA:HB2	1:E:311:ILE:HD11	1.95	0.49
1:E:343:ASP:OD2	1:E:372:ARG:NH2	2.45	0.49
1:F:317:ASP:OD1	1:F:318:SER:N	2.46	0.49
2:G:546:LEU:HD12	2:G:547:LEU:N	2.27	0.49
1:A:243:ILE:HG23	1:A:245:ILE:HG22	1.94	0.49
1:C:770:SER:OG	1:C:773:GLU:OE1	2.31	0.49
2:G:184:GLU:N	2:G:184:GLU:OE1	2.46	0.49
1:A:644:LEU:HD12	1:A:652:LEU:HD21	1.95	0.49
1:F:405:ASP:O	1:F:408:ALA:N	2.42	0.49
3:H:284:THR:HG23	3:H:286:ASP:OD1	2.13	0.49
1:C:314:ASP:OD1	1:C:315:GLU:N	2.45	0.49
1:C:621:MET:SD	1:C:621:MET:N	2.76	0.49
1:A:258:GLY:N	5:A:901:ATP:O1B	2.41	0.49
3:H:299:LEU:HD12	3:H:299:LEU:N	2.28	0.49
1:A:709:ILE:HG21	1:B:513:TYR:HE1	1.78	0.48
1:B:314:ASP:OD1	1:B:315:GLU:N	2.46	0.48
1:D:557:LEU:HD23	1:D:557:LEU:H	1.77	0.48
1:B:395:THR:HG23	1:B:395:THR:O	2.13	0.48
4:J:136:ILE:HD11	4:J:171:LEU:CD2	2.44	0.48
1:B:323:ARG:NH2	1:B:336:SER:OG	2.47	0.48
1:A:648:ARG:O	1:A:650:ASP:N	2.46	0.48
1:C:433:ILE:CD1	1:D:239:LEU:HD13	2.44	0.48
1:C:486:TRP:HH2	1:C:541:VAL:HG22	1.79	0.48
1:F:74:ARG:NH2	1:F:272:THR:O	2.46	0.48
1:F:753:ILE:HD12	1:F:753:ILE:N	2.29	0.48
1:D:360:PRO:O	1:D:368:ARG:NH2	2.47	0.47
1:D:513:TYR:O	1:D:517:GLY:N	2.38	0.47
1:E:401:ALA:O	1:E:404:VAL:HG13	2.14	0.47
1:E:503:VAL:HG13	1:E:504:GLU:N	2.29	0.47
2:G:434:VAL:HG23	2:G:434:VAL:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:331:ASP:HA	2:G:339:VAL:HG12	1.96	0.47
1:A:168:MET:HA	1:A:168:MET:HE2	1.95	0.47
1:E:359:ARG:NH1	1:E:566:GLU:O	2.46	0.47
1:F:489:VAL:HG12	1:F:536:LEU:CD2	2.40	0.47
1:A:96:ARG:NE	1:A:100:ASN:OD1	2.43	0.47
1:E:537:LEU:O	1:E:541:VAL:HG23	2.13	0.47
1:F:214:ASP:OD1	1:F:215:ASP:N	2.48	0.47
4:K:255:THR:OG1	4:K:256:LEU:N	2.46	0.47
1:B:709:ILE:CD1	1:C:518:LEU:HD12	2.42	0.47
1:E:424:LEU:C	1:E:424:LEU:HD23	2.34	0.47
1:F:331:GLU:OE1	1:F:331:GLU:N	2.43	0.47
1:F:503:VAL:HG13	1:F:504:GLU:N	2.30	0.47
2:G:504:LEU:HD12	2:G:532:TYR:HE2	1.78	0.47
1:A:479:VAL:HG12	1:A:550:ILE:CD1	2.44	0.47
1:D:386:GLY:O	1:D:390:VAL:HG23	2.15	0.47
4:K:202:GLN:O	4:K:264:GLU:HA	2.15	0.47
4:K:215:LEU:HD22	4:K:217:VAL:HG12	1.96	0.47
1:A:259:THR:O	1:A:259:THR:HG22	2.15	0.47
1:A:666:ILE:O	1:A:670:GLN:NE2	2.48	0.47
1:D:230:VAL:HG12	1:D:230:VAL:O	2.14	0.47
1:A:211:VAL:HG23	1:A:211:VAL:O	2.14	0.47
1:B:122:THR:HG22	1:B:179:GLU:C	2.36	0.47
1:B:503:VAL:HG13	1:B:504:GLU:N	2.30	0.47
1:D:666:ILE:HD11	6:D:902:ADP:C6	2.50	0.47
1:F:259:THR:O	1:F:259:THR:HG22	2.15	0.47
1:F:648:ARG:O	1:F:650:ASP:N	2.48	0.47
1:F:750:VAL:HG13	1:F:750:VAL:O	2.14	0.47
1:A:181:GLU:CB	1:A:182:GLU:HA	2.34	0.47
1:B:263:LEU:HD23	1:B:263:LEU:C	2.35	0.47
1:C:216:ILE:N	1:C:216:ILE:HD12	2.30	0.47
1:E:668:ASN:O	1:E:672:ARG:NH1	2.48	0.47
4:K:219:SER:O	4:K:256:LEU:HG	2.15	0.46
1:E:367:LEU:O	1:E:373:PHE:N	2.47	0.46
1:A:128:PRO:C	1:A:129:ILE:HD13	2.35	0.46
1:B:643:ILE:HG22	1:B:643:ILE:O	2.15	0.46
1:C:386:GLY:O	1:C:390:VAL:HG23	2.14	0.46
2:G:542:ASP:OD1	2:G:542:ASP:N	2.49	0.46
1:B:24:THR:O	1:B:24:THR:HG22	2.14	0.46
1:B:479:VAL:HG12	1:B:550:ILE:CD1	2.46	0.46
1:D:448:ASP:OD1	1:D:449:ALA:N	2.48	0.46
1:B:37:LEU:HD23	1:B:39:ASP:OD2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:207:THR:HG22	4:K:208:LEU:N	2.31	0.46
1:D:211:VAL:HG23	1:D:211:VAL:O	2.16	0.46
1:D:675:PRO:O	1:D:676:LEU:HD23	2.16	0.46
1:E:525:LEU:HB2	1:E:649:LEU:HD11	1.97	0.46
4:K:223:ILE:HB	4:K:252:ASP:HA	1.98	0.46
1:A:637:ASP:OD1	1:A:637:ASP:N	2.48	0.46
2:G:255:THR:HG23	2:G:257:MET:H	1.80	0.46
1:F:201:ARG:NH1	1:F:205:GLU:OE2	2.49	0.46
2:G:263:MET:HE1	2:G:281:VAL:HG11	1.98	0.46
4:K:243:LEU:N	4:K:243:LEU:HD22	2.31	0.46
1:A:402:ASP:OD1	1:A:403:ASP:N	2.49	0.45
1:A:49:ILE:CD1	1:A:94:ILE:HD11	2.45	0.45
1:A:263:LEU:O	1:A:263:LEU:HD23	2.16	0.45
1:D:279:ILE:HG22	1:D:280:ASN:O	2.16	0.45
2:G:571:THR:HG22	4:K:247:GLY:N	2.32	0.45
1:A:163:VAL:O	1:A:165:ARG:NH1	2.49	0.45
1:B:499:LEU:CD2	1:B:537:LEU:HD21	2.46	0.45
1:B:482:VAL:HG23	1:B:543:THR:HG22	1.98	0.45
2:G:308:LEU:C	2:G:308:LEU:HD23	2.37	0.45
4:J:148:LYS:O	4:J:150:LEU:HD12	2.16	0.45
1:C:372:ARG:O	1:C:374:ASP:N	2.49	0.45
1:C:374:ASP:OD1	1:C:375:ARG:N	2.48	0.45
1:D:368:ARG:NE	1:D:376:GLU:OE2	2.50	0.45
1:E:234:LEU:HD22	1:E:350:ASN:HB3	1.97	0.45
1:E:345:MET:SD	1:E:351:VAL:HG11	2.56	0.45
1:E:374:ASP:OD1	1:E:375:ARG:N	2.50	0.45
1:A:452:LEU:HA	1:A:455:LEU:HD23	1.99	0.45
1:A:614:LEU:HD23	1:A:614:LEU:O	2.17	0.45
1:C:582:THR:HG22	1:C:584:VAL:HG23	1.97	0.45
1:B:627:VAL:HG12	1:B:627:VAL:O	2.17	0.45
1:E:232:LEU:HB2	1:E:233:PRO:HD3	1.99	0.45
2:G:253:ARG:NH2	4:I:46:ALA:O	2.50	0.45
2:G:563:LEU:O	2:G:566:SER:OG	2.08	0.45
1:C:278:LEU:HD23	1:C:279:ILE:N	2.32	0.45
1:D:338:LEU:O	1:D:338:LEU:HD23	2.17	0.45
1:D:586:LEU:N	1:D:586:LEU:HD12	2.32	0.45
1:A:697:LEU:O	1:A:701:VAL:HG23	2.17	0.45
1:C:313:ILE:HG22	1:C:314:ASP:N	2.32	0.45
1:D:615:LEU:HD23	1:D:643:ILE:HD13	1.98	0.45
1:B:77:THR:HG22	1:B:78:VAL:N	2.32	0.44
1:B:366:ALA:O	1:B:372:ARG:NH1	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ALA:CB	1:C:311:ILE:HD11	2.47	0.44
1:D:670:GLN:OE1	1:D:698:LEU:HA	2.17	0.44
1:D:697:LEU:H	1:D:697:LEU:HD22	1.82	0.44
4:K:215:LEU:HD23	4:K:216:GLU:H	1.79	0.44
1:A:130:ALA:HA	1:A:133:ILE:HG12	1.99	0.44
1:A:256:PRO:O	1:A:259:THR:OG1	2.23	0.44
1:A:711:ASP:OD2	1:A:757:HIS:NE2	2.50	0.44
1:C:424:LEU:C	1:C:424:LEU:HD23	2.37	0.44
1:C:499:LEU:HD21	1:C:541:VAL:HG21	1.99	0.44
1:E:664:LEU:HD22	1:E:682:LEU:HD21	1.98	0.44
1:F:360:PRO:O	1:F:368:ARG:NH2	2.51	0.44
1:A:94:ILE:HD12	1:A:94:ILE:N	2.33	0.44
1:C:215:ASP:C	1:C:216:ILE:HD12	2.37	0.44
1:C:593:ALA:O	1:C:638:GLN:NE2	2.48	0.44
2:G:418:THR:HG22	3:H:290:ALA:H	1.82	0.44
4:K:252:ASP:OD1	4:K:252:ASP:N	2.51	0.44
4:K:258:ASP:OD1	4:K:259:TYR:N	2.50	0.44
1:A:713:ILE:HD11	1:B:512:GLN:NE2	2.32	0.44
1:D:372:ARG:O	1:D:374:ASP:N	2.51	0.44
2:G:415:SER:OG	3:H:291:LYS:NZ	2.49	0.44
1:B:511:ASP:OD1	1:B:512:GLN:N	2.50	0.44
1:C:466:LEU:HD23	1:C:466:LEU:O	2.18	0.44
4:J:170:VAL:HG12	4:J:171:LEU:N	2.33	0.44
1:A:249:ARG:NH2	1:A:347:ALA:O	2.50	0.44
1:A:129:ILE:O	1:A:132:THR:OG1	2.28	0.44
1:B:348:ARG:O	1:B:348:ARG:NE	2.51	0.44
1:B:412:GLU:OE2	1:B:463:ARG:NH1	2.51	0.44
1:D:676:LEU:HD22	1:D:753:ILE:HB	1.99	0.44
1:F:313:ILE:HG22	1:F:314:ASP:N	2.33	0.44
2:G:572:LEU:C	2:G:572:LEU:HD23	2.38	0.44
1:B:417:VAL:HG12	1:B:418:GLY:H	1.82	0.43
1:B:590:ASP:OD1	1:B:590:ASP:N	2.51	0.43
1:C:415:GLY:HA3	1:C:474:LEU:HD11	2.00	0.43
1:E:378:ASP:OD1	1:E:379:ILE:N	2.51	0.43
1:F:499:LEU:O	1:F:503:VAL:HG12	2.18	0.43
1:C:230:VAL:HG12	1:C:230:VAL:O	2.19	0.43
1:C:321:PRO:HG3	1:C:326:THR:HG21	1.96	0.43
4:J:136:ILE:HG23	4:J:136:ILE:O	2.18	0.43
1:C:447:ILE:HG21	1:C:452:LEU:HD21	2.00	0.43
1:D:381:ILE:N	1:D:381:ILE:HD12	2.33	0.43
1:D:676:LEU:CD2	1:D:753:ILE:HD13	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:LEU:O	1:F:263:LEU:HD23	2.18	0.43
1:F:754:THR:OG1	1:F:756:GLU:OE2	2.37	0.43
4:K:267:LEU:HD12	4:K:267:LEU:N	2.33	0.43
1:B:34:ASN:HD22	1:B:111:THR:HG22	1.83	0.43
1:B:492:LEU:HD12	1:B:492:LEU:N	2.33	0.43
1:C:213:TYR:HA	1:C:216:ILE:HD13	2.00	0.43
1:C:607:SER:N	1:C:611:VAL:HG23	2.33	0.43
2:G:313:GLN:NE2	2:G:534:ASN:OD1	2.42	0.43
1:B:615:LEU:HD21	1:B:643:ILE:HD13	2.01	0.43
1:B:685:ILE:HD11	1:B:758:PHE:HB3	2.00	0.43
1:C:263:LEU:C	1:C:263:LEU:HD23	2.37	0.43
1:F:282:PRO:O	1:F:286:SER:N	2.50	0.43
1:F:529:PRO:O	1:F:532:THR:HG23	2.19	0.43
1:A:231:GLU:CD	1:A:272:THR:HG22	2.39	0.43
1:A:479:VAL:HG12	1:A:550:ILE:HG12	2.01	0.43
1:D:381:ILE:CD1	1:D:478:VAL:HG11	2.49	0.43
1:D:416:TYR:OH	1:D:469:SER:OG	2.29	0.43
1:F:614:LEU:HD23	1:F:614:LEU:O	2.19	0.43
1:B:177:ASP:OD1	1:B:178:VAL:N	2.52	0.43
1:D:663:ARG:NE	1:D:689:THR:O	2.52	0.43
1:F:537:LEU:O	1:F:541:VAL:HG23	2.18	0.43
2:G:271:ASP:OD1	2:G:271:ASP:N	2.40	0.43
1:B:452:LEU:CD2	1:C:239:LEU:HD23	2.47	0.43
1:B:642:ALA:O	1:B:645:ARG:NE	2.47	0.43
1:D:587:ASP:OD1	1:D:587:ASP:N	2.51	0.43
1:E:753:ILE:N	1:E:753:ILE:HD12	2.34	0.43
2:G:280:VAL:O	2:G:280:VAL:HG23	2.18	0.43
1:B:256:PRO:O	1:B:259:THR:OG1	2.19	0.43
1:B:404:VAL:HG22	1:B:406:LEU:CD1	2.49	0.43
1:D:263:LEU:HD23	1:D:263:LEU:C	2.40	0.43
1:A:313:ILE:HG22	1:A:314:ASP:N	2.34	0.43
1:A:645:ARG:NE	1:A:645:ARG:HA	2.34	0.43
2:G:228:GLN:OE1	4:I:26:VAL:HG13	2.19	0.43
1:D:698:LEU:C	1:D:698:LEU:HD23	2.39	0.42
1:F:773:GLU:OE2	1:F:776:ARG:NH2	2.45	0.42
1:B:328:GLY:O	1:B:329:GLU:HB3	2.20	0.42
1:C:448:ASP:OD1	1:C:449:ALA:N	2.52	0.42
1:F:682:LEU:HD12	1:F:682:LEU:N	2.34	0.42
1:A:232:LEU:HB2	1:A:233:PRO:HD3	2.01	0.42
1:E:682:LEU:C	1:E:682:LEU:HD23	2.39	0.42
2:G:290:HIS:CG	4:J:107:THR:HG21	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:324:LEU:HD23	2:G:324:LEU:H	1.84	0.42
2:G:454:LYS:HB3	2:G:455:PRO:HD3	2.00	0.42
1:A:317:ASP:OD1	1:A:318:SER:N	2.52	0.42
1:A:513:TYR:O	1:A:517:GLY:N	2.52	0.42
1:B:705:ALA:CB	1:C:518:LEU:HD11	2.46	0.42
1:C:542:ALA:HB2	1:C:583:VAL:HG11	2.02	0.42
1:C:635:ARG:HE	1:C:635:ARG:HA	1.84	0.42
1:E:231:GLU:O	1:E:235:ARG:N	2.43	0.42
1:F:291:GLU:O	1:F:294:SER:OG	2.30	0.42
1:F:503:VAL:HG11	1:F:541:VAL:HG13	2.02	0.42
1:C:587:ASP:OD1	1:C:588:GLU:N	2.53	0.42
1:D:278:LEU:HD23	1:D:278:LEU:C	2.39	0.42
4:J:114:THR:C	4:J:115:LEU:HD23	2.39	0.42
1:A:74:ARG:NH2	1:A:272:THR:O	2.45	0.42
1:C:216:ILE:HG22	1:C:217:GLY:N	2.35	0.42
1:F:549:PHE:C	1:F:550:ILE:HD13	2.40	0.42
1:A:243:ILE:CG2	1:A:245:ILE:HG22	2.50	0.42
1:A:479:VAL:HG12	1:A:550:ILE:HD11	2.02	0.42
1:C:614:LEU:HD23	1:C:614:LEU:C	2.40	0.42
1:C:709:ILE:HD11	1:D:516:PHE:CD1	2.55	0.42
1:D:676:LEU:HD23	1:D:753:ILE:HD13	2.02	0.42
1:E:335:VAL:O	1:E:339:LEU:HD13	2.19	0.42
1:C:332:ARG:HA	1:C:335:VAL:HG12	2.01	0.42
1:D:588:GLU:O	1:D:591:SER:OG	2.31	0.42
1:E:525:LEU:HB2	1:E:649:LEU:HD21	2.02	0.42
1:E:671:LEU:O	1:E:674:THR:OG1	2.33	0.42
1:A:36:LEU:HD23	1:A:37:LEU:O	2.20	0.42
1:A:252:LEU:HD22	1:A:254:TYR:HD2	1.85	0.42
1:B:252:LEU:C	1:B:252:LEU:HD23	2.41	0.42
1:D:499:LEU:HD11	1:D:541:VAL:HG21	2.02	0.42
1:E:252:LEU:HD23	1:E:252:LEU:C	2.40	0.42
1:E:359:ARG:NH2	1:E:567:SER:HA	2.34	0.42
1:A:39:ASP:O	1:A:99:ARG:NH1	2.53	0.41
1:A:302:GLU:OE2	1:A:306:ASN:ND2	2.53	0.41
1:A:476:GLU:N	1:A:476:GLU:OE1	2.53	0.41
1:B:433:ILE:HD11	1:C:243:ILE:HD12	2.02	0.41
1:C:615:LEU:HD21	1:C:643:ILE:CD1	2.50	0.41
1:E:685:ILE:O	1:E:689:THR:HG23	2.19	0.41
2:G:389:ASN:ND2	2:G:393:GLU:OE1	2.52	0.41
1:F:232:LEU:HB2	1:F:233:PRO:HD3	2.02	0.41
1:D:229:MET:SD	1:D:251:VAL:HG22	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:761:ALA:O	1:D:765:ALA:N	2.44	0.41
1:F:263:LEU:HD23	1:F:263:LEU:C	2.41	0.41
2:G:107:ARG:HG2	2:G:109:GLY:N	2.36	0.41
4:K:256:LEU:O	4:K:260:ASN:N	2.53	0.41
1:A:129:ILE:HG23	1:A:199:ILE:O	2.20	0.41
1:F:417:VAL:HG12	1:F:418:GLY:N	2.36	0.41
2:G:546:LEU:HD12	2:G:546:LEU:C	2.40	0.41
1:A:78:VAL:C	1:A:79:LEU:HD12	2.41	0.41
1:C:633:THR:OG1	1:C:634:ASN:N	2.52	0.41
1:C:658:PRO:O	1:C:663:ARG:NH1	2.54	0.41
2:G:505:LYS:O	2:G:506:LYS:C	2.59	0.41
1:A:77:THR:HG23	1:A:79:LEU:HD13	2.02	0.41
1:A:129:ILE:HG22	1:A:131:ASP:OD1	2.20	0.41
1:B:124:ILE:HG23	1:B:190:THR:HG21	2.03	0.41
1:B:653:ILE:HD12	1:B:653:ILE:N	2.35	0.41
2:G:568:GLY:O	2:G:571:THR:OG1	2.35	0.41
2:G:572:LEU:HD23	2:G:572:LEU:O	2.21	0.41
1:B:209:ASN:OD1	1:B:266:ARG:NH1	2.54	0.41
1:C:533:GLY:HA2	6:C:902:ADP:H5'1	2.03	0.41
1:E:282:PRO:O	1:E:286:SER:N	2.54	0.41
1:F:528:GLY:O	1:F:634:ASN:ND2	2.44	0.41
1:A:310:ILE:HD11	1:A:354:ILE:HD12	2.03	0.41
1:A:549:PHE:HE1	1:A:551:SER:HG	1.68	0.41
1:B:479:VAL:O	1:B:479:VAL:HG23	2.21	0.41
1:D:330:VAL:O	1:D:334:VAL:HG23	2.20	0.41
1:D:569:ILE:HG21	1:D:613:GLN:HB3	2.02	0.41
1:E:308:PRO:HA	1:E:350:ASN:O	2.21	0.41
1:E:637:ASP:OD1	1:E:638:GLN:N	2.54	0.41
4:K:202:GLN:O	4:K:264:GLU:CA	2.69	0.41
1:B:409:LEU:HD11	1:B:459:MET:SD	2.61	0.41
1:A:146:LYS:HB2	1:A:147:PRO:HD3	2.03	0.40
1:A:229:MET:SD	1:A:375:ARG:NE	2.94	0.40
1:B:248:PRO:HB3	1:B:375:ARG:HE	1.86	0.40
1:B:489:VAL:HG12	1:B:490:GLY:N	2.36	0.40
1:C:474:LEU:N	1:C:474:LEU:HD12	2.36	0.40
1:A:136:ILE:HD12	1:A:169:ARG:CG	2.52	0.40
1:A:264:MET:CE	1:A:379:ILE:HD13	2.52	0.40
1:A:278:LEU:C	1:A:278:LEU:HD23	2.41	0.40
1:B:65:ASP:OD1	1:B:65:ASP:N	2.53	0.40
1:C:252:LEU:C	1:C:252:LEU:HD23	2.41	0.40
1:E:484:VAL:H	1:E:543:THR:HG21	1.83	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:587:ASP:OD1	1:E:588:GLU:N	2.54	0.40
1:A:447:ILE:HD13	1:A:452:LEU:HD21	2.03	0.40
1:B:368:ARG:NH2	1:B:376:GLU:OE2	2.53	0.40
1:E:409:LEU:O	1:E:413:THR:HG23	2.22	0.40
2:G:369:SER:OG	2:G:370:LYS:N	2.54	0.40
1:A:405:ASP:O	1:A:408:ALA:N	2.52	0.40
1:B:140:LEU:N	1:B:140:LEU:HD22	2.36	0.40
1:C:442:LEU:HD12	1:C:443:ASP:N	2.35	0.40
2:G:106:HIS:CG	2:G:107:ARG:N	2.90	0.40
1:B:31:LYS:NZ	1:B:32:LYS:O	2.48	0.40
1:C:535:THR:O	1:C:539:LYS:HG2	2.22	0.40
1:F:387:ARG:NE	1:F:413:THR:O	2.55	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	706/838 (84%)	682 (97%)	24 (3%)	0	100	100
1	B	710/838 (85%)	678 (96%)	32 (4%)	0	100	100
1	C	545/838 (65%)	515 (94%)	29 (5%)	1 (0%)	47	81
1	D	535/838 (64%)	517 (97%)	18 (3%)	0	100	100
1	E	524/838 (62%)	502 (96%)	22 (4%)	0	100	100
1	F	539/838 (64%)	518 (96%)	21 (4%)	0	100	100
2	G	473/583 (81%)	421 (89%)	51 (11%)	1 (0%)	47	81
3	H	58/363 (16%)	51 (88%)	7 (12%)	0	100	100
4	I	36/76 (47%)	30 (83%)	6 (17%)	0	100	100
4	J	74/76 (97%)	69 (93%)	5 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
All	All	4274/6202 (69%)	4052 (95%)	220 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	476	GLU
1	C	608	ASP

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	603/697 (86%)	598 (99%)	5 (1%)	81	91
1	B	606/697 (87%)	600 (99%)	6 (1%)	76	88
1	C	463/697 (66%)	459 (99%)	4 (1%)	78	90
1	D	455/697 (65%)	454 (100%)	1 (0%)	93	98
1	E	441/697 (63%)	439 (100%)	2 (0%)	88	94
1	F	460/697 (66%)	456 (99%)	4 (1%)	78	90
2	G	426/518 (82%)	419 (98%)	7 (2%)	62	83
3	H	53/315 (17%)	52 (98%)	1 (2%)	57	80
4	I	35/69 (51%)	34 (97%)	1 (3%)	42	71
4	J	69/69 (100%)	66 (96%)	3 (4%)	29	62
4	K	69/69 (100%)	67 (97%)	2 (3%)	42	71
All	All	3680/5222 (70%)	3644 (99%)	36 (1%)	77	88

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ARG
1	A	499	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	504	GLU
1	A	624	LYS
1	A	710	LYS
1	B	158	LYS
1	B	223	MET
1	B	348	ARG
1	B	551	SER
1	B	624	LYS
1	B	673	LYS
1	C	223	MET
1	C	323	ARG
1	C	368	ARG
1	C	577	ARG
1	D	564	GLU
1	E	673	LYS
1	E	782	GLN
1	F	254	TYR
1	F	348	ARG
1	F	703	ARG
1	F	707	TYR
2	G	148	CYS
2	G	204	CYS
2	G	504	LEU
2	G	516	ASP
2	G	543	GLU
2	G	549	GLU
2	G	574	MET
3	H	284	THR
4	I	39	ASP
4	J	107	THR
4	J	122	THR
4	J	124	ASP
4	K	264	GLU
4	K	274	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	670	GLN
1	C	612	ASN
1	E	509	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	ATP	B	901	-	26,33,33	0.63	0	31,52,52	1.08	2 (6%)
6	ADP	B	902	-	24,29,29	0.69	0	29,45,45	0.76	1 (3%)
6	ADP	A	902	-	24,29,29	0.69	0	29,45,45	0.75	1 (3%)
6	ADP	F	902	-	24,29,29	0.94	1 (4%)	29,45,45	1.45	4 (13%)
5	ATP	D	901	-	26,33,33	0.62	0	31,52,52	1.07	2 (6%)
6	ADP	E	902	-	24,29,29	0.67	0	29,45,45	0.78	1 (3%)
5	ATP	C	901	-	26,33,33	0.63	0	31,52,52	1.07	2 (6%)
6	ADP	D	902	-	24,29,29	0.68	0	29,45,45	0.81	1 (3%)
5	ATP	A	901	-	26,33,33	0.63	0	31,52,52	1.06	2 (6%)
6	ADP	C	902	-	24,29,29	0.67	0	29,45,45	0.81	1 (3%)
6	ADP	E	901	-	24,29,29	0.73	0	29,45,45	0.87	2 (6%)
5	ATP	F	901	-	26,33,33	0.64	0	31,52,52	1.06	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	B	901	-	-	9/18/38/38	0/3/3/3
6	ADP	B	902	-	-	1/12/32/32	0/3/3/3
6	ADP	A	902	-	-	1/12/32/32	0/3/3/3
6	ADP	F	902	-	-	2/12/32/32	0/3/3/3
5	ATP	D	901	-	-	3/18/38/38	0/3/3/3
6	ADP	E	902	-	-	2/12/32/32	0/3/3/3
5	ATP	C	901	-	-	4/18/38/38	0/3/3/3
6	ADP	D	902	-	-	2/12/32/32	0/3/3/3
5	ATP	A	901	-	-	8/18/38/38	0/3/3/3
6	ADP	C	902	-	-	1/12/32/32	0/3/3/3
6	ADP	E	901	-	-	1/12/32/32	0/3/3/3
5	ATP	F	901	-	-	7/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	902	ADP	C5-C4	2.34	1.47	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	902	ADP	N3-C2-N1	-3.61	123.04	128.68
6	F	902	ADP	PA-O3A-PB	-3.50	120.81	132.83
6	F	902	ADP	C3'-C2'-C1'	2.83	105.25	100.98
6	F	902	ADP	C4-C5-N7	-2.63	106.66	109.40
6	B	902	ADP	C5-C6-N6	2.40	124.00	120.35
6	E	901	ADP	PA-O3A-PB	-2.34	124.78	132.83
5	F	901	ATP	C5-C6-N6	2.33	123.89	120.35
6	D	902	ADP	C5-C6-N6	2.32	123.88	120.35
6	A	902	ADP	C5-C6-N6	2.32	123.87	120.35
5	C	901	ATP	C5-C6-N6	2.28	123.82	120.35
5	D	901	ATP	C5-C6-N6	2.28	123.82	120.35
5	B	901	ATP	C5-C6-N6	2.26	123.79	120.35
5	A	901	ATP	C5-C6-N6	2.26	123.78	120.35
6	E	902	ADP	C5-C6-N6	2.25	123.78	120.35
6	C	902	ADP	C5-C6-N6	2.11	123.57	120.35
5	F	901	ATP	PB-O3B-PG	2.04	139.84	132.83
5	D	901	ATP	PB-O3B-PG	2.04	139.82	132.83
6	E	901	ADP	C5-C6-N6	2.04	123.45	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	901	ATP	PB-O3B-PG	2.04	139.82	132.83
5	A	901	ATP	PB-O3B-PG	2.02	139.77	132.83
5	C	901	ATP	PB-O3B-PG	2.02	139.76	132.83

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	ATP	PB-O3B-PG-O3G
5	B	901	ATP	C5'-O5'-PA-O2A
5	B	901	ATP	O4'-C4'-C5'-O5'
5	C	901	ATP	PB-O3B-PG-O2G
5	F	901	ATP	C4'-C5'-O5'-PA
6	D	902	ADP	C3'-C4'-C5'-O5'
6	F	902	ADP	C3'-C4'-C5'-O5'
5	B	901	ATP	C3'-C4'-C5'-O5'
5	C	901	ATP	O4'-C4'-C5'-O5'
5	D	901	ATP	O4'-C4'-C5'-O5'
5	F	901	ATP	O4'-C4'-C5'-O5'
6	D	902	ADP	O4'-C4'-C5'-O5'
6	F	902	ADP	O4'-C4'-C5'-O5'
5	A	901	ATP	C4'-C5'-O5'-PA
5	F	901	ATP	PB-O3B-PG-O1G
5	F	901	ATP	PB-O3A-PA-O1A
5	C	901	ATP	C4'-C5'-O5'-PA
5	D	901	ATP	C4'-C5'-O5'-PA
5	B	901	ATP	C5'-O5'-PA-O3A
5	B	901	ATP	C5'-O5'-PA-O1A
5	D	901	ATP	PB-O3B-PG-O1G
5	B	901	ATP	PA-O3A-PB-O1B
6	C	902	ADP	O4'-C4'-C5'-O5'
6	E	901	ADP	O4'-C4'-C5'-O5'
5	A	901	ATP	PB-O3B-PG-O1G
5	C	901	ATP	PB-O3B-PG-O1G
6	B	902	ADP	O4'-C4'-C5'-O5'
5	A	901	ATP	C3'-C4'-C5'-O5'
5	A	901	ATP	O4'-C4'-C5'-O5'
6	A	902	ADP	O4'-C4'-C5'-O5'
5	A	901	ATP	PB-O3B-PG-O2G
5	A	901	ATP	PB-O3B-PG-O3G
5	B	901	ATP	PB-O3B-PG-O2G
5	F	901	ATP	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

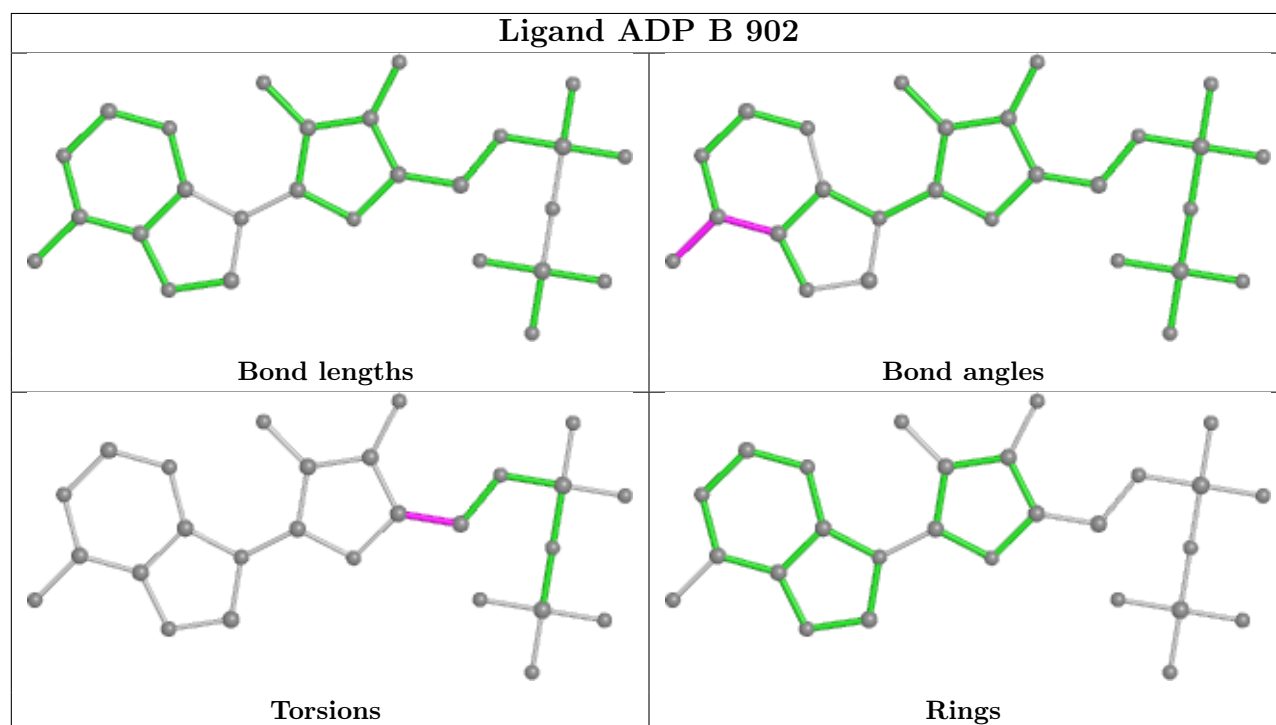
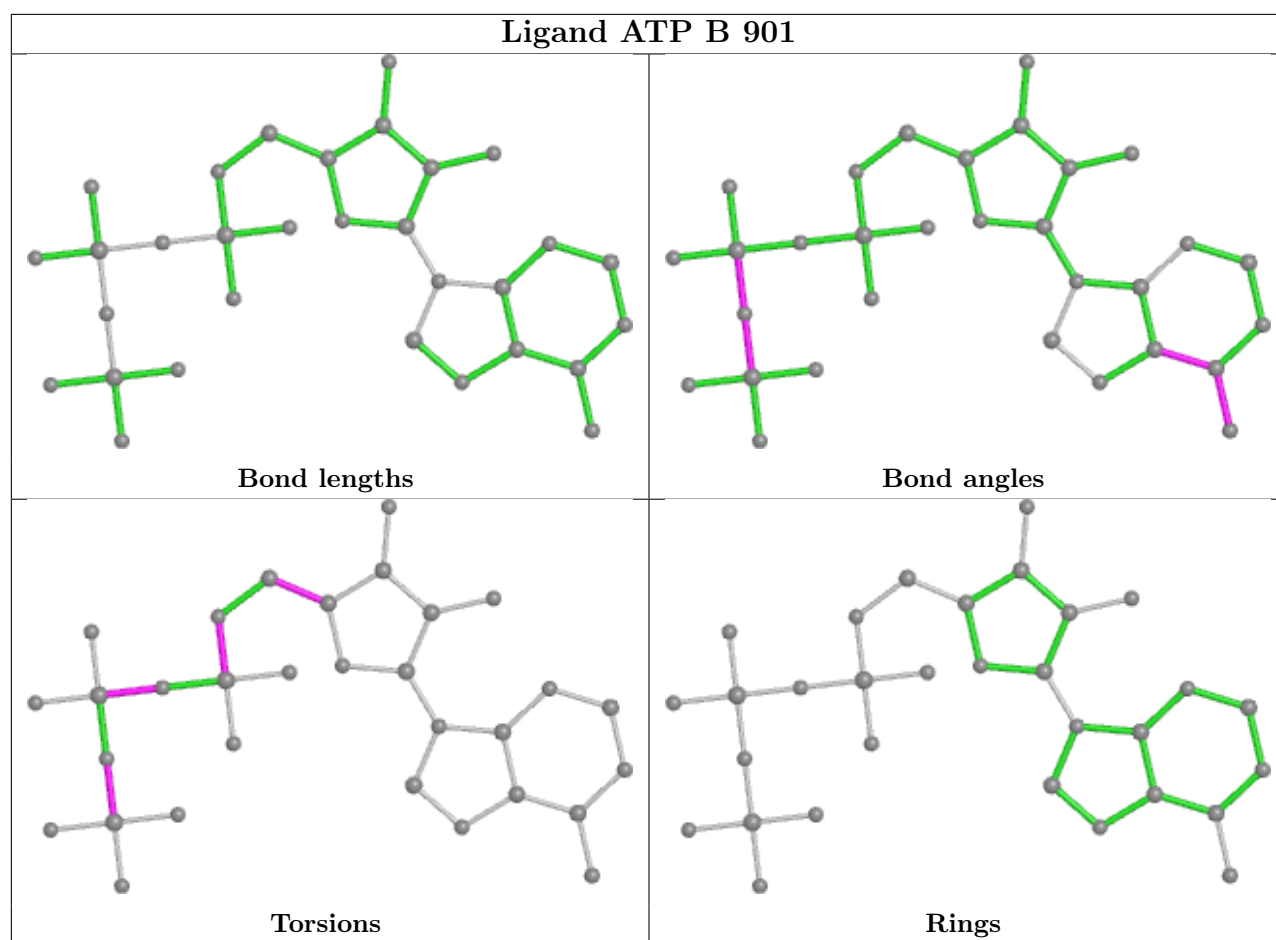
Mol	Chain	Res	Type	Atoms
5	A	901	ATP	C5'-O5'-PA-O3A
6	E	902	ADP	O4'-C4'-C5'-O5'
5	A	901	ATP	PA-O3A-PB-O2B
5	F	901	ATP	PB-O3A-PA-O2A
5	F	901	ATP	C5'-O5'-PA-O1A
5	B	901	ATP	PB-O3B-PG-O1G
6	E	902	ADP	PA-O3A-PB-O1B

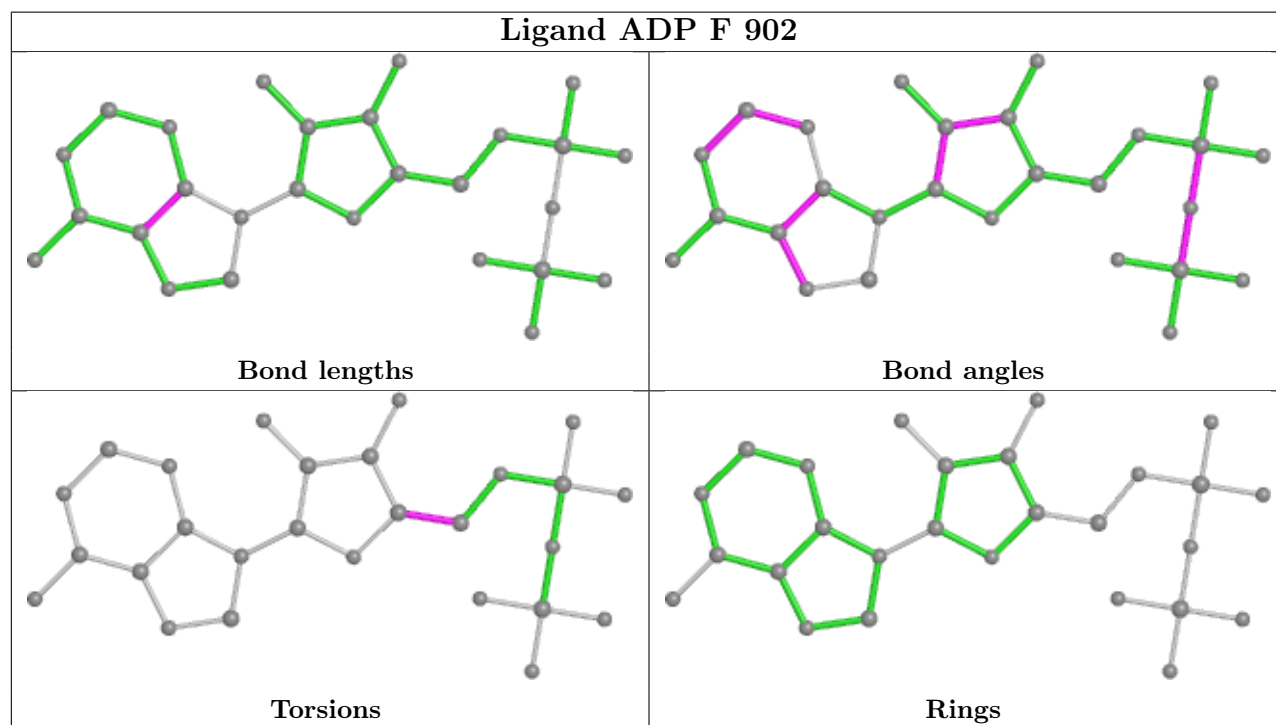
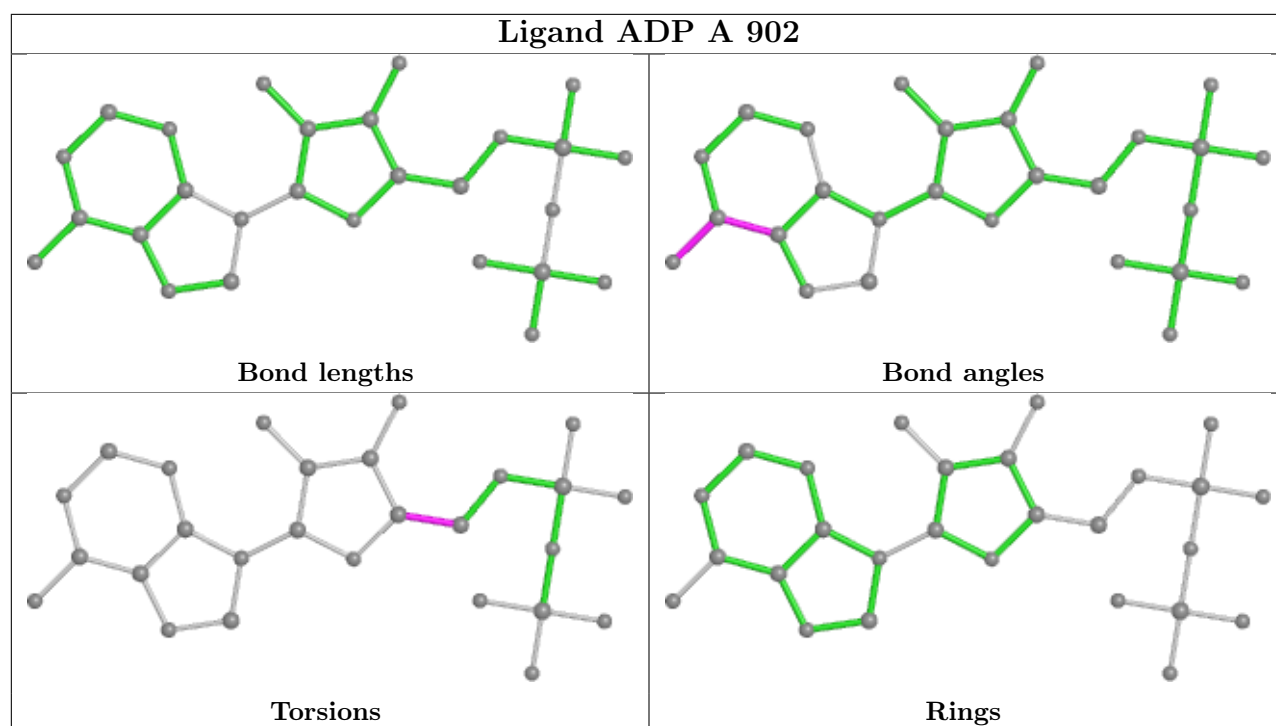
There are no ring outliers.

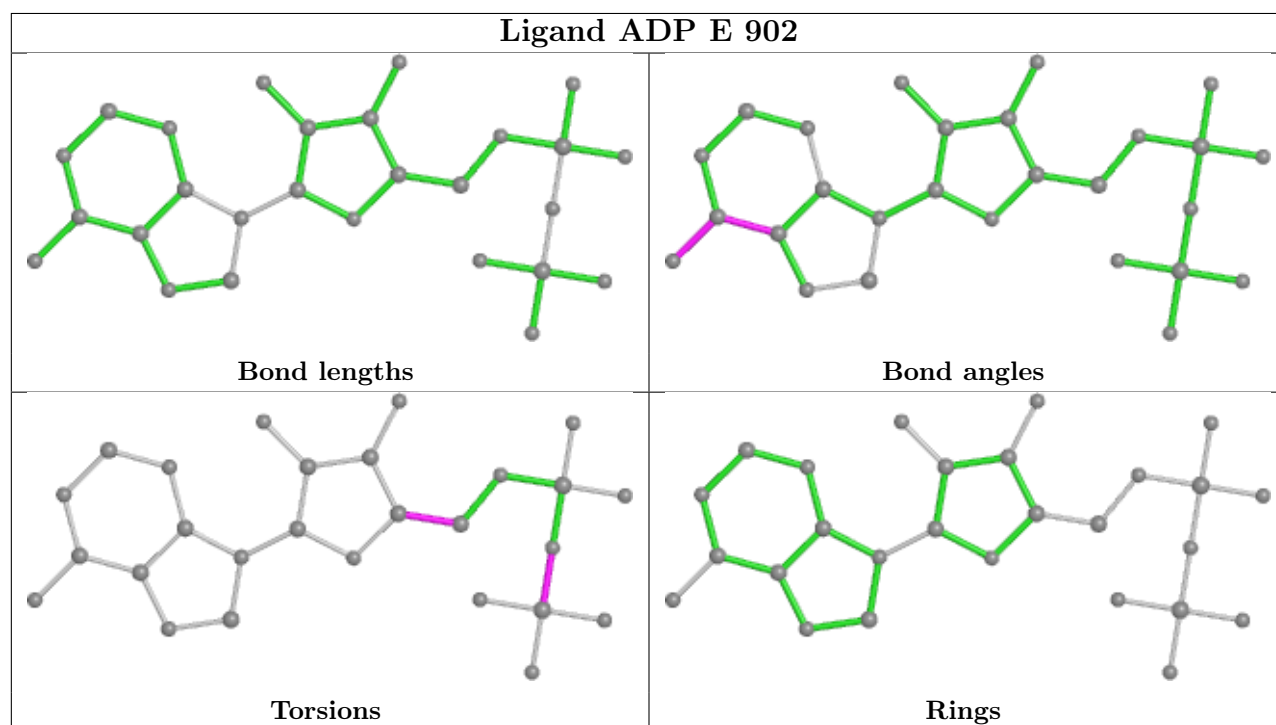
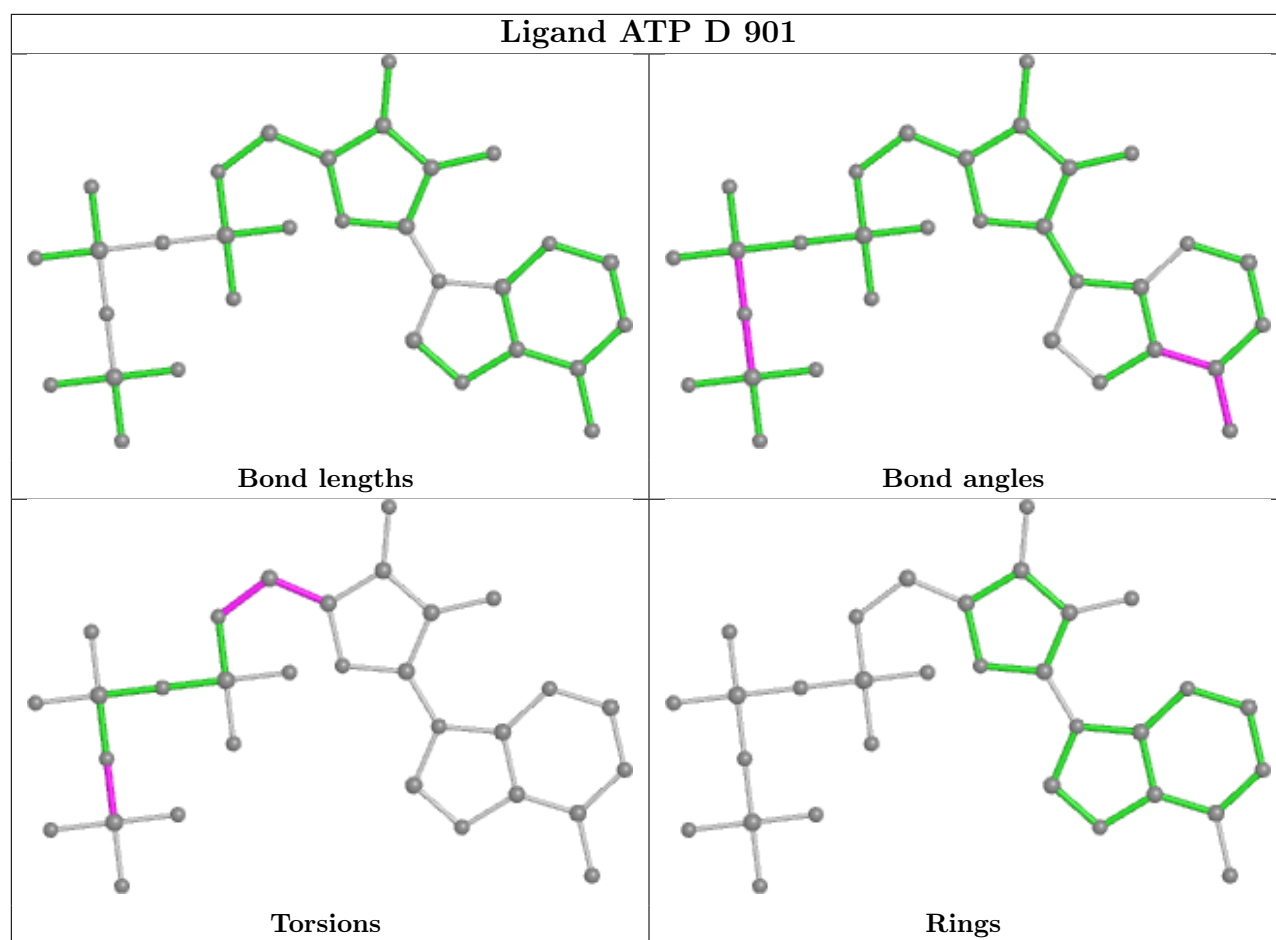
7 monomers are involved in 9 short contacts:

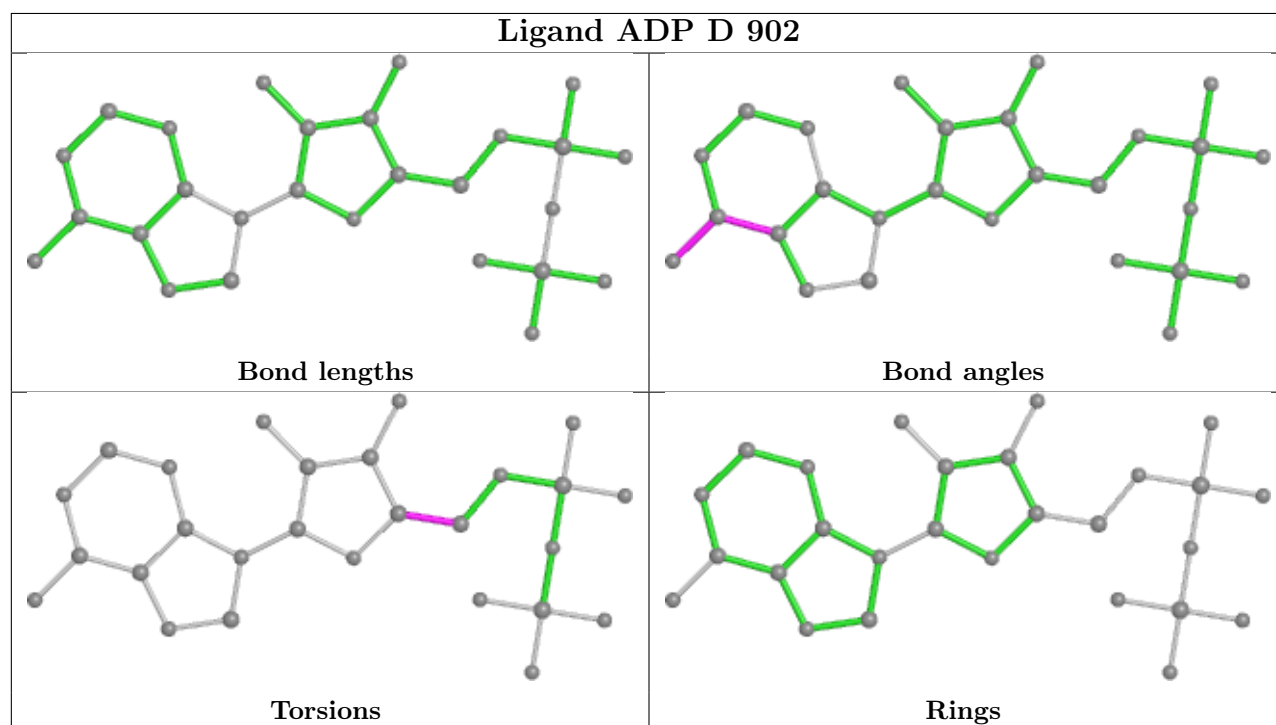
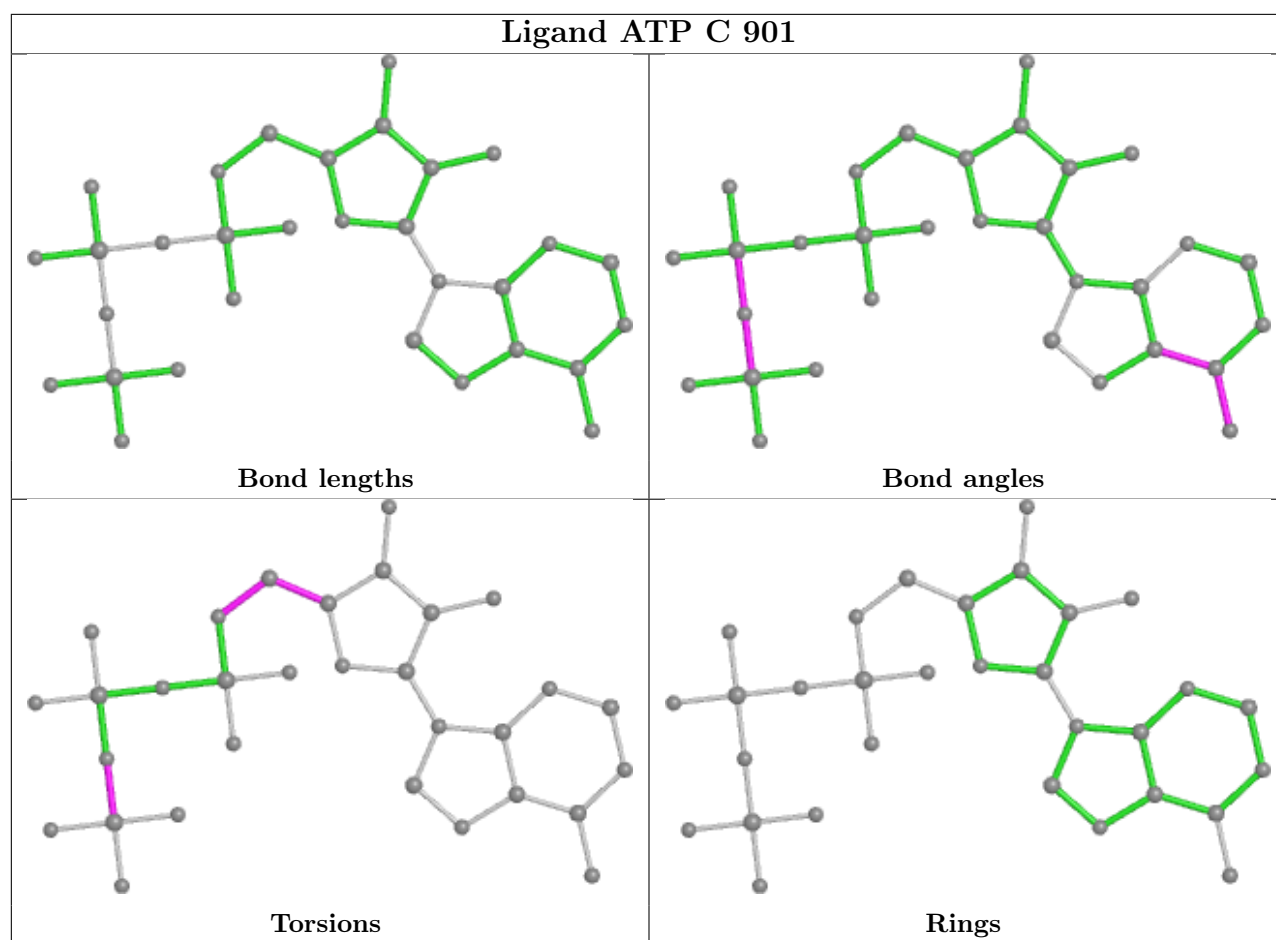
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	901	ATP	2	0
6	A	902	ADP	1	0
5	D	901	ATP	1	0
5	C	901	ATP	1	0
6	D	902	ADP	1	0
5	A	901	ATP	2	0
6	C	902	ADP	1	0

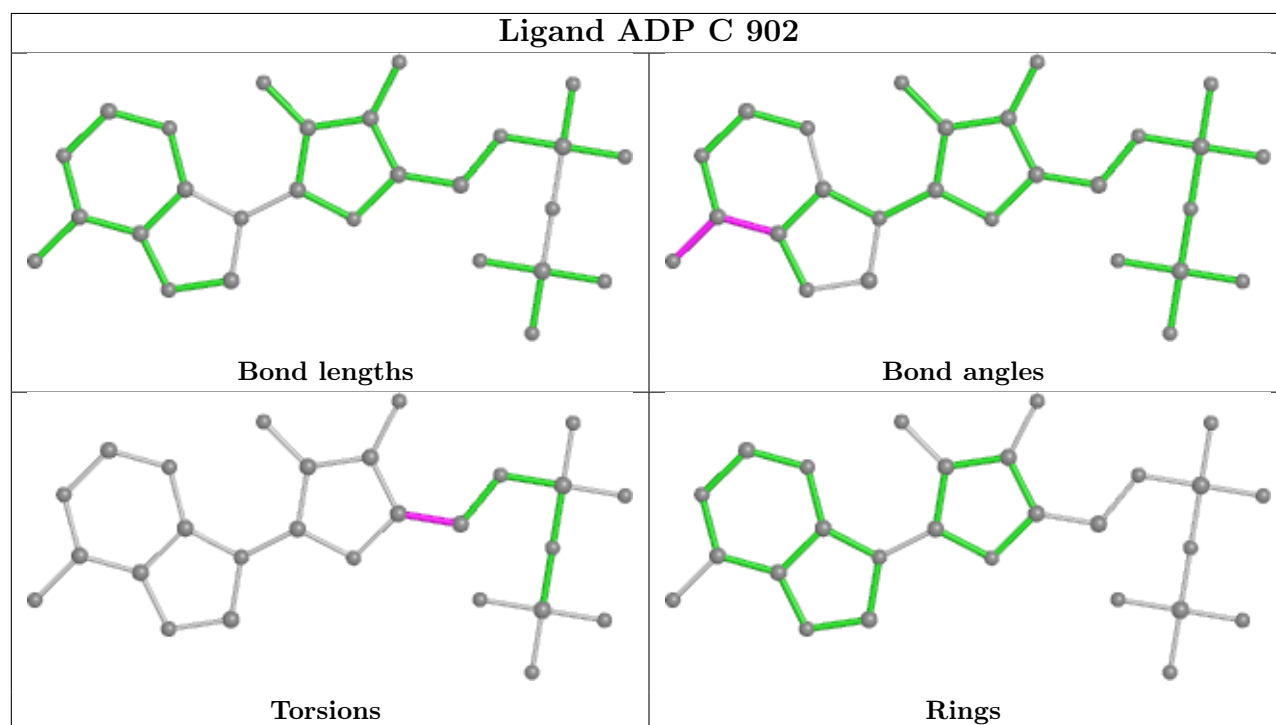
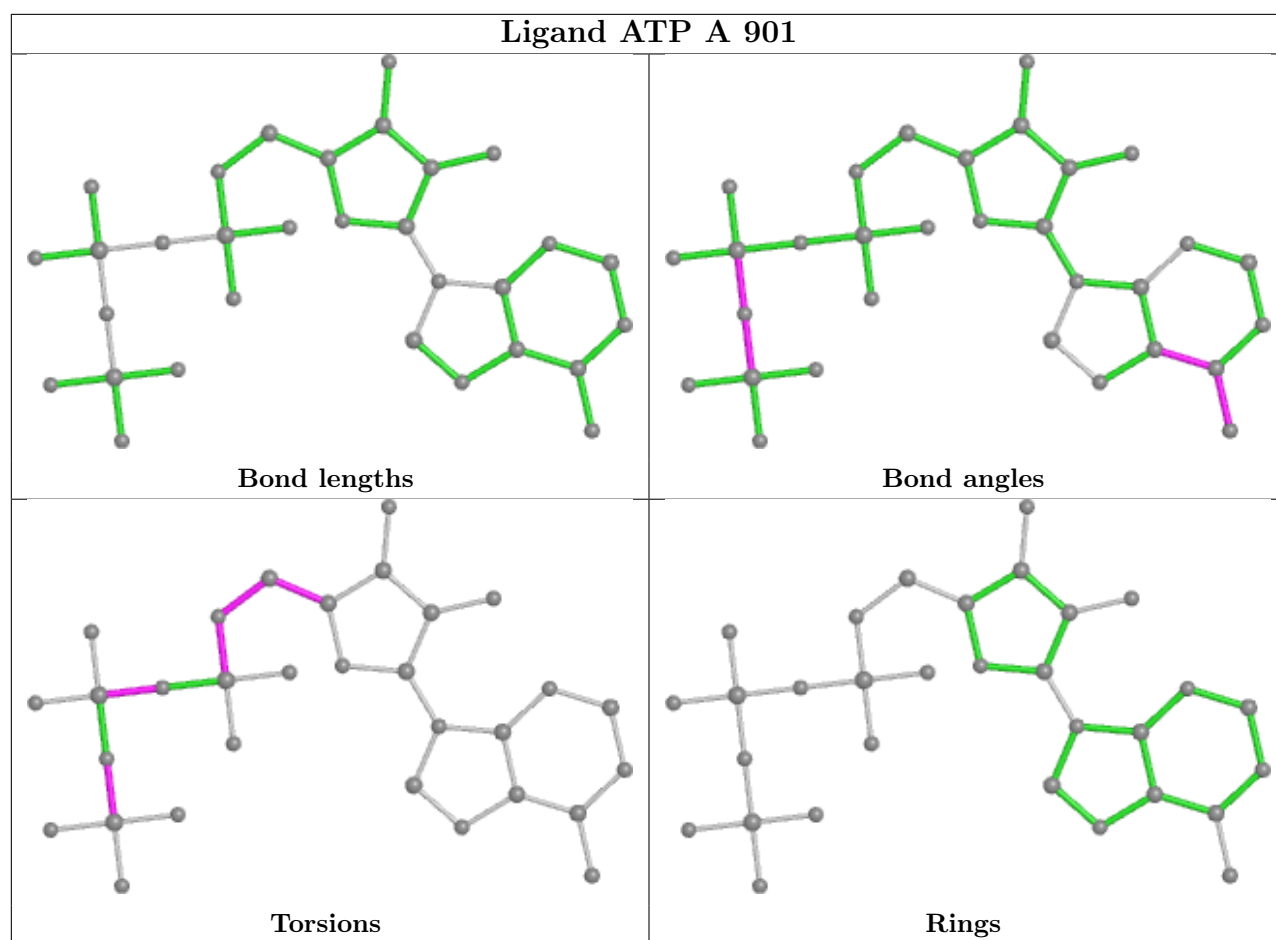
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

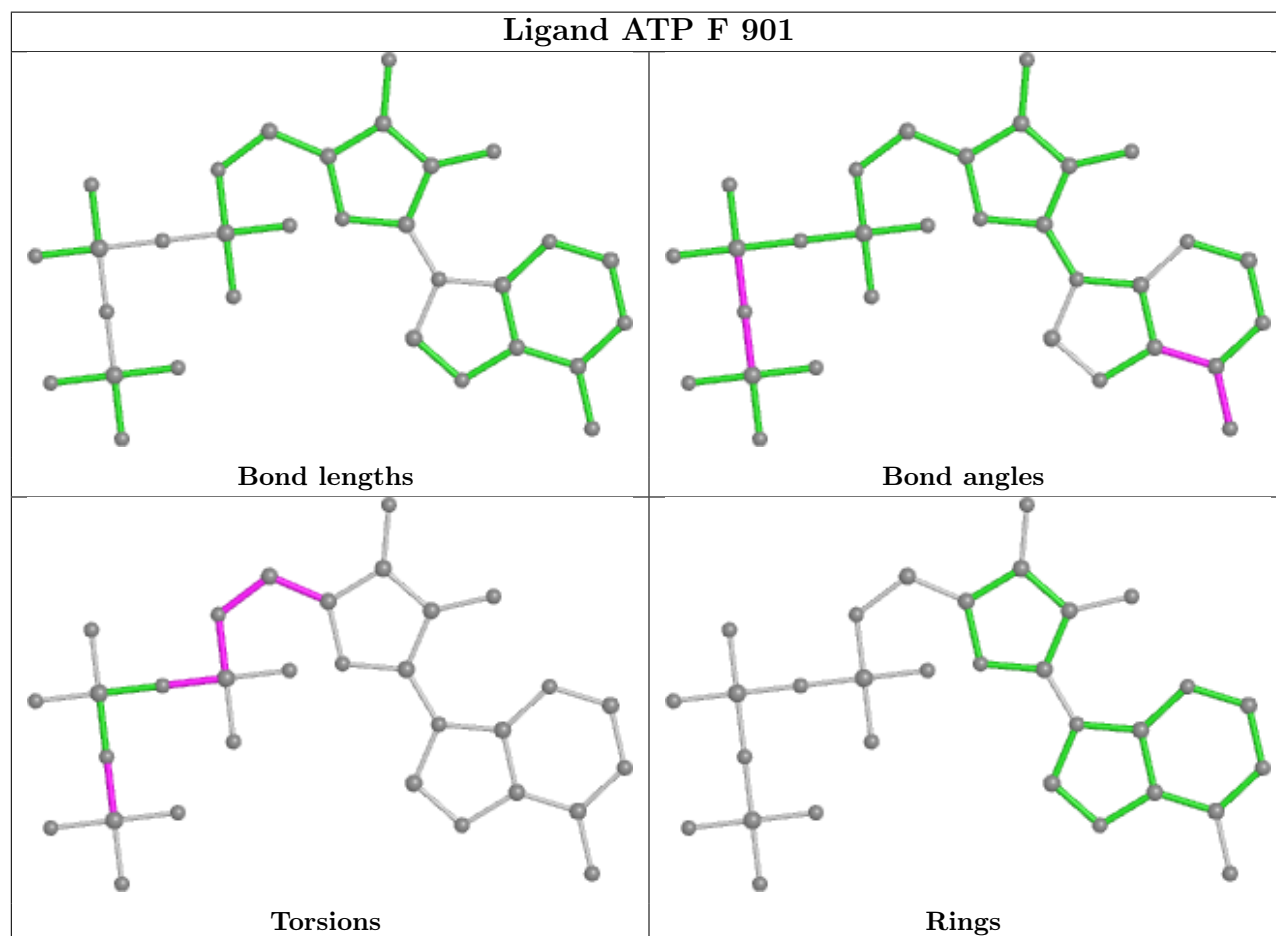
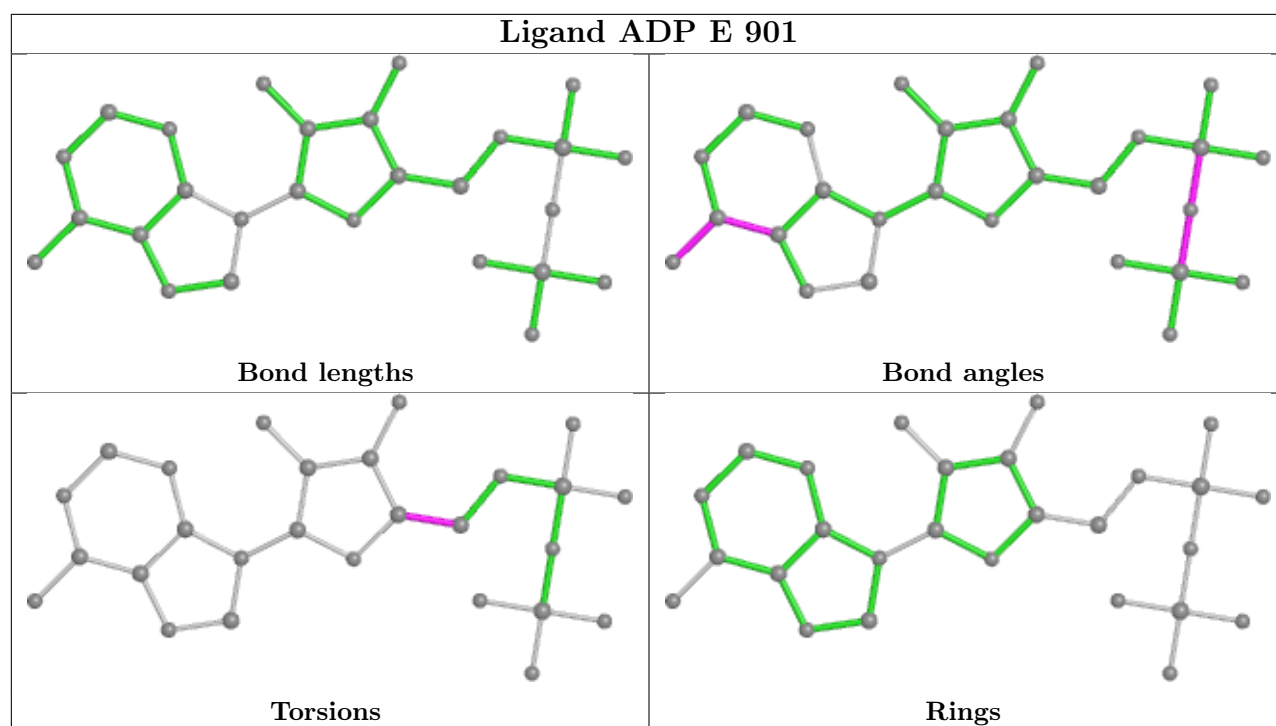












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

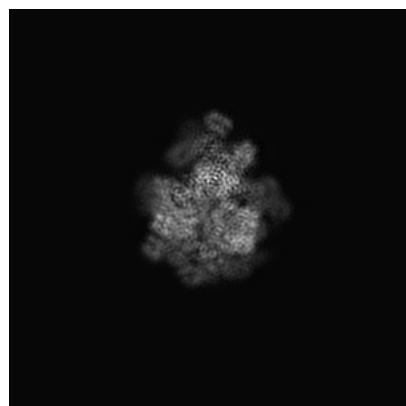
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27277. These allow visual inspection of the internal detail of the map and identification of artifacts.

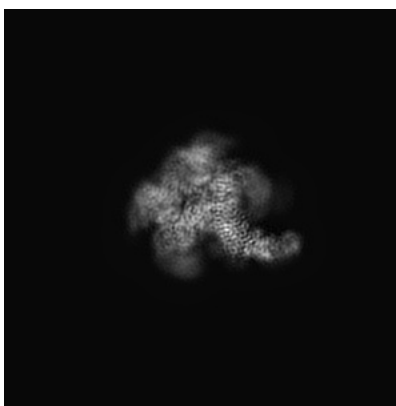
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

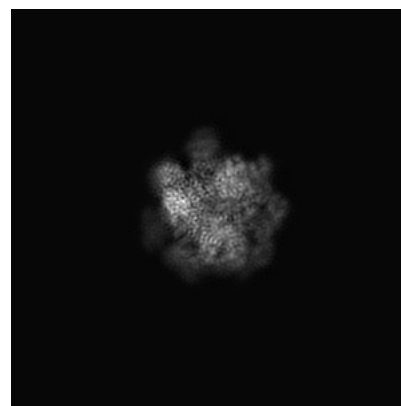
6.1.1 Primary map



X

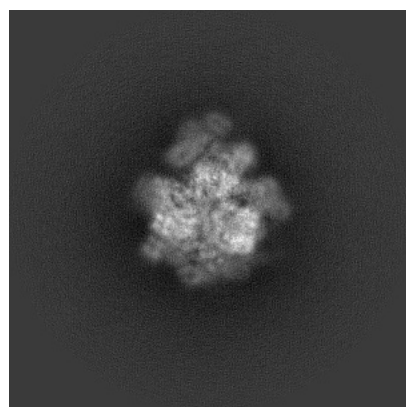


Y

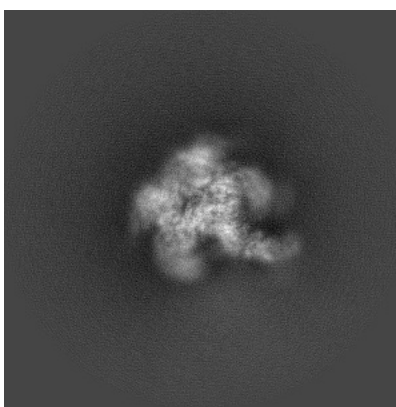


Z

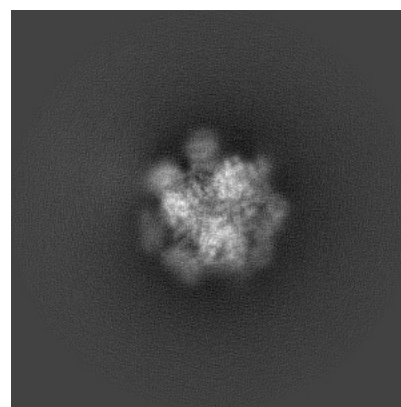
6.1.2 Raw map



X



Y

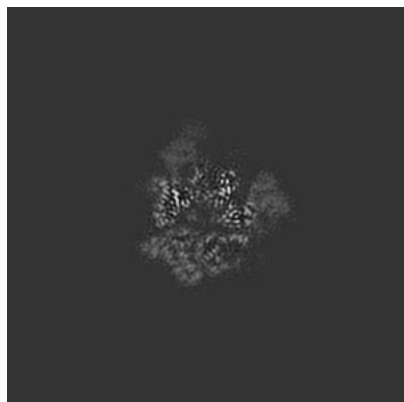


Z

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

6.2 Central slices [i](#)

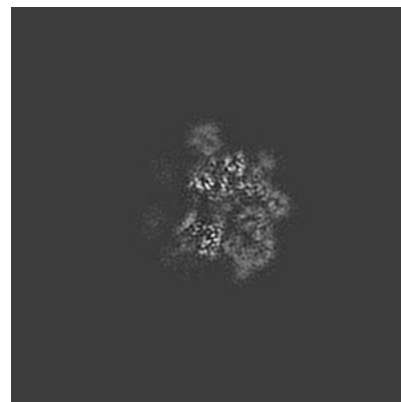
6.2.1 Primary map



X Index: 192

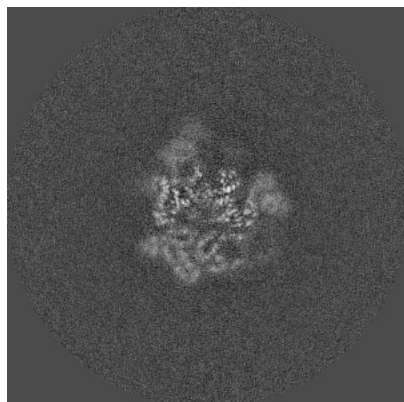


Y Index: 192

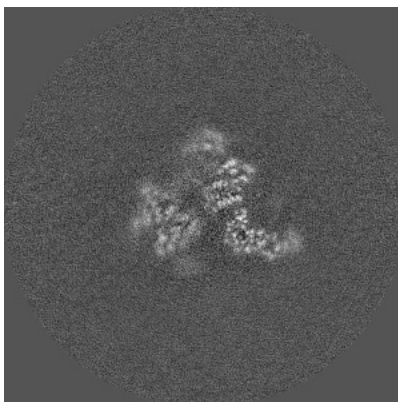


Z Index: 192

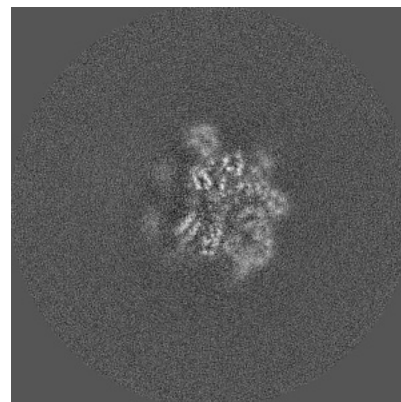
6.2.2 Raw map



X Index: 192



Y Index: 192

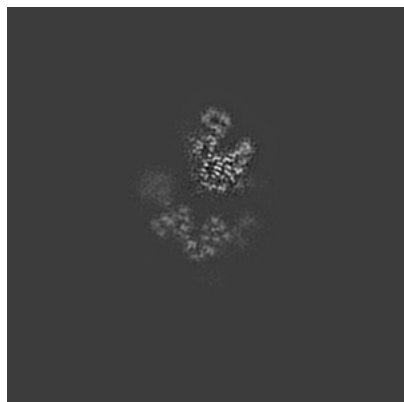


Z Index: 192

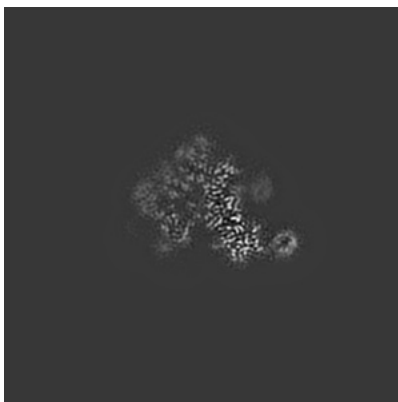
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

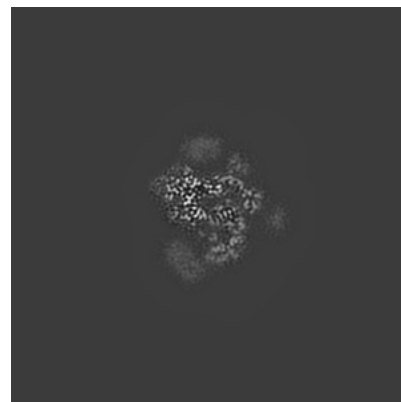
6.3.1 Primary map



X Index: 161

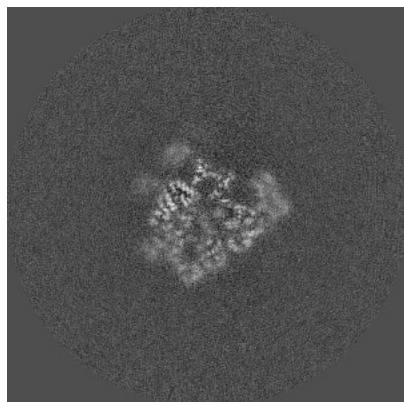


Y Index: 206

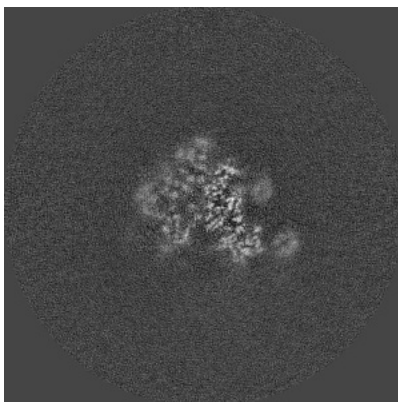


Z Index: 217

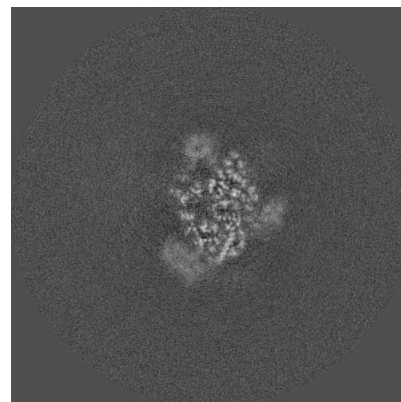
6.3.2 Raw map



X Index: 185



Y Index: 206

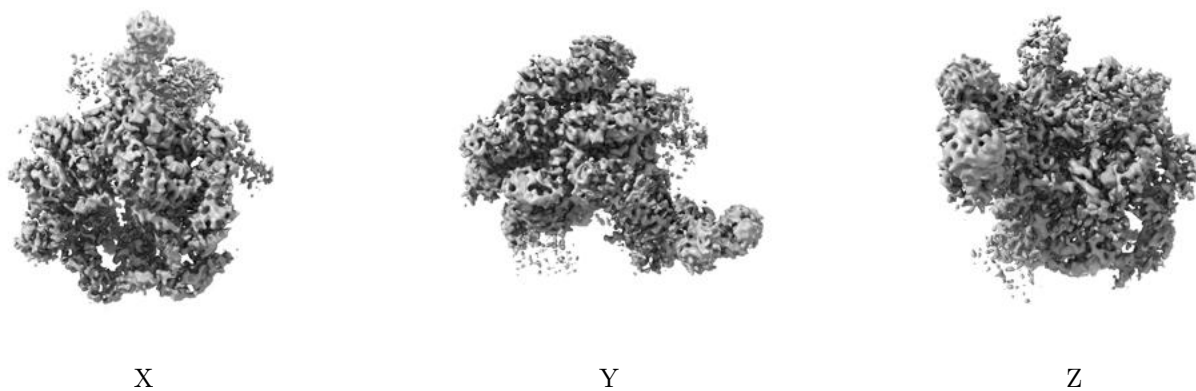


Z Index: 209

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 9.0. 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.

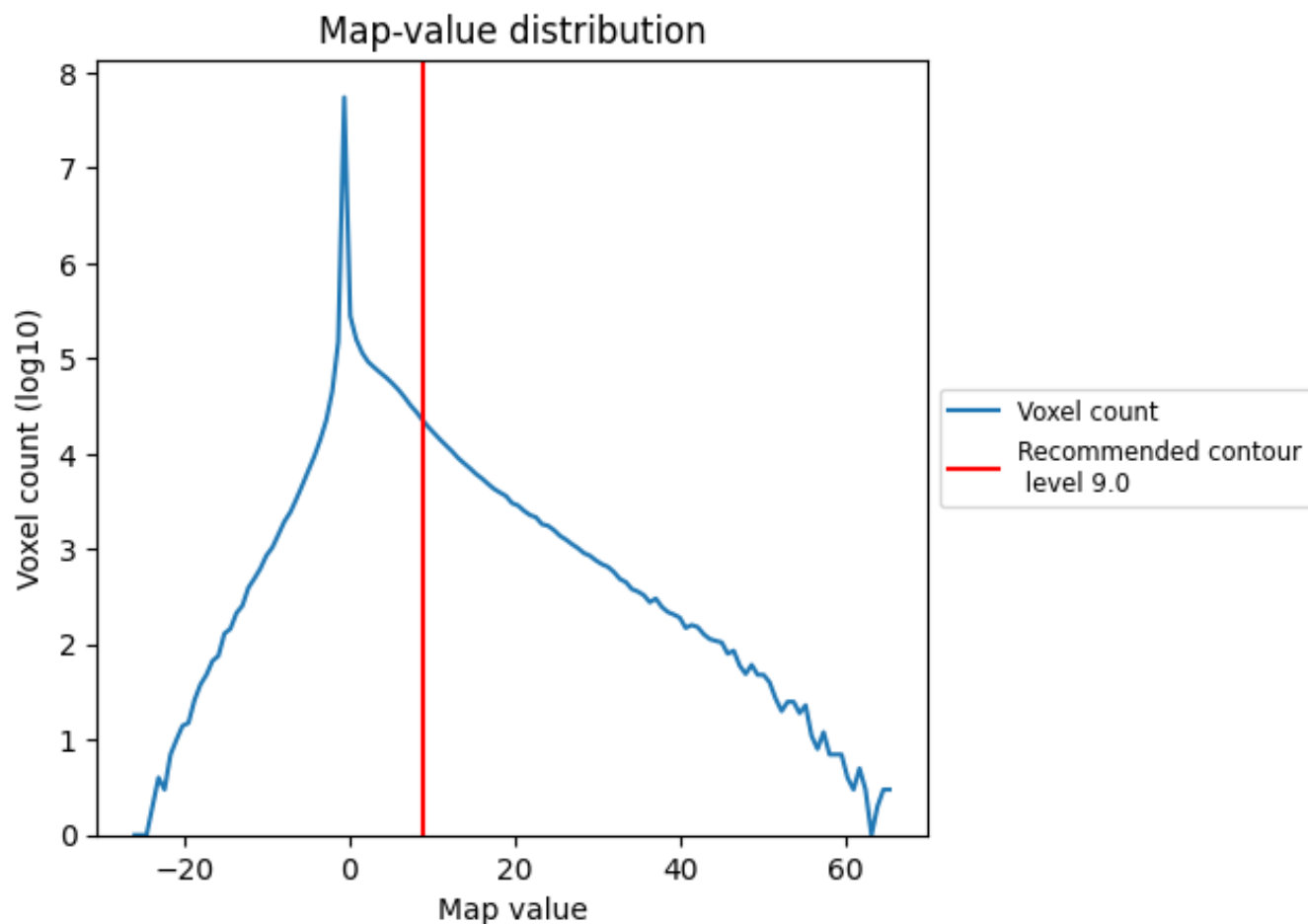
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

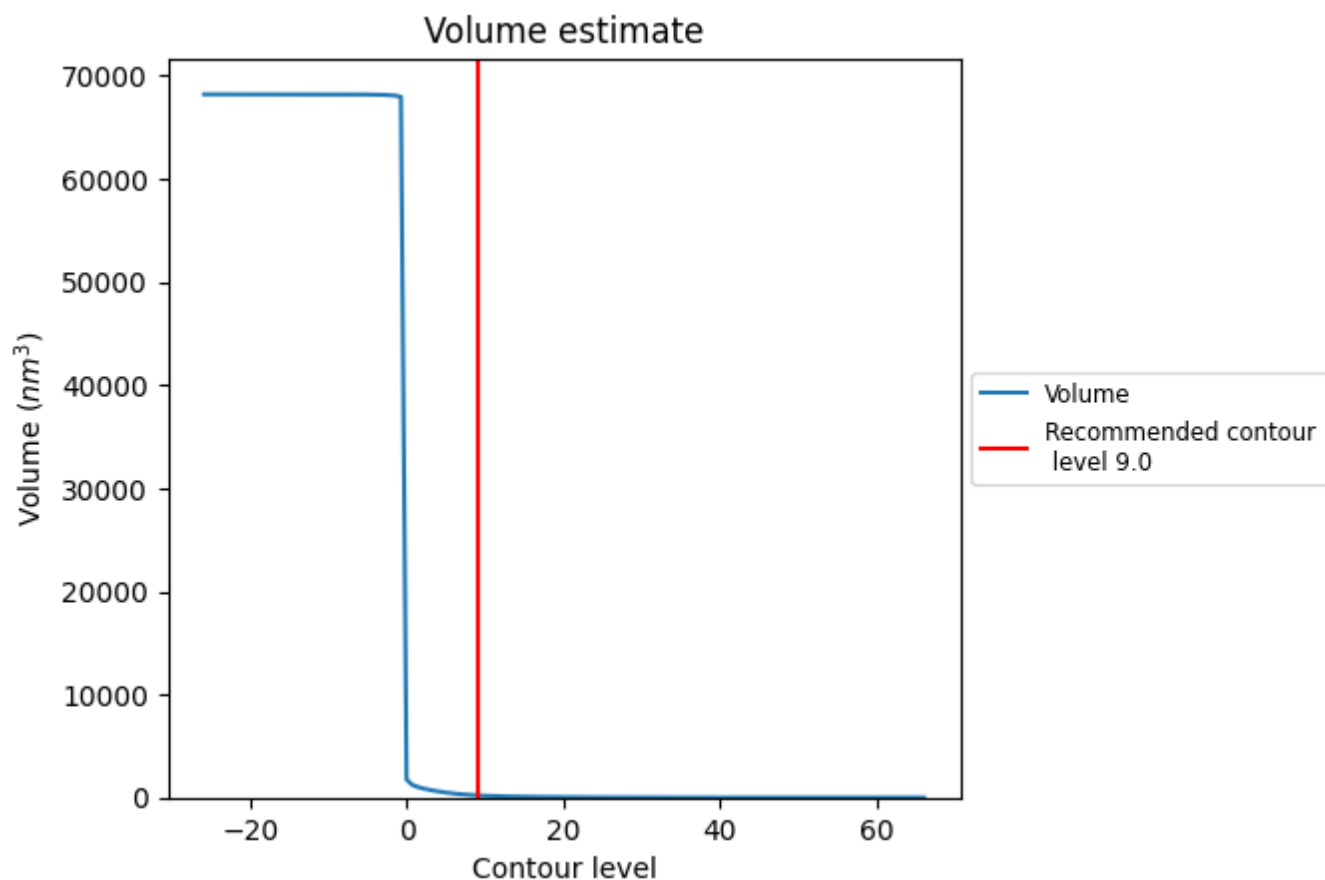
This section contains the results of statistical analysis of the map.

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.

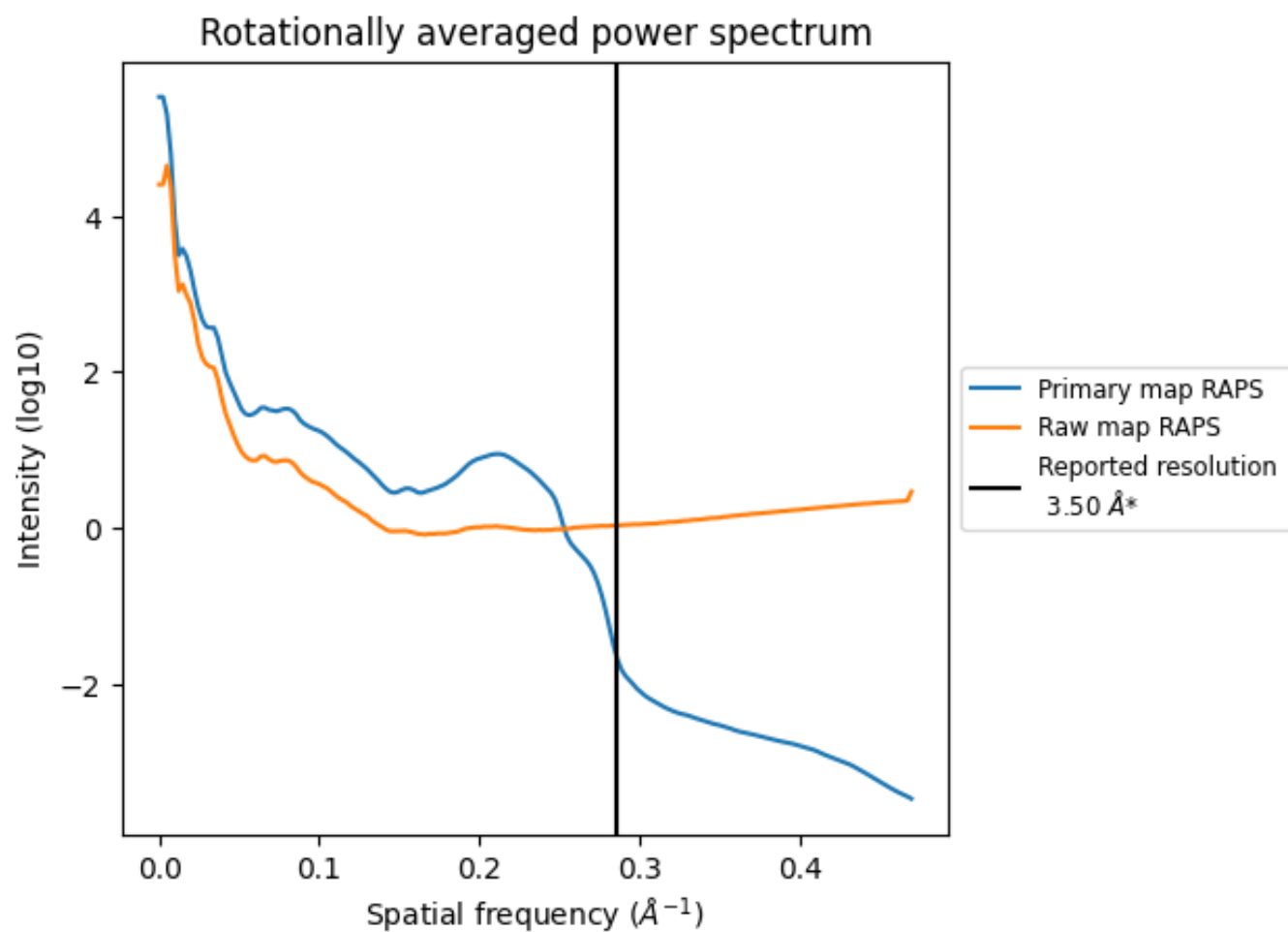
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm^3 ; this corresponds to an approximate mass of 191 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 ⓘ

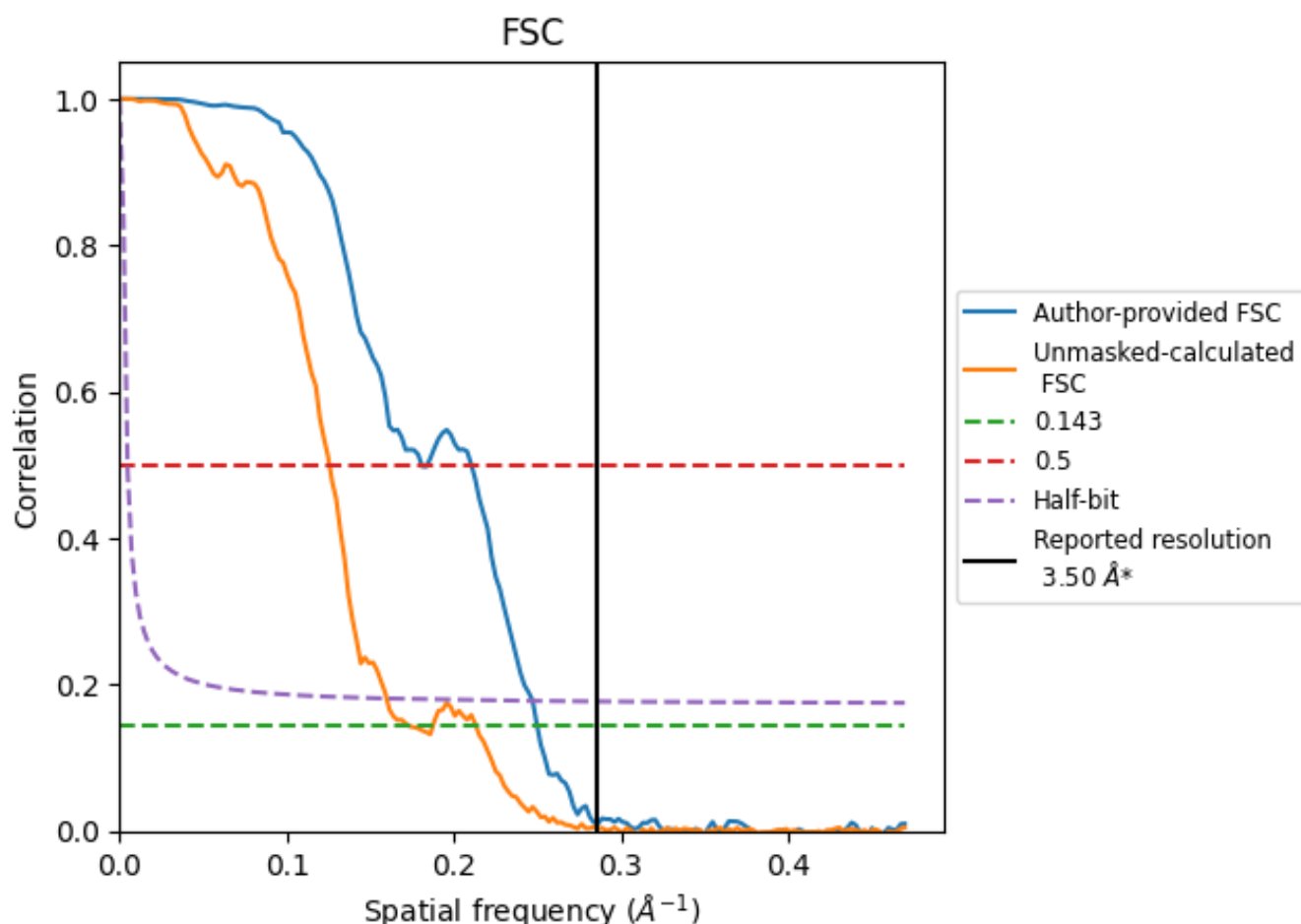


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	4.00	5.53	4.05
Unmasked-calculated*	5.77	7.96	6.25

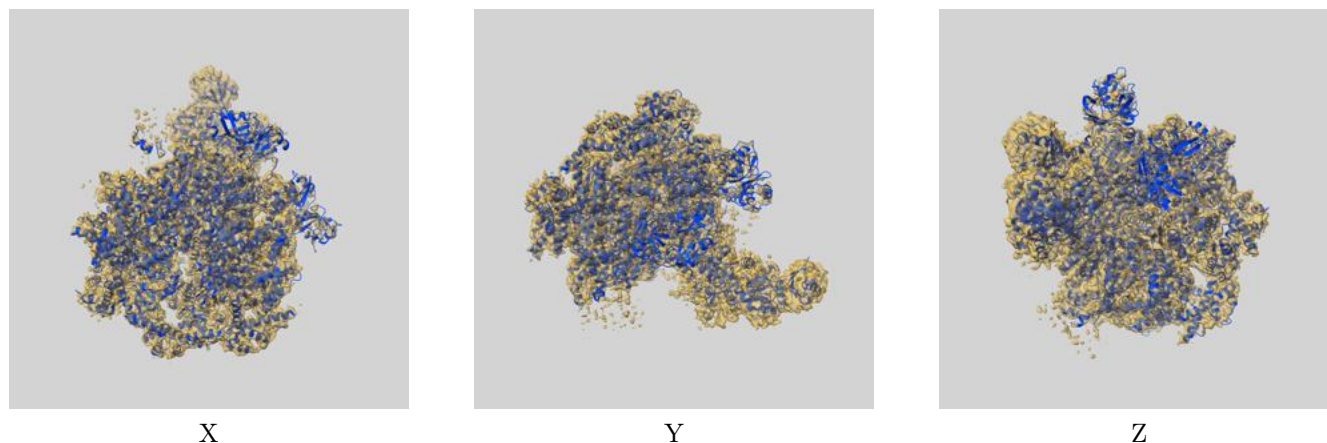
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 3.5 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.77 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

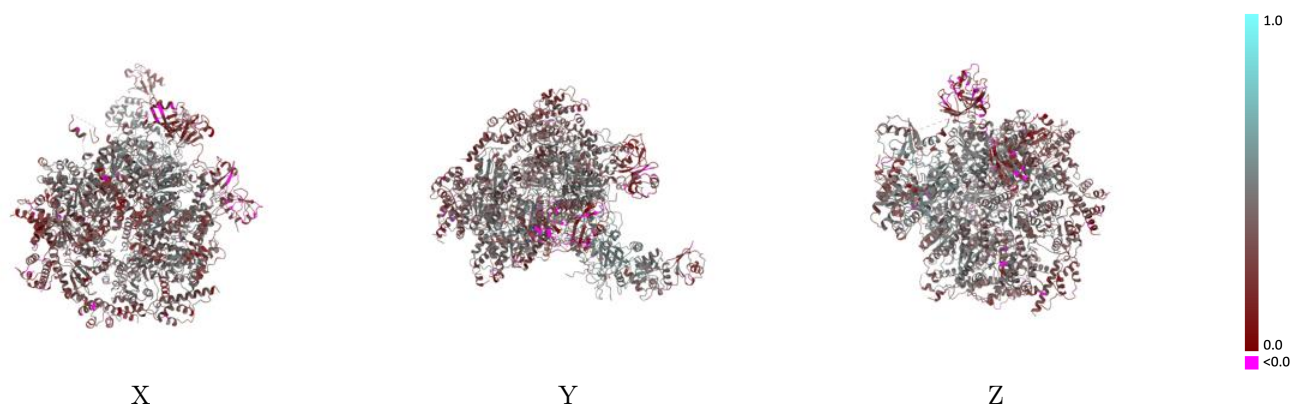
This section contains information regarding the fit between EMDB map EMD-27277 and PDB model 8DAV. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



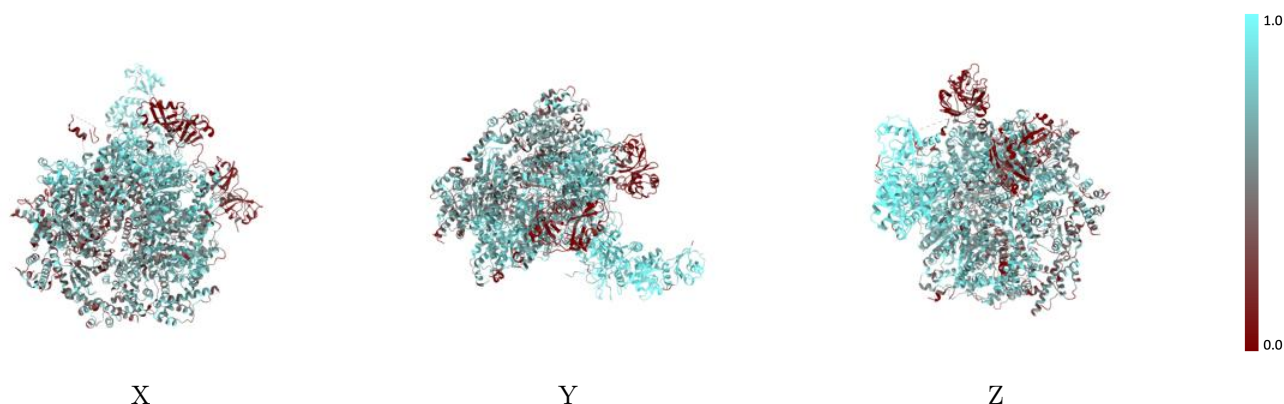
The images above show the 3D surface view of the map at the recommended contour level 9.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



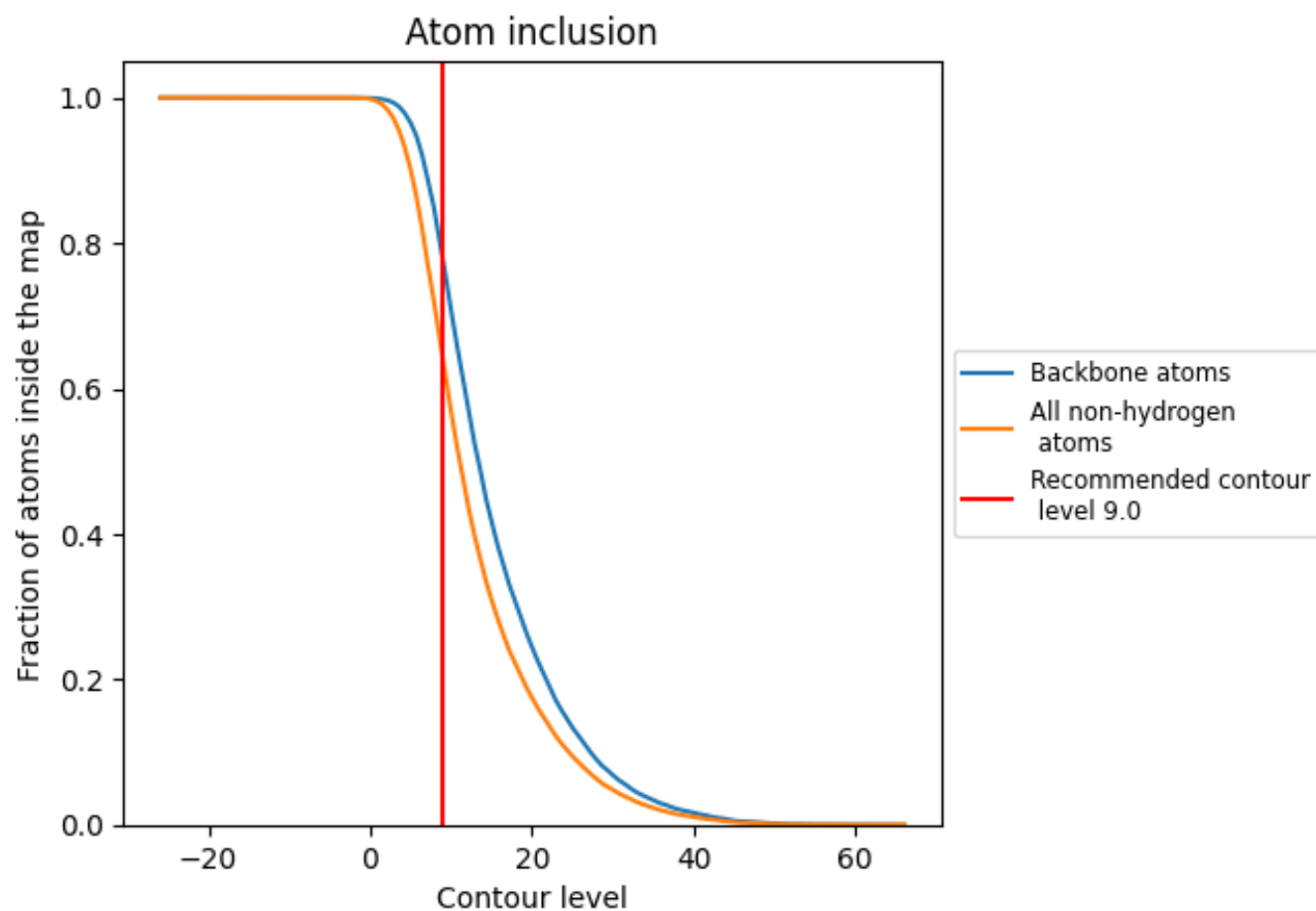
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 64% 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 (9.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6396	<div></div> 0.3740
A	<div></div> 0.5548	<div></div> 0.3430
B	<div></div> 0.5439	<div></div> 0.3470
C	<div></div> 0.6124	<div></div> 0.3660
D	<div></div> 0.6072	<div></div> 0.3590
E	<div></div> 0.6236	<div></div> 0.3500
F	<div></div> 0.6450	<div></div> 0.3810
G	<div></div> 0.8768	<div></div> 0.4930
H	<div></div> 0.7881	<div></div> 0.4610
I	<div></div> 0.7534	<div></div> 0.4970
J	<div></div> 0.9509	<div></div> 0.4370
K	<div></div> 0.8257	<div></div> 0.2690

1.0
0.0
<0.0